DICTIONARY of FOOD COMPOUNDS with CD-ROM

Additives, Flavors, and Ingredients

Edited by
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CHAPMAN & HALL/CRC

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Preface

For some years, those involved in food chemistry and technology have felt the need for a comprehensive and well-organised reference source documenting the whole range of substances on which they may need information during their day-to-day work. While there are many valuable compilations and tabulations of particular areas (e.g., permitted food additives or natural flavourings), there has been nothing available that is truly comprehensive. In addition, the existing reference works have mostly evolved as traditional books, with their associated shortcomings in terms of indexing and expense of updating.

With the increasing and sometimes contradictory demands of the consumer market today, the need for the best up-to-date and accurate information has never been greater. This is perhaps not the place to digress into the debate on "Chemicals in Food;" anyone in the position of reading this preface will be quite aware of most of the issues involved, and will have his or her own views. What is certain, however, is that whatever direction one approaches the debate from, it is a sterile and unproductive one unless there is good information about the true state of the science. And that science is of course by no means limited to food technology. Any participant in the debate who is ignorant about the effects of the natural products in the foods we eat is seriously misinformed.

Chapman & Hall in its role as a chemical information specialist is uniquely able to provide a technology capable of aiding the compilation and publication of such a comprehensive reference source. The company's experience in database publishing in chemistry goes back to the late 1970s when compilation of the first electronic edition of the *Dictionary of Organic Compounds* was begun. Since that time, a series of high-quality searchable data compilations has appeared at regular intervals. In due course, it only remained to put this technical expertise together with the specialist knowledge of an experienced international Editorial Board with overall responsibility for content, and a team of contributors with knowledge of particular areas of food components.

The resulting *Dictionary of Food Compounds* is available both in hard copy and electronically as a CD-ROM product. Each has its own advantages. There is nothing to rival the ease of consulting a book version for quick queries and for browsing to get an overall view of the whole field. On the other hand, the electronic version is searchable by chemical substructure as well as text and, for obvious reasons, is much more easily updated so that the user can get a very rapid summary of new developments in the science. The *Dictionary* is aimed not only at food scientists and technologists, but at the wide range of people whose work brings them into contact with the regulatory aspects of food supply and monitoring.

The book and CD-ROM versions are complementary. The important thing for the user to be assured of is that the *Dictionary of Food Compounds* is an ongoing project which the Publishers hope and expect will become a central feature of the information needs of everyone involved in food.

Every effort has been taken to ensure the accuracy of the information contained in DFC. Any errors or omissions should be communicated to the Publishers, who will also be pleased to receive any comments about the coverage, and especially suggestions for its expansion.

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Introduction

Users interested in more detailed factual information on topics outlined below are referred to *The Organic Chemist's Desk Reference* (Rhodes, P.A., Chapman & Hall, 1995).

1. USING DFC

The arrangement of entries is alphabetical by name. The criteria governing the choice of entry name are described below. Many compounds in DFC are present as derivatives of a parent. The CD-ROM version can be searched by all names given throughout the dictionary, whether entry names, synonyms or derivative names.

Every entry is assigned a DFC number to assist ready location. The DFC number consists of a letter of the alphabet followed by a number, e.g., A-124. All index entries refer to the DFC number.

2. COMPOUND SELECTION AND PRESENTATION

The selection of compounds for DFC is broad. Included are all compounds or group of compounds of interest or potential interest to the food industry in its widest connotation. Compounds need not have been exactly defined structurally to be included.

A full description of the scope of compounds included can be gained by perusing the headings in the Type of Compound Index, since virtually every compound or group of compounds included is listed under at least one of the headings.

Printed DFC contains a number of derivatives that are not of direct food interest, but are included because they have been used for chemical characterisation of the main entry compound. However, the number of these is strictly limited. In contrast, the version of an entry on the CD-ROM, where space is not a limitation, is the full version as present on the Chapman & Hall Chemical Database and may include many more derivatives not thought to be of current food interest. When using the CD-ROM, the possibilities for flexible searching are such that the portion of the entry most relevant to food science can rapidly be homed in on.

DFC contains many natural products known to occur in food plants for which no specific food-related information, such as flavour or toxicity, appears to be available. In such cases, the decision to include them has been based on the species information given in the entry. If one or more of the species recorded is a food plant or other food source, the compound has been selected for inclusion in the DFC dataset. The label "food plant" is broadly defined and includes edible wild foods as well as established crop foods, also toxic plants of potential interest to nutritionists. Where there is some doubt about whether a particular plant is of food significance, it has generally been included. The sources used to validate food plant information include the CropSEARCH database (http://www.hort.purdue.edu/newcrop/, Purdue University, US) and the Plants for a Future database (http://www.scs.leeds.ac.uk/pfaf/, Leeds University, UK), and the titles: *World Economic Plants — A Standard Reference* (Wiersema, J.H. and León, B., CRC Press, 1999); *Fenaroli's Handbook of Flavor Ingredients,* 4th ed., (Burdock, G.A., CRC Press, 2002); *Encyclopedia of Food and Color Additives* (Burdock, G.A., CRC Press, 1997); *Handbook of Nutraceuticals and Functional Foods* (Wildman, R.E.C., CRC Press, 2000).

3. THE TYPE OF COMPOUND INDEX

This is a most important feature of DFC. Every compound of food interest included in the dictionary is indexed under at least one heading, but usually two or more. The headings are of six types.

Structural headings (WA) classify naturally occurring food constituents under one of 30 headings according to their chemical structure, such as:

WA 1100 — Natural food colourants (betalaines)
WA 5100 — Food sugars (disaccharides)

Deliberate food additive headings (WC) refer to the various functions performed by such additives, such as:

WC 0700 — Antioxidants
WC 2100 — Curing agent

Food flavour and odour headings (WE) are self-explanatory and may refer to natural, nature-identical or synthetic odours and flavours

Food contaminant headings (WG) classify all undesirable/unintended compounds present in foods, such as:

WG 1000 — Animal feed contaminants
WG 3500 — Food allergens

Food source headings (WI) classify food compounds, both natural and processing-derived, by their food source. Examples are:

WI 1000 — Cereals and bakery products
WI 6000 — Dairy products

Food function headings (WK) are self-explanatory and include for example

WK 1500 — Antimutagenic agents
WK 6500 — Nutriceuticals

Once again, compounds classified under these headings may be natural, synthetic or nature-identical.

On the CD-ROM, a combination of these headings with other types of compound codes provides powerful search possibilities.

4. OTHER SEARCH POSSIBILITIES FROM THE CD-ROM VERSION

Space considerations have precluded the inclusion of indexes other than the Type of Compound Index and the Name Index in the hard-copy version of DFC. These were considered to be the most useful types of indexing for users primarily wishing to locate food-related information. Other types of search (e.g., by molecular formula and/or CAS registry number) are readily carried out on the CD-ROM version, which is also searchable by chemical structure or substructure. Full details of how to do this are given in the CD-ROM Help file.

5. LITERATURE COVERAGE

In compiling this edition, the primary literature has been surveyed to 2001. Any future editions are likely to be in electronic format for ease of updating.

6. ORGANISATION OF ENTRIES

Figure 1 illustrates the format of a typical entry within which the individual types of data have been labelled.

6.1 Chemical names and synonyms

6.1.1 DFC name

The DFC name is that chosen to head each entry and is that which, in the opinion of the Editors, is the one most likely to be known by, and of use to, most readers.

The American spelling "sulf-" is used throughout in preference to the British "sulph-."

DFC does not seek to establish standards of nomenclature, and the adoption of a particular name as entry name does not imply endorsement in any way. However, the DFC dataset was carefully reviewed before publication in order to give a high degree of internal consistency in the choice of entry names.

Users interested in a fuller explanation of nomenclature policy and nomenclature rules in general are referred to *The Organic Chemist's Desk Reference*.

6.1.2 Synonyms

Nearly all entries and derivatives are accompanied by various synonyms. These come from a variety of sources.

Chemical Abstracts Services (CAS) names. CAS assigns a unique name to every chemical substance. Because of the necessity to employ strict nomenclature rules to arrive at such a unique name, CAS names are often cumbersome and, in addition, many CAS parent names are relatively unfamiliar to many potential DFC users (e.g., benzenamine for aniline and 1-methylethyl for isopropyl). If the CAS name is not the entry name, DFC will often give it as a synonym if it is not too cumbersome for effective use.

The names in use by CAS for organic compounds have been largely unchanged since the beginning of the 9th collective index period in 1972 and are followed by the suffix **9CI**. This suffix means that the name is one in use by CAS since 1972 and does not necessarily mean that the compound can be found in the 9th collective index of CAS, which covers 1972 to 1976 only.

Names in use by CAS before 1972 may also be given. Names from the 8th collective index period (1967 to 1971) are usually suffixed **8CI**, but names used before 1967 are not specially labelled.

Other chemical names not corresponding to any found in CAS also may be given; these have either been found in the chemical/food literature or have been added editorially for consistency or clarity. Some compounds, particularly natural products, possess trivial names. A favoured trivial name will appear in boldface.

Trade names, generic names and names allocated by regulatory bodies are invariably given. Their names may be invented names (e.g., for pesticides) or may be serial numbers (e.g., the E numbers). Examples of such bodies are the Flavor and Extract Manufacturers' Association (FEMA) and the EU Commission (E numbers). Also included are those recommended by the British Pharmaceutical Commission as British Approved Names (BAN), the United States Adopted Name Review Board (USAN), the British Standards Institute (BSI) or the World Health Organisation as an International Nonproprietary Name (INN). No distinction is made between International Nonproprietary Names which are currently proposed (pINN) and those which are recommended (rINN).

Names which are known to be duplicated within the chemical literature are marked with the symbol ‡.

6.2 CAS Registry Numbers

CAS numbers are identifying numbers allocated to each distinctly definable chemical substance indexed by CAS since 1965 (plus some retrospective allocation of numbers by CAS to compounds from earlier index periods). The numbers have no chemical significance, but they provide a label for each substance independent of any system of nomenclature. They are extensively used for exchanging information between individuals and databases. The numbers take the form NNNNNN-NN-R, where the total number of digits is five or more and R is a check digit.

For practical purposes, CAS numbers have certain shortcomings arising from their free allocation, resulting in one substance having more than one potential number. Duplication may arise for one of several reasons to do with

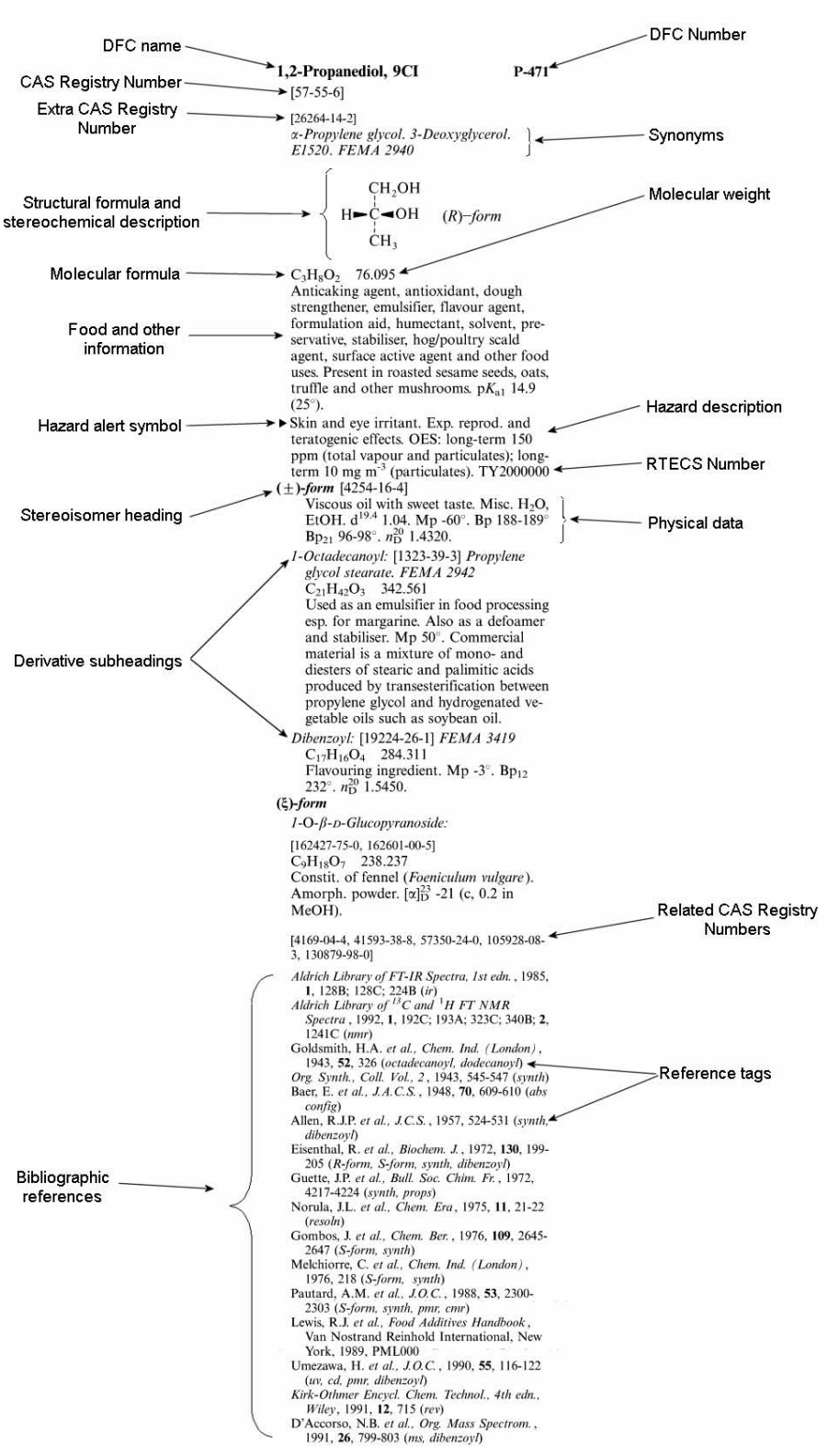


FIGURE 1 The format of a typical entry in DFC.

the detailed chemistry of the substance (e.g., tautomerism, solvent formation, partially unspecified stereochemistry). There are also replaced numbers. For this reason, DFC entries will often contain one or more *Additional CAS numbers* which may help the user to obtain further information about the substance, especially by online searching.

Some entries in DFC refer to families of compounds, especially natural products. An example is the entry for the group of peptide hormones, Relaxins. Here, general information applies to all the species variants, plus a significant number of additional CAS numbers which may refer to additional members of the group that are less well documented or characterised.

Clearly, the additional CAS numbers given in DFC have to be used with care. Their inclusion in the entry is the result of an editorial decision by the DFC contributor that they refer to what is essentially the same substance, but this decision may be a subjective one. Care has been taken to ensure that the main CAS number given in DFC for each substance is the correct one.

Further information on CAS number allocation policy can be obtained from CAS indexes or *The Organic Chemist's Desk Reference*.

6.3 Structural formulae

Every attempt has been made to present the structures of chemical substances as accurately as possible according to best current practice and recommendations of IUPAC (The International Union of Pure and Applied Chemistry). As much consistency as possible has been aimed at between closely related structures. For example, all sugars are shown as Haworth formulae and, whenever possible in complex structures, the rings are oriented in the standard Haworth convention so that structural comparisons can be quickly made.

6.4 Molecular formula and molecular weight

The elements in the molecular formula are given according to the Hill convention (C, H, then other elements in alphabetical order). The molecular weights given are formula weights (or more strictly, molar masses in Daltons) and are rounded to three places in decimals. In the case of some high molecular mass substances, such as proteins, the value quoted may be that taken from an original literature source and may be an aggregate molar mass.

6.5 Food Information

The information given on the food uses of many of the substances included in DFC is of key importance and has, as far as possible, been based on critical sources. However, in the case of compounds that have become of interest only recently, or for which little information is available, the information may be based on journal references only, in which case the reference will normally be given.

In a few cases, the only information that can be found that a compound is of food-related significance is the fact that the compound has been included in a database such as EAFUS Food Additive Database, and there appears to be no published literature supporting that inclusion. This fact will normally be noted in the entry.

DFC also contains much information on the nonfood uses of compounds. This information is of obvious potential use when it is identified for example as a food contaminant.

6.6 Physical data

DFC gives the following physical characteristics of substances, when available: appearance, melting point, boiling point, optical rotation, density, refractive index, solubility, pKa. All of these fields are searchable by numerical value (including range searching) in the CD-ROM version of DFC.

6.6.1 Appearance

Organic compounds are considered to be colourless unless otherwise stated. Where the compound contains a chromophore which would be expected to lead to visible colour, but no colour is mentioned in the literature, the DFC entry will mention this fact if it has been noticed by the contributor. An indication of crystal form and of recrystallisation solvent is often given but these are imprecise items of data; most compounds can be crystallised from several solvent systems and the crystal form often varies. In the case of the small number of compounds where crystal behaviour has been intensively studied (e.g., pharmaceuticals), it is found that polymorphism is a very common phenomenon and there is no reason to believe that it is not widespread among organic compounds generally.

6.6.2 Melting points and boiling points

The policy followed in the case of conflicting data is as follows:

(a) Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted.
(b) Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure), the lower figure is given in parentheses, thus Mp 139° (134-135°).
(c) Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted without parentheses, thus Mp 142°, Mp 205-206°.
(d) Known cases of polymorphism or double melting points are noted.

Boiling point determination is less precise than that of melting points and conflicting boiling point data are not usually reported except when there appears to be a serious discrepancy between the different authors.

6.6.3 Optical rotations

These are given wherever possible and normally refer to what the DFC contributor believes to be the best characterised sample of highest chemical and optical purity. Where available, an indication of the optical purity (op) or enantiomeric excess (ee) of the sample measured follows the specific rotation value.

Specific rotations are dimensionless numbers and the degree sign that was formerly universal in the literature has been discontinued.

6.6.4 Densities and refractive indexes

Densities and refractive indexes are now of less importance for the identification of liquids than has been the case in the past, but are quoted for common or industrially important substances, such as solvents, or where no boiling point can be found in the literature.

Densities and refractive indexes are not quoted where the determination appears to refer to an undefined mixture of stereoisomers.

6.6.5 Solubilities

Solubilities are given only where the solubility is unusual for a compound. Typical organic compounds are soluble in the usual organic solvents, such as ether and chloroform, and virtually insoluble in water. The presence of polar groups (OH, NH_2, and especially COOH, SO_3H and NR_3^+) increases water solubility.

6.6.6 pK_a values

pK_a values are given for both acids and bases. The pK_b of a base can be obtained by subtracting its pK_a from 14.17 (at 20°) or from 14.00 (at 25°).

6.7 Spectroscopic data

Many DFC entries include ultraviolet spectra which are presented in the format:

[neutral] λ_{max} 198 (log ε 1.55); 224 (sh) (log ε 0.61); 241 (sh) (log ε 0.55) (H_2O) (Berdy)

where ε is the absorption coefficient for a given UV maxima value (λ_{max}). A description of the solvent conditions used, if reported in the literature, is listed at the beginning and end of the UV data in parentheses. All peak absorptions cited are maxima unless otherwise described, e.g., shoulder/inflection (sh) and end absorption (end). In addition, UV data may be followed by the term "Berdy" or "DEREP" indicating from which database the data originated. The absence of either of these terms implies that the data was abstracted from the primary literature.

On the CD-ROM, all the λ_{max} values are indexed in the UV Maxima field and can be searched for numerically including range searching. Similarly, the solvent data associated with the UV data are indexed in the UV Solvent field.

6.8 Hazard and toxicity information

6.8.1 General

Toxicity and hazard information is highlighted by the symbol ► and has been selected to assist in risk assessments for experimental, manufacturing and manipulative procedures with chemicals.

Physical, ***reactive*** and ***toxic*** properties all contribute to the hazard associated with a particular chemical. As part of the ***physical data***, flash points, explosive limits and autoignition temperatures have been included where appropriate. Flammable classifications, which are based on flash point measurements and boiling points, are also mentioned, and the opportunity has been taken to include UK occupational exposure limits or, for some compounds, threshold limit values published by the American Conference of Governmental Industrial Hygienists (ACGIH). For the ***reactive*** hazards, a brief comment is made on any explosive (or violent polymerisation) properties and aspects of the chemical reactivity of a substance which are of concern. These include the potential for peroxidation, oxidising/reducing properties and incompatibility with commonly available chemicals. ***Toxicity*** information has been chosen to show hazardous effects from short-term or long-term exposure. Observations from human exposure are summarised if available (including possible adverse effects of drugs), otherwise experimental (exp.) tests are quoted. Included in the toxicity data are the results of irritancy tests, acute lethality data, target organ toxicity, and carcinogenic and reproductive properties, where appropriate. Those chemicals which have been classified by the International Agency for Research on Cancer (IARC) as *human carcinogens*, *probable human carcinogens* or *possible human carcinogens* have been identified in DFC accordingly.

The Publishers cannot be held responsible for any inaccuracies in the reported information, neither does the omission of hazard data in the *Dictionary* imply an absence of this data from the literature. Widely recognised hazards are included, however, and where possible key toxicity reviews are identified in the references. Further advice on the storage, handling and disposal of chemicals is given in *The Organic Chemist's Desk Reference*.

Finally, it should be emphasised that any chemical has the potential for harm if it is carelessly used.

6.8.2 RTECS® Accession Numbers*

Many entries in DFC contain one or more RTECS® Accession Numbers. Possession of these numbers allows users to locate toxicity information on relevant substances from the NIOSH *Registry of Toxic Effects of Chemical Substances*, which is a compendium of toxicity data extracted from the scientific literature.

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* RTECS® Accession Numbers are compiled and distributed by the National Institute for Occupational Safety and Health Service of the U.S. Department of Health and Human Services of The United States of America. All rights reserved (1996)

For each Accession Number, the RTECS® database provides the following data when available: substance prime name and synonyms; data when the substance record was last updated; CAS Registry Number; molecular weight and formula; reproductive, tumorigenic, and toxic dose data; and citations to aquatic toxicity ratings, IARC reviews, ACGIH Threshold Limit Values, toxicological reviews, existing Federal standards, the NIOSH criteria document program for recommended standards, the NIOSH current intelligence program, the NCI Carcinogenesis Testing Program, and the EPA Toxic Substance Control Act inventory. Each data line and citation is referenced to the source from which the information was extracted.

6.9 Bibliographic references

The selection of references is made with the aim of facilitating entry into the chemical and food literature for the user who wishes to locate more detailed information about a particular compound. In general and where possible, recent references are preferred to older ones.

In the printed DFC, the reference selection has been edited to include only those references that are most relevant to each entry. In particular, many references which refer to derivatives that are not of food significance have been omitted from the entry. All of these references can be seen on the CD-ROM version, which contains the complete entries as currently recorded on the Chapman & Hall Chemical Database.

References are given in date order except for references to spectroscopic library collections, which sort at the top of the list, and those to hazard/toxicity sources, which sort at the bottom.

The content of most references is indicated by means of a reference tag. An explanation of standard abbreviations used in reference tags is given in Section 7.2. If a reference tag is considered to be of particular importance, e.g., for an important synthesis or review, it will appear in **boldface** type.

6.9.1 Journal abbreviations

In general these are uniform with the *Chemical Abstracts Service Source Index* (CASSI) listing except for a short list of very common journals where we have been able to save a considerable amount of space by using well understood short-form abbreviations. A list of these follows:

DFC Abbreviation	CASSI Name
Acta Cryst. (and sections thereof)	Acta Crystallogr. (and sections thereof)
Annalen	Liebigs Ann. Chem.
Chem. Comm.	J. Chem. Soc., Chem. Commun.
J.A.C.S.	J. Am. Chem. Soc.
J.C.S. (and various subsections thereof)	J. Chem. Soc. (and various subsections thereof)
J. Het. Chem.	J. Heterocycl. Chem.
J.O.C.	J. Org. Chem.
Tet. Lett.	Tetrahedron Lett.

7. ABBREVIATIONS

7.1 General

The following is a selection of the most common database abbreviations used:

Abbreviation	Name
[α]	specific rotation
abs config	absolute configuration
Ac	acetyl
acc	according
AcOH	acetic acid
Ac_2O	acetic anhydride
ACGIH	American Conference of Governmental Industrial Hygienists
ADI	Acceptable Daily Intake
alk	alkaline
amorph	amorphous
amt	amount
anal	analytical applications, analysis of detection
anhyd	anhydrous
aq	aqueous
BAN	British Approved Name
bibl	bibliography
biosynth	biosynthesis
Bp	boiling point
bwd	bird (wild)
c	concentration
ca	(*circa*) about
cd	circular dichroism
CAS	Chemical Abstracts Service
chromatog	chromatography
cmr	carbon (^{13}C) nuclear magnetic resonance
CNS	central nervous system
col	colour, coloration
coml	commercial(ly)
compd	compound
conc	concentrated
config	configuration
conformn	conformation
constit	constituent
cryst struct	X-ray crystal structure determination
d	density
dck	duck
dec	decomposes, decomposition
degradn	degradation
deg	degree
deriv(s)	derivative(s)
detn	detection, determination
dil	dilute, dilution
dimorph	dimorphic
diss	dissolves, dissolved
dist(n)	distil, distillation
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
ee	enantiomeric excess
epr	electron paramagnetic (spin) resonance

Abbreviation	Name
equilib	equilibrium
esp	especially
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol
EtOH aq	aqueous ethanol
exp	experimental
FEMA	Flavor and Extract Manufacturers' Association
fl p	flash point
fluor	fluoresces, fluorescence
formn	formation
Fp	freezing point
g	gram
glc	gas liquid chromatography
Glc	β-D-glucopyranosyl
gpg	guinea pig
GRAS	Generally Recognised As Safe
ham	hamster
haz	hazard
hplc	high performance liquid chromatography
hydrol	hydrolyses, hydrolysed, hydrolysis
ihl	inhalation
ims	intramuscular
INN	International Nonproprietary Name
intermed	intermediate
ipr	intraperitoneal
ir	infra-red spectrum
isol(n)	isolation, isolated
isom	isomerism, isomers, isomerises
ivn	intravenous
JAN	Japanese Accepted Name
JMAF	Japanese Ministry for Agriculture, Forestry and Fisheries
LC	lethal concentration
LD	lethal dose: LD_{50}, a dose which is lethal to 50% of the animals tested
M	molecular weight (formula weight)
manuf	manufacturer, manufactured
max	maximum
Me	methyl
MeOH	methanol
Me_2CO	acetone
MEL	maximum exposure limit
metab	metabolite, metabolism
misc	miscible
mixt	mixture
mky	monkey
mod	moderately
Mp	melting point
ms	mass spectrum
mus	mouse
n	index of refraction, e.g. n_D^{20} for 20° and sodium light
nmr	nuclear magnetic resonance spectrum (general)
obt	obtained
oc	open cup
occup	occupational
OES	Occupational Exposure Standard
op	optical purity
ord	optical rotatory dispersion
orl	oral
Ph	phenyl (C_6H_5)
pharmacol	pharmacology
pmr	proton (^1H) nuclear magnetic resonance
polarog	polarography
polym	polymerises, polymer
ppd	precipitated
ppm	parts per million
props	properties
purifn	purification
Py	pyridine
rbt	rabbit
ref	reference
resoln	resolution
rev	review
rt	room temperature
scu	subcutaneous
sepn	separation
skn	skin
sl	slightly
sol	soluble
soln	solution
solv	solvent
sp	species (singular)
spar	sparingly
spp	species (plural)
ssp	subspecies
subl	sublimation, sublimes
synth	synthesis
tautom	tautomerism
THF	tetrahydrofuran
tlc	thin layer chromatography
TLV	Threshold Limit Value
tox	toxicity
unsatd	unsaturated
USAN	United States Adopted Name
uv	ultraviolet spectrum
v	very
var	variety
vis	visible
vol	volume

7.2 Reference Tags

The following is a selection of the most common Reference Tag abbreviations used:

Abbreviation	Name
abs config	absolute configuration
anal	analysis
bibl	bibliography
biodistribn	biodistribution

Abbreviation	Name
biosynth	biosynthesis
cd	circular dichroism
chromatog	chromatography
cmr	^{13}C nuclear magnetic resonance spectrum
config	configuration
conformn	conformation
cryst struct	X-ray crystal structure determination
deriv(s)	derivative(s)
detn	determination, detection
dsc	differential scanning calorimetry
dta	differential thermal analysis
ed	electron diffraction
electrochem	electrochemistry, cyclic voltammetry
em	electron microscopy
epr	electron paramagnetic (spin) resonance spectrum
esca	electron spectroscopy for chemical analysis
exafs	extended X-ray diffraction fine structure
fab-ms	fast atom bombardment mass spectroscopy
glc	gas-liquid chromatography
haz	hazard
hplc	high performance liquid chromatography
ir	infrared spectrum
isol	isolation
isom	isomerism
manuf	manufacture
metab	metabolism
mineral	mineralogy
ms	mass spectrum
nmr	nuclear magnetic resonance spectrum
occur	occurrence
ord	optical rotatory dispersion
pe	photoelectron spectroscopy
pharmacol	pharmacology
photol	photolysis
pmr	proton (^{1}H) nuclear magnetic resonance spectrum
polarog	polarography
powder struct	X-ray powder structure determination
props	properties (chemical or physical)
Raman	Raman spectrum
resoln	resolution
rev	review
sepn	separation
soly	solubility
spectra	°
struct	structure
synonyms	°
synth	synthesis
tautom	tautomerism
tga	thermogravimetric analysis
theory	MO calculations etc.
tlc	thin layer chromatography
tox	toxicity
trans	transition(s)
use(s)	°
uv	ultraviolet spectrum
uv-vis	ultraviolet visible spectrum

8. THE CD-ROM VERSION OF DFC

Printed DFC is accompanied by a CD-ROM version. This electronic version has a number of advantages over the print version:

(a) It can be searched more flexibly, as detailed above.
(b) It contains the full version of entries that have been shortened (by the omission of less-relevant derivatives and references) in the printed work.

Once installed, a User manual and Help file providing additional information on data content and guide to searching are available from the Chapman & Hall/CRC folder in the Start Menu and from the Help menu on the CD-ROM.

When accessing the *Dictionary of Food Compounds on CD-ROM,* the first screen that is obtained is the Search Form window (Figure 2).

The Search Form window is split into three panes:

1. Structure Search pane – allowing structure and substructure searching.
2. Search Terms pane – search from one or more of the 29 available data/text fields.
3. Index pane – displays the indexed terms within a selected field.

From the Search Form window, design your search profile using text, structure or text/structure searching. Once your search has been performed, the resultant hits are listed alphabetically by chemical name in the Hit List screen. Clicking on any one of the hits in the hit list screen will result in that entry being displayed in the Entry Display screen (Figure 3).

Any comments and suggestions for inclusion may be sent to:

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Email:swalford@crcpress.com

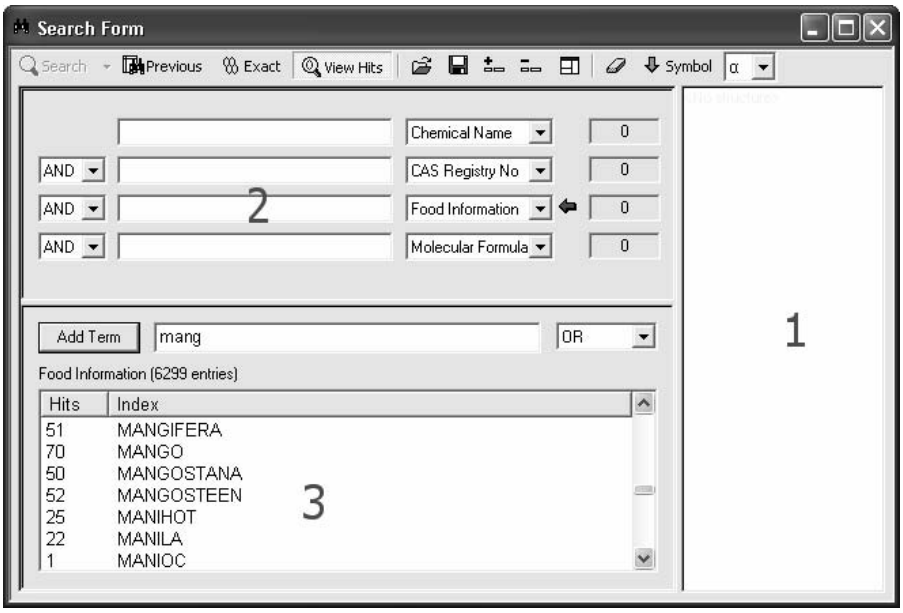


FIGURE 2 Search Form Window.

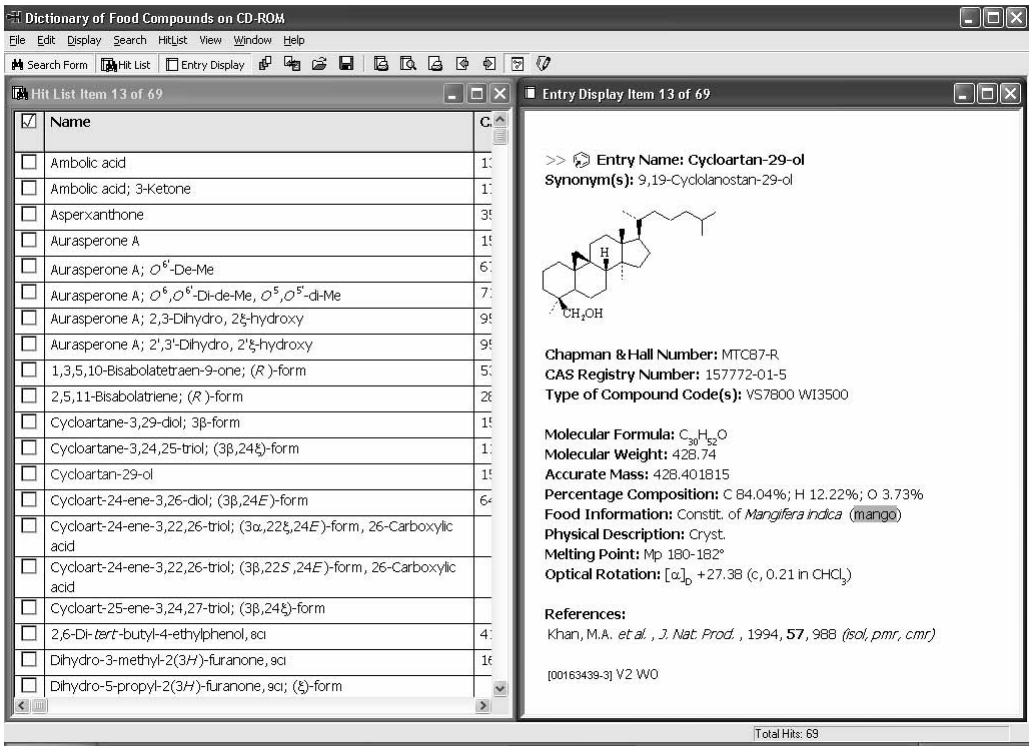
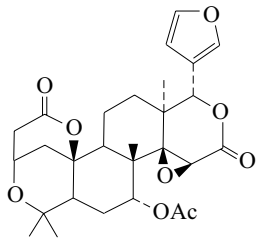


FIGURE 3 Hit List and Entry Display screens.

1(10→19)-Abeo-7-acetoxyisoobacun-3,10-olide A-1

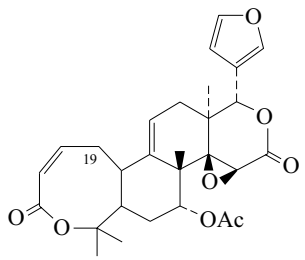


$C_{28}H_{34}O_9$ 514.571

(7α,10β)-*form* [85643-98-7]
Constit. of the fruits of a *Citrus-Poncirus* hybrid. Cryst. (MeOH). Mp 271-274°.

Bennett, R.D. *et al., Phytochemistry*, 1982, **21**, 2349

1(10→19)-Abeo-7-acetoxyobacun-9(11)-ene A-2



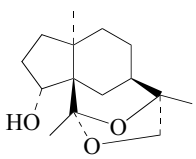
$C_{28}H_{32}O_8$ 496.556

7α-*form* [85643-97-6]
Constit. of the fruits of a *Citrus-Poncirus* hybrid.

Bennett, R.D. *et al., Phytochemistry*, 1982, **21**, 2349

3(4→5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol A-3

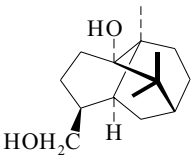
[210106-16-4]



$C_{15}H_{24}O_3$ 252.353
Constit. of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{21}$ +15 (c, 0.04 in $CHCl_3$).

Ohira, S. *et al., Phytochemistry*, 1998, **47**, 1577-1581

5(1→10)-Abeo-1,12-patchoulanediol A-4

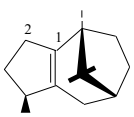


$C_{15}H_{26}O_2$ 238.369
Constit. of *Pogostemon cablin* (patchouli). Cryst. (hexane/C_6H_6). Mp 132.5-133°.

Trifilieff, E. *et al., Phytochemistry*, 1980, **19**, 2467 (*isol, struct*)
Niwa, H. *et al., Tet. Lett.*, 1984, **25**, 2797 (*synth*)

11(1→10)-Abeo-1(5)-patchoulene A-5

[514-51-2]
1,2,3,4,5,6,7,8-Octahydro-1,4,9,9-tetramethyl-4,7-methanoazulene, 9CI. ***β-Patchoulene***



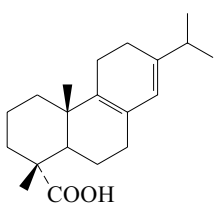
$C_{15}H_{24}$ 204.355
Constit. of guaiac wood oil (*Bulnesia sarmienti*). Oil. $Bp_{0.6}$ 66.8°. $[\alpha]_D^{30}$ -42.6 (c, 10.5 in $CHCl_3$). n_D^{25} 1.4978.

$\Delta^{1,2}$-Isomer: [53823-16-8] *11(1→10)-Abeo-1-patchoulene.* ***δ-Patchoulene***
$C_{15}H_{24}$ 204.355
Constit. of *Pogostemon cablin* (patchouli). Oil. $[\alpha]_D^{25}$ -61.7 (EtOH).

Büchi, G. *et al., J.A.C.S.*, 1961, **83**, 927 (*isol, struct*)
Bates, R.B. *et al., J.A.C.S.*, 1962, **84**, 1307 (*synth*)
Narayanan, C.S. *et al., Tetrahedron*, 1964, **20**, 963 (*isol*)
Mookherjee, B.D. *et al., J. Agric. Food Chem.*, 1974, **22**, 771 (*δ-Patchoulene*)
Akhita, A. *et al., Phytochemistry*, 1987, **26**, 2705 (*biosynth*)

8,13-Abietadien-18-oic acid A-6

[1945-53-5]
Palustric acid



$C_{20}H_{30}O_2$ 302.456
Constit. of *Pinus palustris* (pitch pine). Cryst. (MeOH). Mp 162-167°. $[\alpha]_D$ +71.6 (EtOH). λ_{max} 265 (NaOH) (Berdy).

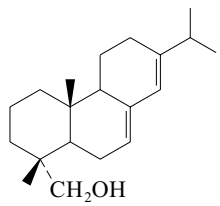
18-Aldehyde: [13508-03-7] *8,13-Abietadien-18-al.* ***Palustral***
$C_{20}H_{30}O$ 286.456
Isol. from *Pinus koraiensis* (Korean pine) and other conifers. Cryst. (EtOH). $[\alpha]_D^{20}$ +59 (c, 4.24 in $CHCl_3$).

8α,9α:13α,14α-Diepoxide: ***8,9:13,14-Diepoxy-18-abietanoic acid***
$C_{20}H_{30}O_4$ 334.455
Cryst. (diisopropyl ether) (as Me ester). Mp 130-132° (Me ester).

Wenkert, E. *et al., J.A.C.S.*, 1964, **86**, 2038
Radulgin, V.A. *et al., Khim. Prir. Soedin.*, 1974, **10**, 674; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 696 (*Palustral*)
Delgado, G. *et al., Phytochemistry*, 1994, **37**, 1119 (*diepoxide*)

7,13-Abietadien-18-ol A-7

[666-84-2]
Abietinol



$C_{20}H_{32}O$ 288.472
Isol. from *Pinus sylvestris* (Scotch pine). Cryst. or oil. Mp 85.5-87°. $[\alpha]_D$ -132.5 (c, 2 in EtOH). $[\alpha]_D$ -73 ($CHCl_3$).

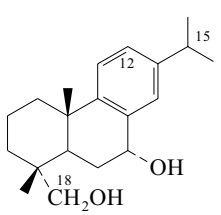
18-Tigloyl:
$C_{25}H_{38}O_2$ 370.574
Gum.

18-Aldehyde: [6704-50-3] *7,13-Abietadien-18-al.* ***Abietinal***
$C_{20}H_{30}O$ 286.456
Constit. of *Pinus sylvestris* (Scotch pine). Cryst. or oil. Mp 45-48°. $[\alpha]_D$ -116 ($CHCl_3$).

18-Carboxylic acid: See 7,13-Abietadien-18-oic acid in *The Combined Chemical Dictionary.*

Erdtman, H. *et al., Acta Chem. Scand.*, 1963, **17**, 1826
Chirkova, M.A. *et al., Khim. Prir. Soedin.*, 1966, **2**, 99; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 77
Caputo, R. *et al., Gazz. Chim. Ital.*, 1974, **104**, 491
Caputo, R. *et al., Phytochemistry*, 1974, **13**, 471
San Feliciano, A. *et al., Magn. Reson. Chem.*, 1993, **31**, 841 (*cmr*)
Lu, T. *et al., Phytochemistry*, 1995, **38**, 451 (*isol, pmr, cmr*)

8,11,13-Abietatriene-7,18-diol A-8



$C_{20}H_{30}O_2$ 302.456

7α-*form* [26920-04-7]
Needles (Me_2CO). Mp 89°. $[\alpha]_D^{20}$ -3.3 (c, 0.46 in EtOH).

18-Ac, 7-ketone: [33980-73-3] ***Pomiferin G***

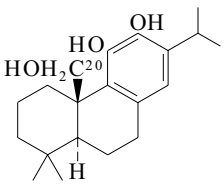
$C_{22}H_{30}O_3$ 342.477
Amorph.

18-Aldehyde, 7-ketone: [96888-45-8] *7-Oxo-8,11,13-abietatrien-18-al*. ***Suginal***
$C_{20}H_{26}O_2$ 298.424
Cryst. Mp 227° dec. $[\alpha]_D^{15}$ -100.5 (c, 1 in $CHCl_3$).

18-Aldehyde, 7-ketone, 12-hydroxy: ***12-Hydroxy-7-oxo-8,11,13-abietatrien-18-al***
$C_{20}H_{26}O_3$ 314.424
Constit. of *Salvia sclarea* (clary sage). Amorph.

Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 229
Kuo, Y.-H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3195 (*Suginal*)
Barrero, A.F. *et al., Phytochemistry*, 1992, **31**, 615 (*isol, pmr, cmr*)
Topcu, G. *et al., Phytochemistry*, 1994, **36**, 743 (*isol, pmr, cmr*)
Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 971 (*12-Hydroxy-7-oxo-8,11,13-abietatrien-18-al*)

8,11,13-Abietatriene-11,12,20-triol A-9



$C_{20}H_{30}O_3$ 318.455
Amorph. solid.

20-Carboxylic acid: [3650-09-7] *11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid*. ***Carnosic acid***. *Deoxypicrosalvinic acid. Salvin*†
$C_{20}H_{28}O_4$ 332.439
Isol. from *Salvia officinalis* (sage) and *Rosamarinus officinalis* (rosemary). Cryst. (hexane). Sol. Et_2O, MeOH, bases, $CHCl_3$; poorly sol. H_2O. Mp 185-190° dec. $[\alpha]_D^{23}$ +191 (c, 1.07 in MeOH). λ_{max} 212 (ϵ 21500); 233 (ϵ 9650); 284 (ϵ 1690) (EtOH) (Berdy).

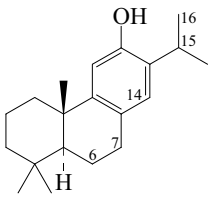
20-Carboxylic acid, di-Ac:
Needles (hexane). Mp 212-217° (196-215° dec.). $[\alpha]_D^{22}$ +139 (c, 1.15 in $CHCl_3$).

20-Carboxylic acid, 11-Me ether: [313050-47-4] ***12-Hydroxy-11-methoxy-8,11,13-abietatrien-20-oic acid***
$C_{21}H_{30}O_4$ 346.466
Constit. of *Citrus* roots infected by nematode *Tylenchulus semipenetrans*. Amorph. solid. Mp 140-141°. $[\alpha]_D^{20}$ +12.1 (c, 0.28 in $CHCl_3$).

12-Me ether, 20-carboxylic acid, 20→11 lactone: ***12-Methoxy-8,11,13-abietatrien-20,11-olide***
$C_{21}H_{28}O_3$ 328.45
Constit. of *Salvia officinalis* (sage). Cryst. (petrol). Mp 112-114°.

Linde, H. *et al., Helv. Chim. Acta*, 1964, **47**, 1234 (*isol, uv, ir, pmr*)
Wenkert, E. *et al., J.O.C.*, 1965, **30**, 2931 (*isol, ir, pmr, config*)
Narayanan, C.R. *et al., Tet. Lett.*, 1965, 3647 (*struct*)
Meyer, W.L. *et al., Tet. Lett.*, 1966, 4261 (*synth*)
Dentali, S.J. *et al., Phytochemistry*, 1990, **29**, 993 (*isol*)
González, A.G. *et al., Phytochemistry*, 1991, **30**, 4067 (*isol, pmr, cmr*)
Djarmati, Z. *et al., Phytochemistry*, 1992, **31**, 1307 (*isol, pmr, cmr, cryst struct*)
Luis, J.G. *et al., Nat. Prod. Lett.*, 2000, **14**, 379-385 (*20-acid-11-Me ether*)

8,11,13-Abietatrien-12-ol A-10



5α-*form*

$C_{20}H_{30}O$ 286.456

5α-*form* [514-62-5]
Ferruginol†
Oil. $Bp_{0.3}$ 175°. $[\alpha]_D^{16}$ +40.6 (EtOH).

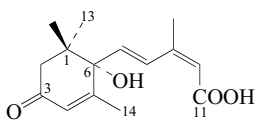
6,7-Didehydro: [34539-84-9] *6,8,11,13-Abietatetraen-12-ol*. ***Δ⁶-Dehydroferruginol***. *6,7-Didehydroferruginol*
$C_{20}H_{28}O$ 284.441
Isol. from woods of *Juniperus communis* (juniper). Light yellow solid. $[\alpha]_D^{20}$ -60 (EtOH).

Briggs, L.H. *et al., Tetrahedron*, 1959, **7**, 270-276 (*Dehydroferruginol*)
González, A.G. *et al., Phytochemistry*, 1992, **31**, 1691-1695 (*6,7-Didehydroferruginol*)

Abscisic acid A-11

[7773-56-0]

[2228-72-0, 52392-36-6]
5-(1-Hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-2,4-pentadienoic acid, 9CI. Abscisin II. Dormin



(*S*)-*form*

$C_{15}H_{20}O_4$ 264.321
Terpenoid (cyclofarnesane) numbering shown. Other schemes freq. encountered. Used to regulate ripening of fruit. λ_{max} 252 (ϵ 25200) (no solvent reported) (Derep). λ_{max} 244 (ϵ 25000) (EtOH/NaOH) (Derep). λ_{max} 245 (sh) (ϵ); 260 (ϵ 21300) (EtOH) (Derep).
►RZ2475100

(*S*)-*form* [21293-29-8]

[72029-68-6, 72029-69-7]
Constit. of cabbage, potato, lemon etc.. Cryst. ($CHCl_3$/petrol). Mp 160-161°. $[\alpha]_D$ +430. The incorrect abs. config. was formerly assigned.

β-D-Glucopyranosyl ester: [21414-42-6] ***Abscisyl β-D-glucopyranoside***
$C_{21}H_{30}O_9$ 426.463
Mp 114°. $[\alpha]_D^{17}$ +180 (c, 0.35 in EtOH).

11-Aldehyde: [41944-86-9] ***Abscisic aldehyde***
$C_{15}H_{20}O_3$ 248.321
Cryst. (CH_2Cl_2/hexane). Mp 127-128°. $[\alpha]_D^{20}$ +450.5 (c,1 in EtOH).

3α-Alcohol: [84026-26-6] ***4′-Dihydroabscisic acid***
$C_{15}H_{22}O_4$ 266.336
Isol. from immature seeds of broad bean (*Vicia faba*).

3β-Alcohol: [85718-96-3]
$C_{15}H_{22}O_4$ 266.336
λ_{max} 265 (EtOH) (Berdy).

13-Hydroxy: [25841-53-6] *13-Hydroxyabscisic acid*
$C_{15}H_{20}O_5$ 280.32
Constit. of cowpea (*Vigna unguiculata*) fruits.

13-Hydroxy, 13-O-(3-hydroxy-3-methylglutaroyl): [69790-31-4]

[69790-32-5] ***9′-(3-Hydroxy-3-methylglutaroyloxy)abscisic acid***. *β-Hydroxy-β-methylglutarylhydroxyabscisic acid. HMG-HOABA*
$C_{21}H_{28}O_9$ 424.447
Gum. $[\alpha]_D^{20}$ +560 (c, 0.013 in EtOH).

13-Hydroxy, 13-O-(3-hydroxy-3-methylglutaroyl), 5′-Me ester: [111672-32-3] ***MeHMG-HOABA***
$C_{22}H_{30}O_9$ 438.474
$[\alpha]_D^{15}$ +243 (c, 0.15 in MeOH).

13-Hydroxy, 3-alcohol:Pisumic acid
$C_{15}H_{22}O_5$ 282.336
Isol. from peas (*Pisum sativum*) irrigated with (±)-abscisic acid. Tentative struct..

14-Hydroxy: [91897-25-5] ***Nigellic acid***
$C_{15}H_{20}O_5$ 280.32
Isol. from leaves of *Vicia faba*. Mp 185-187°.

(±)-*form* [14375-45-2]
Mp 188-190°.

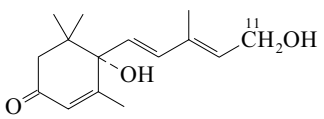
[6735-04-2, 6755-41-5, 14398-53-9, 14674-85-2, 40331-02-0, 58801-55-1, 69350-43-2, 69350-44-3, 78340-30-4, 79199-48-7, 97806-70-7]

Cornforth, J. *et al., Nature (London)*, 1965, **206**, 715 (*synth*)
Koreeda, M. *et al., J.A.C.S.*, 1973, **95**, 239-240 (*synth*)
Milborrow, B.V. *et al., Phytochemistry*, 1975, **14**, 2403-2405 (*biosynth*)
Shibasaki, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 315-322 (*synth*)
Mayer, H.J. *et al., Helv. Chim. Acta*, 1976, **59**, 1424-1427 (*synth, uv, pmr, ms*)
Burden, R.S. *et al., Pure Appl. Chem.*, 1976, **47**, 203 (*rev*)
Ueda, H. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 1506-1509 (*cryst struct*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1978, **61**, 2616-2627 (*synth, aldehyde*)
Hirai, N. *et al., Phytochemistry*, 1978, **17**, 1625-1627; 1981, **20**, 1867-1869 (*HMG-HOABA*)
Adesomoju, A.A. *et al., Phytochemistry*, 1980, **19**, 223-225 (*13-Hydroxyabscisic acid*)
Norman, S.M. *et al., Phytochemistry*, 1981, **20**, 2343-2344 (*biosynth*)
Neill, S.J. *et al., Phytochemistry*, 1982, **21**, 61-65; 1983, **22**, 2469 (*biosynth*)
Dathe, W. *et al., Phytochemistry*, 1982, **21**, 1798-1799 (*4′-Dihydroabscisic acid*)
Lehmann, H. *et al., Phytochemistry*, 1983, **22**, 1277-1278; 1988, **27**, 677-678 (*Nigellic acid*)

Takeda, N. *et al., Agric. Biol. Chem.*, 1984, **48**, 685-694; 1986, **50**, 2295-2230; 1987, **51**, 2351-2357 (*HMG-HOABA, MeHMG-HOABA*)
Bennet, R.D. *et al., Phytochemistry*, 1984, **23**, 1913-1915; 1990, **29**, 3473-3477 (*biosynth*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 245-249 (*biosynth*)
Tietz, D. *et al., Physiol. Plant.*, 1985, **65**, 171-176 (*Pisumic acid*)
Constantino, M.G. *et al., J.O.C.*, 1986, **51**, 253-254 (*synth, ir, pmr, ms*)
Boyer, G.L. *et al., Phytochemistry*, 1986, **25**, 1103-1105 (*Nigellic acid*)
Hirai, N. *et al., Phytochemistry*, 1986, **25**, 1865-1868 (*biosynth*)
Southwick, S.M. *et al., Plant Physiol.*, 1986, **81**, 323-325 (*glucopyranosyl ester*)
Okamoto, M. *et al., Phytochemistry*, 1987, **26**, 1269-1271; 1988, **27**, 2099-2103 (*3β-alcohol, biosynth*)
Soukup, M. *et al., Helv. Chim. Acta*, 1989, **72**, 361-364 (*synth*)
Willows, R.D. *et al., Phytochemistry*, 1989, **28**, 2641-2642; 1992, **31**, 2649-2653; 1993, **34**, 233-237 (*biosynth, pmr, Abscisic aldehyde*)
Abrams, S.R. *et al., Phytochemistry*, 1989, **28**, 2885-2889 (*pmr*)
Parry, A.D. *et al., Phytochemistry*, 1991, **30**, 815-821 (*biosynth*)
Cornforth, J. *et al., Aust. J. Chem.*, 1992, **45**, 179-185 (*synth*)
Hampson, C.R. *et al., Phytochemistry*, 1992, **31**, 2645-2648 (*13-Hydroxyabscisic acid*)
Sakai, K. *et al., Tetrahedron*, 1992, **48**, 8229-8238 (*synth*)
Yamamoto, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 992-993 (*synth*)
Yamauchi, S. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1968 (*glucopyranosyl ester*)
Milborrow, B.V. *et al., Phytochemistry*, 1997, **45**, 257-260 (*biosynth*)
Yamamoto, H. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 2000, **42**, 271-276 (*biosynth*)

Abscisic alcohol A-12

[113472-20-1]



$C_{15}H_{22}O_3$ 250.337
Constit. of quince (*Cydonia oblonga*) fruit.

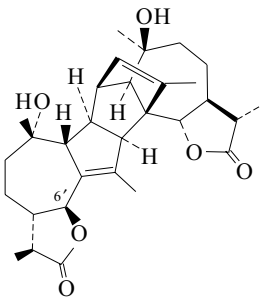
11-O-β-D-Glucopyranoside: [145153-00-0]
$C_{21}H_{32}O_8$ 412.479
Constit. of quince (*Cydonia oblonga*) fruit.

9,10-Dihydro: ***9,10-Dihydroabscisic alcohol***. *2,3-Dihydroabscisic alcohol*
$C_{15}H_{24}O_3$ 252.353
Constit. of starfruit *Averrhoa carambola*. $[\alpha]_D$ +49.7 (c, 0.0018 in EtOH).

Lutz, A. *et al., J. Agric. Food Chem.*, 1992, **40**, 116 (*isol, pmr, cmr*)
Lutz, A. *et al., Phytochemistry*, 1993, **32**, 57; 1994, **36**, 811 (*isol, pmr, cmr, cd*)

Absinthin A-13

[1362-42-1]



$C_{30}H_{40}O_6$ 496.642
Constit. of *Artemisia absinthium* (wormwood). Orange-yellow needles. Mp 182-183° dec. $[\alpha]_D$ +180.

6′-Epimer: [11029-90-6] ***Isoabsinthin***
$C_{30}H_{40}O_6$ 496.642
Constit. of *Artemisia absinthium* (wormwood). Cryst. (MeOH). Mp 172-174°.

11-Epimer: ***11-Epiabsinthin***
$C_{30}H_{40}O_6$ 496.642
Oil. $[\alpha]_D^{24}$ +159 (c, 0.34 in $CHCl_3$).

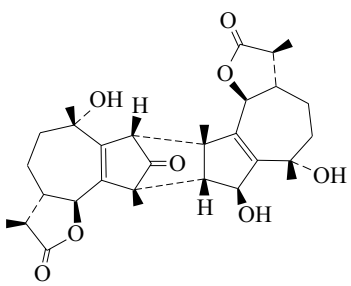
10′,11′-Diepimer: ***10′,11′-Epiabsinthin***
$C_{30}H_{40}O_6$ 496.642
Oil. $[\alpha]_D^{24}$ +107 (c, 0.62 in $CHCl_3$).

10′,11,11′-Triepimer: ***10′,11,11′-Epiabsinthin***
$C_{30}H_{40}O_6$ 496.642
Oil. $[\alpha]_D^{24}$ +46 (c, 0.35 in $CHCl_3$).

Kasymov, Sh.Z. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1979, 430-435 (*isol*)
Beauhaire, J. *et al., Tet. Lett.*, 1980, **21**, 3191; 1981, **22**, 2269 (*isol, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1985, **24**, 1009 (*isol, derivs*)
Ma, C.-M. *et al., J. Nat. Prod.*, 2000, **63**, 1626-1629 (*activity*)

Absintholide A-14

[91997-90-9]

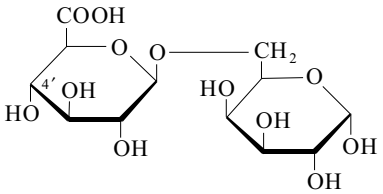


$C_{30}H_{38}O_8$ 526.625
Constit. of *Artemisia absinthium* (wormwood). Cryst. (C_6H_6). Mp 227-228°. $[\alpha]_D^{25}$ +127 (c, 1.3 in $CHCl_3$).

Beauhaire, J. *et al., Tet. Lett.*, 1984, **25**, 2751

Acaciabiuronic acid A-15

[7264-19-9]
6-O-β-D-Glucopyranuronosyl-D-galactose, 9CI, 8CI



α-Pyranose-*form*

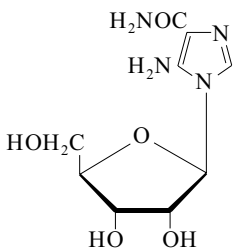
$C_{12}H_{20}O_{12}$ 356.283
Probably the commonest aldobiouronic acid present as a structural unit in plant gums. Isol. from partial acid hydrolysates from the following plants; black wattle (*Acacia mollissima*), *Acacia senegal*, *Acacia pycnantha*, *Acacia karroo*, *Acacia cyanophylla*, egg plum (*Prunus domestica*), almond (*Prunus amygdalus*), peach (*Prunus persica*), *Anogeissus lattifolia* (gum ghatti), *Vigilia oroboides*, *Afraegle paniculata*, *Ferula* and *Chorisia* spp. Also isol. from hydrolysates of maritime pine (*Pinus pinaster*) hemicellulose and wheat straw. Mp 118-119° (hydrate). $[\alpha]_D$ +11.6 → -8.6 (H_2O).

[1693-80-7, 5566-99-4]

Hotchkiss, R.D. *et al., J. Biol. Chem.*, 1936, **115**, 285 (*deriv*)
Goebel, W.F. *et al., J. Biol. Chem.*, 1938, **124**, 207 (*isol*)
Aspinall, G.O. *et al., J.C.S.*, 1955, 1160; 1961, 3461 (*isol*)
Mukherjee, S. *et al., J.A.C.S.*, 1958, **80**, 2536 (*isol*)
Jones, J.K.N. *et al., Can. J. Chem.*, 1961, **39**, 162 (*isol*)
Bailey, R.W. *et al., Oligosaccharides*, Pergamon Press, London, 1965, **4**, 134 (*occur*)
Peciar, C. *et al., Chem. Zvesti*, 1974, **28**, 83 (*config, pmr*)
Di Fabio, J.L. *et al., Carbohydr. Res.*, 1982, **99**, 41 (*isol*)

Acadesine, BAN, INN, USAN A-16

[2627-69-2]
*5-Amino-1-ribofuranosyl-1*H*-imidazole-4-carboxamide, 9CI. AICA-Riboside. AICAR. GP 1-110*



$C_9H_{14}N_4O_5$ 258.233
Pink rosettes (EtOH). Sol. H_2O. Mp 215-216° dec. $[\alpha]_D^{27}$ -62.4 (c, 0.5 in H_2O). Log P -2.97 (calc).

5′-Phosphate: [3031-94-5]
$C_9H_{15}N_4O_8P$ 338.213
Produced by the action of brewer's yeast on the riboside. The 5′-phosphate and its nontoxic salts are potent flavour enhancers of soups, canned foods, beverages, etc. Converted by Bratton-Marshall reagents to a purple dye with

λ_{max} 540 nm λ_{max} 268 (ε 12800) (H_2O).

Greenberg, G.R. *et al., J. Biol. Chem.*, 1956, **219**, 411; 423 (*isol*)
Burrows, I.E. *et al., J.C.S.(C)*, 1967, 1088 (*synth, phosphate*)
U.S. Pat., 1967, 3 355 301; *CA*, **68**, 28636q (*use*)
Panzica, R.P. *et al., J.O.C.*, 1971, **36**, 1594 (*synth*)
Panzica, R.P. *et al., J. Het. Chem.*, 1972, **9**, 623 (*synth, tri-Ac, tetra-Ac*)
Ivanovics, G.A. *et al., J.O.C.*, 1974, **39**, 3651 (*synth*)
Adamiak, D.A. *et al., Acta Cryst. B*, 1979, **35**, 924 (*cryst struct*)
Sabina, R.L. *et al., J. Biol. Chem.*, 1982, **257**, 10178 (*metab*)
Ferris, J.P. *et al., J.O.C.*, 1985, **50**, 747 (*synth, uv, pmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1329

Acemannan, INN, USAN A-17

[110042-95-0]

Carrisyn. Polymannoacetate

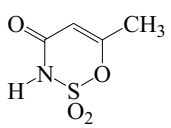
Long chain polymer consisting of linear (1→4)-D-mannopyranosyl units, randomly acetylated (0.8 Ac per monomer) MW >10000 Dalton. Constit. of leaf juice of *Aloe barbadensis*. Used in flavouring. Fluffy amorph. powder.

Pat. Coop. Treaty (WIPO), 1987, 0 052, (*Carrington Lab*); *CA*, **107**, 183550z (*extraction*)
Womble, D. *et al., Int. J. Immunopharmacol.*, 1988, **10**, 967; *CA*, **110**, 50917q (*activity*)
Pat. Coop. Treaty (WIPO), 1990, 01 253, (*Carrington Lab*); *CA*, **114**, 55783k (*prep, activity*)
Fogleman, R.W. *et al., Vet. Hum. Toxicol.*, 1992, **34**, 144; 201 tox
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 536

Acesulfame, BAN, INN A-18

[33665-90-6]

6-Methyl-1,2,3-oxathiazin-4(3H)-one 2,2-dioxide, 9CI. 3,4-Dihydro-6-methyl-1,2,3-oxathiazin-4-one 2,2-dioxide



$C_4H_5NO_4S$ 163.154

Non-nutritive sweetener. Needles ($CHCl_3$ or C_6H_6). Mp 123-123.5°.

K salt: [55589-62-3] *Acesulfame K. E950. Hoe 095K. H 733293*
ADI 15 mg/kg (1991). Intense-type sweetener permitted at 300-5500 ppm in foods. Sweetness approx. 200 × sucrose. Cryst. Mp 225° dec. (on slow heating).

Ger. Pat., 1971, 2 001 017-1193; *CA*, **75**, 129843e (*synth, ir*)
Paulus, E.F. *et al., Acta Cryst. B*, 1975, **31**, 1191-1993 (*cryst struct*)
Clauss, K. *et al., Z. Lebensm.-Unters. -Forsch.*, 1976, **162**, 37-40 (*synth, use*)
Von Rymon Lipinski, G.-W. *et al., Chem. Ind. (London)*, 1983, 427-432 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AAF900
Mayer, D.G. *et al., Acesulfame-K*, M. Dekker, New York, 1991, (*book*)
Von Rymon Lipinski, G.-W. *et al., Food Sci. Technol.*, 1991, **48**, 11-28 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 3-4
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1353
Ager, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAF900

Acetal R A-19

[7493-57-4]

Acetaldehyde phenethyl propyl acetal. Propyl phenethyl acetal. Pepital. [2-(1-Propoxyethoxy)ethyl]benzene, 9CI. FEMA 2004

$PhCH_2CH_2OCH(CH_3)OCH_2CH_2CH_3$

$C_{13}H_{20}O_2$ 208.3

(±)-*form*

Flavouring ingredient with a green pepper taste; useful in vegetable as fruit flavours. Liq. with powerful leafy odour. d_{25}^{25} 0.95. n_D^{20} 1.4800.

Arctander, S. *et al., Perfume and Flavor Chemicals*, Steffen Arctander, 1969, **1**, (*rev*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 109S; *CA*, **117**, 211063 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 10-11 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 6 (*use*)

Acetaldehyde, 9CI A-20

[75-07-0]

Ethanal. FEMA 2003

H_3CCHO

C_2H_4O 44.053

For enol form see Ethenol, E-246.

Flavouring agent and adjuvant used to impart orange, apple and butter flavours; component of food flavourings added to milk products, baked goods, fruit juices, candy, desserts and soft drinks. Liq. with a pungent fruity odour. Misc. H_2O, org. solvs. d_4^{20} 0.78. Mp -121°. Bp 21°. n_D^{20} 1.3316. pK_{a1} 13.57 (25°,hydrate). Vp 900 mmHg (25°). Readily polymerises. At low temps., cationic or anionic polym. gives poly(acetaldehyde). At higher temps. cyclisation to the cyclic trimer, paraldehyde, and the cyclic tetramer, metaldehyde, occurs. The trimer may be formed on standing; redistn. regenerates acetaldehyde. Ceiling temp. for polym. T_c-39° (pure liq.). Crit. point 181.5°/63.2 atm..

▶ Extremely flammable, fl. p.-38°, autoignition temp. 140/175°. Reacts violently with a range of organic and inorganic substances. Possible human carcinogen. Skin and severe eye irritant. A systemic irritant by inhalation. High vapour conc. narcotic preceded by sore throat and headache. Exp. carcinogen and teratogen. Exp. reprod. effects. AB1925000

Di-Me acetal: [534-15-6] *1,1-Dimethoxyethane, 9CI. FEMA 3426*
$C_4H_{10}O_2$ 90.122
Flavouring ingredient. Sol. H_2O, EtOH, Et_2O, Me_2CO, $CHCl_3$. Mp -113.2°. Bp 64.5°. n_D^{20} 1.3668.

▶ Highly flammable, fl. p. 1°. AB2825000

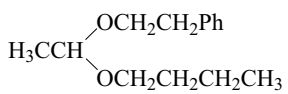
[631-59-4, 1019-57-4, 1632-89-9, 25473-09-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 214A; 465B; **2**, 921A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 348C; 727A; **3**, 487A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 551A; 1577A (*ir*)
Wertheim, E. *et al., J.A.C.S.*, 1922, **44**, 2658 (*synth*)
Kalinowski, H.O. *et al., Org. Magn. Reson.*, 1974, **6**, 305 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AAG250
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 94 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 3; 171
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 9-10; 841-842
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 47
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0776
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 2
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAG250; AAH250; DOO600
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 283 (*tox, rev*)

Acetaldehyde butyl phenethyl acetal A-21

[64577-91-9]

[2-(1-Butoxyethoxy)ethyl]benzene, 9CI. FEMA 3125



$C_{14}H_{22}O_2$ 222.327

Flavour ingredient with a green pepper taste; useful in vegetable as fruit flavours. Liq.

Zyryanova, N.Ya. *et al., CA*, 1978, **89**, 117528g (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 4 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 10 (*use*)

Acetamide, 9CI A-22

[60-35-5]

Ethanamide. Methanecarboxamide

H_3CCONH_2

C_2H_5NO 59.068

Deliquescent, hexagonal cryst. Odourless when pure but usually has characteristic "mouse" odour. V. sol. H_2O, EtOH; sol.

$CHCl_3$; prac. insol. Et_2O. Mp 82-83°. Bp 222° Bp_5 92°. pK_{a1} -1.4 (25°). Triboluminescent.

▶ Fl. p. >104°. Possible human carcinogen. Irritant. Exp. carcinogen (v. large dose). Exp. reprod. and teratogenic effects (large doses). AB4025000

N-*(13-Methyltetradecyl):* [64317-66-4]
Capsiamide
$C_{17}H_{35}NO$ 269.47
Constit. of fruit of hot pepper varieties of *Capsicum annuum*.

Takahashi, M. *et al., Yakugaku Zasshi*, 1977, **97**, 758 (*Capsiamide*)

Acetic acid, 9CI, USAN A-23

[64-19-7]
Ethanoic acid. Methanecarboxylic acid. E260. FEMA 2006

H_3CCOOH

$C_2H_4O_2$ 60.052

Many esters (acetates) are known apart from those cross-referenced below. Most are recorded as Ac derivs. of the relevant alcohols. Salts are included in the *Dictionary of Inorganic Compounds*. Has been used as a food preservative since antiquity. Used in - and contributes to - the flavour of pickles, sauces, mayonnaise and salad dressings. Acts synergistically with lactic and sorbic acid, and is more effective against yeasts and bacteria than against moulds. Used in food processing as a flavour enhancer, flavouring agent, pH control agent, pickling agent, solvent and formulation aid. Liq. or cryst. with pungent vinegar odour. Misc. H_2O, EtOH, Et_2O; sol. most org. solvs.; insol. CS_2. d_4^{20} 1.05. Mp 16.7°. Bp_{31} 30° Bp 118°. n_D^{20} 1.3718. n_D^{25} 1.3696. pK_a 4.76 (20°,H_2O). pK_a 4.78 (25°). Vp 15.5 mmHg (25°). Molecular Fp depression 39, molecular Bp elevation 29.9. Dissolves elemental S.

▶ Flammable, fl. p. 39°, autoignition temp. 463°. Reacts violently with some oxidants. Corrosive and irritating to all tissues. Exp. reprod. effects. OES: long-term 10 ppm; short-term 15 ppm. AF1340000

Me ester: Methyl acetate, M-279

Et ester: Ethyl acetate, E-259

Vinyl ester: Ethenol, E-246

Isopropyl ester: Isopropyl acetate, I-116

Benzyl ester: Benzyl acetate, B-43

Ph ester: Phenyl acetate, P-255

Fluoride: See Acetyl fluoride in *The Combined Chemical Dictionary.*

Chloride: See Acetyl chloride in *The Combined Chemical Dictionary.*

Bromide: See Acetyl bromide in *The Combined Chemical Dictionary.*

Iodide: See Acetyl iodide in *The Combined Chemical Dictionary.*

Amide: Acetamide, A-22

Methylamide: See *N*-Methylacetamide in *The Combined Chemical Dictionary.*

Dimethylamide: See *N*,*N*-Dimethylacetamide in *The Combined Chemical Dictionary.*

Hydrazide: [1068-57-1] *Acethydrazide. Acetylhydrazide. Acetylhydrazine*
$C_2H_6N_2O$ 74.082
Needles (EtOH). Sol. H_2O, EtOH, Et_2O. Mp 67°. Bp_{18} 127°. pK_{a2} 13.04 (25°,NH). Reduces $NH_3.AgNO_3$.

▶ AI1225000

Nitrile: See Acetonitrile in *The Combined Chemical Dictionary.*

Anhydride: Acetic anhydride, A-24

[71-50-1, 758-12-3, 1186-52-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 481B; 768B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 751A; 1254C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 573B (*ir*)
Kolbe, H. *et al., Ann. Chim. Farm.*, 1845, **54**, 145 (*synth*)
Thompson, C.D. *et al., Anal. Chem.*, 1970, **42**, 1474 (*detn, H_2O*)
Perrin, D.D. *et al., Masking and Demasking of Chemical Reactions*, Interscience, New York, 1970,
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 682 (*occur*)
Lowry, R.P. *et al., Hydrocarbon Process.*, 1974, **53**, 103 (*rev, bibl*)
Michael, R.P. *et al., Science (Washington, D.C.)*, 1974, 1217
Preti, G. *et al., J. Chem. Ecol.*, 1975, **1**, 361
Couperus, P.A. *et al., Org. Magn. Reson.*, 1978, **11**, 590 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 121 (*rev, bibl*)
Acetic Acid and its Derivatives, (eds. Agreda, V.H. *et al*), M. Dekker, N.Y., 1993, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1329
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 11-13 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 6
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 13-17
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4909
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 47
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0781
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 5; 11
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAT250; ACM750

Acetic anhydride, 9CI A-24

[108-24-7]

$H_3CCO–O–COCH_3$

$C_4H_6O_3$ 102.09

Esterification agent for use in prepn. of modified food starch and for acetylation of monoglycerides. Liq. with pungent, irritating odour. Spar. sol. H_2O, sol. org. solvs. d_4^{15} 1.09. Mp -73°. Bp 139.55° Bp_{15} 44°. Aq. soln. reacts neutral and is very slowly hyd. to acetic acid.

▶ Flammable, fl. p. 49°, autoignition temp. 316/390°. Reacts violently with some oxidants. Acid-catalysed hydrolysis can be violent. Vapour is a severe irritant of eyes, mucous membranes and skin. Contact with liq. causes burns and blisters of the skin, and can damage eyes. OES: short-term 5 ppm. AK1925000

[16649-49-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 711A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1165A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 760C (*ir*)
Orshansky, J. *et al., Chem. Ind. (London)*, 1944, 382 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 1
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 142 (*rev, bibl*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 13-21 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 17-18
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 9 (*occur*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 48
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1437
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 6
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAX500

Acetone A-25

[67-64-1]
2-Propanone, 9CI. Dimethyl ketone. FEMA 3326

H_3CCOCH_3

C_3H_6O 58.08

Solvent used in food processing as a colour diluent, flavour ingredient, etc.. Volatile liq. Misc. H_2O, org. solvs. d_{25}^{25} 0.79. Mp -94°. Bp 56.2°. n_D^{20} 1.3588. Crit. temp. 246.1°.

▶ Highly flammable, fl. p. -19°, autoignition temp. 538°. Reacts vigorously with $CHCl_3$ in presence of base. Liquid is severe eye irritant and defats skin. High vapour conc. irritate respiratory tract. Inhalation of vapour initially causes excitement followed by CNS depression with headache, restlessness and fatigue. Coma may result. Exp. reprod. effects by inhalation. OES: long-term 750 ppm; short-term 1500 ppm. AL3150000

[666-52-4, 43022-03-3]

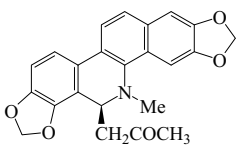
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 219D; 220A; 405A; **2**, 921B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 351C; 352A; 631A; **3**, 487B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 289A; 487A; 1577B (*ir*)
Org. Synth., 1970, **50**, 3 (*synth*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH-Weinheim, 1985, **A1**, 79 (*rev*)
Kamar, A. *et al., Can. J. Chem.*, 1986, **64**, 1979 (*ms*)
Nyquist, R.A. *et al., Appl. Spectrosc.*, 1990, **44**, 433 (*ir*)

Hayashi, S. *et al., Anal. Sci.*, 1991, **7**, 955 (*pmr, cmr*)
O'Toole, L. *et al., J. Chem. Soc., Faraday Trans.*, 1991, **87**, 3343 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 176 (*rev, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1099
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 7
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 20-22
Allan, D.R. *et al., Chem. Comm.*, 1999, 751-752 (*cryst struct*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 49
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1146
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 7
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABC750; ABF000; ABD250; TFQ250; DOM400
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 149 (*tox, rev*)

8-Acetonyldihydrosanguinarine A-26

[37687-34-6]

6-Acetonylsanguinarine. 6-Acetonyldihydrosanguinarine



(*S*)-*form*

$C_{23}H_{19}NO_5$ 389.407

(*S*)-*form*

Needles ($CHCl_3$/EtOH). Mp 209-210°. $[\alpha]_D^{20}$ +25.3 (c, 0.02 in $CHCl_3$). λ_{max} 232 (log ϵ 4.4); 282 (log ϵ 4.6); 323 (log ϵ 4.8) ($CHCl_3$).

(ξ)-*form*

Alkaloid from *Papaver somniferum* (opium poppy). Pale yellow needles (MeOH/$CHCl_3$). Mp 194-195.5°.

Furuya, T. *et al., Phytochemistry*, 1972, **11**, 3041-3044 (*isol, uv, ir, pmr, ms, struct, synth*)
Döpke, W. *et al., Z. Chem.*, 1976, **16**, 54-55 (*occur, uv, ir, pmr, ms, struct*)
Castedo, L. *et al., Heterocycles*, 1981, **16**, 533-536 (*occur*)
Koul, S. *et al., Planta Med.*, 2002, **68**, 262-265 (*isol, pmr, cmr, ms*)

Acetophenone, 8CI A-27

[98-86-2]

1-Phenylethanone, 9CI. Methyl phenyl ketone. Hypnone. Acetylbenzene. FEMA 2009

$PhCOCH_3$

C_8H_8O 120.151

Flavouring ingredient used in fruit flavours; leavening agent. Plates (freq. obt. as liq.) with penetrating sweet odour. Sol. EtOH, Et_2O; insol. H_2O. d_4^{20} 1.03. Mp 20°. Bp 202° Bp_5 67°. n_D^{20} 1.5342. pK_{a1} -6.4 (25°, H_2SO_4 aq.). For enol form see 1-Phenylethenol in The Combined Chemical Dictionary.

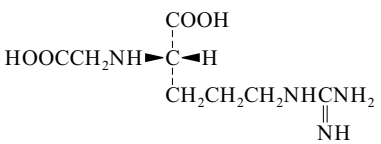
▶ Fl. p. 77°, autoignition temp. 570°. Skin and severe eye irritant. LD_{50} (rat, orl) 815 mg/kg. AM5250000

[19547-00-3, 59130-82-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 8B
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 802A
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1228B (*ir*)
Registry of Mass Spectral Data, Wiley-Interscience, 180 (*ms*)
Sadtler Standard C-13 NMR Spectra, 550 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 953 (*uv*)
Org. Synth., Coll. Vol., 1, 1932, 109 (*synth*)
Adv. Chem. Ser., 1955, **15**, 353 (***props***)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 99 (*rev, tox*)
Taylor, R. *et al., J.C.S. Perkin 2*, 1988, 737 (*synth, pmr*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 8
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 23-24
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 9
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABH000

Acetopine A-28

N^2-*(Carboxymethyl)-arginine, 9CI. Demethyloctopine*



$C_8H_{16}N_4O_4$ 232.239

(*S*)-*form* [18416-86-9]

L-form

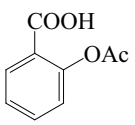
Isol. from calluses of soybean plant and cotton (*Gossypium hirsutum*). Cryst. (EtOH aq.). Mp 281-282°. $[\alpha]_D^{24}$ +24 (c, 2.5 in H_2O).

Herbst, R.M. *et al., J.O.C.*, 1946, **11**, 368 (*synth*)
Christou, P. *et al., Plant Physiol.*, 1986, **82**, 218 (*isol*)

2-Acetoxybenzoic acid A-29

[50-78-2]

2-Acetyloxybenzoic acid, 9CI. Salicylic acid acetate, 8CI. Acetylsalicylic acid. ***Aspirin, BAN, USAN***



$C_9H_8O_4$ 180.16

Constit. of *Glycyrrhiza glabra* var. *typica* (licorice) roots. Cryst. Mp 135° (rapid heat) Fp 118. pK_a 3.38 (25°, 1*M* KCl). Log P 1.02 (calc). Ca salt used in combination with urea as Carbaspirin calcium, USAN.

▶ Dust explosion haz. Irritant. Main adverse effects are gastrointestinal, with other dose dependent systemic effects. LD_{50} (rat, orl) 200 mg/kg. Exp. teratogenic effects. OES: long-term 5 mg m^{-3}. VO0700000

Me ester: [580-02-9]
$C_{10}H_{10}O_4$ 194.187
Cryst. (petrol). Mp 49°.

Et ester: [529-68-0]
$C_{11}H_{12}O_4$ 208.213
Liq. Bp 289° Bp 272°.

Propyl ester: [60310-03-4]
$C_{12}H_{14}O_4$ 222.24
Light yellow liq. Bp 289° Bp_{10} 162-164°.

Butyl ester: [52602-16-1]
$C_{13}H_{16}O_4$ 236.267
Liq. Bp_1 128-130°.

Ph ester: [134-55-4] *Acetylsalol. Phennin. Spiroform. Vesipyrin*
$C_{15}H_{12}O_4$ 256.257
Cryst. (EtOH). Mp 97°. Bp_{11} 197-198°.
Log P 3.15 (calc).

4-(Acetylamino)phenyl ester: See Benorilate in *The Combined Chemical Dictionary.*

2-[(Nitrooxy)methyl]phenyl ester: See 2-[(Nitroxy)methyl]phenyl 2-(acetyloxy)benzoate in *The Combined Chemical Dictionary.*

Chloride: [5538-51-2]
$C_9H_7ClO_3$ 198.605
Solid. Mp 43-46°. $Bp_{0.01}$ 86°.

Nitrile: [5715-02-6]
$C_9H_7NO_2$ 161.16
Liq. Bp_{17} 140°.

Anhydride: [1466-82-6]
$C_{18}H_{14}O_7$ 342.304
Mp 85°.

▶ VO0710000

Phenylalaninamide: See Aspirin phenylalanine in *The Combined Chemical Dictionary.*

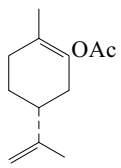
[493-53-8, 5749-67-7, 37933-78-1]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1293B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 315D (*ir*)
Ciusa, R. *et al., Chem. Zentralbl.*, 1943, **2**, 615 (*synth*)
Libermann, S. *et al., Bull. Soc. Chim. Fr.*, 1958, 185 (*synth, nitrile*)
Campini, G. *et al., Ann. Chim. (Rome)*, 1964, **54**, 975 (*synth, anhydride*)
Henriques, H.P. *et al., Mikrochim. Acta*, 1971, 807 (*detn, Mn*)
Scott, K. *et al., J. Magn. Reson.*, 1972, **6**, 55 (*nmr*)
Rüchardt, C. *et al., Annalen*, 1974, 15 (*chloride*)
Ali, S.L. *et al., Pharm. Ztg.*, 1976, **121**, 621 (*esters, synth, ir, pmr*)
Florey, K. *et al., Anal. Profiles Drug Subst.*, 1979, **8**, 1 (*rev*)
Mitscher, L.A. *et al., J. Nat. Prod.*, 1980, **43**, 259 (*occur*)
Byrn, S.R. *et al., J. Pharm. Sci.*, 1981, **70**, 280 (*cryst struct, anhydride*)
Barnett, H.J.M. *et al., Acetylsalicylic Acid*, Raven Press, N.Y., 1982, (*book*)
Collier, H.O.J. *et al., Discoveries Pharmacol.*, 1984, **2**, 555 (*rev, pharmacol*)
Hallam, J. *et al., Int. Congr. Symp. Ser. R. Soc. Med.*, 1984, (*rev*)

Kim, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2641 (*cryst struct*)
Chang, C.J. *et al., Magn. Reson. Chem.*, 1986, **24**, 768 (*cmr*)
Pelz, J. *et al., Pharmazie*, 1986, **41**, 733 (*history*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1120 (*synonyms*)
Bundgaard, H. *et al., J. Med. Chem.*, 1989, **32**, 727 (*esters, synth, props*)
Vane, J.R. *et al., Aspirin and Other Salicylates*, Ed., Chapman and Hall, 1992, (*book*)
Liebeskind, L.S. *et al., J.O.C.*, 1993, **58**, 3543 (*chloride*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 3
Benefic. Toxic Eff. Aspirin, (ed., Feinman, S.E.), CRC Press, 1994,
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADA725
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2937
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 17

2-Acetoxy-*p*-mentha-1,8-diene A-30

[1134-96-9]



$C_{12}H_{18}O_2$ 194.273

Enol acetate of *p*-Menth-8-en-2-one.

(R)-form

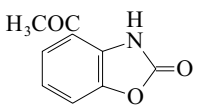
Isol. from grapefruit oil. Oil. $[\alpha]_D^{24}$ +77.

Fairlie, J.C. *et al., Chem. Comm.*, 1969, 1196 (*synth*)
Moshonas, M.G. *et al., J. Agric. Food Chem.*, 1971, **19**, 769 (*isol*)

4-Acetyl-2(3*H*)-benzoxazolone, 9CI A-31

[70735-79-4]

4-Acetylbenzoxazolin-2-one



$C_9H_7NO_3$ 177.159

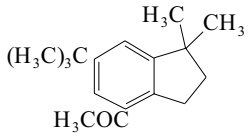
Found in kernels of *Zea mays* (sweet corn). Needles (Me_2CO aq.). Mp 217-218°. λ_{max} 250 (ϵ 9777); 320 (ϵ 5128) (MeOH) (Berdy). λ_{max} 268 (ϵ 8912); 351 (ϵ 7413) (MeOH-NaOH) (Berdy).

Fielder, D.A. *et al., Tet. Lett.*, 1994, **35**, 521-524 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Fielder, D.A. *et al., J. Nat. Prod.*, 1995, **58**, 456-458 (*synth*)
Escobar, C.A. *et al., J. Het. Chem.*, 1997, **34**, 1407-1414 (*synth*)
Kluge, M. *et al., J. Nat. Prod.*, 1998, **61**, 821-822 (*synth*)

4-Acetyl-6-*tert*-butyl-1,1-dimethylindane A-32

[13171-00-1]

*1-[6-(1,1-Dimethylethyl)-2,3-dihydro-1,1-dimethyl-1*H*-inden-4-yl]ethanone, 9CI. 6-*tert*-Butyl-1,1-dimethyl-4-indanyl methyl ketone, 8CI. Celestolide. Chrysolide. Musk celestolide. Esperone. FEMA 3653*



$C_{17}H_{24}O$ 244.376

Flavouring ingredient. Cryst. (MeOH). Mp 77.2-77.9°.

Semicarbazone:

Cryst. (EtOH). Mp 168-168.6°.

2,4-Dinitrophenylhydrazone:

Cryst. (MeOH). Mp 180-181°.

Beets, M.G.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 854-871 (*synth, struct*)
Ferrero, C. *et al., Helv. Chim. Acta*, 1959, **42**, 2111-2121 (*synth*)
U.S. Pat., 1959, 2 899 358; *CA*, **54**, 1475 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1976, **14**, 669 (*rev, tox*)
De Ridder, D.J.A. *et al., Acta Cryst. C*, 1992, **48**, 140-142 (*cryst struct*)
Kagabu, S. *et al., J. Chem. Educ.*, 1992, **69**, 420-421 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 10
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 27

Acetylcholine(1+) A-33

[51-84-3]

*2-Acetyloxy-*N,N,N*-trimethylethanaminium, 9CI. Choline acetate*

$Me_3N^{\oplus}CH_2CH_2OAc$

$C_7H_{16}NO_2^{\oplus}$ 146.209

Occurs in *Capsella bursa-pastoris* (shepherd's purse). Easily hyd. by alkalis, and *in vivo* by cholinesterases.

▶ FZ9700000

Chloride: [60-31-1] ***Acetylcholine chloride, BAN, INN, USAN.*** *Miochol. Ovisot*

$C_7H_{16}ClNO_2$ 181.662

V. deliquescent cryst. powder. Sol. H_2O. Mp 149-152°.

▶ LD_{50} (rat, orl) 2500 mg/kg. LD_{50} (rat, ivn) 22 mg/kg. FZ9800000

Bromide: [66-23-9]

$C_7H_{16}BrNO_2$ 226.113

Deliquescent prisms (EtOH). Mp 143°.

▶ FZ9680000

Iodide: [2260-50-6]

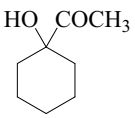
$C_7H_{16}INO_2$ 273.113

Mp 161°.

▶ KH3300000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1078A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 678C; 678D; 679A (*ir*)
Dudley, H.W. *et al., Biochem. J.*, 1929, **23**, 1064 (*synth, bibl*)
Marquardt, P. *et al., Arzneim.-Forsch.*, 1956, **6**, 168; 309 (*biosynth*)
Culvenor, C.C.J. *et al., Chem. Comm.*, 1966, 537 (*pmr*)
Beveridge, D.L. *et al., J.A.C.S.*, 1971, **93**, 3759 (*struct*)
Micelson, M.J. *et al., Acetylcholine; Approach of Mol. Mech. of Action*, Pergamon, 1974,
Hanin, I. *et al., Choline Acetylcholine: Handb. Chem. Assay Methods*, Raven Press, NY, 1974, (*anal*)
Svinning, T. *et al., Acta Cryst. B*, 1975, **31**, 1581 (*cryst struct*)
Sax, M. *et al., Acta Cryst. B*, 1976, **32**, 1953 (*conformn*)
Takasuka, M. *et al., J.C.S. Perkin 2*, 1982, 585 (*ir*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1112
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABO000; CMF250

1-Acetylcyclohexanol A-34



$C_8H_{14}O_2$ 142.197

Ac: [52789-73-8] *1-[1-(Acetyloxy)-1-cyclohexyl]ethanone, 9CI. 1-Acetylcyclohexyl acetate. FEMA 3701*

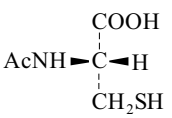
$C_{10}H_{16}O_3$ 184.235

Flavourant for food and tobacco. Oily liq. with sweet, fruity/floral odour. . Bp_2 105° (Kugelrohr).

U.S. Pat., 1982, 4 327 749; *CA*, **97**, 91810f (*synth, use*)
Fukuda, Y. *et al., J.O.C.*, 1991, **56**, 3729-3731 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1066-1067 (*use*)

N-Acetylcysteine A-35

2-Acetamido-3-mercaptopropanoic acid. ***Acetylcysteine, BAN, INN, USAN***



$C_5H_9NO_3S$ 163.197

Log P -0.64 (calc).

▶ Adverse effects reported when used therapeutically. LD_{50} (rat, orl) 5050 mg/kg. HA1660000

(R)-form [616-91-1]

L-form. Airbron. Fabrol. Mucomyst. Parvolex. Respaire. Fluimucil. NSC 111180

Effective inhibitor of enzymic browning in foods. Cryst. (H_2O). Mp 109-110°. $[\alpha]_D$ +5 (c, 3 in H_2O). Pharmacol. active isomer.

(±)-form

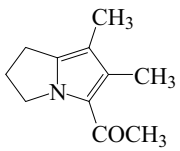
Cryst. (EtOH). Mp 124.5-125.5°. pK_a 9.52 (30°,SH, 0.3*M* KCl).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1282B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 786D (*ir*)
Smith, H.A. *et al., J.O.C.*, 1961, **26**, 820 (*synth*)

U.S. Pat., 1965, 3 184 505; *CA*, **63**, 7107 (*synth*)
Ohta, G. *et al., Chem. Pharm. Bull.*, 1967, **15**, 644 (*synth*)
Martin, T.A. *et al., J. Med. Chem.*, 1968, **11**, 625 (*synth*)
Suzuki, N. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3155 (*synth*)
McKinney, G.R. *et al., Pharmacol. Biochem. Prop. Drug Subst.*, 1979, **2**, 479 (*rev, pharmacol*)
Hopkins, S.J. *et al., Drugs of Today (Barcelona)*, 1980, **16**, 41 (*rev*)
Takusagawa, F. *et al., Acta Cryst. B*, 1981, **37**, 1591 (*cryst struct*)
Naulet, N. *et al., Org. Magn. Reson.*, 1983, **21**, 564 (*N-15 nmr*)
Van der Kuy, A. *et al., Pharm. Weekbl.*, 1986, 121; 646; 649; 663 (*pharmacol, rev*)
De Vries, N. *et al., J. Cell Biochem.*, (Suppl. 17F), 1993, 270 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 741
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACH000

5-Acetyl-2,3-dihydro-6,7-dimethyl-1*H*-pyrrolizine A-36

[97073-03-5]
*1-(2,3-Dihydro-6,7-dimethyl-1*H*-pyrrolizin-5-yl)ethanone*



$C_{11}H_{15}NO$ 177.246
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)
Debrauwer, L. *et al., Bull. Soc. Chim. Fr.*, 1991, 244-254 (*occur*)

7-Acetyl-2,3-dihydro-5,6-dimethyl-1*H*-pyrrolizine A-37

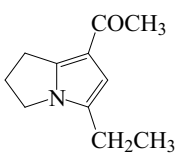
*1-(2,3-Dihydro-5,6-dimethyl-1*H*-pyrrolizin-7-yl)ethanone*

$C_{11}H_{15}NO$ 177.246
Proline- or lysine-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)
Hill, V.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3675-3681 (*occur*)

7-Acetyl-2,3-dihydro-5-ethyl-1*H*-pyrrolizine A-38

[97073-13-7]
*1-(2,3-Dihydro-5-ethyl-1*H*-pyrrolizin-7-yl)ethanone*

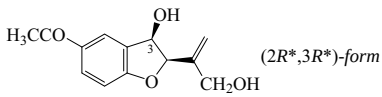


$C_{11}H_{15}NO$ 177.246
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr*)

5-Acetyl-2,3-dihydro-3-hydroxy-2-[1-(hydroxymethyl)ethenyl]benzofuran A-39

10-Hydroxytoxol



$C_{13}H_{14}O_4$ 234.251

(2R,3R)-form
cis-*form*

2′-O-β-D-Glucopyranoside:
$C_{19}H_{24}O_9$ 396.393
Amorph. powder. $[\alpha]_D$ -5 (c, 0.1 in MeOH). λ_{max} 222 ; 274 (MeOH).

2′-Ac: [75680-15-8] ***10-Acetoxytoxol***
$C_{15}H_{16}O_5$ 276.288
Constit. of *Helichrysum italicum* (curry plant). Needles ($CHCl_3$/Et_2O). Mp 110°. λ_{max} 275 (log ϵ 4.09) ($CHCl_3$).

Di-Ac:
$C_{17}H_{18}O_6$ 318.326
Gum.

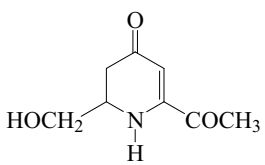
(2R*,3S*)-form
trans-*form*

3-O-Angeloyl:
$C_{18}H_{20}O_5$ 316.353

Haensel, R. *et al., Phytochemistry*, 1980, **19**, 639-644 (*2′-Ac*)
De Guttierrez, A.N. *et al., Phytochemistry*, 1995, **39**, 795-800 (*isol, pmr, ms*)
De Lampasona, M.E.P. *et al., Phytochemistry*, 1997, **46**, 1077-1080 (*di-Ac*)
Gongora, L. *et al., Phytochemistry*, 2002, **59**, 857-860 (*Phagnalon glucoside*)

6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1*H*)-pyridinone, 9CI A-40

[214218-63-0]

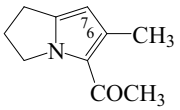


$C_8H_{11}NO_3$ 169.18
Minor product from the Maillard reaction of xylose and glycine. Pale yellow solid.

Ames, J.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 438-443 (*formn, pmr, cmr, ms*)

5-Acetyl-2,3-dihydro-6-methyl-1*H*-pyrrolizine A-41

[55041-86-6]
*1-(2,3-Dihydro-6-methyl-1*H*-pyrrolizin-5-yl)ethanone, 9CI*



$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product. Constit. of beer and malt aroma. Characterised spectroscopically.

Shigematsu, H. *et al., J. Agric. Food Chem.*, 1975, **23**, 233-237 (*occur, ms, pmr*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923; 1993, **41**, 547-553 (*occur, ms, pmr*)

5-Acetyl-2,3-dihydro-7-methyl-1*H*-pyrrolizine A-42

[80933-77-3]
*1-(2,3-Dihydro-7-methyl-1*H*-pyrrolizin-5-yl)ethanone*

$C_{10}H_{13}NO$ 163.219
Proline- or lysine-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923; 1993, **41**, 547-553 (*occur, ms*)
Hill, V.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3675-3681 (*occur*)

7-Acetyl-2,3-dihydro-5-methyl-1*H*-pyrrolizine A-43

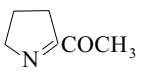
[97073-06-8]
*1-(2,3-Dihydro-5-methyl-1*H*-pyrrolizin-7-yl)ethanone*

$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr*)

5-Acetyl-3,4-dihydro-2*H*-pyrrole A-44

[85213-22-5]
*1-(3,4-Dihydro-2*H*-pyrrol-5-yl)ethanone, 9CI. 2-Acetyl-1-pyrroline*

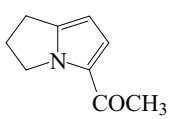


C_6H_9NO 111.143
Key flavour/aroma component of cooked rice, wheatbread crust, popcorn, sweetcorn and roasted sesame. Liq. with popcorn odour. Bp_{15} 26-28°. Unstable. Odour threshold of 0.02ng/L in air.

Buttery, R.G. *et al., Chem. Ind. (London)*, 1982, 958; 1983, 478 (*isol, synth*)
Favino, T.F. *et al., J.O.C.*, 1996, **61**, 8975-8979 (*synth, pmr, bibl*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619; 2270-2277 (***synth, ms, bibl***)

5-Acetyl-2,3-dihydro-1*H*-pyrrolizine A-45

[55041-85-5]
*1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)ethanone, 9CI*



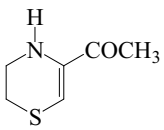
$C_9H_{11}NO$ 149.192
Proline-derived Maillard product. Constit. of popcorn, beer and cooked asparagus

aroma. Mp 45.5°.

Shigematsu, H. *et al., J. Agric. Food Chem.*, 1975, **23**, 233-237 (*occur, synth, uv, ms*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1997, **45**, 837-843 (*occur, ms*)
Chen, W.C. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur, ms*)
Miranda, L.D. *et al., Tet. Lett.*, 2000, **41**, 3035-3038 (*synth, ir, pmr*)

5-Acetyl-2,3-dihydro-1,4-thiazine A-46

[164524-93-0]
*1-(3,4-Dihydro-2*H*-1,4-thiazin-5-yl)ethanone, 9CI*

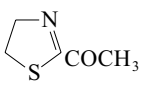


C_6H_9NOS 143.209
Formed by thermal treatment of cysteine and ribose mixtures.. Liq. with intense roasty, popcorn-like odour. Mp 171-172° (as hydrochloride). Odour threshold 0.06 ng/L in air.

Hofman, T. *et al., J. Agric. Food Chem.*, 1995, **43**, 2187-2194 (*occur*)
De Kimpe, N.G. *et al., J. Agric. Food Chem.*, 1998, **46**, 2278-2281 (*synth, pmr, cmr*)

2-Acetyl-4,5-dihydrothiazole A-47

[29926-41-8]
1-(4,5-Dihydro-2-thiazolyl)ethanone, 9CI. Methyl 2-thiazolin-2-yl ketone, 8CI. 2-Acetyl-2-thiazoline. FEMA 3817

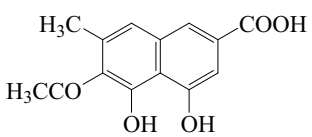


C_5H_7NOS 129.182
Reported in beef broth, roast beef and overpasteurized beer. Roasted meat-like flavour ingredient. Oil or cryst. with onion/grassy odour. Mp 25-26°. Bp_{11} 94°. n_D^{20} 1.5294.

Oxime: [37112-89-3]
$C_5H_8N_2OS$ 144.197
Cryst. (CCl_4). Mp 178-179° dec.

Doornbos, T. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1972, **91**, 711 (*synth, deriv, ir, pmr, uv, ms*)
U.S. Pat., 1973, 3 778 518; *CA*, **80**, 69405e (*props*)
Sakaguchi, M. *et al., J. Agric. Food Chem.*, 1978, **26**, 1179-1183 (*occur*)
Hofmann, T. *et al., J. Agric. Food Chem.*, 1995, **43**, 2946-2950 (*occur*)

6-Acetyl-4,5-dihydroxy-7-methyl-2-naphthalenecarboxylic acid A-48



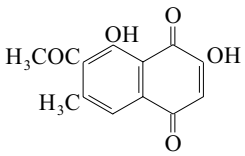
$C_{14}H_{12}O_5$ 260.246

4-O-β-D-Glucopyranoside: ***Rumexoside***
$C_{20}H_{22}O_{10}$ 422.388
Constit. of the roots of *Rumex patientia* (patience dock). Amorph. λ_{max} 224 ; 260 ; 301 ; 334 (MeOH).

Demirezer, O. *et al., Phytochemistry*, 2001, **56**, 399-402

7-Acetyl-2,8-dihydroxy-6-methyl-1,4-naphthoquinone A-49

[80597-54-2]



$C_{13}H_{10}O_5$ 246.219
Yellow solid. Mp 206-209° dec.

2-Me ether: [64756-97-4] *7-Acetyl-8-hydroxy-2-methoxy-6-methyl-1,4-naphthoquinone.* ***Orientalone***
$C_{14}H_{12}O_5$ 260.246
Constit. of *Prunus cerasoides* (wild Himalayan cherry). Yellow-orange cryst. (C_6H_6/petrol). Mp 191-192°.

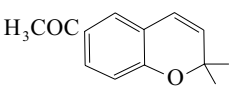
8-Me ether: [95455-42-8] *7-Acetyl-2-hydroxy-8-methoxy-6-methyl-1,4-naphthoquinone*
$C_{14}H_{12}O_5$ 260.246
Yellow solid. Mp 173-177° dec.

Di-Me ether: [80597-53-1] *7-Acetyl-2,8-dimethoxy-6-methyl-1,4-naphthoquinone*
$C_{15}H_{14}O_5$ 274.273
Yellow solid. Mp 182-184°.

Sharma, M. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 544; 1978, **16**, 289 (*Orientalone*)
Jung, M.E. *et al., Tetrahedron*, 1984, **40**, 4751 (*synth, pmr, cmr*)
Garg, M. *et al., Proc. Natl. Acad. Sci., India, Sect. A*, 1985, **55**, 95 (*Orientalone*)

6-Acetyl-2,2-dimethyl-2*H*-1-benzopyran A-50

[19013-07-1]
*1-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)ethanone, 9CI. 6-Acetyl-2,2-dimethyl-3-chromene. Demethoxyencecalin*



$C_{13}H_{14}O_2$ 202.252
Constit. of *Helianthus annuus* (sunflower). Oil. $Bp_{0.05}$ 95°.

2,4-Dinitrophenylhydrazone: [26932-01-4]
Mp 230-232° dec.

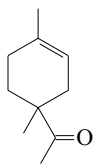
3,4-Dihydro: [32333-31-6] *6-Acetyl-3,4-dihydro-2,2-dimethyl-2*H*-1-benzopyran. 6-Acetyl-2,2-dimethylchroman*
$C_{13}H_{16}O_2$ 204.268
Mp 90-91°.

1′-Alcohol: [71822-00-9] *6-(1-Hydroxyethyl)-2,2-dimethyl-2*H*-1-benzopyran. α,2,2-Trimethyl-2*H*-1-benzopyran-6-methanol, 9CI. Demethoxyencecalinol*
$C_{13}H_{16}O_2$ 204.268
Constit. of *Helianthus annuus* (sunflower). Oil.

Arnoue, A. *et al., Tet. Lett.*, 1967, 4201 (*pmr*)
Bohlmann, F. *et al., Chem. Ber.*, 1970, **103**, 90; 1972, **105**, 863 (*isol, pmr, synth*)
Naidu, M.V. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 73 (*synth, pmr, deriv*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 281 (*isol, ir, pmr, ms, deriv*)
Yamaguchi, S. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 442 (*synth, pmr*)
Varga, E. *et al., Fitoterapia*, 1984, **55**, 307 (*isol*)
Ahluwalia, V.K. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 1124 (*synth, pmr*)
Satoh, A. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 664 (*isol, activity*)

4-Acetyl-1,4-dimethyl-1-cyclohexene A-51

[43219-68-7]
1-(1,4-Dimethyl-3-cyclohexenyl)ethanone. FEMA 3449

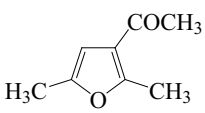


$C_{10}H_{16}O$ 152.236
Occurs in juniper oil. Flavouring ingredient. Oil. Bp 208-211°. $[\alpha]_D^{20}$ +2.1 (c, 1 in CCl_4).

Thomas, A.F. *et al., Helv. Chim. Acta*, 1973, **56**, 1800 (*isol*)
Kreiser, W. *et al., Helv. Chim. Acta*, 1974, **57**, 164 (*synth*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 932 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 172
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 845

3-Acetyl-2,5-dimethylfuran A-52

[10599-70-9]
1-(2,5-Dimethyl-3-furanyl)ethanone, 9CI. 2,5-Dimethyl-3-furyl methyl ketone, 8CI. FEMA 3391



$C_8H_{10}O_2$ 138.166
Flavouring ingredient. d_4^{25} 1.03. $Bp_{0.25}$ 62°. n_D^{20} 1.4850.

Oxime:
$C_8H_{11}NO_2$ 153.18
Cryst. (EtOH aq.). Mp 78°.

Phenylhydrazone:
Cryst. (EtOH aq.). Mp 137°.

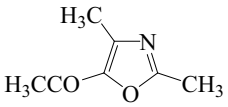
2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 194-195°.

Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)
Yanami, T. *et al., J.C.S. Perkin 1*, 1978, 1144 (*synth, pmr, uv*)
Kretchmer, R.H. *et al., J.O.C.*, 1978, **43**, 4596 (*synth*)

Baciocchi, E. *et al., Synth. Commun.*, 1988, **18**, 1841 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 10
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 27-28

5-Acetyl-2,4-dimethyloxazole A-53

[23012-25-1]
1-(2,4-Dimethyl-5-oxazolyl)ethanone, 9CI



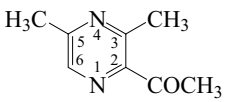
$C_7H_9NO_2$ 139.154
Constit. of Arabica coffee and baked potato aromas.

2,4-Dinitrophenylhydrazone:
Red cryst. (Me_2CO/DMF). Mp 204-205°.

Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, coffee*)
Padwa, A. *et al., J.A.C.S.*, 1975, **97**, 6484-6491 (*synth, pmr, uv, ir*)
Coleman, E.C. *et al., J. Agric. Food Chem.*, 1981, **29**, 42-48 (*isol, potato*)

2-Acetyl-3,5-dimethylpyrazine A-54

[54300-08-2]
1-(3,5-Dimethylpyrazinyl)ethanone, 9CI



$C_8H_{10}N_2O$ 150.18
Normally obt. as a mixt. with 2-Acetyl-3,6-dimethylpyrazine, A-55 to which the Bp and FEMA number refer. Constit. of wood smoke and coffee aroma. Component of FEMA 3327. Bp_7 70°.

Vitzthum, O.G. *et al., Z. Lebensm.-Unters. - Forsch.*, 1974, **156**, 300-307 (*occur*)
Wolt, J. *et al., J.O.C.*, 1975, **40**, 1178-1179 (*synth*)
Maga, J.A. *et al., Flavour Fragrance J.*, 1985, **1**, 37-42 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 20 (*FEMA 3327*)

2-Acetyl-3,6-dimethylpyrazine A-55

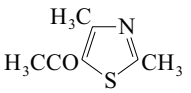
[54300-09-3]
1-(3,6-Dimethylpyrazinyl)ethanone, 9CI

$C_8H_{10}N_2O$ 150.18
Normally obt. as a mixt. with 2-Acetyl-3,5-dimethylpyrazine, A-54.. Component of coffee aroma.

Vitzthum, O.G. *et al., Z. Lebensm.-Unters. - Forsch.*, 1974, **156**, 300-307 (*occur*)
Sakamoto, T. *et al., Synthesis*, 1984, 245-247 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 1974, 20 (*FEMA 3327*)

5-Acetyl-2,4-dimethylthiazole A-56

[38205-60-6]
1-(2,4-Dimethyl-5-thiazolyl)ethanone, 9CI. 2,4-Dimethyl-5-thiazolyl methyl ketone. FEMA 3267



C_7H_9NOS 155.22
Flavouring ingredient. Bp 228-230°. n_D^{20} 1.5436.

Hydrochloride: [88323-87-9]
Cryst. (EtOH aq.). Mp 180°.

Picrate:
Mp 184-185°.

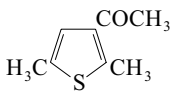
Oxime: [40236-03-1]
$C_7H_{10}N_2OS$ 170.235
Cryst. (EtOH aq. or C_6H_6). Mp 134°.

Semicarbazone:
Mp 230°.

Ganapathi, K. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1945, **22**, 343; *CA*, **40**, 4058^2 (*synth*)
Beraud, J. *et al., Bull. Soc. Chim. Fr.*, 1962, 2072 (*synth*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264 (*ms*)
Mane, R.A. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 690 (*oxime*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 173
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 844-845

3-Acetyl-2,5-dimethylthiophene A-57

[2530-10-1]
1-(2,5-Dimethyl-3-thienyl)ethanone, 9CI. 2,5-Dimethyl-3-thienyl methyl ketone, 8CI. FEMA 3527



$C_8H_{10}OS$ 154.232
Flavouring ingredient. Bp_{15} 105-108°. n_D^{20} 1.5440.

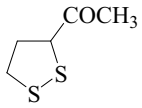
▶ OB2888000

S,S-*Dioxide:*
$C_8H_{10}O_3S$ 186.231
Cryst. Mp 124°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1473D; **2**, 597C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 54C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1473D (*ir*)
Glaze, A.P. *et al., J.C.S. Perkin 1*, 1985, 957 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 11
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 28-29
Rozen, S. *et al., J.O.C.*, 1997, **62**, 1457-1462 (*dioxide, synth, ir, pmr*)

3-Acetyl-1,2-dithiolane A-58

[89712-89-0]
1-(1,2-Dithian-3-yl)ethanone

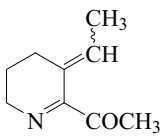


$C_5H_8OS_2$ 148.25
Produced by thermal degradation of thiamine and by Maillard reaction of cysteine. Component of model meat aroma systems. Characterised spectroscopically.

Schmidt, U. *et al., Annalen*, 1963, **670**, 157-168 (*synth, uv*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, synth, pmr, ms*)
Zhang, Y. *et al., J. Agric. Food Chem.*, 1991, **39**, 760-763 (*occur*)

2-Acetyl-3-ethylidene-3,4,5,6-tetrahydropyridine A-59

[118355-72-9]
1-(3-Ethylidene-3,4,5,6-tetrahydro-2-pyridinyl)ethanone

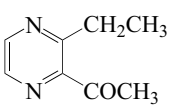


$C_9H_{13}NO$ 151.208
Proline or lysine-derived Maillard product. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*occur, ms, pmr*)
Hill, V.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3675-3681 (*occur*)

2-Acetyl-3-ethylpyrazine A-60

[32974-92-8]
1-(3-Ethylpyrazinyl)ethanone, 9CI. FEMA 3250

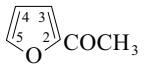


$C_8H_{10}N_2O$ 150.18
Flavouring ingredient. Liq. Bp_6 77°. n_D 1.5142.

Ger. Pat., 1971, 2 166 323; *CA*, **80**, 108574f (*synth*)
Mookherjee, B.D. *et al., J.O.C.*, 1972, **37**, 511 (*synth, ir, pmr, ms*)
Wolt, J. *et al., J.O.C.*, 1975, **40**, 1178
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 12
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 29-30

2-Acetylfuran A-61

[1192-62-7]
1-(2-Furanyl)ethanone, 9CI. 2-Acetofurone. α-Furyl methyl ketone. FEMA 3163



$C_6H_6O_2$ 110.112
Present in cooked apple, morello cherry, wine grapes, peach, strawberry, plum, rabbiteye blueberry, asparagus, kohlrabi, baked potato, pineapple, bread products, rice, yoghurt, wines, soybean, black tea and calamus (European origin). Contributes to aroma of many foods and beverages. Used in flavour compositions. Liq. or cryst. with sweet balsamic odour. Mp 33°. Bp 173° Bp_{10} 67°.

▶ OB3870000

Oxime:
$C_6H_7NO_2$ 125.127
Prisms (Et_2O/petrol). Mp 104°.

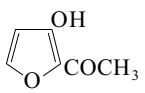
Phenylhydrazone: [61726-90-7]
Yellow plates (EtOH aq.). Mp 86.5°.

Semicarbazone:
Plates (MeOH). Mp 150°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 583B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 23A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1457A (*ir*)
Hartough, H. *et al., J.A.C.S.*, 1947, **69**, 1012 (*synth*)
Angelelli, J.M. *et al., Tetrahedron*, 1972, **28**, 2037 (*ir*)
Chadwick, D. *et al., Tet. Lett.*, 1974, 3183 (*nmr*)
Milstein, D. *et al., J.O.C.*, 1979, **44**, 1613 (*synth*)
Okubo, J. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 2067 (*uv*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1153-1154 (*use, occur*)

2-Acetyl-3-hydroxyfuran A-62

[3420-59-5]
Isomaltol



$C_6H_6O_3$ 126.112
Cryst. (H_2O or Et_2O). Mp 98-103°. Subl.18 115. pK_a 5.7.

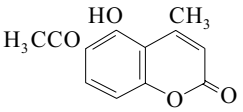
O-*α-D-Glucopyranoside:* [85559-61-1]
$C_{12}H_{16}O_8$ 288.254
Constit. of the roots of *Eleutherococcus senticosus* (Siberian ginseng).

Me ether: [3420-58-4]
$C_7H_8O_3$ 140.138
Prisms (Et_2O). Mp 101-102°.

Hodge, J.E. *et al., Cereal Chem.*, 1961, **38**, 207 (*synth, ir, uv*)
Fisher, B.E. *et al., J.O.C.*, 1964, **29**, 776-781 (*ir, struct*)
Weeks, P.D. *et al., J.O.C.*, 1980, **45**, 1109-1113 (*use*)
Fox, R.C. *et al., Synth. Commun.*, 1999, **29**, 989-1001 (*synth, pmr, cmr*)
Li, X.-C. *et al., Planta Med.*, 2001, **67**, 776-778 (*glucoside*)

6-Acetyl-5-hydroxy-4-methyl-2*H*-1-benzopyran-2-one, 9CI A-63

[36695-19-9]
6-Acetyl-5-hydroxy-4-methylcoumarin. ***Liqcoumarin***



$C_{12}H_{10}O_4$ 218.209
Isol. from *Glycyrrhiza glabra* (licorice). Cryst. Mp 165-166°.

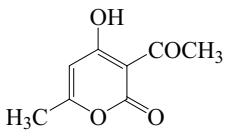
O-*Benzoyl:*
Cryst. Mp 115-116°.

Wadodkar, P.N. *et al., Indian J. Chem.*, 1972, **10**, 145
Bhardwaj, D.K. *et al., Phytochemistry*, 1976, **15**, 1182 (*isol*)

3-Acetyl-4-hydroxy-6-methyl-2*H*-pyran-2-one, 9CI A-64

[771-03-9]

[85-25-6, 520-45-6]
Dehydroacetic acid. Dehydracetic acid



$C_8H_8O_4$ 168.149
Fungicide used against moulds on fresh and dried fruit. Now superseded. Rhombic needles or plates (EtOH). Sol. H_2O, EtOH, Me_2CO, Et_2O. Mp 109°. Bp 270° Bp_5 132-133°. pK_a 5.12 (25°). λ_{max} 223 ; 308 (MeOH) (Berdy).

▶ LD_{50} (rat, orl) 500 mg/kg.

Na salt: [4418-26-2]
Used as a preservative for cut or peeled squash. Mp 284-287°.

▶ UP8225000

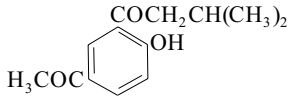
Oxime:
$C_8H_9NO_4$ 183.163
Mp 153-154°.

Anilide:
$C_{14}H_{13}NO_3$ 243.262
Mp 115°.

Berson, J.A. *et al., J.A.C.S.*, 1952, **74**, 5172 (*uv*)
Kiang, A. *et al., J.C.S.*, 1965, 2283 (*synth*)
Royals, E.E. *et al., J.O.C.*, 1965, **30**, 1255 (*uv, ir, pmr, struct*)
Manku, G.S. *et al., Anal. Chim. Acta*, 1971, **54**, 181 (*use*)
Manku, G.S. *et al., Talanta*, 1971, **18**, 1079 (*use*)
Rivera, C. *et al., Experientia*, 1976, **32**, 1490 (*isol*)
Ohta, S. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2762 (*synth, ir, pmr*)
Tan, S.-F. *et al., J.C.S. Perkin 2*, 1982, 513; 1984, 1317 (*ir, pmr, uv, cmr, tautom*)
Pesticide Manual, 9th edn., 1991, No. 3870
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 788-789; 2549-2550
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFW500; SGD000

1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone, 9CI A-65

[62458-64-4]
4′-Hydroxy-3′-isovalerylacetophenone



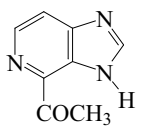
$C_{13}H_{16}O_3$ 220.268
Constit. of *Polymnia sonchifolia* (yacon). Cryst. Mp 94.5-96°. λ_{max} 242 (ε 15200); 271 (ε 5800) (MeOH).

Me ether: [51995-98-3] *1-(5-Acetyl-2-methoxyphenyl)-3-methyl-1-butanone, 9CI. 3-Isovaleroyl-4-methoxyacetophenone.* ***Espeletone***
$C_{14}H_{18}O_3$ 234.294
Oil.

Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 3035; 1977, **110**, 295; 1980, **113**, 261 (*isol, ms, ir, pmr, synth*)
Takasugi, M. *et al., Phytochemistry*, 1996, **43**, 1019 (*isol, uv, ir, pmr, cmr, ms*)

4-Acetylimidazo[4,5-*c*]pyridine A-66

[146874-38-6]
1-(1H-Imidazo[4,5-c]pyridin-4-yl)ethanone, 9CI. 2-Acetylpyrido[3,4-d]imidazole (incorr.)

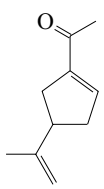


$C_8H_7N_3O$ 161.163
3*H*-form shown. Maillard prod. derived from histidine and glucose. Solid. Characterised spectroscopically.

Gi, U.-S. *et al., J. Agric. Food Chem.*, 1993, **41**, 644-646; 1995, **43**, 2226-2230 (*isol, ms, pmr, ir*)

1-Acetyl-4-isopropenylcyclopentene A-67

[2704-76-9]
1-[4-(1-Methylethenyl)-1-cyclopenten-1-yl]ethanone, 9CI



$C_{10}H_{14}O$ 150.22
Isol. from oil of *Eucalyptus globulus* (Tasmanian blue gum). Oil. Bp_{738} 225-225.5° $Bp_{1.5}$ 67-68°. $n_D^{24.5}$ 1.4965.

2,4-Dinitrophenylhydrazone:
Red plates (EtOH). Mp 178-180°.

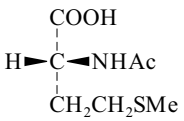
Semicarbazone:
Cryst. (MeOH). Mp 195-196°.

Schmidt, H. *et al., Chem. Ber.*, 1947, **80**, 528; 533 (*isol*)

Wolinsky, J. *et al., J.A.C.S.*, 1960, **82**, 636 (*struct, synth*)
Conia, J.M. *et al., Bull. Soc. Chim. Fr.*, 1964, 1963 (*synth, uv, ir, pmr*)
Vig, P. *et al., Indian J. Chem.*, 1968, **6**, 564 (*synth*)

N-Acetylmethionine, 9CI A-68

2-(Acetylamino)-4-(methylthio)butanoic acid. Aminotylon. Methionamine. Thiomedon-Amp



(*R*)-*form*

$C_7H_{13}NO_3S$ 191.251

(*R*)-*form* [1509-92-8]
Cryst. (EtOAc or H_2O). Mp 104-105°. $[\alpha]_D^{25}$ +20.3 (c, 4 in H_2O).

(*S*)-*form* [65-82-7]
Nutrient supplement used as a source of L-methionine. Mp 104°. $[\alpha]_D^{25}$ -20.3.
► PD0480000

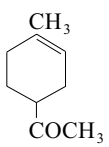
(±)-*form* [1115-47-5]
Cryst. (H_2O). Mp 114-115°.
► PD0500000

4-Acetamidophenyl ester: See Sumacetamol in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 784D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1280A (*nmr*)
Wheeler, G.P. *et al., J.A.C.S.*, 1951, **73**, 4604 (*synth*)
U.S. Pat., 1962, 3 028 395; *CA*, **57**, 16742 (*resoln*)
Heyns, K. *et al., Annalen*, 1963, **667**, 194 (*ms*)
U.K. Pat., 1967, 1 072 876; *CA*, **67**, 114015 (*resoln*)
Jung, G. *et al., Eur. J. Biochem.*, 1973, **35**, 436 (*cd*)
Rotruck, J.T. *et al., J. Nutr.*, 1975, **105**, 331 (*metab*)
Hawkes, G.E. *et al., Nature (London)*, 1975, **257**, 767 (*N-15 nmr*)
Boggs, R.W. *et al., Adv. Exp. Med. Biol.*, 1978, **105**, 571 (*props*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982,
Ponnuswamy, M.N. *et al., Acta Cryst. C*, 1985, **41**, 917 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 30-31
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACQ275

4-Acetyl-1-methylcyclohexene A-69

[6090-09-1]
*1-(4-Methyl-3-cyclohexen-1-yl)ethanone, 9CI. 1′,2′,3′,6′-Tetrahydro-4′-methylacetophenone. Tetrahydro-*p*-acetyltoluene*



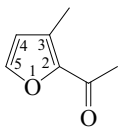
$C_9H_{14}O$ 138.209
Flavouring ingredient. Isol. from the famine food *Santalum album* (sandalwood). Oil. Bp 205-206°.

[70286-20-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **3**, 530D (*ir*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1973, **56**, 1800 (*synth, struct*)
Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*synth*)

2-Acetyl-3-methylfuran A-70

[13101-45-6]
1-(3-Methyl-2-furanyl)ethanone, 9CI. Methyl (3-methyl-2-furyl) ketone, 8CI



$C_7H_8O_2$ 124.139
Present in oils of *Perilla frutescens* and *Elsholtzia ciliata* and sesame oil. Bp_{20} 116-119° Bp_{10} 60°.

[119363-99-4]

Ueda, T. *et al., Nippon Kagaku Zasshi*, 1960, **81**, 1756 (*isol*)
Fujita, Y. *et al., Nippon Kagaku Zasshi*, 1966, **87**, 1361 (*isol*)
Kutney, J.P. *et al., Tetrahedron*, 1971, **27**, 3323 (*synth, ir, uv, pmr*)

2-Acetyl-5-methylfuran A-71

[1193-79-9]
1-(5-Methyl-2-furanyl)ethanone, 9CI. Methyl (5-methyl-2-furyl) ketone, 8CI. FEMA 3069

$C_7H_8O_2$ 124.139
Isol. from raisins, roasted onion, French fried potato, tomato, smoked fatty fish, cooked beef, fried cured pork, beer, spirits, black tea, wild rice, squid and coffee aroma. Organoleptic and flavouring agent. d_4^{20} 1.07. Bp_{10} 80°. n_D^{20} 1.5138.
► LT8528000

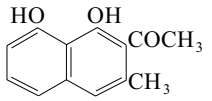
Semicarbazone:
Mp 190.5-191.5°.

[73750-15-9]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 23C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1457C (*ir*)
Farrer, M.W. *et al., J.A.C.S.*, 1950, **72**, 3695 (*synth*)
Morizur, J.P. *et al., Bull. Soc. Chim. Fr.*, 1966, 2296 (*pmr*)
Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*isol*)
Ferretti, A. *et al., J. Agric. Food Chem.*, 1970, **18**, 13 (*isol*)
Scholz, S. *et al., Annalen*, 1985, 1935 (*synth, pmr, cmr, ir*)
Boykin, D.W. *et al., J. Het. Chem.*, 1988, **25**, 643 (*O-17 nmr*)
Farmer, L.J. *et al., J. Sci. Food Agric.*, 1989, **49**, 347
Baig, M.A. *et al., J.C.S. Perkin 2*, 1989, 1981 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 32-33 (*use, occur*)

2-Acetyl-3-methyl-1,8-naphthalenediol A-72

[3785-24-8]
1-(1,8-Dihydroxy-3-methyl-2-naphthalenyl)ethanone, 9CI. 2-Acetyl-1,8-dihydroxy-3-methylnaphthalene. ***Musizin****. Dianellidin. Nepodin*



$C_{13}H_{12}O_3$ 216.236
Yellow needles (EtOH or petrol/C_6H_6). Mp 164-165° (evac. tube).

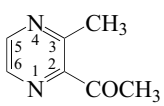
8-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]: ***Orientaloside***
$C_{25}H_{32}O_{13}$ 540.52
Constit. of the roots of *Rumex patientia* (patience dock). Amorph. λ_{max} 225 ; 260 ; 301 ; 333 ; 345 (MeOH).

4-Chloro, 8-O-β-D-glucopyranoside: ***Patientoside A***
$C_{19}H_{21}ClO_8$ 412.823
Constit. of the roots of *Rumex patientia* (patience dock). Pale yellow powder. $[\alpha]_D^{20}$ -109.7 (c, 0.75 in MeOH). λ_{max} 234 (log ϵ 3.97); 312 (log ϵ 3.73); 339 (log ϵ 3.69) (MeOH).

Kuruuzum, A. *et al., J. Nat. Prod.*, 2001, **64**, 688-690 (*Patientoside A*)
Demirezer, O. *et al., Phytochemistry*, 2001, **56**, 399-402 (*Orientaloside*)

2-Acetyl-3-methylpyrazine A-73

[23787-80-6]
1-(3-Methylpyrazinyl)ethanone, 9CI. Methyl (3-methylpyrazinyl) ketone, 8CI

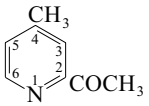


$C_7H_8N_2O$ 136.153
Aroma constit. of spiny lobster (*Panulirus argus*) roasted sesame seed. Liq. with burnt, popcorn-like odour. d 1.11. $Bp_{0.5}$ 56°. n_D^{20} 1.5216. Odour threshold 2 x 10^{-2} ppm in H_2O.

Mookherjee, B.D. *et al., J.O.C.*, 1972, **37**, 511-513 (*synth, ir, pmr, ms*)
Wolt, J. *et al., J.O.C.*, 1975, **40**, 1178-1179 (*synth, pmr, ms*)
Mihara, S. *et al., J. Agric. Food Chem.*, 1988, **36**, 1242-1247 (*props*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*glc, occur*)
Cadwallader, K.R. *et al., J. Agric. Food Chem.*, 1995, **43**, 2432-2437 (*detn, occur*)

2-Acetyl-4-methylpyridine A-74

[59576-26-0]
1-(4-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 4-methyl-2-pyridyl ketone, 8CI. 2-Acetyl-4-picoline



C_8H_9NO 135.165
Component of fig leaf absolute (*Ficus carica*). Cryst. (petrol). Sol. EtOH. Mp 33-34°. Bp_{15} 95-97°.

*Oxime (*E-*):* [23089-35-2]
$C_8H_{10}N_2O$ 150.18
Cryst. (C_6H_6/petrol). Mp 98-99° Mp 125-128°.

Semicarbazone:
Solid. Mp 195-198°.

[18103-84-9]

Case, F.H. *et al., J.A.C.S.*, 1956, **78**, 5842 (*synth*)
Nishimoto, N. *et al., Yakugaku Zasshi*, 1961, **81**, 88; *CA*, **55**, 13421b (*synth*)
Case, F.H. *et al., J. Het. Chem.*, 1968, **5**, 161 (*synth, oxime*)
Schilt, A. *et al., Talanta*, 1969, **16**, 448 (*detn, Co, Cu, Fe*)

2-Acetyl-5-methylpyridine A-75

[5308-63-4]
1-(5-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 5-methyl-2-pyridyl ketone, 8CI. 2-Acetyl-5-picoline

C_8H_9NO 135.165
Component of roasting coffee aroma. Liq. $Bp_{0.1}$ 60-70°.

Crabb, T.A. *et al., Org. Magn. Reson.*, 1982, **20**, 242 (*synth*)
U.S. Pat., 1986, 4 574 125; *CA*, **105**, 635x (*synth*)

2-Acetyl-6-methylpyridine A-76

[6940-57-4]
1-(6-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 6-methyl-2-pyridyl ketone, 8CI. 6-Acetyl-2-picoline

C_8H_9NO 135.165
Minor component of rum. Flavour modifying agent for coffee. Liq. Bp_1 46°.

*Oxime (*E-*):* [23089-39-6]
$C_8H_{10}N_2O$ 150.18
Cryst. (petrol). Sol. EtOH. Mp 49-50°.

Dimethylhydrazone: [33785-80-7]
$C_{10}H_{15}N_3O$ 193.248
Liq. $Bp_{0.1}$ 53-54°. n_D^{26} 1.5370.

[18103-88-3]

Case, F.H. *et al., J. Het. Chem.*, 1968, **5**, 161 (*synth, oxime*)
Schilt, A. *et al., Talanta*, 1969, **16**, 448 (*detn, Cu*)
Newkome, G.R. *et al., J.O.C.*, 1972, **37**, 1329 (*deriv*)
Zanger, M. *et al., Anal. Chem.*, 1974, **46**, 2042 (*pmr*)
Amin, H.B. *et al., J.C.S. Perkin 2*, 1979, 624 (*synth*)

4-Acetyl-2-methylpyridine A-77

[2732-28-7]
1-(2-Methyl-4-pyridinyl)ethanone, 9CI. Methyl 2-methyl-4-pyridyl ketone, 8CI. 4-Acetyl-2-picoline

C_8H_9NO 135.165
Component of roasting coffee aroma. Liq. Bp_{10} 120-124° Bp_4 130°.

Picrate: [31931-61-0]
Solid (EtOH). Mp 174-175°.

[80882-67-3]

Suzuki, Y. *et al., Yakugaku Zasshi*, 1961, **81**, 795; *CA*, **55**, 24742d (*synth*)
Eilhauer, H.D. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1965, **298**, 131 (*synth*)
Govindachari, T.R. *et al., Indian J. Chem.*, 1966, **4**, 398 (*synth*)

4-Acetyl-3-methylpyridine A-78

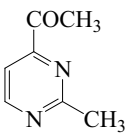
[82352-00-9]
1-(3-Methyl-4-pyridinyl)ethanone, 9CI. Methyl 3-methyl-4-pyridyl ketone, 8CI. 4-Acetyl-3-picoline

C_8H_9NO 135.165
Component of roasting coffee aroma. Bp_1 93-95°.

Hibino, S. *et al., J. Het. Chem.*, 1990, **27**, 1751 (*synth, pmr, ms*)

4-Acetyl-2-methylpyrimidine A-79

[67860-38-2]
1-(2-Methyl-4-pyrimidinyl)ethanone, 9CI. FEMA 3654

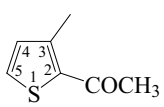


$C_7H_8N_2O$ 136.153
Flavouring ingredient. Present in cooked meats. Liq. d_4^{20} 1.1. Bp_{10} 85-90°. n_D^{20} 1.5039.

Ger. Pat., 1977, 2 800 443; *CA*, **89**, 163595z (*synth, use*)
Sakamoto, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 4554-4560 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 14 (*props, use*)

2-Acetyl-3-methylthiophene A-80

[13679-72-6]
1-(3-Methyl-2-thienyl)ethanone, 9CI. Methyl 3-methyl-2-thienyl ketone, 8CI



C_7H_8OS 140.206
Flavouring ingredient with a honey-like flavour. Bp 216° Bp_{14} 98-99°. n_D^{20} 1.5620.

Oxime:
C_7H_9NOS 155.22
Mp 85-86°.

Demuth, R. *et al., Ber.*, 1885, **18**, 3026 (*synth*)
Von Gerlach, M. *et al., Annalen*, 1892, **267**, 153 (*synth, oxime*)

2-Acetyl-5-methylthiophene A-81

[13679-74-8]
1-(5-Methyl-2-thienyl)ethanone, 9CI. Methyl 5-methyl-2-thienyl ketone

C_7H_8OS 140.206
Organoleptic. Constit. of coffee aroma.. Mp 25°. Bp 232-233° Bp_8 98-100°.

▶ OB4972000

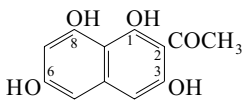
Oxime: [1956-44-1]
C_7H_9NOS 155.22
Mp 125°.

Semicarbazone:
Mp 215-217° dec.

Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*isol*)
Kaper, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1970, **81**, 825 (*uv*)
Bagli, J. *et al., J. Med. Chem.*, 1976, **19**, 876 (*synth*)
Drage, J.S. *et al., Organometallics*, 1985, **4**, 389 (*synth, pmr*)
Spinelli, D. *et al., Acta Chem. Scand.*, 1993, **47**, 160 (*cmr, O-17 nmr*)

2-Acetyl-1,3,6,8-naphthalenetetrol A-82

2-Acetyl-1,3,6,8-tetrahydroxynaphthalene



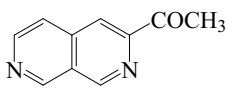
$C_{12}H_{10}O_5$ 234.208

1,6-Di-Me ether, 3-O-β-D-apiofuranoside, 8-O-β-D-glucopyranoside: [170384-73-3]
Cassitoroside
$C_{25}H_{32}O_{14}$ 556.519
Constit. of the seeds of *Cassia tora* (charota). Pale yellow needles. Mp 234-236°.

Choi, J.S. *et al., Phytochemistry*, 1995, **40**, 997 (*isol, pmr, cmr*)

3-Acetyl-2,7-naphthyridine A-83

[73607-00-8]
1-(2,7-Naphthyridin-3-yl)ethanone, 9CI

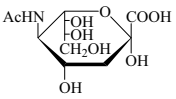


$C_{10}H_8N_2O$ 172.186
Alkaloid from valerian *(Valeriana officinalis)*.

Janot, M.M. *et al., Ann. Pharm. Fr.*, 1979, **37**, 413-420 (*isol, cryst struct*)
Barbu, E. *et al., Heterocycl. Commun.*, 2000, **6**, 25-28 (*synth*)

N-Acetylneuraminic acid A-84

[131-48-6]
*5-(Acetylamino)-3,5-dideoxy-D-*glycero-*D-*galacto-*2-nonulosonic acid, 9CI.* O-*Sialic acid.* ***Aceneuramic acid, INN.*** *Lactaminic acid. Gynaminic acid. Serolactaminic acid. KI 111. NANA. Neu5Ac. Neu5NAc*



α-D-Pyranose-*form*

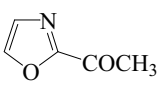
$C_{11}H_{19}NO_9$ 309.272
Isol. from eggs, milk and colostrum by acid or enzymic hydrol. of the constit. sialoproteins and oligosaccharides. Most abundant source is the nest cementing glycoprotein of the Chinese swiftlet used in birdsnest soup. Mp 185-187° dec. $[\alpha]_D^{22}$ -32 (H_2O). The only sialic acid formed in human tissues. Store below 0° in the dark.

[19342-33-7, 126934-33-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 758C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1239A (*nmr*)
Gottschalk, A. *et al., The Chemistry and Biology of Sialic Acids and Related Substances*, Cambridge Univ. Press, London, 1960, (*rev*)
Blix, G. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 246 (*isol*)
O'Connell, A.M. *et al., Acta Cryst. B*, 1973, **29**, 2320 (*cryst struct*)
Codington, J.F. *et al., Methods Carbohydr. Chem.*, 1976, **7**, 226 (*isol, detn*)
Martin, J.E. *et al., Carbohydr. Res.*, 1977, **56**, 432 (*isol*)
Jaques, L.W. *et al., J. Biol. Chem.*, 1977, **252**, 4533 (*cmr*)
Czarniecki, M.F. *et al., J.A.C.S.*, 1977, **99**, 8273 (*isol, cmr*)
Benzing-Nguyen, L. *et al., J.O.C.*, 1978, **43**, 551 (*synth, cmr*)
Friebolin, H. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 208 (*equilib*)
Schauer, R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1982, **40**, 131 (*rev*)
Sialic Acids: Chem. Metab. and Function, (Ed. Schauer, R.), Springer-Verlag, Vienna, 1982, 5 (*rev*)
Csuk, R. *et al., Helv. Chim. Acta*, 1988, **71**, 609 (*synth*)
Prytulla, A. *et al., Magn. Reson. Chem.*, 1990, **28**, 888 (*cmr, pmr*)
Kragl, U. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 827 (*enzymic synth*)
De Ninno, M.P. *et al., Synthesis*, 1991, 583 (*synth, gly, rev*)
Bodenmüller, A. *et al., Annalen*, 1994, 541 (*synth*)
Kragl, U. *et al., Ann. N.Y. Acad. Sci.*, 1995, **750**, 300 (***synth***)
Chan, T.H. *et al., J.O.C.*, 1995, **60**, 4228 (*synth*)
Maru, I. *et al., Carbohydr. Res.*, 1998, **306**, 575-578 (***synth***)
Banwell, M. *et al., J.C.S. Perkin 1*, 1998, 2251-2252 (*synth*)
Ooi, H.C. *et al., Aust. J. Chem.*, 1999, **52**, 937-940 (*synth*)

2-Acetyloxazole A-85

[77311-07-0]
1-(2-Oxazolyl)ethanone, 9CI

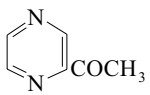


$C_5H_5NO_2$ 111.1
Constit. of roasted peanuts and cocoa beans. No synth. reported. Identification of the food product was by ms only with no indication of whether a reference sample was available.

Ho, C.-T. *et al., J. Food Sci.*, 1981, **47**, 127-133 (*occur, ms*)
Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur*)

2-Acetylpyrazine A-86

[22047-25-2]
Methyl pyrazinyl ketone. 1-Pyrazinylethanone. FEMA 3126



$C_6H_6N_2O$ 122.126
Flavouring ingredient. Component of roasted sesame seed aroma. Cream cryst. with popcorn-like flavour. Mp 75-77°.

2-Thiazolylhydrazone: [73568-92-0]
$C_9H_9N_5S$ 219.27
Cryst. (EtOH). Sol. common org. solvs. Mp 210°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 844A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 407C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1562B (*ir*)
Kushner, S. *et al., J.A.C.S.*, 1952, **74**, 3617-3621 (*synth, deriv*)
Schilt, A.A. *et al., Talanta*, 1980, **27**, 55-58 (*thiazolylhydrazone, use*)
Easmon, J. *et al., J. Med. Chem.*, 1992, **35**, 3288-3296 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 14
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 34
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADA350

2-Acetylpyridine A-87

[1122-62-9]
1-(2-Pyridinyl)ethanone, 9CI. Methyl 2-pyridyl ketone. 2-Acetopyridine. FEMA 3251



C_7H_7NO 121.138
Organoleptic. Flavouring agent. Present in wheat bread, cooked beef, roast lamb, grape brandies, roast peanut, roast filbert, beer, cocoa, black tea, coriander seed and other foodstuffs. Liq. with roasted odour. Bp 192°. n_D^{20} 1.5203. pK_a 2.64 (25°). Turns yellow in air.

Hydrochloride:
Mp 183-185° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 779A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 310A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1542B (*ir*)
Miyajama, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 429 (*cmr*)
Lesman, T. *et al., Org. Mass Spectrom.*, 1973, **7**, 1321 (*ms*)
Seth-Paul, W.A. *et al., Spectrochim. Acta A*, 1974, **30**, 1817 (*ir*)
Reimann, E. *et al., Annalen*, 1976, 1351 (*synth*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 35 (*occur*)
Girardot, M. *et al., J.O.C.*, 1998, **63**, 10063-10068 (*synth*)

3-Acetylpyridine A-88

[350-03-8]
1-(3-Pyridinyl)ethanone, 9CI. Methyl 3-pyridyl ketone. 3-Acetopyridine. FEMA 3424

C_7H_7NO 121.138
Organoleptic, flavouring ingredient. Liq. Sol. H_2O. Bp 220° Bp_{12} 106°. pK_a 3.26 (25°). Yellows in air..

▶ OB5425000

Hydrochloride:
Mp 80° dec.

Oxime: [5973-83-1]
$C_7H_8N_2O$ 136.153
Mp 130.5°.

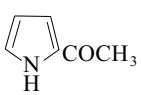
▶ OB5600000

Phenylhydrazone:
Mp 137°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 780C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 312B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1543A (*ir*)
Scott, F.L. *et al., J.O.C.*, 1957, **22**, 1568 (*synth*)
Katritzky, A.R. *et al., J.C.S.*, 1958, 3165 (*uv*)
Kavalewski, V.J. *et al., J. Chem. Phys.*, 1962, **36**, 266 (*pmr*)
Miyajama, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 429 (*cmr*)
Lesman, T. *et al., Org. Mass Spectrom.*, 1973, **7**, 1321 (*ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 35-36; *Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press*, 1995, **2**, 15
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABI000

2-Acetylpyrrole A-89

[1072-83-9]
1-(1H-Pyrrol-2-yl)ethanone, 9CI. Methyl 2-pyrrolyl ketone. 2-Acetopyrrole. Pseudoacetylpyrrole. FEMA 3202



C_6H_7NO 109.127
Organoleptic which contributes to many aromas, including roasted filbert. Present in cooked apple, asparagus, wheat bread, tea, roasted peanut, popcorn, potato chips, licorice, Chinese boxthorn and other foodstuffs. Cryst. (petrol) with bread-like odour. Sol. H_2O. Mp 90°. Bp 220°. λ_{max} 247 ; 287 (MeOH) (Berdy).

N-*Me:* [932-16-1] *2-Acetyl-1-methylpyrrole. FEMA 3184*
C_7H_9NO 123.154
Flavouring ingredient. Bp 200-202°. n_D^{20}

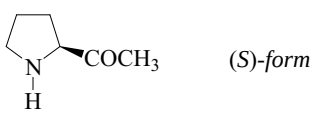
1.5420.

N-*Et:* [39741-41-8] *2-Acetyl-1-ethylpyrrole. FEMA 3147*
$C_8H_{11}NO$ 137.181
Flavouring ingredient. Bp_{12} 82°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 567D; 568A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 5B; 5C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1447B; 1447C (*ir*)
Cionga, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1935, **200**, 780 (*isol*)
Sugisawa, H. *et al., Chem. Ind. (London)*, 1958, 887 (*synth*)
Budzikiewicz, H. *et al., J.C.S.*, 1964, 1949 (*ms*)
Abraham, R.J. *et al., J.C.S. Perkin 2*, 1974, 1004 (*cmr*)
Sannai, A. *et al., Agric. Biol. Chem.*, 1983, **47**, 2397 (*isol*)
Miyayawa, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 2925; 1984, **48**, 2847 (*isol*)
Kakushima, M. *et al., J.O.C.*, 1983, **48**, 3214 (*synth*)
Garrido, D.O.A. *et al., J.O.C.*, 1984, **49**, 2619 (*synth*)
Anderson, H.J. *et al., Can. J. Chem.*, 1985, **63**, 896 (*synth*)
Eyley, S.C. *et al., Tet. Lett.*, 1985, **26**, 4649 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ADA 375
Pindur, H. *et al., J. Het. Chem.*, 1989, **26**, 1563 (*ir*)
Kuroda, Y. *et al., Tet. Lett.*, 1989, **30**, 2411 (*synth*)
Ito, M. *et al., Agric. Biol. Chem.*, 1991, **55**, 2117 (*isol, props*)
Goldberg, Yu. *et al., Synth. Commun.*, 1991, **21**, 557 (*N-alkyl derivs, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 215; 468; 560
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 944; 1709; 1853-1854 (*occur, props, use*)

2-Acetylpyrrolidine A-90

[60026-20-2]
1-(2-Pyrrolidinyl)ethanone, 9CI



(*S*)-*form*

$C_6H_{11}NO$
Aroma constit. of wheat bread crust. Proposed precursor of the roasty-popcorn flavour material 5-Acetyl-3,4-dihydro-2*H*-pyrrole, A-44 formed in food processing. Undergoes ready air oxidn. to 5-Acetyl-3,4-dihydro-2*H*-pyrrole, A-44.

(*S*)-*form* [120966-82-7]

[90427-71-7]
$[\alpha]_D^{25}$ -2.4 (c, 3 in 2*M* HCl).

N-tert-*Butyloxycarbonyl:*
$C_{11}H_{19}NO_3$ 213.276
Cryst. (pentane). Mp 38°. $[\alpha]_D^{25}$ -57.8 (c, 4.3 in $CHCl_3$).

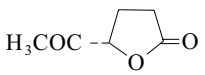
N-*Benzyl:*
$C_{13}H_{17}NO$ 203.283
$Bp_{0.01}$ 85° (bulb). $[\alpha]_D^{25}$ -81.2 (c, 1.04 in EtOH).

(±)-*form*
N-*Me:* [54969-35-6] *2-Acetyl-1-methylpyrrolidine*
$C_7H_{13}NO$ 127.186
Bp_{14} 58-59°.

Duhamel, L. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1974, **279**, 1159-1161 (*N-Me*)
Fittkau, S. *et al., J. Prakt. Chem.*, 1986, **328**, 529-538 (*S-form, synth*)
Goldstein, S.W. *et al., J.O.C.*, 1992, **57**, 1179-1190 (*S-form, derivs*)
Hofmann, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619 (*synth, ms*)

5-Acetyltetrahydro-2(3*H*)-furanone, 9CI A-91

[29393-32-6]
5-Oxo-4-hexanolide. ***Solerone***



(*S*)-*form*

$C_6H_8O_3$ 128.127

(*S*)-*form* [61262-92-8]
$Bp_{0.2}$ 83°. $[\alpha]_D^{25}$ +13.4 (c, 0.25 in MeOH).

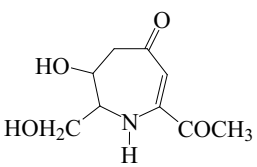
(±)-*form* [69308-41-4]
$Bp_{1.2}$ 102-104°.

(ξ)-*form*
Aroma constit. of wine esp. sherry. Formed during fermentation.

Augustyn, D.P.H. *et al., J. Agric. Food Chem.*, 1971, **19**, 1128 (*synth, struct*)
Yanrad, S.-I. *et al., Tet. Lett.*, 1976, 2557 (*synth*)
Jensen, J.E. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 457 (*synth, ir, pmr*)

2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4*H*-azepine-4-one A-92

[220662-48-6, 220662-49-7]

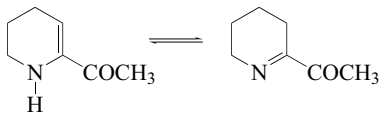


$C_9H_{13}NO_4$ 199.206
Minor product from the Maillard reaction of xylose and glycine. Yellow solid. Isol. as *cis*/*trans*- mixt..

Ames, J.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 438-443 (*formn, pmr, cmr, ms*)

6-Acetyl-1,2,3,4-tetrahydropyridine A-93

[27300-27-2]
Methyl 3,4,5,6-tetrahydro-2-pyridyl ketone, 8CI. 2-Acetyl-3,4,5,6-tetrahydropyridine. 2-Acetyl-Δ^1-piperideine. 2-Acetyl-Δ^2-piperideine. 1-(1,2,3,4-Tetrahydro-2-pyridinyl)ethanone



1*H*-*form* 3*H*-*form*

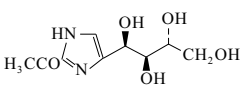
$C_7H_{11}NO$ 125.17
Tautomeric, 1*H*-form predominates *ca.* 2:1. Responsible for mousy taint in wines. Constit. of wheat, popcorn and bread aroma. Unstable liq. Bp_3 65-67°. Odour threshold 0.06 ng/L in air.

Hydrochloride:
Mp 112-119°.

Hunter, I.R. *et al., Cereal Chem.*, 1969, **46**, 189 (*isol*)
Büchi, G. *et al., J.O.C.*, 1971, **36**, 609 (*ir, uv, pmr, ms, synth*)
Strauss, C.R. *et al., Chem. Ind. (London)*, 1984, 109 (*isol*)
De Kimpe, N. *et al., J.O.C.*, 1993, **58**, 2904 (*synth, pmr, cmr, ms*)
De Kimpe, N. *et al., Tetrahedron*, 1995, **51**, 2387 (*synth*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619; 2270-2277 (***synth, ms, bibl***)

2-Acetyl-4(5)-(1,2,3,4-tetrahydroxybutyl)imidazole A-94

[95120-07-3]
*1-[4-(1,2,3,4-Tetrahydroxybutyl)-1*H*-imidazol-2-yl]ethanone, 9CI*



(1*R*,2*S*,3*R*)-*form*

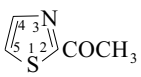
$C_9H_{14}N_2O_5$ 230.22

(1*R*,2*S*,3*R*)-*form* [94944-70-4]
Minor component of Caramel Colour III. Cryst. (H_2O). Mp 232-233°. $[\alpha]_D^{25}$ -12 (c, 1.17 in 1M HCl).

Kröplien, U. *et al., J.O.C.*, 1985, **50**, 1131 (*isol, struct*)
Halweg, K.M. *et al., J.O.C.*, 1985, **50**, 1133 (*synth, uv, pmr, cmr, ir*)
Sweeny, J.G. *et al., J.O.C.*, 1985, **50**, 1133 (*synth, pmr, uv, ir, cmr, abs config*)

2-Acetylthiazole A-95

[24295-03-2]
1-(2-Thiazolyl)ethanone, 9CI. Methyl 2-thiazolyl ketone, 8CI. FEMA 3328



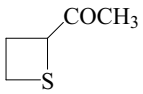
C_5H_5NOS 127.167
Important flavour component; antioxidant. Present in asparagus, kohlrabi, cooked potatoes, roast turkey, raw chicken, cooked beef, pork liver, beer, whisky, heated beans, various mushrooms, rice bran and maize. Mp 64.5-65.5°. Bp_{15} 98-102°.

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1494D (*ir*)
Hartman, G.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1030 (*isol*)

Medici, A. *et al., Tet. Lett.*, 1983, **24**, 2901 (*synth*)
Dondoni, A. *et al., J.O.C.*, 1991, **56**, 5294 (*synth, ir, pmr, cmr*)

2-Acetylthietane A-96

[119209-96-0]
1-(2-Thietanyl)ethanone, 9CI



C_5H_8OS 116.184

(±)-form
Bp_7 49°.

(ξ)-form
Thiamine thermal degradation product formed in meat aroma model systems.
Yonemoto, H. *et al., Yakugaku Zasshi*, 1957, **77**, 1128-1132; *CA*, **52**, 5421b (*synth*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, pmr, ms*)

2-Acetylthiophene A-97

[88-15-3]
1-(2-Thienyl)ethanone, 9CI. Methyl 2-thienyl ketone. 2-Acetothienone



C_6H_6OS 126.179
Organoleptic which contributes to several aromas. Liq. d^{24} 1.17. Mp 9°. Bp 213-214° Bp_{13} 94.5-96.5°.
► LD_{50} (mus, ipr) 40 mg/kg. OB6300000

E-Oxime: [92313-54-7]
C_6H_7NOS 141.193
Cryst. (EtOAc/hexane). Mp 113-114°.

Z-Oxime: [92313-45-6]
C_6H_7NOS 141.193
Cryst. (EtOAc/hexane). Mp 84-85°.

Phenylhydrazone: [55968-17-7]
Yellow cryst. (EtOH). Mp 96°.

Semicarbazone: [3771-70-8]
Plates (C_6H_6). Mp 190-191°.

[39709-34-7]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 53A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 596C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1472C (*ir*)
Hartough, H.D. *et al., J.A.C.S.*, 1947, **69**, 1012 (*synth*)
Bohlmann, F. *et al., Chem. Ber.*, 1964, **97**, 2135 (*isol, ir, uv, pmr*)
Nishiwaki, T. *et al., Tetrahedron*, 1967, **23**, 2979 (*ms*)
Martin, M.L. *et al., Bull. Soc. Chim. Fr.*, 1968, 698 (*pmr*)
Zeisberg, R. *et al., Chem. Ber.*, 1975, **108**, 1040 (*cmr, struct*)
Conde, S. *et al., J. Het. Chem.*, 1985, **22**, 301 (*oximes, config, pmr*)
Keumi, T. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 455 (*synth*)
Goda, H. *et al., Synthesis*, 1992, 849 (*synth*)
Spinelli, D. *et al., Acta Chem. Scand.*, 1993, **47**, 160 (*cmr, O-17 nmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABI500

3-Acetylthiophene A-98

[1468-83-3]
1-(3-Thienyl)ethanone, 9CI. Methyl 3-thienyl ketone. 3-Acetothienone

C_6H_6OS 126.179
Maillard product; organoleptic. Mp 61-62°. Bp_5 78-79°.

Phenylhydrazone:
Mp 114°.

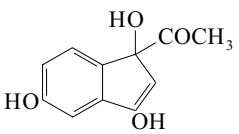
Semicarbazone:
Mp 173-174°.

[39709-34-7]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 54B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 597B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1473C (*ir*)
Macdowell, D.W.H. *et al., J. Het. Chem.*, 1965, **2**, 44 (*synth*)
Clarke, J.A. *et al., Tet. Lett.*, 1975, 4705 (*synth*)
Macco, A.A. *et al., J.O.C.*, 1978, **43**, 1591 (*synth, pmr*)
Collins, S. *et al., J.O.C.*, 1990, **55**, 3565 (*synth*)

1-Acetyl-1,3,5-trihydroxy-1*H*-indene A-99

*1-Acetyl-1*H*-indene-1,3,5-triol, 9CI*

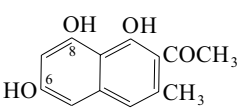


$C_{11}H_{10}O_4$ 206.198

3,5-Di-Me ether: [151466-74-9] *1-Acetyl-1-hydroxy-3,5-dimethoxy-1*H*-indene.* ***Coixinden B***
$C_{13}H_{14}O_4$ 234.251
Constit. of *Coix lacrima-jobi* var. *mayuen*.
Ishiguro, Y. *et al., Chem. Lett.*, 1993, 1139 (*isol*)

2-Acetyl-1,6,8-trihydroxy-3-methylnaphthalene A-100

[23520-25-4]
1-(1,6,8-Trihydroxy-3-methyl-2-naphthalenyl)ethanone, 9CI. 1′,6′,8′-Trihydroxy-3′-methyl-2′-acetonaphthone, 8CI. 7-Acetyl-6-methyl-1,3,8-naphthalenetriol. 6-Hydroxymusizin



$C_{13}H_{12}O_4$ 232.235

8-O-β-D-Glucopyranoside: [23566-96-3]
$C_{19}H_{22}O_9$ 394.377
Isol. from the rhubarb Rhei rhizoma. Needles (EtOAc). Mp 214-215° (207°).

6-Me ether: [22649-04-3] *2-Acetyl-1,8-dihydroxy-6-methoxy-3-methylnaphthalene.* ***Torachrysone.*** *Nakahalene*
$C_{14}H_{14}O_4$ 246.262
Isol. from seeds of *Cassia tora* (charota). Yellow needles (C_6H_6). Mp 214-215° dec. (207-208°).

6-Me ether, di-Ac: [22649-05-4]
$C_{18}H_{18}O_6$ 330.337
Plates (EtOH). Mp 181-182°.

6-Me ether, 8-O-β-D-glucopyranoside: [64032-49-1] ***Torachrysone 8-glucoside***
$C_{20}H_{24}O_9$ 408.404
Isol. from Rhei rhizoma. Needles + $1H_2O$ (MeOH). Mp 150-152°. $[\alpha]_D^{21}$ -109 (c, 0.5 in MeOH).

6-Me ether, 8-O-(6-O-oxalyl-β-D-glucopyranoside): [64078-76-8] ***Torachrysone 8-(6-oxalylglucoside)***
$C_{22}H_{24}O_{12}$ 480.424
Constit. of a Rhei sp.. Pale yellow powder. $[\alpha]_D^{18}$ -102 (c, 0.25 in H_2O).

6-Me ether, 8-O-[β-D-xylopyranosyl-(1→6)-β-D- glucopyranoside]: [150566-02-2]
$C_{25}H_{32}O_{13}$ 540.52
Orange needles ($CHCl_3$/MeOH). Mp 252-253°.

6-Me ether, 8-O-[β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]: [245724-11-2] ***Torachrysone 8-(2-apiosylglucoside)***
$C_{25}H_{32}O_{13}$ 540.52
Constit. of the seeds of *Cassia tora* (charota). Pale yellow powder. $[\alpha]_D$ -23.4 (c, 0.1 in Py). λ_{max} 233 (log ε 4.41); 262 (log ε 4.09); 306 (log ε 3.58); 323 (log ε 3.59); 337 (log ε 3.64) (MeOH).

6-Me ether, 8-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [245724-09-8] ***Torachrysone 8-β-gentiobioside***
$C_{26}H_{34}O_{14}$ 570.546
Constit. of the seeds of *Cassia tora* (charota). Needles (MeOH). Mp 221°. $[\alpha]_D$ -18.7 (c, 0.1 in MeOH). λ_{max} 236 (log ε 4.38); 263 (log ε 4.19); 310 (log ε 3.59); 324 (log ε 3.59); 339 (log ε 3.59) (MeOH).

6-Me ether, 8-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [245724-10-1]
$C_{38}H_{54}O_{24}$ 894.83
Constit. of the seeds of *Cassia tora* (charota). Pale yellow powder. $[\alpha]_D$ -9 (c, 0.1 in Py). λ_{max} 236 (log ε 4.48); 262 (log ε 4.24); 312 (log ε 3.64); 325 (log ε 3.65); 340 (log ε 3.65) (MeOH).

8-Me ether: [173867-28-2] *2-Acetyl-1,6-dihydroxy-8-methoxy-3-methylnaphthalene. Tinnevellin.* ***Isotorachrysone***
$C_{14}H_{14}O_4$ 246.262
Yellow needles ($CHCl_3$/MeOH). Mp 219°.

8-Me ether, 6-O-β-D-glucopyranoside: [80358-06-1]
$C_{20}H_{24}O_9$ 408.404
Pale yellow powder. Mp 175°.

6,8-Di-Me ether: [22699-07-6] *2-Acetyl-1-hydroxy-6,8-dimethoxy-3-methylnaphthalene. 1-(1-Hydroxy-6,8-dimethoxy-3-methyl-2-napthalenyl)ethanone, 9CI. 2-Acetyl-6,8-dimethoxy-1-naphthol*
$C_{15}H_{16}O_4$ 260.289

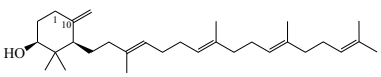
Needles. Mp 98-99°.

Tri-Me ether: [22649-03-2]
$C_{16}H_{18}O_4$ 274.316
Tiny plates (MeOH aq.). Mp 63-64°.

Shibata, S. *et al., Chem. Pharm. Bull.*, 1969, **17**, 454-475 (*Torachrysone, isol*)
Brown, K.S. *et al., Tet. Lett.*, 1969, 471-476 (*8-glucoside, isol*)
Harris, T.M. *et al., J.A.C.S.*, 1975, **97**, 3270-3271 (*synth*)
Dreyer, D.L. *et al., J.A.C.S.*, 1975, **97**, 4985-4990 (*3,8-di-Me ether, isol*)
Tsuboi, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2708-2712 (*6-Me 8-glucosides*)
Yamasaki, K. *et al., Tet. Lett.*, 1977, 1231-1234 (*cmr, glucosides*)
Lemli, J. *et al., Planta Med.*, 1981, **43**, 11-17 (*Tinnevellin glucoside*)
Gill, M. *et al., Prog. Chem. Org. Nat. Prod.*, 1987, **51**, 121-122 (*3,8-di-Me ether, occur*)
Wei, B.-L. *et al., J. Nat. Prod.*, 1992, **55**, 967-969 (*Nakahalene*)
Lin, C.N. *et al., Phytochemistry*, 1993, **33**, 905-908 (*6-Me ether, 8-xylosylglucoside*)
Lin, C.-N. *et al., J. Nat. Prod.*, 1995, **58**, 1934-1940 (*Isotorachrysone*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1121-1127 (*Torachrysone glycosides, activity*)

Achilleol A A-101

[125287-06-1]



$C_{30}H_{50}O$ 426.724
$[\alpha]_D$ -10.9 (c, 0.9 in $CHCl_3$).

Dodecanoyl: [213007-57-9]
$C_{42}H_{72}O_2$ 609.03

Tetradecanoyl: [213007-39-7]
$C_{44}H_{76}O_2$ 637.083

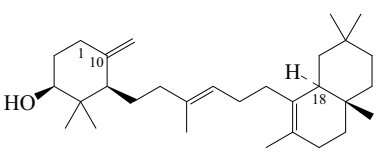
Hexadecanoyl: [213007-45-5]
$C_{46}H_{80}O_2$ 665.137

$\Delta^{1(10)}$-Isomer: [220359-76-2] ***Camelliol C***
$C_{30}H_{50}O$ 426.724
Constit. of sasanqua oil (*Camellia sasanqua*). Gum. $[\alpha]_D^{25}$ -12.9 (c, 0.2 in $CHCl_3$).

Barrero, A.F. *et al., Tet. Lett.*, 1989, **30**, 3351-3352 (*Achilleol A*)
Barrero, A.F. *et al., Phytochemistry*, 1998, **48**, 1237-1240 (*esters*)
Akihisa, T. *et al., J. Nat. Prod.*, 1999, **62**, 265-268 (*Camelliol C*)
Joubert, B.M. *et al., Org. Lett.*, 2000, **2**, 339-341 (*biosynth*)

Achilleol B A-102

[132922-73-7]



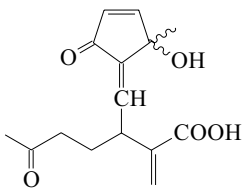
$C_{30}H_{50}O$ 426.724
Viscous oil. $[\alpha]_D$ -8.1 (c, 1 in $CHCl_3$).

$\Delta^{1(10)}$-Isomer, 18-epimer: [220359-69-3] ***Camelliol A***
$C_{30}H_{50}O$ 426.724
Constit. of Sasanqua oil (*Camellia sasanqua*). Gum. $[\alpha]_D^{25}$ +4 (c, 0.2 in $CHCl_3$).

Barrero, A.F. *et al., Tetrahedron*, 1990, **46**, 8161-8168 (*isol, ir, pmr, cmr, ms*)
Akihisa, T. *et al., J. Nat. Prod.*, 1999, **62**, 265-268 (*Camelliol A*)

Achimilic acid A-103

[110732-04-2]
3-[(2-Hydroxy-2-methyl-5-oxo-3-cyclopenten-1-ylidene)methyl]-2-methylene-6-oxoheptanoic acid, 9CI



$C_{15}H_{18}O_5$ 278.304
Isol. from *Achillea millefolium* (yarrow). Obt. as mixture of diastereoisomers.

Me ester:
$C_{16}H_{20}O_5$ 292.331
Cryst. (Et_2O/pentane). Mp 76-77°. $[\alpha]_D$ -23.6 ($CHCl_3$).

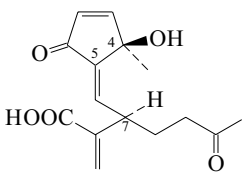
Me ester, stereoisomer (1):Achimilic acid B methyl ester
$C_{16}H_{20}O_5$ 292.331
Oil. $[\alpha]_D$ -78.2 ($CHCl_3$).

Me ester, stereoisomer (2):Achimilic acid C methyl ester
$C_{16}H_{20}O_5$ 292.331
Oil. $[\alpha]_D$ -87.3 ($CHCl_3$).

Japan. Pat., 1987, 87 81 349; *CA*, **107**, 161673 (*isol, cmr, ir, uv, ms*)

Achimillic acid A A-104

[157184-04-8]



$C_{15}H_{18}O_5$ 278.304
Constit. of *Achillea millefolium* (yarrow). Needles (as Me ester). Mp 76-77° (Me ester). $[\alpha]_D$ -23.6 (c, 1 in $CHCl_3$) (Me ester). λ_{max} 245 (ϵ) (EtOH) (Derep).

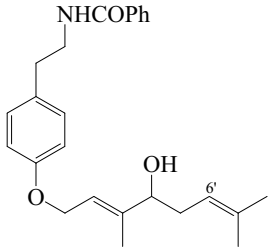
5Z-Isomer: [157184-05-9] ***Achimillic acid B***
$C_{15}H_{18}O_5$ 278.304
Constit. of *Achillea millefolium* (yarrow). Oil (as Me ester). $[\alpha]_D$ -78.2 (c, 1 in $CHCl_3$) (Me ester). λ_{max} 245 (ϵ) (EtOH) (Derep).

4-Epimer: [157184-06-0] ***Achimillic acid C***
$C_{15}H_{18}O_5$ 278.304
Constit. of *Achillea millefolium* (yarrow). Oil (as Me ester). $[\alpha]_D$ -87.3 (c, 1 in $CHCl_3$) (Me ester). λ_{max} 245 (ϵ) (EtOH) (Derep).

Tozyo, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1096 (*isol, pmr, cmr, cryst struct*)

Acidissiminol A-105

[126006-00-6]



$C_{25}H_{31}NO_3$ 393.525
Alkaloid from the fruit of *Limonia acidissima* (wood apple). Cryst. (EtOAc/hexane). Mp 85-87°.

O-*Ac:* [33055-26-4] **N-*Benzoyl-4-(4-acetoxyneryloxy)phenethylamine***
$C_{27}H_{33}NO_4$ 435.562
Cryst. (EtOAc/hexane). V. sol. MeOH. Mp 64-65°. Opt. inactive. Related to Severine.

O-*Octadecanoyl:* [126005-91-2] ***Acidissiminin***
$C_{43}H_{65}NO_4$ 659.991
Alkaloid from the fruits of *Limonia acidissima* (wood apple). Amorph. solid (EtOAc/hexane). Mp 65°. $[\alpha]_D$ 0 ($CHCl_3$). λ_{max} 225 (ϵ); 277 (sh) (ϵ); 286 (ϵ) (MeOH) (Derep).

6′,7′-Epoxide: [139165-01-8]

[33055-25-3] ***Acidissiminol epoxide***. *Severine*
$C_{25}H_{31}NO_4$ 409.524
Alkaloid from fruits of *Limonia acidissima* (wood apple). Cryst. (MeOH). Mp 146-149° (141-143°). Severine originally considered to be a diol with formula $C_{25}H_{33}NO_4$. Identity of Acidissiminol epoxide and Severine not confirmed; stereochem. not established.

6′,7′-Epoxide, octadecanoyl: [139083-09-3] ***Acidissiminin epoxide***. *Severine palmitate*
$C_{43}H_{65}NO_5$ 675.99
Alkaloid from the fruit of *Limonia acidissima* (wood apple). Cryst. (C_6H_6/hexane). Mp 105-106° Mp 113-114°. Identity of Acidissiminin epoxide and Severin palmitate not definitely establ. Mps are similar.

6′,7′-Dihydro, 6′,7′-dihydroxy: [160387-10-0] ***Dihydroxyacidissiminol***
$C_{25}H_{33}NO_5$ 427.539
Alkaloid from fruits of *Limonia acidissima* (wood apple). Amorph. semi-solid.

Dreyer, D.L. *et al., Tetrahedron*, 1967, **23**, 4613; 1970, **26**, 5745; 1980, **36**, 827 (*Severine, Severine palmitate, N-Benzoyl-4-(4-acetoxyneryloxy)phenethylamine*)
Ghosh, P. *et al., J. Nat. Prod.*, 1989, **52**, 1323; 1991, **54**, 1389 (*Acidissiminol, Acidissiminin*)
Ghosh, P. *et al., Phytochemistry*, 1994, **37**, 757 (*Dihydroxyacidissiminol, Acidissiminol epoxide*)

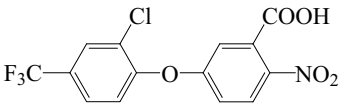
Acidophilucin A A-106

[137699-22-0]
Prod. by *Lactobacillus acidophilus* LAPT 1060. Bacteriocin.

Toba, T. *et al., Lett. Appl. Microbiol.*, 1991, **12**, 106-108 (*isol*)

Acifluorfen, ANSI, BSI, ISO, WSSA A-107

[50594-66-6]
5-[2-Chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid, 9CI. Tackle 25



$C_{14}H_7ClF_3NO_5$ 361.661
Selective pre- and post-emergence herbicide. Used on soybeans and peanuts. Off-white solid. Mp 151.5-157° (140-150°) Mp 240°.

▶ Skin and eye irritant. LD_{50} (rat, orl) 2025 mg/kg. DG5643070

Na salt: [62476-59-9] *Acifluorfen sodium. Blazer. Scifluorfen. RH 6201*
Powder. Mp 124-125°.

▶ DG5643200

Me ester: [50594-67-7] *Acifluorfen methyl*
$C_{15}H_9ClF_3NO_5$ 375.688

Carboxymethyl ester: [77501-60-1] ***Fluoroglycofen, ANSI, BSI***. O-*[5-(2-Chloro-α,α,α-trifluoro-*p*-tolyloxy)-2-nitrobenzoyl]glycolic acid*

2-Ethoxy-2-oxoethyl ester: [77501-90-7] ***Fluoroglycofen-ethyl***
$C_{18}H_{13}ClF_3NO_7$ 447.751
Dark amber solid. d^{25} 1.01. Mp 65°.

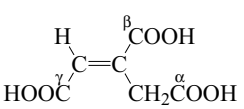
▶ LD_{50} (rat, orl) 1500 mg/kg. DG5643100

Nitrile: [50594-65-5]
Cryst. Mp 95-103°.

Ger. Pat., 1973, 2 311 638; *CA*, **80**, 3253 (*synth*)
Johnson, W.O. *et al., J. Agric. Food Chem.*, 1978, **26**, 285 (*synth, props*)
Eur. Pat., 1980, 20 052; *CA*, **94**, 191 921 (*synth, activity, Fluoroglycofen*)
Orr, G.L. *et al., ACS Symp. Ser.*, 1982, **181**, 131 (*rev*)
Lee, G.H. *et al., J. Agric. Food Chem.*, 1985, **33**, 499 (*pmr, cmr*)
Kennard, C.H.L. *et al., Aust. J. Chem.*, 1987, **40**, 1131 (*cryst struct*)
Teasdale, J.R. *et al., Weed Technol.*, 1987, **1**, 165 (*activity, Fluoroglycofen*)
Maigrot, P.H. *et al., Proc. Br. Crop Prot. Conf. Weeds*, 1989, 47 (*activity, Fluoroglycofen-Et*)
Pesticide Manual, 9th edn., 1991, No. 40; No. 6565
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A788

Aconitic acid A-108

[499-12-7]
1-Propene-1,2,3-tricarboxylic acid, 9CI. Achilleaic acid. Citridinic acid. Equisetic acid. Pyrocitric acid. 3-Carboxy-2-pentenedioic acid. FEMA 2010



(*E*)-*form*

$C_6H_6O_6$ 174.11
▶ UD2380000

Mixed Et esters:Ethyl aconitate. FEMA 2417
$C_8H_{10}O_6$ 202.163
Flavouring ingredient. Prepd. as mixt. of mono-, di- and triesters by acid-catalysed esterification of aconitic acid with EtOH or by heating, Tri-Et ester. Oily liq. with sweet, fruity odour and flavour. Mp 260°.

(E)-form [4023-65-8]
Isol. from *Asarum europaeum*, from cane-sugar molasses, roasted chicory root, roasted malt barley, passion fruit, sorghum root and sugar beet. Flavouring agent used in fruit flavours and alcoholic beverages. Leaflets (H_2O). Sol. H_2O, EtOH. Mp 194-195° dec. pK_{a2} 4.46 (25°). Decarboxylates at Mp to Methylenebutanedioic acid, M-403. Mp variable with rate of heating.

Tri-Et ester: [68077-28-1]

[5349-99-5]
$C_{12}H_{18}O_6$ 258.271
Bp_{18} 172°.

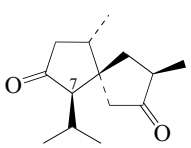
(Z)-form [585-84-2]
Present in apple fruits, maple syrup and passion fruit juice. Mp 125°. Gives (*E*)-form on heating.

[1321-30-8, 5349-99-5, 20820-77-3, 65629-33-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 505D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 789B; 789C (*nmr*)
Malachowski, R. *et al., Ber.*, 1928, **61**, 2521 (*synth, props*)
Org. Synth., Coll. Vol., 2, 1943, 12 (*synth*)
Miller, R.E. *et al., Adv. Carbohydr. Chem.*, 1951, **6**, 231 (*rev*)
Klostergaard, H. *et al., J.O.C.*, 1958, **23**, 108-110 (*tri-Et ester*)
Krogh, A. *et al., Acta Chem. Scand.*, 1969, **23**, 2932 (*isol*)
Bartos, J. *et al., Pure Appl. Chem.*, 1984, **56**, 467 (*use*)
Barlianto, H. *et al., Z. Lebensm.-Unters. -Forsch.*, 1994, **198**, 215-222 (*occur, glc, ms*)
Nagel, N. *et al., Acta Cryst. C*, 1996, **52**, 2912-2915 (*cryst struct, Z-form*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 38; 944-945 (*mixed Et esters*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 30-31; 514-515 (*mixed Et esters*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4974
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADH000

3,8-Acoranedione A-109

[10121-28-5]
Acorone



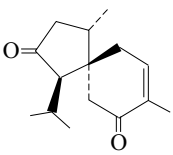
$C_{15}H_{24}O_2$ 236.353
Constit. of *Acorus calamus* (sweet flag). Cryst. (heptane). Mp 100°. $[\alpha]_D^{15}$ +139.5 (EtOH).

*7-Epimer:**Epiacorone***
$C_{15}H_{24}O_2$ 236.353
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D$ -53.9 (c, 0.54 in MeOH).

McEachan, C.E. *et al., J.C.S.(C)*, 1966, 579 (*cryst struct*)
Andersen, N.H. *et al., Tet. Lett.*, 1972, 899 (*abs config*)
Marx, J.N. *et al., J.O.C.*, 1975, **40**, 1602 (*synth*)
McCrae, D.A. *et al., J.O.C.*, 1977, **42**, 1607 (*synth*)
Ackroyd, J. *et al., Helv. Chim. Acta*, 1985, **68**, 338 (*synth*)
Rao, G.S.R.S. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 783 (*synth*)
Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175 (*isol, pmr, cmr*)
Srikrishna, A. *et al., Tet. Lett.*, 1996, **37**, 1683 (*synth*)
Biju, P.J. *et al., Tet. Lett.*, 1999, **40**, 2405-2406 (*synth*)
Srikrishna, A. *et al., Tetrahedron*, 2000, **56**, 8189-8195 (*synth*)

4-Acorene-3,8-dione A-110

[33983-45-8]
Acoronene



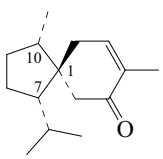
$C_{15}H_{22}O_2$ 234.338
Constit. of *Acorus calamus* (sweet flag). Cryst. (hexane). Mp 69°. $[\alpha]_D$ +66.8 (c, 1 in dioxan). $[\alpha]_D$ -104 (c, 0.12 in MeOH).

*7-Epimer:**Epiacoronene***
$C_{15}H_{22}O_2$ 234.338
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D$ -96 (c, 0.12 in MeOH). λ_{max} 238 (ε 3640) (MeOH).

Minato, H. *et al., Chem. Pharm. Bull.*, 1971, **19**, 638
Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175 (*isol, pmr, cmr*)

4-Acoren-3-one A-111

[5956-05-8]
Acorenone



$C_{15}H_{24}O$ 220.354
Constit. of carrot (*Daucus carota*) and *Acorus calamus* (sweet flag). Oil. $Bp_{0.1}$ 61°. $[\alpha]_D^{20}$ -22.3. n_D^{20} 1.5039.

1-Epimer: [21653-33-8] *3-Acoren-5-one.* ***Acorenone B***
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D$ +12.3 (c, 0.25 in $CHCl_3$).

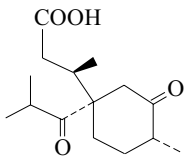
1,7-Diepimer: [311350-99-9] ***10-Epi-3-acoren-5-one***
$C_{15}H_{24}O$ 220.354

McClure, R.J. *et al., Chem. Comm.*, 1968, 1135

(*cryst struct*)
Trost, B.M. *et al., J.A.C.S.*, 1975, **97**, 5873 (*synth*)
Oppolzer, W. *et al., Helv. Chim. Acta*, 1977, **60**, 2388 (*synth*)
Lange, G.L. *et al., Tet. Lett.*, 1977, 4479 (*synth*)
Rascher, W. *et al., Tetrahedron*, 1977, **33**, 575 (*synth*)
Naegeli, P. *et al., Tet. Lett.*, 1978, 2127 (*synth*)
White, J.D. *et al., J.A.C.S.*, 1981, **103**, 1813 (*synth*)
Baldwin, S.W. *et al., Tet. Lett.*, 1982, **23**, 1235 (*synth*)
Iwata, C. *et al., Chem. Comm.*, 1984, 781 (*synth*)
Nagumo, S. *et al., Chem. Comm.*, 1990, 1778 (*synth*)
Kido, F. *et al., J.C.S. Perkin 1*, 1992, 229 (*synth, bibl*)
Wu, C.-L. *et al., J. Chin. Chem. Soc. (Taipei)*, 1995, **42**, 597 (*isol, pmr, cmr*)
Weyerstahl, P. *et al., Flavour Fragrance J.*, 2000, **15**, 61-83 (*1,7-diepimer*)

Acoric acid A-112

[5956-06-9]

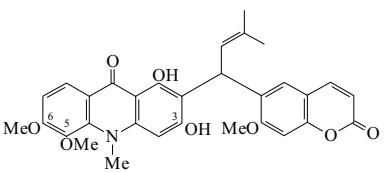


$C_{15}H_{24}O_4$ 268.352
Constit. of *Acorus calamus* (sweet flag). Cryst. (Et_2O/petrol). Mp 166-168°. $[\alpha]_D^{25}$ +27 (c, 1 in $CHCl_3$). Log P 1.53 (calc).

Birch, A.J. *et al., J.C.S.*, 1964, 2923 (*isol*)
Birch, A.J. *et al., J.C.S. Perkin 1*, 1972, 1186 (*synth*)
Rao, G.S.R.S. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 1089 (*synth*)
Ramanathan, H. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 901 (*synth*)

Acrimarine A A-113

[119152-47-5]



$C_{31}H_{29}NO_8$ 543.572
Pale yellow oil. $[\alpha]_D$ -9.76 (c, 0.082 in $CHCl_3$).

3-Me ether: ***Acrimarine N***
$C_{32}H_{31}NO_8$ 557.599
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisi*) x Dancy tangerine (*Citrus tangerina*)]. Yellow oil. Opt. inactive.

3-Me ether, N-*de-Me:* [119152-48-6] ***Acrimarine B***
$C_{31}H_{29}NO_8$ 543.572
Yellow prisms (Me_2CO). Mp 288-290°. $[\alpha]_D$ -7.14 (c, 0.056 in $CHCl_3$).

O^6*-De-Me:* [147395-91-3] ***Acrimarine K***
$C_{30}H_{27}NO_8$ 529.545
Yellow oil. $[\alpha]_D^{25}$ 0 (c, 0.0695 in $CHCl_3$).

O^6*-De-Me, 3-Me ether:* [129722-89-0] ***Acrimarine F***
$C_{31}H_{29}NO_8$ 543.572
Pale yellow powder.

O^6*-De-Me, 3-Me ether,* N^6*-de-Me:* [129722-88-9] ***Acrimarine E***
$C_{30}H_{27}NO_8$ 529.545
Pale yellow prisms (Me_2CO). Mp 274-276°. $[\alpha]_D$ +20.1 (c, 0.05 in Me_2CO).

6-Demethoxy, O^5*-de-Me:* [129722-97-0] ***Acrimarine G***
$C_{29}H_{25}NO_7$ 499.519
Yellow oil. $[\alpha]_D$ +8 (c, 0.075 in $CHCl_3$).

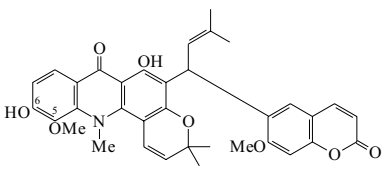
6-Demethoxy, O^5*-de-Me, 3-Me ether:* [132185-44-5] ***Acrimarine H***
$C_{30}H_{27}NO_7$ 513.546
Alkaloid from roots of *Citrus* spp.. Yellow oil. $[\alpha]_D$ 0 (Me_2CO).

Bis(demethoxy): [147513-68-6] ***Acrimarine M***
$C_{29}H_{25}NO_6$ 483.52
Yellow oil. $[\alpha]_D^{25}$ 0 (c, 0.052 in $CHCl_3$).

Ito, C. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2586 (*Acrimarine H*)
Furukawa, H. *et al., J.C.S. Perkin 1*, 1990, 1593 (*isol, pmr, cmr, struct*)
Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2363 (*Acrimarine K, Acrimarine M*)
Takemura, Y. *et al., Heterocycles*, 1994, **38**, 1937 (*Acrimarine N*)

Acrimarine J A-114

[147395-90-2]

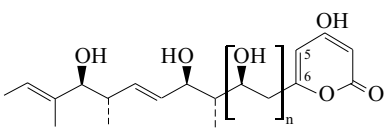


$C_{35}H_{33}NO_8$ 595.648
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisii*) × Dancy tangerine (*Citrus tangerina*)]. Yellow oil. $[\alpha]_D^{28}$ 0 (c, 0.106 in $CHCl_3$).

6-Deoxy, O^5*-de-Me:* [147395-89-9] ***Acrimarine I***
$C_{34}H_{31}NO_7$ 565.621
Alkaloid from roots of Yalaha. Yellow oil. $[\alpha]_D^{26}$ +27.8 (c, 0.036 in $CHCl_3$).

Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2363 (*isol, uv, ir, pmr, cmr, ms, struct*)

ACRL Toxins A-115



Toxin II, n = 0
Toxin III, n= 1
Toxin IV, n = 2

ACRL Toxin II [101951-84-2]

$C_{17}H_{24}O_5$ 308.374
Prod. by the fungus *Alternaria citri* on rough lemon. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 67-68°. $[\alpha]_D$ +5 (c, 0.25 in MeOH). λ_{max} 277 (ε 4100) (MeOH) (Berdy). λ_{max} 285 (MeOH-HCl) (Berdy).

ACRL Toxin III [101951-97-7]

$C_{19}H_{28}O_6$ 352.427
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 142-145°. $[\alpha]_D$ -17 (c, 0.60 in MeOH). λ_{max} 280 (MeOH) (Berdy).

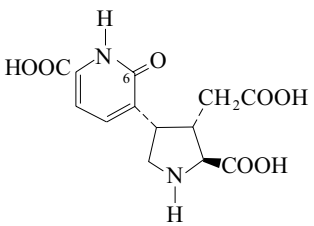
5,6-Dihydro: [98353-41-4] ***ACRL Toxin I***
$C_{19}H_{30}O_6$ 354.442
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 192-196°. Major phytotoxic component λ_{max} 245 (ε 9500) (MeOH) (Berdy). λ_{max} 236 (MeOH-HCl) (Berdy).

ACRL toxin IV [101951-98-8]
$C_{21}H_{32}O_7$ 396.48
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 102-105°. $[\alpha]_D$ -11 (c, 0.30 in MeOH). λ_{max} 280 (MeOH) (Berdy).

Gardner, J.M. *et al., Phytochemistry*, 1985, **24**, 2861; 1986, **25**, 69 (*isol, ACRL Toxin I*)
Kono, Y. *et al., Phytochemistry*, 1985, **24**, 2869; 1986, **25**, 69 (*isol, struct, abs config*)
Lichtenthaler, F.W. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 1339 (*synth*)
Mulzer, J. *et al., Angew. Chem., Int. Ed.*, 1993, **32**, 1452 (*synth*)
Munchhof, M.J. *et al., J.O.C.*, 1994, **59**, 7566 (*synth*)
Paterson, I. *et al., Synthesis*, 1998, 639-652 (*synth*)

Acromelic acid A A-116

[86630-09-3]
5-[5-Carboxy-4-(carboxymethyl)-3-pyrrolidinyl]-1,6-dihydro-6-oxo-2-pyridinecarboxylic acid, 9CI. Acromelinic acid A



$C_{13}H_{14}N_2O_7$ 310.263
Cryst. Sol. H_2O; poorly sol. Me_2CO, hexane. Mp 310°. $[\alpha]_D$ +27.8 (c, 0.35 in H_2O). Struct. established by synth. Phys. props. are of synthetic material λ_{max} 240 (ε 4370); 315 (ε 8910) (pH 2) (Derep). λ_{max} 241 (ε 5130); 312 (ε 9120) (pH 12) (Derep). λ_{max} 243 (ε 5500); 315 (ε 9550) (H_2O pH 7) (Derep). λ_{max} 242 ; 317 (pH 7 buffer) (Berdy). λ_{max} 240 ; 313 (pH 2 buffer) (Berdy). λ_{max} 241 ; 312 (pH 12 buffer) (Berdy). λ_{max} 240 (ε 5130); 313 (ε 9550) (H_2O) (Berdy).

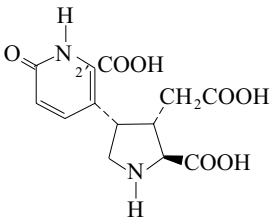
6-Deoxo, 5,6-didehydro: [102329-71-5] ***Acromelic acid D***
$C_{13}H_{14}N_2O_6$ 294.263
Sol. H_2O. $[\alpha]_D$ +17.6 (c, 0.07 in H_2O). λ_{max} 221 ; 269 (H_2O) (Berdy).

6-Deoxo, 5,6-didehydro, 4-decarboxy, 6-carboxy: [145237-01-0] *Acromelic acid E*
$C_{13}H_{14}N_2O_6$ 294.263
Sol. H_2O. λ_{max} 266 (H_2O) (Berdy).

Takano, S. *et al., J.A.C.S.*, 1987, **109**, 5523 (*synth*)
Konno, K. *et al., J.A.C.S.*, 1988, **110**, 4807; 6926 (*isol, synth, ir, uv, pmr*)
Takano, S. *et al., Heterocycles*, 1989, **29**, 1473 (*synth, bibl*)
Fushiya, S. *et al., Heterocycles*, 1992, **34**, 1277 (*isol, pmr, cd, struct*)
Barco, A. *et al., Gazz. Chim. Ital.*, 1993, **123**, 185 (*synth*)
Baldwin, J.E. *et al., Tetrahedron*, 1998, **54**, 7465-7484 (*synth*)

Acromelic acid B A-117

[86630-10-6]
3-[5-Carboxy-4-(carboxymethyl)-3-pyrrolidinyl]-1,6-dihydro-6-oxo-2-pyridinecarboxylic acid, 9CI. Acromelinic acid B

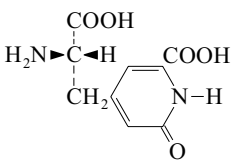


$C_{13}H_{14}N_2O_7$ 310.263
Amorph. powder. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D$ +50.1 (c, 0.45 in H_2O). Struct. established by synth. Phys. props. are of synthetic material λ_{max} 231 (ϵ); 308 (ϵ) (pH 2) (Derep). λ_{max} 241 (ϵ); 311 (ϵ) (pH 12) (Derep). λ_{max} 227 (ϵ); 300 (ϵ) (pH 7) (Derep). λ_{max} 236 (ϵ 6320); 302 (ϵ 2920) (MeOH) (Berdy).

2′-Decarboxy: [133740-47-3] ***Acromelic acid C***
$C_{12}H_{14}N_2O_5$ 266.253
Powder. $[\alpha]_D$ +31.9 (c, 0.23 in H_2O). λ_{max} 230 (ϵ 11000); 302 (ϵ 6150) (MeOH) (Derep). λ_{max} 230 (ϵ 10592); 301 (ϵ 6150) (H_2O) (Berdy).
▶ LD_{50} (mus, ipr) 10 mg/kg.
Hashimoto, K. *et al., Chem. Lett.*, 1986, 1399 (*synth, uv, ir, cd, abs config*)
Konno, K. *et al., J.A.C.S.*, 1988, **110**, 4807; 6926 (*isol, uv, pmr, synth, struct*)
Takano, S. *et al., Heterocycles*, 1989, **29**, 1473 (*synth, bibl*)
Fushiya, S. *et al., Tet. Lett.*, 1990, **31**, 3901 (*Acromelic acid C*)

Acromelobic acid A-118

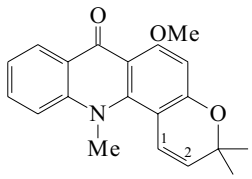
[158703-45-8]
α-Amino-6-carboxy-1,2-dihydro-2-oxo-4-pyridinepropanoic acid. 3-(2-Carboxy-6-oxo-4-pyridinyl)alanine



$C_9H_{10}N_2O_5$ 226.188
Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. λ_{max} 230 (ϵ 1660); 310 (ϵ 1230) (H_2O) (Berdy).
(S)-form [142179-90-6]
L-form
$[\alpha]_D^{22}$ -131 (c, 0.05 in H_2O). λ_{max} 230 (log ϵ 3.22); 310 (log ϵ 3.09) (H_2O).
Yamano, K. *et al., Tetrahedron*, 1993, **49**, 2427-2436 (*isol, uv, pmr*)
Baldwin, J.E. *et al., Tet. Lett.*, 1994, **35**, 6575-6576 (*synth*)
Adamcyzk, M. *et al., Tetrahedron*, 2002, **58**, 6943-6950 (*synth, pmr, cmr*)

Acronycine A-119

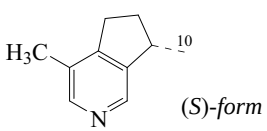
[7008-42-6]
*3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7H-pyrano[2,3-c]acridin-7-one, 9CI, 8CI. **Acronine, INN, USAN**. NSC 403169. Compound 42339*



$C_{20}H_{19}NO_3$ 321.375
Never marketed.
Yellow needles (EtOH). Mp 175-176°. Log P 3.7 (calc). λ_{max} 280 (ϵ 39800); 291 (ϵ 34700); 304 (ϵ 19100); 392 (ϵ 6920) (EtOH) (Derep). λ_{max} 224 (ϵ 24500); 281 (ϵ 48000); 293 (ϵ 43500); 308 (ϵ 40700); 380 (ϵ 10250) (MeOH) (Berdy).
▶ LD_{50} (mus, orl) 522 mg/kg. Exp. carcinogenic data. UQ0330000

O-*De-Me, 5-methoxy:* ***5-Methoxynoracronycine***
$C_{20}H_{19}NO_4$ 337.374
Alkaloid from the bark of *Citrus junos* (yuzu). Light-yellow prisms. Mp 146-148°.
Ju-ichi, M. *et al., Heterocycles*, 1986, **24**, 1595 (*5-Methoxynoracronycine*)

Actinidine A-120

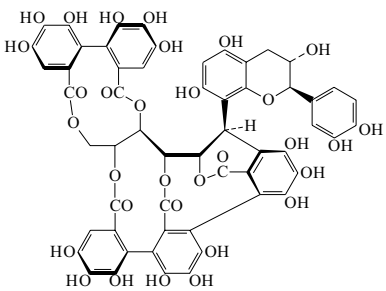


(S)-form

$C_{10}H_{13}N$ 147.219
(R)-form [15524-81-9]
Liq. Bp_{10} 92-94°. $[\alpha]_D^{20}$ +10.8 (c, 0.36 in $CHCl_3$).
Picrate:
Mp 146-147°.
(S)-form [524-03-8]
Alkaloid from *Actinidia arguta* (taravine) and *Valeriana officinalis* (valerian). Oil. Bp_9 100-103°. $[\alpha]_D^{11}$ -7.2 ($CHCl_3$).
Picrate:
Mp 143°.
N-*(4-Hydroxyphenethyl):* [15794-92-0] **N-*(p-Hydroxyphenethyl)actinidine***
$C_{18}H_{22}NO^{\oplus}$ 268.378
Quaternary alkaloid from the roots of *Valeriana officinalis* (valerian). Mp 201-203° dec. (as chloride). $[\alpha]_D^{22}$ +50.5 (MeOH).
N-*(4-Hydroxyphenethyl), picrate:*
Mp 151-152°.
10-Acetoxy: ***10-Acetoxyactinidine***
$C_{12}H_{15}NO_2$ 205.256
Amorph. solid. Stereochem. not certain.
(±)-*form* [79254-93-6]
Oil. Bp_9 100-103°.
Picrate:
Mp 146-146.5°.
Sakan, T. *et al., Bull. Chem. Soc. Jpn.*, 1959, **32**, 315; 1155; 1960, **33**, 712 (*uv, ir, isol, struct, synth*)
Djerassi, C. *et al., Chem. Ind. (London)*, 1961, 210 (*pmr*)
Torssell, K. *et al., Acta Chem. Scand.*, 1967, **21**, 53 (*N-4-Hydroxyphenethylactinidine*)
Cavill, G.W.K. *et al., Aust. J. Chem.*, 1967, **20**, 349 (*synth, uv, pmr*)
Johnson, R.D. *et al., Phytochemistry*, 1971, **10**, 3334 (*isol, ms*)
Wheeler, J.W. *et al., J. Chem. Ecol.*, 1977, **3**, 241
Wuest, J.D. *et al., J.O.C.*, 1977, **42**, 2111 (*synth*)
Nitta, M. *et al., Chem. Lett.*, 1981, 933 (*synth*)
Davies, L.B. *et al., J.C.S. Perkin 1*, 1981, 1909 (*synth, uv, ir, pmr, ms*)
Tomalski, M.D. *et al., J. Chem. Ecol.*, 1987, **13**, 253 (*ms*)
Cossy, J. *et al., Tet. Lett.*, 1988, **29**, 6113 (*synth*)
Ranarivelo, Y. *et al., Heterocycles*, 1990, **31**, 1727 (*synth*)
Cossy, J. *et al., J.O.C.*, 1993, **58**, 2351 (*synth*)
Shiao, M.J. *et al., J.O.C.*, 1993, **58**, 3162 (*synth*)
Stepanov, A.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **47**, 2286-2291 (*synth*)
Jones, K. *et al., Tetrahedron*, 1998, **54**, 2275-2280 (*synth*)
Bianco, A. *et al., Nat. Prod. Lett.*, 2002, **16**, 77-80 (*10-Acetoxyactinidine*)

Acutissimin A A-121

[108906-66-7]

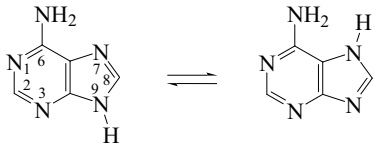


$C_{56}H_{38}O_{31}$ 1206.898
Isol. from *Castanea crenata* (Japanese chestnut). Off-white amorph. powder + $3^1/_2$ or $5H_2O$. $[\alpha]_D^{32}$ -74 (c, 1.2 in Me_2CO). λ_{max} 225 (ϵ 85100); 275 (ϵ 28800) (MeOH) (Berdy).
Ishimaru, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 602 (*isol, uv, cd, pmr, cmr*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2151 (*struct*)

Adenine, JAN, USAN A-122

[73-24-5]

1H-Purin-6-amine, 9CI. 6-Aminopurine. Vitamin B_4



9H-form *7H-form*

$C_5H_5N_5$ 135.128

9*H*-form is favoured in free base. CAS refers mainly to 1*H* struct. which is not in reality a favoured tautomer. Widespread throughout animal and plant tissue, purine components of DNA, RNA, and coenzymes. Vitamin. Needles + $3H_2O$ (H_2O). Mp 360-365° (anhyd.) dec. pK_{a1} 4.12; pK_{a2} 9.83 (25°).

▶ Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 745 mg/kg. AU6125000

Hydrochloride: [2922-28-3]
Cryst. + $0.5H_2O$. Mp 285°.

Sulfate: [321-30-2]

[6509-19-9]
Mp 285° dec.

▶ AU7140000

6N-Benzyl: [1214-39-7] N-*Benzyladenine, 8CI. 6-Benzylaminopurine. Cytokinin B. BAP*
$C_{12}H_{11}N_5$ 225.252
Cryst. (C_6H_6). Mp 229°.

▶ AU6252200

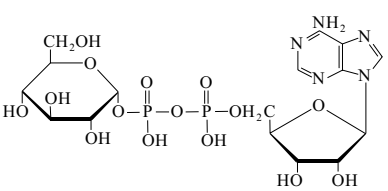
[2312-73-4, 6055-72-7]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 589C; 589D; 590C (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 708A; 713C; 713D; 714D (*ir*)
Traube, W. *et al., Annalen*, 1904, **331**, 64-88 (*synth*)
Skinner, C.G. *et al., J.A.C.S.*, 1955, **77**, 6692-6693 (*Cytokinin B*)

Adenosine 5′-diphosphate glucose A-123

[2140-58-1]

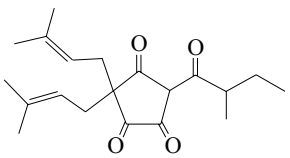
Adenosine 5′-(trihydrogen diphosphate) mono-α-D-glucopyranosyl ester, 9CI. ADPG



$C_{16}H_{25}N_5O_{15}P_2$ 589.345
Present in ripening cereal grains. λ_{max} 257 nm (pH 2) λ_{max} 259 (ε 15400) (H_2O) (as di-K salt). λ_{max} 257 (dil. acid) (pH2).

Roseman, S. *et al., J.A.C.S.*, 1961, **83**, 659
Murata, T. *et al., Arch. Biochem. Biophys.*, 1964, **106**, 371 (*isol, synth*)
Frydman, R.B. *et al., Biochim. Biophys. Acta*, 1966, **113**, 620 (*occur*)
Krauss, G. *et al., J. Chromatogr.*, 1973, **76**, 248 (*chromatog*)
Sarma, R.H. *et al., FEBS Lett.*, 1973, **36**, 157 (*nmr*)
Lee, C.H. *et al., Biochemistry*, 1976, **15**, 697 (*conformn, pmr*)

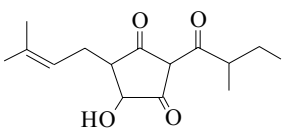
Adhulupone A-124



$C_{20}H_{28}O_4$ 332.439
Minor constit. of hops. Oil. $Bp_{0.007}$ 130°.

Brown, P.M. *et al., J.C.S.*, 1964, 4774 (*struct*)
Gienapp, E. *et al., Nahrung*, 1975, **19**, 697 (*struct*)

Adhumulinic acid A-125

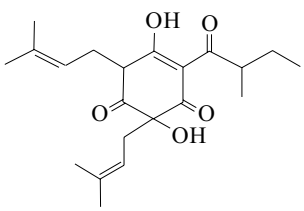


$C_{15}H_{22}O_4$ 266.336
Constit. of hops. Cryst. (petrol). Mp 83°.

Rigby, F.L. *et al., J.A.C.S.*, 1955, **77**, 2828

Adhumulone A-126

[28374-89-2]



$C_{21}H_{30}O_5$ 362.465
Tautomeric. Constit. of hops. Viscous oil. Sol. MeOH, Et_2O; fairly sol. H_2O. $[\alpha]_D$ -187 (MeOH). λ_{max} 236 ; 288 ; 323 (HCl) (Berdy). λ_{max} 325 ; 360 (NaOH) (Berdy).

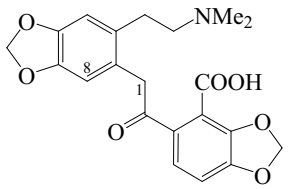
[31769-65-0, 71800-99-2]

Molyneux, R.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 1201

Adlumidiceine A-127

[51059-65-5]

5-[[6-[2-(Dimethylamino)ethyl]-1,3-benzodioxol-5-yl]acetyl]-1,3-benzodioxole-4-carboxylic acid, 9CI



$C_{21}H_{21}NO_7$ 399.399
Alkaloid from *Papaver rhoeas* (corn poppy). Cryst. (MeOH). Mp 244-246°.

1-Hydroxy, Me ester: [169626-17-9] ***Paprafumine***
$C_{22}H_{23}NO_8$ 429.426
Amorph. solid. Shown in the paper as the enediol tautomer.

1-Oxo: [59443-00-4] ***Narceimine***. *Bicucullinine. Alkaloid F450*
$C_{21}H_{19}NO_8$ 413.383
Mp 268° (259-260°).

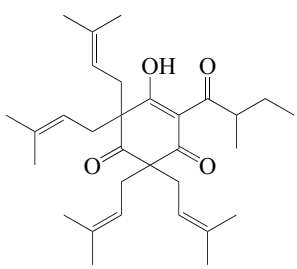
1-Oxo, Me ester:
Mp 188°.

1-Hydroxy: [116368-95-7] ***Narceimicine***
$C_{21}H_{21}NO_8$ 415.399
Pale-yellow granules (MeOH aq.). Mp 242-246° dec. Shown in the paper as the enediol tautomer.

Preininger, V. *et al., Phytochemistry*, 1973, **12**, 2513 (*ir, uv, pmr, ms, struct*)
Preininger, V. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 699 (*ir, uv, pmr, ms, struct*)
Rodrigo, R.G.A. *et al., Can. J. Chem.*, 1976, **54**, 471 (*isol, ir, pmr, cmr, ms, struct, Narceimine*)
Seth, K.K. *et al., Chem. Ind. (London)*, 1979, 744 (*ir, uv, pmr, ms, struct, Narceimine*)
Popova, M.E. *et al., Planta Med.*, 1982, **45**, 120 (*isol*)
Tripathi, Y.C. *et al., Phytochemistry*, 1988, **27**, 1918 (*Narceimicine, isol, ir, uv, pmr, ms, struct*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1995, **40**, 593 (*Parafumine*)

Adlupone A-128

[16595-43-0]

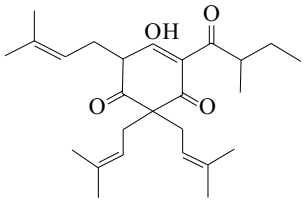


$C_{31}H_{46}O_4$ 482.702
Constit. of hops. Mp 45°. $Bp_{0.002}$ 150-155° (bath).

Laws, D.R.J. *et al., J.C.S.*, 1965, 6542-6543 (*synth*)

Adlupulone A-129

[28374-71-2]

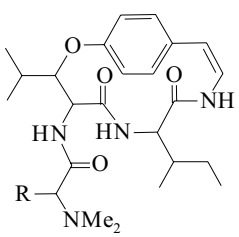


$C_{26}H_{38}O_4$ 414.584
Constit. of hops. Cryst. (MeOH). Sol. MeOH, Et_2O; fairly sol. H_2O. Mp 82-83°.

Howard, G.A. *et al., J.C.S.*, 1955, 174 (*struct*)
Brown, P.M. *et al., J.C.S.*, 1964, 4774 (*synth*)
Kowaka, M. *et al., Proc. Conv. - Inst. Brew. (Aust. N.Z. Sect.)*, 1970, **11**, 35; *CA*, **74**, 98087j (*isol*)

Adouetine X A-130

[19542-37-1]
2-(Dimethylamino)-4-methyl-N-*[3-(1-methylethyl)-7-(1-methylpropyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]-hexadeca-10,12,14,15-tetraen-4-yl]pentanamide, 9CI. Ceanothamine B*



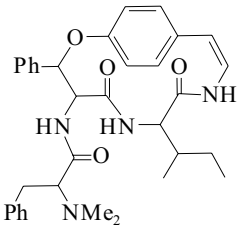
R = $CH_2CH(CH_3)_2$

$C_{28}H_{44}N_4O_4$ 500.68
Alkaloid from *Ceanothus americanus* (New Jersey tea) and *Zizyphus jujuba* var. *inermis*. Needles (MeOH or CH_2Cl_2/EtOAc). Mp 279-280.5°. $[\alpha]_D^{25}$ -370 (c, 0.205 in $CHCl_3$).

Païs, M. *et al., Ann. Pharm. Fr.*, 1963, **21**, 139; *CA*, **59**, 5215c (*isol, ir, pmr*)
Warnhoff, E.W. *et al., Can. J. Chem.*, 1965, **43**, 2594 (*isol, uv, ms, pmr*)
Païs, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 1145 (*uv, ir, pmr, ms, struct*)
Servis, R.E. *et al., J.A.C.S.*, 1969, **91**, 5619 (*isol, ms*)
Branch, G.B. *et al., Aust. J. Chem.*, 1972, **25**, 2209 (*isol*)
Otsuka, H. *et al., Phytochemistry*, 1974, **13**, 2016 (*isol, ir, pmr, ms*)

Adouetine Y A-131

[19542-38-2]
α-(Dimethylamino)-N-*[7-(1-methylpropyl)-5,8-dioxo-3-phenyl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]benzenepropanamide, 9CI*

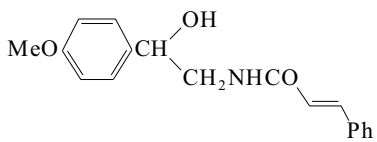


$C_{34}H_{40}N_4O_4$ 568.714
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Cryst. (MeOH or $CHCl_3/Et_2O$). Mp 292°. $[\alpha]_D$ -230 ($CHCl_3$/MeOH 9:1).

Païs, M. *et al., Ann. Pharm. Fr.*, 1963, **21**, 139 (*isol, ir, pmr*)
Païs, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 1145 (*uv, ir, pmr, ms, struct*)
Servis, R.E. *et al., J.A.C.S.*, 1969, **91**, 5619 (*isol, ms*)

Aegeline A-132

[456-12-2]
N-*[2-Hydroxy-2-(4-methoxyphenyl)ethyl]-3-phenyl-2-propenamide, 9CI. Egeline, 8CI.* N-*β*-Hydroxy-*β*-p-*methoxyphenethylcinnamamide.* N-*Cinnamoyl-2-hydroxy-2-(4-methoxyphenyl)ethylamine. Cinnamic acid 2-hydroxy-2-(*p-*methoxyphenyl)ethylamide*



$C_{18}H_{19}NO_3$ 297.353
Originally assigned the formula $C_{18}H_{18}O_4$.

(+)-form [15298-36-9]
Cryst. (EtOH). Mp 196-197°. $[\alpha]_D^{22}$ +36 (c, 0.4 in $CHCl_3$). $[\alpha]_D^{21}$ -48.1 (c, 0.5 in EtOH).

(-)-form [15298-37-0]
Cryst. (EtOH). Mp 196-197°. $[\alpha]_D$ -35.1 ($CHCl_3$). $[\alpha]_D$ +47.5 (c, 0.5 in EtOH).

(±)-form [37791-13-2]
Alkaloid from the leaves of *Aegle marmelos* (bael). Cryst. (EtOH/EtOAc). Mp 176° (173-175°).

Ac:
Plates (EtOAc). Mp 124°.

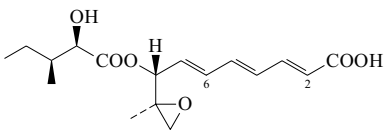
Dihydro:
Plates (EtOH/EtOAc). Mp 140°.

Me ether: [70546-93-9] N-*[2-Methoxy-2-(4-methoxyphenyl)ethyl]cinnamide.* Aegle marmelos *Alkaloid D*
$C_{19}H_{21}NO_3$ 311.38
Isol. from *Aegle marmelos* (bael). Cryst. (C_6H_6/hexane). Mp 135°. Artifact.

Et ether: [70546-94-0] N-*[2-Ethoxy-2-(4-methoxyphenyl)ethyl]cinnamide.* Aegle marmelos *Alkaloid B*
$C_{20}H_{23}NO_3$ 325.407
Isol. from *Aegle marmelos* (bael). Cryst. (C_6H_6/hexane). Mp 99-100°. Artifact.

Chatterjee, A. *et al., J. Indian Chem. Soc.*, 1952, **29**, 425 (*isol*)
Chakravarti, R.N. *et al., Chem. Ind. (London)*, 1955, 1632 (*struct*)
Chatterjee, A. *et al., J.O.C.*, 1959, **24**, 687 (*isol, uv, ir, struct, synth*)
Albónico, S.M. *et al., J.C.S.(C)*, 1967, 1327 (*synth*)
Della Casa de Marcano, D. *et al., Phytochemistry*, 1972, **11**, 1531 (*isol*)
Manandhar, M.D. *et al., Phytochemistry*, 1978, **17**, 1814 (*derivs*)
Patra, A. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 385 (*isol, uv, ir*)
Swinehart, J. *et al., Phytochemistry*, 1980, **19**, 1219 (*isol*)
Patra, A. *et al., Org. Magn. Reson.*, 1981, **16**, 65 (*cmr*)
Sharma, B.R. *et al., Phytochemistry*, 1981, **20**, 2606 (*isol*)
Somanathan, R. *et al., Synth. Commun.*, 1983, **13**, 273 (*synth, ir, ms, pmr, cmr*)
Brown, R.F.C. *et al., Tetrahedron: Asymmetry*, 1993, **4**, 205 (*synth*)

AF Toxin II A-133



(2*E*,4*E*,6*E*)-*form*

$C_{17}H_{24}O_6$ 324.373
Prod. by *Alternaria alternata* on strawberry. Phytotoxin specific to strawberry and pear. Not related to AF Toxin.

(2E,4E,6E)-form [104420-17-9]
AF Toxin IIc
Oil (as Et ester). $[\alpha]_D^{23}$ -4.4 (c, 0.9 in EtOH) (Et ester). λ_{max} 289 (ε 27000) (MeOH) (Derep).

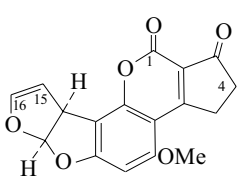
(2E,4E,6Z)-form [104363-99-7]
AF Toxin IIa
Oil (as Et ester). $[\alpha]_D^{23}$ +153 (c, 0.78 in EtOH) (Et ester). Major component of AF toxin complex λ_{max} 289 (ε 27000) (MeOH) (Derep).

(2E,4Z,6E)-form
AF Toxin IIb
λ_{max} 289 (ε 27000) (MeOH) (Derep).

Maekawa, N. *et al., Nippon Shokubutsu Byori Gakkaiho*, 1984, **50**, 610 (*props*)
Nakatsuka, S.-I. *et al., Tet. Lett.*, 1986, **27**, 2753 (*isol, struct*)
Irie, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2545 (*synth*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1991, 1511 (*synth*)

Aflatoxin B_1 A-134

*2,3,6*a,*9*a-*Tetrahydro-4-methoxycyclopenta[*c*]furo[3,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 9CI. Aflatoxin FB_1. Aflatoxin B*



(−)-*form*

$C_{17}H_{12}O_6$ 312.278
Sol. MeOH, $CHCl_3$; poorly sol. hexane. λ_{max} 220 (ε 25600); 265 (ε 13400); 362 (ε 21800) (MeOH) (Berdy). λ_{max} 223 (ε

25100); 265 (ϵ 13400); 362 (ϵ 21800) (EtOH) (Berdy).

▶ LD_{50} (mus, orl) 1 mg/kg. GY1925000

(-)-*form* [1162-65-8]
Prod. by *Aspergillus flavus* and *Aspergillus parasiticus*. Toxin causing Turkey X disease. One of the most potent carcinogens known in animals. Potential food contaminant esp. in grains and nuts. Cryst. exhibiting blue fluor. Mp 268-269° dec. $[\alpha]_D^{25}$ -562 (c, 0.115 in $CHCl_3$).

▶ Human and exp. carcinogen; LD_{50} (rat, orl) 5 mg/kg. Exp. reprod. and teratogenic effects. Hepatotoxic. Crystalline material, e.g. from preparative tlc plates, presents an inhalation hazard because the crystals develop electrostatic charge and cling to dust particles.

O-*De-Me:* [32215-02-4] ***Aflatoxin P_1***
$C_{16}H_{10}O_6$ 298.251
Metab. of Aflatoxin B_1. Pale yellow needles (MeOH/C_6H_6/hexane). Mp 320°. $[\alpha]_D^{20}$ -574 (c, 0.08 in MeOH).

▶ GY1775000

15α,16α-Epoxide: [67337-06-8]
$C_{17}H_{12}O_7$ 328.278
Prob. ultimate carcinogen of Aflatoxin B_1. Cryst. (Me_2CO/CH_2Cl_2). Mp 300° (phase transition at 230°). Stable at -10°, fairly stable at r.t..

▶ Presumed highly toxic and carcinogenic.

15,16-Dihydro: [7220-81-7] ***Aflatoxin B_2***
$C_{17}H_{14}O_6$ 314.294
Metab. of *Aspergillus flavus*. Yellow cryst. with blue fluor. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 310° dec. $[\alpha]_D^{23}$ -492 (c, 0.1 in $CHCl_3$). λ_{max} 222 (ϵ 19600); 265 (ϵ 9200); 363 (ϵ 14700) (MeOH) (Berdy). λ_{max} 220 (ϵ 20800); 265 (ϵ 12700); 363 (ϵ 24000) (EtOH) (Berdy).

▶ Human and exp. carcinogen. LD_{50} (dck, orl) 1.7 mg/kg. Hepatotoxic. GY1722000

15,16-Dihydro, 16-hydroxy: [17878-54-5] ***Aflatoxin B_{2a}***. *Dihydrohydroxyaflatoxin B_1*
$C_{17}H_{14}O_7$ 330.293
Metab. of *Aspergillus flavus*. Cryst. with blue fluor. ($CHCl_3$). Mp 217° (240° dec.).

▶ GY1718000

15,16-Dihydro, 16-methoxy: [20421-12-9] ***Aflatoxin Ex_2B_1***
$C_{18}H_{16}O_7$ 344.32
Metab. of *Aspergillus flavus*. Cryst. ($CHCl_3$). Mp 240°.

15,16-Dihydro, 16-ethoxy: [23402-20-2] ***Aflatoxin ExB_2***
$C_{19}H_{18}O_7$ 358.347
Isol. from *Aspergillus flavus*. Cryst. Mp 245°.

4-Hydroxy: [104700-21-2] ***Aflatoxin M_4***
$C_{17}H_{12}O_7$ 328.278
Isol. from cultures of *Aspergillus parasiticus*. Cryst.

(±)-*form* [10279-73-9]
Mp 255-256°.

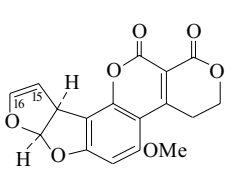
15,16-Dihydro:
Cryst. with blue fluor. ($CHCl_3$/MeOH). Mp 303-306° dec.

[42583-46-0]

Asao, T. *et al., J.A.C.S.*, 1963, **85**, 1705; 1965, **87**, 882 (*struct, isol, ir, uv, ms, nmr*)
Dutton, M.F. *et al., Biochem. J.*, 1966, **101**, 21P (*deriv*)
Brechbühler, S. *et al., J.O.C.*, 1967, **32**, 2641 (*abs config*)
Roberts, J.C. *et al., J.C.S.(C)*, 1968, 22 (*synth, uv, ir, ms*)
Dutton, M.F. *et al., Chem. Ind. (London)*, 1969, 983 (*Aflatoxin Ex_2B_1, Aflatoxin ExB_2*)
Heathcote, J.G. *et al., Tetrahedron*, 1969, **25**, 1497 (*biosynth*)
v. Soest, T.C. *et al., Acta Cryst. B*, 1970, **26**, 1940; 1947 (*cryst struct*)
Büchi, G. *et al., J.A.C.S.*, 1971, **93**, 746 (*synth, uv, ms*)
Heathcote, J.B. *et al., Chem. Ind. (London)*, 1976, 270 (*biosynth*)
IARC Monog., 1976, **10**, 51; *Suppl.* 6, 40; 46; *Suppl.* 7, 83 (*rev, tox*)
Pachler, K.G.R. *et al., J.C.S. Perkin 1*, 1976, 1182 (*cmr, biosynth*)
Cox, R.H. *et al., J.O.C.*, 1977, **42**, 112 (*cmr*)
Heathcote, J.G. *et al., Aflatoxins, Chemical and Biological Aspects*, Elsevier, 1978, (*book*)
Simpson, T.J. *et al., Chem. Comm.*, 1982, 631; 1983, 338 (*biosynth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Moss, E.J. *et al., Biochem. Pharmacol.*, 1985, **34**, 3193 (*metab*)
Castellino, A.J. *et al., J.O.C.*, 1986, **51**, 1006 (*synth*)
Lafont, P. *et al., Microbiol., Aliments, Nutr.*, 1986, **4**, 65 (*Aflatoxin M_4*)
Townsend, C.A. *et al., Pure Appl. Chem.*, 1986, **58**, 227 (*biosynth*)
Weeratunga, G. *et al., Chem. Comm.*, 1988, 721 (*Aflatoxin B_2*)
Baertschi, S.W. *et al., J.A.C.S.*, 1988, **110**, 7929 (*epoxide*)
Townsend, C.A. *et al., J.C.S. Perkin 1*, 1988, 839 (*biosynth*)
Sloan, C.P. *et al., Tet. Lett.*, 1988, **29**, 4685 (*synth*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 114 (*rev*)
Horne, S. *et al., Chem. Comm.*, 1990, 39 (*Aflatoxin B_2, synth*)
Bhatnager, D. *et al., Biochemistry*, 1991, **30**, 4343 (*biosynth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1332
Koreeda, M. *et al., Synlett*, 1993, 555 (*synth, Aflatoxin B_2*)
Iyer, R.S. *et al., J.A.C.S.*, 1994, **116**, 1603 (*haz*)
Civitello, E.R. *et al., J.O.C.*, 1994, **59**, 3775 (*synth, bibl*)
Chatterjee, M. *et al., J.O.C.*, 1994, **59**, 4424 (*biosynth*)
Toxicol. Aflatoxins, (eds. Eaton, D.L. *et al*), Academic Press, London, 1994,
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 3; 15; 34; 51
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEU250; AEU750

Aflatoxin G_1 A-135

[1165-39-5]
Aflatoxin G



Absolute configuration

$C_{17}H_{12}O_7$ 328.278
Mycotoxin prod. by *Aspergillus flavus* and *Aspergillus parasiticus*. Needles (MeOH) exhibiting green fluor. Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 257-259° (247-250°). $[\alpha]_D^{23}$ -556 (c, 0.1 in $CHCl_3$). λ_{max} 235 (ϵ 21200); 262 (ϵ 26300); 358 (ϵ 14000) (MeOH) (Berdy). λ_{max} 243 (ϵ 11500); 257 (ϵ 9900); 264 (ϵ 10000); 362 (ϵ 16100) (EtOH) (Berdy).

▶ Human and exp. carcinogen. LD_{50} (dck, orl) 0.79 mg/kg. LV1720000

15,16-Dihydro: [7241-98-7] ***Aflatoxin G_2***
$C_{17}H_{14}O_7$ 330.293
Minor mycotoxin prod. by *Aspergillus flavus*. Cryst. with green fluor. (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 237-240°. $[\alpha]_D^{23}$ -473 (c, 0.084 in $CHCl_3$). λ_{max} 223 ; 265 (ϵ 11200); 363 (ϵ 19300) (EtOH) (Berdy).

▶ LD_{50} (dck, orl) 2.45 mg/kg. LV1700000

15,16-Dihydro, 16-hydroxy: [20421-10-7] ***Aflatoxin G_{2a}***
$C_{17}H_{14}O_8$ 346.293
Mycotoxin prod. by *Aspergillus flavus*. Cryst. with green fluor. Mp 190° dec.

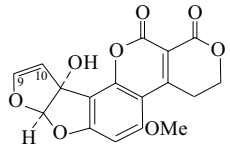
▶ LV1690000

15,16-Dihydro, 16-ethoxy: [23402-21-3] *Aflatoxin ExG*
$C_{19}H_{18}O_8$ 374.346
Mp 203°.

Nesbitt, B.E. *et al., Nature (London)*, 1962, **195**, 1062 (*isol*)
Asao, T. *et al., J.A.C.S.*, 1963, **85**, 1706; 1965, **87**, 882 (*isol, uv, ir, ms, nmr, struct*)
Dutton, M.F. *et al., Biochem. J.*, 1966, **101**, 21P (*deriv*)
Brechbühler, S. *et al., J.O.C.*, 1967, **32**, 2641 (*abs config*)
Dutton, M.F. *et al., Chem. Ind. (London)*, 1969, 983 (*Aflatoxin ExG*)
Büchi, G. *et al., J.A.C.S.*, 1971, **93**, 746 (*uv, ms, synth*)
Heathcote, J.G. *et al., Chem. Ind. (London)*, 1976, 270 (*biosynth*)
IARC Monog., 1976, **10**, 51; 1992, **56**, 245; *Suppl.* 6, 49; *Suppl.* 7, 83 (*rev, tox*)
Cox, R.H. *et al., J.O.C.*, 1977, **42**, 112 (*cmr*)
Heathcote, J.G. *et al., Aflatoxins, Chemical and Biological Aspects*, Elsevier, 1978, (*prop*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 114 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1332
Civitello, E.R. *et al., J.O.C.*, 1994, **59**, 3775 (*synth, bibl*)
Toxicol. Aflatoxins, Eaton, D.L., *et al* Eds., Academic Press, London, 1994,
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 25; 45; 55
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEV000; AEV500

Aflatoxin GM_1 A-136

[23532-00-5]
*3,4,7*a,*10*a-*Tetrahydro-10*a-*hydroxy-5-methoxy-1*H,*12*H-*furo[3′,2′:4,5]furo[2,3-*h*]pyrano[3,4-*c*][1]benzopyran-1,12-dione, 9CI*



Absolute configuration

$C_{17}H_{12}O_8$ 344.277
Mycotoxin prod. by *Aspergillus flavus*. Cryst. ($CHCl_3$). Mp 276°.

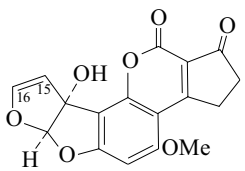
Ac:
Mp 280°.

9,10-Dihydro: ***Aflatoxin GM₂***
$C_{17}H_{14}O_8$ 346.293
Minor mycotoxin of *Aspergillus flavus*. Mp 270-272°.

Heathcote, J.G. *et al., Tetrahedron*, 1969, **25**, 1497 (*isol, uv, struct*)
IARC Monog., 1972, **1**, 145; 1976, **10**, 51; *Suppl.* 7, 83 (*rev, tox*)
Heathcote, J.G. *et al., Biochem. Soc. Trans.*, 1974, **2**, 301 (*deriv*)
Heathcote, J.G. *et al., Chem. Ind. (London)*, 1976, 270 (*synth*)
Heathcote, J.G. *et al., Aflatoxins, Chemical and Biological Aspects*, Elsevier, 1978, (*rev*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 114 (*rev*)
Toxicol. Aflatoxins, (eds. Eaton, D.L. *et al*), Academic Press, London, 1994,

Aflatoxin M_1 A-137

[6795-23-9]



$C_{17}H_{12}O_7$ 328.278
Minor mycotoxin of *Aspergillus flavus*, also found in the milk of cows and sheep fed toxic meal. Metab. of Aflatoxin B_1, . Cryst. (MeOH) exhibiting blue-violet fluor. Mp 299° dec. $[\alpha]_D^{20}$ -280 (c, 0.1 in DMF). λ_{max} 235 (ϵ 21200); 262 (ϵ 16300); 358 (ϵ 14000) (MeOH) (Berdy). λ_{max} 226 ; 265 ; 357 (EtOH) (Berdy).

▶ Exp. carcinogen. Hepatotoxic. Less potent carcinogen then Aflatoxin B_1. GY1880000

15,16-Dihydro: [6885-57-0] ***Aflatoxin M₂***
$C_{17}H_{14}O_7$ 330.293
Trace mycotoxin of *Aspergillus flavus*. Cryst. with violet fluor. (MeOH/$CHCl_3$). Mp 293° dec.

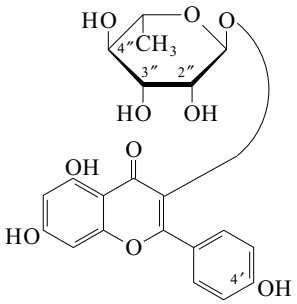
▶ GY1720000

15,16-Dihydro, 16-hydroxy: [36601-31-7] *Aflatoxin M_{2a}*
$C_{17}H_{14}O_8$ 346.293

Holzapfel, C.W. *et al., Tet. Lett.*, 1966, 2799 (*isol, struct*)
Büchi, G. *et al., J.A.C.S.*, 1969, **91**, 5408; 1971, **93**, 746 (*uv, ms, nmr, synth*)
Stack, M.E. *et al., J. Assoc. Off. Anal. Chem.*, 1972, **55**, 313 (*Aflatoxin M_{2a}*)
Heathcote, J.G. *et al., Chem. Ind. (London)*, 1976, 270 (*biosynth*)
IARC Monog., 1976, **10**, 51; *Suppl.*, **6**, 55; *Suppl.*, **7**, 83 (*rev, tox*)
Heathcote, J.G. *et al., Aflatoxins, Chemical and Biological Aspects*, Elsevier, 1978, (*rev*)
Büchi, G. *et al., J.A.C.S.*, 1981, **103**, 3497 (*synth*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 114 (*rev*)
Toxicol. Aflatoxins, Eaton, D.L., *et al* Eds., Academic Press, London, 1994,
Kraus, G.A. *et al., Tet. Lett.*, 1999, **40**, 8513-8514 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 29; 49
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEW000

Afzelin A-138

[482-39-3]
3-O-α-L-Rhamnopyranosyloxy-4′,5,7-trihydroxyflavone. Kaempferol 3-α-L-rhamnoside. Afzeloside. Kaempferin



$C_{21}H_{20}O_{10}$ 432.383
Yellow prisms + $1^1/_2H_2O$ (EtOH aq.). Mp 172-174°.

O″-Sulfate: [62794-01-8]
$C_{21}H_{20}O_{13}S$ 512.447

7-O-α-L-Arabinopyranoside: [71801-95-1]
$C_{26}H_{28}O_{14}$ 564.499

7-O-α-L-Rhamnopyranoside: [482-38-2] ***Kaempferitrin****. Kaempferol 3,7-dirhamnoside. Lespedin*
$C_{27}H_{30}O_{14}$ 578.526
Needles + $4H_2O$. Mp 202-203° (185-186°).

▶ DJ2977500

7-O-[β-D-Xylopyranosyl-(1→2)-α-L-rhamnopyranoside]:
$C_{32}H_{38}O_{18}$ 710.641
Amorph. yellow powder. λ_{max} 238 (sh) ; 269 ; 310 (sh) ; 358 (MeOH).

7-O-[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranoside]: [156980-60-8] ***Grosvenorin***
$C_{33}H_{40}O_{19}$ 740.668

7-O-[α-L-Rhamnopyranosyl-(1→3)-α-L-rhamnopyranoside]: [117628-05-4]
$C_{33}H_{40}O_{18}$ 724.668

2″-Ac: [135618-15-4] ***2″-O-Acetylafzelin***
$C_{23}H_{22}O_{11}$ 474.42
Constit. of *Zingiber zerumbet* (wild ginger). Yellow amorph. solid. $[\alpha]_D^{20}$ -93 (c, 1 in Me_2CO).

3″-Ac: [135618-16-5] ***3″-O-Acetylafzelin***
$C_{23}H_{22}O_{11}$ 474.42
Constit. of *Zingiber zerumbet* (wild ginger). Yellow powder. Mp 117°. $[\alpha]_D^{20}$ -126 (c, 1 in Me_2CO).

4″-Ac: [135618-17-6] ***4″-O-Acetylafzelin***
$C_{23}H_{22}O_{11}$ 474.42
Constit. of *Zingiber zerumbet* (wild ginger). Yellow powder. Mp 199-201°. $[\alpha]_D^{14}$ -119 (c, 1 in MeOH).

2″,4″-Di-Ac: [133882-73-2] ***2″,4″-Diacetylafzelin***
$C_{25}H_{24}O_{12}$ 516.457
Constit. of *Zingiber zerumbet* (wild ginger). Pale yellow amorph. solid. Mp 111°. $[\alpha]_D^{18}$ -95 (c, 1.0 in Me_2CO).

3″,4″-Di-Ac: [77307-50-7] ***3″,4″-Diacetylafzelin***
$C_{25}H_{24}O_{12}$ 516.457
Constit. of *Zingiber zerumbet* (wild ginger). Pale yellow amorph. solid. Mp 154°. $[\alpha]_D^{18}$ -125.4 (c, 0.7 in Me_2CO). λ_{max} 266 (ϵ 23600); 345 (ϵ 16200) (EtOH) (Berdy). λ_{max} 276 (ϵ 28200); 327 (ϵ 15100); 396 (ϵ 26300) (EtOH/NaOH) (Berdy).

2″-O-(4-Hydroxycinnamoyl):
$C_{30}H_{26}O_{12}$ 578.528*E*- and *Z*-isomers isol. from *P. acerifolia*.

4″-O-(4-Hydroxycinnamoyl): ***4″-O-p-Coumaroylafzelin***
$C_{30}H_{26}O_{12}$ 578.528

2″,3″-Bis-O-(4-hydroxy-E-cinnamoyl): ***2″,3″-Di-O-p-coumaroylafzelin***
$C_{39}H_{32}O_{14}$ 724.673
Constit. of the flowers of *Foeniculum vulgare* (fennel). Amorph. yellow powder. Mp 190-193°. λ_{max} 268 (sh) (log ϵ 4.48); 300 (sh) (log ϵ 4.73); 312 (log ϵ 4.76) (MeOH).

2″,4″-Bis-O-(4-hydroxy-E-cinnamoyl): [163434-73-9] ***2″,4″-Di-O-p-coumaroylafzelin***
$C_{39}H_{32}O_{14}$ 724.673
Yellow powder. λ_{max} 270 ; 316 (MeOH) (Berdy).

2″,4″-Bis-O-(4-hydroxy-Z-cinnamoyl):
$C_{39}H_{32}O_{14}$ 724.673
Constit. of *Laurus nobilis* (bay laurel). Yellow powder.

3″,4″-Bis-O-(4-hydroxycinnamoyl): ***3″,4″-Di-O-p-coumaroylafzelin***
$C_{39}H_{32}O_{14}$ 724.673

Bis-O-(4-hydroxycinnamoyl):Kaempferol 3-(2,3-dicoumaroylrhamnoside). ***Platanoside***†
$C_{39}H_{32}O_{14}$ 724.673
Yellow powder.

O″-β-D-Xylopyranosyl:
$C_{26}H_{28}O_{14}$ 564.499

2″-β-D-Glucopyranosyl: [142451-65-8]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Ginkgo biloba* (ginkgo).

2″-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl]:
$C_{36}H_{36}O_{17}$ 740.67
Isol. from *Ginkgo biloba* (ginkgo).

4″-O-β-D-Glucopyranosyl: [52657-01-9] ***Multiflorin B***
$C_{27}H_{30}O_{15}$ 594.525

4″-β-D-Glucopyranosyl, 2″ or 3″-O-Ac: [61358-52-9] ***Multiflorin A***
$C_{29}H_{32}O_{16}$ 636.562

3″-α-L-Rhamnopyranosyl: [151746-85-9]
$C_{27}H_{30}O_{14}$ 578.526

2″,3″-Di-β-D-glucopyranosyl:
$C_{33}H_{40}O_{20}$ 756.667
λ_{max} 268 ; 315 (sh) ; 347 (no solvent reported).

2″-[β-D-Glucopyranosyl-(1→4)-4-hydroxycinnamoyl-(→6)-β-D-glucopyranosyl]: [142997-34-0]
$C_{42}H_{46}O_{22}$ 902.812
Isol. from *Ginkgo biloba* (ginkgo).

King, F.E. *et al., J.C.S.*, 1950, 168 (*isol*)
Vermes, B. *et al., Phytochemistry*, 1976, **15**, 1320 (*synth*)
Takagi, S. *et al., Yakugaku Zasshi*, 1976, **96**, 1217; 1977, **97**, 109; 1979, **99**, 439 (*Multiflorin*)
Wilkins, C.K. *et al., Phytochemistry*, 1977, **16**, 144 (*sulfate*)
Yamasaki, K. *et al., Tet. Lett.*, 1977, 1231 (*cmr, Multiflorin*)
Hiraoka, A. *et al., Biochem. Syst. Ecol.*, 1978, **6**, 171 (*O″-xyloside*)
Imperato, F. *et al., Experientia*, 1979, **35**, 1134 (*7-arabinoside*)
Itokawa, H. *et al., Chem. Lett.*, 1982, 49 (*ms*)
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1982, **18**, 695; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 658 (*pmr*)
Kaouadji, M. *et al., Phytochemistry*, 1990, **29**, 2295 (*Platanoside*)
Nakatani, N. *et al., Agric. Biol. Chem.*, 1991, **55**, 455 (*diacetates*)
Masuda, T. *et al., Phytochemistry*, 1991, **30**, 2391 (*acetates*)
Hasler, A. *et al., Phytochemistry*, 1992, **31**, 1391 (*2″-glucosides*)
Kaouadji, M. *et al., J. Nat. Prod.*, 1993, **56**, 1618 (*2″-coumaroyl derivs*)
Sticher, O. *et al., Planta Med.*, 1993, **59**, 2
Mitrokotsa, D. *et al., Planta Med.*, 1993, **59**, 517 (*2″-coumarate*)
Si, J.Y. *et al., Yaoxue Xuebao*, 1994, **29**, 158 (*Grosvenorin*)
Bloor, S.J. *et al., Phytochemistry*, 1995, **38**, 1033 (*2″,4″-Dicoumaroylafzelin*)
Garcez, W.S. *et al., Phytochemistry*, 1995, **39**, 815 (*4″-Coumaroylafzelin*)
Fiorini, C. *et al., Phytochemistry*, 1998, **47**, 821-824 (*Coumaroylafzelins*)
El-Sayed, N.H. *et al., Phytochemistry*, 1999, **51**, 591-593 (*7-xylosylrhamnoside*)
Norbaek, R. *et al., Phytochemistry*, 1999, **51**, 1113-1119 (*2″,3″-diglucosyl*)
Soliman, F.M. *et al., Molecules*, 2002, **7**, 245-251 (*2″,3″-Dicoumaroylafzelin*)

Agar A-139

[9002-18-0]
Agar-agar. Gum agar. Gelose. Japan agar. Bengal isinglass. Ceylon isinglass. Chinese isinglass. Japan isinglass. FEMA 2012. E406

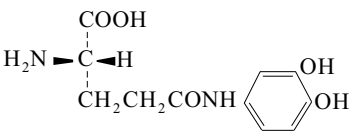
See also Agarose, A-142. Consists of a mixt. of 2 polysaccharides, Agarose A-142 and Agaropectin, which has essentially the same struct. except that a variable proportion of the sugars in the polymer are replaced by 4,6-*O*-(1-carboxyethylidene)galactose or by sulfated or methylated sugar residues such as to retain the alternating sequence of 3-linked β-D- and 4-linked α-L- units. An important thickener, stabiliser and gelling agent in the food industry. Strips or fine powder. Sl. sol. in hot H_2O.

▶ AW7950000

Clark, R.E. *et al., Analyst (London)*, 1937, **62**, 661 (*detn, Sn*)
Bogan, E.J. *et al., Ind. Eng. Chem., Anal. Ed.*, 1942, **14**, 849 (*detn, $SO_4^{2\ominus}$*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1948, **4**, (*use*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 65 (*purifn*)
Duckworth, M. *et al., Carbohydr. Res.*, 1971, **18**, 1 (*struct, bibl*)
Davidson, R.L. *et al., Handb. Water-Soluble Gums Resins*, McGraw-Hill, N.Y., 1980, 7/1 (*rev*)
Glickmann, M. *et al., Food Hydrocolloids*, CRC Press, Boca Raton, Florida, 1983, **2**, 73 (*rev*)
Rochas, C. *et al., Carbohydr. Res.*, 1994, **253**, 69 (*bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 53-56 (*use, props*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1470
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEX250

Agaridoxin A-140

[58298-77-4]
N-*(3,4-Dihydroxyphenyl)glutamine, 9CI. 3,4-Dihydroxy(γ-glutamyl)anilide*



$C_{11}H_{14}N_2O_5$ 254.242

▶ MA2276100

(*S*)-*form*

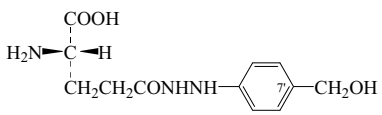
L-form

Constit. of *Agaricus campestris* (field mushroom). Grey-white powder (MeOH aq.). Mp 220-221°. Darkens in air.

Szent-Gyorgyi, A. *et al., J.O.C.*, 1976, **41**, 1603 (*synth*)

Agaritine A-141

[2757-90-6]
β-N-(γ-Glutamyl)-4-hydroxymethylphenylhydrazine. Glutamic acid 5-2-(α-hydroxy-p-tolyl)hydrazide, 8CI



$C_{12}H_{17}N_3O_4$ 267.284

▶ MA1284000

(*S*)-*form*

L-form

Constit. of some members of the family Agaricaceae, notably *Agaricus bisporus* (button mushroom). Cryst. (EtOH/butanol). Sol. MeOH, H_2O; poorly sol. EtOAc, hexane. Mp 205-209° dec. $[\alpha]_D^{25}$ +7 (c, 0.8 in H_2O). pK_{a1} 3.4; pK_{a2} 8.86 (H_2O). λ_{max} 237 (ε 12000); 280 (ε 1400) (H_2O) (Berdy).

▶ A procarcinogen.

7′-Aldehyde: [114847-20-0] N^2-*(γ-Glutamyl)-4-formylphenylhydrazine.* ***Agaritinal***
$C_{12}H_{15}N_3O_4$ 265.268
Isol. from *Agaricus campestris* (field mushroom). Sol. H_2O, MeOH. λ_{max} 248 (ε 5750); 385 (ε 20000) (MeOH) (Berdy). λ_{max} 231 (ε 6200); 313 (ε 15500) (H_2O) (Berdy). λ_{max} 231 (ε 6200); 313 (ε 15500) (HCl) (Berdy).

7′-Carboxylic acid: [69644-85-5] N^2-*(γ-Glutamyl)-4-carboxyphenylhydrazine*
$C_{12}H_{15}N_3O_5$ 281.268
Isol. from *Agaricus bisporus* (button mushroom). Mp 175°. Isomer of Anthglutin.

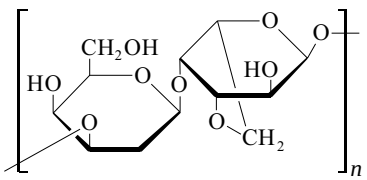
▶ MA0955600

Daniels, E.G. *et al., J.O.C.*, 1962, **27**, 3229 (*isol, synth*)
Levenberg, B. *et al., J. Biol. Chem.*, 1964, **239**, 2267 (*isol, struct*)
Chauhan, Y.S. *et al., J. Agric. Food Chem.*, 1984, **32**, 676; 1985, **33**, 817 (*deriv*)
Datta, S. *et al., Helv. Chim. Acta*, 1987, **70**, 1261 (*synth, ir, pmr, bibl*)
Chulia, A.J. *et al., Phytochemistry*, 1988, **27**, 929 (*Agaritinal*)
Baumgartner, D. *et al., Phytochemistry*, 1998, **49**, 465-474 (*biosynth*)
Espin, J.C. *et al., Phytochemistry*, 1999, **50**, 555-563 (*activity*)

Agarose A-142

[9012-36-6]

[9036-61-7]
Neutral agarose. Indubiose A4



See also Agar, A-139. Composed of repeating units of β-D-Galp (1→4) 3,6-anhydro-α-L-Galp(1→3). Has a domain struct. of double helixes aggregating into a three-dimensional framework holding water molecules.There are two other polysaccharides in agar, one is similar to agarose but with 4,6-acetals of pyruvic acid at some of the D-galactose units. The other contains fewer 3,6-anhydro-L-galactose units and is sulfated.

Poly(6-aminohexyl) ether: [58856-73-8] *Agarose (6-aminohexyl)carbamimidate. Sepharose AH*Non-stoichiometric.

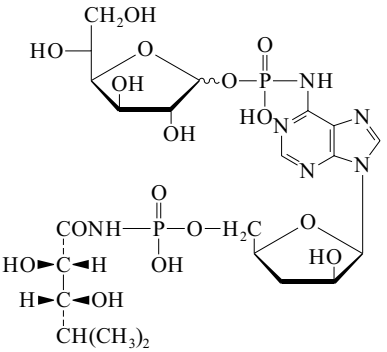
Poly(5-carboxypentyl) ether: [55128-01-3] Non-stoichiometric.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 201C; 201D (*ir*)
Hegenauer, J.C. *et al., Biochim. Biophys. Acta*, 1965, **111**, 334 (*isol*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 65 (*purifn*)
Percival, E. *et al., The Carbohydrates*, 1970, **2B**, 553
Batey, J.F. *et al., Carbohydr. Res.*, 1975, **43**, 133
Turvey, J.R. *et al., Carbohydr. Res.*, 1976, **49**, 419
Rees, D. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 214
Taylor, J.L. *et al., J. Chromatogr.*, 1983, **257**, 275-284 (*5-carboxypentyl ether*)
Szewezyk, A. *et al., Biochim. Biophys. Acta*, 1987, **89**, 252-260 (*6-aminohexyl ether*)
Kiwitt-Haschemie, K. *et al., Carbohydr. Res.*, 1993, **248**, 267

Arndt, E.R. *et al., Carbohydr. Res.*, 1997, **303**, 73-78 (*cd, struct*)
Gamini, A. *et al., Carbohydr. Res.*, 1997, **304**, 293-302 (*pmr, cmr, conformn*)

Agrocin 84, 9CI A-143

[59111-78-3]



$C_{22}H_{36}N_6O_{16}P_2$ 702.504

Nucleotide antibiotic. Bacteriocin active against *Agrobacterium tumefaciens*. λ_{max} 270 (ϵ 19000) (pH 1) (Derep). λ_{max} 264 (ϵ 19500); 270 (sh) (ϵ 15000) (pH 7 H_2O) (Derep). λ_{max} (H_2O) (Berdy). λ_{max} 270 (pH 1 buffer) (Berdy).

Heip, J. *et al., Arch. Int. Physiol. Biochim.*, 1975, **83**, 974 (*isol*)
Roberts, W.P. *et al., Nature (London)*, 1977, **265**, 379 (*struct*)
Das, P.K. *et al., J. Antibiot.*, 1978, **31**, 490 (*props*)
Thompson, R.J. *et al., Antimicrob. Agents Chemother.*, 1979, **16**, 293 (*isol, props*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711 (*rev*)
Filippov, D. *et al., Tet. Lett.*, 1998, **39**, 4891-4894 (*partial synth*)

Agrocin C58 A-144

[98667-77-7]

Struct. unknown. Bacteriocin prod. by *Agrobacterium tumefaciens*.

Necasek, J. *et al., Folia Microbiol. (Prague)*, 1985, **30**, 353-358

Agrocin D286 A-145

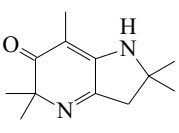
[86337-94-2]

Bacteriocin. Struct. unknown. Bacteriocin prod. by *Agrobacterium tumefaciens*. Sol. H_2O. λ_{max} 264 (H_2O).

Hendson, M. *et al., Appl. Environ. Microbiol.*, 1983, **45**, 1526-1532

Agrocybenine A-146

[178764-92-6]
1,2,3,5-Tetrahydro-2,2,5,5,7-pentamethyl-6H-pyrrolo[2,3-b]pyridin-6-one, 9CI



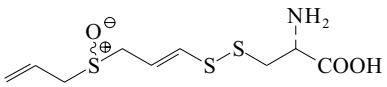
$C_{12}H_{18}N_2O$ 206.287

Alkaloid from the edible Korean mushroom yangimatusutake (*Agrocybe cylindracea*). Yellow powder. λ_{max} 223 (ϵ 16800); 333 (ϵ 9200) (MeOH).

Koshino, H. *et al., Tet. Lett.*, 1996, **37**, 4549 (*isol, uv, ir, pmr, cmr, N-15 nmr, struct*)

Ajocysteine A-147

2-Amino-4,5,9-trithia-6,11-dodecadienoic acid 9-oxide



$C_9H_{15}NO_3S_3$ 281.42

Constit. of garlic (*Allium sativum*). No phys. props. reported.

Lawson, L.D. *et al., Planta Med. (Suppl.)*, 1993, **59**, A688 (*isol*)

Ajoene A-148

[92285-01-3]
2-Propenyl 3-(2-propenylsulfinyl)-1-propenyl disulfide, 9CI. 4,5,9-Trithia-1,6,11-dodecatriene 9-oxide. Allyl 3-allylsulfinyl-1-propenyl disulfide

$H_2C{=}CHCH_2^9S(O)CH_2CH{=}CH\text{-}S\text{-}CH_2CH{=}CH_2$

$C_9H_{14}OS_3$ 234.407

Isol. from garlic (*Allium sativum*) extracts. Nutriceutical with anti-cancer props.. λ_{max} 240 (MeOH) (Berdy).

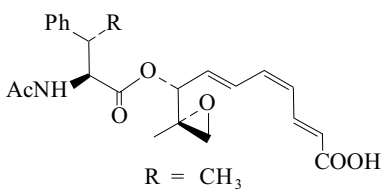
9-Oxide: [118590-71-9] *2-Propenyl 3-(2-propenylsulfonyl)-1-propenyl disulfide, 9CI. Allyl 3-(allylsulfonyl)-1-propenyl disulfide*
$C_9H_{14}O_2S_3$ 250.406
Isol. from garlic.

[72869-75-1, 92284-99-6, 92285-00-2]

Block, E. *et al., J.A.C.S.*, 1986, **108**, 7045-7055 (*synth*)
Gallwitz, H. *et al., J. Med. Chem.*, 1999, **42**, 364-372 (*props*)

AK toxin I A-149

[85146-09-4]
N-*Acetyl-β-methyl-L-phenylalanine 7-carboxy-1-(2-methyloxiranyl)-2,4,6-heptatrienyl ester, 9CI*



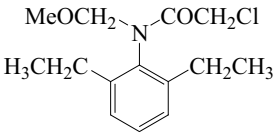
$C_{23}H_{27}NO_6$ 413.469

Prod. by *Alternaria alternata* Japanese pear pathotype. Cryst. (MeOH). Mp 168° dec. $[\alpha]_D^{25}$ +164 (c, 0.128 in MeOH). λ_{max} 285 (ϵ 27600) (MeOH) (Derep). λ_{max} 284 (ϵ 27600) (MeOH) (Berdy).

Nakashima, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 807 (*isol, struct, props*)
Uemura, I. *et al., Tetrahedron*, 2002, **58**, 2351 (*synth*)

Alachlor, ANSI, BSI, ISO, JMAF, WSSA A-150

[15972-60-8]
2-Chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide, 9CI. 2-Chloro-2′,6′-diethyl-N-(methoxymethyl)acetanilide. Alagan. Alanex. Alatox. Bullet. Lasso. Pillarzo. Ralchlor. Satochlor. Alapaz. Nitala



$C_{14}H_{20}ClNO_2$ 269.77

Selective preemergent herbicide used on food crops. Cryst. Spar. sol. H_2O; sol. Me_2CO, C_6H_6, EtOH, EtOAc. Mp 39.5-41.5°.

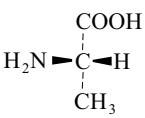
▶ LD_{50} (rat, orl) 1200 mg/kg. Possible skin allergen. AE1225000

[8070-94-8]

U.K. Pat., 1961, 1 008 851; *CA*, **59**, 11330h
Burow, M.D. *et al., Cryst. Struct. Commun.*, 1982, **11**, 747 (*cryst struct*)
Huppatz, J.L. *et al., Pestic. Sci.*, 1982, **13**, 78 (*synth, activity*)
Voyksner, R.D. *et al., J. Chromatogr.*, 1984, **312**, 221 (*hplc*)
Kimmel, E.C. *et al., J. Agric. Food Chem.*, 1986, **34**, 157 (*metab*)
Supreck, J.F. *et al., J. Assoc. Off. Anal. Chem.*, 1987, **70**, 1014 (*gc*)
Chesters, G. *et al., Rev. Environ. Contam. Toxicol.*, 1989, **110**, 1 (*rev*)
Venkov, A.P. *et al., Synth. Commun.*, 1989, **19**, 2133 (*synth, pmr, ir*)
Dangerous Prop. Ind. Mater. Rep., 1990, **10**, 23 (*rev, tox*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A4
Warner, J.M. *et al., Compr. Anal. Profiles Important Pestic.*, 1993, 109 (*rev*)
Pesticide Manual, 11th edn., 1997, No. 14 (*props, use*)
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1341
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CFX000

Alanine, INN, USAN A-151

2-Aminopropanoic acid, 9CI. α-Alanine. Ala



(S)-form

$C_3H_7NO_2$ 89.094

(S)-form [56-41-7]
L-form
Dietary supplement, nutrient. Insol. EtOH; sol. H_2O (16.5g/100ml at 25°). Mp 297° dec. $[\alpha]_D$ +14.6 (c, 1 in 5*M* HCl). $[\alpha]_D$ +1.8 (c, 1 in H_2O). pK_{a1} 2.34; pK_{a2} 9.69 (NH_2). Isoelectric point 6.01. Sweet taste.

▶ AY2990000

N-*(5-Methyl-3-oxohexyl)*:N-*(5-Methyl-3-*

oxohexyl)alanine
$C_{10}H_{19}NO_3$ 201.265
Constit. of false sago (*Cycas circinalis*) (Cycadaceae). Amorph. solid. $[\alpha]_D$ +100 (c, 1.1 in H_2O).

(±)-*form* [302-72-7]
Dietary supplement, nutrient, sweetening flavour enhancer in pickling spice mixts.. Sweet tasting needles or prisms. Spar. sol. H_2O; insol. Et_2O. Mp 295° dec.

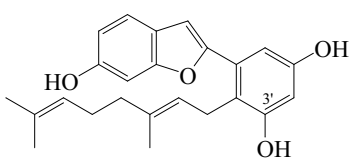
► AY2980000

[2134-48-7, 2491-20-5, 3082-75-5, 17831-01-5, 33208-99-0, 34404-37-0, 95596-57-9, 98204-12-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 570D; 571A; 571B; 672A; 672B; 672C; **2**, 260D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 868C; 869B; 1069B; 1069C (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 20 (*synth*)
Biochem. Prep., 1949, **1**, 9
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1819 (*rev*)
Kost, A.N. *et al., Chem. Ind. (London)*, 1966, 1496 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 16; **5**, 6; **6**, 10 (*use*)
Cavanaugh, J.R. *et al., J.A.C.S.*, 1967, **89**, 1558 (*pmr*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Lehmann, M.S. *et al., J.A.C.S.*, 1972, **94**, 2657 (*cryst struct*)
Okawara, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 869 (*synth*)
Kopitsya, T.P. *et al., Khim. Prir. Soedin.*, 1973, **9**, 656; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 619 (*resoln*)
Kiyooka, S. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1897 (*synth*)
Krapcho, A. *et al., Tet. Lett.*, 1976, 2205 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AFH600; AFH625
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1035
Li, C.-J. *et al., Phytochemistry*, 1996, **42**, 443 (*N-5-methyl-3-oxohexyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 57-59 (*use, props*)
Rosado, M.T.S. *et al., J. Mol. Struct.*, 1997, 410-411; 343-348 (*Raman, ir*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFH600; AFH625

Albafuran A A-152

[84323-14-8]
4-(3,7-Dimethyl-2,6-octadienyl)-5-(6-hydroxy-2-benzofuranyl)-1,3-benzenediol, 9CI. 2-[3,5-Dihydroxy-2-(3,7-dimethyl-2,6-octadienyl)phenyl]-6-hydroxybenzofuran



$C_{24}H_{26}O_4$ 378.467
Constit. of white mulberry (*Morus alba*). Cryst. Poorly sol. hexane. Mp 150-150.5°. λ_{max} 214 (ϵ 40300); 312 (ϵ 27300) (EtOH) (Berdy).

3′-Me ether: [68978-04-1] ***Mulberrofuran A***
$C_{25}H_{28}O_4$ 392.494
Constit. of white mulberry (*Morus alba*). Cryst. λ_{max} 216 (ϵ 32500); 311 (ϵ 23400) (EtOH). λ_{max} 328 (ϵ 23400) (EtOH-NaOH) (Berdy).

Nomura, T. *et al., Heterocycles*, 1978, **9**, 1593-1601 (*Mulberrofuran A*)
Takasugi, M. *et al., Chem. Lett.*, 1982, 1221-1222 (*Albafuran A*)

Albafuran B A-153

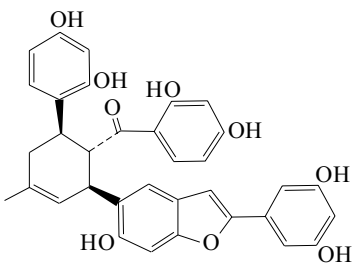
[84323-15-9]
2-(3,7-Dimethyl-2,6-octadienyl)-5-(6-hydroxy-2-benzofuranyl)-1,3-benzenediol, 9CI. 2-[3,5-Dihydroxy-4-(3,7-dimethyl-2,6-octadienyl)phenyl]-6-hydroxybenzofuran

$C_{24}H_{26}O_4$ 378.467
Antifungal constit. of white mulberry (*Morus alba*). Cryst. Poorly sol. hexane. Mp 158-158.5°. λ_{max} 219 (ϵ 27000); 320 (ϵ 34000); 335 (ϵ 29000) (EtOH) (Berdy).

Takasugi, M. *et al., Chem. Lett.*, 1982, 1221

Albafuran C A-154

[84323-16-0]

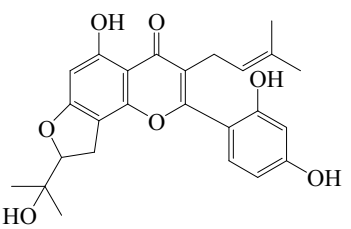


$C_{34}H_{28}O_9$ 580.59
Constit. of white mulberry bark *Morus alba* (famine food). Amorph. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. hexane. $[\alpha]_D$ -302 (EtOH). λ_{max} 216 (ϵ 47000); 284 (ϵ 22300); 294 (ϵ 19600); 322 (ϵ 31700); 336 (ϵ 25700) (EtOH) (Berdy).

Takasugi, M. *et al., Chem. Lett.*, 1982, 1223

Albanin C A-155

[73343-43-8]

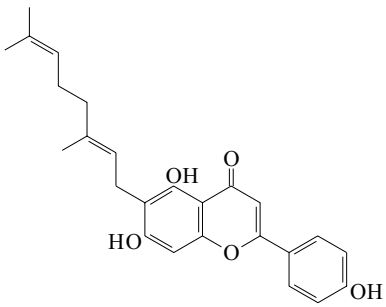


$C_{25}H_{26}O_7$ 438.476
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*.

Takasugi, M. *et al., CA*, 1980, **92**, 160540d (*isol*)

Albanin D A-156

[134955-26-3]
6-(3,7-Dimethyl-2,6-octadienyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 6-Geranyl-4′,5,7-trihydroxyflavone. 6-Geranylapigenin

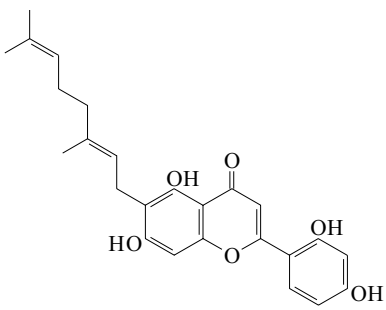


$C_{25}H_{26}O_5$ 406.477
Struct. revised in 1991. Isol. from *Morus alba* (white mulberry). Pale yellow prisms (Me_2CO). Mp 205-207°. λ_{max} 255 ; 288 ; 355 (EtOH) (Berdy).

Fukai, T. *et al., Heterocycles*, 1991, **32**, 499 (*synth, pmr, struct*)

Albanin E A-157

[134955-27-4]
2-(2,4-Dihydroxyphenyl)-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. 6-Geranyl-2′,4′,5,7-tetrahydroxyflavone. 6-Geranylnorartocarpetin

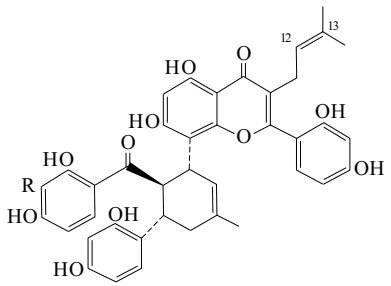


$C_{25}H_{26}O_6$ 422.477
Struct. revised in 1991. Isol. from *Morus alba* (white mulberry). Pale yellow prisms (C_6H_6/Me_2CO). Mp 174-177°. λ_{max} 269 (ϵ 13100); 348 (ϵ 11400) (MeOH) (Berdy). λ_{max} 213 ; 252 ; 271 ; 355 (EtOH) (Berdy).

Fukai, T. *et al., Heterocycles*, 1991, **32**, 499 (*synth, pmr, struct*)

Albanin F A-158

[75629-19-5]
Kuwanon G. Moracenin B



R = H

$C_{40}H_{36}O_{11}$ 692.718

Abs. configs. do not appear certain. All isolates strongly laevorotatory. Authors' numbering shown. Constit. of white mulberry bark (*Morus alba*) (famine food). Amorph. $[\alpha]_D$ -529 (MeOH). Log P 5.13 (calc).

12,13-Dihydro, 13-hydroxy: [78277-79-9]
Moracenin D
$C_{40}H_{38}O_{12}$ 710.733
Yellow amorph. powder. $[\alpha]_D^{18}$ -419 (c, 0.16 in MeOH). $[\alpha]_D$ -388 (c, 0.25 in MeOH). Log P 3.41 (calc).

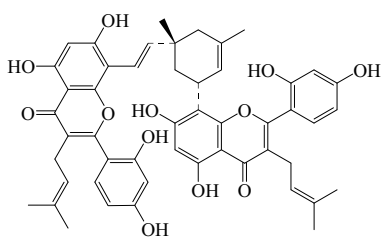
Takasugi, M. *et al., Chem. Lett.*, 1980, 1577
Oshima, Y. *et al., Heterocycles*, 1981, **16**, 979 (*Moracenin D*)
Nomura, T. *et al., Heterocycles*, 1981, **16**, 983 (*Moracenin D*)
Nomura, T. *et al., Planta Med.*, 1983, **49**, 90; 1984, **50**, 127 (*isol*)
Hano, Y. *et al., Heterocycles*, 1988, **27**, 2315 (*abs config*)
Takayama, M. *et al., Rapid Commun. Mass Spectrom.*, 1995, **9**, 383 (*ms*)

Albanin G A-159

[76472-87-2]
Kuwanon H. Moracenin A
As Albanin F, A-158 with
R = $(H_3C)_2C{=}CHCH_2$–
$C_{45}H_{44}O_{11}$ 760.836
Constit. of white mulberry (*Morus alba*). $[\alpha]_D$ -455 (MeOH). Log P 7.13 (uncertain value) (calc).

Takasugi, M. *et al., Chem. Lett.*, 1980, 1577
Nomura, T. *et al., Planta Med.*, 1983, **49**, 90; 1984, **50**, 127 (*isol*)

Albanin H A-160

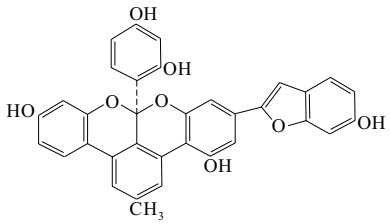


$C_{50}H_{48}O_{12}$ 840.922
Constit. of *Morus alba* (white mulberry). Yellow cryst. Mp 215° dec. Racemic.

Nomura, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **53**, 87-201 (*rev*)

Albanol B A-161

[87084-99-9]



$C_{34}H_{22}O_8$ 558.543

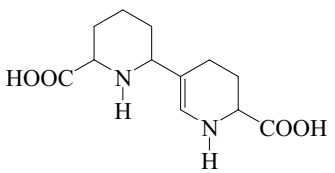
Artifact derived from Mulberrofuran I. Constit. of bark of white mulberry *Morus alba* (famine food). Yellow plates. Mp 248° dec.

Rao, A.V.R. *et al., Tet. Lett.*, 1983, **24**, 3013
Hano, Y. *et al., Heterocycles*, 1989, **28**, 745

Aldosine A-162

[142759-11-3]

[173449-61-1, 173653-73-1]
5-(6-Carboxy-2-piperidinyl)-1,2,3,4-tetrahydro-2-pyridinecarboxylic acid, 9CI

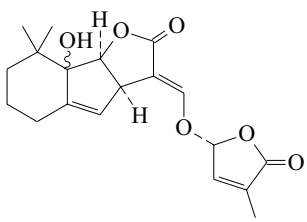


$C_{12}H_{18}N_2O_4$ 254.285
Hydrol. product from the aldol crosslinks of bovine elastin and collagen.

Suyama, K. *et al., Agric. Biol. Chem.*, 1991, **55**, 3147-3149
Nakamura, F. *et al., Arch. Biochem. Biophys.*, 1996, **325**, 167-173

Alectrol A-163

[143572-84-3]



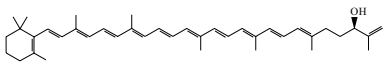
$C_{19}H_{22}O_6$ 346.379

Struct. has been proven to be incorrect (1998) by synthesis. Revised struct. not reported. Isol. from the roots of *Vigna unguiculata* (genuine host plant for *Alectra* spp.). Similar to Strigol, S-251.

Mueller, S. *et al., J. Plant Growth Regul.*, 1992, **11**, 77 (*isol*)
Mori, K. *et al., Tet. Lett.*, 1998, **39**, 6023-6026 (*struct*)
Matsui, J. *et al., Eur. J. Org. Chem.*, 1999, 2195-2199 (*struct*)

Aleuriaxanthin A-164

[51599-07-6]
1′,16′-Didehydro-1′,2′-dihydro-β,ψ-caroten-2′-ol



$C_{40}H_{56}O$ 552.882
Constit. of *Aleuria aurantia* (orange cup). Cryst. (Et_2O/petrol). Mp 122-122.5°.

Ac: [51276-30-3]
Purple prisms. Mp 134.5-135.5°.

Liaaen-Jensen, S. *et al., Phytochemistry*, 1965, **4**, 925 (*occur*)
Kjosen, H. *et al., Acta Chem. Scand.*, 1973, **27**, 2495 (*synth, uv, ir, pmr*)
Arpin, N. *et al., Phytochemistry*, 1973, **12**, 2751 (*struct, pmr, ir, uv*)
Buchecker, R. *et al., Phytochemistry*, 1976, **15**, 1013 (*struct*)
Eschenmoser, W. *et al., Helv. Chim. Acta*, 1983, **66**, 82 (*synth*)

Alexomycin, USAN A-165

[165101-50-8]
U 82127. PNU 82127

Mixt. composed mainly of isolate 10381b which contains several cyclic sulfur peptides prod. by *Streptomyces arginensis*. Veterinary growth promoter used for poultry and swine.

Cromwell, G.L. *et al., J. Anim. Sci.*, 1996, **74**, 1284-1287 (*activity*)
Cho, B.-Y. *et al., J. Chromatogr., B: Biomed. Appl.*, 1997, **67**, 163-174 (*anal*)
Marshall, S.A. *et al., Diagn. Microbiol. Infect. Dis.*, 1999, **33**, 181-186 (*activity*)

Alfalfone A-166

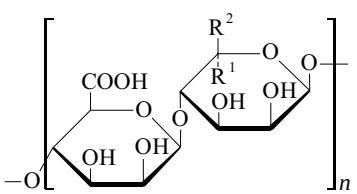
$C_{21}H_{42}O$ 310.562

Ketone of unknown struct.. Constit. of the meal of *Medicago sativa* (alfalfa). Powder. Mp 88.5-88.8°.

Jacobson, C.A. *et al., J.A.C.S.*, 1912, **34**, 300 (*isol*)

Alginic acid, BAN A-167

[9005-32-7]
Gum levan. Levan gum. Kelacid. Norgine. Sazio. E400



R^1 = H, R^2 = COOH
or R^1 = COOH, R^2 = H

$[C_6H_8O_6]$

A polymer consisting of various proportions of β-D-Mannuronic acid and α-L-Guluronic acid linked 1→4 and arranged in a block fashion. Polymeric. Minimum formula given. Alginates are used to improve food texture, e.g. in ice cream, pie fillings. Emulsifier, stabiliser,

thickener. $[\alpha]_D$ -120 (as Na salt in H_2O). Approx. 200 grades of the acid and its salts (ammonium, Ca, K, Na) comly. available. Alginates with the highest guluronic acid content display the strongest gel-forming activity.

▶ AZ5775000

Na salt: [9005-38-3] *Sodium alginate. Algin. E401*
Stabiliser, emulsifier, thickener, formulation aid. Pale yellow-brown powder. Sol. H_2O; poorly sol. EtOH, hexane. λ_{max} 260 (H_2O) (Berdy).

▶ AZ5820000

K salt: [9005-36-1] *Potassium alginate. E402*
Stabiliser, emulsifier, thickener, formulation aid. Insol. EtOH, Et_2O.

Ca salt: [9005-35-0] *Calcium alginate. E404*
Stabiliser, emulsifier, thickener, formulation aid. Sl. sol. EtOH; insol. H_2O, Et_2O.

NH_4 salt: [9005-34-9] *Ammonium alginate. E403*
Stabiliser, emulsifier, thickener, formulation aid. Insol. EtOH, Et_2O.

2-Hydroxypropyl ester:

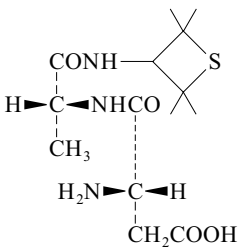
[39306-87-1, 51374-11-9, 52441-26-6, 57762-73-9, 59125-52-9, 95328-14-6] *Propylene glycol alginate. Colloid 602. Dricoid. Kelcoloid. FEMA 2941. E405. Many other trade names*
Stabiliser, emulsifier, thickener, formulation aid, surface active agent and flavouring adjunct or adjuvant for foodstuffs. White to yellowish fibrous or granular powder. Sol. H_2O. Composition varies acc. to the degree of esterification.

[9005-31-6, 9019-42-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1225B (*ir*)
Hirst, E. *et al., Chem. Ind. (London)*, 1963, 257
Haug, A. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 69 (*synth*)
Percival, E. *et al., The Carbohydrates*, (Pigman, W., Ed.), Academic Press, 1970, **2B**, 545
Ger. Pat., 1971, 2 046 966; *CA*, **75**, 22923d (*2-hydroxypropyl ester, manuf*)
Rees, D.A. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 214 (*struct, rev*)
Grasdalen, H. *et al., Carbohydr. Res.*, 1977, **56**, C11; 1981, **89**, 179 (*nmr, cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 45 (*use*)
Cottrell, I.W. *et al., Handb. Water-Soluble Gums Resins*, McGraw-Hill, N.Y., 1980, 2/1-2/43 (*rev*)
Fed. Regist., 1982, **47**, 29946-29952 (*propylene glycol alginate*)
Martin, G. *et al., Sci. Aliments*, 1986, **6**, 473 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AFL000
Beale, J.M. *et al., Environ. Sci. Res.*, 1992, **44**, 209 (*rev, biosynth, struct*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 10-11; 428-430
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1535
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 71-74; 2349-2352 (*props, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFL000; SEH000; CAM200; PKU700

Alitame, USAN A-168

[80863-62-3]
L-α-Aspartyl-N-*(2,2,4,4-tetramethyl-3-thietanyl)-D-alaninamide, 9CI. CP 54802*

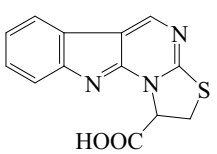


$C_{14}H_{25}N_3O_4S$ 331.435
Sweetening agent. Intensely sweet, approx. 2000 × sucrose.. Solid + $2.5H_2O$. Log P -1.28 (calc). Use currently (1999) permitted in Australia, New Zealand, Indonesia and China.

[99016-42-9]

U.S. Pat., 1983, 4 411 925, (*Pfizer*); *CA*, **101**, 22238 (*synth, use*)
Lawrence, J.F. *et al., J. Assoc. Off. Anal. Chem.*, 1988, **71**, 934-937 (*chromatog*)
Hendrick, M.E. *et al., Food Sci. Technol.*, 1991, **48**, 29-38 (*rev*)
Ager, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*rev*)

Brassica oleracea Alkaloid A-169



$C_{13}H_9N_3O_2S$ 271.299
Alkaloid found on the leaf surfaces of *Brassica oleracea* cv. *botrytis* (cauliflower).

Glycine amide:
$C_{15}H_{12}N_4O_3S$ 328.351
Alkaloid found on the leaf surfaces of *Brassica oleracea* cv. *botrytis* (cauliflower).

Hurter, J. *et al., Phytochemistry*, 1999, **51**, 377-382 (*isol, pmr, cmr, ms*)

Gentiana Alkaloid V A-170

$C_{10}H_9NO_2$ 175.187
Struct. unknown. Monoterpene alkaloid. Alkaloid from *Gentiana lutea* (yellow gentian). Mp 240°.

Marekov, N. *et al., Dokl. Bolg. Akad. Nauk*, 1965, **18**, 999; *CA*, **64**, 11270a (*isol, ir*)
Cordell, G.A. *et al., Alkaloids (N.Y.)*, 1977, **16**, 431 (*rev*)

Rosmarinus officinalis Alkaloid 2 A-171

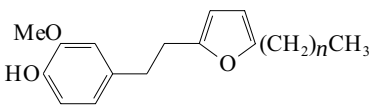
$C_{20}H_{27}NO_4$ 345.438
Struct. unknown. Isol. from rosemary (*Rosmarinus officinalis*) using NH_3 during extraction. Cryst. (toluene). Mp 197-198° dec. $[\alpha]_D$ +36 (c, 1.48 in dioxan). Artifact.

Hydrochloride:
Cryst. (H_2O). Mp 214-216° dec.

N,O,O-*Tri-Ac:*
Cryst. (MeOH). Mp 291-292° dec.

Yakhontova, L.D. *et al., Khim. Prir. Soedin.*, 1967, **3**, 140; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 118

2-Alkyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furans A-172



n = 3, 5, 7

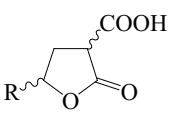
2-Butyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan [143114-90-3]
4-[2-(5-Butyl-2-furanyl)ethyl]-2-methoxyphenol, 9CI
$C_{17}H_{22}O_3$ 274.359
Isol. from dry rhizomes of ginger *Zingiber officinale*. *n* = 3.

2-Hexyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan [143114-91-4]
4-[2-(5-Hexyl-2-furanyl)ethyl]-2-methoxyphenol, 9CI
$C_{19}H_{26}O_3$ 302.413
Isol. from dry rhizomes of ginger *Zingiber officinale*. *n* = 5.

2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]-5-octylfuran [143114-92-5]
4-[2-(5-Octyl-2-furanyl)ethyl]-2-methoxyphenol, 9CI
$C_{21}H_{30}O_3$ 330.466
Isol. from dry rhizomes of ginger *Zingiber officinale*. *n* = 7.

Nakatani, N. *et al., Chem. Express*, 1992, **7**, 221 (*isol, pmr, cmr*)

5-Alkyltetrahydro-2-oxo-3-furancarboxylic acids A-173



5-Butyltetrahydro-2-oxo-3-furancarboxylic acid, 9CI
2-Carboxy-4-octanolide
$C_9H_{14}O_4$ 186.207
Possible latent butter aroma compd.. Mp 48-50°.

5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-6-methyl-4-heptanolide
$C_9H_{14}O_4$ 186.207
Possible latent butter aroma compd.. Mp

51-54°.

5-Pentyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-nonanolide
$C_{10}H_{16}O_4$ 200.234
Possible latent butter aroma compd.. Mp 46-48°.

5-(3*E*-Pentenyl)tetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-7-nonen-4-olide
$C_{10}H_{14}O_4$ 198.218
Possible latent butter aroma compound. Mp 52.5-54°.

5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid, 9CI
2-Carboxy-4-decanolide. α-Carboxy-γ-decalactone
$C_{11}H_{18}O_4$ 214.261
Possible latent butter aroma compd.. Mp 60.5-62.5°.

5-(1,3-Dimethylbutyl)tetrahydro-2-oxo-3-furancarboxylic acid
5-(4-Methyl-2-pentyl)tetrahydro-2-oxo-3-furancarboxylic acid. 2-Carboxy-5,7-dimethyl-4-octanolide
$C_{11}H_{18}O_4$ 214.261
Possible latent butter aroma compd.. Mp 100.5-105°.

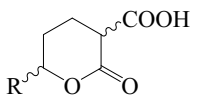
5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-undecanolide
$C_{12}H_{20}O_4$ 228.288
Possible latent butter aroma compd.. Mp 58-60°.

5-Octyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-dodecanolide. α-Carboxy-γ-dodecalactone
$C_{13}H_{22}O_4$ 242.314
Possible latent butter aroma compd.. Mp 68.5-70.5°.

5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-tridecanolide
$C_{14}H_{24}O_4$ 256.341
Possible latent butter aroma compd.. Mp 68.5-69.5°.

Stoll, M. *et al., Nature (London)*, 1964, **202**, 350
Martin, J. *et al., Chem. Comm.*, 1970, 27 (*synth*)

6-Alkyltetrahydro-2-oxo-2*H*-pyran-3-carboxylic acids A-174



See also 5-Alkyltetrahydro-2-oxo-3-furancarboxylic acids, A-173.

6-Butyltetrahydro-2-oxo-2*H*-pyran-3-carboxylic acid
2-Carboxy-5-nonanolide. α-Carboxy-δ-nonalactone
$C_{10}H_{16}O_4$ 200.234
Possible latent butter aroma compd.. Mp 79-80°.

6-Pentyltetrahydro-2-oxo-2*H*-pyran-3-carboxylic acid
2-Carboxy-5-decanolide. α-Carboxy-δ-decalactone
$C_{11}H_{18}O_4$ 214.261
Possible latent butter aroma compd.. Mp 77-78°.

Stoll, M. *et al., Nature (London)*, 1964, **202**, 350 (*synth*)

Allantoic acid A-175

[99-16-1]
Bis[(aminocarbonyl)amino]acetic acid, 9CI. Diureidoacetic acid. Hidantoic acid (obsol.)
$(H_2NCONH)_2CHCOOH$
$C_4H_8N_4O_4$ 176.132
Isol. from coffee beans and leaves. Needles. Spar. sol. H_2O, org. solvs., dil. acids. Mp 173° dec. Sinters at 168°. Hot H_2O → Glyoxylic acid + Urea, U-33.

Et ester: [156217-60-6]
$C_6H_{12}N_4O_4$ 204.185
Needles. Sol. EtOH, hot H_2O. Dec. ca. 200°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 675B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 805D (*ir*)
Behrend, R. *et al., Annalen*, 1909, **365**, 21-37 (*synth*)
Fosse, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1929, **189**, 716-717; 1933, **196**, 1264-1267 (*occur*)
Schlee, D. *et al., Phytochemistry*, 1963, **2**, 231-236 (*biosynth*)
Ringertz, H. *et al., Acta Cryst. B*, 1968, **24**, 1686-1692 (*cryst struct*)

Allicin A-176

[539-86-6]
S-*2-Propenyl 2-propene-1-sulfinothioate, 9CI. Allitridi*
$H_2C{=}CHCH_2\text{-}SO\text{-}S\text{-}CH_2CH{=}CH_2$
$C_6H_{10}OS_2$ 162.276
Isol. from garlic (*Allium sativum*). Nutriceutical. Yellow liq. Sol. H_2O, MeOH, Et_2O; fairly sol. hexane. d 1.11. λ_{max} 202 ; 240 (MeOH) (Berdy).

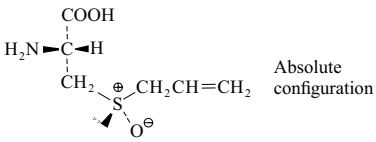
▶ LD_{50} (mus, scu) 120 mg/kg, LD_{50} (mus, ivn) 60 mg/kg. Can cause allergic contact dermatitis in sensitized individuals. UD1900000

[72869-75-1]

Cavallito, C.J. *et al., J.A.C.S.*, 1944, **66**, 1950 (*isol, pharmacol*)
Stoll, A. *et al., Helv. Chim. Acta*, 1948, **31**, 189; 1949, **32**, 197 (*synth*)
Virtanen, A.I. *et al., Angew. Chem., Int. Ed.*, 1962, **1**, 299 (*rev*)
Isenberg, N. *et al., Int. J. Sulfur Chem.*, 1973, **3**, 307 (*rev*)
Papageorgiou, C. *et al., Arch. Dermatol. Res.*, 1983, **275**, 229 (*tox*)
Block, E. *et al., J.A.C.S.*, 1986, **108**, 7045 (*synth, cmr, ir, pmr*)
Mayeux, P.R. *et al., Agents Actions*, 1988, **25**, 182 (*pharmacol*)
Makheja, A.N. *et al., Agents Actions*, 1990, **29**, 360 (*pharmacol*)
Gebhardt, R. *et al., Arzneim.-Forsch.*, 1991, **41**, 800 (*pharmacol*)
Gebhardt, R. *et al., Biochim. Biophys. Acta*, 1994, **1213**, 57 (*pharmacol*)
Calvey, E.M. *et al., J. Chromatogr. Sci.*, 1994, **32**, 93 (*chromatog*)
Block, E. *et al., Sulfur Compds. Foods, 1993*, (Eds. Mussinan, C.J. *et al*), American Chemical Society (*ACS Symp. Ser.* v564 1994), 1994, 63 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFS250

Alliin A-177

3-(2-Propenylsulfinyl)alanine, 9CI. β-Allylsulfenylalanine. S-*Allylcysteine sulfoxide*



$C_6H_{11}NO_3S$ 177.224

(*R*)$_C$(*S*)$_S$-*form* [556-27-4]
Constit. of garlic oil (*Allium sativum*), also from ramsons (*Allium ursinum*). Needles (Me_2CO aq.). Mp 163° dec. $[\alpha]_D^{21}$ +67.7 (c, 2.0 in H_2O). Other stereoisomers have been prepared synthetically.

N-*(1-Deoxy-β-D-fructopyranosyl):*
[149340-22-7]
$C_{12}H_{21}NO_8S$ 339.366
Isol. from garlic (*Allium sativum*). Powder. $[\alpha]_D^{20}$ -25.4 (c, 0.41 in H_2O).

N-*Ac:* [38131-20-3]
Mp 188-198° dec. $[\alpha]_D^{21}$ -29 (c, 1.0 in MeOH).

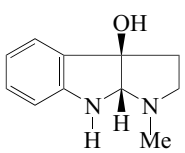
N-*Benzoyl:*
Mp 152-153.5° dec. $[\alpha]_D^{20}$ -6 (c, 1.0 in MeOH).

N-*(4-Nitrobenzoyl):*
Mp 180-182° dec. $[\alpha]_D^{20}$ -9 (c, 1.0 in 0.1*N* NaOH).

Stoll, A. *et al., Helv. Chim. Acta*, 1951, **34**, 481 (*synth*)
Virtanen, A.I. *et al., Angew. Chem., Int. Ed.*, 1962, **1**, 299 (*rev*)
Nishimura, H. *et al., Tetrahedron*, 1972, **28**, 4503 (*ms, ir*)
Freeman, G.G. *et al., Phytochemistry*, 1976, **15**, 521 (*synth*)
Muetsch-Eckner, M. *et al., J. Nat. Prod.*, 1993, **56**, 864 (*N-glycoside*)
Edwards, S.J. *et al., Phytochem. Anal.*, 1994, **5**, 4 (*anal*)
Keusgen, M. *et al., Planta Med.*, 1998, **64**, 736-740 (*anal*)
Kubec, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 428-433 (*occur*)

Alline A-178

[101053-34-3]
2,3,8,8a-Tetrahydro-1-methylpyrrolo[2,3-b]indol-3a(1H)-ol, 9CI



Relative Configuration

$C_{11}H_{14}N_2O$ 190.244

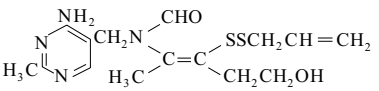
Relative config. only appears to be known. Alkaloid from Chinese chives (*Allium odorum*) and several other *Allium* spp.. Mp 91-92°. $[\alpha]_D$ +136.3 (c, 1.218 in HCl). λ_{max} 245 (log ϵ 3.68); 303 (log ϵ 3.14) (no solvent reported).

Hydrochloride:
Mp 196-197°.

Tashkhodzhaev, B. *et al., Khim. Prir. Soedin.*, 1985, **21**, 687; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 645 (*isol, cryst struct, uv*)
Samikov, K. *et al., Khim. Prir. Soedin.*, 1986, **22**, 383; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 362 (*occur*)
Antsupova, T.P. *et al., Rastit. Resur.*, 1987, **23**, 436; *CA*, **107**, 214830x (*occur*)

Allithiamine A-179

[554-44-9]
N-*[(4-Amino-2-methyl-5-pyrimidinyl)-methyl]*-N-*[4-hydroxy-1-methyl-2-(2-propenyldithio)-1-butenyl]formamide, 9CI*



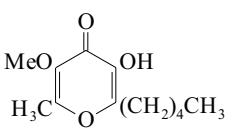
$C_{15}H_{22}N_4O_2S_2$ 354.496

Obt. from garlic (*Allium sativum*). Imparts meaty flavour to foods. Has vitamin B_1 activity. Investigated as a dietary supplement to enhance muscle performance in sports. Cryst. (C_6H_6). Mp 132-133° dec.

Matsukawa, T. *et al., Science (Washington, D.C.)*, 1953, **118**, 325 (*isol, struct*)
Matsukawa, T. *et al., CA*, 1955, **49**, 7572g (*synth*)
Baker, H. *et al., J. Nutr. Sci. Vitaminol.*, Suppl., 1976, **22**, 63-68 (*pharmacol*)
Doyle, M.R. *et al., Int. J. Sport Nutr.*, 1997, **7**, 39-47 (*use*)

Allixin A-180

[125263-70-9]
3-Hydroxy-5-methoxy-6-methyl-2-pentyl-4H-pyran-4-one, 9CI



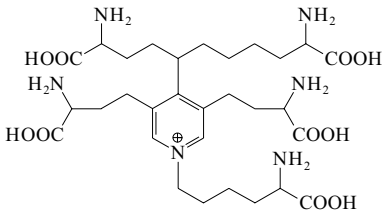
$C_{12}H_{18}O_4$ 226.272

Constit. of garlic (*Allium sativum*). Potential nutriceutical. Needles (MeOH aq.). Mp 80-81°. λ_{max} 279 (no solvent reported).

Kodera, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1656 (*isol, struct*)
Arimoto, H. *et al., Tet. Lett.*, 1997, **38**, 7761-7762 (*synth*)
Matsumura, Y. *et al., Tet. Lett.*, 1998, **39**, 2339-2340 (*synth*)
Kodera, Y. *et al., Chem. Pharm. Bull.*, 2002, **50**, 354-363; 405-407 (*pmr, cmr, ms, pharmacokinet*)

Allodesmosine A-181

[129717-82-4]



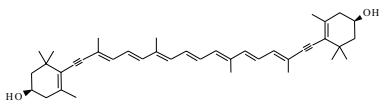
$C_{30}H_{51}N_6O_{10}^{\oplus}$ 655.767

Isol. from hydrolysate of bovine ligamentum nuchae elastin. Amorph. solid with faint yellow tinge. V. hygroscopic. Related to Desmosine, D-93.

Suyuma, K. *et al., Biochem. Biophys. Res. Commun.*, 1990, **170**, 713 (*isol, uv, ms, pmr*)
Nakamura, F. *et al., Agric. Biol. Chem.*, 1991, **55**, 547 (*isol, pmr, ms*)

Alloxanthin A-182

[28380-31-6]
7,7′,8,8′-Tetradehydro-β,β-carotene-3,3′-diol. Cynthiaxanthin. Cryptomonaxanthin. Manixanthin. Pectenoxanthin



$C_{40}H_{52}O_2$ 564.85

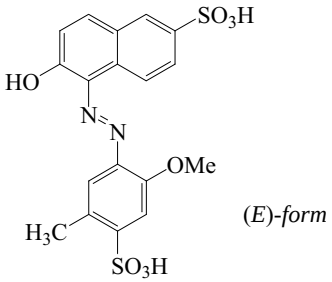
Constit. of many shellfish including the giant scallop (*Pecten maximus*) and edible mussel (*Mytilus edulis*). Reddish needles (Me_2CO/petrol). Mp 188-190° (186-188°).

[26666-93-3, 95343-66-1]

Chapman, D.J. *et al., Phytochemistry*, 1966, **5**, 1331 (*isol*)
Davies, A.J. *et al., Chem. Comm.*, 1967, 941 (*isol*)
De Ville, T.E. *et al., Chem. Comm.*, 1969, 1311 (*struct*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Davies, A.J. *et al., J.C.S. Perkin 1*, 1984, 2147 (*synth*)
Pennington, F.C. *et al., Biochem. Syst. Ecol.*, 1985, **13**, 215 (*isol, cd*)
Matsuno, T *et al., J. Nat. Prod.*, 1985, **48**, 606 (*isol*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv*)

Allura red AC A-183

[25956-17-6]
6-Hydroxy-5-[(2-methoxy-5-methyl-4-sulfophenyl)azo]-2-naphthalenesulfonic acid, 9CI. FD and C Red No. 40. C.I. 16035. C.I. Food Red 17. Allura Red. E129



(*E*)-*form*

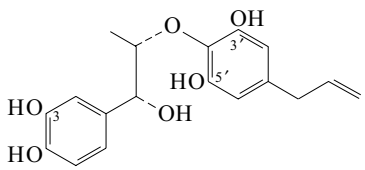
$C_{18}H_{16}N_2O_8S_2$ 452.465

Colour additive used in gelatins, puddings, custards, beverages, sauces, toppings, fruits, dairy products, bakery products, jams, jellies, condiments, meat and poultry. Dark red powder. Strictly the name Allura red AC applies to the disodium salt. Banned in EEC, Norway and Japan.

▶ QK2260000

U.K. Pat., 1970, 1 164 249; *CA*, **72**, 68195 (*synth*)
Borzelleca, J.F. *et al., Food Chem. Toxicol.*, 1989, **27**, 701 (*tox*)
Merck Index, 11th edn., 1989, No. 283
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1078-1080 (*use, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG100

2-(4-Allyl-2,6-dihydroxyphenoxy)-1-(3,4-dihydroxyphenyl)-1-propanol A-184



$C_{18}H_{20}O_6$ 332.352

Neolignan numbering shown.

(R*,S*)-form

3,3′,5′-Tri-Me ether: [52190-21-3] *α-[1-[2,6-Dimethoxy-4-(2-propenyl)phenoxy]ethyl]-4-hydroxy-3-methoxybenzenemethanol, 9CI. 2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol*
$C_{21}H_{26}O_6$ 374.433
From seed kernels of *Myristica fragrans* (nutmeg). Mp 96.5-97.5°.

3,3′,5,5′-Tetra-Me ether: [41535-92-6] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)-1-propanol*
$C_{22}H_{28}O_6$ 388.46
From *Myristica fragrans* (nutmeg). Cryst. Mp 65-66°.

3,4-Methylene, 3′,5′-di-Me ether: [50354-29-5] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-methylenedioxyphenyl)-1-propanol*
$C_{21}H_{24}O_6$ 372.417
Constit. of *Myristica fragrans* (nutmeg). Oil.

3,4-Methylene, 3′,5′-di-Me ether, Ac:
$C_{23}H_{26}O_7$ 414.454

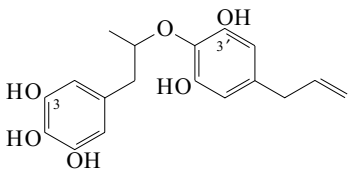
Consit. of *Myristica fragrans* (nutmeg). Oil.

3,4-Methylene, 3′,5′-di-Me ether, benzoyl:
$C_{28}H_{28}O_7$ 476.525
Consit. of *Myristica fragrans* (nutmeg). Oil.

[41535-95-9, 52190-19-9]

Isogai, A. *et al., Agric. Biol. Chem.*, 1973, **37**, 1479 (*isol, ir, uv, pmr, ms*)
Forrest, J.E. *et al., J.C.S. Perkin 1*, 1974, 205 (*isol, uv, pmr, ms*)
Kasahara, H. *et al., Phytochemistry*, 1995, **40**, 1515 (*abs config*)

2-(4-Allyl-2,6-dihydroxyphenoxy)-1-(3,4,5-trihydroxyphenyl)propane A-185



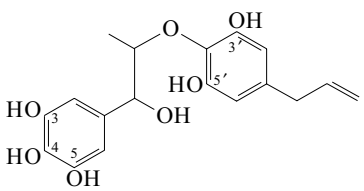
$C_{18}H_{20}O_6$ 332.352
Neolignan numbering shown.

Penta-Me ether: [124151-41-3] ***Virolongin B.*** *β-O-Dilignol*
$C_{23}H_{30}O_6$ 402.486
Constit. of *Myristica fragrans* (nutmeg). Oil. Identity of isolated samples not establ., may not be stereochemically identical.

3,4-Methylene, 3′,5,5′-tri-Me ether: [126223-32-3] ***Virolongin C***
$C_{22}H_{26}O_6$ 386.444
Oil.

Isogai, A. *et al., Agric. Biol. Chem.*, 1973, **37**, 193; 889; 1479 (*isol, struct*)
Forrest, J.E. *et al., J.C.S. Perkin 1*, 1974, 205 (*isol, synth, struct*)
Calvacante, S.H. *et al., Phytochemistry*, 1985, **24**, 1051 (*isol*)
Muhammed, I. *et al., J. Nat. Prod.*, 1989, **52**, 1177 (*isol, pmr, cmr*)

2-(4-Allyl-2,6-dihydroxyphenoxy)-1-(3,4,5-trihydroxyphenyl)-1-propanol A-186



$C_{18}H_{20}O_7$ 348.352
Neolignan numbering shown.

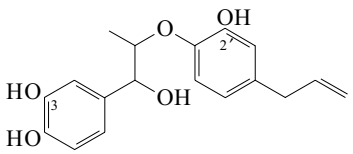
3,3′,4,5′-Tetra-Me ether: [108907-57-9] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3-hydroxy-4,5-dimethoxyphenyl)-1-propanol*
$C_{22}H_{28}O_7$ 404.459
Constit. of oil of *Myristica fragrans* (nutmeg). Oil.

3,3′,5,5′-Tetra-Me ether: [108907-53-5] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(4-hydroxy-3,5-dimethoxyphenyl)-1-propanol*
$C_{22}H_{28}O_7$ 404.459
Constit. of oil of *Myristica fragrans* (nutmeg).

Penta-Me ether: [41551-58-0] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4,5-trimethoxyphenyl)-1-propanol*
$C_{23}H_{30}O_7$ 418.486
Constit. of *Myristica fragrans* (nutmeg). Mp 70-72° (66-66.5°).

Isogai, A. *et al., Agric. Biol. Chem.*, 1973, **37**, 193; 889; 1479
Forrest, J.E. *et al., J.C.S. Perkin 1*, 1974, 205
Hattori, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 668
Zacchino, S.A. *et al., J. Nat. Prod.*, 1988, **51**, 1261 (*synth, ir, pmr, cmr, ms*)

2-(4-Allyl-2-hydroxyphenoxy)-1-(3,4-dihydroxyphenyl)-1-propanol A-187



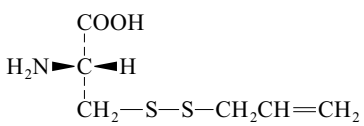
$C_{18}H_{20}O_5$ 316.353
Neolignan numbering shown.

2′,3-Di-Me ether: [108907-55-7] *2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol*
$C_{20}H_{24}O_5$ 344.407
Constit. of *Myristica fragrans* (nutmeg) oil. Oil.

Hattori, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 668

S-(Allylthio)cysteine A-188

[30910-60-2]
3-(2-Propenyldithio)alanine, 9CI. 3-(Allyldithio)alanine, 8CI. 2-Amino-3-(2-propenyldithio)propanoic acid. S-*Allymercaptocysteine. 2-Amino-4,5-dithia-7-heptenoic acid. SAMC*



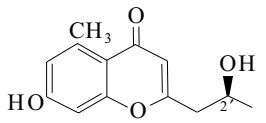
$C_6H_{11}NO_2S_2$ 193.29

(*R*)-*form* [2281-22-3]
L-form
Isol. from garlic (*Allium sativum*). Potential nutriceutical. Plates (Me_2CO aq.). Mp 187-188° dec. $[\alpha]_D^{23.5}$ -107.9 (c, 0.4 in 6*M* HCl).

Cavallito, C.J. *et al., J.A.C.S.*, 1944, **66**, 1952 (*synth*)
Sugii, M. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1114 (*isol, ir, struct*)

Aloesol A-189

[94356-35-1]
7-Hydroxy-2-(2-hydroxypropyl)-5-methyl-4H-1-benzopyran-4-one, 9CI. 7-Hydroxy-2-(2-hydroxypropyl)-5-methylchromone



$C_{13}H_{14}O_4$ 234.251
Constit. of *Aloe* spp. and Chinese rhubarb. Cryst. (AcOH/MeOH). Mp 187.5-189°. $[\alpha]_D^{21}$ +38.4 (c, 0.89 in MeOH).

7-O-β-D-Glucopyranoside: [94356-36-2]
$C_{19}H_{24}O_9$ 396.393
Constit. of rhubarb *Rheum* sp.. Needles + $1H_2O$ (MeOH/$CHCl_3$). Mp 191-193°. $[\alpha]_D^{24}$ -4.3 (c, 0.21 in MeOH).

2′-Ketone: [40738-40-7] ***Aloesone***
$C_{13}H_{12}O_4$ 232.235
Cryst. ($CHCl_3$). Mp 151-152°.

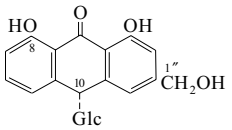
2′-Ketone, 7-O-β-D-glucopyranoside: [128701-04-2]
$C_{19}H_{22}O_9$ 394.377
Constit. of Chinese rhubarb (*Rheum* sp.). Needles (MeOH aq.). Mp 229-230°. $[\alpha]_D^{19}$ -50.6 (c, 0.37 in MeOH).

[104871-04-7, 135096-88-7]

Holdsworth, D.K. *et al., Planta Med.*, 1972, **22**, 54 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3493 (*isol*)
Gramatica, P. *et al., Heterocycles*, 1986, **24**, 743 (*synth*)
Kashiwada, Y. *et al., Phytochemistry*, 1990, **29**, 1007 (*isol, pmr, cmr*)
Che, Q.M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 704 (*occur*)

Aloin, BAN A-190

[8015-61-0]
10-β-D-Glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10H)-anthracenone, 9CI. Barbaloin. Socaloin. Ugandaloin. Jafaloin. Cafaloin



(10*R*)-*form*

$C_{21}H_{22}O_9$ 418.399
Aloin as normally obt. is a mixt. of 10-epimers separable by hplc into Aloin A and the unstable Aloin B. Aloin A can also be obt. by cryst. from MeOH. Constit. of various *Aloe* spp.. Sol. H_2O. Log P -1.88 (calc).
▶ LD_{50} (mus, ivn) 200 mg/kg.

(10*R*)-*form* [28371-16-6]
Aloin B. *Isobarbaloin. β-Barbaloin*
Mp 138-140° (block). $[\alpha]_D^{30}$ -73 (c, 0.5 in MeOH). Negative CD at 295 nm. Pmr δ 5.27 (C-1′). Labile in soln. Isobarbaloin and β-Barbaloin were prob. not homogeneous.

1″-O-α-L-Rhamnopyranoside: [11006-91-0] ***Aloinoside B***
$C_{27}H_{32}O_{13}$ 564.542
Isol. from leaves of *Aloe* cf. *perryi*. Cryst. (Me_2CO aq.). Mp 233°. $[\alpha]_D^{20}$ -45.3 (c, 1.5 in 50% dioxan aq.).

8-O-β-D-Glucopyranoside: [53861-34-0] ***Cascaroside B***

$C_{27}H_{32}O_{14}$ 580.541
Isol. from *Rhamnus purshiana* (Cascara sagrada) bark. Cryst. + $2H_2O$. Mp 175-178°. $[\alpha]_D^{30}$ -104.4 (MeOH). Cascarosides A and B are a pair of 10-epimers corresponding to Aloins A and B but the configurational correspondence of Cascaroside B to Aloin B is not established, i.e. it could be (10*R*-).

*1″-Carboxylic acid, 8-*O*-β-D-glucopyranoside:* [111545-29-0] ***Rheinoside C***
$C_{27}H_{30}O_{15}$ 594.525
Isol. from rhubarb. Pale yellow powder + $2H_2O$. $[\alpha]_D^{25}$ -40 (c, 0.5 in MeOH).

7-Hydroxy: [82461-12-9] ***7-Hydroxyaloin B***
$C_{21}H_{22}O_{10}$ 434.399
Constit. of leaves of *Aloe vera*.

7-Hydroxy, 8-Me ether: ***7-Hydroxy-8-O-methylaloin B***
$C_{22}H_{24}O_{10}$ 448.426
Constit. of leaves of *Aloe vera*. Amorph. yellowish solid. $[\alpha]_D^{25}$ -0.7 (c, 0.1 in MeOH). λ_{max} 204 (log ε 4.4); 221 (log ε 4.35); 294 (log ε 4.09); 345 (log ε 3.82) (MeOH).

*1″-Deoxy, 8-*O*-β-D-glucopyranoside:* [53861-35-1] ***Cascaroside D***
$C_{27}H_{32}O_{13}$ 564.542
From cascara sagrada (*Rhamnus purshiana*) bark.

*1″-Deoxy, 6-hydroxy, 8-*O*-β-D-glucopyranoside:* [164322-83-2] ***Cascaroside F***
$C_{27}H_{32}O_{14}$ 580.541
Constit. of cascara sagrada *Rhamnus purshiana* bark. Mp 176-178°. $[\alpha]_D^{25}$ -69.5 (c, 0.1 in MeOH).

(10*S*)-*form* [1415-73-2]
Aloin A
Yellow needles (EtOH). Sol. H_2O. Mp 148° (block). $[\alpha]_D^{30}$ +10.2 (c, 0.5 in MeOH). Positive CD at 295 nm. Pmr δ 5.13 (C-1′).

▶ LD_{50} (mus, ivn) 200 mg/kg. LZ6520000

*1″-*O*-α-L-Rhamnopyranoside:* [56645-88-6] ***Aloinoside A***
$C_{27}H_{32}O_{13}$ 564.542
Constit. of *Aloe ferox* and other *Aloe* spp.. λ_{max} 236 (ε 22400) (MeOH) (Derep).

*8-*O*-β-D-Glucopyranoside:* [53823-08-8] ***Cascaroside A***
$C_{27}H_{32}O_{14}$ 580.541
Constit. of *Rhamnus purshiana* (Cascara sagrada) bark. Cryst. + $2H_2O$. Mp 184-187°. $[\alpha]_D^{30}$ +36.8 (MeOH).

*1″-Carboxylic acid, 8-*O*-β-D-glucopyranoside:* [111614-11-0] ***Rheinoside D***
$C_{27}H_{30}O_{15}$ 594.525
Constit. of rhubarb. Pale yellow powder + $2^1/_2H_2O$. $[\alpha]_D^{25}$ -56 (c, 0.5 in MeOH).

5-Hydroxy: [138373-23-6] ***5-Hydroxyaloin A***
$C_{21}H_{22}O_{10}$ 434.399
Constit. of *Aloe* spp. leaf. 10*R*-config. (C-10 config. changes with addn. of C-5 hydroxy group).

7-Hydroxy, 8-Me ether: ***7-Hydroxy-8-O-methylaloin A***
$C_{22}H_{24}O_{10}$ 448.426
Constit. of *Aloe vera* leaf. Yellowish needles (Me_2CO/C_6H_6). Mp 218-224°. $[\alpha]_D^{30}$ +27.2 (c, 0.25 in MeOH). λ_{max} 206 (log ε 4.48); 221 (log ε 4.45); 294 (log ε 4.2); 345 (log ε 3.93) (MeOH).

*1″-Deoxy, 8-*O*-β-D-glucopyranoside:* [53823-09-9] ***Cascaroside C***
$C_{27}H_{32}O_{13}$ 564.542
From cascara sagrada *Rhamnus purshiana* bark. Cascarosides C and D are a pair of epimers resembling Cascarosides A and B.

*1″-Deoxy, 6-hydroxy, 8-*O*-β-D-glucopyranoside:* [164178-32-9] ***Cascaroside E***
$C_{27}H_{32}O_{14}$ 580.541
Constit. of cascara sagrada *Rhamnus purshiana* bark. Mp 197-199°. $[\alpha]_D^{25}$ -95.4 (c, 0.1 in MeOH).

(10ξ)-*form*

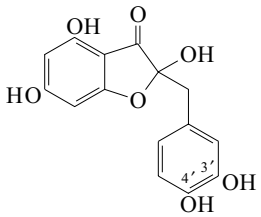
1′-Deoxy: [18262-45-8] ***Chrysaloin***. *11-Deoxyaloin*
$C_{21}H_{22}O_8$ 402.4
Isol. from *Rumex vesicarius* (bladder dock). Yellow powder (EtOAc). Mp 224-225° dec. $[\alpha]_D^{27}$ -9 (c, 1 in EtOH).

[5133-19-7, 73889-54-0, 138373-24-7]

Hay, J.E. *et al., J.C.S.*, 1956, 3141 (*struct, bibl*)
Hörhammer, L. *et al., Z. Naturforsch., B*, 1964, **19**, 222 (*Aloinoside B*)
Piox, A. *et al., Tetrahedron*, 1968, **24**, 3697 (*ms*)
Wagner, H. *et al., Z. Naturforsch., B*, 1976, **31**, 267 (*Cascarosides*)
Hata, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3792 (*Chrysaloin*)
Evans, F.J. *et al., Biomed. Mass Spectrom.*, 1979, **6**, 374 (*ms*)
Auterhoff, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1980, **313**, 113 (*resoln*)
Gruen, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1982, **315**, 231 (*biosynth*)
Minocha, P.K. *et al., Proc. Natl. Acad. Sci., India, Sect. A*, 1982, **52**, 123 (*Deoxyaloin*)
Rauwald, H.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1984, **317**, 362 (*pmr*)
Rauwald, H.W. *et al., Angew. Chem., Int. Ed.*, 1989, **28**, 1528 (*cryst struct, bibl*)
Manitto, P. *et al., J.C.S. Perkin 1*, 1990, 1297; 1993, 1577 (*abs config, pmr, cmr, conformn, Rheinosides, Cascarosides*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 869
Rauwald, H.W. *et al., Z. Naturforsch., C*, 1993, **48**, 1 (*5-Hydroxyaloin A*)
Sigler, A. *et al., Z. Naturforsch., C*, 1994, **49**, 286 (*7-Hydroxyaloin*)
Manitto, P. *et al., J. Nat. Prod.*, 1995, **58**, 419 (*Cascarosides*)
Van Wyk, B.-E. *et al., Planta Med.*, 1995, **61**, 250 (*occur*)
Dagne, E. *et al., Phytochemistry*, 1997, **44**, 1271 (*Microstigmin A, 5-Hydroxyaloin A*)
Holzapfel, C.W. *et al., Phytochemistry*, 1997, **45**, 97 (*isol, derivs*)
Okamura, N. *et al., Phytochemistry*, 1997, **45**, 1519 (*7-Hydroxy-8-methylaloin, 10-Hydroxyaloin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAF825

Alphitonin A-191

[493-36-7]
*2-[(3,4-Dihydroxyphenyl)methyl]-2,4,6-trihydroxy-3(2*H*)-benzofuranone, 9CI. 2,3′,4,4′,6-Pentahydroxybenzylcoumaranone*



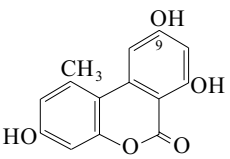
$C_{15}H_{12}O_7$ 304.256
Cryst. (H_2O). Mp 222-223°.

*3′-Deoxy, 6-*O*-β-D-glucopyranoside:* ***Maesopsin 6-glucoside***
$C_{21}H_{22}O_{11}$ 450.398
Constit. of *Ceanothus americanus* (New Jersey tea). Powder (MeOH). $[\alpha]_D^{25}$ -43 (c, 0.9 in MeOH).

Li, X.-C. *et al., Phytochemistry*, 1997, **46**, 97 (*Maesopsin 6-glucoside*)

Alternariol A-192

[641-38-3]
*3,7,9-Trihydroxy-1-methyl-6*H*-dibenzo[b,d]pyran-6-one, 9CI. 3,4′,5-Trihydroxy-6′-methyldibenzo-α-pyrone*



$C_{14}H_{10}O_5$ 258.23
Occurs in mycelium of *Alternaria tenuis* responsible for alternaria cone disorder in hops and fruit spot on papaya (*Carica papaya*) and *Passiflora* spp.. Needles (EtOH aq.). Sol. MeOH, bases, Et_2O; poorly sol. C_6H_6, hexane, H_2O. Mp 350° dec. Subl. 250 *in vacuo*. λ_{max} 213 (ε 21900); 258 (ε 41700); 290 (ε 10500); 303 (ε 11200); 336 (ε 11500) (MeOH) (Derep). λ_{max} 255 ; 288 ; 298 ; 337 (MeOH) (Berdy).

▶ Exp. reprod. and teratogenic effects. HP8757000

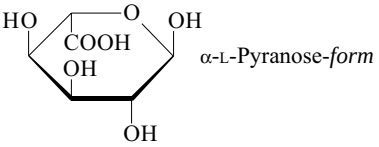
Tri-Ac:
Cryst. (EtOH). Mp 167-169°.

9-Me ether: [26894-49-5] *3,7-Dihydroxy-9-methoxy-1-methyl-6*H*-dibenzo[b,d]pyran-6-one.* ***Djalonensone***
$C_{15}H_{12}O_5$ 272.257
Needles (EtOH or dioxan). Mp 266-268° dec.

Raistrick, H. *et al., Biochem. J.*, 1953, **55**, 421 (*isol*)
Thomas, R. *et al., Proc. Chem. Soc., London*, 1959, 88 (*biosynth*)
Gatenbeck, S. *et al., Acta Chem. Scand.*, 1965, **19**, 65 (*synth*)
Sóti, F. *et al., Chem. Ber.*, 1977, **110**, 979 (*synth*)
Harris, T.M. *et al., J.A.C.S.*, 1977, **99**, 1631 (*synth*)
Abell, C. *et al., Chem. Comm.*, 1982, 1011 (*biosynth*)
Leeper, F.J. *et al., J.C.S. Perkin 1*, 1984, 1053 (*synth*)
DiCosimo, F. *et al., Experientia*, 1985, **41**, 1188
Stinson, E.E. *et al., Can. J. Chem.*, 1986, **64**, 1590 (*biosynth*)
Abell, C. *et al., Chem. Comm.*, 1986, 15 (*synth*)
Dasenbrock, J. *et al., Chem. Comm.*, 1987, 1235 (*biosynth*)

Kanakam, C.C. *et al., J.C.S. Perkin 1*, 1990, 2233 (*synth*)
Onocha, P.A. *et al., Phytochemistry*, 1995, **40**, 1183 (*Djalonensone*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 615; 623
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGW476

Altruronic acid, 9CI A-193



α-L-Pyranose-*form*

$C_6H_{10}O_7$ 194.141

L-*form* [39737-41-2]
Prod. during pectin saponification, by epimerisation of Galacturonic acid. Mp 124-127°. $[\alpha]_D^{18}$ +5.3 (c, 0.568 in H_2O).

[21675-51-4]

Fisher, F.G. *et al., Chem. Ber.*, 1959, **92**, 2184 (*synth*)
Carlsson, B. *et al., Acta Chem. Scand.*, 1969, **23**, 261 (*synth*)
Kjolberg, O. *et al., Acta Chem. Scand.*, 1972, **26**, 3245 (*synth*)
Bilik, V. *et al., Chem. Zvesti*, 1982, **36**, 831 (*synth*)
Zhan, D. *et al., Carbohydr. Res.*, 2001, **330**, 357-363 (*occur*)

Aluminium ammonium sulfate (1:1:2) A-194

[7784-25-0]
Aluminium ammonium bis(sulfate). Burnt ammonium alum. Exsiccated ammonium alum. E523

$NH_4Al(SO_4)_2$

$AlH_4NO_8S_2$ 237.147
Cryst. Dec. at 280°.

Dodecahydrate: [7784-26-1]

[15614-99-0] *Ammonium alum*
$AlH_{28}NO_{20}S_2$ 453.329
Used in foods as a buffer and neutralizing agent. Cryst. (H_2O). Becomes anhyd. at *ca*. 250°.

[15710-63-1]

Franke, W. *et al., Acta Cryst.*, 1965, **19**, 870-871 (*synth, cryst struct*)
Larson, A.C. *et al., Acta Cryst.*, 1967, **22**, 793-800 (*dodecahydrate, cryst struct*)
Venkatesh, G.M. *et al., Indian J. Pure Appl. Phys.*, 1971, **9**, 39-43 (*dodecahydrate, ir*)
Bailey, W.C. *et al., J. Chem. Phys.*, 1974, **60**, 1952-1953 (*dodecahydrate, N-14 nmr*)
Abdeen, A.M. *et al., Z. Kristallogr.*, 1981, **157**, 147-166 (*dodecahydrate, cryst struct*)
Eckert, H. *et al., J.A.C.S.*, 1986, **108**, 2140-2146 (*dodecahydrate, S-33 nmr*)
Bradley, S.M. *et al., Magn. Reson. Chem.*, 1993, **31**, 883-886 (*dodecahydrate, Al-27 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 108

Aluminium calcium silicate A-195

[12251-31-9]
Calcium aluminosilicate. E554

$CaAl_2(SiO_3)_4$

$Al_2CaO_{12}Si_4$ 398.376
Anticaking agent.

Mineral-*form* [1318-80-5]

[11126-82-2, 12026-15-2, 12251-34-2, 12330-25-5, 138329-32-5]
Laumontite

Zeolite-group mineral corresp. to $Al_2Ca(SiO_3)_4.4H_2O$ or $Al_2CaH_8(SiO_4)_4$.A partially dehydrated variety leonhardite also occurs naturally.

Mineral-*form* [12042-71-6]

[82828-52-2]
Wairakite

Zeolite-group mineral corresp. to $Al_2Ca(SiO_3)_4.2H_2O$; Ca analogue of Analcime.

Bartl, H. *et al., Neues Jahrb. Mineral., Monatsh.*, 1967, 33-42; 1970, 298-310 (*cryst struct, laumontite*)
Takeuchi, Y. *et al., Am. Mineral.*, 1979, **64**, 993-1001 (*cryst struct, wairakite*)
Armbruster, J. *et al., Neues Jahrb. Mineral., Monatsh.*, 1992, 385-397 (*cryst struct, leonhardite*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 108-109

Aluminium hydroxide, JAN, USAN A-196

[21645-51-2]

[12252-70-9]

$Al(OH)_3$

AlH_3O_3 78.003
Used in foods as a buffer, neutralising agent or firming agent. White solid (H_2O). Prac. insol. H_2O; sol. conc. aq. acids and alkalis. Forms gel on prolonged contact with H_2O.

► Gastrointestinal disturbances by ingestion.
BD0940000

Gel-*form* [1330-44-5]
Algeldrate. Aluminium hydroxide hydrate. W 4600

Mineral-*form* [14762-49-3]
Gibbsite. Hydragillite
Double layer of close packed OH of held by H bonds with Al in ⅔ octahedral holes.Colourless hexagonal platelets.

Mineral-*form* [20257-20-9]
Bayerite
Layer struct. with O approx. hcp and Al octahedrally coord..White powder, colourless monoclinic cryst.

Mineral-*form* [13840-05-6]
Nordstrandite
Double layers of AlO_6 octahedra with shared edges and corners linked by H bonds.Colourless, beige, pink and pale green cryst.

Mineral-*form*
Doyleite
Creamy or bluish white triclinic cryst.

[37317-08-1]

Thibon, H. *et al., Bull. Soc. Chim. Fr.*, 1951, 384 (*props*)
Calvet, E. *et al., Bull. Soc. Chim. Fr.*, 1953, 99 (*props*)
Brown, J.F. *et al., J.C.S.*, 1953, 84 (*gibbsite, thermal dec*)
van Nordstrand, R.A. *et al., Nature (London)*, 1956, **177**, 713 (*nordstrandite*)
Papeé, D. *et al., Bull. Soc. Chim. Fr.*, 1958, 1301 (*props*)
Kroon, D.J. *et al., Nature (London)*, 1959, **183**, 944 (*gibbsite, bayerite, pmr*)
Wall, J.R.D. *et al., Nature (London)*, 1962, **196**, 264 (*nordstrandite*)
Hathaway, J.C. *et al., Nature (London)*, 1962, **196**, 265 (*nordstrandite*)
Hauschild, U. *et al., Z. Anorg. Allg. Chem.*, 1963, **324**, 15 (*synth, ir, powder struct, props*)
Lippens, C. *et al., Acta Cryst.*, 1964, **17**, 1312 (*phase trans*)
Beretka, J. *et al., J.C.S.(A)*, 1967, 2106 (*bayerite, gibbsite, synth, props*)
Rothbauer, R. *et al., Z. Kristallogr.*, 1967, **125**, 317 (*bayerite, cryst struct, nd*)
Bosmans, H.J. *et al., Acta Cryst. B*, 1970, **26**, 649 (*nordstrandite, cryst struct*)
Sato, T. *et al., Z. Anorg. Allg. Chem.*, 1972, **391**, 69 (*synth*)
Singh, S.S. *et al., Soil Sci. Soc. Am. Proc.*, 1974, **38**, 415 (*soly, gibbsite*)
Saalfield, H.L. *et al., Z. Kristallogr.*, 1974, **139**, 129 (*gibbsite, cryst struct*)
Smyshiyaev, S.I. *et al., Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 528 (*thermodyn data*)
Chang, B.-T. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 1960 (*gibbsite, thermodyn data*)
Aluminium Chems. Sci. and Tech. Handbook, (Hart, D.Le.R., Ed.), Amer. Ceram. Soc., 1990,
Washington, N. *et al., Antacids and Anti-Reflux Agents*, CRC Press, 1991, 8 (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 869
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 110-111
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHC000

Aluminium potassium silicate A-197

[12003-49-5]
Silicic acid (H_4SiO_4) aluminium potassium salt (1:1:1), 10CI. Potassium aluminosilicate ($KAlSiO_4$), 9CI. E555

$AlK(SiO_4)$

$AlKO_4Si$ 158.163
Polymorphic; the 3 common polymorphs are kalsilite, metastable kaliophilite and a high-temp. rhombic phase. All are based on a tridymite framework. Anticaking agent.

Schairer, J.F. *et al., Am. J. Sci.*, 1955, **253**, 681-746 (*synth*)
Deer, W.A. *et al., Rock Forming Minerals*, Longman, 1963, **4**, 231-270 (*mineral*)
Perotta, A.J. *et al., Mineral. Mag.*, 1965, **35**, 588-595 (*kalsilite, cryst struct*)
Abbott, R.N. *et al., Am. Mineral.*, 1984, **69**, 449-457 (*polymorphism*)

Aluminium potassium sulfate ($AlK(SO_4)_2$) A-198

[10043-67-1]

[15007-61-1]
Sulfuric acid, aluminium potassium salt (2:1:1), 8CI. Aluminium potassium sulfate. Anhydrous alum. E522

$KAl(SO_4)_2$

$AlKO_8S_2$ 258.207

Struct. comprises alternate layers of six coordinate $Al^{3\oplus}$ and $K^{\oplus}$ with $SO_4^{2\ominus}$ between.Colourless hexagonal plates (H_2SO_4). Sol. H_2O (7.74 g per 100 cm^3 at 30°); insol. EtOH. Corresp. $NH_4^{\oplus}$, $Rb^{\oplus}$, $Cs^{\oplus}$ salts also descr. ΔH_f° -2470 kJ mol^{-1}; ΔG_f° -2240 kJ mol^{-1}; S° 205 J K^{-1} mol^{-1}.

▶ WS5650000

Dodecahydrate: [7784-24-9] *Potassium alum.* ***Kalinite.*** *Hexaaquaaluminium(3+) hexaaquapotassium(1+) bis(sulfate). α-Alum*

$AlH_{24}KO_{20}S_2$ 474.389

Used as an additive in the bleaching of milk and flour by benzoyl peroxide. Colourless cryst. (H_2O). Sol. H_2O (11 g per 100 cm^3 at 20°); insol. EtOH, Me_2CO. Mp 105°. Dec. on heating (-$9H_2O$ at 64.5°, -$12H_2O$ at 200°).

▶ WS5690000

[14635-80-4]

Lipson, H. *et al., Proc. R. Soc. London, A*, 1935, **148**, 664; **151**, 347 (*cryst struct, dodecahydrate*)
Klug, H.P. *et al., J.A.C.S.*, 1940, **62**, 1492 (*dodecahydrate, cryst struct*)
Young, F.E. *et al., J.A.C.S.*, 1945, **67**, 257 (*synth, thermodyn props*)
Palmer, W.G. *et al., Experimental Inorganic Chemistry*, CUP, 1959, 216 (*synth, dodecahydrate*)
Burns, G. *et al., Phys. Rev.*, 1961, **123**, 64 (*dodecahydrate, pmr*)
Tret'yakov, Yu.D. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1961, 859 (*phase diagram*)
Haussühl, S. *et al., Z. Kristallogr.*, 1961, **116**, 371 (*props*)
Franke, W. *et al., Acta Cryst. B*, 1965, **19**, 870 (*anhydrous, cryst struct*)
Cromer, D.T. *et al., Acta Cryst.*, 1967, **22**, 800 (*nd, dodecahydrate*)
Vandorpe, B. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1968, **266**, 379 (*related compds*)
Manoli, J.-M. *et al., Bull. Soc. Chim. Fr.*, 1970, 98 (*synth, cryst struct*)
Rems, P. *et al., Inorg. Chim. Acta*, 1971, **5**, 33 (*ir*)
Gal, S. *et al., Therm. Anal., Proc. Int. Conf., 3rd, 1971 (1972)*, 1971, **2**, 559; *CA*, 1973, **78**, 131564 (*dodecahydrate, thermal anal*)
Pannetier, G. *et al., Bull. Soc. Chim. Fr.*, 1972, 485 (*analogues*)
Strupler, N. *et al., Bull. Soc. Chim. Fr.*, 1974, 1830 (*dodecahydrate, ir*)
Eysel, H.H. *et al., Z. Anorg. Allg. Chem.*, 1976, **424**, 68 (*Raman*)
Hurlburt, H.Z. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, ; *CA*, 1978, **88**, 193727 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 250
Couchot, P. *et al., Rev. Chim. Miner.*, 1978, **15**, 373 (*anhydrous, ir, Raman*)
Bhat, S.V. *et al., Curr. Sci.*, 1984, **53**, 27 (*Al-27 nmr, anhydrous*)
Eckert, H. *et al., J.A.C.S.*, 1986, **108**, 2140 (*dodecahydrate, S-33 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 115-118
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHF100; AHF200

Aluminium sodium oxide ($AlNaO_2$) A-199

[1302-42-7]

Aluminium sodium oxide†. Sodium aluminium oxide (NaAlO₂). Sodium aluminate (NaAlO₂)

$NaAlO_2$

$AlNaO_2$ 81.97

$NaFeO_2$ type struct.. Food contaminant arising from its use as a boiler water additive in the prepn. of steam for food processing. White cryst. or powder. Mp 1700°. Various hydrated forms known. cf. also Aluminium sodium oxide (Al_5NaO_8). For species in soln. see Aluminate ($Al(OH_4)^{\ominus}$). ΔH_{f298}° -1133.2 kJ mol^{-1}; S° 70.4 J K^{-1} mol^{-1}.

Théry, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1962, **254**, 2782 (*related compds*)
Reid, A.F. *et al., Inorg. Chem.*, 1968, **7**, 443 (*cryst struct*)
Peterson, G.E. *et al., J. Chem. Phys.*, 1969, **51**, 2610 (*Na-23 nqr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 312
Müller, D. *et al., Chem. Phys. Lett.*, 1981, **79**, 59 (*Al-27 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2522

Aluminium sodium silicate A-200

[1302-72-3]

[1344-00-9, 12003-51-9, 12251-27-3]

Sodium aluminium silicate. Sodium aluminosilicate. Nepheline. E554

$Na[AlSiO_4]$

$AlNaO_4Si$ 142.054

Stuffed tridymite struct.. Anticaking agent. White cryst. (aq. melt). Hydrothermal synth. from Na_2O, Al_2O_3, SiO_2 gels.

Barrer, R.M. *et al., J.C.S.*, 1952, 1561 (*synth*)
Hahn, T. *et al., Z. Kristallogr.*, 1955, **106**, 308 (*cryst struct*)
Brinkman, D. *et al., Z. Kristallogr.*, 1972, **135**, 208 (*Na-23, Al-27, Si-29 nmr*)
Klaska, R. *et al., Z. Kristallogr.*, 1975, **142**, 225 (*cryst struct*)
Lippmaa, E. *et al., J.A.C.S.*, 1980, **102**, 4889; 1986, **108**, 1730 (*Si-29, Al-27 nmr*)
Wirsching, U. *et al., Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Klinowski, J. *et al., J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2524-2525

Aluminium sodium sulfate ($AlNa(SO_4)_2$) A-201

[10102-71-3]

Sulfuric acid aluminium sodium salt (2:1:1), 8CI. Aluminium sodium sulfate. Sodium aluminium sulfate. E521

$NaAl(SO_4)_2$

$AlNaO_8S_2$ 242.098

Orthorhombic cryst. V. sol. H_2O (40.9 g per 100 cm^3 at 20°).

Dodecahydrate: [7784-28-3] *Sodium alum. γ-Alum. Hexaaquaaluminium hexaaquasodium sulfate (1:1:2)*

$AlH_{24}NaO_{20}S_2$ 458.281

Food additive in baking powder, firming agent, buffer. May migrate to food from paper/board packaging. Cubic white cryst. Mp 61°. ΔH_f -2353 kJ mol^{-1}. Formulated as $[Na(OH_2)_6][Al(OH_2)_6](SO_4)_2$.

Steele, F.A. *et al., Science (Washington, D.C.)*, 1928, **68**, 156 (*dodecahydrate, synth*)
Lipson, H. *et al., Proc. R. Soc. London, A*, 1935, **151**, 347 (*dodecahydrate, cryst struct*)
Cola, M. *et al., Gazz. Chim. Ital.*, 1960, **90**, 220 (*cryst struct, synth*)
Cromer, D.T. *et al., Acta Cryst.*, 1967, **22**, 182 (*dodecahydrate, cryst struct, nd*)
Petrov, K.I. *et al., Zh. Neorg. Khim.*, 1970, **15**, 2938 (*dodecahydrate, ir*)
Perret, R. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1972, **274**, 366 (*synth*)
Weiden, N. *et al., J. Magn. Reson.*, 1975, **20**, 279 (*dodecahydrate, Na-23, Al-27 nmr*)
Hurlburt, H.Z. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 120; *CA*, 1978, **88**, 193727 (*rev, synth*)
W.H.O. Tech. Rep. Ser., 1978, **631**, 7; *CA*, 1979, **90**, 136443 (*uses*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 244 (*dodecahydrate, rev*)

Aluminium sulfate, USAN A-202

[10043-01-3]

[10124-29-5, 10199-21-0, 16828-11-8, 17927-65-0]

Alunogenite. E520

$Al_2(SO_4)_3$

$Al_2O_{12}S_3$ 342.154

Used in foods as a firming agent. White solid. Forms complex series of hydrates. Dec. at 450° to amorphous Al_2O_3 with high surface area. ΔH_{f298}° -3435 kJ mol^{-1}. $Al(HSO_4)_3$ also known.

▶ BD1700000

Heptadecahydrate: ***Alunogen***
Colourless cryst.

Octadecahydrate: [7784-31-8]
Colourless hygroscopic cryst. (H_2O). Exact amount of H_2O uncertain. Gives anhydrous salt during 24h at 380°.

▶ WS5697000

Sodium alum: Aluminium sodium sulfate ($AlNa(SO_4)_2$), A-201

Potassium alum: Aluminium potassium sulfate ($AlK(SO_4)_2$), A-198

Caesium alum: See Aluminium caesium sulfate dodecahydrate in *The Combined Chemical Dictionary.*

Young, F.E. *et al., J.A.C.S.*, 1945, **67**, 257 (*synth, thermodyn data*)
Bassett, H. *et al., J.C.S.*, 1949, 2239 (*synth, phase diagram, powder struct, hydrates, props*)
Kellogg, H.H. *et al., Trans. Metall. Soc. AIME*, 1964, **230**, 1622 (*thermodyn data*)
Vandorpe, B. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1973, **277**, 1121 (*related compd*)
Akitt, J.W. *et al., J.C.S. Dalton*, 1973, 1226 (*Al-27 nmr*)
Knutsen, G.F. *et al., J. Electrochem. Soc.*, 1978, **125**, 327 (*dec*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 120-122
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHG750

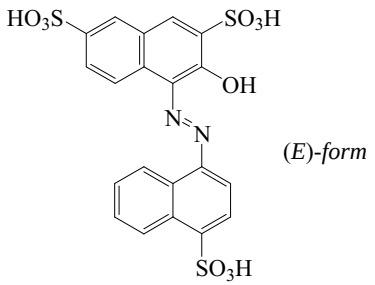
Amaranth A-203

[642-59-1]

[915-67-3]

3-Hydroxy-4-[(4-sulfo-1-naphthalenyl)azo]-2,7-naphthalenedisulfonic acid, 9CI. C.I. Acid red 27, 8CI. Amaranth R.

Amaranth S. Azorubine S. Bordeaux S. C.I. 16185. C.I. Food Red 9. FD and C Red No. 2. E123



(*E*)-form

$C_{20}H_{14}N_2O_{10}S_3$ 538.536

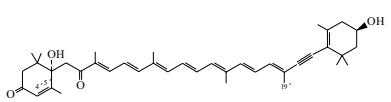
Usually obt. as tri-Na salt, to which most synonyms refer. Used in food colouring. Dark red-brown powder (as tri-Na salt). Sol. H_2O, EtOH, 2-ethoxyethanol. Banned by FDA for use in food, drugs and cosmetics. Permitted in the UK and some other countries.

▶ Exp. weak reprod. and teratogenic effects (conflicting data).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 988B (*ir*)
Knecht, O. *et al., J. Soc. Dyers Colour.*, 1886, **2**, 24 (*synth*)
Lambert, J.L. *et al., Anal. Chem.*, 1954, **26**, 558-560; 1955, **27**, 800-801 (*detn, F,S*)
Nursten, H.E. *et al., J. Soc. Dyers Colour.*, 1973, **89**, 49-53 (*synth*)
Marmion, D.M. *et al., J. Assoc. Off. Anal. Chem.*, 1974, **57**, 495-507 (*synth*)
IARC Monog., 1975, **8**, 41; *Suppl.* 7, 56 (*rev, tox*)
Fogg, A.G. *et al., Analyst (London)*, 1979, **104**, 723-729 (*anal*)
Clode, S.A. *et al., Food Chem. Toxicol.*, 1987, **25**, 937-946 (*tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 698
Merck Index, 12th edn., 1996, No. 391
Yamada, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 494-499 (*hplc, pmr, cmr*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 92
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG020

Amarouciaxanthin B A-204

[92121-55-6]
7,8-Didehydro-7′,8′-dihydro-3,6′-dihydroxy-β,ε-carotene-3′,8′-dione. Sidnyaxanthin



$C_{40}H_{52}O_4$ 596.848
Dark reddish cryst. (Et_2O); reddish needles (petrol/Et_2O). Sol. MeOH, hexane; poorly sol. H_2O. Mp 88-89° Mp 154°. $[\alpha]_D$ +1.6 (c, 0.9 in $CHCl_3$). λ_{max} 230 ; 281 ; 463 (Et_2O) (Berdy).

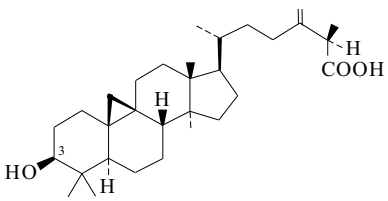
4,5β-Dihydro: [50906-60-0] *7,8-Didehydro-5′,6′,7′,8′-tetrahydro-3,6′-dihydroxy-β,β-carotene-3,8-dione.* ***Isomytiloxanthin***
$C_{40}H_{54}O_4$ 598.864
Isol. from the edible mussel (*Mytilus edulis*). Red gum. Tentative abs. config. λ_{max} 451 (no solvent reported).

19′-Hexanoyloxy, 4,5β-dihydro: ***19′-Hexanoyloxymytiloxanthin***
$C_{46}H_{64}O_6$ 713.008
Isol. from the edible mussel (*Mytilus edulis*).

Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Belaud, C. *et al., Tet. Lett.*, 1984, **25**, 3087 (*isol, struct*)
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606 (*isol, struct*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*19′-Hexanoyloxymytiloxanthin*)
Khare, A. *et al., J.C.S. Perkin 1*, 1988, 1389 (*isol, struct*)

Ambolic acid A-205

[13878-93-8]
*3β-Hydroxy-24-methylene-25*R*-cycloartan-26-oic acid*



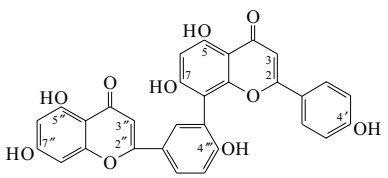
$C_{31}H_{50}O_3$ 470.734
Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$). Mp 168-170°. $[\alpha]_D$ +32.6 (c, 0.5 in $CHCl_3$).

3-Ketone: [17984-17-7] ***Ambonic acid***
$C_{31}H_{48}O_3$ 468.718
Constit. of *Mangifera indica* (mango). Cryst. (Et_2O/hexane). Mp 149-150°. $[\alpha]_D$ +9.4 (c, 0.7 in $CHCl_3$).

Corsano, S. *et al., Chem. Comm.*, 1968, 738 (*isol*)
Singh, C. *et al., Tetrahedron*, 1977, **33**, 817 (*synth*)

Amentoflavone A-206

[1617-53-4]
4′,4‴,5,5″,7,7″-Hexahydroxy-3‴,8-biflavone, 8CI. 4′,5,7-Trihydroxyflavone(3′→8)-4′,5,7-trihydroxyflavone. 3′,8-Bi[4′,5,7-trihydroxyflavone]



$C_{30}H_{18}O_{10}$ 538.466
Numbering of the rings in the names of derivs. does not always follow the scheme shown here. Obt. from *Viburnum prunifolium* (black haw). Yellow cryst. (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 300°. $[\alpha]_D^{40}$ +9. Log P 1.7 (calc). Opt. rotn. of derivs. is variable owing to atropisomerism λ_{max} 270 (ε 41600); 338 (ε 38900) (EtOH) (Berdy).

4‴-Me ether: [521-32-4] ***Bilobetin***
$C_{31}H_{20}O_{10}$ 552.493
From *Ginkgo biloba* (ginkgo). Cryst. Mp 320° dec. Softens at 245-53°, resolidifies at 278°.

4‴,7″-Di-Me ether: [481-46-9] ***Ginkgetin***
$C_{32}H_{22}O_{10}$ 566.52
From *Ginkgo biloba* (ginkgo). Yellow plates (Me_2CO). Mp 336° Mp 350°.

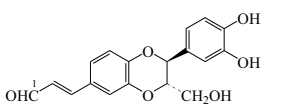
4′,4‴-Di-Me ether: [548-19-6] ***Isoginkgetin***
$C_{32}H_{22}O_{10}$ 566.52
From leaves of *Ginkgo biloba* (ginkgo). Yellow cryst. (Me_2CO). Mp 210°. Effervesces at 226°, resolidifies and remelts at 245-7° λ_{max} 213 (ε 90000); 271 (ε 42000); 330 (ε 36500) (EtOH) (Berdy). λ_{max} 280 (ε 53000); 376 (ε 24300) (EtOH/NaOH) (Berdy).

5‴-Methoxy, 4‴-Me ether: [77053-35-1] ***5′-Methoxybilobetin***
$C_{32}H_{22}O_{11}$ 582.519
Isol. from *Ginkgo biloba* (ginkgo). Yellow cryst. (EtOH aq.). Mp 251°.

Nakazawa, K. *et al., Chem. Pharm. Bull.*, 1962, **10**, 1032 (*synth, derivs*)
Baker, W. *et al., J.C.S.*, 1963, 1477 (*isol, struct, derivs*)
Batterham, R. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr, derivs*)
Beckmann, S. *et al., Phytochemistry*, 1971, **10**, 245 (*derivs*)
Ilyas, N. *et al., Phytochemistry*, 1978, **17**, 987 (*derivs*)
Joly, M. *et al., Phytochemistry*, 1980, **19**, 1999 (*5′-Methoxybilobetin*)
Ahmad, I. *et al., Phytochemistry*, 1981, **20**, 1169 (*deriv*)
Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 919 (*derivs*)
Kamil, M. *et al., Phytochemistry*, 1987, **26**, 1171 (*deriv*)
Konda, Y. *et al., J. Het. Chem.*, 1995, **32**, 1531 (*Ginkgetin, Sciadopitysin, cryst struct, pmr, cmr*)
Reddy, B.P. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 283 (*Ginkgetin, Sciadopitysin*)
Muranaka, T. *et al., CA*, 1999, **130**, 322915n

Americanin A A-207

[69506-79-2]
3-[2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3-hydroxymethyl-1,4-benzodioxin-6-yl]-2-propenal, 9CI



Absolute Configuration

$C_{18}H_{16}O_6$ 328.321
Constit. of *Phytolacca americana* (pokeberry). Yellow plates (MeOH). Mp 246-247°. $[\alpha]_D^{17}$ +23.7.

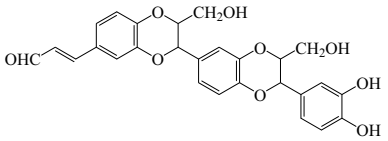
1-Alcohol: [133838-65-0] ***Americanol A***
$C_{18}H_{18}O_6$ 330.337
Isol. from seeds of *Phytolacca americana* (pokeberry). Prisms (Me_2CO/EtOAc). Mp 125-128°. Racemic.

Woo, W.S. *et al., Tet. Lett.*, 1978, 3239 (*isol*)
Antus, S. *et al., Annalen*, 1986, 647 (*struct*)
Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 252 (*Americanol A*)
She, X.G. *et al., J. Chem. Res., Synop.*, 1998, 436-437 (*synth*)

Takahashi, H. *et al., Heterocycles*, 2002, **56**, 245-256 (*Americanol A, synth*)
Waibel, R. *et al., Phytochemistry*, 2003, **62**, 805-811 (*isol, pmr, cmr, struct*)

Americanin B A-208

[77053-44-2]



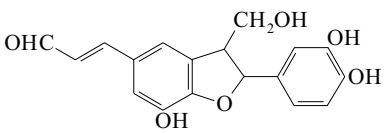
$C_{27}H_{24}O_9$ 492.481
Constit. of the seeds of *Phytolacca americana* (pokeberry). Mp 258-260°. $[\alpha]_D^{17}$ +1.7 (c, 0.3 in Py).

9-Alcohol: [362606-64-2] ***Artabotrycinol. Isoamericanol B***
$C_{27}H_{26}O_9$ 494.497
Cryst. (MeOH). Mp 194-196°. $[\alpha]_D^{20}$ -7 (c, 0.03 in MeOH). λ_{max} 236 (sh) ; 282 (MeOH).

Woo, W.S. *et al., Tet. Lett.*, 1980, **21**, 4255-4258
Yu, J.-G. *et al., Yaoxue Xuebao*, 2001, **36**, 281-286 (*isol, pmr, cmr, Artabotrycinol*)

Americanin D A-209

[77053-45-3]

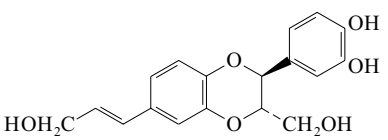


$C_{18}H_{16}O_6$ 328.321
Constit. of *Phytolacca americana* (pokeberry). Cryst. Mp 197-200°.

[106622-79-1]

Woo, W.S. *et al., Tet. Lett.*, 1980, **21**, 4255 (*isol, pmr, cmr*)

Americanol A-210

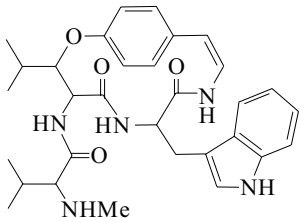


$C_{18}H_{18}O_6$ 330.337
Constit. of *Phytolacca americana* (pokeberry). Cryst. (EtOAc/Me_2CO). Mp 125-128°.

Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 252 (*isol, pmr, cmr*)

Americine A-211

[18867-84-0]
N-[7-(1H-Indol-3-ylmethyl)-3-(1-methylethyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-3-methyl-2-(methylamino)butanamide, 9CI



$C_{31}H_{39}N_5O_4$ 545.68
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Mp 135.5-137°. $[\alpha]_D^{20}$ -198 (c, 0.51 in MeOH).

N-*Me:* [70403-89-3] ***5-β-Indolylmethyl-8N-(N,N-dimethylvalyl)-9-isopropylphencyclopeptine***
$C_{32}H_{41}N_5O_4$ 559.707
Mp 233° (229°).

Klein, F.K. *et al., J.A.C.S.*, 1968, **90**, 2398 (*isol, uv, ir, pmr, ms, struct*)
Lagarias, J.C. *et al., J. Nat. Prod.*, 1979, **42**, 220; 663 (*deriv*)

Amino (methoxysulfinyl) pentasulfide, 9CI A-212

[198898-37-2]
Methyl 5-aminopentasulfide 1-sulfinate
$H_2N–S–S–S–S–S(O)–OMe$
$CH_5NO_2S_6$ 255.452
Constit. of *Moringa oleifera* (horseradish tree).

Faizi, S. *et al., J. Nat. Prod.*, 1997, **60**, 1317-1321 (*isol, ms*)

2′-Aminoacetophenone, 8CI A-213

[551-93-9]
1-(2-Aminophenyl)ethanone, 9CI. FEMA 3906



C_8H_9NO 135.165
Flavour compd. in stale dried milk. Responsible for the foxy odour of Concord grape (*Vitis lambrusca*). Flavour ingredient. Cryst. with grape-like odour. Mp 20°. Bp 250-252° slight dec. Bp_{12} 130°. Steam-volatile.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 47C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 868C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1262D (*ir*)
Simpson, J.C.E. *et al., J.C.S.*, 1945, 646 (*synth, bibl*)
Leonard, N.J. *et al., J.O.C.*, 1946, **11**, 405 (*synth*)
Parks, O.W. *et al., Nature (London)*, 1964, **202**, 185 (*isol*)
Kozlov, N.S. *et al., CA*, 1969, **71**, 12833 (*synth*)
Arnold, R.G. *et al., J. Dairy Sci.*, 1969, **52**, 1097 (*occur*)
East Ger. Pat., 1971, 82 135; *CA*, **76**, 99347 (*synth*)
Blum, M.S. *et al., Experientia*, 1981, **37**, 816 (*isol*)
Shure, K.B. *et al., J. Agric. Food Chem.*, 1994, **42**, 350-353 (*occur*)

2-Aminoacetophenone, 8CI A-214

[613-89-8]
2-Amino-1-phenylethanone, 9CI. Phenacylamine. Phenomydrol. Benzoylmethylamine
$PhCOCH_2NH_2$
C_8H_9NO 135.165
Component of tortilla aroma and of other corn flour products. Aroma threshold 0.2 ppb in H_2O.

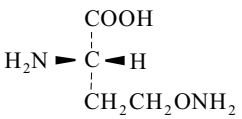
▶ Exp. reprod. effects. AM5775000

[25384-14-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 46D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 867A (*nmr*)
Tiffeneau, M. *et al., Bull. Soc. Chim. Fr.*, 1931, **49**, 1761 (*rev*)
Stalham, F.S. *et al., J.C.S.*, 1951, 213 (*synth*)
Bellamy, L.J. *et al., Spectrochim. Acta A*, 1972, **28**, 1869 (*ir*)
Yamaguchi, K. *et al., J. Agric. Food Chem.*, 1979, **27**, 847 (*isol*)
Abdalla, G.M. *et al., J. Het. Chem.*, 1987, **24**, 297 (*synth, ir, pmr*)
Yamagama, C. *et al., Aust. J. Chem.*, 1989, **42**, 463 (*N-15 nmr*)
Baumstark, A.L. *et al., Chem. Comm.*, 1989, 767 (*O-17 nmr*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1994, **42**, 1-2 (*occur, anal*)
Shure, K.B. *et al., J. Agric. Food Chem.*, 1994, **42**, 350 (*isol*)

2-Amino-4-(aminooxy)butanoic acid, 8CI A-215

O-*Aminohomoserine, 9CI.* ***Canaline***



(*S*)-*form*

$C_4H_{10}N_2O_3$ 134.135

(S)-form [496-93-5]
L-form
Present in *Canavalia ensiformis* (Jackbean). Needles (EtOH). Mp 214° dec. $[\alpha]_D^{21}$ -8.31.

Hydrochloride (1:2):
Cryst. (EtOH). Mp 166° dec.

Picrate:
Mp 192-193° dec.

Dibenzoyl:
Mp 99° dec.

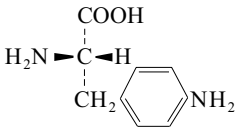
(±)-form [15985-61-2]
Cryst. (Me_2CO/EtOH/H_2O). Mp 195° dec. pK_{a3} 9.2 (25°).

Me ester:
$C_5H_{12}N_2O_3$ 148.161
Mp 165° dec. (as hydrochloride).

Gilon, C. *et al., Tetrahedron*, 1967, **23**, 4441 (*synth*)
Rahiala, E.-L. *et al., Acta Chem. Scand.*, 1973, **27**, 3861 (*synth*)
Williamson, J.D. *et al., Life Sci.*, 1974, **14**, 2481 (*isol*)
Rosenthal, G.A. *et al., Life Sci.*, 1978, **23**, 93 (*rev*)
Ozinskas, A.J. *et al., J.O.C.*, 1986, **51**, 5047 (*synth*)
Barlos, K. *et al., Annalen*, 1986, 287

2-Amino-3-(4-aminophenyl)-propanoic acid A-216

α,4-Diaminobenzenepropanoic acid. 4-Aminophenylalanine, 9CI



(*S*)-form

$C_9H_{12}N_2O_2$ 180.206

(*R*)-form [102281-45-8]
D-form
Mp 245-248° Mp 268-270°. $[\alpha]_D^{20}$ +37 (c, 2 in H_2O).

Me ester:
$C_{10}H_{14}N_2O_2$ 194.233
$[\alpha]_D$ -5.9 (c, 2.02 in H_2O). Hygroscopic.

$N^2,N^{4'}$-*Di-Ac, Me ester:*
$C_{14}H_{18}N_2O_4$ 278.307
Yellow powder. $[\alpha]_D$ -40.1 (c, 0.85 in MeOH).

(*S*)-form [943-80-6] *L-form*
Constit. of the famine food *Vigna vexillata*. Needles (H_2O). Mp 260-264° dec. $[\alpha]_D^{23}$ +1 (c, 0.3 in H_2O). $[\alpha]_{580}^{23}$ +28 (c, 0.3 in 1*N* HCl).

$N^2,N^{4'},N^{4'}$-*Tri-Me:3-(4-Dimethylamino-phenyl)-2-methylaminopropanoic acid.* p-*Dimethylamino*-N-*methylphenylalanine*
$C_{12}H_{18}N_2O_2$ 222.286
Needles + $^1/_2H_2O$ (EtOH aq.). Mp 208°. $[\alpha]_D^{20}$ +22.6 (c, 0.5 in 1*M* HCl). $[\alpha]_D$ -3.2 (c, 1.076 in H_2O).

(±)-form [2922-41-0]
Cryst. (EtOH aq.). Mp 248°.

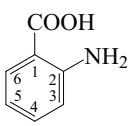
$N^2,N^{4'},N^{4'}$-*Tri-Me:*
Needles. Mp 214°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 257D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1192A (*nmr*)
Pedrazzali, A. *et al., Helv. Chim. Acta*, 1957, **40**, 80 (*synth, resoln*)
Eastwood, F.W. *et al., J.C.S.*, 1960, 2286
Georges, J. *et al., Bull. Soc. Chim. Fr.*, 1965, 2252
Dardenne, G.A. *et al., Phytochemistry*, 1972, **11**, 2567
Patel, V.F. *et al., J. Med. Chem.*, 1999, **42**, 2588-2603 (*R-form, Me ester, di-Ac, Me ester di-Ac, synth, pmr, ir, cmr*)

2-Aminobenzoic acid, 9CI A-217

[118-92-3]

[1321-11-5]
Anthranilic acid, 8CI. Vitamin L_1



$C_7H_7NO_2$ 137.138
Leaflets. Sol. hot H_2O, EtOH, Et_2O. Mp 144-148°. pK_{a1} 1.97; pK_{a2} 4.79 (25°). pK_{a1} 2.17; pK_{a2} 4.85 (25°, 0.1*M* KCl). Sublimes, triboluminescent λ_{max} 218 (ε 20200); 248 (ε 7000); 335 (ε 4700) (MeOH) (Berdy).

▶ LD_{50} (mus, orl) 1400 mg/kg. Exp. reprod. effects. CB2450000

β-D-Glucopyranosyl ester:β-D-Glucopyranosyl anthranilate
$C_{13}H_{17}NO_7$ 299.28
Constit. of the fruit of piñuela *Bromelia plumieri*.

Me ester: [134-20-3] *Methyl 2-aminobenzoate. FEMA 2682*
$C_8H_9NO_2$ 151.165
Found in essential oils, including bergamot, orange peel, lemon peel, jasmine, ylang-ylang and neroli. Also present in concord grape, strawberry, star fruit, wines, cocoa, black tea and rice bran. Flavouring agent. Cryst. Mp 24-25°. Bp_{15} 133.5°. pK_a 2.32 (25°, 1% EtOH aq.). Steam-volatile.

▶ Skin irritant. LD_{50} (rat, orl) 2910 mg/kg. Exp. reprod. effects. CB3325000

Et ester: [87-25-2] *Ethyl 2-aminobenzoate. FEMA 2421*
$C_9H_{11}NO_2$ 165.191
Flavouring ingredient. Present in orange juice, orange peel and concord grape. Liq. with faint orange-flower odour and flavour. d_4^{20} 1.12. Mp 13°. Bp 266-268° Bp_{15} 145-147°.

▶ DG2448000

2-Methylpropyl ester: [7779-77-3] *2-Methylpropyl 2-aminobenzoate. Isobutyl anthranilate. FEMA 2182*
$C_{11}H_{15}NO_2$ 193.245
Used in food flavouring. Liq. d 1.06. Bp 270° $Bp_{13.5}$ 169-170°.

2-Propenyl ester: [7493-63-2] *2-Propenyl 2-aminobenzoate. Allyl anthranilate. FEMA 2020*
$C_{10}H_{11}NO_2$ 177.202
Flavour ingredient. Bp_2 105°.

Butyl ester: [7756-96-9] *Butyl 2-aminobenzoate. FEMA 2181*
$C_{11}H_{15}NO_2$ 193.245
Used in fruit food flavouring. d 1.07. Bp 182°.

(Z)-3-Hexenyl ester: [65405-76-7] cis-*3-Hexenyl 2-aminobenzoate. FEMA 3925*
$C_{13}H_{17}NO_2$ 219.283
Flavouring ingredient for baked goods and candies. Bp_5 160°.

Cyclohexyl ester: [7779-16-0] *Cyclohexyl 2-aminobenzoate. Cyclohexyl anthranilate. FEMA 2350*
$C_{13}H_{17}NO_2$ 219.283
Flavouring ingredient. Liq. with a sweet, fruity taste. $d^{15.5}$ 1.02. Bp 318°.

2-Phenylethyl ester: [133-18-6] *2-Phenylethyl 2-aminobenzoate. Phenethyl anthranilate. FEMA 2859*
$C_{15}H_{15}NO_2$ 241.289
Flavouring ingredient. Cryst. Mp 42°. Bp 324°.

2-Naphthyl ester: [63449-68-3] *2-Naphthalenol 2-aminobenzoate. β-Naphthyl anthranilate. FEMA 2767*
$C_{17}H_{13}NO_2$ 263.295
Flavouring ingredient for beverages, baked goods and candies. Mp 118°. Bp 340°.

Amide: [88-68-6] *2-Aminobenzamide. Anthranilamide*
$C_7H_8N_2O$ 136.153
Acetaldehyde scavenger for polyethylene beverage bottles. Leaflets. Mp 109-111.5° dec.

▶ CU8993000

N-*(Carboxyacetyl):* [53947-84-5] *2-[(Carboxyacetyl)amino]benzoic acid, 9CI. 2-(Malonylamino)benzoic acid*
$C_{10}H_9NO_5$ 223.185
Isol. from the leaves of the peanut (*Arachis hypogaea*). Cryst. (Me_2CO/hexane). Mp 190-192°.

N-*Me, 2-methylpropyl ester:* [65505-24-0] *Isobutyl* N-*methylanthranilate*
$C_{12}H_{17}NO_2$ 207.272
Possible flavour ingredient; reported in food additive surveys.

N-*Et, Et ester:* [38446-21-8] *Ethyl* N-*ethylanthranilate*
$C_{11}H_{15}NO_2$ 193.245
Possibly used as a flavouring agent; listed in the FDA inventory of substances added to food.

[552-37-4, 99196-74-4, 99196-75-5, 99197-00-9, 117808-63-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 189A; 301D; 302A; 368D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1066B; 1262B; 1262C; 1390C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1371A; 1371B (*ir*)
Bredt, J. *et al., Ber.*, 1900, **33**, 29 (*2-methylpropyl ester*)
Smith, P.A.S. *et al., J.A.C.S.*, 1954, **76**, 431 (*synth*)
Adv. Chem. Ser., 1955, **15**, 513; 514 (*props, Me ester, Et ester*)
Forbes, W.F. *et al., Can. J. Chem.*, 1958, **36**, 1371 (*uv*)
Staiger, R.P. *et al., J.O.C.*, 1959, **24**, 1214-1219 (*2-naphthyl ester*)
Evans, H.B. *et al., J. Phys. Chem.*, 1968, **72**, 2552 (*pmr*)
Dhaneshwar, N.N. *et al., Acta Cryst. B*, 1972, **28**, 647 (*cryst struct*)
Kimura, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1507 (*2-malonylaminobenzoic acid*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 935 (*rev, tox, Me ester*)
Errede, L.A. *et al., J.O.C.*, 1976, **41**, 1763 (*synth*)
IARC Monog., 1978, **16**, 265; *Suppl.* 7, 57 (*rev, tox*)
Parada, F. *et al., Phytochemistry*, 1996, **42**, 871 (*glucosyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 80; 751; 949; 981-982; 1445; 1456; 1717; 2156-2157 (*esters*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 38-39; 186-187; 365; 518-519; 760; 868-869; 1071-1072; 1278-1279; 1439 (*esters, use*)
Osvath, R. *et al., Food Chem. News*, 2001, **43(26)**, 30 (*amide, use*)

4-Aminobenzoic acid, 9CI A-218

[150-13-0]

[1321-11-5]
Vitamin H'. Aminobenzoic acid, USAN. PABA

$C_7H_7NO_2$ 137.138
Listed in the EAFUS Food Additive Database (Jan. 2001) but with no reported use. Prisms. Sol. H_2O, alkalis, EtOH, Et_2O, C_6H_6. Mp 188-188.5°. pK_{a1} 2.5;

pK_{a2} 4.87 (25°). Log P 0.98 (calc). Discolours to orange on exp. to air and light.

► Can cause contact and photocontact allergic dermatitis from topical use. LD_{50} (rbt, orl) 1830 mg/kg. Exp. reprod. effects. DG1400000

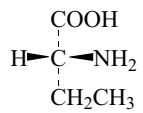
[138-84-1, 515-74-2, 555-06-6, 577-48-0, 64059-66-1, 75106-10-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 198C; 199A; 199C; 303A; 361B; 382D; 450D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1085B; 1086A; 1086C; 1264A; 1264B; 1371C; 1395C; 1413A; 1521B; 1524A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1372A; 1372B (*ir*)
Registry of Mass Spectral Data, Wiley-Interscience, 290 (*ms*)
Sadtler Standard C-13 NMR Spectra, 3466; 6429 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 15745; 16313 (*uv*)
Kremer, C.B. *et al., J. Chem. Educ.*, 1956, **33**, 71-72 (*synth*)
IARC Monog., 1978, **16**, 249; *Suppl.* 7, 56 (*rev, tox*)
Dewick, P.M. *et al., Nat. Prod. Rep.*, 1993, **10**, 233-263 (*biosynth*)

2-Aminobutanoic acid, 9CI A-219

[80-60-4]

[28805-76-7]
α-Aminobutyric acid. Butyrine. Quadrin



(*R*)-*form*

$C_4H_9NO_2$ 103.121

(*R*)-*form* [2623-91-8]
D-form
Constit. of seedlings of *Glycine max* (soybean), *Dolichos lablab* (hyacinth bean), *Canavalia gladiata* (swordbean), *Arachis hypogaea* (peanut), *Pisum sativum* (pea), *Phaseolus vulgaris* (kidney bean) and *Vigna sesquipedalis* (asparagus bean) after hydrol.. Leaflets (EtOH aq.). Mp 292° dec. $[\alpha]_D^{20}$ -7.86 (H_2O) (5*M* HCl).

Hydrochloride: [67607-42-5]
$[\alpha]_D^{20}$ +14.1.

Me ester: [74645-03-7]
$C_5H_{11}NO_2$ 117.147
Bp_{15} 62°. $[\alpha]_D^{25}$ -19.44 (neat).

Me ester, hydrochoride: [85774-09-0]
Cryst. (MeOH/Et_2O). Mp 150°.

N-*Formyl:*
$C_5H_9NO_3$ 131.131
Cryst. (EtOH). Mp 126°. $[\alpha]_D^{20}$ +27.98 (H_2O).

(*S*)-*form* [1492-24-6] *L-form*
Leaflets (EtOH aq.). Mp 292° dec. (303° in sealed tube). $[\alpha]_D^{20}$ +8 (H_2O) (5*M* HCl).

Hydrochloride: [5959-29-5]
Needles. $[\alpha]_D^{20}$ -14.

N-*Formyl:*
Cryst. (EtOH). Mp 126°. $[\alpha]_D^{20}$ -27.74 (H_2O).

(±)-*form* [2835-81-6]
Mp 304° (307° in sealed tube).

Hydrochloride: [40522-79-0]
Cryst.(EtOH aq.). Mp 179-180° (>230°).

Me ester: [2483-62-7]
Mp 139° (as hydrochloride).

Et ester:
$C_6H_{13}NO_2$ 131.174
Oil. Bp_{11} 61-62° (Bp_{16} 58°).

Et ester, hydrochloride:
Mp 148-150°.

Amide:
$C_4H_{10}N_2O$ 102.136
Prisms. Mp 74-75°.

Nitrile: [40651-89-6] *2-Aminobutanenitrile. 2-Cyanopropylamine*
$C_4H_8N_2$ 84.121
Mp 144-145° (as hydrochloride).

N-*Formyl:* [82413-57-8]
Needles (EtOH). Mp 153°.

N-*Benzoyl:* [5468-52-0]
$C_{11}H_{13}NO_3$ 207.229
Mp 145-146°.

N-*Me:* [70606-05-2] *2-(Methylamino)butanoic acid*
$C_5H_{11}NO_2$ 117.147
Prisms + $1H_2O$. V. sol. H_2O; insol. Et_2O. Mp 248° subl. Sweet taste.

N-*Me; hydrochloride:*
Mp 150° dec.

N-*Me, Me ester:*
$C_6H_{13}NO_2$ 131.174
Bp_{30} 64.5°.

N-*Di-Me:2-(Dimethylamino)butanoic acid*
$C_6H_{13}NO_2$ 131.174
Hygroscopic needles. Sol. H_2O. Mp 179°.

N-*Ph:* [67832-70-6] *2-Anilinobutanoic acid*
$C_{10}H_{13}NO_2$ 179.218
Cryst. (MeOH/$CHCl_3$). Mp 141°.

N-*Ph, Et ester:* [73717-57-4]
$C_{12}H_{17}NO_2$ 207.272
Mp 26°. Bp 278°.

N-*Ph, amide:*
$C_{10}H_{14}N_2O$ 178.233
Mp 123°.

N-*Ph, nitrile:* [85599-84-4]
$C_{10}H_{12}N_2$ 160.218
Needles. Mp 39°.

N-*(2,4-Dinitrophenyl):* [31356-29-3]
Mp 143°.

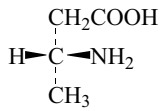
[4470-69-3, 5959-30-8, 6367-34-6, 7324-11-0, 7682-18-0, 7682-20-4, 15399-11-8, 15399-22-1, 21685-47-2, 22621-37-0, 26815-92-9, 39540-29-9, 40916-98-1, 53726-14-0, 55410-21-4, 56545-22-3, 67942-91-0, 73689-74-4, 87068-75-5, 91462-82-7, 93554-80-4, 103765-03-3, 104652-77-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 572C; 572D; 573A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 871B; 871C; 872A (*nmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2381
Junk, J.G. *et al., J.A.C.S.*, 1963, **85**, 839 (*ms*)
Pachler, K.G.R. *et al., Spectrochim. Acta*, 1963, **19**, 2085 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Ronwin, E. *et al., Can. J. Chem.*, 1968, **46**, 3013 (*ir*)
Akimoto, T. *et al., Acta Cryst. B*, 1972, **28**, 3106 (*cryst struct*)
Harada, K. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 191; 1865 (*synth*)
Ogawa, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 1661 (*occur*)
Glowiak, T. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1978, **26**, 43 (*cryst struct*)
Cooper, A.J.L. *et al., J. Biol. Chem.*, 1979, **254**, 2748 (*synth*)
Compagnone, R.S. *et al., J.O.C.*, 1986, **51**, 1713 (*synth, pmr*)
Chenault, H.K. *et al., J.O.C.*, 1987, **52**, 2608 (*resoln, pmr*)
Stirling, I.R. *et al., J.C.S. Perkin 1*, 1997, 677-680 (*synth*)

3-Aminobutanoic acid, 9CI A-220

[541-48-0]

[28805-76-7]
β-Homoalanine



(*R*)-*form*

$C_4H_9NO_2$ 103.121
Prod. by *Oryza sativa* (rice).

(*R*)-*form* [3775-73-3]
Prisms (MeOH). Mp 218-219°. $[\alpha]_D^{23}$ -39 (c, 0.4 in H_2O) (op).

(*S*)-*form* [3775-72-2]
Prisms (MeOH). Mp 215° (220° dec.). $[\alpha]_D^{20}$ +35.3 (H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 577B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 877B (*nmr*)
Aldrich Library of NMR Spectra, **3**, 4C (*pmr*)
Skita, A. *et al., Annalen*, 1927, **453**, 206 (*synth*)
Furukawa, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1319-1325; 1978, **26**, 260-263 (*synth*)
Griesbeck, A. *et al., Helv. Chim. Acta*, 1987, **70**, 1326-1332 (*synth*)
Gmeiner, P. *et al., Annalen*, 1991, 501-502 (*synth*)
Bringmann, G. *et al., Synthesis*, 1991, 829-831 (*synth, ir, pmr*)
Davies, S.G. *et al., Chem. Comm.*, 1995, 1109-1110 (*synth*)
Cimarelli, C. *et al., Synth. Commun.*, 2001, **31**, 2943-2953 (*R-form, synth, ir, pmr, cmr*)
Agami, C. *et al., Tetrahedron*, 2001, **57**, 195-200 (*S-form, synth*)

(4-Aminobutyl)guanidine, 9CI A-221

[306-60-5]
4-Guanidinobutylamine. 1-Amino-4-guanidinobutane. ***Agmatine***
$HN{=}^{6}C(NH_2)NH(CH_2)_3CH_2NH_2$
$C_5H_{14}N_4$ 130.192
Mp 101.5-103°.

Sulfate: [2482-00-0]
Cryst. Mp 229° (224-225°).

N^{1}-*(4-Hydroxy-*E*-cinnamoyl):* [7295-86-5]
N^{1}-trans-p-*Coumaroylagmatine.* 4-Hydroxycinnamoylagmatine
$C_{14}H_{20}N_4O_2$ 276.338
Isol. from barley seedlings. Sol. H_2O. Mp 215-217° (as picrate). λ_{max} 229 (ε 33100); 300 (ε 26300) (H_2O) (Berdy).

N^1-*(4-Hydroxy-Z-cinnamoyl)*:**N^1-cis-p-*Coumaroylagmatine***
$C_{14}H_{20}N_4O_2$ 276.338
Syrup or powder. λ_{max} 278 (ε 2000) (H_2O).

N^1-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl)*:**N^1-trans-*Feruloylagmatine***
$C_{15}H_{22}N_4O_3$ 306.364
Isol. from *Triticum aestivum* (wheat) exposed to low temps..

N^1-*(3,4-Dimethoxycinnamoyl)*:**N^1-*(3,4-Dimethoxycinnamoyl)agmatine***
$C_{16}H_{24}N_4O_3$ 320.391

N^6-*Me:* [77414-15-4] N-*(4-Aminobutyl)*-N′-*methylguanidine.* **N^6-*Methylagmatine***
$C_6H_{16}N_4$ 144.219
Isol. from soybean and alfalfa.

N^6-*(3-Methyl-2-butenyl)*:**N^6-*(3-Methyl-2-butenyl)agmatine***. N^6-*Prenylagmatine*
$C_{10}H_{22}N_4$ 198.311

N^6-*(3-Methyl-2-butenyl), N^{ξ}-(3,4-dimethoxycinnamoyl):* See Caracasanamide in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 821B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1330A (*nmr*)
Kossel, A. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1910, **66**, 257; **68**, 170 (*isol, struct, synth*)
Heyl, F.W. *et al., J.A.C.S.*, 1919, **41**, 681 (*isol*)
Stoessl, A. *et al., Phytochemistry*, 1965, **4**, 973 (*isol, uv, struct, synth, N-coumaroyl*)
Boldt, A. *et al., Phytochemistry*, 1971, **10**, 731 (*biosynth*)
Smith, T.A. *et al., Phytochemistry*, 1978, **17**, 1093 (*occur, N-coumaroyl*)
Kowabata, T. *et al., CA*, 1979, **89**, 178349 (*isol*)
Bird, C.R. *et al., Phytochemistry*, 1981, **20**, 2345 (*biosynth, N-coumaroyl*)
Chandrasekhar, K. *et al., Acta Cryst. B*, 1982, **38**, 2538 (*cryst struct*)
Cho, Y.B. *et al., Anal. Biochem.*, 1987, **160**, 429 (*N^6-Methylagmatine*)
Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1313 (*N^6-Methylagmatine*)
Mitchinson, A. *et al., Chem. Comm.*, 1994, 2613 (*synth*)
Ueda, M. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2133-2137 (*Z-coumaroyl*)
Reis, D.J. *et al., Ann. N.Y. Acad. Sci.*, 1999, **881**, 65-80 (*rev, activity*)
Monache, G.D. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3249-3254 (*Prenylagmatine, Dimethoxycinnamoylagmatine*)
Jin, S. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1614-1617 (*Feruloylagmatine*)
Fairbanks, C.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 10584-10589 (*pharmacol*)
Reis, D.J. *et al., Trends Pharmacol. Sci.*, 2000, **21**, 187-193 (*pharmacol, rev*)
Demady, D.R. *et al., Mol. Pharmacol.*, 2001, **59**, 24-29 (*pharmacol*)

(4-Aminobutyl)urea, 8CI A-222

[6851-51-0]
N-*Carbamoylputrescine*
$H_2NCH_2(CH_2)_3NHCONH_2$
$C_5H_{13}N_3O$ 131.177
Alkaloid from *Hordeum vulgare* (barley) and *Sesamum indicum* (sesame).

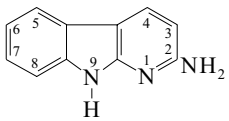
Hydrochloride:
Mp 185-186°.

Dipicrate:
Mp 164-165°.

Linneweh, F. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1932, **205**, 126; *CA*, **26**, 3276 (*synth*)
Smith, T.A. *et al., Phytochemistry*, 1964, **3**, 23 (*occur, synth*)
Crocomo, O.J. *et al., Phytochemistry*, 1970, **9**, 1487 (*occur*)

2-Amino-α-carboline A-223

[26148-68-5]
9H-Pyrido[2,3-b]indol-2-amine. 3-Amino-3-carboline (obsol.)



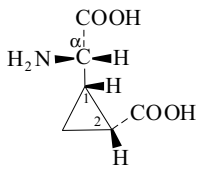
$C_{11}H_9N_3$ 183.212
Found in cooked foods as pyrol. prod. of tryptophan. Cryst. ($CHCl_3$/hexane or EtOH). Mp 202-203°.
▶ Exp. carcinogen and mutagen. UU9351600

N^2-*Me:* [26148-70-9]
$C_{12}H_{11}N_3$ 197.239
Cryst. (C_6H_6/petrol). Mp 156-157°.

Stephenson, L. *et al., J.C.S.(C)*, 1970, 1355 (*synth*)
Yoshida, D. *et al., Biochem. Biophys. Res. Commun.*, 1978, **83**, 915 (*cryst struct, tox*)
Matsumoto, T. *et al., Agric. Biol. Chem.*, 1979, **43**, 675 (*synth*)
Yoshida, D. *et al., Agric. Biol. Chem.*, 1979, **43**, 1769
Hibino, S. *et al., Chem. Pharm. Bull.*, 1991, **39**, 79 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJD750

α-Amino-2-carboxycyclopropaneacetic acid, 8CI A-224

2-(Carboxycyclopropyl)glycine. 3,4-Methanoglutamic acid



(α*S*,1*S*,2*R*)-*form*

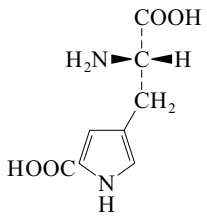
$C_6H_9NO_4$ 159.141
(α*S*,1*S*,2*R*)-*form* [117857-95-1]
L-cis-*form*
Cryst. (EtOH/Me_2CO/H_2O). $[\alpha]_D^{20}$ +25 (c, 1 in H_2O). $[\alpha]_D$ +58 (c, 0.5 in 5*M* HCl).
(α*S*,1*S*,2*S*)-*form* [117857-93-9]
L-trans-*form*. *L-CCG-I*
Isol. from seeds of *Blighia sapida* (akee apple). Cryst. $[\alpha]_D^{20}$ +107 (c, 2 in H_2O). $[\alpha]_D$ +146 (c, 1 in 5*M* HCl). Pharmacol. active isomer.
(α*S*,1*R*,2*S*)-*form* [117857-96-2]

[22255-17-0, 22255-18-1]

Fowden, L. *et al., Phytochemistry*, 1969, **8**, 437 (*isol, struct, pmr, ms, cryst struct*)
Fowden, L. *et al., J.C.S.(C)*, 1971, 833 (*cd, ord*)
Kurokawa, N. *et al., Tet. Lett.*, 1985, **26**, 83 (*synth, pmr*)
Yamanoi, K. *et al., Tet. Lett.*, 1988, **29**, 1181 (*synth, biochem*)
Stammer, H. *et al., Tetrahedron*, 1990, **46**, 2231 (*rev*)
Starratt, A.N. *et al., Phytochemistry*, 1995, **40**, 479 (*isol, bibl*)
Sagnard, I. *et al., Tet. Lett.*, 1995, **36**, 3149 (*synth*)

4-(2-Amino-2-carboxyethyl)-1*H*-pyrrole-2-carboxylic acid A-225

3-(2-Carboxy-4-pyrrolyl)alanine. 2-Amino-3-(2-carboxy-4-pyrrolyl)propanoic acid

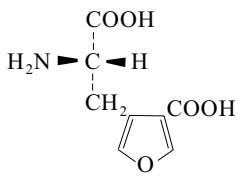


$C_8H_{10}N_2O_4$ 198.178
(*S*)-*form* [137309-97-8]
L-*form*
Mp 200-202° dec.
(±)-*form*
Mp 200-202° dec.

Yamano, K. *et al., Tetrahedron*, 1992, **48**, 1457 (*isol, synth, struct*)

α-Amino-4-carboxy-3-furanpropanoic acid, 9CI A-226

3-(3-Carboxy-4-furanyl)alanine

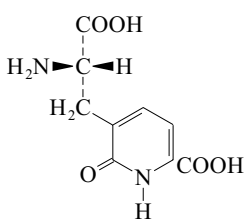


$C_8H_9NO_5$ 199.163
(*S*)-*form* [54836-90-7]
Isol. from the unpalatable mushrooms *Phyllotopsis nidulans* and *Tricholomopsis rutilans*. Cryst. (Me_2CO). Mp 227-228°.

Hatanaka, S. *et al., Mushroom Sci.*, (Publ. 1976), (Part 1), 1974, **9**, 809 (*isol*)
Doyle, R.R. *et al., Phytochemistry*, 1974, **13**, 2813 (*isol, struct*)

α-Amino-6-carboxy-2-oxo-3-pyridinepropanoic acid A-227

3-(6-Carboxy-2-oxo-4-pyridinyl)alanine



$C_9H_{10}N_2O_5$ 226.188
Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. λ_{max} 241 (ε 12000); 315 (ε 13500)

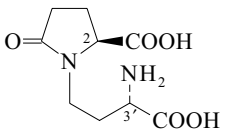
(H_2O) (Berdy).

(*S*)-*form* [148001-20-1]
$[\alpha]_D^{23}$ -5.8 (c, 0.13 in H_2O).

Yamano, K. *et al., Heterocycles*, 1993, **35**, 125 (*isol, struct*)
Yamano, K. *et al., Tetrahedron*, 1993, **49**, 2427 (*isol*)

α-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid, 9CI A-228

[115553-99-6]
1-(3-Amino-3-carboxypropyl)-5-oxo-2-pyrrolidinecarboxyic acid. Lp-2



(2*S*,3′*S*)-*form*

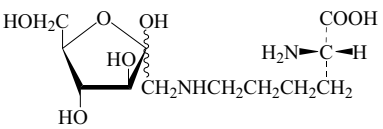
$C_9H_{14}N_2O_5$ 230.22

(2*S*,3′*S*)-*form*
Amino acid from the basidiomycete *Lactarius piperatus*. Amorph. solid. Sol. H_2O. $[\alpha]_D$ -17.5 (c, 0.939 in H_2O).

Fushiya, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1366 (*isol, ir, pmr, cmr, synth*)

1-[(5-Amino-5-carboxypentyl)amino]-1-deoxyfructose, 9CI A-229

[21291-40-7]
N^6-*(1-Deoxyfructos-1-yl)lysine. ϵ-Fructoselysine. ϵ-Deoxyfructosyllysine*



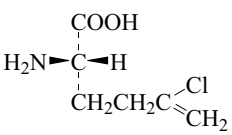
$C_{12}H_{24}N_2O_7$ 308.331
Amadori rearrangement prod. found in heated milk and other foodstuffs.

Acetate salt: [23931-62-6]
Mp 53-55°.

Finot, P.A. *et al., Helv. Chim. Acta*, 1969, **52**, 1488-1495 (*synth*)
Steinig, J. *et al., Z. Lebensm.-Unters. -Forsch.*, 1982, **174**, 453-457 (*synth, ms, detn*)
Dyer, D.G. *et al., J. Clin. Invest.*, 1993, **91**, 2463-2469; 2470-2478

2-Amino-5-chloro-5-hexenoic acid A-230

[66157-56-0]

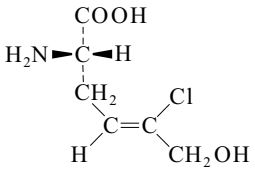


(*S*)-*form*

$C_6H_{10}ClNO_2$ 163.603

(*S*)-*form*
Japan. Pat., 1977, 77 148 019; *CA*, **88**, 149206w (*isol, ir*)
Hatanaka, S.-I. *et al., Phytochemistry*, 1998, **49**, 573-578 (*isol, synth, pmr, ms*)

2-Amino-5-chloro-6-hydroxy-4-hexenoic acid A-231



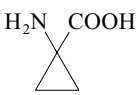
$C_6H_{10}ClNO_3$ 179.603

(*S*,*Z*)-*form* [108101-63-9]
Sol. H_2O; poorly sol. butanol, hexane. Mp 200-212° dec. $[\alpha]_D^{20}$ -17.9 (c, 0.19 in H_2O). λ_{max} (H_2O) (Berdy).

Ohta, T. *et al., Phytochemistry*, 1987, **26**, 565 (*isol*)

1-Aminocyclopropanecarboxylic acid, 9CI A-232

[22059-21-8]



$C_4H_7NO_2$ 101.105
Biosynth. precursor of Ethylene, E-301 in plants. Isol. from apple and pear juice and cranberries. Cryst. (EtOH aq.). Mp 229-231°.

▶ GZ1110000

N-*Malonyl:* [80550-27-2] *1-(Malonylamino)cyclopropanecarboxylic acid. MACC*
$C_7H_9NO_5$ 187.152
Constit. of numerous plant spp. including wheat, tomato and sweet corn. Mp 158-160°.

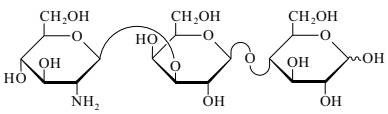
N-*(L-γ-Glutamyl):* [171437-78-8] *1-(γ-Glutamylamino)cyclopropanecarboxylic acid*
$C_9H_{14}N_2O_5$ 230.22
Isol. from tomato fruit (*Lycopersicon esculentum*).

[72784-48-6]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 884A; 884B (*nmr*)
Vähätalo, M.L. *et al., Acta Chem. Scand.*, 1957, **11**, 741-743 (*isol*)
Berlinguet, L. *et al., Nature (London)*, 1962, **194**, 1082-1083 (*activity*)
Bregovec, I. *et al., Monatsh. Chem.*, 1972, **103**, 288-291 (*synth*)
Kollonitsch, J. *et al., J.O.C.*, 1979, **44**, 771-777 (*synth*)
Ger. Pat., 1982, 3 122 240; *CA*, **98**, 88868w (*synth*)
Baldwin, J.E. *et al., Chem. Comm.*, 1985, 206-207 (*props*)
Schöllkopf, U. *et al., Angew. Chem., Int. Ed.*, 1986, **25**, 754-755 (*synth*)
Isogai, K. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2839-2842 (*synth, pmr, ir*)
Yang, S.F. *et al., Conjugated Plant Horm.: Proc. Int. Symp., 1986 (1987)*, 1986, 92-101 (*rev*)
Amrhein, N. *et al., Conjugated Plant Horm.: Proc. Int. Symp., 1986 (1987)*, 1986, 102-110 (*rev*)
Wiesendanger, R. *et al., Experientia*, 1986, **42**, 207-209 (*biosynth*)
Strazewski, P. *et al., Synthesis*, 1987, 298-299 (*synth, pmr, cmr, ms*)
Wheeler, T.N. *et al., Synth. Commun.*, 1988, **18**, 141-149 (*synth, pmr, cmr*)
Vaidyanathan, G. *et al., J.O.C.*, 1989, **54**, 1810-1815; 1815-1820 (*synth, Me ester, N,N-dibenzyl, N,N-di-Me, N-Me, N-benzyl, bibl*)
Salaün, J. *et al., J.O.C.*, 1990, **55**, 4276-4281 (*synth, pmr*)
Stammer, H. *et al., Tetrahedron*, 1990, **46**, 2231-2254 (*rev*)
Cativiela, C. *et al., Synth. Commun.*, 1992, **22**, 2955-2963 (*synth*)
Alami, A. *et al., Bull. Soc. Chim. Fr.*, 1993, **130**, 5-24 (*rev*)
Angus, P.M. *et al., Chem. Comm.*, 1993, 979-980 (*synth*)
Zhu, X. *et al., Synth. Commun.*, 1998, **28**, 3159-3162 (*synth, ir, pmr, ms*)
Pirrung, M.C. *et al., Acc. Chem. Res.*, 1999, **32**, 711-718 (*rev*)
Fulop, F. *et al., Chem. Rev.*, 2001, **101**, 2181-2204 (*rev*)

2-Amino-2-deoxy-β-D-gluco-pyranosyl-(1→3)-β-D-galactopyranosyl-(1→4)-D-glucose A-233

3^2-Glucosaminyllactose



Pyranose-*form*

$C_{18}H_{33}NO_{15}$ 503.456

N-*Ac:* [75645-27-1] *2-Acetamido-2-deoxy-β-D-glucopyranosyl-(1→3)-β-D-galactopyranosyl-(1→4)-D-glucose. 3^2-β-N-Acetylglucosaminyllactose. Lacto-N-triose II*
$C_{20}H_{35}NO_{16}$ 545.494
Isol. from the partial acid hydrolysates of the tetra and higher saccharides obt. from human milk; does not occur free in milk. Mp 201-202°. $[\alpha]_D$ +40.7 (in H_2O).

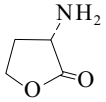
N-*Ac, phenylosazone:*
Mp 230°.

[24741-60-4]

Kuhn, R. *et al., Chem. Ber.*, 1958, **91**, 364; 1960, **93**, 647; 1962, **95**, 513; 518 (*isol*)
Okuyama, T. *et al., CA*, 1961, **55**, 18817; 1962, **57**, 8880 (*isol*)
Acher, A.J. *et al., J.O.C.*, 1970, **35**, 2436 (*synth*)
Koenderman, A.H.L. *et al., Biomed. Chromatogr.*, 1986, **1**, 104; *CA*, **106**, 191579k (*synth*)

3-Aminodihydro-2(3*H*)-furanone, 9CI, 8CI A-234

[1192-20-7]
2-Amino-4-butanolide. 2-Amino-4-hydroxybutanoic acid lactone. Homoserine lactone. α-Amino-γ-butyrolactone



(*S*)-*form*

$C_4H_7NO_2$ 101.105

(*S*)-*form* [2185-02-6]
L-*form*
Constit. of pea *Pisum sativum* seedlings. May be an artifact but most recent work

indicates that it is prob. a genuine nat. prod..

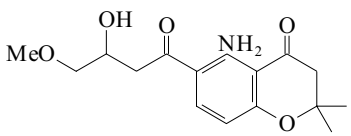
N-*(3-Hydroxy-7-tetradecenoyl)(3*R,*7*Z*-):* [172617-17-3] *Small bacteriocin*
$C_{18}H_{31}NO_4$ 325.447
Bacteriocin. Prod. by *Rhizobium leguminosarum*.

[2185-03-7, 51744-82-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 700C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1139C (*nmr*)
Weiss, S. *et al., J.A.C.S.*, 1951, **73**, 2497
Saarivirta, M. *et al., Acta Chem. Scand.*, 1965, **19**, 1008 (*isol*)
Jošt, K. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 2365 (*synth*)
Natelson, S. *et al., Microchem. J.*, 1982, **27**, 466 (*occur*)
Japan. Pat., 1983, 83 096 079; *CA*, **99**, 174212 (*isol, uv, ir, pmr, cmr, deriv*)
McGarvey, G.J. *et al., J.A.C.S.*, 1986, **108**, 4943 (*synth, pmr, ir*)
Buchardt, O. *et al., Synthesis*, 1993, 1065 (*pmr*)
Shiraiwa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2322-2325 (*resoln*)
Schripsema, J. *et al., J. Bacteriol.*, 1996, **178**, 366-371 (*3-hydroxytetradecenoyl*)

5-Amino-2,3-dihydro-6-(3-hydroxy-4-methoxy-1-oxobutyl)-2,2-dimethyl-4*H*-1-benzopyran-4-one, 9CI A-235

[130767-47-4]
*5-Amino-2,3-dihydro-6-(3-hydroxy-4-methoxybutanoyl)-2,2-dimethyl-4*H*-4-chromanone*

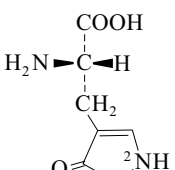


$C_{16}H_{21}NO_5$ 307.346
Isol. from rice cultures of *Fusarium equiseti*.

Xie, W. *et al., Appl. Environ. Microbiol.*, 1990, **56**, 2946 (*isol, pmr, ms*)

α-Amino-2,5-dihydro-5-oxo-4-isoxazolepropanoic acid, 9CI A-236

α-Amino-5-oxo-3-isoxazoline-4-propionic acid, 8CI. 3-(Isoxazolin-5-on-4-yl)alanine. 4-Alanyl-3-isovalin-5-one. TAN 950A. Antibiotic TAN 950A



$C_6H_8N_2O_4$ 172.14
Exists in tautomeric equilibrium with Antibiotic TAN 950B.λ_{max} 253 (ε 8060) (H_2O) (Derep).

(*S*)-*form* [127607-88-9]
L-form
Powder + $1H_2O$ (as Na salt). Sol. H_2O, DMSO, DMF; poorly sol. Me_2CO, $CHCl_3$, EtOAc. $[\alpha]_D^{23}$ -69.5 (c, 0.52 in H_2O) (as Na salt). λ_{max} 253 (E1%/1cm 380) (H_2O) (Berdy). λ_{max} 259 (E1%/1cm 421) (HCl) (Berdy).

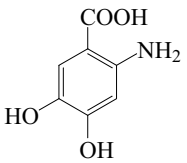
N^2-*β-D-Glucosyl:* [29790-46-3]
$C_{12}H_{18}N_2O_9$ 334.282
Isol. from *Pisum sativum* (peas). Cryst. (MeOH/propanol). Mp 182° dec.

[130620-29-0, 130621-41-9, 130621-42-0, 130621-61-3]

Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1970, **40**, 557; 1974, **61**, 155 (*isol, struct, uv, pmr, ir*)
Murakoshi, I. *et al., Phytochemistry*, 1975, **14**, 1515 (*biosynth*)
Iwama, T. *et al., Eur. J. Pharmacol.*, 1991, **197**, 187 (*props*)
Tsubotani, S. *et al., Tetrahedron*, 1991, **47**, 8079-8090 (*synth, cryst struct*)
Hakoda, S. *et al., J. Antibiot.*, 1992, **45**, 854 (*isol*)

2-Amino-4,5-dihydroxybenzoic acid A-237

[114874-99-6]
6-Aminoprotocatechuic acid. 4,5-Dihydroxyanthranilic acid



$C_7H_7NO_4$ 169.137

N-*Et, amide:* [127793-87-7] *2-(Ethylamino)-4,5-dihydroxybenzamide, 9CI*
$C_9H_{12}N_2O_3$ 196.205
Alkaloid from *Piper nigrum* (pepper).

4-Me ether, N-*(4-hydroxy-3-methoxy-E-cinnamoyl):* [154992-25-3] ***Avenanthramide 2***
$C_{18}H_{17}NO_7$ 359.335
Constit. of *Avena sativa* (oat).

Di-Me ether: [5653-40-7] *2-Amino-4,5-dimethoxybenzoic acid. 6-Aminoveratric acid*
$C_9H_{11}NO_4$ 197.19
Needles (EtOAc). Mp 186°.

Di-Me ether, Me ester: [26759-46-6]
$C_{10}H_{13}NO_4$ 211.217
Plates (C_6H_6). Mp 133°.

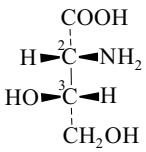
Di-Me ether, nitrile: [26961-27-3] *2-Cyano-4,5-dimethoxyaniline*
$C_9H_{10}N_2O_2$ 178.19
Cryst. (MeOH). Mp 99-100°.

4-Benzyl ether, 5-Me ether:
$C_{15}H_{15}NO_4$ 273.288
Yellow solid. Mp 159-161°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 233A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1150B; 1541A (*nmr*)
Fetscher, C.A. *et al., J.O.C.*, 1939, **4**, 71 (*synth*)
McKee, R.L. *et al., J.A.C.S.*, 1946, **68**, 1902 (*nitrile, synth*)
Wilson, C.V. *et al., J.A.C.S.*, 1948, **70**, 1901 (*nitrile, synth*)
Carpenter, P.D. *et al., J.C.S. Perkin 1*, 1979, 103 (*Me ester, synth, pmr*)
Bandyopadhyay, C. *et al., J. Agric. Food Chem.*, 1990, **38**, 1696-1699 (*N-Et amide*)
Dimberg, L.H. *et al., Cereal Chem.*, 1993, **70**, 637-641 (*Avenanthramide 2*)
Alvi, K.A. *et al., J. Antibiot.*, 1997, **50**, 264-266 (*isol*)
Hu, W.-P. *et al., J.O.C.*, 2001, **66**, 2881-2883 (*4-benzyl-5-Me ether, pmr, cmr*)

2-Amino-3,4-dihydroxybutanoic acid A-238

[104111-37-7]
4-Hydroxythreonine



(2*R*,3*R*)-*form*

$C_4H_9NO_4$ 135.119
The stereoisomers can be named as 4-hydroxythreonines or 4-hydroxyallothreonines, but a change of Cahn-Ingold-Prelog priorities can lead to confusion.

(2*R*,3*R*)-*form* [21768-44-5]
(+)-threo-*form*
Isol. from the mushroom *Lyophyllum ulmarium*. Mp 214-215° (194°). $[\alpha]_D^{23}$ +13.6 (c, 4.8 in H_2O).

Lactone: [21768-48-9]
$C_4H_7NO_3$ 117.104
Cryst. (as hydrochloride). Mp 176.5° (hydrochloride). $[\alpha]_D^{23}$ -56.6 (c, 1.5 in H_2O).

4-Et ether: [98644-37-2] *2-Amino-4-ethoxy-3-hydroxybutanoic acid*
$C_6H_{13}NO_4$ 163.173
Isol. from the mushroom *Lyophyllum ulmarium*.

(2*R*,3*S*)-*form* [21768-46-7]
(-)-erythro-*form*
Mp 194-195° dec. $[\alpha]_D^{23}$ +11.3 (c, 1.5 in H_2O).

Lactone:
Mp 176° dec. (as hydrochloride). $[\alpha]_D^{23}$ +55.6 (c, 1.5 in H_2O).

(2*S*,3*S*)-*form* [21768-43-4] *(-)*-threo-*form*
Needles (EtOH aq.). Sol. EtOH; fairly sol. H_2O; poorly sol. butanol, hexane. Mp 210° dec. (194-195°). $[\alpha]_D^{25}$ -13.3 (c, 1 in H_2O). λ_{max} (H_2O) (Berdy).

Lactone:
Mp 173-174° dec. (as hydrochloride). $[\alpha]_D^{23}$ -26.2 (c, 1 in H_2O).

Niemann, C. *et al., J. Biol. Chem.*, 1942, **143**, 191 (*synth*)
Hamel, E.E. *et al., J.A.C.S.*, 1953, **75**, 1362 (*config*)
Okawa, K. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2720 (*resoln*)
Westley, J.W. *et al., J. Antibiot.*, 1971, **24**, 330-331 (*isol*)
Katz, E. *et al., J. Antibiot.*, 1974, **27**, 952
Ogawa, T. *et al., Phytochemistry*, 1984, **23**, 684-686; 1985, **24**, 1837-1838 (*isol*)
Pirrung, M.C. *et al., Bioorg. Med. Chem. Lett.*, 1993, **3**, 2095-2098 (*synth, abs config*)
Cativiela, C. *et al., Tetrahedron*, 1996, **52**, 9563-9574 (*synth*)

2-Amino-3,4-dihydroxypentanedioic acid A-239

3,4-Dihydroxyglutamic acid

HOOCCH(OH)CH(OH)CH(NH_2)COOH

$C_5H_9NO_6$ 179.129

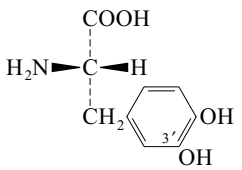
Isol. from *Lepidium sativum* (garden cress) and *Rheum rhaponticum* (rhubarb). The (2*S*,3*S*,4*R*)- and (2*S*,3*S*,4*S*)-stereoisomers have been synthesised, but the abs. config. of the natural product is currently (2001) unknown.

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1957, **11**, 182 (*isol*)
Mueller, A.L. *et al., Acta Chem. Scand.*, 1965, **19**, 1987 (*isol*)
Dauban, P. *et al., Tetrahedron*, 1999, **55**, 7589-7600 (*synth*)
Oba, M. *et al., Tet. Lett.*, 2001, **42**, 5901-5902 (*synth*)

2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid A-240

[587-45-1]

3-Hydroxytyrosine, 9CI. 3,4-Dihydroxyphenylalanine. DOPA



(*S*)-*form*

$C_9H_{11}NO_4$ 197.19Log P -2.82 (uncertain value) (calc).

(*S*)-*form* [59-92-7]

L-*form*. ***Levodopa, BAN, INN, JAN, USAN***. *Bendopa. Brocadopa. Dopar. Larodopa. Levopa. Veldopa. Many other names*

Occurs in seedlings and pods of *Vicia faba*. Prisms, needles (H_2O + SO_2) or plates (EtOH aq.). Mp 285.5° dec. $[\alpha]_D^{20}$ -12.15 (c, 4 in 1*N* HCl). Pharmacol. active isomer. Rapidly turns green in air, aq. solns. darken in air. Green col. with $FeCl_3$. Reduces $AgNO_3$, NH_3 and acid $KMnO_4$. Component of Sinemet. High-mol.-wt. polymers have been synth..

▶ Systemic (e.g. CNS) and adverse effects when used therapeutically. LD_{50} (rat, orl) 1780 mg/kg. Exp. reprod. and teratogenic effects. AY5600000

3′-O-β-D-Glucopyranoside: [2275-95-8]

$C_{15}H_{21}NO_9$ 359.332

Isol. from *Pisum sativum* (peas) and *Vicia faba*. Resin or syrup.

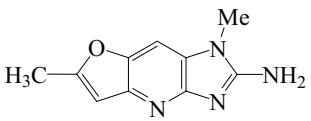
[57308-51-7, 127441-81-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 257A; 257B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1190A; 1190B (*nmr*)
Andrews, R.S. *et al., Nature (London)*, 1965, **205**, 1213 (*glucoside*)
Vorbruggen, H. *et al., Chem. Ber.*, 1972, **105**, 1168 (*synth*)
Griffith, T. *et al., Phytochemistry*, 1973, **12**, 1651 (*biosynth*)
Mostad, A. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 1161 (*cryst struct*)
Renth, E.-O. *et al., Angew. Chem., Int. Ed.*, 1975, **14**, 361 (*synth*)
Bartholini, G. *et al., Pharmacol. Ther., Part B*, 1975, **1**, 407 (*rev, pharmacol*)
Gomez, R. *et al., Anal. Profiles Drug Subst.*, 1976, **5**, 189 (*rev*)
Dardenne, G. *et al., Phytochemistry*, 1977, **16**, 1822 (*deriv*)
Danishevsky, S. *et al., Tetrahedron*, 1981, **37**, 4081 (*synth*)
Nutt, J.G. *et al., Clin. Neuropharmacol.*, 1984, **7**, 35 (*rev, metab*)

2-Amino-1,6-dimethylfuro[3,2-*e*]imidazo[4,5-*b*]pyridine A-241

[132898-08-9]

*1,6-Dimethyl-1*H*-furo[2,3-*b*]imidazo[4,5-e]pyridin-2-amine, 9CI*



$C_{10}H_{10}N_4O$ 202.215

Isolated from cooked meats.

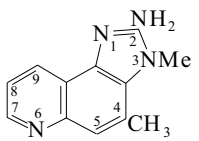
▶ Mutagenic.

Pais, P. *et al., J. Agric. Food Chem.*, 2000, **48**, 1721-1726 (*isol, struct*)

2-Amino-3,4-dimethylimidazo[4,5-*f*]quinoline A-242

[77094-11-2]

Me-IQ



$C_{12}H_{12}N_4$ 212.254

Isol. from sardines, beef extract and hamburger, probably widely distributed in cooked foods. Mp 296-298° (sealed tube). λ_{max} 219 ; 265 ; 332 (no solvent reported).

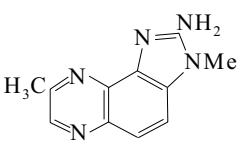
▶ Highly mutagenic. Exp. carcinogenic data. NJ5907000

Kasai, H. *et al., Chem. Lett.*, 1980, 1391 (*struct, bibl*)
Kasai, H. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2233
Adolfsson, L. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 157 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*carcinogenicity*)
IARC Monog., 1986, **40**, 275; *Suppl.* 7, 65 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJQ600

2-Amino-3,8-dimethyl-3*H*-imidazo[4,5-*f*]quinoxaline A-243

[77500-04-0]

*3,8-Dimethyl-3*H*-imidazo[4,5-f]quinoxalin-2-amine, 9CI. MeIQx*



$C_{11}H_{11}N_5$ 213.241

Food-related mutagen isol. from cooked meats (esp. grilled/barbecued). Cryst. (Py). Mp 295-300° (sealed tube).

▶ Highly mutagenic. Exp. carcinogenic data. NJ5925500

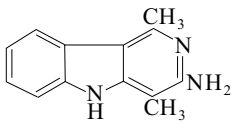
Kasai, H. *et al., Chem. Lett.*, 1981, 675 (*synth*)
IARC Monog., 1986, **40**, 283; *Suppl.* 7, 65 (*rev, tox*)
Knapp, S. *et al., Tetrahedron*, 1989, **45**, 1293 (*synth*)
Grivas, S. *et al., Acta Chem. Scand.*, 1993, **43**, 521 (*synth, pmr, ms*)
Knize, M.G. *et al., J. Agric. Food Chem.*, 1998, **46**, 4648-4651 (*hplc*)
De Meester, C. *et al., Z. Lebensm.-Unters. -Forsch.*, 1998, **207**, 441-447 (*hplc*)
Fukushima, S. *et al., Cancer Lett. (Shannon, Irel.)*, 1999, **143**, 157-159 (*tox*)
Schut, H.A. *et al., Carcinogenesis (London)*, 1999, **20**, 353-368 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJQ675

3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole A-244

[62450-06-0]

[68808-54-8]

*1,4-Dimethyl-5*H*-pyrido[4,3-b]indol-3-amine, 9CI. 3-Amino-1,4-dimethyl-γ-carboline. Trp-P1*



$C_{13}H_{13}N_3$ 211.266

Powerful mutacarcinogen found in cooked foods. Pale-brown needles or small prisms (EtOAc)(as acetate salt). Mp 252-262° (acetate salt).

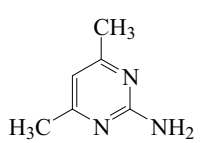
▶ Highly mutagenic. Possible human carcinogen. LD_{50} (rat, orl) 100 mg/kg. Exp. carcinogen. UU9351900

Kosuge, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 611 (*isol, cryst struct, spectra*)
IARC Monog., 1983, **31**, 247; *Suppl.* 7, 73 (*rev, tox*)
Akimoto, H. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 123 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*tox*)
Stavric, B. *et al., Food Chem. Toxicol.*, 1994, **32**, 977 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJR500; TNX275

2-Amino-4,6-dimethylpyrimidine A-245

[767-15-7]

4,6-Dimethyl-2-pyrimidinamine, 9CI



$C_6H_9N_3$ 123.157

Cryst. (H_2O). Mod. sol. H_2O, EtOH;

insol. Et_2O. Mp 153° (149-150°). Distils undec..

2-N-*Ac:* [15755-12-1]
$C_8H_{11}N_3O$ 165.194
Mp 124°.

2-N-*Me:* [15231-64-8]
$C_7H_{11}N_3$ 137.184
Cryst. (petrol). Mp 98°.

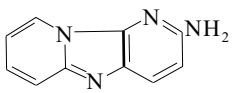
2-N-*Ph:* [53112-28-0] *2-Anilino-4,6-dimethylpyrimidine.* ***Pyrimethanil, BSI.*** *Mythos. Scala. SN 100309. ZK 100309*
$C_{12}H_{13}N_3$ 199.255
Fungicide used on grape vines. Cryst. (toluene). Mp 88-89°.

▶ LD_{50} (rat, orl) 4150-5971 mg/kg.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 701D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 822D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1555A (*ir*)
Hale, W.J. *et al., J.A.C.S.*, 1918, **40**, 1046 (*synth*)
Short, L.N. *et al., J.C.S.*, 1952, 168 (*ir*)
Alberola, A. *et al., Synth. Commun.*, 1987, **17**, 1309 (*synth*)
Neumann, G.L. *et al., Brighton Crop Prot. Conf. - Pests Dis.*, 1992, **1**, 395-402 (*pyrimethanil*)
Cobras, P. *et al., J. Agric. Food Chem.*, 1997, **45**, 2708-2710 (*pyrimethanil, detn*)
Pesticide Manual, 12th edn., 2000, No. 674 (*Pyrimethanil*)

2-Aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole A-246

[67730-10-3]
*Dipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, 9CI. Glu-P-2*



$C_{10}H_8N_4$ 184.2
Parent compd. of a group of potent mutagens found in cooked foods.

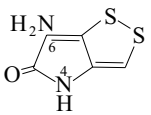
▶ Possible human carcinogen. Exp. carcinogen. Mutagen. JM5615000

Hydrobromide:
Mp 286-287°.

Takeda, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2924 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*tox*)
IARC Monog., 1986, **40**, 235; *Suppl.* 7, 64 (*rev, tox*)
Stavric, B. *et al., Food Chem. Toxicol.*, 1994, **32**, 997 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DWW700

6-Amino-1,2-dithiolo[4,3-*b*]pyrrol-5(4*H*)-one, 9CI A-247

[488-03-9]
Holothin



$C_5H_4N_2OS_2$ 172.231
Greenish-black cryst. (as hydrochloride). Mp 300° (hydrochloride).

▶ AB7450000

4-Me, N^6*-Ac:* [87-11-6] ***Thiolutin.*** N-*Acetylpyrrothine. Farcinicine. Acetopyrrothine*
$C_8H_8N_2O_2S_2$ 228.295
Isol. from several strains of *Streptomyces albus* and *Streptomyces pimprina*. Antibiotic which inhibits microbiological growth in beer. Brilliant yellow needles (1-butanol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, C_6H_6, Et_2O, hexane. Mp 273-276° dec. $Bp_{0.1}$ 200° subl.. λ_{max} 248 (ϵ 6300); 311 (ϵ 5700); 388 (ϵ 10800) (MeOH) (Derep). λ_{max} 250 (ϵ 6030); 311 (ϵ 5600); 388 (ϵ 10960) (MeOH) (Berdy).

▶ LD_{50} (mus, scu) 25 mg/kg. JP1355000

Celmer, W.D. *et al., J.A.C.S.*, 1952, **74**, 6304; 1955, **77**, 2861 (*Pyrrothine, Aureothricin, Thiolutin, isol, ir, uv, struct*)
Hagio, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1484 (*Holothin, Thiolutin, Aureothricin, synth, ir, uv, pmr*)
Ninomiya, Y.T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3157-3162 (*Pyrrothine, Thiolutin, props, ms*)
Deb, P.R. *et al., Curr. Sci. (India)*, 1984, **53**, 659 (*Thiolutin, props*)
Lamari, L. *et al., J. Antibiot.*, 2002, **55**, 696-701; 702-706 (*Saccharothrix pyrrothines*)

2-Aminoethanesulfonic acid, 9CI A-248

[107-35-7]
Taurine, 8CI, INN. *Aminoethylsulfonic acid. Ethylaminesulfonic acid. FEMA 3813*
$H_2NCH_2CH_2SO_3H$
$C_2H_7NO_3S$ 125.148
Essential nutrient obt. from diet and by *in vivo* synth. from methionine and cysteine. Present in meats, fish, legumes, human milk, molluscs and other foodstuffs. Dietary supplement, e.g. in Red Bull drink. Monoclinic prismatic rods with sharp taste. Sol. H_2O, insol. EtOH. Mp 328° (320-325° dec.). pK_{a1} 1.5; pK_{a2} 8.74. Dec. at 300°.

▶ LD_{50} (mus, scu) 6000 mg/kg. WX0175000

Amide: [4378-70-5]
$C_2H_8N_2O_2S$ 124.163
Plates (EtOH) (as hydrochloride). Mp 133° (hydrochloride).

N-*Me:* [107-68-6]
$C_3H_9NO_3S$ 139.175
Prisms. V. sol. H_2O, insol. EtOH, Et_2O. Mp 241-242°.

N,N-*Di-Me:* [637-95-6]
$C_4H_{11}NO_3S$ 153.202
Prisms (MeOH). V. sol. H_2O, AcOH, insol. EtOH, Et_2O. Mp 315-316° dec.

N,N-*Bis(2-chloromethyl):* [98277-87-3] *Taumustine*
$C_6H_{13}Cl_2NO_3S$ 250.145
Cryst. (H_2O). Mp 178-180°.

N-*(2,3-Dihydroxypropyl):* [65222-42-6] N-*Glyceryltaurine*
$C_5H_{13}NO_5S$ 199.227
Cryst. (EtOH aq.). Mp 163-164°. $[\alpha]_D^{23}$ -21 (H_2O).

[4316-74-9, 7347-25-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 890A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1433C (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 563; 564 (*synth*)
Ishidate, M. *et al., Chem. Pharm. Bull.*, 1954, **2**, 275 (*synth*)
Lindberg, B. *et al., Acta Chem. Scand.*, 1955, **9**, 1093; 1323 (*isol, derivs*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1956, **10**, 1097 (*Glyceryltaurine*)
Sutherland, H.H. *et al., Acta Cryst.*, 1963, **16**, 897 (*cryst struct*)
Huxtable, R. *et al., Taurine, [Int. Symp.], 1st, 1975 (1976)*, (Eds.), Raven Press, New York, 1975, (*book*)
Hashem, K.M.E. *et al., Bull. Soc. Chim. Belg.*, 1985, **94**, 735 (*cmr*)
Taurine: Nutritional Value and Mechanisms of Action, (eds. Lombardini, J.B. *et al*), Plenum Press, 1992, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1419
Merck Index, 12th edn., 1996, No 9241
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1665-1666 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TAG750

2-Aminoethanol, 9CI A-249

[141-43-5]
2-Hydroxyethylamine. Ethanolamine. Monoethanolamine. Colamine
$H_2NCH_2CH_2OH$
C_2H_7NO 61.083
Used in flume water for washing sugar beets prior to the slicing operation. Viscous, hygroscopic liq. Misc. H_2O, MeOH, Me_2CO; spar. sol. C_6H_6, Et_2O. d_4^{25} 1.01. Mp 10.5°. Bp 171°. n_D^{20} 1.4539. pK_a 9.47. Vp 0.48 mmHg (20°).

▶ Fl. p. 85°, autoignition temp. 410°. Corrosive and irritating to skin, eyes and mucous membranes. LD_{50} (rat, orl) 1720 mg/kg. Exp. teratogen. OES: long-term 3 ppm; short-term 6 ppm. KJ5775000

O-*Ac:* [1854-30-4] **O-*Acetylethanolamine.*** *2-Acetoxyethylamine*
$C_4H_9NO_2$ 103.121
Isol. from seeds of *Lens culinaris* (lentil), also present in other Leguminosae. $Bp_{0.3}$ 134-135°.

N,N-*Di-Et:* [100-37-8] *2-Diethylaminoethanol, 9CI. 2-Hydroxytriethylamine*
$C_6H_{15}NO$ 117.191
Boiler water additive. Sol. H_2O. Bp 163° Bp_{35} 75°.

▶ Skin and severe eye irritant. Adverse gastrointestinal effects by inhalation. LD_{50} (rat, orl) 1300 mg/kg. LD_{50} (gpg, skn) 884 mg/kg. OES: long-term 10 ppm (Sk). KK5075000

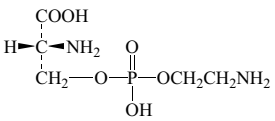
[96-80-0, 20739-39-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 334A; 334B; 339D; 340A; 340C; 756B; 904B; 1280A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 535B; 543A; 543B; 544A; 545B; 545C; **2**, 457B; 591A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 423D; 430A; 430B; 430D; 432B; 1112C (*ir*)
Putokhin, N. *et al., CA*, 1929, **23**, 2938 (*synth*)

Sarneski, J.E. *et al., Anal. Chem.*, 1975, **47**, 2116 (*cmr*)
Voronkov, M.G. *et al., Zh. Obshch. Khim.*, 1978, **48**, 429 (*ms*)
Hayman, A.R. *et al., Phytochemistry*, 1987, **26**, 839 (*O-Acetylethanolamine*)
Van Oycke, S. *et al., Bull. Soc. Chim. Belg.*, 1988, **97**, 297-311 (*isol*)
Mootz, D. *et al., Acta Cryst. C*, 1989, **45**, 754 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1703
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 813; 1904-1905
Liu, J. *et al., J.O.C.*, 2001, 5655-5663 (*OAc, synth, pmr*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0889
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 447; 578
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BQC000; DNP000; HKM000; MGG000; INN400; DHO500; EGA500; DDU600; EEC600

2-Aminoethyl seryl phosphate A-250

[17871-37-3, 18635-48-8]
Serine ethanolamine phosphodiester. SEP



(*R*)-*form*

$C_5H_{13}N_2O_6P$ 228.141

(*R*)-*form* [16106-04-0]
D-form
Cryst. (MeOH aq.). Mp 143-144° (dec.). $[\alpha]_D^{23}$ +18.2 (c, 0.7 in H_2O).

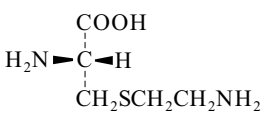
(*S*)-*form* [1186-34-1]
L-form
Isol. from numerous animals incl. chicken, fish and reptiles. Needles (MeOH aq.). Mp 142-143° (dec.). $[\alpha]_D^{23}$ -15 (c, 2 in H_2O).

(±)-*form* [114760-94-0]
Prisms (EtOH aq.). Mp 193-194° (dec.).

Ennor, A.H. *et al., J. Biochem. (Tokyo)*, 1960, **75**, 179-182
Beatty, I.M. *et al., J.A.C.S.*, 1960, **82**, 4983-4989 (*synth*)
Rosenberg, H. *et al., J. Biochem. (Tokyo)*, 1961, **50**, 81-84 (*occur, biosynth*)
Allen, A.K. *et al., Biochim. Biophys. Acta*, 1968, **151**, 504-519; **152**, 208-210 (*biosynth*)
Euerby, M.R. *et al., J. Chem. Res., Synop.*, 1988, 394-395 (*synth, pmr, cmr, ms*)
Merchant, T.E. *et al., J. Lipid Res.*, 1990, **31**, 479-486 (*P-31 nmr*)

S-(2-Aminoethyl)cysteine, 9CI A-251

[617-71-0]
3-[(2-Aminoethyl)thio]alanine, 8CI. Thialysine. Thiosine

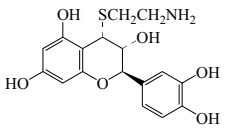


$C_5H_{12}N_2O_2S$ 164.228

(*R*)-*form* [2936-69-8]
L-form
Isol. from the edible mushroom *Rozites caperta*. Sol. H_2O; fairly sol. MeOH; poorly sol. Me_2CO, hexane.
► LD_{50} (mus, ipr) 300 mg/kg.

Matsumoto, N. *et al., CA*, 1985, **103**, 3724 (*isol*)

4-(2-Aminoethylthio)-3,3′,4′,5,7-pentahydroxyflavan A-252



(2*R*,3*R*,4*S*)-*form*

$C_{17}H_{19}NO_6S$ 365.406

(2*R*,3*R*,4*S*)-*form*
4β-(2-Aminoethylthio)catechin
Constit. of *Vitis vinifera* (wine grape).

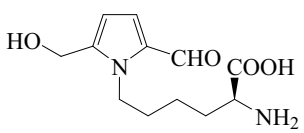
(2*R*,3*S*,4*S*)-*form*
4β-(2-Aminoethylthio)epicatechin
Constit. of *Vitis vinifera* (wine grape).

3-O-(3,4,5-Trihydroxybenzoyl):
$C_{24}H_{23}NO_{10}S$ 517.512
Constit. of *Vitis vinifera* (wine grape).

Torres, J.L. *et al., J. Agric. Food Chem.*, 2001, **49**, 4627-4634

α-Amino-2-formyl-5-(hydroxymethyl)-1*H*-pyrrole-1-hexanoic acid, 9CI A-253

[126255-18-3]
2-Formyl-5-(hydroxymethyl)pyrrole-1-norleucine. Lysylpyrroaldehyde. ϵ-Pyrrolelysine (incorr.)

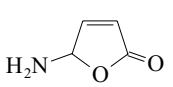


$C_{12}H_{18}N_2O_4$ 254.285

(*S*)-*form* [74509-14-1]
Pyrraline
Maillard prod. obt. by reacn. between, and, . Syrup.
► Mutagenic props..

Nakayama, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 1201-1202 (*synth, uv, ms, pmr, cmr*)
Miller, R. *et al., Acta Chem. Scand., Ser. B*, 1984, **38**, 689-694; 1985, **39**, 717-723 (*synth, pmr, cmr*)
Schloesser, U. *et al., Z. Lebensm.-Unters. -Forsch.*, 1989, **189**, 138-140 (*synth*)
Henle, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1996, **202**, 72-74 (*synth, bibl*)

5-Amino-2(5*H*)-furanone A-254



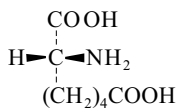
$C_4H_5NO_2$ 99.089
Parent compd. not known.

(±)-*form*
N-*Ac:* [16275-44-8] N-*(2,5-Dihydro-5-oxo-2-furanyl)acetamide, 9CI. 4-Acetamido-4-hydroxy-2-butenoic acid γ-lactone. 4-Acetamido-2-buten-4-olide*
$C_6H_7NO_3$ 141.126
Cryst. (EtOAc/cyclohexane). Mp 116.5-118.5°.
► LU3455000

Yates, S.G. *et al., Tet. Lett.*, 1967, 621 (*spectra*)
Yates, S.G. *et al., Microb. Toxins*, (eds. Kadis, S. *et al*), Academic Press, N.Y., 1971, 198 (*rev*)
Grove, M.D. *et al., J.O.C.*, 1973, **38**, 815 (*bibl*)
Ružic-Toroš, Z. *et al., Acta Cryst. B*, 1982, **38**, 1664 (*cryst struct*)
Valla, A. *et al., Bull. Soc. Chim. Fr.*, 1997, **134**, 601-603 (*synth, pmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 898

2-Aminoheptanedioic acid, 8CI A-255

[3721-85-5]
α-Aminopimelic acid



(*R*)-*form*

$C_7H_{13}NO_4$ 175.184
Isol. from *Ceratonia siliqua* (carob).

(*R*)-*form* [32224-57-0]
D-form
Cryst. (EtOH). Mp 219-220° dec. $[\alpha]_D^{25}$ -21 (c, 0.1 in 5*M* HCl). $[\alpha]_D^{26}$ -45.5 (c, 0.1 in 1*M* HCl). Rare occurrence of a D-aminoacid in higher plants. Forms a monohydrate.

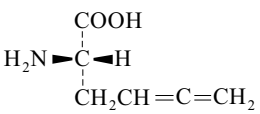
(*S*)-*form* [26630-55-7]
L-form
Microcryst. Mp 204°. $[\alpha]_D^{25}$ +21.6 (c, 0.1 in 5*M* HCl). $[\alpha]_D^{26}$ +45 (c, 0.1 in 1*M* HCl). Forms a monohydrate.

(±)-*form* [627-76-9]
Mp 225°.

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1954, **8**, 1085; 1725 (*isol*)
Wade, R. *et al., J.A.C.S.*, 1957, **79**, 648 (*synth*)
Farkašová, H. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 3117 (*synth*)
Jošt, K. *et al., Coll. Czech. Chem. Comm.*, 1971, **36**, 2795
Lerch, Ev. *et al., Helv. Chim. Acta*, 1974, **57**, 1584 (*ms, nmr*)
Rosowsky, A. *et al., J. Het. Chem.*, 1976, **13**, 729
Rabenstein, D.L. *et al., J. Magn. Reson.*, 1976, **24**, 27 (*nmr*)
Murakami, N. *et al., Phytochemistry*, 1983, **22**, 2735; 1985, **24**, 2291 (*isol, abs config*)
Phan, T. *et al., J.O.C.*, 1994, **59**, 3676 (*synth, pmr, cmr*)

2-Amino-4,5-hexadienoic acid, 9CI A-256

[18751-91-2]



(*S*)-*form*

$C_6H_9NO_2$ 127.143
Sol. H_2O; fairly sol. MeOH; poorly sol.

MeOH, hexane.

(S)-form [22260-39-5]
Mp 174° dec. $[\alpha]_D^{22}$ -52.1 (c, 0.8 in H_2O).

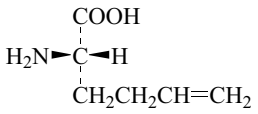
(±)-form [52521-29-6]
Powder.

3,5-Dinitrophenyl:
Yellow needles (EtOH aq.). Mp 177-180°.

Black, D.K. *et al., J.C.S.(C)*, 1968, 283 (*synth*)
Chilton, W.S. *et al., Tet. Lett.*, 1968, 6283 (*isol, struct*)
Baldwin, J.E. *et al., Chem. Comm.*, 1984, 1284 (*synth*)
Hatanaka, S.-I. *et al., Phytochemistry*, 1998, **49**, 573-578 (*isol, bibl*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)

2-Amino-5-hexenoic acid, 9CI A-257

[16258-05-2]



(*S*)-*form*

$C_6H_{11}NO_2$ 129.158
Cryst. (H_2O). Mp 252-255°.

(S)-form [90989-12-1]
Powder. Mp 248° (dec.). $[\alpha]_D^{20}$ +13.6 (c, 0.9 in H_2O).

N-*Ac:*
$C_8H_{13}NO_3$ 171.196
Solid. Mp 114-116°. $[\alpha]_D^{20}$ -42.77 (c, 1.41 in $CHCl_3$) (78% ee).

(±)-form
Cryst. (H_2O). Mp 275-276° (252-255°) dec.

Benzyl ester:
$C_{13}H_{17}NO_2$ 219.283
Oil.

Nitrile: [84673-59-6]
$C_6H_{10}N_2$ 110.158
No phys. props. reported.

N-*Ac:* [142034-37-5]
Solid. Mp 113.5-115°.

N-*Ac, Me ester:*
$C_9H_{15}NO_3$ 185.222
Fine needles (Et_2O/pentane). Mp 59.5-60.5°.

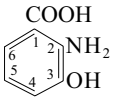
N-tert-*Butyloxycarbonyl:*
$C_{11}H_{19}NO_4$ 229.275
Solid (pentane). Mp 59-62°.

[103067-78-3, 141362-49-4, 142034-37-5]

Drinkwater, D.J. *et al., J.C.S.(C)*, 1971, 1305-1307 (*synth*)
Kennewell, P.D. *et al., J.C.S. Perkin 1*, 1982, 2553-2556 (*synth, ir, pmr*)
Bajgrowicz, J.A. *et al., Tetrahedron*, 1985, **41**, 1833-1843 (*nitrile*)
Baldwin, J.E. *et al., Chem. Comm.*, 1986, 273-275 (*synth*)
Baldwin, J.E. *et al., J. Chem. Res., Synop.*, 1992, 173; *J. Chem. Res., Miniprint*, 1992, 1517-1526 (*synth, S-form, pmr, cmr, ir, ms*)
Hatanaka, S.-I. *et al., Mycoscience*, 1994, **35**, 391 (*isol*)
Biagini, S.C.G. *et al., J.C.S. Perkin 1*, 1998, 2485-2499 (*synth, derivs, ir, pmr, ms*)
Collet, S. *et al., J.C.S. Perkin 1*, 2000, 177-182 (*S-form, synth, pmr, cmr*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)

2-Amino-3-hydroxybenzoic acid A-258

[548-93-6]
3-Hydroxyanthranilic acid



$C_7H_7NO_3$ 153.137
Isol. from *Brassica oleracea* (cauliflower). Leaflets (H_2O). Mp 164°. pK_{a2} 5.19; pK_{a3} 10.12 (20°).

▶ Exp. carcinogen. DG2625000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 206C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1098C; 1123C (*nmr*)
CRC Atlas of Spectral Data and Physical Constants, b842 (*uv, ir*)
Muelle, F. *et al., Planta*, 1961, **57**, 403-477 (*isol*)
Munsche, D. *et al., Phytochemistry*, 1965, **4**, 705-712 (*biosynth*)
Kuznezova, L.E. *et al., Nature (London)*, 1969, **222**, 484-485 (*props*)
Mohr, N. *et al., Annalen*, 1981, 1515-1518 (*isol*)
Okabe, N. *et al., Acta Cryst. C*, 1996, **52**, 2345-2347 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKE750

2-Amino-4-hydroxybenzoic acid A-259

[38160-63-3]
4-Hydroxyanthranilic acid

$C_7H_7NO_3$ 153.137
Needles (H_2O). Mp 148° (dec.).

Hydrochloride:
Needles.

Me ester:
$C_8H_9NO_3$ 167.164
Needles. Mp 132-133°.

Me ether: [4294-95-5] *2-Amino-4-methoxybenzoic acid. 2-Aminoanisic acid. 4-Methoxyanthranilic acid*
$C_8H_9NO_3$ 167.164
Plates (EtOH). Mp 166° (dec.) Mp 190°. pK_{a1} 2.06; pK_{a2} 4.88 (25°, 0.1*M* KCl).

N-*(4-Hydroxycinnamoyl)* (E-)*:4-Hydroxy*-N-*(4-hydroxycinnamoyl)anthranilic acid.* ***Avenanthramide G***
$C_{16}H_{13}NO_5$ 299.282
Stress metab. in oats (*Avena sativa*) induced by Victorin M. Cryst. + ¼ MeOH (MeOH/1% AcOH aq.). Mp 290-291°.

CRC Atlas of Spectral Data and Physical Constants, b843 (*uv*)
Drain, D.G. *et al., J.C.S.*, 1949, 1489 (*synth*)
van der Stelt, C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **72**, 195 (*synth*)
Jilek, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 519 (*synth, uv, ir, pmr, deriv*)
Paulidis, V.H. *et al., Synth. Commun.*, 1994, **24**, 533 (*Me ether, synth, ir, pmr, cmr*)
Miyagawa, H. *et al., Phytochemistry*, 1996, **41**, 1473 (*Avenanthramide G*)
Boojamra, C.G. *et al., J.O.C.*, 1997, **62**, 1240-1256 (*Me ether*)

2-Amino-5-hydroxybenzoic acid A-260

[394-31-0]
5-Hydroxyanthranilic acid

$C_7H_7NO_3$ 153.137
Violet cryst. (H_2O). Mp 252° dec. pK_{a1} 2.72; pK_{a2} 5.37 (25°, 0.1*M* KCl). Log P 0.66 (calc).

N-*(4-Hydroxycinnamoyl)* (E-)*:* [108605-70-5] *5-Hydroxy*-N-*(4-hydroxycinnamoyl)anthranilic acid.* ***Avenanthramide A****. Avenalumin I*
$C_{16}H_{13}NO_5$ 299.282
Isol. from the grains of oats (*Avena sativa*). Pale yellow needles (Me_2CO aq.). Mp 277°. Darkens at 235°. Originally descr. as Avenalumin I, given the wrong struct. λ_{max} 320 (ϵ 15400); 344 (ϵ 13400) (MeOH/HCl) (Derep). λ_{max} 366 (ϵ 16600) (MeOH/NaOH) (Derep). λ_{max} 317 (ϵ 15200); 336 (ϵ 15900) (MeOH) (Derep).

N-*(4-Hydroxycinnamoyl)* (Z-)*:* [116764-20-6]
$C_{16}H_{13}NO_5$ 299.282
Isol. from oats (*Avena sativa*).

N-*(3,4-Dihydroxycinnamoyl)* (E-)*:*N-*(3,4-Dihydroxycinnamoyl)-5-hydroxyanthranilic acid.* ***Avenanthramide C***
$C_{16}H_{13}NO_6$ 315.282
Isol. from oat grains.

N-*(3,4-Dihydroxycinnamoyl)* (Z-)*:* [116764-22-8]
$C_{16}H_{13}NO_6$ 315.282
Isol. from oats (*Avena sativa*).

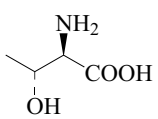
N-*(4-Hydroxy-3-methoxycinnamoyl)* (E-)*:* [108605-69-2] N-*Feruloyl-5-hydroxyanthranilic acid.* ***Avenanthramide B****. Avenanthramide 1*
$C_{17}H_{15}NO_6$ 329.309
Isol. from oat grains. Long pale yellow needles (Me_2CO aq.). Sol. EtOAc, Et_2O, H_2O-Me_2CO; poorly sol. $CHCl_3$, C_6H_6, H_2O. Mp 246°. λ_{max} 228 ; 315 ; 361 ; 392 (MeOH-NAOH) (Berdy).

N-*(4-Hydroxy-3-methoxycinnamoyl)* (Z-)*:* [116764-21-7]
$C_{17}H_{15}NO_6$ 329.309
Isol. from oats (*Avena sativa*).

Collins, F.W. *et al., J. Agric. Food Chem.*, 1989, **37**, 60 (*Avenanthramides*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth, Avenanthramides*)
Dimberg, L.H. *et al., Cereal Chem.*, 1993, **70**, 637-641 (*Avenanthramides*)

2-Amino-3-hydroxybutanoic acid A-261

[36676-50-3]
Threonine, 9CI. Thr



(2*R*,3*R*)-*form*

$C_4H_9NO_3$ 119.12

(2S,3R)-form [72-19-5]
L-Threonine
From wide variety of protein hydroly-

sates. Dietary supplement, nutrient. Cryst. (EtOH aq.). Sol. H_2O (20.5 g/100 ml at 25°). Mp 251-253° dec. $[\alpha]_D^{26}$ -33.9 (H_2O). pK_{a2} 9.62 (NH_2). Isoelectric point 6.16. Sweet taste.

► LD_{50} (rat, ipr) 3098 mg/kg. XO8590000

[2676-21-3, 4385-90-4, 62076-66-8, 71292-23-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 581A; 581B; 581C; 582A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 881C; 882A; 882B (*nmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2238-2258
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679-681 (*cd*)
Aruldhas, G. *et al., Spectrochim. Acta A*, 1967, **23**, 1345-1350 (*pmr*)
Pachler, K.G.R. *et al., Spectrochim. Acta A*, 1968, **24**, 1311-1316 (*pmr*)
Mallikarjunan, M. *et al., Acta Cryst. B*, 1969, **25**, 220-227 (*abs config*)
Maldonado, P. *et al., Bull. Soc. Chim. Fr.*, 1971, 2933-2938 (*synth*)
Swaminathan, P. *et al., Acta Cryst. B*, 1975, **31**, 217-221 (*2S,3S-form, cryst struct*)
Soukup, M. *et al., Helv. Chim. Acta*, 1987, **70**, 232-236 (*2S,3R-form, synth*)
Seebach, D. *et al., Helv. Chim. Acta*, 1987, **70**, 237-261 (*2S,3R-form, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TFU750
Jung, M.E. *et al., Tet. Lett.*, 1989, **30**, 6637-6640 (*synth*)
Shiraiwa, T. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 3296-3299; 1994, **67**, 1899-1903 (*resoln*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1050
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFU750

2-Amino-4-hydroxybutanoic acid A-262

[498-19-1]
Homoserine, 9CI

$C_4H_9NO_3$ 119.12

(*S*)-*form* [672-15-1]
L-form
Present in germinating peas, Jack bean seeds (*Canavalia ensiformis*) and the seedlings of many leguminous plants. Mp 203° dec. $[\alpha]_D^{26}$ -8.8 (c, 5 in H_2O).

O-*Ac:* [7540-67-2] *4-Acetoxy-2-aminobutanoic acid.* O-*Acetylhomoserine. Homoserine acetate*
$C_6H_{11}NO_4$ 161.157
Found in green tissues of pea (*Pisum sativum*). Mp 200°. $[\alpha]_D^{20}$ +4.5 (c, 4 in H_2O).

(±)-*form* [1927-25-9]
Needles (EtOH aq.). Mp 186-188° dec. Readily lactonises.

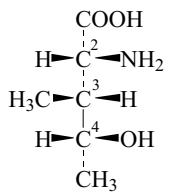
O-*Ac:* [6232-10-6]
Found in *Pisum sativum* (peas). Plates (EtOH). Mp 183-185°.

[53949-21-6, 55596-53-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 580C; 580D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 880B; 880C; 881A (*nmr*)
de Wald, H.A. *et al., J.A.C.S.*, 1959, **81**, 4367 (*acetate*)
Guenther, D. *et al., Chem. Ber.*, 1964, **97**, 159 (*synth*)
Kollonitsch, A. *et al., J.A.C.S.*, 1964, **86**, 1857 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1965, **3**, 2612 (*synth*)
Grobbelaar, N. *et al., Phytochemistry*, 1969, **8**, 553 (*acetate*)
Miyoshi, M. *et al., Chem. Lett.*, 1973, 5 (*abs config*)
Lawrence, J.M. *et al., Phytochemistry*, 1973, **12**, 2207 (*isol*)
Curran, W.V. *et al., Prep. Biochem.*, 1981, **11**, 269 (*resoln*)
Baldwin, J.E. *et al., Tetrahedron*, 1988, **44**, 637 (*synth*)
Seebach, D. *et al., Annalen*, 1989, 1215 (*synth*)
Shiraiwa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2322-2325 (*R-form, S-form, synth*)

2-Amino-4-hydroxy-3-methylpentanoic acid A-263

[50764-07-3]
2-Amino-2,3,5-trideoxy-3-methylpentonic acid. 4-Hydroxyisoleucine


(2*R*,3*R*,4*R*)-*form*

$C_6H_{13}NO_3$ 147.174

(2*R*,3*R*,4*R*)-*form*
D-xylo-*form*
Minor amino acid constit. of *Trigonella foenum-graecum* (fenugreek) seeds. $[\alpha]_D^{20}$ +1 (c, 1 in H_2O).

1,4-Lactone:3-Aminodihydro-4,5-dimethyl-2(3H)-furanone
$C_6H_{11}NO_2$ 129.158
Cryst. (EtOH/petrol) (as hydrochloride). Mp 222° (hydrochloride). $[\alpha]_D^{25}$ +88.7 (c, 1 in MeOH).

1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 140°. $[\alpha]_D^{25}$ +88 (c, 1 in DMSO).

(2*R*,3*R*,4*S*)-*form* *L*-lyxo-*form*

1,4-Lactone:
Cryst. (as hydrochloride). Mp 170-175° (hydrochloride).

1,4-Lactone, N-*Ac:* [60010-74-4] *3-Acetamidodihydro-4,5-dimethyl-2(3H)-furanone.* ***Desmodilactone***
$C_8H_{13}NO_3$ 171.196
Cryst. Mp 84-85°. $[\alpha]_D^{18}$ -16.4 (c, 0.11 in MeOH).

(2*S*,3*R*,4*R*)-*form* *D*-lyxo-*form*

1,4-Lactone:
Needles (EtOH/petrol) (as hydrochloride). Mp 255° (hydrochloride). $[\alpha]_D^{25}$ +24.3 (c, 1 in MeOH).

1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 141°.

(2*S*,3*R*,4*S*)-*form* *L*-ribo-*form*
Major constit. of *Trigonella foenum-graecum* (fenugreek). $[\alpha]_D^{20}$ +31 (c, 1 in H_2O). Stereochem. revised in 1989.

1,4-Lactone:
Needles (EtOH/petrol) (as hydrochloride). Mp 230° (hydrochloride). $[\alpha]_D^{25}$ -15.5 (c, 1 in MeOH).

1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 94°.

(2*S*,3*S*,4*R*)-*form* [21704-86-9] *D*-arabino-*form*
Mp 205-207°. $[\alpha]_D^{27}$ +2.9 (c, 0.1 in H_2O). λ_{max} 197 (ε 250) (H_2O).

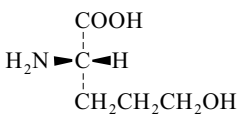
1,4-Lactone: [71392-28-4]

[90693-46-2]
Powder (as hydrochloride). Mp 212-215° (hydrochloride). $[\alpha]_D^{25}$ -14.8 (c, 0.7 in MeOH).

Fowden, L. *et al., Phytochemistry*, 1973, **12**, 1707
Gieren, A. *et al., Annalen*, 1974, 1561-1569 (*synth*)
Hasan, M. *et al., Annalen*, 1976, 781-787 (*lactone, synth, pmr*)
Raffauf, R.F. *et al., J.O.C.*, 1984, **49**, 2714-2718 (*isol, pmr*)
Alcock, N.W. *et al., Phytochemistry*, 1989, **28**, 1835
Yang, J. *et al., Yaoxue Xuebao*, 1993, **28**, 197-201; *CA*, **119**, 156209m (*Desmodilactone*)
Wang, Q. *et al., Eur. J. Org. Chem.*, 2002, 834-839 (*synth, pmr, cmr*)

2-Amino-5-hydroxypentanoic acid, 9CI A-264

2-Amino-5-hydroxyvaleric acid. Pentahomoserine. 5-Hydroxynorvaline


(*S*)-*form*

$C_5H_{11}NO_3$ 133.147

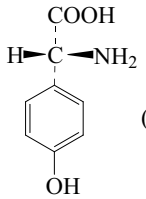
(*S*)-*form*
L-form
Present in jack bean seeds (*Canavalia ensiformis*). Mp 231.5°. $[\alpha]_D^{25}$ +22.6 (c, 2 in 0.5*M* HCl).

(±)-*form*
Needles (MeOH aq.). Sol. H_2O; spar. sol. EtOH, Me_2CO. Mp 223-224°.

Sörensen, S.P.L. *et al., Chem. Zentralbl.*, 1905, **2**, 398
Thompson, J.F. *et al., J. Biol. Chem.*, 1964, **239**, 1122 (*isol, synth*)
Barlos, K. *et al., Chem. Comm.*, 1987, 1583 (*synth, bibl*)
Hill, R.E. *et al., J. Nat. Prod.*, 1993, **56**, 1246 (*isol, ms, synth*)
Garcia, M. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 991-994 (*S-form, synth, pmr, cmr, ms*)

2-Amino-2-(4-hydroxyphenyl)acetic acid A-265

[938-97-6]
α-Amino-4-hydroxybenzeneacetic acid, 9CI. 2-(p-Hydroxyphenyl)glycine, 8CI. ***Oxfenicine, BAN, INN, USAN***



(*R*)-*form*

$C_8H_9NO_3$ 167.164
Never marketed

(*R*)-*form* [22818-40-2]
D-form
Cryst. Mp 240° dec. $[\alpha]_D^{25}$ -158.4 (c, 1 in 1M HCl).

N-tert-*Butyloxycarbonyl:* [27460-85-1]
$C_{13}H_{17}NO_5$ 267.281
Cryst. (EtOAc). Mp 199° (dec. from 160°). $[\alpha]_D^{24}$ -130 (c, 1.08 in EtOH).

(*S*)-*form* [32462-30-9] *UK 25842*

Me ether: [24593-48-4] *2-Amino-2-(4-methoxyphenyl)acetic acid*
$C_9H_{11}NO_3$ 181.191
Mp 260° dec. $[\alpha]_D^{20}$ +139.1 (c, 1 in 1*M* HCl) (96.5% ee).

(±)-*form* [6324-01-2]
Plates (H_2O). Spar. sol. H_2O, insol. Et_2O. Dec. at 200° without melting.

Amide: [72151-95-2]

[73226-87-6]
$C_8H_{10}N_2O_2$ 166.179
Mp 135-136°.

N-*Carbamoyl:* [32507-69-0]

[72500-37-9]
$C_9H_{10}N_2O_4$ 210.189
Isol. from leaves of *Vicia faba*.

Me ether: [19789-59-4]

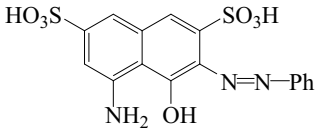
[2540-53-6]
Mp 200° dec.

Meldola, R. *et al., J.C.S.*, 1917, **111**, 551-553 (*synth*)
Lomakina, N.N. *et al., Khim. Prir. Soedin.*, 1969, **5**, 43-46; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 36 (*occur, abs config*)
Larsen, P.O. *et al., Biochim. Biophys. Acta*, 1975, **381**, 397-408 (*isol*)
Smith, G.A. *et al., J.C.S. Perkin 1*, 1975, 2108-2115 (*isol*)
Yamada, S. *et al., Agric. Biol. Chem.*, 1979, **43**, 395-396 (*synth*)
Blackburn, K.J. *et al., Br. J. Pharmacol.*, 1979, **66**, 443P-444P (*pharmacol*)
McGahren, W.J. *et al., J.A.C.S.*, 1980, **102**, 1671-1684 (*isol*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13061
Yoshioka, R. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 649-652 (*resoln, bibl*)
Salituro, G.M. *et al., J.A.C.S.*, 1990, **112**, 760-770 (*N-tert-butyloxycarbonyl*)
Bhattacharya, A. *et al., Synth. Commun.*, 1994, **24**, 2449-2459 (*resoln, pmr, cmr*)
Beller, M. *et al., Chem. Eur. J.*, 1998, **4**, 935-941 (*Me ether, synth, ir, pmr*)

5-Amino-4-hydroxy-3-(phenylazo)-2,7-naphthalenedisulfonic acid, 9CI A-266

[2203-16-9]

[3567-66-6, 112524-65-9, 126212-64-4]
Acid Fuchsin Fast B. Acid Fuchsine D. Azofuchsin. Fast Acid Magenta. C.I. Acid Red 33. C.I. Food Red 12. C.I. 17200. D and C Red No. 33

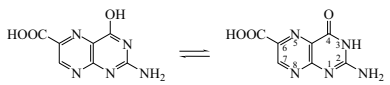


$C_{16}H_{13}N_3O_7S_2$ 423.427
Normally encountered as Na salt, to which the trade names refer. Food dye. Na salt sol. H_2O. Exists in soln. as an equilib. mixt. of azo and hydrazone tautomers with the naphthoquinone hydrazone predominating.

Krasovitskii, B.M. *et al., Ukr. Khim. Zh. (Russ. edn.)*, 1961, **27**, 94-97 (*synth, uv*)
Colour Index, 3rd edn., 1971, **4**, 4105 (*synth*)
Lycka, A. *et al., Dyes Pigm.*, 1987, **8**, 315-325 (*pmr, cmr, N-15 nmr, tautom*)

2-Amino-4-hydroxy-6-pteridinecarboxylic acid A-267

[948-60-7]
2-Amino-1,4-dihydro-4-oxo-6-pteridinecarboxylic acid. 2-Amino-4(3H)-pteridinone-6-carboxylic acid. Pterin-6-carboxylic acid. Ranachrome 5



$C_7H_5N_5O_3$ 207.148
Isol. from various biol. sources incl. fish and soybeans. Cream cryst. Mp 360°.

Me ester: [31010-61-4]
$C_8H_7N_5O_3$ 221.175
Cryst. (DMF). Mp 285° dec.

2-N-*Ac:* [31010-65-8]
$C_9H_7N_5O_4$ 249.185
Cryst. (MeOH). Mp 210°.

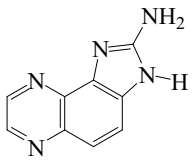
2-N-*Ac, Me ester:* [31010-67-0]
$C_{10}H_9N_5O_4$ 263.212
Mp 283°.

7,8-Dihydro: ***7,8-Dihydropterin-6-carboxylic acid***
$C_7H_8N_5O_3$ 210.172

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 896C (*ir*)
Baugh, C.M. *et al., J.O.C.*, 1964, **29**, 3610 (*synth*)
Pfleiderer, W. *et al., Annalen*, 1970, **741**, 64 (*synth, derivs*)
Iwanami, Y. *et al., Tet. Lett.*, 1972, 3219 (*ms*)
Nair, M.G. *et al., J.O.C.*, 1973, **38**, 2185 (*synth*)
Mengel, R. *et al., Chem. Ber.*, 1978, **111**, 3790 (*synth*)
Kohashi, M. *et al., J. Biochem. (Tokyo)*, 1980, **87**, 1581 (*isol*)
Zeitler, M. *et al., Methods Enzymol.*, 1986, **122**, 273 (*isol*)
Sato, N. *et al., J. Het. Chem.*, 1988, **25**, 1737 (*synth, derivs*)
Suga, T. *et al., J. Nat. Prod.*, 1988, **51**, 713 (*isol*)
Kuse, M. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 1037-1040 (*7,8-dihydro*)

2-Amino-3*H*-imidazo[4,5-*f*]quinoxaline A-268

*3*H-*Imidazo[4,5-f]quinoxalin-2-amine, 9CI*



$C_9H_7N_5$ 185.188

3H*-*form

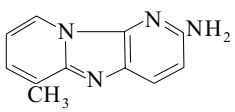
3-Me: [108354-47-8] *3-Methyl-3H-imidazo[4,5-f]quinoxalin-2-amine. 2-Amino-3-methyl-3H-imidazo[4,5-f]quinoxaline. Iqx*
$C_{10}H_9N_5$ 199.215
Mutagen found in cooked beef and pork.

▶ Mutagenic.

Grivas, S. *et al., Acta Chem. Scand.*, 1993, **47**, 521-528 (*synth*)
Solyakov, A. *et al., Food Chem. Toxicol.*, 1999, **32**, 1-11 (*occur*)
Guy, P.A. *et al., J. Chromatogr.*, 2000, **883**, 89-102 (*occur*)

2-Amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole A-269

[67730-11-4]
6-Methyldipyrido[1,2-a:3′,2′-d]imidazol-2-amine, 9CI. Glu-P-1



$C_{11}H_{10}N_4$ 198.227
Powerful mutagen presumed present in cooked foods. Yellow prisms (MeOH/EtOAc).

▶ Highly mutagenic. Possible human carcinogen. Exp. carcinogen. JM5620000

Hydrobromide: [68739-12-8]
Cryst. + $1H_2O$. Mp 290-292°.

Takeda, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2924
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*tox*)
IARC Monog., 1986, **40**, 223; *Suppl.* 7, 64 (*rev, tox*)
Stavric, B. *et al., Food Chem. Toxicol.*, 1994, **32**, 997 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKS250

4-Amino-2-methylenebutanoic acid, 9CI A-270

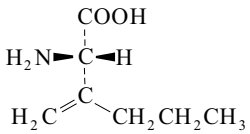
[65370-67-4]
γ-Amino-α-methylenebutyric acid
$H_2C{=}C(COOH)CH_2CH_2NH_2$
$C_5H_9NO_2$ 115.132
Found in *Arachis hypogaea* (peanut). Cryst. (EtOH aq. or EtOH/Me_2CO). Mp 152° dec Mp 170-179° dec.

Fowden, L. *et al., Biochem. J.*, 1953, **55**, 548
Marcus, A. *et al., Arch. Biochem. Biophys.*, 1963, **100**, 80

Hatanaka, S. *et al., Phytochemistry*, 1977, **16**, 1820 (*synth, nmr*)

2-Amino-3-methylenehexanoic acid A-271

3-Methylenenorleucine, 8CI. 2-Amino-3-propyl-3-butenoic acid



$C_7H_{13}NO_2$ 143.185

(*S*)-*form* [29784-96-1]

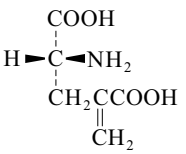
L-form

Found in carpophores of *Amanita vaginata* (grisette). Cryst. (EtOH aq.). Mp 171°. $[\alpha]_D^{20}$ +158 (c, 0.51 in 1*M* HCl). $[\alpha]_D^{20}$ +148 (c, 0.56 in H_2O).

Vervier, R. *et al., Phytochemistry*, 1970, **9**, 2059

2-Amino-4-methylenepentanedioic acid A-272

4-Methyleneglutamic acid. 4-Amino-1-butene-2,4-dicarboxylic acid. 2-Amino-4-methyleneglutaric acid



(*R*)-*form*

$C_6H_9NO_4$ 159.141

(*R*)-*form* [2517-06-8]

D-form

$[\alpha]_D$ -13.7 (5*M* HCl).

(*S*)-*form* [16804-57-2]

L-form

Constit. of peanuts (*Arachis hypogaea*) and other plants, notably tulips and hops. $[\alpha]_D$ +13.7 (5*M* HCl).

γ-Amide:γ-Methyleneglutamine

$C_6H_{10}N_2O_3$ 158.157

Amorph. $[\alpha]_D^{18}$ 0 (H_2O). $[\alpha]_D$ +21 (6*M* HCl).

(±)-*form* [7150-74-5]

Mp 203-210° dec.

Hydrochloride:

Mp 179-180° dec.

N-*Ac:*

$C_8H_{11}NO_5$ 201.179

Mp 88.5°.

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1955, **9**, 553 (*isol*)

Marcus, A. *et al., Arch. Biochem. Biophys.*, 1963, **100**, 80 (*synth*)

Blake, J. *et al., Biochem. J.*, 1964, **92**, 136 (*isol, abs config*)

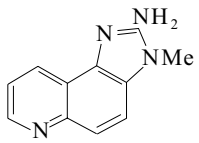
Meier, L.K. *et al., Phytochemistry*, 1979, **18**, 1173 (*isol*)

Moody, C.M. *et al., J.C.S. Perkin 1*, 1997, 3519-3530 (*synth, ir, pmr, cmr*)

2-Amino-3-methylimidazo[4,5-*f*]quinoline A-273

[76180-96-6]

IQ



$C_{11}H_{10}N_4$ 198.227

Isol. from cooked foods, e.g. sardines, beef extract. Cryst. (MeOH aq.). Mp 300°.

▶ Highly mutagenic. Possible human carcinogen. Exp. carcinogen. NJ5910000

Kasai, H. *et al., J.C.S. Perkin 1*, 1981, 2290

Adolfsson, L. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 157 (*synth*)

Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*carcinogenicity*)

IARC Monog., 1986, **40**, 261; *Suppl.* 7, 64 (*rev, tox*)

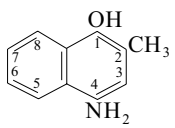
Ronne, E. *et al., Acta Chem. Scand.*, 1994, **48**, 823 (*synth, bibl*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKT600

4-Amino-2-methyl-1-naphthol, 8CI A-274

[83-70-5]

4-Amino-2-methyl-1-naphthalenol, 9CI. Vitamin K_5



$C_{11}H_{11}NO$ 173.214

Vitamin. Used as a food preservative. Log P 1.92 (calc).

▶ LD_{50} (mus, ipr) 250 mg/kg. QL3350000

Hydrochloride: [130-24-5] *Synkamine. Kayvisyn*

Needles (HCl aq.). Mp 280-282° dec. (darkens at 260°).

N-*Ac:* [523-68-2] *4-Acetamido-2-methyl-1-naphthol.* ***Acetyl-Vitamin K_5***. *Kavitrat. K-Vitrat*

$C_{13}H_{13}NO_2$ 215.251

Prothrombogenic vitamin. Needles. Mp 208-210°. Log P 2.17 (calc).

Sah, P.P.T. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1941, **60**, 373 (*synth*)

Veldstra, H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1943, **62**, 75 (*synth*)

Gaultier, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1967, **264**, 766 (*cryst struct*)

Madelmont, J.C. *et al., J. Labelled Compd. Radiopharm.*, 1978, **14**, 281 (*synth*)

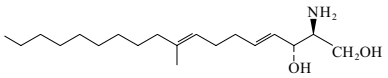
Prenzel, U. *et al., J. Chromatogr.*, 1982, **242**, 9 (*hplc*)

Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 7909

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKX500

2-Amino-9-methyl-4,8-octadecadiene-1,3-diol A-275

9-Methyl-4,8-sphingadienine



$C_{19}H_{37}NO_2$ 311.507

(2*S*,3*R*,4*E*,8*E*)-*form*

N-*Hexadecanoyl, 1*-O-α-D-*glucopyranoside:* ***Thraustochytroside B***

$C_{41}H_{77}NO_8$ 712.061

Amorph. solid.

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-β-D-*glucopyranoside:* [88642-46-0] ***Cerebroside B***

$C_{41}H_{77}NO_9$ 728.061

From *Clitocybe* spp.. Mp 180-190°. $[\alpha]_D^{20}$ +5.2 (c, 1 in MeOH). $[\alpha]_D^{19}$ -7.4 (c, 0.3 in $CHCl_3$).

N-*(2*R*-Hydroxy-3-hexadecenoyl), 1*-O-β-D-*glucopyranoside:* [115681-40-8] ***Cerebroside A***

$C_{41}H_{75}NO_9$ 726.045

Cryst. Sol. MeOH. Mp 170-178°. $[\alpha]_D^{20}$ -6.7 (c, 1 in MeOH).

N-*(2*R*-Hydroxyoctadecanoyl):* ***Lactariamide B***

$C_{37}H_{71}NO_4$ 593.972

Isol. from the fungus *Lactarius volemus* (tawny milkcap mushroom). Amorph. powder. $[\alpha]_D^{20}$ +8.4 (c, 0.39 in MeOH). Stereochem. not confirmed.

N-*(2*R*-Hydroxyoctadecanoyl), 1*-O-β-D-*glucopyranoside:* [113773-89-0] ***Cerebroside D***

$C_{43}H_{81}NO_9$ 756.114

Cryst. Sol. MeOH. Mp 178-189°. $[\alpha]_D^{20}$ +4.9 (c, 1 in MeOH).

N-*(2*R*-Hydroxy-3-octadecenoyl), 1*-O-β-D-*glucopyranoside:* [98677-33-9] ***Cerebroside C***

$C_{43}H_{79}NO_9$ 754.098

Cryst. Mp 159-169°. $[\alpha]_D^{20}$ -6.2 (c, 1 in MeOH).

N-*(2*R*-Hydroxytetradecanoyl):*

$C_{33}H_{63}NO_4$ 537.865

Amorph. powder. $[\alpha]_D^{20}$ +6.3 (c, 0.2 in $CHCl_3$).

N-*(2*R*-Hydroxypentadecanoyl):*

$C_{34}H_{65}NO_4$ 551.892

Amorph. powder. $[\alpha]_D^{21}$ +7 (c, 0.1 in $CHCl_3$).

N-*Hexadecanoyl:*

$C_{35}H_{67}NO_3$ 549.919

Amorph. powder. $[\alpha]_D^{21}$ -11.6 (c, 0.09 in $CHCl_3$).

N-*(2*R*-Hydroxyhexadecanoyl):*

$C_{35}H_{67}NO_4$ 565.919

Isol. from the mushroom *Lepista nuda* (wood blewit). Amorph. powder. $[\alpha]_D^{19}$ +7.5 (c, 0.1 in $CHCl_3$).

N-*(2*R*-Hydroxyheptadecanoyl), 1*-O-β-D-*glucopyranoside:* [120029-71-2]

$C_{42}H_{79}NO_9$ 742.087

Amorph. powder. Mp 154-156°. $[\alpha]_D^{26}$ +4.9 (c, 0.4 in MeOH).

N-*(9Z,12Z-Octadecadienoyl):*

$C_{37}H_{67}NO_3$ 573.941

Amorph. powder. $[\alpha]_D^{30}$ -13.3 (c, 0.08 in

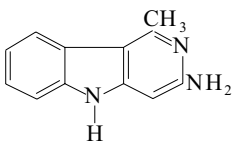
$CHCl_3$).

Kawai, G. *et al., Biochim. Biophys. Acta*, 1982, **719**, 612; 1983, **754**, 243 (*isol*)
Kawai, G. *et al., Agric. Biol. Chem.*, 1985, **49**, 2137 (*isol, pmr*)
Kawai, G. *et al., J. Lipid Res.*, 1985, **26**, 338 (*struct*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 2369; 2379 (*synth*)
Kawai, G. *et al., J. Biol. Chem.*, 1986, **261**, 779-784 (*isol*)
Fogeldal, M. *et al., CA*, 1987, **160**, 29746 (*isol*)
Sitrin, R.D. *et al., J. Antibiot.*, 1988, **41**, 469 (*isol, pmr, cmr, ms, struct*)
Striegler, S. *et al., Monatsh. Chem.*, 1996, **127**, 755-761 (*activity*)
Koga, Y. *et al., J. Biol. Chem.*, 1998, **273**, 31985-31991 (*activity, pmr, cmr*)
Jenkins, K.M. *et al., Tet. Lett.*, 1999, **40**, 7637-7640 (*Thraustochytroside B*)
Wang, X.-Z. *et al., J.O.C.*, 2000, **65**, 8146-8151 (*synth*)
Yue, J.-M. *et al., J. Nat. Prod.*, 2001, **64**, 1246-1248 (*Lactariamide B*)
Gao, J.M. *et al., Lipids*, 2001, **36**, 521-527 (*Polyporus ceramide*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2002, **50**, 681-684 (*hexadecanoyl, 2-hydroxyacyl, octadecadienoyl*)

3-Amino-1-methyl-5*H*-pyrido[4,3-*b*]indole A-276

[62450-07-1]

[72254-58-1]
*1-Methyl-5*H*-pyrido[3,4-*b*]indol-1-amine, 9CI. Trp-P2*



$C_{12}H_{11}N_3$ 197.239
Isol. from protein pyrolysates contg. tryptophan. Mutagenic potential food contaminant. Prisms (as acetate salt). Mp 242-247° (acetate salt).

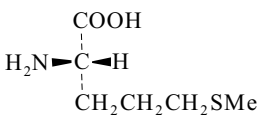
▶ Possible human carcinogen. Exp. carcinogen and mutagen. UU9354000

[75074-77-0]

IARC Monog., 1983, **31**, 255; *Suppl*. 7, 73 (*rev, tox*)
Akimoto, H. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 123 (*synth, bibl, ir, uv*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALD500; ALE750

2-Amino-5-(methylthio)pentanoic acid A-277

[5632-95-1]
5-(Methylthio)norvaline, 9CI, 8CI. Homomethionine



(*S*)-*form*

$C_6H_{13}NO_2S$ 163.24

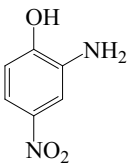
(*S*)-*form* [25148-30-5]
L-form
Isol. from cabbage and horseradish. Plates (EtOH aq.). Mp 235° Mp 247-248° dec. $[\alpha]_D^{25.5}$ +21 (c, 0.3 in 6*M* HCl).

(±)-*form* [6094-76-4]
Hexagonal plates (EtOH). Mp 247-248°.

Kjaer, A. *et al., Acta Chem. Scand.*, 1955, **9**, 721 (*synth*)
Sugii, M. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1115 (*isol*)
Suketa, Y. *et al., Chem. Pharm. Bull.*, 1970, **18**, 249 (*isol, ord, biosynth*)
Vriesema, B.K. *et al., Tet. Lett.*, 1986, **27**, 2045 (*resoln, cd, abs config*)

2-Amino-4-nitrophenol, 9CI A-278

[99-57-0]



$C_6H_6N_2O_3$ 154.125
Orange prisms. Mp 142-143° Mp 176-177° Mp 195-198°.

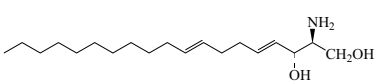
▶ Eye irritant. LD_{50} (mus, orl) 850 mg/kg. Exp. neoplastic agent. SJ6300000

Propyl ether: [553-79-7] *5-Nitro-2-propoxyaniline. P 4000*
$C_9H_{12}N_2O_3$ 196.205
Once proposed for use as an artificial sweetener but now prohibited from use in food.

Propyl ether, N-*Ac:* [553-20-8] N-*(5-Nitro-2-propoxyphenyl)acetamide, 9CI. 5′-Nitro-2′-propoxyacetanilide, 8CI. Acetylaminonitropropoxybenzene.* ***Falimint***
$C_{11}H_{14}N_2O_4$ 238.243
Sweetening agent. Cryst. Mp 102-103° Mp 202-203°.

U.K. Pat., 1948, 597 835; *CA*, **42**, 5050i (*synth, Falimint*)
Hannig, E. *et al., Arzneim.-Forsch.*, 1953, **3**, 310 (*pharmacol, Falimint*)
Becher, M. *et al., Pharmazie*, 1989, **44**, 56; 1990, **45**, 440; 534 (*metab, Falimint*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2079 (*propyl ether*)

2-Amino-4,8-nonadecadiene-1,3-diol A-279



$C_{19}H_{37}NO_2$ 311.507

(2*S*,3*R*,4*E*,8*E*)-*form*

N-*(2*R*-Hydroxytetradecanoyl), 1*-O-*β*-*D*-glucopyranoside:* [189272-90-0] ***Lucyobroside***
$C_{39}H_{73}NO_9$ 700.007
Constit. of *Luffa cylindrica* (smooth luffa). Mp 140-142°.

Fang, Z. *et al., CA*, 1997, **126**, 303677n (*isol, struct, Lucyobroside*)

2-Amino-11-nonadecene-1,3,4-triol A-280

$H_3C(CH_2)_6CH=CH(CH_2)_6CH(OH)CH(OH)CH(NH_2)-)CH_2OH$

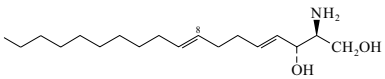
$C_{19}H_{39}NO_3$ 329.522

N-*(2-Hydroxyeicosanoyl), 1*-O-*β*-*D*-*glucopyranoside:* [230295-19-9] ***Culinariside***
$C_{45}H_{87}NO_{10}$ 802.183
Constit. of the seeds of *Lens culinaris* (lentil). Stereochem. not determined.

Hong, Y. *et al., J. Chin. Pharm. Sci.*, 1999, **8**, 8-10

2-Amino-4,8-octadecadiene-1,3-diol A-281

4,8-Sphingadiene. 4,8-Octadecasphingadiene



(2*S*,3*R*,4*E*,8*E*)-*form*

$C_{18}H_{35}NO_2$ 297.48

(2*S*,3*R*,4*E*,8*E*)-*form*

N-*Hexadecanoyl:* [141980-53-2]
$C_{34}H_{65}NO_3$ 535.892
Isol. from *Vigna angularis* (azuki bean). Solid. Mp 82-83°. $[\alpha]_D^{25}$ -8 (c, 0.5 in $CHCl_3$).

N-*(2*R*-Hydroxytetradecanoyl), 1*-O-*β*-*D*-*glucopyranoside:AS 1-1*
$C_{38}H_{71}NO_9$ 685.98
Isol. from garlic bulbs. Amorph. powder. Mp 197-200°. $[\alpha]_D^{28}$ +5.2 (c, 0.25 in propanol).

N-*(2*R*-Hydroxypentadecanoyl), 1*-O-*β*-*D*-*glucopyranoside:AS 1-2*
$C_{39}H_{73}NO_9$ 700.007
Isol. from garlic bulbs. Amorph. powder. Mp 195-200°. $[\alpha]_D^{28}$ +8.8 (c, 0.13 in 1-propanol).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β*-*D*-*glucopyranoside:* [114297-20-0] ***Soyacerebroside I**. AS 1-4*
$C_{40}H_{75}NO_9$ 714.034
Isol. from *Tetragonia tetragonoides* (New Zealand spinach), *Glycine max* (soybean) and bulbs of *Allium sativum* var. *sativum* (garlic). Hygroscopic granules or amorph. solid. Mp 184-186° Mp 193-197°. $[\alpha]_D^{24}$ +10.5 (c, 0.30 in MeOH/$CHCl_3$, 3:2).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*sulfate:*
$C_{34}H_{65}NO_7S$ 631.956
$[\alpha]_D$ +17 (c, 0.06 in MeOH).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β*-*D*-*glucopyranoside:* ***Typhoniside A***
$C_{46}H_{87}NO_9$ 798.195
Amorph. powder. Mp 172-174°.

N-*Me,* N-*hexadecanoyl:*
$C_{35}H_{67}NO_3$ 549.919
Amorph. powder. Mp 86°. $[\alpha]_D^{27}$ +20.1 (c, 0.01 in $CHCl_3$).

N-*Me,* N-*octadecanoyl, 1*-O-*sulfate:* ***Hariamide***
$C_{37}H_{71}NO_6S$ 658.037
Cryst. Mp 165°. $[\alpha]_D^{27}$ +11.3 (c, 0.01 in

MeOH).

(2*S*,3*R*,4*E*,8*Z*)-*form*

N-*Hexadecanoyl, 1*-O-*β*-D-*glucopyranoside:* [127842-89-1]
$C_{40}H_{75}NO_8$ 698.034
Constit. of *Lycium chinense* (Chinese boxthorn). Amorph. powder. $[\alpha]_D^{25}$ +1.2 (c, 0.1 in MeOH).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β*-D-*glucopyranoside:* [115074-93-6] ***Soyacerebroside II***. *AS 1-3*
$C_{40}H_{75}NO_9$ 714.034
Isol. from *Tetragonia tetragonoides* (New Zealand spinach), *Glycine max* (soybean) and bulbs of *Allium sativum* var. *sativum* (garlic). Hygroscopic granules or amorph. solid. Mp 192-194° (183°). $[\alpha]_D^{24}$ +13.4 (c, 0.43 in MeOH/$CHCl_3$ 3:2) (+4.6).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Stenochlaena cerebroside***
$C_{48}H_{91}NO_9$ 826.248
$[\alpha]_D^{25}$ +7.9 (c, 0.09 in MeOH).

N-*(15*E*-Tetracosenoyl), 1*-O-*β*-D-*glucopyranoside:* [204126-76-1] *CE 1-2*
$C_{48}H_{89}NO_8$ 808.233
Amorph. powder. Mp 136-137°. $[\alpha]_D$ -1.9 (c, 0.33 in 1-propanol).

(2ξ,3ξ,4*E*,8*E*)-*form*

N-*Hexadecanoyl:* [124787-56-0] ***Sinumeramide***
$C_{34}H_{65}NO_3$ 535.892
Cryst. ($CHCl_3$/MeOH). Mp 98-100°. $[\alpha]_D^{25}$ +2.8 (c, 0.5 in $CHCl_3$).

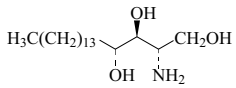
N-*Nonadecanoyl:* ***Humesamide***
$C_{37}H_{71}NO_3$ 577.973
Amorph. solid. Mp 79-80°.

[127912-01-0]

Mori, K. *et al., Annalen*, 1988, 807 (*abs config, ir, pmr, cmr, synth, bibl, Soyacerebroside*)
Kodato, S. *et al., Tetrahedron*, 1989, **45**, 7263 (*Sinumeramide*)
Su, J. *et al., CA*, 1990, **112**, 52558 (*isol, Sinumeramide*)
Shibuya, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2933 (*Soyacerebrosides*)
Shibuya, H. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1534 (*synth*)
Shin, J. *et al., J. Nat. Prod.*, 1995, **58**, 948-953 (*N-hexadecanoyl*)
Kim, S.Y. *et al., J. Nat. Prod.*, 1997, **60**, 274-276
Babu, U.V. *et al., J. Nat. Prod.*, 1997, **60**, 1307-1309 (*Hariamide*)
Ojika, M. *et al., Tet. Lett.*, 1997, **38**, 4235-4238 (*N-hydroxyhexadecanoyl 1-sulfate*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1153-1156 (*AS compounds*)
Yamada, K. *et al., Eur. J. Org. Chem.*, 1998, 371-378 (*CE 1-2*)
Liu, H. *et al., Phytochemistry*, 1998, **49**, 2403-2408 (*Stenochlaena cerebroside*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 457-460 (*N-hexadecanoyl*)
Wang, M.Y. *et al., Chin. Chem. Lett.*, 2000, **11**, 783-784 (*Hamesamide*)
Wang, X.-Z. *et al., J.O.C.*, 2000, **65**, 8146-8151 (*synth*)
Murakami, T. *et al., Tetrahedron*, 2000, **56**, 533-545 (*synth*)
Chen, X. *et al., Tet. Lett.*, 2002, **43**, 3529-3532 (*Typhoniside A*)

2-Amino-1,3,4-octadecanetriol, 8CI A-282

C_{18}-Phytosphingosine. 4-Hydroxysphinganine



(2*S*,3*S*,4*R*)-*form*

$C_{18}H_{39}NO_3$ 317.511
Amorph. powder. $[\alpha]_D$ +9.4 (c, 0.21 in Py).

(2*S*,3*S*,4*R*)-*form* [554-62-1]
D-ribo-*form*
Mp 103° (95-97°). $[\alpha]_D^{20}$ +10.3 (Py) (+8.5).

N-*Hexadexanoyl:* ***Armillaramide***
$C_{34}H_{69}NO_4$ 555.923
Isol. from *Armillaria mellea* (honey mushroom). Amorph. powder. Mp 113-117°. $[\alpha]_D^{26}$ +14.3 (c, 0.21 in Py).

N-*(2*R*-Hydroxydocosanoyl):*
$C_{40}H_{81}NO_5$ 656.084
Isol. from the mushroom *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{22}$ +12.9 (c, 0.1 in Py).

N-*(2*R*-Hydroxytricosanoyl):*
$C_{41}H_{83}NO_5$ 670.11
Isol. from the mushroom *Grifola frondosa* (maitake) and the truffle *Tuber indicum*. Amorph. powder. $[\alpha]_D^{20}$ +14.9 (c, 0.07 in Py).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-*glucopyranoside:* [193412-78-1] ***Regulosside C***
$C_{48}H_{95}NO_{10}$ 846.279

N-*(2*R*-Hydroxypentacosanoyl):*
$C_{43}H_{87}NO_5$ 698.164
Isol. from the mushroom *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{21}$ +13.8 (c, 0.1 in Py).

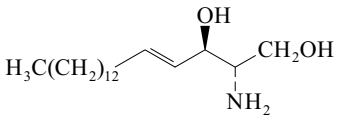
N-*(2*R*-Hydroxyhexacosanoyl):*
$C_{44}H_{89}NO_5$ 712.191
Isol. from the mushroom *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{22}$ +11.1 (c, 0.1 in Py).

(2ξ,3ξ,4ξ)-*form*

N-*(2ξ,3ξ-Dihydroxy-?-tetracosenoyl):* [260545-65-1] ***Tuberceramide***
$C_{42}H_{83}NO_6$ 698.121
Constit. of the seeds of *Allium tuberosum* (Chinese chives). Posn. of double bond not determined.

Prostenik, M. *et al., Tetrahedron*, 1965, **21**, 651
Gigg, J. *et al., J.C.S.(C)*, 1966, 1872; 1876
Schmidt, R.R. *et al., Carbohydr. Res.*, 1988, **174**, 169 (*synth, stereoisomers*)
Lin, G. *et al., Tetrahedron*, 1996, **52**, 2187-2192 (*synth*)
Zou, Z.-M. *et al., J. Asian Nat. Prod. Res.*, 1999, **2**, 55-61 (*Tuberceramide*)
Gao, J.M. *et al., Chin. Chem. Lett.*, 2001, **12**, 139-140 (*Armillaramide*)

2-Amino-4-octadecene-1,3-diol, 9CI A-283



(2*S*,3*R*,4*E*)-*form*

$C_{18}H_{37}NO_2$ 299.496Many syntheses reported of various stereoisomers. See Miyata *et al* (1996) for a listing of recent ones.

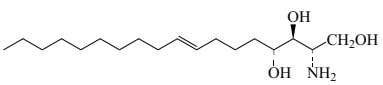
(2*S*,3*R*,4*E*)-*form* [123-78-4]
D-erythro-trans-*form*. *Sphing-4-enine*. *C_{18}-Sphingosine*
Cryst. (Et_2O). Mp 80-84° (79-81°).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β*-D-*glucopyranoside: AS 1-5*
$C_{40}H_{77}NO_9$ 716.05
Constit. of *Allium sativum* (garlic) bulbs. Amorph. powder. Mp 205-210°. $[\alpha]_D^{28}$ +8.3 (c, 0.15 in propanol).

Inagaki, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1153-1156 (*AS 1-5*)

2-Amino-8-octadecene-1,3,4-triol, 9CI A-284

[81520-97-0]



(2*S*,3*S*,4*R*,8*E*)-*form*

$C_{18}H_{37}NO_3$ 315.495

(2*S*,3*S*,4*R*,8*E*)-*form* [3687-54-5]
D-ribo-trans-*form*. *Dehydrophytosphingosine*
Present in soybean phospholipids. Cryst. (Et_2O). Mp 92-94°. $[\alpha]_D^{25}$ +8.5 (c, 1.2 in EtOH).

N-*Benzoyl:*
Cryst. (Me_2CO). Mp 128-129°.

N-*Benzoyl, tri-Ac:*
Cryst. (hexane). Mp 77-78°. $[\alpha]_D^{25}$ +10 (c, 0.76 in $CHCl_3$).

N-*(2-Hydroxyhexadecanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Araliacerebroside***
$C_{40}H_{77}NO_{10}$ 732.049
Constit. of the root bark of *Aralia elata* (Japanese angelica tree). Amorph. powder. Mp 215-216°. $[\alpha]_D^{20}$ +14.6 (c, 0.53 in MeOH).

(2*S*,3*S*,4*R*,8*Z*)-*form*

N-*Hexadecanoyl, 1*-O-*β*-D-*glucopyranoside:* ***Pokeweedcerebroside 1***
$C_{40}H_{77}NO_9$ 716.05

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Pokeweedcerebroside 2***
$C_{40}H_{77}NO_{10}$ 732.049

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Pokeweedcerebroside 3***
$C_{46}H_{89}NO_{10}$ 816.21

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Pokeweedcerebroside 4***
$C_{47}H_{91}NO_{10}$ 830.237

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-

glucopyranoside: ***Pokeweedcerebroside 5***
$C_{48}H_{93}NO_{10}$ 844.263

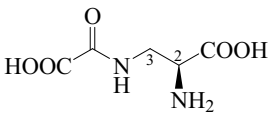
N-*(2*R*-Hydroxypentacosanoyl), 1*-O-*β*-D-*glucopyranoside:* ***Pokeweedcerebroside 6***
$C_{49}H_{95}NO_{10}$ 858.29

[25277-37-6, 51153-53-8]

Prostenik, M. *et al., Naturwissenschaften*, 1961, **48**, 500 (*struct*)
Carter, H.E. *et al., Biochemistry*, 1963, **2**, 389 (*isol, struct*)
Kang, S.S. *et al., J. Nat. Prod.*, 1999, **62**, 1059-1060 (*Araliacerebroside*)
Kang, S.S. *et al., Chem. Pharm. Bull.*, 2001, **49**, 321-323 (*Pokeweedcerebrosides*)

2-Amino-3-(oxalylamino)propanoic acid A-285

[7554-90-7]
*3-[(Carboxycarbonyl)amino]alanine, 9CI. (2-Amino-2-carboxyethyl)oxamic acid, 8CI. 2,3-Diamino-3-*N*-oxalylpropanoic acid.* ***Dencichin***



$C_5H_8N_2O_5$ 176.129

(*S*)-*form* [5302-45-4]
L-form
Isol. from *Panax notoginseng* (sanchi). Cryst. (H_2O) (dimorph.). Mp 206° dec. $[\alpha]_D^{27}$ -36.9 (c, 0.66 in 4*N* HCl).
► Neurotoxin. RO4555000

[58086-31-0, 61238-52-6, 120963-05-5]

Rao, S.L.R. *et al., Biochemistry*, 1964, **3**, 432 (*isol, synth*)
Murti, V.V.S. *et al., Phytochemistry*, 1964, **3**, 73 (*ir*)
Bell, E.A. *et al., Phytochemistry*, 1966, **5**, 1211 (*occur*)
Rao, S.L.N. *et al., Biochemistry*, 1975, **14**, 5218 (*synth*)
O'Brien, P. *et al., Phytochemistry*, 1982, **21**, 2001 (*dimorphism, ir, bibl*)
Rutter, J. *et al., New Sci.*, 23rd Aug., 1984, 23 (*rev*)
Euerby, M.R. *et al., J. Chromatogr.*, 1989, **466**, 407 (*hplc, resoln*)
Bridges, R.J. *et al., J. Neurosci.*, 1989, **9**, 2073 (*props*)
Davis, A.J. *et al., J. Inorg. Biochem.*, 1990, **39**, 209 (*isol*)
Lambein, F. *et al., Phytochemistry*, 1990, **29**, 3793 (*biosynth, bibl*)
Davis, A.J. *et al., Phytochemistry*, 1991, **30**, 3635 (*cryst struct*)

3-Amino-2-(oxalylamino)propanoic acid A-286

[7554-89-4]
*3-Amino-*N*-(carboxycarbonyl)alanine, 9CI. (2-Amino-1-carboxyethyl)oxamic acid, 8CI. 2,3-Diamino-2-*N*-oxalylpropanoic acid*

$C_5H_8N_2O_5$ 176.129

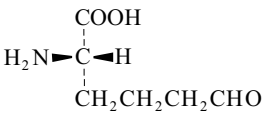
(*S*)-*form* [61277-72-3]
L-form
Present in seeds of *Lathyrus sativus* (chickling pea). Cryst. + ½H_2O. Mp 170-172°. $[\alpha]_D^{21}$ +14.7 (c, 2 in 1*M* KOH).

[61238-53-7]

Bell, E.A. *et al., Phytochemistry*, 1966, **5**, 1211 (*isol*)
Roy, D.N. *et al., Curr. Sci.*, 1968, **37**, 395 (*isol*)
Wu, G. *et al., Phytochemistry*, 1976, **15**, 1257 (*synth*)

2-Amino-6-oxohexanoic acid A-287

[1962-83-0]
6-Oxonorleucine, 9CI. 5-Formylnorvaline, 8CI. α-Aminoadipic semialdehyde. 2-Aminoadipaldehydic acid. Allysine



(*S*)-*form*

$C_6H_{11}NO_3$ 145.158
In equil. with the anhydro-form 2,3,4,5-Tetrahydro-2-pyridinecarboxylic acid.Does not show typical aldehyde reactions.

(*S*)-*form*
L-form
Found in collagen, elastin and heart muscle. $[\alpha]_D^{25}$ -5.1 (c, 3 in H_2O) (ca. 90% pure).

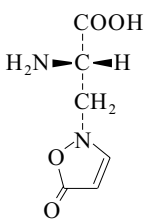
(±)-*form* Obt. only in soln..
2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 116-117°. Formed only slowly (5 days at 5°).

N-*Ac:*
$C_8H_{13}NO_4$ 187.195
Mp 95-96°.

Aspen, A.J. *et al., Biochemistry*, 1962, **1**, 600
Basso, L.V. *et al., J. Biol. Chem.*, 1962, **237**, 2239
Rodwell, V.W. *et al., Methods Enzymol., Part B*, 1971, **17**, 188 (*synth, bibl*)

α-Amino-5-oxo-2(5*H*)-isoxazolepropanoic acid, 9CI A-288

α-Amino-5-oxo-3-oxazoline-2-propionic acid, 8CI. β-(Isoxazolin-5-on-2-yl)alanine. 2-Alanyl-3-isoxazolin-5-one



$C_6H_8N_2O_4$ 172.14

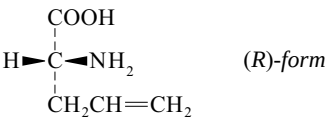
(*S*)-*form* [59476-61-8]
L-form
Amino acid from the roots of pea seedlings (*Pisum* spp.). Fairly sol. H_2O. Mp 203-205° dec. $[\alpha]_D^{20}$ -62 (c, 1.4 in H_2O). Base-labile λ_{max} 265 (ε 12300) (pH 2 buffer) (Berdy). λ_{max} 267 (ε 13190) (pH 10 buffer) (Berdy).

N-*(4-Amino-4-carboxybutanoyl):* [142115-24-0] *γ-Glutamyl-β-(isoxazolin-5-on-2-yl)alanine*
$C_{11}H_{15}N_3O_7$ 301.255
Constit. of *Lens culinaris* (lentil). Cryst. (Me_2CO aq.).

Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1969, **37**, 375 (*isol*)
Lambein, F. *et al., Heterocycles*, 1976, **4**, 567 (*isol*)
Baldwin, J.E. *et al., Tet. Lett.*, 1985, **26**, 5931 (*synth, pmr, ir*)
Lambein, F. *et al., Phytochemistry*, 1992, **31**, 887 (*glutamyl deriv*)
Kuo, Y.-H *et al., Phytochemistry*, 1998, **49**, 43-48 (*occur, metab, biosynth*)

2-Amino-4-pentenoic acid, 9CI A-289

[1069-48-3]
Allylglycine. 2-(2-Propenyl)glycine



(*R*)-*form*

$C_5H_9NO_2$ 115.132

(*R*)-*form* [54594-06-8]
D-form
Cryst. (EtOH aq.). Mp 240-241° dec. $[\alpha]_D^{24}$ +37.8 (c, 4 in H_2O). $[\alpha]_D^{24}$ +5.7 (c, 2 in 6*M* HCl).

N-*Ac:* [121786-40-1]
$C_7H_{11}NO_3$ 157.169
Cryst. (Me_2CO/petrol). $[\alpha]_D^{22}$ -42 (c, 4 in H_2O).

(*S*)-*form* [16338-48-0] *L-form*
Cryst. (EtOH aq.). Mp 275-280° (241-243°) dec. $[\alpha]_D^{24}$ -37.1 (c, 4 in H_2O). $[\alpha]_D^{24}$ -5.7 (c, 2 in 6*M* HCl).

N-tert-*Butyloxycarbonyl:* [90600-20-7]
$C_{10}H_{17}NO_4$ 215.249
Viscous oil. $[\alpha]_D^{23}$ +11.9 (c, 1.4 in MeOH). $[\alpha]_D^{23}$ -3.9 (c, 1 in CH_2Cl_2).

(±)-*form* [7685-44-1]
Cryst. (MeOH). Mp 243-245° dec.

Me ester: [70837-19-3]
$C_6H_{11}NO_2$ 129.158
Liq. $Bp_{1.1}$ 69-70°.

Et ester: [89077-49-6]

[68843-72-1]
$C_7H_{13}NO_2$ 143.185
Liq. Bp_{15} 75-78°.

N-*Ac:* [50299-14-4]
Mp 114°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 574D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 874C; 875A (*nmr*)
Black, S. *et al., J. Biol. Chem.*, 1955, **213**, 39-50 (*synth, resoln*)
Japan. Pat., 1977, 77 54 085; *CA*, **87**, 150205 (*isol*)
Yaozhong, J. *et al., Synth. Commun.*, 1989, **19**, 881-888 (*synth, ir, pmr*)
Sasaki, N.A. *et al., Tet. Lett.*, 1989, **30**, 1943-1946 (*synth*)
Mooiweer, H.H. *et al., Tetrahedron*, 1989, **45**, 4627-4636 (*synth, ir, pmr*)
Broxterman, Q.B. *et al., J.O.C.*, 1992, **57**, 6286-6294 (*resoln, pmr, cmr*)
Dragovich, P.S. *et al., J. Med. Chem.*, 1996, **39**, 1872-1884 (*Me ester, synth, ir, pmr*)
Org. Synth., 1999, **76**, 57-76 (*synth, ir, pmr, cmr*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)

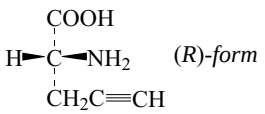
(5-Aminopentyl)guanidine, 9CI A-290

[18431-52-2]
1-Amino-5-guanidinopentane. ***Homoagmatine***
$HN{=}C(NH_2)NH(CH_2)_4CH_2NH_2$
$C_6H_{16}N_4$ 144.219
Constit. of *Lathyrus sativus* (chickling pea).

Ramakrishna, S. *et al., Phytochemistry*, 1973, **12**, 2691 (*isol, synth, ir*)

2-Amino-4-pentynoic acid, 9CI A-291

Propargylglycine



(*R*)-*form*

$C_5H_7NO_2$ 113.116
Sol. H_2O; poorly sol. butanol, hexane.

(*R*)-*form* [23235-03-2]
Mp 221° dec. $[\alpha]_D^{25}$ +25.7 (c, 0.8 in H_2O).

(*S*)-*form* [23235-01-0]
L-*form*
Mp 230° (dec. from 210°) (248-249° dec.). $[\alpha]_D^{20}$ -35 (c, 1 in H_2O).

N-*Phthaloyl, dicyclohexylamine salt:*
Mp 205°. $[\alpha]_D^{20}$ -29.4 (c, 1 in EtOH).

N-*Phthaloyl, Me ester:*
Cryst. (petrol). Mp 112°. $[\alpha]_D^{20}$ -63.2 (c, 1 in EtOH).

(±)-*form* [50428-03-0]
Mp 235-237° dec.

Hydrochloride: [61172-65-4]
Cryst. (2-propanol/diisopropyl ether). Mp 195°.

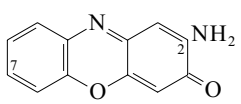
N-*Phthaloyl,* tert-*butyl ester:*
Mp 97°.

[198774-27-5]

Scannell, J.P. *et al., J. Antibiot.*, 1971, **24**, 239-244 (*isol, synth*)
Tun-kyi, A. *et al., Helv. Chim. Acta*, 1976, **59**, 2181-2183 (*synth*)
Fauchére, J.-L. *et al., Helv. Chim. Acta*, 1979, **62**, 1385-1395 (*synth, resoln*)
Diuric, S. *et al., Tet. Lett.*, 1981, **22**, 1787-1790 (*synth*)
Church, N.J. *et al., J.C.S. Perkin 1*, 1998, 1475-1482 (*R-form, S-form, synth, pmr, ir*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)

2-Amino-3*H*-phenoxazin-3-one, 9CI, 8CI A-292

[1916-59-2]
Questiomycin A. *AV toxin C*



$C_{12}H_8N_2O_2$ 212.207
Isol. from *Calocybe gambosa* (St George's mushroom). Dark-brown or red cryst. (EtOH). Sol. EtOH. Subl. 255-257. Sometimes occurs in amorph. form with Mp 296-297°. E° + 0.372V (pH 0.92, 23°) λ_{max} 235 (ε 28400); 467 (ε 1700) (0.25*N* HCl) (Derep). λ_{max} 335 (ε 1230) (0.1*N* KOH) (Derep). λ_{max} 240 (ε 26300); 435 (ε 2330) (pH 7.4) (Derep).

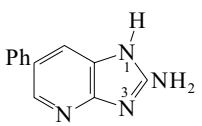
▶ LD_{50} (mus, ipr) 200 mg/kg. SP7695000

N-*Ac:* [1916-55-8] N-*(3-Oxo-3*H*-phenoxazin-2-yl)acetamide, 9CI.* ***2-Acetamido-3H-phenoxazin-3-one***
$C_{14}H_{10}N_2O_3$ 254.245
Orange cryst. Sol. EtOH, Et_2O, C_6H_6, MeOH; poorly sol. H_2O. Subl. 165. E° + 0.375V (pH 0.84, 23°) λ_{max} 240 (E1%/1cm 1400); 405 (E1%/1cm 1100) (EtOH) (Berdy).

N-*β-D-Glucopyranosyl:* **N-*β*-D-Glucopyranosylquestiomycin A**
$C_{18}H_{18}N_2O_7$ 374.349
Red powder. Sol. DMSO, Py; fairly sol. MeOH; poorly sol. $CHCl_3$, EtOAc. $[\alpha]_D^{28}$ +16.5 (c, 0.1 in Py). Mp >195° dec. λ_{max} 240 (log ε 4.33); 423 (log ε 4.23) (MeOH).

Fischer, O. *et al., Ber.*, 1961, **27**, 2784 (*synth*)
Gerber, N.N. *et al., Biochemistry*, 1964, **3**, 598; 1966, **5**, 3824 (*isol, uv, ir*)
Gerber, N.N. *et al., J.O.C.*, 1967, **32**, 4055 (*isol, uv, ir, bibl*)
Ruzička, E. *et al., Mikrochim. Acta*, 1967, 277 (*use*)
Ruzička, E. *et al., CA*, 1968, **69**, 40930j (*stannometry*)
Ikekawa, T. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1705 (*synth, ir*)
Sullivan, G. *et al., J. Pharm. Sci.*, 1971, **60**, 1097 (*isol*)
Baer, H. *et al., Pharmazie*, 1971, **26**, 108; 314 (*isol*)
Hishida, T. *et al., Chem. Lett.*, 1974, 293 (*synth*)
Schlunegger, U.V. *et al., Helv. Chim. Acta*, 1976, **59**, 1383 (*isol*)
Motohashi, N. *et al., Yakugaku Zasshi*, 1983, **103**, 364 (*synth, props*)
Bolognese, A. *et al., J. Het. Chem.*, 1986, **23**, 1003 (*synth, pmr, uv, deriv*)
Kinjo, J. *et al., Tet. Lett.*, 1987, **28**, 3697 (*isol*)
Simandi, L.I. *et al., Tet. Lett.*, 1993, **34**, 717 (*synth*)
Igarashi, Y. *et al., J. Antibiot.*, 1998, **51**, 915-920 (*Glucosylquestiomycin A*)
Kim, D.S. *et al., Planta Med.*, 2000, **66**, 78 (*Questiomycin A, isol, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QCJ275

2-Amino-6-phenylimidazo[4,5-*b*]pyridine A-293



1*H*-*form*

$C_{12}H_{10}N_4$ 210.238

1*H*-*form*

1-Me: [105650-23-5] *1-Methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridin-2-amine, 9CI. 2-Amino-1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridine. PhIP*
$C_{13}H_{12}N_4$ 224.265
Food-related mutagen, reported to be the most abundant heterocyclic amine found in cooked meat and fish. Solid. Mp 327-328°.

▶ Mutagen. Exp. carcinogen.

3*H*-*form*

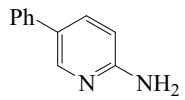
*3-Me:2-Amino-3-methyl-6-phenyl-3*H*-imidazo[4,5-*b*]pyridine*
$C_{13}H_{12}N_4$ 224.265
Mp 217°.

▶ Mutagen.

Knize, M.G. *et al., Heterocycles*, 1986, **24**, 1815 (*synth, ir, uv, pmr, cmr*)
Lindström, S. *et al., Acta Chem. Scand.*, 1993, **47**, 805; 1995, **49**, 361 (*synth, bibl*)
Lang, N.P. *et al., Cancer Lett. (Shannon, Irel.)*, 1999, **143**, 135-138 (*metab*)

2-Amino-5-phenylpyridine, 8CI A-294

[33421-40-8]
5-Phenyl-2-pyridinamine, 9CI. Phe-P-1



$C_{11}H_{10}N_2$ 170.213
Mutagen found in cooked food. Cryst. (H_2O). Mp 136-137° (134-135°).

▶ Mutagen. US2145000

N-*Acetoxy:* [124392-12-7]

[189894-03-9] *2-Acetoxyamino-5-phenylpyridine. 5-Phenyl-2(1*H*)-pyridinone,* O-*acetyloxime, 9CI*
$C_{13}H_{12}N_2O_2$ 228.25
Cryst. Mp 124-126°.

▶ Proximate carcinogen of the parent compd..

Beyer, H. *et al., Chem. Ber.*, 1958, **91**, 247-256 (*synth, ir*)
Butler, D.E. *et al., J. Med. Chem.*, 1971, **14**, 575 (*synth*)
Kosuge, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 611 (*tox*)
U.S. Pat., 1983, 4 386 209; *CA*, **100**, P6343u (*synth*)
Stavenuiter, J.F.C. *et al., Carcinogenesis (London)*, 1985, **6**, 13-19 (*synth, pmr, ms*)
Lutgerink, J.T. *et al., Carcinogenesis (London)*, 1989, **10**, 1957-1960 (*N-acetyloxy, synth, pmr, ms*)
Ojala, W.H. *et al., Acta Cryst. C*, 1997, **53**, 634-637 (*N-acetyloxy, cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALY000

3-Aminopropanoic acid A-295

[107-95-9]
β-Alanine, 9CI. FEMA 3252
$H_2NCH_2CH_2COOH$
$C_3H_7NO_2$ 89.094
Widely distributed in plants including algae, fungi and many higher plants. Flavouring ingredient. Cryst. (H_2O). Sol. H_2O; almost insol. Et_2O, Me_2CO. Mp 200° (197-198°). pK_{a1} 3.7; pK_{a2} 10.1 (30°).

Nitrile: [151-18-8] *3-Aminopropanenitrile, 9CI. 3-Cyanopropylamine. β-Aminopropionitrile*
$C_3H_6N_2$ 70.094
Constit. of chickling pea (*Lathyrus sativus*). Bp_{23} 89° $Bp_{0.1}$ 50-55°.

▶ LD_{50} (mus, ipr) 1152 mg/kg. Exp. reprod. and teratogenic effects. Polymerizes to an

explosive yellow solid. Storage hazard. UG0350000

N-*Benzoyl:* [3440-28-6] N-*Benzoyl-β-alanine, 9CI.* ***Betamipron, INN.*** *3-Benzamidopropanoic acid*
$C_{10}H_{11}NO_3$ 193.202
Artificial sweetener. Leaflets or prisms (H_2O). Mp 120°. Log P 0.69 (calc).

▶ AY3272500

Org. Synth., *Coll. Vol. 3*, 1955, 93 (*3-Aminopropanenitrile*)
Kircz, M. *et al., Rev. Chim. (Bucharest)*, 1959, **10**, 78 (*rev*)
Jose, P. *et al., Acta Cryst. C*, 1965, **18**, 806 (*cryst struct*)
Voellmin, J. *et al., Microchem. J.*, 1966, **11**, 73 (*ms*)
Zilkha, A. *et al., J.O.C.*, 1968, **33**, 1686 (*synth*)
Becke, F. *et al., Annalen*, 1970, **735**, 27 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2425 (*occur*)
Shirai, T. *et al., Synth. Prod. Util. Amino Acids*, (Kaneko, T. *et al*, Ed.), Kodansha, Ltd., Tokyo, 1974, 67 (*rev*)
Garrigou-Lagrange, C. *et al., Can. J. Chem.*, 1978, **56**, 663 (*ir, Raman*)
Blagoeva, I. *et al., Synthesis*, 1982, 967 (*synth*)
Ishibashi, N. *et al., Agric. Biol. Chem.*, 1988, **52**, 819 (*synth, use, Betamipron*)
Tamura, M. *et al., J. Agric. Food Chem.*, 1989, **37**, 737; 1990, **38**, 1368 (*synth, activity, Betamipron*)
Barluenga, J. *et al., Tetrahedron*, 1989, **45**, 2183 (*synth, Betamipron*)
Rosado, M.T.S. *et al., J. Mol. Struct.*, 1997, 343-348; 410-411 (*Raman, ir*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1139
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 212
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AMB500; DPU000; AMB750

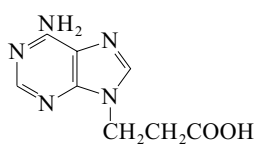
(3-Aminopropoxy)guanidine, 9CI A-296

[97091-01-5]
γ-Guanidinooxypropylamine
$HN{=}C(NH_2)NHOCH_2CH_2CH_2NH_2$
$C_4H_{12}N_4O$ 132.165
Constit. of *Canavalia gladiata* (sword-bean).

Hamana, K. *et al., Biochem. Biophys. Res. Commun.*, 1985, **129**, 46 (*isol*)
Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1311 (*isol*)

6-Amino-9*H*-purine-9-propanoic acid, 9CI A-297

[4244-47-7]
3-(9-Adeninyl)propionic acid



$C_8H_9N_5O_2$ 207.191
Isol. from *Lentinus edodes* (shiitake). Mp 277-278° dec. λ_{max} 262 (ε 14400) (0.1*N* NaOH). λ_{max} 259 (ε 13800) (0.1*N* HCl).

Me ester: [70259-15-3]
$C_9H_{11}N_5O_2$ 221.218
Cryst. (Et_2O/MeOH). Mp 182-183°.

Et ester: [7083-40-1]
$C_{10}H_{13}N_5O_2$ 235.245
Solid. Mp 167-168°.

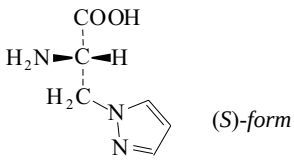
Nitrile: [4244-45-5] *6-Amino-9-(2-cyanoethyl)purine*
$C_8H_8N_6$ 188.191
Solid (H_2O). Mp 258-261° (245-247°).

Lira, E.P. *et al., J.O.C.*, 1966, **31**, 2188-2191 (*acid, nitrile, synth*)
Chakraborti, S.K. *et al., Indian J. Chem.*, 1969, **7**, 426 (*synth*)
Saito, Y. *et al., Tet. Lett.*, 1970, 4863 (*isol, struct, synth*)
Holy, A. *et al., Coll. Czech. Chem. Comm.*, 1978, **43**, 3444-3465 (*synth*)
Poritere, S.E. *et al., Khim. Geterotsikl. Soedin.*, 1982, 539-541; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1982, 415-417 (*nitrile*)

2-Amino-3-(1-pyrazolyl)propanoic acid A-298

[10162-27-3]

[28024-60-4]
*α-Amino-1*H*-pyrazole-1-propanoic acid, 9CI. β-Pyrazol-1-ylalanine*



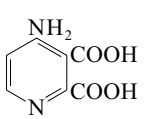
(*S*)-*form*

$C_6H_9N_3O_2$ 155.156
(***S*)-*form*** [2734-48-7]
L-form
Amino acid present in seeds of *Citrullus vulgaris* (watermelon). Cryst. (EtOH aq.). Mp 243° dec. $[\alpha]_D^{20}$ -73 (c, 3.4 in H_2O).

Noe, F.F. *et al., Biochem. J.*, 1960, **77**, 543 (*isol, synth*)
Sugimoto, N. *et al., Tetrahedron*, 1960, **11**, 231 (*synth*)
Dunnill, P.M. *et al., Biochem. J.*, 1963, **86**, 388 (*isol*)
Takeshita, M. *et al., J. Biol. Chem.*, 1963, **238**, 660 (*isol, synth*)
Dunnill, P.M. *et al., Phytochemistry*, 1965, **4**, 933 (*occur*)
Frisch, D.M. *et al., Phytochemistry*, 1967, **6**, 921 (*biosynth*)
Murakoshi, I. *et al., Chem. Pharm. Bull.*, 1972, **20**, 609; 1980, **34**, 1473 (*synth*)
Brown, E.G. *et al., Phytochemistry*, 1982, **21**, 863 (*biosynth*)
Arnold, L.D. *et al., J.A.C.S.*, 1988, **110**, 2237-2241 (*synth, pmr*)

4-Amino-2,3-pyridinedicarboxylic acid, 9CI A-299

[122475-55-2]

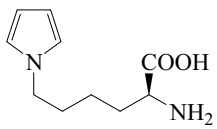


$C_7H_6N_2O_4$ 182.135
Cryst. (H_2O). Sol. H_2O, MeOH; poorly sol. Me_2CO, hexane. λ_{max} 262 (ε 9550) (0.1*N* HCl) (Derep). λ_{max} 245 (sh) (ε 8710); 290 (ε 2090) (H_2O at pH 11) (Derep). λ_{max} 265 (ε 9120) (H_2O pH 7) (Derep). λ_{max} 252 (ε 10000) (MeOH) (Berdy). λ_{max} 265 (ε 9800); 290 (ε 2080) (H_2O) (Berdy).

Hirayama, F. *et al., Phytochemistry*, 1989, **28**, 1133 (*isol, uv, ir, pmr, cmr, ms, synth, struct*)

α-Amino-1*H*-pyrrole-1-hexanoic acid, 9CI A-300

N$^{\epsilon}$-*Pyrrolylnorleucine. Pyrrole-1-norleucine. 1-(5′-Amino-5′-carboxypentyl)pyrrole*

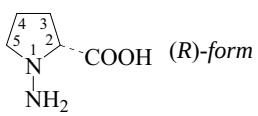


$C_{10}H_{16}N_2O_2$
(***S*)-*form*** [156539-32-1]
L-form
Widely distributed in fresh foodstuffs, e.g. meats, fish, vegetables, nuts, and processed foods. Component of nonenzymic browning reaction models. Characterised spectroscopically.

Chiang, G.H. *et al., J. Agric. Food Chem.*, 1988, **36**, 506-509 (*hplc, occur*)
Zamora, R. *et al., Lipids*, 1994, **29**, 243-249; 1995, **30**, 477-483 (*synth, detn, pmr, cmr*)
Zamora, R. *et al., Biochim. Biophys. Acta*, 1995, **1258**, 319-327 (*formn*)
Hidalgo, F.J. *et al., J. Agric. Food Chem.*, 1995, **43**, 1023-1028 (*occur, formn*)
Zamora, R. *et al., J. Agric. Food Chem.*, 1999, **47**, 1942-1947 (*occur*)

1-Amino-2-pyrrolidinecarboxylic acid A-301

1-Aminoproline, 9CI



(*R*)-*form*

$C_5H_{10}N_2O_2$ 130.146Log P -0.97 (calc).
(***R*)-*form*** [10139-05-6]
D-form
Obt. from linseed meal. Pale yellow cryst. (EtOH). Mp 155° dec. $[\alpha]_D^{25}$ +113 (c, 2 in 0.5M HCl).

▶ TW3588500

N-*γ-L-Glutamyl:* [10139-06-7] *1-[N-(γ-L-Glutamyl)amino]-D-proline.* ***Linatine***
$C_{10}H_{17}N_3O_5$ 259.261
Isol. from *Linum usitatissimum* (flax). Amorph. solid. Sol. H_2O; poorly sol. butanol, hexane. $[\alpha]_D^{24}$ +46.4 (c, 2.75 in H_2O).

▶ MA2275500

(***S*)-*form*** [15265-22-2]
L-form
Mp 155-156°. $[\alpha]_D^{24}$ -111 (c, 1.6 in 0.5*M* HCl).

Parsons, J.L. *et al., Antimicrob. Agents Chemother.*, 1967, 415

Klosterman, H.J. *et al., Biochemistry*, 1967, **6**, 170 (*synth*)
Achiwa, K. *et al., Tet. Lett.*, 1974, 1799 (*synth*)
Klosterman, H.J. *et al., Methods Enzymol.*, 1979, **62**, 483 (*props*)

3-Amino-2-pyrrolidinecarboxylic acid A-302

[24279-08-1]
3-Aminoproline, 9CI

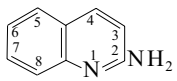
$C_5H_{10}N_2O_2$ 130.146

(2*S*,3*R*)-*form* [25876-88-4]
L-cis-*form*
Isol. from *Morchella esculenta* (common morel). Pale yellow powder (H_2O). Mp 215° (190°). $[\alpha]_D^{20}$ +22.5 (c, 0.9 in 6*M* HCl).

Baldwin, J.E. *et al., Tetrahedron*, 1995, **51**, 5169 (*synth, pmr, 2S,3R-form*)

2-Aminoquinoline A-303

[580-22-3]
2-Quinolinamine, 9CI. α-Aminoquinoline



$C_9H_8N_2$ 144.176
Alkaloid from the mushroom *Leucopaxillus aebissimus* var. *paradoxus* form *albiformis* (of unknown palatability). Cryst. (H_2O). Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 131.5-132.5° (129°). pK_a 7.3 (20°).

▶ VA9621800

Picrate:
Mp 266-267°.

Methochloride:
Cryst. + 1H_2O. Mp 268°.

Methiodide:
Cryst. (H_2O). Mp 247°.

N-*Ac:*
$C_{11}H_{10}N_2O$ 186.213
Mp 88-90°.

N-*Ph:* [5468-85-9] *2-Anilinoquinoline*
$C_{15}H_{12}N_2$ 220.273
Cryst. (EtOH). Mp 98°.

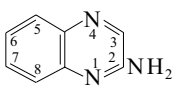
N-*Ph, 1-oxide:*
$C_{15}H_{12}N_2O$ 236.273
Mp 211-212°.

N-*Nitro:2-Nitraminoquinoline. 2-Quinolylnitramine*
$C_9H_7N_3O_2$ 189.173
Yellow needles (AcOH). Mp 223-225°. Turns red in air.

Tschitschibabin, A.E. *et al., Ber.*, 1925, **58**, 803
Steck, E.A. *et al., J.A.C.S.*, 1948, **70**, 3397 (*synth*)
Dymek, W. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1964, **38**, 925 (*2-Anilinoquinoline*)
Kametani, T. *et al., J. Het. Chem.*, 1965, **2**, 330 (*synth*)
Cook, M.J. *et al., J.C.S. Perkin 2*, 1973, 1080 (*tautom*)
Tondys, H. *et al., J. Het. Chem.*, 1985, **22**, 353 (*synth*)
Pfister, J.R. *et al., J. Nat. Prod.*, 1988, **51**, 969 (*isol, cmr, pmr*)
Yamada, M. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 1821 (*uv*)
Strekowski, L. *et al., Synth. Commun.*, 1994, **24**, 2387 (*N-Ac*)
Campagnone, R.S. *et al., Synth. Commun.*, 1997, **27**, 1631-1641 (*synth, ir, pmr, cmr*)

2-Aminoquinoxaline A-304

[5424-05-5]
2-Quinoxalinamine, 9CI



$C_8H_7N_3$ 145.163
Mp 155-156°. pK_a 3.93 (20°). Subl. *in vacuo*.

2-N-*Ac:* [6479-24-9]
$C_{10}H_9N_3O$ 187.201
Yellow. Mp 192.3-193.5°.

1-N-*Oxide:* [6479-23-8]
$C_8H_7N_3O$ 161.163
Mp 187-188°.

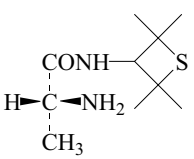
N-*(4-Aminobenzenesulfonyl):* [59-40-5] *4-Amino-*N*-2-quinoxalinylbenzenesulfonamide, 9CI.* ***Sulfaquinoxaline, BAN, INN.*** *Avicocid. Aviochina. Embazin. Italquina. Kokozigal S. Nococcin. Quinoxipra C. Sulfabenzpyrazine. Sulfa-Q. Sulquin. Compound 3-120*
$C_{14}H_{12}N_4O_2S$ 300.34
Antimicrobial, coccidiostat for vet. use. Potential food contaminant in animal products arising from its veterinary use. Sol. alkalis. Mp 247-248°. Log P 1.66 (calc). Freq. used as Na salt.

▶ LD_{50} (rat, orl) 1370 mg/kg. WP2100000

[967-80-6]

Weijlard, J. *et al., J.A.C.S.*, 1944, **66**, 1957
Elina, A.S. *et al., Zh. Obshch. Khim.*, 1963, **33**, 1954; *CA*, **59**, 12807
Ryley, J.F. *et al., Parasitology*, 1968, **58**, 215 (*sulfaquinoxaline, use*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 205
Combs, M.T. *et al., J. Agric. Food Chem.*, 1997, **45**, 1779-1783 (*sulfaquinoxaline, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QTS000

2-Amino-*N*-(2,2,4,4-tetramethyl-3-thietanyl)propanamide, 9CI A-305

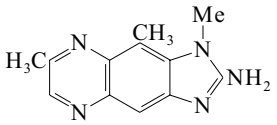


$C_{10}H_{20}N_2OS$ 216.347

(*R*)-*form* [80875-07-6]
Aqueous degradn. prod. of Alitame, A-168. Oil.

Eur. Pat., 1989, 325 485; *CA*, **112**, 77948d (*synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*occur*)

2-Amino-1,7,9-trimethylimidazo[4,5-*g*]quinoxaline A-306



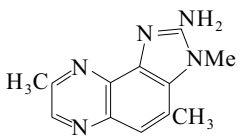
$C_{12}H_{13}N_5$ 227.268
Isol. from beef extract. Mp 250°.

▶ Mutagenic.

Achiwa, I. *et al., Chem. Pharm. Bull.*, 1994, **42**, 408 (*synth, pmr, uv*)

2-Amino-3,4,8-trimethyl-3*H*-imidazo[4,5-*f*]quinoxaline A-307

[95896-78-9]
*3,4,8-Trimethyl-3*H*-imidazo[4,5-*f*]quinoxalin-2-amine, 9CI. 4,8-Di-MeIQx*



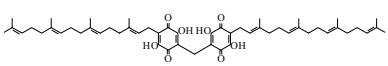
$C_{12}H_{13}N_5$ 227.268
Pyrolysis prod. from creatine, threonine and glucose in cooked food. Mp 300°.

▶ Mutagen. NJ5920400

Knapp, S. *et al., Tetrahedron*, 1989, **45**, 1293 (*synth*)
Grivas, S. *et al., Acta Chem. Scand.*, 1993, **47**, 521 (*synth, pmr, ms*)

Amitenone A-308

[21682-47-3]
2,2′-Methylenebis[3,6-dihydroxy-5-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)]-2,5-cyclohexadiene-1,4-dione, 9CI. Methylenebis[2,5-dihydroxy-4-geranylgeranyl-3,6-benzoquinone]



$C_{53}H_{72}O_8$ 837.147
Pigment from the edible mushroom Amitake (*Suillus bovinus*). Yellow-orange cryst. Mp 187-188°.

Minami, K. *et al., Tet. Lett.*, 1968, 5067 (*isol, struct*)
Azawa, K. *et al., Mokuzai Gakkaishi*, 1971, **17**, 384; *CA*, **76**, 59139 (*struct, synth*)

AML 1 A-309

[125147-23-1]

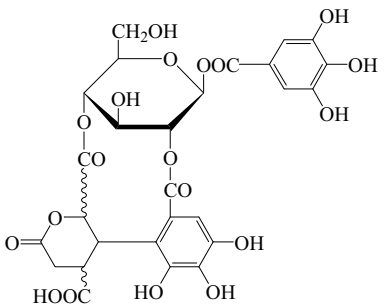
$C_{35}H_{62}O_4$ 546.872

Acetogenin. Struct. unknown. Constit. of *Annona muricata* (soursop). Powder. Sol. MeOH, hexane; poorly sol. H_2O.

Japan. Pat., 1989, 89 50 892; *CA*, **112**, 72327r

Amlaic acid A-310

[17278-02-3]



$C_{27}H_{24}O_{19}$ 652.475

Constit. of the leaves of *Phyllanthus emblica* (emblic). Cryst. (butanol/Et_2O). Mp 206°. $[\alpha]_D$ -289.

Theresa, Y.M. *et al., Leather Sci. (Madras)*, 1967, **14**, 16-17; *CA*, **67**, 88373r

Ammonium acetate A-311

[631-61-8]

NH_4OAc

$C_2H_7NO_2$ 77.083

Struct. is a 3-D H-bonded network with each O atom accepting 2 H bonds. Listed in the EAFUS Food Additive Database (Jan 2001) but with no reported use. Hygroscopic cryst. Mp 114°.

Zuffanti, S. *et al., J.A.C.S.*, 1941, **63**, 3123-3124 (*synth*)
Gutowsky, H.S. *et al., J. Chem. Phys.*, 1954, **22**, 1782-1783 (*pmr*)
Schmidt, B.M. *et al., J. Mol. Spectrosc.*, 1958, **2**, 539-550 (*N-14 nmr*)
Vratny, F. *et al., Anal. Chem.*, 1961, **33**, 1455 (*ir*)
Nahringbauer, I. *et al., Acta Cryst.*, 1967, **23**, 956-965 (*cryst struct*)

Ammonium carbonate, USAN A-312

[10361-29-2]

[8000-73-5]

Carbonic acid ammonium salt. Diammonium carbonate. Sal volatile. Hartshorn. E503

$(NH_4)_2CO_3$

$CH_8N_2O_3$ 96.086

As normally obt., contains large amounts of, from which it is formed on hydration. Used in baking powder. Colourless cryst. Strong odour of NH_3. Sharp taste. V. sol. H_2O. Mp 58° dec. Dec. in air → NH_3 + CO_2 + H_2O. Converts to, Mono-NH_4 salt. The name E503 is also used for Mono-NH_4 salt.

► LD_{50} (mus, ivn) 96 mg/kg. BP1925000

Monohydrate: [16799-91-0]
$CH_{10}N_2O_4$ 114.101
Colourless cubes. V. sol. cold H_2O; dec. hot H_2O.

Compd. with H_2O_2: [76261-70-6] *Ammonium carbonate peroxohydrate*
$CH_{10}N_2O_5$ 130.1
Colourless cryst.

[506-87-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1272B (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1964, **8/IA**, 459 (*rev*)
Jones, D.P. *et al., J.C.S. Dalton*, 1980, 2526 (*synth, ir, Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 743
Merck Index, 12th edn., 1996, No. 534
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANE000

Ammonium chloride A-313

($(NH_4)Cl$), 11CI, JAN, USAN

[12125-02-9]

Sal ammoniac. Amchlor. Darammon. Ammonium muriate. Salmiac

$[NH_4]Cl$

ClH_4N 53.491

Has CsCl struct. below 184.3° and NaCl above this temp.. Dough conditioner, dough strengthener, flavour enhancer, leavening agent, processing aid and yeast food. Hygroscopic white solid. V. sol. H_2O. V.p. 758 mm at 338°. Subl. when heated.

► Irritant. BP4550000

[12015-14-4]

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1521D (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 150 (*bibl*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1964, **8/I**, *Part* 1; 378 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 520 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 135-136
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANE500

Ammonium hydroxide A-314

($(NH_4)(OH)$), 11CI, 10CI, 9CI

[1336-21-6]

Ammonium hydroxide. Ammonia aqueous. Aqua ammonia. E527

$NH_3.H_2O$ rather than NH_4OH

H_5NO 35.046

Name given to aq. soln. of Ammonia. Used in food processing as a leavening agent, pH control agent, surface-finishing agent, and boiler water additive. Colourless liq. Sol. H_2O. d^{20} 0.89. Mp -77°.

► Corrosive. V. pungent odour, poison by ingestion. Severe eye irritant. Can inflict burns. BQ9625000

Penta-deutero compd.: [12168-30-8]
D_5NO 40.077

Mellor Compr. Treat. Inorg. Theor. Chem., 1928, 194; 1964, **8/I**, 311 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 42 (*bibl*)
Herber, R.H. *et al., Inorg. Isot. Synth.*, Benjamin, 1962, 47 (*deutero deriv*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 224 (*struct, rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 137-138
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANK250

Ammonium phosphate A-315

($(NH_4)(H_2PO_4)$)

[7722-76-1]

[10124-31-9]

Monoammonium phosphate, 9CI, 8CI. Ammonium phosphate†. Ammonium dihydrogenphosphate

$(NH_4)(H_2PO_4)$

H_6NO_4P 115.025

Thermally the most stable of the ammonium orthophosphates. Each NH_4 cation is coordinated by 8 oxygens forming two interpenetrating tetragonal disphenoids. Mean P–O 153.7 pm. Used in food as a source of acidity, pH control agent, buffering agent, leavening agent, dough strengthener and nutrient source; also used as a yeast nutrient in wine production and to start secondary fermentations in the production of sparkling wines. Colourless, transparent tetragonal prisms (H_2O). Mp 190°. Low temp. orthorhombic, antiferroelectric phase transforms at -125° (rising temp.) into tetragonal, paraelectric phase.

[93454-15-0, 93454-16-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1266C (*ir*)
Miller, F.A. *et al., Spectrochim. Acta A*, 1960, **16**, 135 (*ir*)
Kolomiichuk, V.N. *et al., Kristallografiya*, 1968, **13**, 519; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1968, **13**, 4221 (*ed*)
Mullin, J.W. *et al., J. Appl. Chem.*, 1970, **20**, 153 (*synth*)
Khan, A.A. *et al., Acta Cryst. B*, 1973, **29**, 2721 (*cryst struct*)
Nicholson, J.Y. *et al., J. Chem. Phys.*, 1974, **60**, 715 (*pmr*)
Ratcliffe, C.I. *et al., Chem. Phys. Lett.*, 1985, **120**, 427 (*N-15 nmr*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Bréhat, F. *et al., J. Phys. C: Solid State Phys.*, 1986, **19**, 6893 (*ir*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Mohanial, S.K. *et al., Cryst. Res. Technol.*, 1987, **22**, 21 (*synth*)
Pastor, A.C. *et al., Ferroelectrics*, 1987, **71**, 61 (*rev*)
Cerreta, M.K. *et al., J. Cryst. Growth*, 1987, **84**, 577 (*Raman*)
Hattori, T. *et al., J. Phys. Soc. Jpn.*, 1987, **56**, 781 (*Raman*)
Fukami, T. *et al., J. Phys. Soc. Jpn.*, 1987, **56**, 2223; 4388 (*cryst struct*)
Kim, J.J. *et al., Phys. Rev. B*, 1987, **36**, 5651 (*Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 142-143

Ammonium phosphate A-316

($(NH_4)_2HPO_4$)

[7783-28-0]

[10124-31-9]

Diammonium phosphate, 9CI, 8CI. Diammonium hydrogen phosphate ($(NH_4)_2HPO_4$). Ammonium phosphate, USAN

$(NH_4)_2HPO_4$

$H_9N_2O_4P$ 132.056

Struct. has discrete $PO_4H^{2\ominus}$ and $NH_4^{\oplus}$

tetrahedra with P–O 151.9-158.7 pm, angle: OPO 103.6-113.2°. Dough strengthener, firming agent, leavening agent, pH control agent, processing aid, nutrient source, yeast nutrient and a starter for secondary fermentation in the production of sparkling wines. Mp 185° dec.

▶ TB9375000

α-form

High temp.-form

Orthorhombic cell at 120°.Reverts to β-form at *ca*. 100°.

β-form

Low temp.-form

Monoclinic cell.Colourless cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1266D (*ir*)
Thompson, H.L. *et al., Ind. Eng. Chem.*, 1950, **42**, 2176 (*props, manuf*)
Smith, P. *et al., Acta Cryst.*, 1957, **10**, 709 (*cryst struct*)
Coates, R.V. *et al., Acta Cryst.*, 1967, **23**, 504 (*synth, cryst struct*)
Nabiev, M.N. *et al., Zh. Neorg. Khim.*, 1969, **14**, 2950; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 1556 (*synth, props*)
Khan, A.A. *et al., Acta Cryst. B*, 1972, **28**, 2065 (*cryst struct*)
Hamann, S.D. *et al., Aust. J. Chem.*, 1978, **31**, 11 (*ir*)
Neels, J. *et al., Z. Anorg. Allg. Chem.*, 1982, **495**, 65 (*P-31 nmr*)
Ratcliffe, C.I. *et al., Chem. Phys. Lett.*, 1983, **99**, 177 (*N-15 nmr*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 338 (*P-31 nmr*)
Videnova-Adrabinska, V. *et al., J. Mol. Struct.*, 1988, **175**, 295 (*ir, Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 140-145
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANR500

Ammonium sulfide ($(NH_4)_2S$), 10CI, 9CI A-317

[12135-76-1]

Diammonium sulfide. FEMA 2053

$[NH_4]_2S$

H_8N_2S 68.143

Flavouring ingredient. Used in baked goods, meat products, condiments and gravies. Below -18° stable. Yellow hygroscopic cryst. Sol. H_2O. Dec. to NH_3 + NH_4SH, polysulfides.

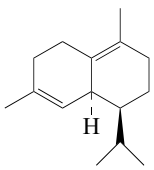
▶ Toxic. Pyrophoric in air. BS4920000

Mellor Compr. Treat. Inorg. Theor. Chem., 1928, **2**, 645; *Part 1*, 1964, **8/1**, 469 (*rev*)
Merck Index, 11th edn., 1989, No. 585 (*props, uses*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 197-199 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 35
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 146-147
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 7th edn., Van Nostrand Reinhold*, 1989, 243; 244 (*haz*)

1(10),4-Amorphadiene A-318

[189165-79-5]

δ-Amorphene



$C_{15}H_{24}$ 204.355

Constit. of *Leptospermum scoparium* (red tea).

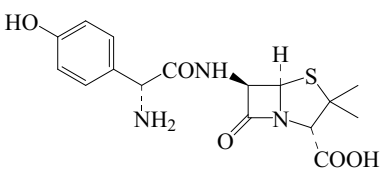
Melching, S. *et al., Phytochemistry*, 1997, **44**, 1291-1296 (*isol, pmr, ms, gc*)

Amoxicillin, INN, JAN, USAN A-319

[26787-78-0]

[61336-70-7]

6-[[Amino(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 9CI. 6-(α-Amino-4-hydroxyphenylacetamido)-penicillanic acid. ρ-Hydroxyampicillin. ***Amoxycillin, BAN****. Almodan. Amix. Amopen. Amoram. Amoxid. Amoxil. Amoxymed. Amrit. Biomox. Cemoxin. Clamoxyl (SKB). Flemoxin. Galenamox. Imacillin. Polymox. Rimoxallin. Sauracillin. Trimox. Wymox. BRL 2333. Many other names*



$C_{16}H_{19}N_3O_5S$ 365.409

Potential contaminant in cow's milk arising from its veterinary use. Marketed drug. Worldwide 145th best selling prescription drug ($0.32 bn) (SmithKline Beecham) (1999, Pharma Business)Cryst. + $3H_2O$. Sol. H_2O. $[\alpha]_D^{20}$ +246 (c, 0.1 in H_2O). Log P -1.94 (uncertain value) (calc).

▶ Hypersensitivity reactions and gastrointestinal effects reported when used therapeutically. LD_{50} (rat, ipr) 2870 mg/kg (trihydrate). XH8300000

Na salt: [34642-77-8] ***Amoxicillin sodium, USAN***Used in combination with clavulanate potassium and marketed as Augmentin.

2-Naphthalenesulfonate:

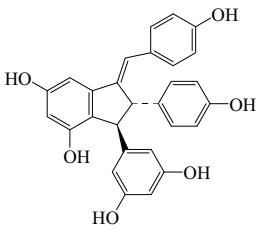
Mp 194° dec.

[79198-29-1]

Neu, H. *et al., Antimicrob. Agents Chemother.*, 1970, 407; 411; 416; 423, (*props*)
U.K. Pat., 1970, 1 241 844; *CA*, **72**, 90447 (*synth*)
Long, A. *et al., J.C.S.(C)*, 1971, 1920 (*synth*)
Boles, M.O. *et al., Acta Cryst. B*, 1978, **34**, 461 (*cryst struct*)
Bhattacharyya, P.K. *et al., Anal. Profiles Drug Subst.*, 1978, **7**, 19 (*rev*)
Owen, R.T. *et al., Drugs of Today (Barcelona)*, 1980, **16**, 163 (*rev, pharmacol*)
Bird, A.E. *et al., J.C.S. Perkin 1*, 1982, 563 (*pmr, cd*)
Kawamori, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 2503 (*biosynth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 4027 (*synonyms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, A0A100
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **3**, 129 (*rev*)
Vega, J.M. *et al., Allergy*, 1994, **49**, 317 (*tox*)
Bird, A.E. *et al., Anal. Profiles Drug Subst.*, 1994, **23**, 1 (*rev*)
Aguilar, L. *et al., Antimicrob. Agents Chemother.*, 1997, **41**, 1403-1405 (*amoxicillin sodium-clavulanic acid*)
Ang, C.Y.W. *et al., J. Agric. Food Chem.*, 1997, **45**, 4351-4356 (*occur, anal*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 151
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, A0A100

Ampelopsin D A-320

[149418-37-1]



Absolute Configuration

$C_{28}H_{22}O_6$ 454.478

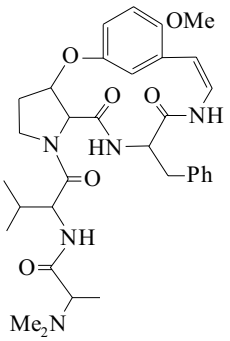
Constit. of *Vitis vinifera* (wine grape). Amorph. powder. $[\alpha]_D^{22}$ -5 (c, 0.27 in MeOH).

Oshima, Y. *et al., Phytochemistry*, 1993, **33**, 179-182 (*isol, pmr, cmr*)
Adesanya, S.A. *et al., J. Nat. Prod.*, 1999, **62**, 1694-1695 (*struct*)
Niwa, M. *et al., Heterocycles*, 2000, **53**, 1475-1478 (*pmr, cmr, abs config*)
Takaya, Y. *et al., Tetrahedron*, 2002, **58**, 7259-7265 (*abs config*)

Amphibine H A-321

[52659-55-9]

*2-(Dimethylamino)-*N*-[2-methyl-1-[[3,3a,12,13,14,15,16,16*a*-octahydro-8-methoxy-13,16-dioxo-14-(phenylmethyl)-5,9-metheno-9*H*-pyrrolo[3,2-*b*][1,5,8]oxadiazacyclopentadecin-1(2*H*)-yl]carbonyl]propyl]propanamide, 9CI*



$C_{33}H_{43}N_5O_6$ 605.733

Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Cryst. ($CHCl_3$/petrol). Mp 205°. $[\alpha]_D^{20}$ -570 (c, 0.12 in MeOH).

N-*De-Me:* [53947-96-9] ***Nummularine B***. N-*Demethylamphibine H*. *Daechuine S27*

$C_{32}H_{41}N_5O_6$ 591.706

Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Needles (MeOH). Mp 230-231°. $[\alpha]_D^{20}$ -390 (c, 0.2 in $CHCl_3$).

N-*De-Me,* N-*formyl:* [99694-95-8] ***Nummularine T***

$C_{33}H_{41}N_5O_7$ 619.716

Granules (MeOH). Mp 188-190°.

Dihydro:

Needles (CH_2Cl_2/Me_2CO). Mp 281°. $[\alpha]_D^{20}$ -381 (c, 0.15 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1974, **107**, 686; 3180 (*isol, uv, ir, pmr, ms, struct*)

Tschesche, R. *et al., Phytochemistry*, 1976, **15**, 541; 1979, **18**, 702 (*isol*)

Pandey, V.B. *et al., Phytochemistry*, 1984, **23**, 2118 (*isol*)

Han, B.H. *et al., Pure Appl. Chem.*, 1989, **61**, 443 (*isol, Nummularine B*)

Pandey, V.B. *et al., Planta Med.*, 1990, **56**, 649 (*activity*)

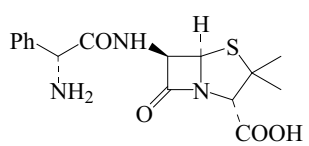
Singh, B. *et al., Phytochemistry*, 1995, **38**, 271 (*Nummularine T*)

Ampicillin, BAN, INN, JAN, USAN A-322

[69-53-4]

[7177-48-2]

6-[(Aminophenylacetyl)amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]-heptane-2-carboxylic acid, 9CI. D-α-Aminobenzylpenicillin. 6-(α-Aminophenylacetamido)penicillanic acid. Amblosin. Amfipen. Binotal. Magnapen. Marcillin. Omnipen. Penbristol. Pentritin. Penicline. Tolomol. Viccillin. Vidocillin. Vidopen. AY 6108. BRL 1341. NSC 528986



$C_{16}H_{19}N_3O_4S$ 349.41

Semisynthetic penicillin. Potential contaminant of cow's milk arising from its veterinary use. Marketed drug.

Worldwide 92nd best selling prescription drug (as Unasyn in combination with) ($0.33 bn) (Pfizer) (1996, PharmaBusiness)Mp 199-202° dec. $[\alpha]_D^{23}$ +287.9 (H_2O). pK_{a1} 2.52; pK_{a2} 7.24 (25°). Log P -1.27 (uncertain value) (calc). Constit. of Unasyn.

▶ Hypersensitivity reactions reported when used therapeutically. LD_{50} (rat, ipr) 4500 mg/kg. Exp. teratogen. XH8350000

Na salt: [69-52-3] *Ampicillin sodium, USAN. Omnipen. Embacillin C*

▶ LD_{50} (mus, ipr) 3480 mg/kg. XH8400000

(5-Methyl-2-oxo-1,3-dioxol-4-yl)methyl ester: See Lenampicillin in *The Combined Chemical Dictionary.*

[94935-63-4]

Doyle, F. *et al., J.C.S.*, 1962, 1440 (*synth*)

Austin, K. *et al., Nature (London)*, 1965, **208**, 99

Ivashkiv, E. *et al., Anal. Profiles Drug Subst.*, 1973, **2**, 1 (*rev*)

Boles, M. *et al., Acta Cryst. B*, 1976, **32**, 2279; 1978, **34**, 461 (*cryst struct*)

Kaifež, F. *et al., J. Het. Chem.*, 1976, **13**, 561 (*synth*)

Bird, A.E. *et al., J.C.S. Perkin 1*, 1982, 563 (*pmr, cd*)

Akita, H. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4317 (*synth*)

Humber, D.C. *et al., Tetrahedron*, 1984, **40**, 4153 (*synth*)

Cooper, J. *et al., Tetrahedron*, 1984, **40**, 4153 (*synth*)

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 4026 (*synonyms*)

IARC Monog., 1990, **50**, 153 (*rev, tox*)

Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **3**, 129 (*rev*)

Ang, C.Y.W. *et al., J. Agric. Food Chem.*, 1997, **45**, 4351-4356 (*occur, anal*)

Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 153; 154

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AIV500; SEQ000; AOD125

α-Amylase A-323

[9000-90-2]

Alpha Amylase, USAN. Fortizyme. Amylopsin. Buclamase. Maxilase. Amylase THC250. Glycogenase. 1,4-K-D-Glucan glucanohydrolase. E.C. 3.2.1.1

Enzyme which hydrolyses 1,4-α-glycosidic linkages in starch, glycogen and related polysaccharides; starch is converted into maltose and dextrins. Used for the hydrolysis of starch in the sugar, brewing and distilling industries. Improves baking quality and fermentation. A concentrate of amylolytic enzymes of bacterial or animal origin.

Manners, D.J. *et al., Adv. Carbohydr. Chem.*, 1962, **17**, 371-430 (*rev*)

Thoma, J.A. *et al., Enzymes (3rd edn.)*, 1971, **5**, 115 (*rev*)

Pierrot, M. *et al., FEBS Lett.*, 1977, **79**, 105 (*cryst struct*)

Ingle, M.B. *et al., Adv. Appl. Microbiol.*, 1978, **24**, 257 (*rev, bacterial amylase*)

Karn, R.C. *et al., Adv. Comp. Physiol. Biochem.*, 1978, **7**, 1 (*rev, animal amylase*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1337

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 149-153

β-Amylase, 9CI A-324

[9000-91-3]

1,4-D-Glucan maltohydrolase. Saccharogen amylase. Glycogenase. E.C. 3.2.1.2

Tetrameric enzyme, MW 206 000 ± 1000; tryptophan residues are involved at the active site. Used in the prodn. of alcoholic beverages and sugar syrups. Releases successive maltose units from the non-reducing end of a polysaccharide chain by hydrolysis of α-(1→4)-glucan linkages; acts on starch, glycogen and related polysaccharides.

Manners, D.J. *et al., Adv. Carbohydr. Chem.*, 1962, **17**, 371-430 (*rev*)

Thoma, J. *et al., The Enzymes*, (Boyer, P. Ed.), 3rd Edn., Academic Press, N.Y., 1971, **5**, 115-189 (*rev*)

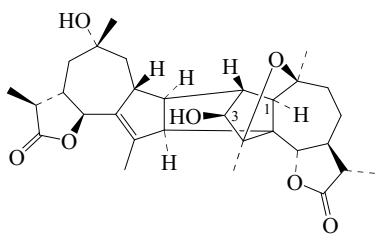
Vihinen, M. *et al., Crit. Rev. Biochem. Mol. Biol.*, 1989, **24**, 329-418 (*rev*)

Ray, R.R. *et al., J. Chem. Res., Miniprint*, 1996, **22**, 181-199 (*rev*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 151-152 (*use*)

Anabsin A-325

[72542-39-3]



$C_{30}H_{40}O_7$ 512.642

Constit. of *Artemisia absinthium* (wormwood). Cryst. Mp 276° dec. $[\alpha]_D^{25}$ +110 (c, 1.7 in Me_2CO).

3-Deoxy: [6903-12-4] ***Anabsinthin***

$C_{30}H_{40}O_6$ 496.642

Isol. from *Artemisia absinthium* (wormwood). Cryst. (C_6H_6). Mp 267° (260°). $[\alpha]_D^{20}$ +113 ($CHCl_3$).

3-Deoxy, 1α-hydroxy: [244179-05-3] ***Seemarin***

$C_{30}H_{40}O_7$ 512.642

Cryst. Mp 256-257°. $[\alpha]_D$ +114.5 (c, 0.1 in MeOH/$CHCl_3$).

10′,11′-Diepimer, 3-deoxy: [314763-54-7] ***Caruifolin D***

$C_{30}H_{40}O_6$ 496.642

Amorph. powder. $[\alpha]_D^{24}$ +108 (c, 0.29 in $CHCl_3$).

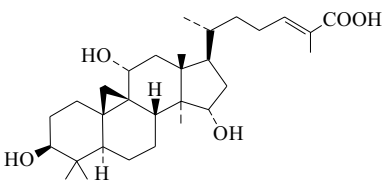
Kasyrov, Sh.Z. *et al., Khim. Prir. Soedin.*, 1979, **15**, 495; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 430 (*struct, bibl*)

Ullah, N. *et al., Phytochemistry*, 1999, **51**, 559-562 (*Seemarin, Anabsinthin*)

Ma, C.-M. *et al., J. Nat. Prod.*, 2000, **63**, 1626-1629 (*Caruifolin D*)

Ananasic acid A-326

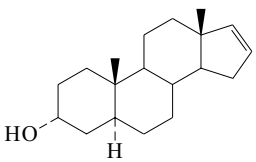
[60877-02-3]
*3β,11α,15α-Trihydroxycycloart-24*E*-en-26-oic acid*



$C_{30}H_{48}O_5$ 488.706
Constit. of pineapple stems. Cryst. (MeOH). Mp 194-197.5°. $[\alpha]_D^{25}$ +4.23.

Takata, R.H. *et al., Tetrahedron*, 1976, **32**, 1077

Androst-16-en-3-ol, 9CI A-327



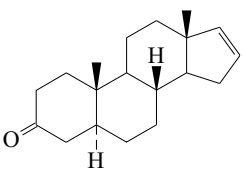
(3α,5α)-*form*

$C_{19}H_{30}O$ 274.445

(3α,5α)-*form* [1153-51-1]
Aroma substance from the Perigord truffle tuber. Cryst. (petrol). Mp 143.5-144°. $[\alpha]_D^{20}$ +15 (c, 1.33 in $CHCl_3$).

Ruzicka, L. *et al., Helv. Chim. Acta*, 1943, **26**, 975; 1947, **30**, 3080
Prelog, V. *et al., Helv. Chim. Acta*, 1945, **28**, 618
Fishman, J. *et al., J.O.C.*, 1963, **28**, 1443 (*synth, 3α,5α-form*)
Hudec, J. *et al., Tetrahedron*, 1976, **32**, 2475 (*ord, cd*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1983, **66**, 192 (*synth, ir, pmr*)

Androst-16-en-3-one A-328



$C_{19}H_{28}O$ 272.43

5α-*form* [18339-16-7]
Androgen metabolite which causes "boar taint" in pigmeat products. Cryst. (pentane). Mp 140-141°. $[\alpha]_D^{17}$ +38 (c, 2.08 in $CHCl_3$).

(5α,13α)-*form* [86335-08-2]
Cryst. (petrol). Mp 120-122°. $[\alpha]_D$ -86.8 (c, 8.5 in $CHCl_3$).

(5α,14β)-*form* [88930-98-7]
Mp 101.5-103°.

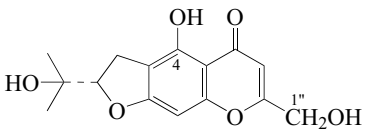
(5β,8α,9β,10α,13α,14β)-*form* [86362-77-8]
Cryst. (pentane). Mp 140-141°. $[\alpha]_D$ -38.5 (c, 1 in $CHCl_3$).

[66263-13-6, 82209-77-6, 82209-82-3, 82209-84-5]

Prelog, V. *et al., Helv. Chim. Acta*, 1944, **27**, 66 (*synth*)
Zalkow, L.H. *et al., Tet. Lett.*, 1964, 217 (*synth*)
Patterson, R.L.S. *et al., J. Sci. Food Agric.*, 1968, **19**, 31 (*occur*)
Kingsbury, A.E. *et al., Horm. Res.*, 1978, **9**, 254 (*metab*)
Kagan, M.Z. *et al., Bioorg. Khim.*, 1979, **5**, 1158 (*synth*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1983, **66**, 192 (*synth, epimers, isomers*)
Turner, A.B. *et al., Tet. Lett.*, 1983, **24**, 4589 (*14β-form*)
Cox, P.J. *et al., Tetrahedron*, 1984, **40**, 3153 (*synth, cryst struct, bibl*)

Angelicain A-329

[64519-22-8]
*2,3-Dihydro-4-hydroxy-7-(hydroxymethyl)-2-(1-hydroxy-1-methylethyl)-5*H*-furo[3,2-*g*][1]benzopyran-5-one, 9CI. Norcimifugin*



$C_{15}H_{16}O_6$ 292.288

(*S*)-*form* [49624-66-0]
Constit. of *Angelica archangelica* (angelica). Cryst. Mp 208-209°. $[\alpha]_D$ +49.

1″-O-β-D-Glucopyranoside: [85889-15-2]
prim-O-*Glucosylangelicain*
$C_{21}H_{26}O_{11}$ 454.43
Needles (EtOH). Mp 130-132°. $[\alpha]_D^{22}$ +13.7 (c, 0.580 in EtOH).

9-O-Angeloyl: [173994-06-4] ***Angeliticin A***
$C_{20}H_{22}O_7$ 374.39
Cryst. Mp 177-178°.

4-Me ether: [37921-38-3] ***Cimifugin***. *Cimitin*
$C_{16}H_{18}O_6$ 306.315
Needles (MeOH). Mp 107-109°. $[\alpha]_D$ +79.2 (c, 0.8 in $CHCl_3$).

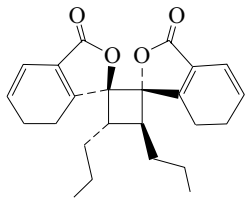
4-Me ether, 1″-O-β-D-glucopyranoside: [80681-45-4]
$C_{22}H_{28}O_{11}$ 468.457
Cryst. ($CHCl_3$). Mp 118-120° (113°-115°). $[\alpha]_D^{24}$ +33.3 (c, 0.6 in $CHCl_3$).

(±)-*form*
Mp 197-198°.

Kondo, Y. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1940 (*isol, abs config, Cimicifugin*)
Kirtany, J.K. *et al., Indian J. Chem.*, 1973, **11**, 505 (*struct*)
Wada, H. *et al., Phytochemistry*, 1974, **13**, 297 (*isol*)
Chatterjee, A. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 212 (*isol*)
Baba, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2565 (*isol, Cimifugin*)
Kozawa, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 64 (*isol*)
Kopp, B. *et al., Helv. Chim. Acta*, 1991, **74**, 611 (*Cimifugin glucoside*)
Lemmich, J. *et al., Phytochemistry*, 1995, **38**, 427 (*glucosides*)
Mi, C.F. *et al., Yaoxue Xuebao*, 1995, **30**, 910 (*Angelicitin A*)
Lal, B. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 881-893 (*isol, synth, pmr, activity*)

Angelicolide A-330

[90826-58-7]

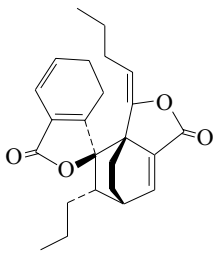


$C_{24}H_{28}O_4$ 380.483
Constit. of roots of *Angelica glauca*. Prisms (Me_2CO/petrol). Mp 157°.

Banerjee, S.K. *et al., Annalen*, 1984, 888 (*cryst struct*)

Angeolide A-331

[81957-73-5]

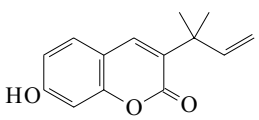


$C_{24}H_{28}O_4$ 380.483
Constit. of *Angelica glauca*. Cryst. (C_6H_6/hexane). Mp 130°. $[\alpha]_D^{25}$ 0 ($CHCl_3$).

Banerjee, S.K. *et al., Annalen*, 1982, 699 (*cryst struct*)

Angustifolin A-332

[56881-08-4]
*3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-2*H*-1-benzopyran-2-one, 9CI. 3-(1,1-Dimethylallyl)-7-hydroxycoumarin*



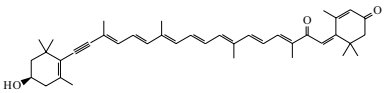
$C_{14}H_{14}O_3$ 230.263
Gum.

Me ether: [20958-63-8] *3-(1,1-Dimethyl-2-propenyl)-7-methoxy-2*H*-1-benzopyran-2-one. 3-(1,1-Dimethylallyl)-7-methoxycoumarin.* ***3-(1,1-Dimethylallyl)herniarin***
$C_{15}H_{16}O_3$ 244.29
Constit. of *Ruta graveolens* (rue). Cryst. (MeOH or hexane). Mp 126-128°.

Reisch, J. *et al., Tet. Lett.*, 1968, 4395 (*isol, deriv*)
Raj, K. *et al., Indian J. Chem.*, 1975, **13**, 404 (*synth*)
Del Castillo, J.B. *et al., Phytochemistry*, 1984, **23**, 2095 (*isol*)
Galán, R.H. *et al., Heterocycles*, 1989, **29**, 297 (*synth*)
Macias, F.A. *et al., Acta Cryst. C*, 1990, **46**, 2482 (*cryst struct*)

Anhydroamarouciaxanthin B A-333

[119286-10-1]
6′,7,7′,8-Tetrahydro-6′,8′-dihydro-3-hydroxy-β,ϵ-carotene-3′,8′-dione

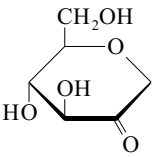


$C_{40}H_{50}O_3$ 578.833
Constit. of *Mytilus edulis* (blue mussel).
λ_{max} 458 ; 485 (hexane).

Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*occur, uv, ms, pmr*)

1,5-Anhydrofructose, 9CI A-334

1,5-Anhydro-arabino-*hex-2-ulose*



$C_6H_{10}O_5$ 162.142
The oxo form illus. is in equilib. with the 2-enol form, the 2,3-enediol form and the 3,3-diol covalent hydrate, which is the predominating species in aq. soln..

D-*form* [75414-43-6]
Isol. from *Morchella vulgaris* (morel).
Amorph. solid. Mp 107-112°. $[\alpha]_D^{20}$ -32.9 (c, 0.86 in H_2O).

Oxime: [75414-31-2]
$C_6H_{11}NO_5$ 177.157
Mp 178-180°. $[\alpha]_D^{21}$ -43 (c, 0.3 in H_2O).

Tri-Ac, oxime: [88851-59-6]

[75414-20-9]
$C_{12}H_{17}NO_8$ 303.268
Mp 89-90°. $[\alpha]_D^{21}$ -52.9 (c, 0.3 in $CHCl_3$).

Tribenzoyl: [75414-32-3] *1,5-Anhydro-3,4,6-tri*-O-*benzoyl*-D-*fructose*
$C_{27}H_{22}O_8$ 474.466
Mp 126-127°. $[\alpha]_D^{20}$ -24 (c, 0.8 in $CHCl_3$).

Tribenzoyl, oxime: [82569-81-1]

[75414-21-0]
$C_{27}H_{23}NO_8$ 489.481
Mp 176-177°. $[\alpha]_D^{21}$ -39 (c, 0.4 in $CHCl_3$).

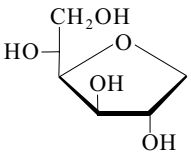
*4,6-Benzylidene, 3-(*tert-*butyldimethylsilyl):* [89872-98-0] *1,5-Anhydro-4,6*-O-*benzylidene-3*-O-*(*tert-*butyldimethylsilyl)*-D-*fructose*
$C_{19}H_{28}O_5Si$ 364.513
Syrup + $1H_2O$. $[\alpha]_D^{20}$ -49.9 (c, 2.7 in $CHCl_3$).

Lichtenthaler, F.W. *et al., Tet. Lett.*, 1980, **21**, 1429-1432 (*synth, tri-Ac, tribenzoyl*)
Tulshian, D.B. *et al., J.O.C.*, 1984, **49**, 2347-2355 (*benzylidene butyldimethylsilyl*)
Deffieux, G. *et al., Phytochemistry*, 1987, **26**, 1391-1393 (*biosynth, isol, oxime, cryst struct*)
Baute, M.A. *et al., Phytochemistry*, 1991, **30**, 1419-1423 (*biosynth*)
Yu, S. *et al., Carbohydr. Res.*, 1998, **305**, 73-82 (*anal, bibl*)
Kopper, S. *et al., Chem. Eur. J.*, 1998, **4**, 2442-2455 (*synth*)
Yamaji, K. *et al., Planta Med.*, 2002, **68**, 16-19 (*activity*)

1,4-Anhydroglucitol, 9CI, 8CI A-335

[27299-12-3]

[12441-09-7]
1,4-Anhydrosorbitol. Arlitan. Sorbitan



$C_6H_{12}O_5$ 164.158

D-*form*
Cryst. (2-propanol). Mp 115-116°. $[\alpha]_D^{27}$ -21.9 (c, 2.5 in H_2O).

6-O-*Dodecanoyl:* [1338-39-2] *Sorbitan monolaurate, BAN, USAN.* ***Sorbitan laurate, INN****. Sorbester P12. Span 20. E493*
$C_{18}H_{34}O_6$ 346.463
Food emulsifier, solubiliser, crystallisation retarder, dough improver, antifoam agent, stabiliser.
▶ Eye irritant. LD_{50} (rat, orl) 33600 mg/kg. WG2920000

6-O-*Hexadecanoyl:* [26266-57-9] *Sorbitan monopalmitate, BAN, USAN.* ***Sorbitan palmitate, INN****. Sorbester P16. Span 40. E495*
$C_{22}H_{42}O_6$ 402.57
Food emulsifier, stabiliser.
▶ WG2932900

6-O-*Octadecanoyl:* [1338-41-6] *Sorbitan monostearate, BAN, USAN.* ***Sorbitan stearate, INN****. Sorbester P18. Span 60. FEMA 3028. E491*
$C_{24}H_{46}O_6$ 430.624
Food emulsifier, stabiliser, defoaming agent, flavouring and flavour modifier, rehydration agent for active dried yeast, coating for fruit and vegetables and other food uses.
▶ Skin irritant. LD_{50} (rat, orl) 31000 mg/kg. WG2933500

6-O-*(9-Octadecenoyl):* [1338-43-8] *Sorbitan monooleate, BAN, USAN.* ***Sorbitan oleate, INN****. Sorbester P17. Span 80. NSC 406239. E494*
$C_{24}H_{44}O_6$ 428.608
Emulsifier and clarification agent in food preparations (sugar liquor or juice).
▶ Skin irritant. WG2932400

3,5,6-Trioctadecanoyl: [26658-19-5] ***Sorbitan tristearate, BAN, USAN****. Sorbester P38. Span 65. E492*
$C_{60}H_{114}O_8$ 963.556
Food emulsifier, stabiliser.

3,5,6-Tris(9-octadecenoyl): [5960-06-5]

[26266-58-0] ***Sorbitan trioleate, BAN, USAN****. Sorbester P37. Span 85*
$C_{60}H_{108}O_8$ 957.508
Food emulsifier.

5,6-O-*Isopropylidene:* [55730-73-9] *1,4-Anhydro-5,6*-O-*isopropylidene*-D-*glucitol*
$C_9H_{16}O_5$ 204.222
Mp 68-70°. $[\alpha]_D^{20}$ -6 (c, 1 in $CHCl_3$).

5,6-O-*Isopropylidene, 2-mesyl:* [55730-74-0] *1,4-Anhydro-5,6*-O-*isopropylidene-2*-O-*mesyl*-D-*glucitol*
$C_{10}H_{18}O_7S$ 282.314
Mp 112°.

5,6-O-*Isopropylidene, 2,3-dimesyl:* [55730-75-1] *1,4-Anhydro-5,6*-O-*isopropylidene-2,3-di*-O-*mesyl*-D-*glucitol*
$C_{11}H_{20}O_9S_2$ 360.406
Mp 163-163.5°.

Tetra-Me:1,4-Anhydro-2,3,5,6-tetra-O-*methyl*-D-*glucitol*
$C_{10}H_{20}O_5$ 220.265
Bp_{14} 170-174°. $[\alpha]_D^{22}$ -43 (c, 4.84 in EtOH).

Mixt. of partial esters, mono- and dianhydrides with oleic acid: [8007-43-0]

[37318-79-9] ***Sorbitan sesquioleate, BAN, USAN****. Arlacel C*
Oily viscous liq.
▶ Potent allergen.

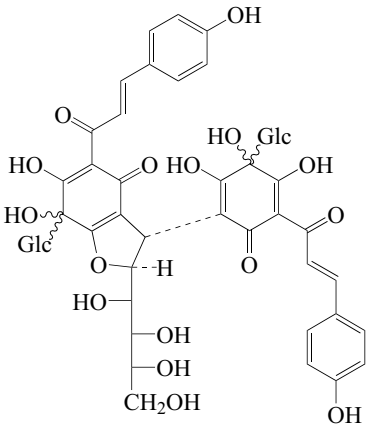
9-Octadecenoyl (2:3):Crill 43. Sorgen 30. Nikkol SO-15
Water in oil emulsifier, wetting agent, pigment dispersant. Mixt. of mono- and diesters of oleic acid.

[36521-89-8, 51938-44-4, 54392-26-6]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1055A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 727B (*ir*)
Goldsmith, H.A. *et al., Chem. Ind. (London)*, 1943, **52**, 326-328 (*sorbitan sesquioleate*)
Soltzberg, S. *et al., J.A.C.S.*, 1946, **68**, 919 (*D-form, synth, D-tetra-Me*)
Sherman, P. *et al., J. Colloid Sci.*, 1953, **8**, 35-37 (*sorbitan sesquioleate*)
Que, L. *et al., Biochemistry*, 1974, **13**, 146 (*cmr*)
Hanessian, S. *et al., Tet. Lett.*, 1974, 3983 (*D-isopropylidene mesyl, D-isopropylidene dimesyl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 332 (*esters, use*)
Sato, S. *et al., Anal. Lett.*, 1981, **14**, 531 (*use*)
Sato, S. *et al., Anal. Chim. Acta*, 1982, **142**, 319 (*use*)
Larni, E. *et al., Contact Dermatitis*, 1988, **19**, 368-371 (*sorbitan sesquioleate*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, SKV100; SKU700
Duclos, A. *et al., Synthesis*, 1994, 1087 (*D-isopropylidene*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 729 (*monooctadecanoate*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2620; 2621-2624 (*monooleate, monostearate, use, props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2620-2624 (*esters*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1328
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKV000; SKV100; SKV150

Anhydrosafflor Yellow B A-336

[184840-84-4]



$C_{48}H_{52}O_{26}$ 1044.923

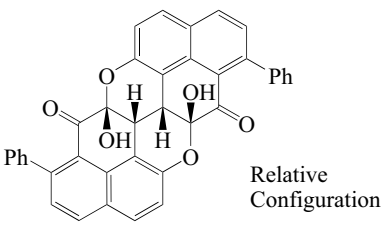
Isol. from fresh florets of safflower (*Carthamus tinctorius*). Amorph. yellow powder. λ_{max} 230 (log ϵ 4.33); 410 (log ϵ 4.62) (MeOH).

Kazuma, K. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1588-1599

Anigorootin A-337

[221287-38-3]

[193892-39-6, 193892-60-3]



Relative Configuration

$C_{38}H_{22}O_6$ 574.588

Phenalene dimer showing 2-fold rotational symmetry. Compd. 2 of Luis *et al*, 1997, has been reassigned this struct. (2002). Constit. of *Musa acuminata* (dwarf banana). Yellow solid. λ_{max} 249 (log ϵ 3.9); 284 (log ϵ 3.4); 358 (log ϵ 1.5); 448 (log ϵ 1.5) (MeOH).

4′-Hydroxy: ***4′-Hydroxyanigorootin***
$C_{38}H_{22}O_7$ 590.588
Constit. of the rhizomes of *Musa acuminata* (dwarf banana). Pale yellow solid. Contains a *p*-hydroxyphenyl residue. Formerly assigned an isomeric struct..

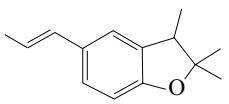
4′,4″-Dihydroxy: ***4′,4″-Dihydroxyanigorootin***
$C_{38}H_{22}O_8$ 606.587
Constit. of the rhizomes of *Musa acuminata* (dwarf banana). Pale yellow solid. Compd. 3 of Luis *et al*, 1997, was reassigned this struct. (2002).

Luis, J.G. *et al., Tetrahedron*, 1997, **53**, 8249-8256 (*isol*)
Hoelscher, D. *et al., Phytochemistry*, 1999, **50**, 155-161 (*isol, uv, ir, pmr, cmr*)
Otalvaro, F. *et al., Phytochemistry*, 2002, **60**, 61-66 (*isol, pmr, cmr, cryst struct*)

Anisoxide A-338

[643-49-2]

2,3-Dihydro-2,2,3-trimethyl-5-(1-propenyl)benzofuran, 9CI



$C_{14}H_{18}O$ 202.296

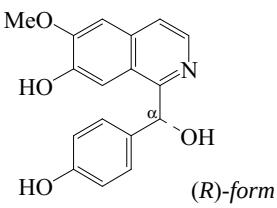
(±)-form

Isol. from oil of star anise (*Illicium verum*) after thermal fractionation. Mp 34-37°. Bp_{14} 142-143°. An artifact resulting from rearr. of Foeniculin (see 4-(1-Propenyl)phenol, P-512).

Jackson, R.W. *et al., J.C.S.*, 1937, 513 (*isol*)
Barton, D.H.R. *et al., J.C.S.*, 1958, 4393 (*synth*)
Okely, H.M. *et al., J.C.S. Perkin 1*, 1981, 897

Annocherine A A-339

Annocherine C



(*R*)-*form*

$C_{17}H_{15}NO_4$ 297.31

Annocherine A was the *S*-enantiomer and Annocherine C the *R*-form.

(R)-form [431982-10-4]

Alkaloid from the leaves of *Annona cherimola* (cherimoya). Yellow amorph. powder. Mp 123-125°. $[\alpha]_D^{25}$ -125 (c, 0.3 in $CHCl_3$). λ_{max} 260 ; 300 ; 331 (MeOH).

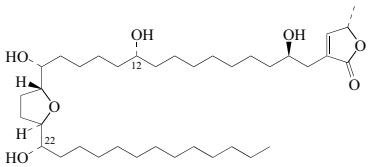
(S)-form

Alkaloid from *Annona cherimola* (cherimoya). Yellow needles. Mp 156-158°. $[\alpha]_D^{24}$ +135 (c, 0.1 in $CHCl_3$). λ_{max} 260 (log ϵ 3.41); 300 (log ϵ 3.1); 330 (log ϵ 3.52) (MeOH).

α-Me ether: ***Annocherine B***
$C_{18}H_{17}NO_4$ 311.337
Alkaloid from *Annona cherimola* (cherimoya). Amorph. yellow powder. Mp 196-198°. $[\alpha]_D^{24}$ +115 (c, 0.1 in $CHCl_3$). λ_{max} 260 (log ϵ 3.32); 300 (log ϵ 3.11); 331 (log ϵ 3.6) (MeOH).

Chen, C.-Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 2001, **48**, 1203-1206 (*Annocherine C*)
Chen, C.-Y. *et al., Phytochemistry*, 2001, **56**, 753-757 (*Annocherine A,B*)

Annoglacin A A-340



Absolute Configuration

$C_{37}H_{68}O_7$ 624.94

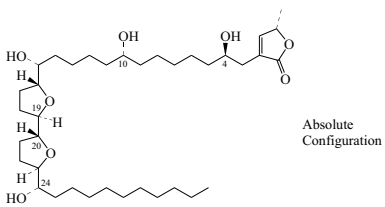
Constit. of the leaves of *Annona glabra* (pond apple). Waxy solid. $[\alpha]_D^{25}$ +15 ($CHCl_3$). λ_{max} 219 (log ϵ 3.62) (MeOH).

22-Epimer: ***Annoglacin B***
$C_{37}H_{68}O_7$ 624.94
Constit. of *Annona glabra* (pond apple). Waxy solid. $[\alpha]_D^{25}$ +15.7 ($CHCl_3$). λ_{max} 218 (log ϵ 3.48) (MeOH).

Liu, X.-X. *et al., Phytochemistry*, 1999, **50**, 815-821 (*isol, uv, ir, pmr, cmr, ms*)

Annoglaucin A-341

[164991-79-1]



Absolute Configuration

$C_{37}H_{66}O_8$ 638.924

Constit. of the seeds of *Annona purpurea* (soncoya). Waxy solid. Mp 58-59°. $[\alpha]_D^{20}$ +15.4 (c, 0.6 in $CHCl_3$). $[\alpha]_D$ +31 (c, 1 in MeOH). λ_{max} 210 (ϵ 10000) (EtOH).

24-Epimer: [249737-62-0] ***Atemoyacin D***
$C_{37}H_{66}O_8$ 638.924
Constit. of the seeds of *Annona atemoya* (custard apple). C-4, C-10 stereochem. not known.

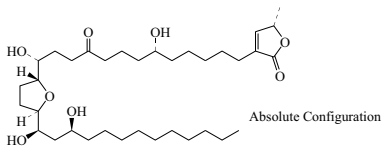
19,20-Diepimer: ***Purpuracenin***
$C_{37}H_{66}O_8$ 638.924
Constit. of the seeds of *Annona purpurea* (soncoya). Pale yellow wax. Mp 42-44°. $[\alpha]_D$ +26 (c, 1 in MeOH). λ_{max} 207 (log ϵ 4.32) (MeOH).

20,24-Diepimer: [184240-39-9] ***10-Hydroxytrilobacin***
$C_{37}H_{66}O_8$ 638.924
Constit. of *Asimina triloba* (pawpaw). Oil. $[\alpha]_D^{22}$ +8.3 (c, 0.36 in $CHCl_3$).

Stereoisomer: [184240-38-8] ***10-Hydroxyasimicin***
$C_{37}H_{66}O_8$ 638.924
Constit. of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D$ +17.3 (c, 0.22 in $CHCl_3$). Epimeric with Annoglaucin at C-24; C-4,C-10 configs. not known.

Etcheverry, S. *et al., Phytochemistry*, 1995, **38**, 1423-1426 (*Annoglaucin*)
He, K. *et al., J. Nat. Prod.*, 1996, **59**, 1029-1034 (*10-Hydroxyasimicin, 10-Hydroxytrilobicin*)
Wu, P. *et al., CA*, 1999, **131**, 334564f (*Atemoyacin D*)
Chavez, D. *et al., Phytochemistry*, 1999, **50**, 823-828 (*Purpuracenin*)

Annoglaxin A-342

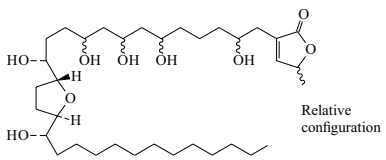


$C_{35}H_{62}O_8$ 610.87
Constit. of the leaves of *Annona glabra* (pond apple). Waxy powder. $[\alpha]_D^{25}$ +14.7 ($CHCl_3$).

Liu, X.-X. *et al., J. Nat. Prod.*, 1999, **62**, 848-852 (*isol, ir, pmr, cmr, ms*)

Annohexocin A-343

[167696-97-1]

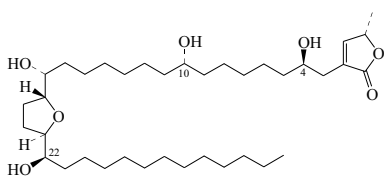


$C_{35}H_{64}O_9$ 628.885
Constit. of the leaves of *Annona muricata* (soursop). Powder. $[\alpha]_D^{22}$ +18.5 (c, 0.3 in $CHCl_3$). λ_{max} 208 (ϵ 1740) (MeOH).

Zeng, L. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 1865-1868 (*isol, uv, pmr, cmr*)

Annomontacin A-344

[137550-92-6]



$C_{37}H_{68}O_7$ 624.94
Solid. Mp 70-72° (34-36°). $[\alpha]_D^{20}$ +81 (c, 1 in MeOH). λ_{max} 224 (ϵ 16600) (MeOH) (Berdy).

4-Deoxy: [189630-57-7] ***4-Deoxyannomontacin***
$C_{37}H_{68}O_6$ 608.941
Wax. $[\alpha]_D^{25}$ +10.9 (c, 0.06 in $CHCl_3$). λ_{max} 228 (log ϵ 2.86) (MeOH).

*10-Deoxy, 15*S*-hydroxy:* ***Asitrilobin C***
$C_{37}H_{68}O_7$ 624.94
Constit. of *Asimina triloba* (pawpaw). Powder. Mp 85.3-86.4°. $[\alpha]_D$ -8 (c, 0.005 in CH_2Cl_2). λ_{max} 226 (log ϵ 3.7) (MeOH).

22-Epimer: [170900-29-5] ***Annomutacin***
$C_{37}H_{68}O_7$ 624.94
Constit. of *Annona muricata* (soursop). $[\alpha]_D$ +60 (c, 0.001 in EtOH). Possesses 4*R*,10ξ -config. λ_{max} 212 (ϵ 9200) (MeOH) (Berdy).

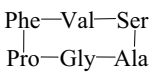
17,18-Diepimer: **cis-*Annomontacin***
$C_{37}H_{68}O_7$ 624.94
Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +36.5 (c, 0.03 in $CHCl_3$). λ_{max} 210 (log ϵ 3.72) (MeOH).

Stereoisomer: ***Asitrilobin A***
$C_{37}H_{68}O_7$ 624.94
Constit. of the seeds of *Asimina triloba* (pawpaw). Amorph. powder. Mp 79.3-82.5°. $[\alpha]_D^{22}$ -2.6 (c, 0.03 in CH_2Cl_2). Partial relative config. is known λ_{max} 226 (log ϵ 4.3) (MeOH).

Jossang, A. *et al., J. Nat. Prod.*, 1991, **54**, 967-971 (*isol, pmr, cmr*)
Fang, X.-P. *et al., J. Nat. Prod.*, 1992, **55**, 1655-1663 (*isol*)
Colman-Saizarbitoria, T.J. *et al., J. Nat. Prod.*, 1994, **57**, 486-493 (*isol*)
Wu, F.E. *et al., J. Nat. Prod.*, 1995, **58**, 1430-1437 (*Annomutacin*)
Alali, F. *et al., Bioorg. Med. Chem.*, 1997, **5**, 549-555 (*4-Deoxyannomontacin*)
Yu, Q. *et al., J.C.S. Perkin 1*, 1999, 1183-1188 (*synth, 4-Deoxyannomontacin*)
Woo, M.-H. *et al., Phytochemistry*, 1999, **50**, 1033-1040 (*Asitrilobin A*)
Woo, M.-H. *et al., Bioorg. Med. Chem.*, 2000, **8**, 285-290 (*Asitrilobin C*)
Liaw, C.-C. *et al., J. Nat. Prod.*, 2002, **65**, 470-475 (*cis-Annomontacin*)

Annomuricatin A A-345

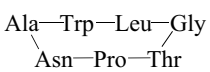
[173994-05-3]



$C_{27}H_{38}N_6O_7$ 558.633
Cyclic peptide. Constit. of the seeds of *Annona muricata* (soursop). Needles (MeOH). Mp 285-287°. $[\alpha]_D^{23}$ +11.28 (c, 0.4 in Py). λ_{max} 202 (ϵ 2800) (EtOH).

Li, C.-M. *et al., Yunnan Zhiwu Yanjiu*, 1995, **17**, 459-462; *CA*, **124**, 170600 (*isol, pmr, ms*)

Annomuricatin B A-346

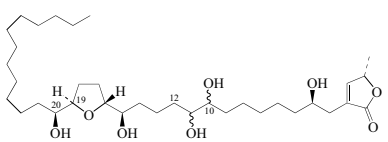


$C_{35}H_{49}N_9O_9$ 739.827
Cyclic peptide. Constit. of the seeds of *Annona muricata* (soursop). Needles ($CHCl_3$/MeOH). Mp 213°. $[\alpha]_D^{19}$ -37.2 (c, 0.5 in MeOH). λ_{max} 204 (log ϵ 3.49); 221 (log ϵ 3.53); 282 (log ϵ 2.65); 290 (log ϵ 2.61) (MeOH).

Li, C.-M. *et al., Phytochemistry*, 1998, **48**, 555-556 (*isol, uv, ir, pmr, cmr, ms*)

Annomuricin A A-347

[167172-78-3]



$C_{35}H_{64}O_8$ 612.886
Constit. of the leaves of *Annona muricata* (soursop). Amorph. powder. $[\alpha]_D^{22}$ -6.4. Possesses *threo*-config. at C-10/C-11. Abs. config. of remainder of struct. is known λ_{max} 220 (ϵ 3100) (MeOH) (Berdy).

11-Deoxy, 12-hydroxy: [167355-38-6] ***Muricatocin B***
$C_{35}H_{64}O_8$ 612.886
Constit. of the leaves of *Annona muricata* (soursop). Powder. $[\alpha]_D^{22}$ +62.5 (c, 0.001 in EtOH). λ_{max} 214 (ϵ 9500) (MeOH).

10- or 11-Epimer: [167355-37-5] ***Annomuricin B***
$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Amorph. powder. $[\alpha]_D^{22}$ -11.7. Possesses *erythro*-config. at C-10/C-11 λ_{max} 220 (ϵ 3000) (MeOH) (Berdy).

10- or 12-Epimer, 11-deoxy, 12-hydroxy: [167355-40-0] ***Muricatocin C***
$C_{35}H_{64}O_8$ 612.886
Constit. of the leaves of *Annona muricata* (soursop). Powder. $[\alpha]_D^{22}$ +32.5 (c, 0.001 in EtOH). λ_{max} 225 (ϵ 9100) (MeOH).

20-Epimer: [167355-39-7] ***Annomuricin C***
$C_{35}H_{64}O_8$ 612.886
Constit. of the leaves of *Annona muricata* (soursop). Powder. $[\alpha]_D^{22}$ +57.7 (c, 0.0005 in EtOH). Possesses *threo*-config. at C-10/C-11 λ_{max} 220 (ϵ 3800) (MeOH).

20-Epimer, 11-deoxy, 12-hydroxy: [167172-79-4] ***Muricatocin A***
$C_{35}H_{64}O_8$ 612.886
Constit. of the leaves of *Annona muricata* (soursop). Powder. $[\alpha]_D^{22}$ +21.8 (c, 0.001 in EtOH). λ_{max} 216 (ϵ 8500) (MeOH).

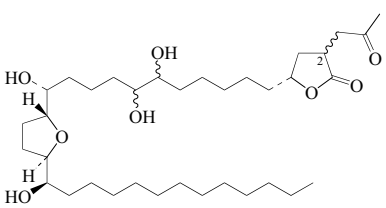
10,20- or 11,20-Diepimer: ***Annomuricin E***
$C_{35}H_{64}O_8$ 612.886
Constit. of the leaves of *Annona muricata* (soursop). Solid. $[\alpha]_D$ +12.5 (c, 0.04 in MeOH). Possesses *erythro*-config. at C-10/C-11 λ_{max} 218 (log ϵ 3.76) (MeOH).

Stereoisomer: [205814-19-3] ***Cheliensisin B***
$C_{35}H_{64}O_8$ 612.886

Wu, F.-E. *et al., J. Nat. Prod.*, 1995, **58**, 830-836; 902-908; 909-915
Li, C. *et al., CA*, 1998, **128**, 280809g (*Cheliensisin B*)
Kim, G.-S. *et al., J. Nat. Prod.*, 1998, **61**, 432-436 (*Annomuricin E*)

Annomuricin-D-one A-348

[184093-47-8, 184093-48-9]



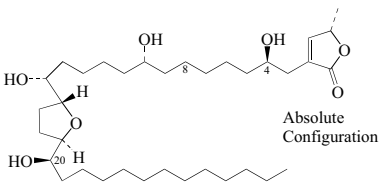
$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Powder. $[\alpha]_D^{25}$ +15 (c, 10 in $CHCl_3$). Obt. as a 1:1 mixture of C-2 epimers λ_{max} 205 (ϵ 7750) (MeOH).

Zeng, L. *et al., J. Nat. Prod.*, 1996, **59**, 1035-1042 (*isol, uv, ir, pmr, cmr, ms*)

Annonacin A-349

[111035-65-5]

[129212-95-9, 152985-32-5]
Annonacin 1. Howiicin A



$C_{35}H_{64}O_7$ 596.886

MF incorr. given as C_{33} in CA. Closely related to Goniothalamicin, G-296. Constit. of *Annona* spp.. Sol. MeOH, C_6H_6, hexane; poorly sol. H_2O. Mp 57° Mp 65-67° Mp 82-83.5°. $[\alpha]_D$ +20.8 (c, 5 in $CHCl_3$). λ_{max} 210 (ϵ 10700) (MeOH) (Derep). λ_{max} 207 (ϵ 15390) (2-propanol) (Berdy).

4-Ac: [183551-74-8] ***4-Acetylannonacin***
$C_{37}H_{66}O_8$ 638.924
Wax. Mp 67-68°. $[\alpha]_D^{21}$ +13 (c, 0.1 in MeOH).

10-Ketone: [123266-21-7] ***Annonacin-10-one***. *Annonacinone*
$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona muricata* (soursop). Cryst. Sol. MeOH, C_6H_6, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O. Mp 73-75°. $[\alpha]_D^{20}$ +31.1 (c, 0.06 in MeOH).

8-Hydroxy: [144182-25-2] ***8-Hydroxyannonacin***. *Gardnerin*
$C_{35}H_{64}O_8$ 612.886
Waxy solid. $[\alpha]_D$ +6.1 (c, 0.12 in MeOH). Stereochem. not confirmed. Stereochem. identity of 8-Hydroxyannonacin and Gardnerin not certain λ_{max} 209 (ϵ 16600) (MeOH) (Berdy).

8-Hydroxy, 10-ketone: ***Montanacin B***
$C_{35}H_{62}O_8$ 610.87
Solid. Stereochem. not fully determined.

4-Deoxy: [133352-34-8]

[152985-34-7] ***Corossoline***. *Howiicin C*
$C_{35}H_{64}O_6$ 580.887
Constit. of *Annona muricata* (soursop). Cryst. (EtOAc). Mp 45-50° Mp 83-85°. $[\alpha]_D$ +24 (c, 3.4 in $CHCl_3$). $[\alpha]_D$ +19 (c, 0.2 in MeOH).

4-Deoxy, 10-ketone: [133352-33-7] ***Corossolone***
$C_{35}H_{62}O_6$ 578.871
Constit. of *Annona muricata* (soursop). Cryst. (EtOAc). Mp 55-57°. $[\alpha]_D$ +15 (c, 0.13 in MeOH). No stereochem. detd..

20-Epimer: [130853-76-8]

[129212-96-0] ***Annonacin A***. *Annonacin 2*
$C_{35}H_{64}O_7$ 596.886
Isol. from *Annona squamosa* (sugar apple). Amorph. $[\alpha]_D^{25}$ +23.8 (c, 0.4 in $CHCl_3$). C-4 and C-10 stereochem. not confirmed.

19,20-Diepimer: [172586-13-9] **cis-*Annonacin***
$C_{35}H_{64}O_7$ 596.886
Constit. of *Annona muricata* (soursop). Amorph. powder. Mp 77°. $[\alpha]_D^{25}$ +10 ($CHCl_3$). λ_{max} 215 (ϵ 9700) (MeOH).

19,20-Diepimer, 10-ketone: [172488-91-4] **cis-*Annonacin-10-one***
$C_{35}H_{62}O_7$ 594.871
Constit. of the seeds of *Annona muricata* (soursop). Amorph. powder. Mp 70°. $[\alpha]_D$ +6.2 (c, 0.07 in $CHCl_3$). λ_{max} 209 (ϵ 8400) (MeOH).

19,20-Diepimer, 8-hydroxy, 10-ketone:- ***Montanacin C***
$C_{35}H_{62}O_8$ 610.87
Solid. Stereochem. not fully determined.

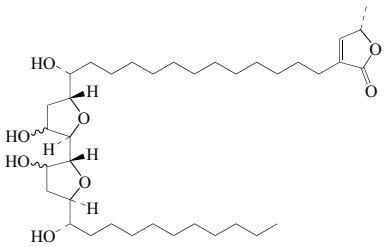
19,20-Diepimer, 4-deoxy, 10-ketone: **cis-*Corossolone***
$C_{35}H_{62}O_6$ 578.871
Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +13.6 (c, 0.1 in MeOH). λ_{max} 210 (log ϵ 3.61) (MeOH).

Stereoisomer, 8-hydroxy: [205814-20-6] ***Cheliensisin C***
$C_{35}H_{64}O_8$ 612.886

McCloud, T.G. *et al., Experientia*, 1987, **43**, 947 (*isol*)
Alkofahi, A. *et al., Experientia*, 1988, **44**, 83 (*isol*)
Xu, L. *et al., J.O.C.*, 1989, **54**, 5418-5421 (*Annonacinone*)
Nonfon, M. *et al., Phytochemistry*, 1990, **29**, 1951 (*isol, struct*)
Lieb, F. *et al., Planta Med.*, 1990, **56**, 317 (*isol, pmr, cmr, struct*)
Jossang, A. *et al., Tet. Lett.*, 1990, **31**, 1861 (*Annonacinone*)
Cortes, D. *et al., Can. J. Chem.*, 1991, **69**, 8-11 (*Corossoline, Corossolone*)
Yu, J.G. *et al., J.O.C.*, 1992, **57**, 6198 (*8-Hydroxyannonacin*)
Zhang, L. *et al., Zhiwu Xuebao*, 1993, **35**, 390; *CA*, **120**, 129491 (*Howiicins*)
Laprevote, D. *et al., Tetrahedron*, 1994, **50**, 8479 (*ms, struct*)
Yao, Z.J. *et al., J.O.C.*, 1995, **60**, 1170-1176 (*Corossoline, synth*)
Makabe, H. *et al., Heterocycles*, 1996, **43**, 2229 (*synth, Corossoline*)
Rieser, M.J. *et al., J. Nat. Prod.*, 1996, **59**, 100 (*cis-Annonacins*)
Ye, Q. *et al., Nat. Prod. Lett.*, 1996, **8**, 291-298 (*4-Acetylannonacin*)
Zeng, L. *et al., Nat. Prod. Rep.*, 1996, **13**, 275-306 (*rev*)
Chen, Y. *et al., Chin. Chem. Lett.*, 1997, **8**, 971-974 (*Gardnerin*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)
Li, C. *et al., CA*, 1998, **128**, 280809g (*Cheliensisin C*)
Hanessian, S. *et al., J.O.C.*, 1998, **63**, 1049-1057 (*synth*)
Yu, Q. *et al., J.O.C.*, 1999, **64**, 2440-2445 (*synth, Corossoline*)
Wang, L.-Q. *et al., Nat. Prod. Lett.*, 2000, **14**, 83-90 (*Montanacins*)
Hu, T.-S. *et al., Org. Lett.*, 2000, **2**, 887-889 (*synth*)
Hu, T.-S. *et al., J.O.C.*, 2001, **66**, 853-861 (*synth*)
Liaw, C.-C. *et al., J. Nat. Prod.*, 2002, **65**, 470-475 (*cis-Corossolone*)

Annonin XIV A-350

[129138-52-9]



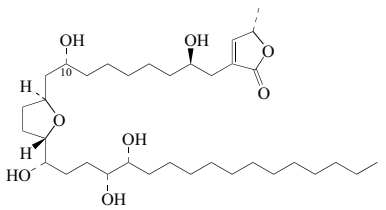
$C_{37}H_{66}O_8$ 638.924

Incorrect struct. has been assigned. Constit. of *Annona squamosa* (sugar apple). Amorph. wax. $[\alpha]_D^{25}$ +15.7 (c, 0.3 in CH_2Cl_2).

Nonfon, M. *et al., Phytochemistry*, 1990, **29**, 1951 (*isol, pmr, cmr, ms*)

Annopentocin A A-351

[184093-44-5]



$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Amorph. powder. $[\alpha]_D^{25}$ +12 (c, 14 in $CHCl_3$). λ_{max} 215 (ϵ 9600) (MeOH). λ_{max} 215 (ϵ 2600) (MeOH) (Berdy).

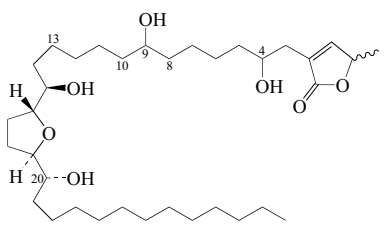
19- or 20-Epimer: [184093-46-7] ***Annopentocin C***
$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Oil. $[\alpha]_D^{25}$ +9 (c, 11 in $CHCl_3$). λ_{max} 214 (ϵ 9750) (MeOH).

19,20-Diepimer: [184093-45-6] ***Annopentocin B***
$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Oil. $[\alpha]_D^{25}$ +15 (c, 10 in $CHCl_3$). λ_{max} 214 (ϵ 9800) (MeOH).

Zeng, L. *et al., J. Nat. Prod.*, 1996, **59**, 1035 (*isol, uv, ir, pmr, cmr, ms*)

Annoreticuin A-352

[142488-56-0]



$C_{35}H_{64}O_7$ 596.886
Acetogenin isol. from *Annona reticulata* (custard apple). Amorph. powder. Mp 75-

77°. $[\alpha]_D^{24}$ +10.5 (c, 0.02 in $CHCl_3$). λ_{max} 210 (ϵ 40100) (EtOH) (Berdy).

9-Ketone: [152369-74-9] ***Annoreticuin-9-one***
$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona reticulata* (custard apple). Amorph. powder. $[\alpha]_D^{25}$ +11.7 (c, 0.02 in $CHCl_3$). λ_{max} 215 (ϵ 2500) (MeOH) (Berdy).

9-Ketone, stereoisomer (1): [191876-89-8] ***Mosin B***
$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona squamosa* (sugar apple). Waxy solid. $[\alpha]_D^{23}$ +11.5 (c, 0.005 in CH_2Cl_2). Abs. config. determined in 2001 λ_{max} 222 (log ϵ 3.57) (MeOH).

9-Ketone, stereoisomer (2): [191936-12-6] ***Mosin C***
$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona squamosa* (sugar apple). Waxy solid. $[\alpha]_D^{23}$ -2.7 (c, 0.007 in CH_2Cl_2). λ_{max} 216 (log ϵ 3.56) (MeOH).

4-Deoxy: [206192-79-2] ***4-Deoxyannoreticuin***
$C_{35}H_{64}O_6$ 580.887
Constit. of *Annona squamosa* (sugar apple). Amorph. powder. $[\alpha]_D^{23}$ +6.8 (c, 0.03 in CH_2Cl_2). λ_{max} 215 (log ϵ 3.5) (MeOH).

4-Deoxy, 19,20-diepimer: [206192-80-5] **cis-*4-Deoxyannoreticuin***
$C_{35}H_{64}O_6$ 580.887
Constit. of *Annona squamosa* (sugar apple). Amorph. powder. $[\alpha]_D^{23}$ +6.8 (c, 0.01 in CH_2Cl_2). λ_{max} 218 (log ϵ 3.61) (MeOH).

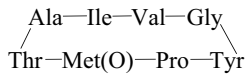
9-Deoxy, 11-oxo: [155709-42-5] ***Reticulacinone***
$C_{35}H_{62}O_7$ 594.871
Isol. from stem bark of *Annona reticulata* (custard apple). Waxy solid.

9-Deoxy, 8,13-dihydroxy: [128741-22-0] ***Annomonicin***
$C_{35}H_{64}O_8$ 612.886
Waxy solid. Sol. MeOH, hexane; poorly sol. H_2O. Mp 45-48°. $[\alpha]_D^{20}$ +4 (c, 1.0 in MeOH). No stereochem. detd. λ_{max} 224 (ϵ 31600) (EtOH) (Derep).

Jossang, A. *et al., Tet. Lett.*, 1990, **31**, 1861-1864 (*Annomonicin*)
Wu, Y.-C. *et al., Heterocycles*, 1992, **34**, 667-674 (*Annoreticuin*)
Chang, F.-R. *et al., J. Nat. Prod.*, 1993, **56**, 1688-1694 (*Annoreticuin-9-one*)
Hisham, A. *et al., Phytochemistry*, 1994, **35**, 1325-1329 (*Reticulacinone*)
Hopp, D.C. *et al., J. Nat. Prod.*, 1997, **60**, 581-586 (*Mosins, Annoreticuin-9-one*)
Hopp, D.C. *et al., Phytochemistry*, 1998, **47**, 803-809 (*4-Deoxyannoreticuin*)
Maezaki, N. *et al., Org. Lett.*, 2001, **3**, 429-432 (*Mosin B, synth, abs config*)

Annosquamosin A A-353

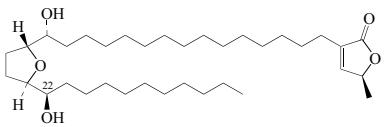
[192584-48-8]



$C_{39}H_{60}N_8O_{11}S$ 849.016
Cyclic peptide. Constit. of the seeds of *Annona squamosa* (sugar apple). Needles (MeOH). Mp 215-216°. $[\alpha]_D^{24}$ -65.3 (c, 0.4 in MeOH).
Chao-Ming, L. *et al., Phytochemistry*, 1997, **45**, 521-523 (*isol, ir, pmr, cmr, ms*)

Annotemoyin 1 A-354

[180892-69-7]



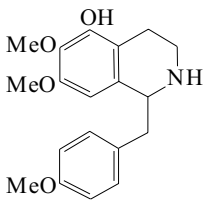
$C_{35}H_{64}O_5$ 564.888
Suggested absolute configuration is shown. Constit. of the seeds of *Annona atemoya* (custard apple). Waxy solid. $[\alpha]_D$ +21 (c, 0.1 in MeOH). λ_{max} 217 (log ϵ 3.63) (EtOH).

22-Epimer: [181377-80-0] ***Annotemoyin 2***
$C_{35}H_{64}O_5$ 564.888
Constit. of the seeds of *Annona atemoya* (custard apple). Waxy solid. $[\alpha]_D$ +20 (c, 0.1 in MeOH). λ_{max} 217 (log ϵ 3.66) (EtOH).

Duret, P. *et al., Nat. Prod. Lett.*, 1996, **8**, 89-95 (*isol, uv, ir, pmr, cmr*)

Anomuricine A-355

[78416-89-4]
1,2,3,4-Tetrahydro-6,7-dimethoxy-1-[(4-methoxyphenyl)methyl]-5-isoquinolinol, 9CI. 1,2,3,4-Tetrahydro-5-hydroxy-6,7-dimethoxy-1-(4-methoxybenzyl)isoquinoline



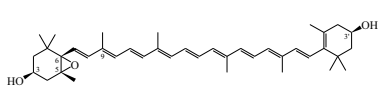
$C_{19}H_{23}NO_4$ 329.395
(ξ)-*form*
Minor alkaloid from the root and stem barks of *Annona muricata* (soursop). Noncryst.

Me ether: [78478-27-0] *1,2,3,4-Tetrahydro-5,6,7-trimethoxy-1-[(4-methoxyphenyl)-methyl]isoquinoline, 9CI.* ***Anomurine***
$C_{20}H_{25}NO_4$ 343.422
Minor alkaloid from the root and stem bark of *Annona muricata* (soursop). Noncryst.

Leboeuf, M. *et al., Planta Med.*, 1981, **42**, 37 (*uv, pmr, ms, struct*)

Antheraxanthin A-356

5,6-Epoxy-5,6-dihydro-β,β-carotene-3,3′-diol, 9CI. Zeaxanthin epoxide. 5,6-Epoxyzeaxanthin

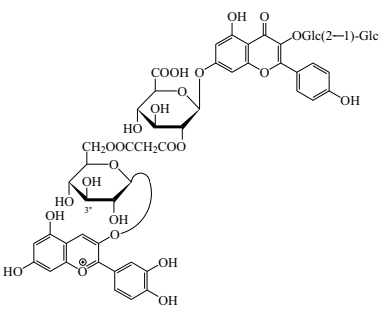


(3S,3′R,5S,6R,9E)-form

$C_{40}H_{56}O_3$ 584.881
(3*S*,3′*R*,5*S*,6*R*,9*E*)-*form* [25494-44-4] ***Antheraxanthin A***
Constit. of *Capsicum* fruit; potential nutriceutical. Cryst. (MeOH). Mp 197°.
(3*S*,3′*R*,5*S*,6*R*,9*Z*)-*form* [68831-78-7] **cis-*Antheraxanthin***
Cryst. (MeOH). Mp 108°.
(3*S*,3′*R*,5*R*,6*S*)-*form* [640-03-9] ***Antheraxanthin B***

λ_{max} 420 ; 445 ; 475 (Et_2O).
Tappi, G. *et al., Helv. Chim. Acta*, 1949, **32**, 50 (*isol*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527 (*synth, pmr, ms, uv, ord*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1841 (*occur*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 2198 (*abs config*)
Molnar, P. *et al., Acta Chim. Hung.*, 1983, **112**, 477 (*cmr*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 231 (*bibl*)
Tsushima, M. *et al., J. Nat. Prod.*, 2000, **63**, 960-964 (*Antheraxanthin B*)

Allium schoenoprasum Anthocyanin-flavonol A-357



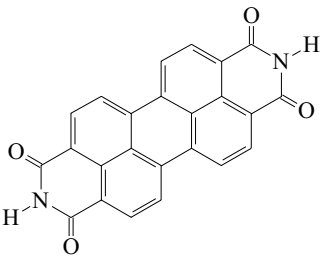
$C_{57}H_{59}O_{35}^{\oplus}$ 1304.072
Constit. of the flowers of *Allium schoenoprasum* (chives).

3″-Ac:
$C_{59}H_{61}O_{36}^{\oplus}$ 1346.109
Constit. of the flowers of *Allium schoenoprasum* (chives).

Fossen, T. *et al., Phytochemistry*, 2000, **54**, 317-323

Anthra[2,1,9-*def*:6,5,10-*d′e′f′*]diisoquinoline-1,3,8,10(2*H*,9*H*)-tetrone, 9CI A-358

[81-33-4]
Perylene-3,4:9,10-tetracarboxdiimide. C.I. Pigment Violet 29



$C_{24}H_{10}N_2O_4$ 390.354

N,N′-*Di-Me:* [5521-31-3] *Indanthrene Red GG. Perylene maroon. C.I. Pigment Red 179. C.I. Vat Red 23*
$C_{26}H_{14}N_2O_4$ 418.408
Red-violet needles.

N,N′-*Bis(tridecyl):* [95689-92-2]
$C_{50}H_{62}N_2O_4$ 755.051
Mp 300°.

N,N′-*Bis(3,5-dimethylphenyl):* [4948-15-6] *C.I. Pigment Red 149*
$C_{40}H_{26}N_2O_4$ 598.656
FDA approved colourant for food contact polymers. Red prisms (quinoline). Mp >300°.

N,N′-*Bis(4-methoxyphenyl):* [6424-77-7] *Indanthrene Scarlet R. Perylene red. Perylene scarlet. C.I. Pigment Red 190. C.I. Vat Red 29*
$C_{38}H_{22}N_2O_6$ 602.602

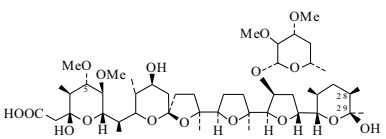
N,N′-*Bis(2-phenylethenyl):* [97540-34-6] *Perylene green*
$C_{40}H_{22}N_2O_4$ 594.625

N-*Amino,* N′-*(1-butylpentyl):*
$C_{33}H_{29}N_3O_4$ 531.61Mp >350°.

Ger. Pat., 1959, 1 115 386; *CA*, **56**, 7244c (*synth*)
Manukian, B.K. *et al., Helv. Chim. Acta*, 1971, **54**, 2924-2929 (*struct, ir, ms, pmr*)
Rademacher, A. *et al., Chem. Ber.*, 1982, **115**, 2927-2934 (*synth, ms*)
Langhals, H. *et al., Chem. Ber.*, 1985, **118**, 4641-4645; 1991, **124**, 529-535 (*synth, ir, uv, pmr*)
Haedicke, E. *et al., Acta Cryst. C*, 1986, **42**, 189-195; 195-198 (*cryst struct*)
Akers, K. *et al., Spectrochim. Acta A*, 1988, **44**, 1129-1135 (*ir, uv, Raman*)
Quante, H. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 1323-1325 (*bibl*)
Langhals, H. *et al., Chem. Eur. J.*, 1998, **4**, 2110-2116 (*N-amino derivs, synth, ir, pmr, cmr, ms, use*)
Osvath, R. *et al., Food Chem. News*, 2001, **43(19)**, 6 (*C.I. Pigment Red 149, use*)

Antibiotic X 14868A A-359

[79356-08-4]
Maduramicin, INN, USAN. *Maduramicin α. Cygro. X 14868A. CL 273703. LL-C 23024α-A. Antibiotic CL 273703. Antibiotic LL-C 23024α-A*



$C_{47}H_{80}O_{17}$ 917.139

Polyether antibiotic. Anibiotic approved as a feed additive for broiler chickens in the UK. Cryst. (EtOAc/hexane) (as Na salt). Mp 193-194° (Na salt). $[\alpha]_D^{25}$ +40.6 (c, 1 in $CHCl_3$).

▶ Cardiotoxic in cattle.

O^5-*De-Me:* [79331-53-6] ***Antibiotic X 14868C.*** *Maduramicin β. LL-C23024B. X 14868C. Antibiotic LL-C23024B*
$C_{46}H_{78}O_{17}$ 903.112
Cryst. (as Na salt). Mp 172-175° (Na salt). $[\alpha]_D^{25}$ +49.6 (c, 1 in $CHCl_3$).

O^{29}-*Me:* [79296-11-0] ***Antibiotic X 14868B.*** *X 14868B*
$C_{48}H_{82}O_{17}$ 931.166
Cryst. (hexane) (as Na salt). Mp 172.5-174° (Na salt). $[\alpha]_D^{25}$ +46.1 (c, 1 in $CHCl_3$).

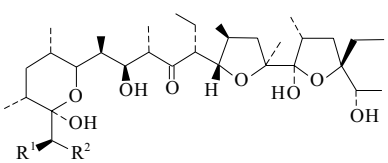
28-Epimer: [79331-54-7] ***Antibiotic X 14868D.*** *X 14868D*
$C_{47}H_{80}O_{17}$ 917.139
Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 194-195° (as Na salt). $[\alpha]_D^{25}$ +41.4 (c, 1 in $CHCl_3$).

[84878-61-5]

Liu, C.-M. *et al., J. Antibiot.*, 1983, **36**, 343 (*isol, struct, props*)
Rajan, S. *et al., J. Antibiot.*, 1984, **37**, 1495; 1651 (*struct, pmr, biosynth*)
Ellestad, G.A. *et al., J. Antibiot.*, 1986, **39**, 447 (*salts, cmr*)
Siegel, M.M. *et al., Biomed. Environ. Mass Spectrom.*, 1987, **14**, 29 (*ms*)
Shlosberg, A. *et al., Vet. Res. Commun.*, 1992, **16**, 45 (*tox*)
Mead, J.R. *et al., Antimicrob. Agents Chemother.*, 1995, **39**, 854 (*activity*)
Kennedy, D.G. *et al., Food Addit. Contam.*, 1997, **14**, 27-33 (*anal*)

Antibiotic X 14889A A-360

[97671-96-0]
X 14889A



$R^1 = CH_3$, $R^2 = H$

$C_{33}H_{60}O_8$ 584.832

Polyether antibiotic. Related to Lysocellin. Ruminant antibiotic feed additive. Cryst. (hexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 149-150°. $[\alpha]_D$ +29.3 (c, 1 in MeOH). $[\alpha]_D$ +6.7 (c, 1 in $CHCl_3$).

Eur. Pat., 1985, 143 438; *CA*, **103**, 86514 (*isol, struct, props*)
Liu, C.-M. *et al., J. Antibiot.*, 1993, **46**, 275; 280 (*isol, cryst struct*)

Antibiotic X 14889C A-361

[97671-95-9]
X 14889C
As Antibiotic X 14889A, A-360 with
R^1 = H, R^2 = COOH

$C_{33}H_{58}O_{10}$ 614.815

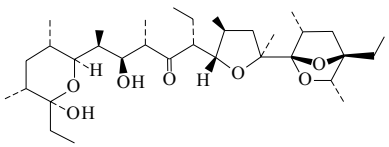
Polyether antibiotic. Related to Lysocellin. Ruminant feed additive. Cryst. $+1H_2O$ (Et_2O/hexane)(as Na salt). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.

▶ LD_{50} (mus, ipr) 120 mg/kg , LD_{50} (mus, orl) 190 mg/kg. OL5820000

Eur. Pat., 1985, 143 438; *CA*, **103**, 86514 (*isol, struct, props*)
Liu, C.-M. *et al., J. Antibiot.*, 1993, **46**, 275; 280 (*isol, cryst struct*)

Antibiotic X 14889D A-362

[97671-94-8]
X 14889D



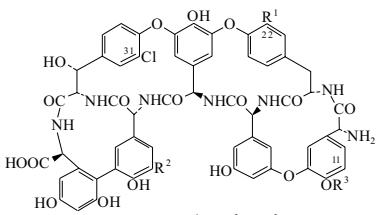
$C_{33}H_{58}O_7$ 566.817

Polyether antibiotic. Ruminant antibiotic feed additive. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 117°. Related to Lysocellin.

Eur. Pat., 1985, 143 438; *CA*, **103**, 86514 (*isol*)
Westley, J.W. *et al., J. Antibiot.*, 1986, **39**, 1704 (*struct*)
Liu, C.-M. *et al., J. Antibiot.*, 1993, **46**, 275; 280 (*isol, cryst struct*)

Antibiotic A 41030 A-363

[89147-18-2]
A 41030



	R^1	R^2	R^3
A	Cl	Cl	H
B	Cl	H	H
C	Cl	Cl	Gal
D	H	Cl	H
E	H	H	H
F	Cl	Cl	Gal-Gal
G	Cl	Cl	Gal-Gal

Glycopeptide antibiotic complex related to Vancomycin. Components D and G have two additional butyl groups each attached to the peptide nucleus at undetermined locations. Prod. by *Streptomyces virginiae*. Growth promotor and feed additive for poultry, swine, and ruminants.

Antibiotic A 41030A [89139-41-3]
22,31,45-Trichloro-7-demethyl-64-O-demethyl-19-deoxyristomycin A aglycone, 9CI

$C_{58}H_{44}Cl_3N_7O_{18}$ 1233.38
Sol. DMSO, MeCN, MeOH-H_2O, DMF, acids, H_2O; fairly sol. Me_2CO, THF, EtOAc; poorly sol. hexane. $[\alpha]_D^{25}$ -19.6 (c, 9.0 in DMSO). pK_{a1} 5.53; pK_{a2} 7.6; pK_{a3} 10.37; pK_{a4} 10.5 (66% DMF). Major component of complex λ_{max} 278 (ε 11100) (MeOH aq.) (Berdy). λ_{max} 278 (ε 11100) (MeOH-HCl) (Berdy). λ_{max} 298 (ε 17200)

(MeOH-NaOH) (Berdy).

► LD_{50} (mus, ipr) 300 - 700 mg/kg. VJ8598600

Antibiotic A 41030B [89139-42-4]
22,31-Dichloro-7-demethyl-64-O-demethyl-19-deoxyristomycin A aglycone. Antibiotic L 17392. A 41030B. L 17392

$C_{58}H_{45}Cl_2N_7O_{18}$ 1198.935
Sol. DMSO, DMF, H_2O, MeCN, MeOH-H_2O, acids; fairly sol. Me_2CO, EtOAc, THF; poorly sol. hexane. pK_{a1} 5.6; pK_{a2} 7.5; pK_{a3} 10 (66% DMF). λ_{max} 278 (ϵ 9600) (MeOH aq.) (Berdy). λ_{max} 278 (ϵ 9600) (MeOH-HCl) (Berdy). λ_{max} 298 (ϵ 16800) (MeOH/NaOH) (Berdy).

► LD_{50} (mus, ipr) 300 - 700 mg/kg. VJ8598000

Antibiotic A 41030C [89140-21-6]
A 41030C

$C_{64}H_{54}Cl_3N_7O_{23}$ 1395.522
Sol. DMSO, DMF, H_2O, MeCN, MeOH-H_2O, acids; fairly sol. Me_2CO, THF, EtOAc; poorly sol. hexane. pK_{a3} 10 (66% DMF). λ_{max} 278 (ϵ 8500) (MeOH aq.) (Berdy). λ_{max} 278 (ϵ 8400) (MeOH/HCl) (Berdy). λ_{max} 298 (ϵ 14000) (MeOH/NaOH) (Berdy).

► LD_{50} (mus, ipr) 300 - 700 mg/kg. VJ8598500

Antibiotic A 41030D
A 41030D

$C_{66}H_{64}Cl_2N_8O_{18}$ 1328.18
Sol. DMSO, acids, MeOH-H_2O, MeCN, H_2O, DMF; fairly sol. Me_2CO, THF, EtOAc; poorly sol. hexane. pK_{a2} 7.6; pK_{a3} 10 (66% DMF). λ_{max} 278 (ϵ 10600) (MeOH aq.) (Berdy). λ_{max} 278 (ϵ 10600) (MeOH/HCl) (Berdy). λ_{max} 298 (ϵ 19900) (MeOH/NaOH) (Berdy).

Antibiotic A 41030E [89139-43-5]
A 41030E

$C_{58}H_{46}ClN_7O_{18}$ 1164.49
Sol. DMSO, MeOH-H_2O, MeCN, H_2O, DMF, acids; fairly sol. Me_2CO, EtOAc, THF; poorly sol. hexane. pK_{a1} 5.8; pK_{a2} 7.7; pK_{a3} 10 (66% DMF). λ_{max} 278 (ϵ 8500) (MeOH aq.) (Berdy). λ_{max} 278 (ϵ 8500) (MeOH/HCl) (Berdy). λ_{max} 298 (ϵ 15500) (MeOH/NaOH) (Berdy).

Antibiotic A 41030F [89140-20-5]
A 41030F

$C_{70}H_{64}Cl_3N_7O_{28}$ 1557.664
Sol. DMSO, H_2O, MeCN, MeOH-H_2O, acids, DMF; fairly sol. Me_2CO, EtOAc, THF; poorly sol. hexane. pK_{a2} 7.1; pK_{a3} 10 (66% DMF). λ_{max} 278 (ϵ 19300) (MeOH aq.) (Berdy). λ_{max} 278 (ϵ 19300) (MeOH/HCl) (Berdy). λ_{max} 298 (ϵ 14500) (MeOH/NaOH) (Berdy).

Antibiotic A 41030G
A 41030G

$C_{78}H_{83}Cl_3N_8O_{28}$ 1686.909
Sol. DMSO, DMF, H_2O, acids, MeCN, MeOH-H_2O; fairly sol. Me_2CO, EtOAc, THF; poorly sol. hexane. pK_{a3} 10.5 (66% DMF). λ_{max} 278 (ϵ 15000) (MeOH aq.) (Berdy). λ_{max} 278 (ϵ 15000) (MeOH/HCl) (Berdy). λ_{max} 298 (ϵ 18000) (MeOH/NaOH) (Berdy).

Eur. Pat., 1983, 90 578; *CA*, **100**, 119330
Boeck, L.D. *et al., J. Antibiot.*, 1985, **38**, 1
Eggert, J.H. *et al., J. Antibiot.*, 1986, **39**, 792 (*isol, struct*)

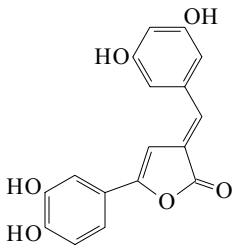
Antibiotic AC1 A-364

Protein, MW 5.4 kDa, comprising a single polypeptide chain. Isol. from *Lactobacillus acidophilus* AC 1. Shows antimicrobial activity.

Mehta, A.M. *et al., Microbios*, 1983, **38**, 73-81

Antibiotic BE 23372M A-365

[145588-13-2]
5-(3,4-Dihydroxyphenyl)-3-[(3,5-dihydroxyphenyl)methylene]-2(3H)-furanone. BE 23372M



$C_{17}H_{12}O_6$ 312.278
Sol. MeOH, DMSO, Me_2CO; fairly sol. $CHCl_3$, EtOAc; poorly sol. hexane. λ_{max} 266 (ϵ 8800); 426 (ϵ 20400) (MeOH) (Derep).

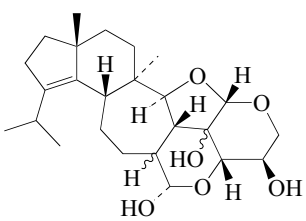
(E)-form

Prod. by *Rhizoctonia solani* found on the bark of *Ginkgo biloba* (ginkgo). Red-orange solid. Mp 265-270° dec. Similar to Aspulvinone G λ_{max} 266 (ϵ 8800); 426 (ϵ 20400) (MeOH).

Japan. Pat., 1992, 92 275 284; *CA*, **118**, 58224 (*isol, pmr, cmr, uv, ir, activity*)
Okabe, T. *et al., J. Antibiot.*, 1994, **47**, 289; 294; 297

Antibiotic CJ 14258 A-366

CJ 14258

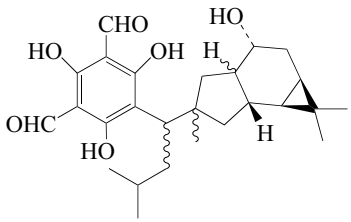


$C_{25}H_{38}O_6$ 434.572
Prod. by *Hericium ramosum*. Powder. $[\alpha]_D^{25}$ -73.4 (c, 0.74 in MeOH).

Saito, T. *et al., J. Antibiot.*, 1998, **51**, 983-990 (*isol, ir, pmr, cmr*)

Antibiotic GR 95647X A-367

GR 95647X



$C_{26}H_{36}O_6$ 444.567
Related to Euglobal V, E-388. Constit. of *Eucalyptus globulus* (Tasmanian blue gum).

Noble, H.M. *et al., Planta Med.*, 1990, **56**, 647 (*isol*)

Raphanus sativus Antifungal peptides A-368

RS-AFP

Highly-basic polypeptides containing 51 amino acids; rich in cysteine. Four components characterised. Isol. from radish seeds (*Raphanus sativus*).

Terras, F.R. *et al., J. Biol. Chem.*, 1992, **267**, 15301-15309 (*AFP 1, AFP 2, isol, struct*)
Terras, F.R. *et al., Plant Cell*, 1995, **7**, 573-588 (*AFP 3, AFP 4, isol, struct*)
Fant, F. *et al., J. Mol. Biol.*, 1998, **279**, 257-270 (*AFP 1, struct*)

Allium cepa Antimicrobial protein 1 A-369

Ace-AMP 1

Cationic protein containing 93 amino acid residues and 4 disulfide bonds. Isol. from onion seeds.

Cammue, B.P. *et al., Plant Physiol.*, 1995, **109**, 445-455 (*isol, struct*)
Tassin, S. *et al., Biochemistry*, 1998, **37**, 3623-3637 (*pmr, soln struct*)

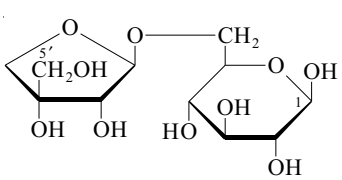
Capsicum annuum Antimicrobial protein 1 A-370

Ca AMP 1

Protein. Shows antifungal activity. Isol. from *Capsicum annuum*.

Pat. Coop. Treaty (WIPO), 1994, 94 11 511; *CA*, **121**, 127853c (*isol*)

6-*O*-β-D-Apiofuranosyl-D-glucose A-371



$C_{11}H_{20}O_{10}$ 312.273

β-D-Pyranose-*form*

1-O-*(3-Methylbutanoyl):* [467242-31-5]
$C_{16}H_{28}O_{11}$ 396.391
Constit. of green coffee beans (*Coffea arabica*).

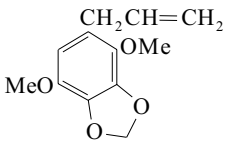
1-O-*(3-Methyl-2-butenoyl):* [467242-32-6]

$C_{16}H_{26}O_{11}$ 394.375
Constit. of green coffee beans (*Coffea arabica*).

1-O-*Benzoyl, 5′*-O-*(3,4-dihydroxycinnamoyl)(*E-*):* [166990-09-6] ***Psydroside***
$C_{27}H_{30}O_{14}$ 578.526
$[\alpha]_D^{25}$ -45 (c, 0.5 in MeOH).
Nahrstedt, A. *et al., Phytochemistry*, 1995, **39**, 375 (*Psydroside*)
Weckerle, B. *et al., Phytochemistry*, 2002, **60**, 409-414 (*coffee constits*)

Apiole A-372

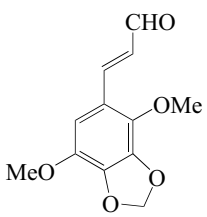
[523-80-8]
4,7-Dimethoxy-5-(2-propenyl)-1,3-benzodioxole, 9CI. 1-Allyl-2,5-dimethoxy-3,4-methylenedioxybenzene. Parsley apiole. Parsley camphor



$C_{12}H_{14}O_4$ 222.24
Occurs in *Sassafras albidum* (sassafras) and *Anethum graveolens* (dill). Needles. d_4^{20} 1.02. Mp 30°. Bp 294° Bp_{33} 179°. Log P 2.5 (calc). 2 unstable modifications Mps. 18° and 27.5° λ_{max} 280 (no solvent reported).
▶ CY2500000
Baker, W. *et al., J.C.S.*, 1938, 1602 (*synth*)
Sethi, M.L. *et al., Phytochemistry*, 1976, **15**, 1773 (*isol*)
Goeckeritz, D. *et al., Pharmazie*, 1979, **34**, 426 (*isol*)
Santos, B.V. de O. *et al., Phytochemistry*, 1998, **49**, 1381-1384 (*isol, uv, pmr, cmr*)
Benevides, P.J.C. *et al., Phytochemistry*, 1999, **52**, 339-343 (*isol, pmr*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1999, **52**, 495-499 (*isol, pmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGE500

Apional A-373

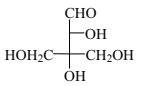
3-(2,5-Dimethoxy-3,4-methylenedioxyphenyl)-2-propenal. 2,5-Dimethoxy-3,4-methylenedioxycinnamaldehyde



$C_{12}H_{12}O_5$ 236.224
Constit. of parsley (*Petroselinum hortense*). Yellow needles (Et_2O). Mp 99°.
Appendino, G. *et al., Phytochemistry*, 1998, **49**, 1719-1722 (*isol, ir, pmr, cmr, ms*)

Apiose, 9CI, 8CI A-374

2,3,4-Trihydroxy-3-(hydroxymethyl)butanal. 3-C-*(Hydroxymethyl)*-glycero-*tetrose. Tetrahydroxyisovaleraldehyde*



D-*form*



β-D-erythro-Tetrofuranose-*form*

$C_5H_{10}O_5$ 150.131
Care needed with naming and numbering of derivs. C-3 is not a chiral centre in the acyclic sugar. In L-Apio-α-D-furanose for example, L- defines the config. at C-2 (L-apiose), while D-defines the config. at C-3 (D-furanosyl stereoisomeric form of L-apiose).

D-*form* [639-97-4]
*(*R*)-form*
First found in parsley as the glycoside Apiin, 2′′-β-D-Apiofuranosyl, also present in celery. Syrup. $[\alpha]_D$ +7.6 (c, 0.7 in H_2O).
Benzylphenylhydrazone:
Cryst. ($CHCl_3$). Mp 138-139°. $[\alpha]_D^{20}$ -94 (c, 4.6 in Py). $[\alpha]_D$ -29 (c, 1.1 in MeOH).
2,3-O-*Isopropylidene:2,3*-O-*Isopropylidene-D-apiose*
$C_8H_{14}O_5$ 190.196
Syrup. $[\alpha]_D$ -35 (c, 0.87 in MeOH).

α-D-*erythro*-Tetrofuranose-*form* [30738-01-3]
D-Apio-α-D-furanose, 9CI. 3-C-*Hydroxymethyl-α-D-*erythro-*tetrofuranose*
1,2-O-*Isopropylidene:* [25018-74-0] *1,2*-O-*Isopropylidene-D-apio-α-D-furanose. 1,2*-O-*Isopropylidene-α-D-*erythro-*tetrofuranose*
$C_8H_{14}O_5$ 190.196
Needles (Et_2O/hexane). Mp 118-120°. $[\alpha]_D^{29}$ +54.5 (c, 0.8 in EtOH).
1,2-O-*Isopropylidene, di-Ac:* [33962-41-3] *1′,3-Di*-O-*acetyl-1,2*-O-*isopropylidene-D-apio-α-D-furanoside. 1′,3-Di*-O-*acetyl-1,2*-O-*isopropylidene-α-D-*erythro-*tetrofuranose*
$C_{12}H_{18}O_7$ 274.27
Needles (hexane). Mp 110-111°. $[\alpha]_D$ +64 (c, 1.4 in $CHCl_3$).
1,2;1′,3-Di-O-*isopropylidene:* [25904-06-7] *1,2:1′,3-Di*-O-*isopropylidene-D-apio-α-D-furanoside. 1,2:1′,3-Di*-O-*isopropylidene-α-D-*erythro-*tetrofuranose*
$C_{11}H_{18}O_5$ 230.26
Cryst. (Et_2O/hexane). Mp 46-49° Mp 52-54°. $[\alpha]_D$ +62.4 (c, 1.0 in $CHCl_3$). $[\alpha]_D^{28}$ +76.5 (c, 3.0 in EtOH).
Me glycoside, 1′,2,3-tri-Me:Methyl 1′,2,3-tri-O-*methyl-D-*apio-*α-D-furanoside. Methyl 3*-C-*(methoxymethyl)-2,3-di*-O-*methyl-α-D-*erythro-*tetrofuranoside*
$C_9H_{18}O_5$ 206.238
$[\alpha]_D^{26}$ +116 ($CHCl_3$).

β-D-*erythro*-Tetrofuranose-*form* [36465-64-2]
D-Apio-β-D-furanose, 9CI. 3-C-*Hydroxymethyl-β-D-*erythro-*tetrofuranose*
Syrup.
2,3-O-*Isopropylidene:* [70147-50-1] *2,3*-O-*Isopropylidene-D-apio-β-D-furanose. 3*-C-*Hydroxymethyl-2,3*-O-*isopropylidene-β-D-*erythro-*tetrofuranose*
$C_8H_{14}O_5$ 190.196
Cryst. (Et_2O/hexane). Mp 72°. $[\alpha]_D$ -40 (c, 1.5 in $CHCl_3$).
Me glycoside, 2,3-O-*isopropylidene, 3′-tosyl:* [32445-78-6] *Methyl 2,3*-O-*Isopropylidene-1′-tosyl-D-apio-β-D-furanoside*
$C_{16}H_{22}O_7S$ 358.412
Cryst. (Et_2O/hexane). Mp 90-91°. $[\alpha]_D^{28}$ -82.1 (c, 4.0 in $CHCl_3$).
Me glycoside, 3′-Me, 2,3-O-*isopropylidene:* [4098-02-6] *Methyl 2,3*-O-*isopropylidene-3′-methyl-D-apio-β-D-furanoside. 2,3*-O-*Isopropylidene-3*-C-*(methoxymethyl)-3*-O-*methyl-β-D-*erythro-*tetrofuranose*
$C_{10}H_{18}O_5$ 218.249
Bp_2 70°. $[\alpha]_D^{25}$ -106 (c, 2.4 in $CHCl_3$).
Me glycoside, 1′,2,3-tri-Me:Methyl 1′,2,3-tri-O-*methyl-D-apio-β-D-furanoside. Methyl 3*-C-*(methoxymethyl)-2,3-di*-O-*methyl-β-D-*erythro-*tetrofuranoside*
$C_9H_{18}O_5$ 206.238
Syrup. $[\alpha]_D$ -79 ($CHCl_3$).

β-L-*threo*-Tetrofuranose-*form*
1,2-O-*Isopropylidene:* [14048-35-2] *1,2*-O-*Isopropylidene-L-apio-β-L-furanose. 1,2*-O-*Isopropylidene-3*-C-*hydroxymethyl-β-L-*threo-*tetrofuranose*
$C_8H_{14}O_5$ 190.196
Needles (CH_2Cl_2/hexane). Mp 124-125°. $[\alpha]_D^{29}$ +46 (c, 1.0 in EtOH).
1,2-O-*Isopropylidene, di-Ac:* [14048-36-3] *1′,3-Di*-O-*acetyl-1,2*-O-*isopropylidene-D-apio-β-L-furanose. 1′,3-Di*-O-*acetyl-1,2*-O-*isopropylidene-β-L-*threo-*tetrofuranose*
$C_{12}H_{18}O_7$ 274.27
Cubes (cyclohexane). Mp 88-89.5°. $[\alpha]_D^{29}$ +75 (c, 1.4 in $CHCl_3$).
1,2-O-*Isopropylidene, 1′-tosyl:1,2*-O-*Isopropylidene-1′*-O-*tosyl-β-D-apio-β-L-furanose. 1,2*-O-*Isopropylidene-1′*-O-*tosyl-β-L-*threo-*tetrofuranose*
$C_{15}H_{20}O_7S$ 344.385
Cryst. (Et_2O). Mp 137-138°. $[\alpha]_D$ +43.2 (c, 4.4 in $CHCl_3$).
1,2:1′,3-Di-O-*isopropylidene:* [14854-36-5]
[34724-16-8] *1,2:1′,3-Di*-O-*isopropylidene-D-apio-β-L-furanose. 1,2:1′,3-Di*-O-*isopropylidene-3*-C-*(hydroxymethyl)-β-L-*threo-*tetrofuranose*
$C_{11}H_{18}O_5$ 230.26
Needles (H_2O/NH_3). Mp 80-82°. $[\alpha]_D^{29}$ +59 (c, 1.0 in EtOH).
1′,3-Di-Me, 1,2-O-*isopropylidene:* [32445-76-4] *1,2*-O-*Isopropylidene-1′,3′-di*-O-*methyl-D-apio-β-L-furanose. 1,2*-O-*Isopropylidene-1′,3′-di*-O-*methyl-β-L-*threo-*tetrofuranose*
$C_{10}H_{18}O_5$ 218.249
Oil. $Bp_{0.1}$ 60°.
1′,3-Dibenzyl, 1,2-O-*isopropylidene:* [34339-65-6] *1′,3-Di*-O-*benzyl-1,2*-O-*isopropylidene-L-apio-β-L-furanose. 1′,3-Di*-O-*benzyl-1,2*-O-*isopropylidene-β-L-*threo-*tetrofuranose*
$C_{22}H_{26}O_5$ 370.444
Mp 38-39°. $[\alpha]_D^{22}$ +54.5 (c, 1.2 in $CHCl_3$).

L-*form* [6477-44-7]
Syrup. $[\alpha]_D^{20}$ -5 (c, 8.0 in H_2O).

Benzylphenylhydrazone:
Cryst. Mp 136-137°. $[\alpha]_D^{20}$ +94 (c, 1.0 in Py).

α-L-*erythro*-Tetrofuranose-*form* *L-Apio-α-L-furanose, 9CI. 3-*C*-Hydroxymethyl-α-L-*erythro-*tetrofuranose*

*1,2-*O*-Isopropylidene:* [22403-90-3] *1,2-*O*-Isopropylidene-L-apio-α-L-furanose*
$C_8H_{14}O_5$ 190.196
Cryst. (EtOAc/hexane). Mp 116-118°. $[\alpha]_D^{20}$ -43.8 (c, 1.5 in EtOH).

*1′,3-Dibenzyl, 1,2-*O*-isopropylidene:1′,3-Di-*O*-benzyl-1,2-*O*-isopropylidene-L-apio-α-L-furanose. 1′,3-Di-*O*-benzyl-1,2-*O*-isopropylidene-α-L-*erythro-*tetrofuranose*
$C_{22}H_{26}O_5$ 370.444
Cryst. (Et_2O/petrol). Mp 60-61°. $[\alpha]_D^{19}$ -58 (c, 1.5 in $CHCl_3$).

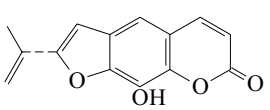
DL-*form* [42927-70-8]
Syrup.

[6477-44-7, 30912-14-2, 41546-43-4, 41546-44-5, 41546-46-7, 41546-47-8, 41546-49-0, 94943-41-6]

Bell, D.J. *et al., J.C.S.*, 1954, 3702 (*isol*)
Weygand, F. *et al., Chem. Ber.*, 1959, **92**, 535 (*L-form*)
Schaffer, R. *et al., J.A.C.S.*, 1959, **81**, 5452 (*L-form*)
Bell, D.J. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 260 (*isol*)
Williams, D.T. *et al., Can. J. Chem.*, 1964, **42**, 69 (*D-form, isol, synth, D-isopropylidene*)
Carey, F.A. *et al., Carbohydr. Res.*, 1966, **2**, 205 (*α-L-fur derivs*)
Ball, D.H. *et al., Carbohydr. Res.*, 1969, **10**, 121; 1971, **17**, 165; 1975, **45**, 91 (*α-D-Me gly tri-Me, β-D-Me gly tri-Me, β-D-Me gly derivs, 1,2;3,3′-diisopropylidene*)
Ezekiel, A.D. *et al., Tet. Lett.*, 1969, 1635 (*α-D-isopropylidene, α-D-isopropylidene di-Ac*)
Overend, W.G. *et al., Carbohydr. Res.*, 1970, **15**, 185 (*L-form*)
Tronchet, J.M.J. *et al., Helv. Chim. Acta*, 1971, **54**, 1466 (*1,2-*O*-isopropylidene*)
Ezekiel, A.D. *et al., J.C.S.(C)*, 1971, 2907 (*β-L-dibenzyl isopropylidene*)
Kinoshita, T. *et al., Carbohydr. Res.*, 1973, **28**, 175 (*β-L-threo-isopropylidene, β-L-threo diisopropylidene*)
Tronchet, J.M.T. *et al., Carbohydr. Res.*, 1974, **33**, 237 (*β-L-threo isopropylidene*)
Watson, R.R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1975, **31**, 135 (***rev***)
Vyas, D.M. *et al., Can. J. Chem.*, 1975, **53**, 2748 (*cmr*)
Ho, P.-T. *et al., Can. J. Chem.*, 1979, **57**, 381 (*D-form, L-form, synth, β-D-isopropylidene*)
Koos, M. *et al., Carbohydr. Res.*, 1986, **146**, 335 (***synth***)
Snyder, J.R. *et al., Carbohydr. Res.*, 1987, **166**, 85 (*DL-form*)

Apiumetin A-375

[70610-24-1]
*2,3-Dihydro-9-hydroxy-2-(1-methylethenyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. Leptophyllidin*



$C_{14}H_{12}O_4$ 244.246

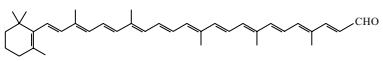
(*R*)-*form*
Constit. of the seeds of *Apium graveolens*. Needles. Mp 198°. $[\alpha]_D^{19}$ -68.29 (c, 0.41 in $CHCl_3$).

O-β-D-Glucopyranoside: [115356-05-3]
$C_{20}H_{22}O_9$ 406.388
Constit. of *Apium graveolens*. Needles (EtOH). Mp 165°. $[\alpha]_D^{20}$ -60 (c, 0.16 in $CHCl_3$).

Garg, S.K. *et al., Phytochemistry*, 1978, **17**, 2135 (*isol, struct*)
Sharma, B.R. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 647 (*Leptophyllidin*)
Ahluwalia, V.K. *et al., Phytochemistry*, 1988, **27**, 1181 (*deriv*)
Elgamal, M.H.A. *et al., Phytochemistry*, 1993, **34**, 819 (*isol, pmr*)

2′-Apo-β-carotenal, 8CI A-376

[5525-46-2]
β-Apo-2′-carotinal

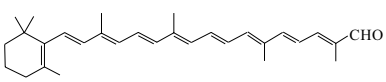


$C_{37}H_{48}O$ 508.786
Trace constit. of *Citrus* spp.. Violet cryst. (petrol). Mp 160-161°. λ_{max} 498 (petrol).

Rüegg, R. *et al., Helv. Chim. Acta*, 1949, **42**, 854 (*synth*)
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951 (*isol*)
Enzell, C.R. *et al., Acta Chem. Scand.*, 1969, **23**, 727 (*ms*)

8′-Apo-β-caroten-8′-al A-377

[1107-26-2]
β-Carotinal. *β-Apo-2-carotinal. C.I. Food Orange 6*



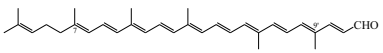
$C_{30}H_{40}O$ 416.645
Constit. of orange peel, spinach, marigolds and egg yolks. Colour additive. Violet cryst. (MeOH). Mp 139°.

8′-Carboxylic acid, Et ester: [1109-11-1]
all-trans *Carophyll yellow. C.I. Food Orange 7*
$C_{32}H_{44}O_2$ 460.698
Colour additive for foods, e.g. egg yolks. Dark red cryst. (CH_2Cl_2/EtOH). Mp 137-138°. λ_{max} 445 ; 470 (petrol).

Rüegg, R. *et al., Helv. Chim. Acta*, 1959, **42**, 854-864 (*synth*)
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951-2965 (*isol*)
Isler, O. *et al., Chimia*, 1961, **15**, 208-226 (*synth*)
Schwieter, H. *et al., Helv. Chim. Acta*, 1966, **49**, 369-390 (*carboxylic acid, Et ester, uv*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367-2390 (*cmr*)
Sharma, R.V. *et al., Biochim. Biophys. Acta*, 1977, **486**, 183-194 (*biochem*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 482 (*bibl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AQO300
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 192-193 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQO300

6′-Apo-ψ-caroten-6′-al A-378

Apo-6′-lycopenal. Lycopenal. Apo-2-lycopenal



(*all-E*)-*form*

$C_{32}H_{42}O$ 442.683

(*all-E*)-*form* [22255-36-3]
Isol. from *Lycopersicon esculentum* (tomato). Dark red plates (EtOH). Mp 147°. λ_{max} 475 (EtOH). λ_{max} 569 (CS_2). λ_{max} 455 ; 486 ; 519 (petrol).

6′-Carboxylic acid, Me ester: [22255-21-6]
Methyl apo-6′-lycopenate. *Methyl 6′-apo-γ-carotenoate, 8CI*
$C_{33}H_{44}O_2$ 472.709
Constit. of the seeds of *Bixia orellana* (annatto). Cryst. (C_6H_6/MeOH). Mp 141-144° (137-145°). λ_{max} 471 ; 503 (petrol). λ_{max} 445 ; 469 (Me_2CO).

(9′*Z*)-*form*
*6′-Carboxylic acid:****6′-Apo-ψ-caroten-6′-oic acid***
$C_{32}H_{42}O_2$ 458.683

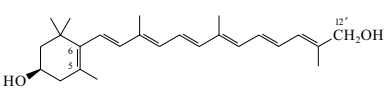
6′-Carboxylic acid, Me ester: [174206-07-6]
Methyl 6′-apo-9′Z-lycopen-6′-oate
$C_{33}H_{44}O_2$ 472.709
Constit. of the seeds of *Bixa orellana* (annatto). λ_{max} 342 ; 360 ; 439 (sh) ; 460 ; 493 (sh) (no solvent reported).

(7*Z*,9*Z*,9′*Z*)-*form*
6′-Carboxylic acid, Me ester: [188738-88-7]
Isol. from the seeds of *Bixa orellana* (annatto).

Kuhn, R. *et al., Ber.*, 1932, **65**, 898 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1939, **22**, 69
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951 (*isol*)
Kjosen, H. *et al., Phytochemistry*, 1969, **8**, 483-491 (*Methyl apo-6′-lycopenate*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759-2764 (*isol*)
Mercadante, A.Z. *et al., Phytochemistry*, 1996, **41**, 1201-1203 (*9Z-carboxylic acid Me ester*)
Mercadante, A.Z. *et al., J. Agric. Food Chem.*, 1997, **45**, 1050-1054 (*7Z,9Z,9′Z-carboxylic acid Me ester*)

12′-Apo-β-carotene-3,12′-diol A-379

[120021-87-6]



$C_{25}H_{36}O_2$ 368.558
Constit. of peaches (*Prunus persica*).

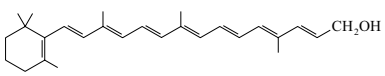
5α,6α-Epoxide: [80952-82-5] *5,6-Epoxy-5,6-dihydro-12′-apo-β-carotene-3,12′-diol.* ***Persicaxanthin***
$C_{25}H_{36}O_3$ 384.558
Isol. from plums *Prunus domestica*. Yellow plates (C_6H_6/petrol). Mp 92°.

12′-Aldehyde, 5α,6α-epoxide:5,6-Epoxy-5,6-dihydro-3β-hydroxy-12′-apo-β-caroten-12′-al. ***Apo-12′-violaxanthal***

$C_{25}H_{34}O_3$ 382.542
Isol. from plums *Prunus domestica*. Yellow pigment.

Gross, J. *et al., Phytochemistry*, 1981, **20**, 2267 (*Persicaxanthin*)
Molnár, P. *et al., Phytochemistry*, 1987, **26**, 1493 (*abs config*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1988, **71**, 1689 (*isol, pmr, uv*)

10′-Apo-β-caroten-10′-ol A-380



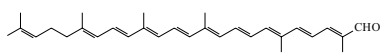
$C_{27}H_{38}O$ 378.597

10′-Aldehyde: [640-49-3] ***10′-Apo-β-caroten-10′-al***. *β-Apo-3-carotenal*
$C_{27}H_{36}O$ 376.581
Constit. of oranges and other citrus fruits. Red cryst. (petrol). Mp 97-98°.

Rüegg, R. *et al., Helv. Chim. Acta*, 1959, **42**, 854 (*synth*)
Yokoyama, H. *et al., Phytochemistry*, 1966, **5**, 1159 (*isol*)
Singh, H. *et al., Biochem. J.*, 1972, **128**, 11P (*synth*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1987, **70**, 1988 (*isol*)

Apo-8′-lycopenal A-381

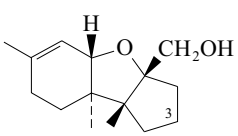
[2213-22-1]
2,6,11,15,19,23-Hexamethyl-2,4,6,8,10,12,14,16,18,22-tetracosadecaenal. 8′-Apo-ψ-caroten-8′-al. Apo-3-lycopenal



$C_{30}H_{40}O$ 416.645
Isol. from *Lycopersicon esculentum* (tomato). Purple plates (C_6H_6/MeOH). Mp 141°. λ_{max} 280 ; 475 ; 505 (cyclohexane).

Karrer, P. *et al., Helv. Chim. Acta*, 1939, **22**, 69 (*synth*)
Surmatis, J.D. *et al., J.O.C.*, 1966, **31**, 186 (*synth*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759 (*isol*)
Johansen, J.E. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 301 (*synth*)

Apotrichothecene A-382



$C_{15}H_{24}O_2$ 236.353
Mycotoxin of *Fusarium culmorum*.

3α-Hydroxy: [104148-45-0] ***Apotrichodiol***. *3-Hydroxyapotrichothecene. Secodeoxysambucinol*
$C_{15}H_{24}O_3$ 252.353
Mycotoxin of *Fusarium culmorum*, *Fusarium sambucinum* and *Fusarium crookwellense*. Glass.

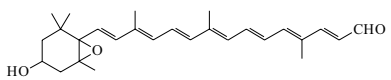
3β-Hydroxy:
$C_{15}H_{24}O_3$ 252.353
Mycotoxin prod. by *Fusarium sambucinum*. Glass. λ_{max} 197 (ε 7800) (MeCN).

3-Oxo: ***3-Ketoapotrichothecene***
$C_{15}H_{22}O_3$ 250.337
Mycotoxin from *Fusarium sambucinum*. Glass. λ_{max} 197 (ε 3600) (MeCN) (Berdy).

Lauren, D.R. *et al., J. Agric. Food Chem.*, 1987, **35**, 884 (*isol*)
Zamir, L.O. *et al., J. Biol. Chem.*, 1987, **262**, 15348; 15354 (*isol, pmr*)
Greenhalgh, R. *et al., J. Agric. Food Chem.*, 1989, **37**, 699 (*cryst struct*)
Sanson, D.R. *et al., J.O.C.*, 1989, **54**, 4313 (*isol, deriv*)
Zamir, L.O. *et al., Tet. Lett.*, 1992, **33**, 5181 (*isol, pmr, cmr*)

Apo-10′-violaxanthal A-383

[17237-68-2]
5,6-Epoxy-5,6-dihydro-3-hydroxy-10′-apo-β,ψ-carotenal, 9CI. 5,6-Epoxy-3-hydroxy-5,6-dihydro-10′-apo-β-caroten-10′-al. Apo-violaxanthinal

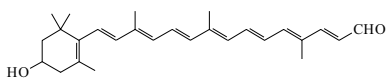


$C_{27}H_{36}O_3$ 408.58
Isol. from Valencia orange peels. λ_{max} 403 ; 424 ; 448 (hexane). λ_{max} 440 (EtOH).

Curl, A.L. *et al., J. Food Sci.*, 1967, **32**, 141 (*isol*)
Gross, J. *et al., Phytochemistry*, 1974, **13**, 1917

10′-Apozeaxanthal A-384

[79709-31-2]
3-Hydroxy-10′-apo-β,ψ-carotenal, 9CI. 3-Hydroxy-β-apo-10′-carotenal. Apo-3-zeaxanthinal

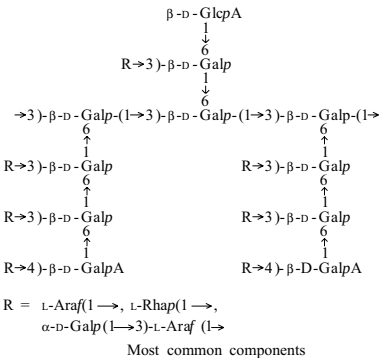


$C_{27}H_{36}O_2$ 392.58
Prob. isol. from Sinton citrangequat. λ_{max} 444 (EtOH).

Yokoyama, H. *et al., Phytochemistry*, 1966, **5**, 1159 (*isol*)
Ellis, P.R. *et al., Helv. Chim. Acta*, 1981, **64**, 1092 (*synth*)

Arabic acid, 9CI, 8CI A-385

[32609-14-6]



A highly branched polysaccharide composed of L-Arabinose, D-Galactose, L-Rhamnose and D-Gluconic acid in an approximate 3:3:1:1 ratio.

Mixed salts: [9000-01-5] *Gum arabic. Australian gum. Acacia gum. Wattle gum. E414. FEMA 2001*
Stabiliser for soft drink and flavour emulsions; encapsulating agent to protect lipid or liposoluble materials that are sensitive to decomposition; texturising or filming agent in confectionary; gelling agent or carrier in reduced calorie applications; clarification and stabilising aid in wines. Yellowish-amber lumps. Dissolves slowly in H_2O.

▶ CE5945000

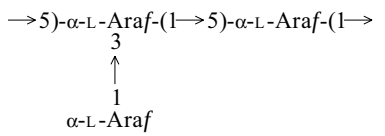
Me ester:
$[\alpha]_D^{19}$ -47 (c, 1.0 in $CHCl_3$).

Per-Ac:
$[\alpha]_D$ -21 (c, 0.94 in $CHCl_3$).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 202A (*ir*)
Smith, F. *et al., J.C.S.*, 1939, 1724; 1940, 1035
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, NY, 1948, **4**, 303 (*use*)
Aspinal, G.O. *et al., J.C.S.*, 1963, 1696
Aspinal, G.O. *et al., The Carbohydrates*, (Pigman, W. *et al*, Ed.), Academic Press, 1970, **2B**, 523
Churms, S.C. *et al., Carbohydr. Res.*, 1983, **123**, 267 (*struct*)
Defaye, J. *et al., Carbohydr. Res.*, 1986, **150**, 221 (*cmr, struct, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1-5 (*Gum arabic*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQQ500

Arabinan, 9CI, 8CI A-386

[11078-27-6]
Araban



Portion of idealised structure

$C_5H_8O_4$ 132.116
A polymer of linearly α-(1→5)-linked L-

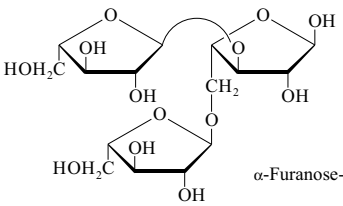
arabinofuranose units with single L-arabinofuranose α-(1→3)-linked to the main chain at intervals. Polymeric. Minimum formula given. Arabinans devoid of other sugars have been isol. from mustard seeds. Heteroarabinans have been found in sugar beet and apples. $[\alpha]_D$ -157. $[\alpha]_D$ -114. $[\alpha]_D$ -129 (H_2O).

Ac:
$[\alpha]_D^{20}$ -90 (Me_2CO).

[9060-75-7]

Hirst, E.L. *et al., J.C.S.*, 1939, 452; 454; 1865
Hirst, E.L. *et al., Adv. Carbohydr. Chem.*, 1947, **2**, 235 (*rev*)
Hirst, E.L. *et al., Biochem. J.*, 1965, **95**, 453 (*isol*)
Roudier, A.J. *et al., Bull. Soc. Chim. Fr.*, 1965, 460
Jones, J.K.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 74 (*synth*)
Aspinal, G.O. *et al., The Carbohydrates*, (Pigman W. etal, Ed.), Academic Press, 1970, **2B**, 517
Radha, A. *et al., Carbohydr. Res.*, 1997, **298**, 105-115 (*cryst struct, conformn*)

α-L-Arabinofuranosyl-(1→3)-[α-L-arabinofuranosyl-(1r5)]-L-arabinose A-387

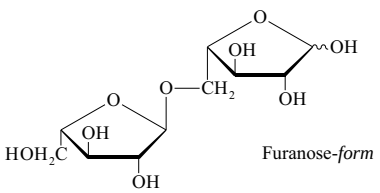


$C_{15}H_{26}O_{13}$ 414.363
Constit. of the anti-complementary arabinogalactan (AG IIb-1), isol. from the roots of *Angelica acutiloba* (Dong Dang Gui).

α-Furanose-*form* [114226-47-0]
Syrup.

Kiyohara, H. *et al., Carbohydr. Res.*, 1987, **167**, 221 (*isol, glc, ms, chromatog*)

5-*O*-α-L-Arabinofuranosyl-L-arabinose A-388

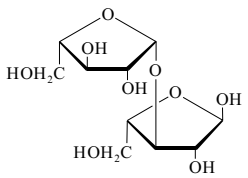


$C_{10}H_{18}O_9$ 282.247
From stem mucilage of *Opuntia ficus-indica* (Indian fig). Isol. from partial acid hydrolysates of sugar beet araban. $[\alpha]_D^{18}$ -87 (c, 0.5 in H_2O). $[\alpha]_D$ -98.4 (H_2O).

Andrews, P. *et al., Chem. Ind. (London)*, 1956, 658 (*isol, sugarbeet*)
Smith, F. *et al., J.C.S.*, 1961, 4892 (*isol*)
Tanaka, M. *et al., Biochim. Biophys. Acta*, 1981, **658**, 377
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol, synth*)

3-*O*-β-L-Arabinofuranosyl-L-arabinose, 9CI A-389

[52287-00-0]
Arabinofuranobiose

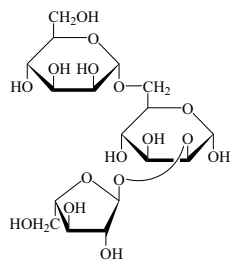


$C_{10}H_{18}O_9$ 282.247
Formed on partial acid hydrolysis of sugar beet araban and certain plant gums. $[\alpha]_D$ +94 (H_2O).

Phenylosazone:
Mp 200°.

Andrews, P. *et al., Chem. Ind. (London)*, 1956, 658 (*isol*)
Aspinall, G.O. *et al., J.C.S.*, 1959, 1697 (*isol*)
Sarkar, M. *et al., Indian J. Chem.*, 1974, **11**, 1129
Sarkar, M. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 369 (*isol, pmr*)

α-L-Arabinofuranosyl-(1→2)-[α-D-mannopyranosyl-(1→6)]-D-mannose A-390



$C_{17}H_{30}O_{15}$ 474.415
Residue present in tomato oligosaccharides.

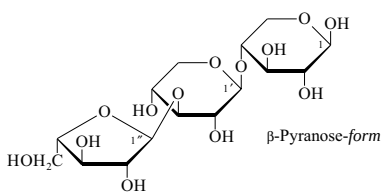
α-*form*

Allyl glycoside:
Amorph. solid. $[\alpha]_D$ +8 (c, 1 in H_2O).

Utille, J.P. *et al., Carbohydr. Res.*, 2000, **329**, 431-439 (*occur, synth*)

α-L-Arabinofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-D-xylose A-391

[66186-04-7]



$C_{15}H_{26}O_{13}$ 414.363
Prod. of partial enzymic hydrol. of xylans found in foods, e.g. rye flour. Pentahydrate. $[\alpha]_D^{20}$ -72 (c, 0.5 in H_2O). $[\alpha]_D$ -15 (H_2O).

Pyranose-*form*

*5″-(4-Hydroxy-*E*-cinnamoyl):* [102254-69-3]
$C_{24}H_{32}O_{15}$ 560.508
Enzym. hydrol. product of bamboo shoot (*Phyllostachys edulis*) cell wall and of barley straw cell walls. Syrup.

α-Pyranose-*form*

Benzyl glycoside, heptabenzyl: [99388-77-9]
$C_{71}H_{74}O_{13}$ 1135.358
$[\alpha]_D^{20}$ +14 (c, 1.5 in $CHCl_3$).

β-Pyranose-*form*

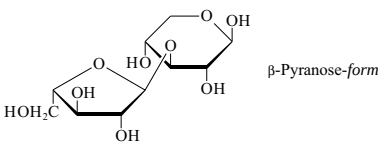
Me glycoside: [93130-20-2] *Methyl α-L-arabinofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-xylopyranoside*
$C_{16}H_{28}O_{13}$ 428.389
Cryst. (MeOH/Me_2CO). Mp 146-147°.
$[\alpha]_D^{22}$ -121 (c, 1.0 in H_2O).

Me glycoside, 2″,3″,4″-tribenzoyl, 2,2′,3,4′-tetra-Ac:
$C_{45}H_{48}O_{20}$ 908.862
Amorph. $[\alpha]_D^{22}$ -48 (c, 1.0 in $CHCl_3$).

Bishop, C.T. *et al., J.A.C.S.*, 1956, **78**, 2840 (*isol*)
Aspinall, G.O. *et al., J.C.S.*, 1960, 3881 (*isol*)
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1983, **47**, 2713
Shambe, T. *et al., Carbohydr. Res.*, 1983, **113**, 125
Hirsch, J. *et al., Carbohydr. Res.*, 1984, **131**, 219 (*β-Me gly synth, cmr*)
Schraml, J. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1605 (*pmr, cmr*)
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1464 (*enzymic synth, α-deriv synth*)
Mueller-Harvey, I. *et al., Carbohydr. Res.*, 1986, **148**, 71 (*coumaroyl, isol, pmr, cmr, ms*)
Ishii, T. *et al., Carbohydr. Res.*, 1990, **206**, 297 (*coumaroyl, isol, cmr, pmr*)

3-*O*-α-L-Arabinofuranosyl-D-xylose, 9CI A-392

[66186-03-6]



$C_{10}H_{18}O_9$ 282.247

β-Pyranose-*form*

Me glycoside: [93130-21-3] *Methyl 3-O-α-L-arabinofuranosyl-β-D-xylopyranoside*
$C_{11}H_{20}O_9$ 296.274
Sesquihydrate. $[\alpha]_D^{20}$ -113 (c, 1.2 in H_2O).

Me glycoside, pentabenzyl: [99388-70-2] *Methyl 2,4-di-O-benzyl-3-O-(2,3,5-tri-O-benzyl-α-L-arabinofuranosyl)-β-D-xylopyranoside*
$C_{46}H_{50}O_9$ 746.896
$[\alpha]_D^{20}$ -7 (c, 1.1 in $CHCl_3$).

*2′-O-(4-Hydroxy-3-methoxycinnamoyl)(*E*-):*
$C_{20}H_{26}O_{12}$ 458.418
Isol. from corn hulls. Powder. λ_{max} 230 ; 279 (MeOH).

*2′-Me ether, 5′-O-(4-hydroxy-3-methoxycinnamoyl)(*E*):*
$C_{21}H_{28}O_{12}$ 472.445
Isol. from corn hulls. Powder. λ_{max} 228 ; 284 (MeOH).

2′-Me ether, 5′-O-(4-hydroxy-3-

methoxycinnamoyl)(Z-):
$C_{21}H_{28}O_{12}$ 472.445
Isol. from corn hulls. Powder. λ_{max} 215 ; 272 (MeOH).

Kusakabe, I. *et al., Nippon Nogei Kagaku Kaishi*, 1977, **51**, 669; *CA*, **88**, 147669a (*isol*)
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1983, **47**, 2713
Sahrami, J. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1605 (*nmr*)
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1464 (*Me gly*)
Hosny, M. *et al., J. Nat. Prod.*, 1997, **60**, 219 (*feruloyl derivs*)

Arabinogalactan A-393

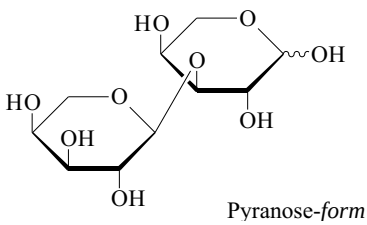
[9036-66-2]
D-Galacto-L-arabinan. Larch gum. FEMA 3254

A complex polymer of arabinose and galactose in a 1:6 ratio. Emulsifier, stabiliser.

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 194-195

3-*O*-α-L-Arabinopyranosyl-L-arabinose, 9CI A-394

[79435-28-2]



Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247
Hydrolytic product of the mucilage from the stems of *Opuntia ficus-indica* (Indian fig). Syrup. $[\alpha]_D$ +76 (c, 0.63 in H_2O).

α-Pyranose-*form*

Me glycoside: [105261-00-5] *Methyl 3-O-α-L-arabinopyranosyl-α-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
Mp 211°. $[\alpha]_D$ +34.4 (c, 3.9 in H_2O).

Me glycoside, penta-Ac: [105453-49-4] *Methyl 2,4-di-O-acetyl-3-O-(2,3,4-tri-O-acetyl-α-L-arabinopyranosyl)-α-L-arabinopyranoside, 9CI*
$C_{21}H_{30}O_{14}$ 506.46
Mp 70°. $[\alpha]_D$ +1.78 (c, 4.8 in $CHCl_3$).

β-Pyranose-*form*

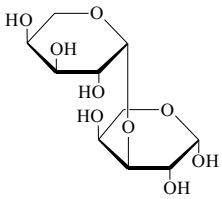
Me glycoside: [105260-96-6] *Methyl 3-O-α-L-arabinopyranosyl-β-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
Mp 194°. $[\alpha]_D$ +156 (c, 0.8 in H_2O).

Me glycoside, penta-Ac: [105260-90-0]
$C_{21}H_{30}O_{14}$ 506.46
Mp 154°. $[\alpha]_D$ +89.3 (c, 2.0 in $CHCl_3$).

McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol, pmr*)
Kochetkov, N.K. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1986, 200 (*Me gly, pmr, cmr*)
Shashkov, A.S. *et al., Magn. Reson. Chem.*, 1988, **26**, 735 (*cmr*)

3-*O*-β-L-Arabinopyranosyl-L-arabinose, 9CI, 8CI A-395

[20546-04-7]
Arabinopyranobiose



β-Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247
Isol. from partial acid hydrolysates of golden apple (*Spondias cytherea*), lemon, peach, cherry. Also major disaccharide product from the acid reversion of L-arabinose. $[\alpha]_D$ +210 (c, 1.0 in H_2O). $[\alpha]_D$ +164 (c, 1.0 in H_2O). $[\alpha]_D$ +193 (c, 3.8 in H_2O).

Phenylosazone:
Mp 235° (221°).

α-Pyranose-*form*

Me glycoside: [105260-99-9] *Methyl 3-O-β-L-arabinopyranosyl-α-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
$[\alpha]_D$ +140 (c, 2.6 in MeOH).

Me glycoside, penta-Ac: [105260-92-2]
$C_{21}H_{30}O_{14}$ 506.46
$[\alpha]_D$ +115 (c, 2.3 in $CHCl_3$).

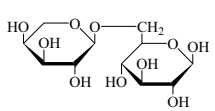
β-Pyranose-*form*

Me glycoside, penta-Ac: [105260-89-7]
Mp 211°. $[\alpha]_D$ +148 (c, 0.3 in $CHCl_3$).

Jones, J.K.N. *et al., J.C.S.*, 1953, 1672; 1958, 27 (*isol, synth*)
Andrews, P.A. *et al., J.C.S.*, 1953, 4090
Aspinall, G.O. *et al., J.C.S.*, 1955, 1106; 1965, 2685 (*isol*)
Smith, F. *et al., Chemistry of Plant Gums and Mucilages*, Reinhold, New York, 1959,
Haq, S. *et al., Can. J. Chem.*, 1961, **39**, 1563 (*isol*)
Chalk, R.C. *et al., Can. J. Chem.*, 1968, **46**, 2311 (*isol*)
Aspinall, G.O. *et al., Carbohydr. Res.*, 1968, **7**, 421 (*isol*)
Kubala, J. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 2809 (*isol*)
Kochetkov, N.K. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1986, 200 (*deriv, synth, pmr, cmr*)
Shashkov, A.S. *et al., Magn. Reson. Chem.*, 1988, **26**, 735 (*cmr*)
Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, R.), Sheffield Academic Press, 1998, 29-53 (*rev*)

6-*O*-α-L-Arabinopyranosyl-D-glucose, 9CI, 8CI A-396

[14116-69-9]
Vicianose



α-D-Pyranose-*form*

$C_{11}H_{20}O_{10}$ 312.273
Mp 210° dec. $[\alpha]_D^{20}$ +56.5 → +39.7 (H_2O).

β-Pyranose-*form*

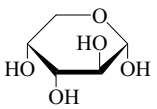
Hepta-Ac: [14260-08-3]
$C_{25}H_{34}O_{17}$ 606.533
Mp 158.5-160.5°. $[\alpha]_D$ +15 ($CHCl_3$).

Benzyl glycoside: [148031-67-8] ***Benzyl β-vicianoside***
$C_{18}H_{26}O_{10}$ 402.397
Constit. of the fruit of *Passiflora edulis* (passion fruit).

Helferich, B. *et al., Annalen*, 1928, **465**, 166 (*synth*)
Kochetkov, N.K. *et al., Zh. Obshch. Khim.*, 1967, **37**, 338; *CA*, **67**, 108856f (*synth*)
Psenak, M. *et al., Planta Med.*, 1972, **22**, 93; *CA*, **77**, 149673u (*isol*)
Balan, N.F. *et al., Bioorg. Khim.*, 1980, **5**, 1657; *CA*, **94**, 103719m (*hepta-Ac*)
Bartlett, P.A. *et al., J.A.C.S.*, 1980, **102**, 337 (*synth*)
Paterson, I. *et al., Tetrahedron*, 1985, **41**, 3569 (*rev*)
Pearson, A.J. *et al., Chem. Comm.*, 1988, 442 (*synth, bibl*)
Chassagne, D. *et al., Phytochemistry*, 1996, **41**, 1497-1500 (*benzyl glycoside*)

Arabinose A-397

[147-81-9]
Aloinose. Aloe sugar. Pectinose



α-D-Pyranose-*form*

$C_5H_{10}O_5$ 150.131

L-*form* [5328-37-0]

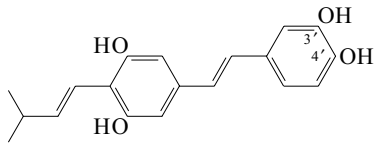
[87-72-9]
FEMA 3255
Flavouring agent. Mp 160°. $[\alpha]_D^{20}$ +190.6 → +104.5 (c, 4 in H_2O). Sweetness = 0.37 × sucrose.

[1768-95-2, 28697-53-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 188D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 293B (*nmr*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 120 (*rev*)
White, E.V. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 76 (*synth, L-form*)
Staněk, J. *et al., The Monosaccharides*, Academic Press, 1963, (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 583; 584 (*occur*)
Schaffer, R. *et al., The Carbohydrates*, 1972, **1A**, 69 (*occur*)
Benesi, A.J. *et al., Carbohydr. Res.*, 1994, **258**, 27 (*pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 48
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 196

Arachidin I A-398

[79147-73-2]
4-[2-[3,5-Dihydroxy-4-(3-methyl-1-butenyl)phenyl]ethenyl]-1,2-benzenediol, 9CI. 3,3′,4′,5-Tetrahydroxy-4-(3-methyl-1-butenyl)stilbene



$C_{19}H_{20}O_4$ 312.365

Stilbene numbering shown.

(E,E)-form [98391-38-9]

Constit. of peanuts (*Arachis hypogaea*).

3′-Deoxy: [87320-15-8] *5-[2-(4-Hydroxyphenyl)ethenyl]-2-(3-methyl-1-butenyl)-1,3-benzenediol, 9CI. 3,4′,5-Trihydroxy-4-(3-methyl-1-butenyl)stilbene.* ***Arachidin III***

$C_{19}H_{20}O_3$ 296.365

Isol. from peanuts (*Arachis hypogaea*).

3′-Deoxy, 2′-hydroxy:2′,3,4′,5-Tetrahydroxy-4-(3-methyl-1-butenyl)-stilbene

$C_{19}H_{20}O_4$ 312.365

Constit. of *Artocarpus integer* (champedak). Pale orange powder. Mp 191-193°. λ_{max} 217 (log ϵ 4.1); 243 (log ϵ 3.9); 311 (log ϵ 4); 345 (log ϵ 4.2) (MeOH).

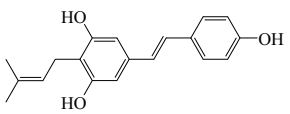
[79147-71-0]

Keen, N.T. *et al., Phytochemistry*, 1976, **15**, 1794 (*isol*)
Aguamah, G.E. *et al., Phytochemistry*, 1981, **20**, 1381 (*isol*)
Wotton, H.R. *et al., J. Gen. Microbiol.*, 1985, **131**, 487 (*isol*)
Boonlaksiri, C. *et al., Phytochemistry*, 2000, **54**, 415-417 (*3′-deoxy-2′-hydroxy*)

Arachidin II A-399

[79147-72-1]

5-[2-(4-Hydroxyphenyl)ethenyl]-2-(3-methyl-2-butenyl)-1,3-benzenediol, 9CI. 3,4′,5-Trihydroxy-4-prenylstilbene



(*E*)-*form*

$C_{19}H_{20}O_3$ 296.365

(E)-form [61517-87-1]

Constit. of peanuts (*Arachis hypogaea*). Yellow oil.

3,5-Di-Me ether: ***4′-Hydroxy-3,5-dimethoxy-4-prenylstilbene***

$C_{21}H_{24}O_3$ 324.419

Yellowish oil. λ_{max} 313 (log ϵ 4.2); 325 (log ϵ 4.21) (MeOH).

Tri-Me ether: [56866-27-4] ***3,4′,5-Trimethoxy-4-prenylstilbene***

$C_{22}H_{26}O_3$ 338.446

Cryst. Mp 92-94°.

2′-Hydroxy: [69065-16-3] *2′,3,4′,5-Tetrahydroxy-4-prenylstilbene*

$C_{19}H_{20}O_4$ 312.365

Constit. of *Artocarpus incisus* (breadfruit) and *Morus alba* (white mulberry). Mp 196-197°. λ_{max} 220 (ϵ 28100); 240 (sh) (ϵ 19700); 294 (sh) (ϵ 21300); 303 (ϵ 23100); 330 (ϵ 33100) (EtOH).

(Z)-form [61517-88-2]

Constit. of peanuts (*Arachis hypogaea*). Yellow oil.

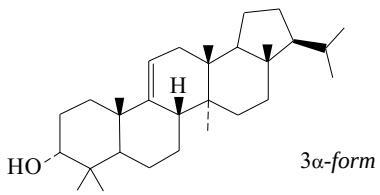
Braz Filho, R. *et al., Phytochemistry*, 1975, **14**, 1454 (*deriv*)
Keen, N.T. *et al., Phytochemistry*, 1976, **15**, 1794 (*isol*)
Takasugi, M. *et al., Chem. Lett.*, 1978, 1241-1242 (*2′,3,4′,5-Tetrahydroxy-4-prenylstilbene*)
Aguamah, G.E. *et al., Phytochemistry*, 1981, **20**, 1381 (*isol*)
Magalhaes, A.F. *et al., Phytochemistry*, 2001, **57**, 77-89 (*3,5-di-Me ether*)

Arachidoside A-400

Struct. unknown. Flavonoid glucoside. Poss. a glycoside of Dihydroisorhamnetin (See 3,3′,4′,5,7-Pentahydroxyflavanone, P-109). Isol. from shells of peanuts (*Arachis hypogaea*). Brown-red powder.

Tuyeau, F. *et al., C. R. Hebd. Seances Acad. Sci.*, 1947, **224**, 290

9(11)-Arborinen-3-ol A-401



3α-*form*

$C_{30}H_{50}O$ 426.724

(3β,21βH)-form [90582-44-8]

Sorghumol

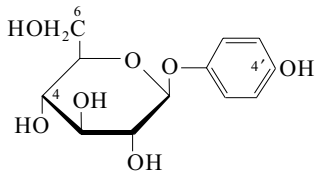
Constit. of *Sorghum bicolor* (sorghum). Cryst. Mp 277-282°.

Nes, W.D. *et al., Chem. Comm.*, 1984, 223 (*Sorghumol*)

Arbutin A-402

[497-76-7]

4-Hydroxyphenyl β-D-glucopyranoside, 9CI, 8CI. Hydroquinone-glucose. Arbutoside. Ericolin



$C_{12}H_{16}O_7$ 272.254

Glucoside in pear leaves (*Pyrus communis*). Mp 142-143°. $[\alpha]_D^{18}$ -60.34 (H_2O). Log P -1.83 (calc). λ_{max} 291 (MeOH) (Berdy). λ_{max} 294 (EtOH) (Berdy).

▶ Exp. reprod. and teratogenic effects (v. large doses). CE8863000

2-Ac: [15794-91-9] ***2-O-Acetylarbutin***. *Isopyroside*

$C_{14}H_{18}O_8$ 314.291

Constit. of *Vaccinium vacillans* (blueberry). Cryst. Mp 172-174°. $[\alpha]_D^{22}$ -22. $[\alpha]_D$ -21.2 (c, 0.9 in MeOH).

6-Ac: [10338-88-2] ***6-O-Acetylarbutin***. *Pyroside*

$C_{14}H_{18}O_8$ 314.291

Constit. of the leaves of immature pear (*Pyrus communis*) and mountain cranberry (*Vaccinium vitis-idaea*). Mp 214-216°. $[\alpha]_D^{23}$ -58.8 (c, 2.0 in H_2O).

2-O-(3,4-Dihydroxy-E-cinnamoyl): [230955-36-9]

[14477-53-3] ***2-O-Caffeoylarbutin***

$C_{21}H_{22}O_{10}$ 434.399

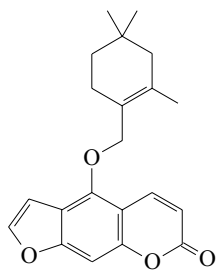
Isol. from leaves of *Vaccinium vitis-idaea* (mountain cranberry). Prisms. Mp 165°.

Bradfield, F.J. *et al., J.C.S.*, 1952, 4740
Haslam, E. *et al., J.C.S.*, Suppl. I, 1964, 5649-5654 (*2-O-Caffeoylarbutin*)
Durkee, A.B. *et al., J. Food Sci.*, 1968, **33**, 461 (*isol, deriv*)
Haslam, E. *et al., Tetrahedron*, 1968, **24**, 4015 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 204; 205; 2610 (*occur*)
Perol, G.W. *et al., J.C.S. Perkin 1*, 1979, 239 (*synth, pmr*)
Lutterbach, R. *et al., Helv. Chim. Acta*, 1992, **75**, 2009 (*isol*)
Jeo, W.K. *et al., Nat. Prod. Sci.*, 1999, **5**, 60-63 (*2′-Caffeoylarbutin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HIH100

Archangelin A-403

[21174-75-4]

4-[(2,4,4-Trimethyl-1-cyclohexen-1-yl)-methoxy]-7H-furo[3,2-g][1]benzopyran-7-one, 9CI. Iselin



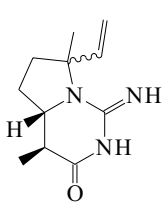
$C_{21}H_{22}O_4$ 338.402

Constit. of the root of *Angelica archangelica* (angelica). Thick rods (MeOH). Mp 132°. $[\alpha]_D^{30}$ +14 ($CHCl_3$).

Chatterjee, A. *et al., Tet. Lett.*, 1964, 1961 (*isol, struct*)
Chatterjee, A. *et al., Indian J. Chem.*, 1968, **6**, 415 (*isol, struct*)
Bates, R.B. *et al., Tet. Lett.*, 1972, 3811 (*rev*)
Dukhovlinova, L.I. *et al., Khim. Prir. Soedin.*, 1974, **10**, 308; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 316 (*isol*)
Magotra, D. *et al., Acta Cryst. C*, 1995, **51**, 2196 (*cryst struct*)

Arenaine A-404

[35471-10-4]



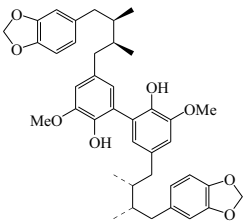
Relative configuration

$C_{11}H_{17}N_3O$ 207.275

Alkaloid from seeds of *Plantago arenaria* (sand plantain). Mp 208-210°. $[\alpha]_D^{22}$ +305 (c, 1.7 in $CHCl_3$).

Rabaron, A. *et al., J.A.C.S.*, 1971, **93**, 6270 (*uv, ir, pmr, cmr, struct*)

Argenteane A-405



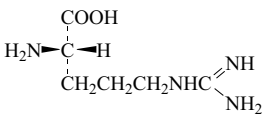
Relative Configuration

$C_{40}H_{46}O_8$ 654.799
Constit. of mace, *Myristica argentea*. Oil. λ_{max} 220 (log ϵ 1.53); 250 (sh) ; 289 (log ϵ 1.04) (MeOH).

Filleur, F. *et al., Nat. Prod. Lett.*, 2002, **16**, 1-7 (*isol, pmr, cmr*)

Arginine, INN, USAN A-406

[7004-12-8]
2-Amino-5-[(aminoiminomethyl)amino]-pentanoic acid. 2-Amino-5-guanidinovaleric acid. Arg



(*S*)-*form*

$C_6H_{14}N_4O_2$ 174.202Log P -4.79 (calc).

(*S*)-*form* [74-79-3]
L-form. L-Arginine. FEMA 3819
Dietary supplement, nutrient. Plates or prisms + $2H_2O$ (H_2O), plates (EtOH). Sol. H_2O (15.0g/100g at 21°). Mp 207° Mp 244° dec. (anhyd. 105°). $[\alpha]_D$ +21.8 (H_2O). $[\alpha]_D^{25}$ +48.1 (c, 1 in 5*M* HCl). pK_{a3} 12.48 (guanido). Isoelectric point 10.76. Bitter taste. *N*-Protected derivs. useful in peptide synth. have been listed alphabetically elsewhere.

▶ CF1934200

Hydrochloride: [1119-34-2]

[15595-35-4] ***Arginine hydrochloride, USAN***
Dietary supplement, nutrient. Mp 222° dec. (235°). $[\alpha]_D^{20}$ +12.1 (H_2O).

▶ LD_{50} (rat, orl) 12000 mg/kg. Exp. teratogen. CF1995500

N^2-*(3-Carboxypropanoyl):* [2478-02-6] **N^2-*Succinoylarginine***
$C_{10}H_{18}N_4O_5$ 274.276
Constit. of the shoots of pear trees.

N^2-*Oxalyl:* [90250-86-5] **N^2-*Oxalylarginine***
$C_8H_{14}N_4O_5$ 246.222
Constit. of the shoots of apple and pear trees (*Malus* spp.).

N^2-*(3-Carboxy-2-hydroxypropanoyl):* [87605-92-3] **N^2-*(2-Hydroxysuccinoyl)arginine***. N^2-*(3-Carboxy-2-hydroxy-1-oxopropyl)arginine*
$C_{10}H_{18}N_4O_6$ 290.275
Constit. of the seeds of *Vicia faba* and the shoots of apple and pear trees.

N^2-*(3-Carboxy-3-hydroxypropanoyl):* [90250-85-4] **N^2-*(3-Hydroxysuccinoyl)arginine***
$C_{10}H_{18}N_4O_6$ 290.275
Constit. of the shoots of apple and pear trees.

N^2-*[3-Carboxy-2-(carboxymethyl)-2-hydroxypropanoyl]:* [87605-91-2] **N^2-*(2-Carboxymethyl-2-hydroxysuccinoyl)arginine***
$C_{12}H_{20}N_4O_8$ 348.312
Constit. of the shoots of apple and pear trees.

N^2-*β-D-Fructopyranos-1-yl:* [162966-07-6] N^2-*Fructopyranosylarginine. UK III*
$C_{12}H_{24}N_4O_7$ 336.344
Constit. of Korean red ginseng.

N^2-*[α-D-Glucopyranosyl-(1→4)-β-D-fructopyranos-1-yl]:* [162966-06-5]

[185351-34-2] N^2-*Maltulosylarginine. UK II*
$C_{18}H_{34}N_4O_{12}$ 498.486
Constit. of Korean red ginseng. Powder. Mp 158-160°.

[14975-30-5, 32042-43-6, 50912-92-0, 63238-98-2, 78851-84-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 785A; 785D; 786A; 786B; **2**, 259C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1281A (*nmr*)
Org. Synth., 1932, **12**, 4 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1841 (*rev*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Bak, B. *et al., J. Mol. Spectrosc.*, 1968, **26**, 78 (*pmr*)
Voelter, W. *et al., Z. Naturforsch., B*, 1971, **26**, 213 (*cmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2392 (*occur*)
Lehmann, M.S. *et al., J.C.S. Perkin 2*, 1973, 133 (*cryst struct*)
Torgerson, D.F. *et al., Biochem. Biophys. Res. Commun.*, 1974, **60**, 616 (*ms*)
Kasai, T. *et al., Phytochemistry*, 1983, **22**, 147-149; 1984, **23**, 19-22 (*N-succinoyl derivs*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AQV 980; AQW 000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 197-198
Zheng, Y.-N. *et al., J. Chin. Pharm. Sci.*, 1998, **7**, 7-10 (*Maltulosylarginine*)

Argon A-407

[7440-37-1]
E938

Ar

Ar 39.948

Atomic No. 18. Ground state electron config. [Ne]$3s^23p^6$. Discovered in air in 1894 by Sir W. Ramsey and M.W. Travers. There are 8 isotopes of which 3 are natural. Abundance: 9300 ppm in air (by vol.). Solid state struct. is ccp or hcp (metastable). Inert atmosphere for wine and fruit or vegetable juice containers. Generally recognised as safe (GRAS) in the USA. Colourless, odourless, tasteless, monatomic gas. Forms no true chemical compds. Forms clathrates with H_2O and hydroquinone. Forms complex with HBr. Sol. H_2O (33.6 cm^3 kg^{-1} at 20°). Mp -189.4°. Bp -185.9°. Forms clathrate compds. with phenols.

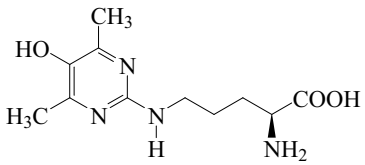
▶ CF2300000

[11130-84-0, 12595-59-4, 12650-44-1, 14343-01-2, 14791-69-6, 14864-12-1, 15056-24-3, 15099-26-0, 15801-88-4, 16249-22-2, 16740-17-3, 16904-17-9, 16941-40-5, 16941-44-9, 17428-37-4, 17596-58-6, 18973-74-5, 20499-74-5, 26603-53-2, 34247-59-1, 37352-46-8, 61762-54-7]

Mellor Compr. Treat. Inorg. Theor. Chem., 1927, **7**, 889 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 1, *Suppl. Vol.*, 1970, 16; 133 (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 139 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 249 (*rev, bibl*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 1042 (*rev*)
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 24; 235
Osvath, R. *et al., Food Chem. News*, 2000, **42**, 3-5 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQW250

Argpyrimidine A-408

N^5-*(5-Hydroxy-4,6-dimethyl-2-pyrimidinyl)ornithine*

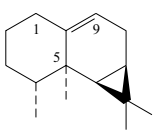


$C_{11}H_{18}N_4O_3$ 254.288

(*S*)-*form*
Found in beer.

Glomb, M.A. *et al., J. Agric. Food Chem.*, 2001, **49**, 366-372 (*isol, synth, ms*)

9-Aristolene A-409



$C_{15}H_{24}$ 204.355

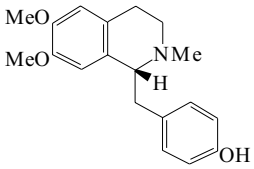
(+)-*form* [27862-07-3]
ent-*9-Aristolene*. ***α-Ferulene***
Oil. Bp_8 110°. $[\alpha]_D$ +68 (neat). $[\alpha]_D$ +40 (c, 0.1 in $CHCl_3$).

(-)-*form* [6831-16-9]
Aristolene
Constit. of calarene from sweet flag oil. Oil. $[\alpha]_D$ -98.7 (neat).

Pesnelle, P. *et al., Bull. Soc. Chim. Fr.*, 1963, 912 (*isol*)
Carboni, S. *et al., Tet. Lett.*, 1965, 3017 (*isol*)
Weinheimer, A.J. *et al., Chem. Comm.*, 1968, 1070 (*isol*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)

Armepavine A-410

4-[(1,2,3,4-Tetrahydro-6,7-dimethoxy-2-methyl-1-isoquinolinyl)methyl]phenol, 9CI. 1,2,3,4-Tetrahydro-1-(4-hydroxybenzyl)-6,7-dimethoxyisoquinoline. Evoeuropine



(*R*)-*form*

$C_{19}H_{23}NO_3$ 313.396

(*S*)-*form*

Mp 149-150°. $[\alpha]_D^{20}$ +118 ($CHCl_3$).

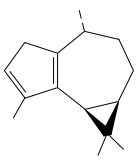
Me ether: [3423-02-7] ***(+)-O-Methylarmepavine***

$C_{20}H_{25}NO_3$ 327.422

Alkaloid from *Annona squamosa* (sugar apple). Cryst. (petrol). Mp 60-62°. $[\alpha]_D^{20}$ +85.

Marion, L. *et al., J.O.C.*, 1950, **15**, 216 (*deriv, synth*)
Tomita, M. *et al., Chem. Pharm. Bull.*, 1953, **1**, 10 (*deriv, synth*)
Ferrari, C. *et al., Tetrahedron*, 1962, **18**, 419 (*deriv, synth*)
Kapadia, G.J. *et al., J. Pharm. Sci.*, 1964, **53**, 1140 (*deriv, isol, pmr, struct*)
Bishay, D.W. *et al., Phytochemistry*, 1973, **12**, 693 (*isol, uv, ir, pmr, ms*)
Sheth, J.P. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 595 (*deriv, synth, ms*)
Shono, T. *et al., Tet. Lett.*, 1978, 4819 (*deriv, synth*)
Torres, R. *et al., J. Nat. Prod.*, 1979, **42**, 430 (*deriv, isol, uv, ir, pmr, ms*)
Bhaumik, P.K. *et al., Phytochemistry*, 1979, **18**, 1584 (*deriv, isol, uv, pmr*)

1(5),3-Aromadendradiene A-411



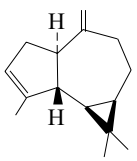
$C_{15}H_{22}$ 202.339

(6α,7α,10α)-*form* [111778-06-4]

Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Flavouring agent. Oil.

Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753

3,10(14)-Aromadendradiene A-412



$C_{15}H_{22}$ 202.339

(1α,5β,6α,7α)-*form* [53526-64-0]

β-Spathulene

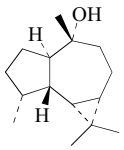
Constit. of the the oil of *Schinus molle* (California peppertree).

Terhune, S.J. *et al., Phytochemistry*, 1974, **13**, 865

10-Aromadendranol A-413

[19078-39-8]

*Decahydro-1,1,4,7-tetramethyl-1*H*-cyclo-prop[e]azulen-4-ol, 9CI*



(1α,4α,5β,6α,7α,10α)-*form*

$C_{15}H_{26}O$ 222.37

(1α,4α,5β,6α,7α,10α)-*form* [489-41-8]

Globulol

Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Needles (EtOH aq.). Mp 88.5°. Bp 283°. $[\alpha]_D^{20}$ -35.3 ($CHCl_3$).

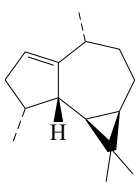
(1β,4α,5β,6β,7β,10α)-*form* [577-27-5]

Ledol. *Ledum camphor. Porschcamphor*

Constit. of *Valeriana officinalis* (valerian), *Piper* spp. and others. Cryst. (petrol). Mp 105°. Bp 282-283°. $[\alpha]_D$ +8 (EtOH). Stereochem. revised in 2000.

Birch, A.J. *et al., Aust. J. Chem.*, 1955, **8**, 550 (*isol*)
Büchi, G. *et al., Tet. Lett.*, 1959, **No. 6**, 14 (*struct, synth*)
Graham, B.A. *et al., Aust. J. Chem.*, 1960, **13**, 372 (*struct*)
Büchi, G. *et al., J.A.C.S.*, 1969, **91**, 6473 (*synth, abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1908 (*occur*)
Marshall, J.A. *et al., J.O.C.*, 1974, **39**, 1971 (*synth*)
Pakrashi, S.C. *et al., J.O.C.*, 1980, **45**, 4765 (*isol*)
El-Seedi, H. *et al., Phytochemistry*, 1994, **35**, 1495 (*Ledol, cmr*)
Wassmuth-Wagner, I. *et al., Planta Med.*, 1995, **61**, 196 (*pmr, cmr*)
Gwaltney, S.L. *et al., Tet. Lett.*, 1996, **37**, 949 (*synth*)
Topçu, G. *et al., Phytochemistry*, 1997, **44**, 1393 (*Ledol, pmr, cmr*)
Cao, S.-G. *et al., Nat. Prod. Lett.*, 2000, **14**, 447-452 (*Ledol, synth*)
Kaplan, M.A.C. *et al., Phytochemistry*, 2000, **55**, 749-753 (*Ledol, struct, bibl*)

1-Aromadendrene A-414



$C_{15}H_{24}$ 204.355

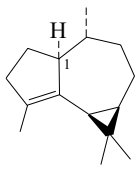
(4α,5β,6α,7α,10α)-*form* [111821-79-5]

Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ +42 (c, 0.2 in pentane).

Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1243 (*synth*)

4-Aromadendrene A-415



(1α,6α,7α,10α)-*for*

$C_{15}H_{24}$ 204.355

(1α,6α,7α,10α)-*form* [112421-19-9]

1-Epi-α-gurjunene

Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ -68 (c, 0.2 in pentane).

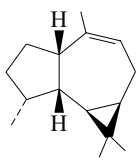
(1β,6α,7α,10α)-*form* [489-40-7]

α-Gurjunene. *Gurjunene*

Oil. Bp_{10} 114-116° Bp_3 75-77°. $[\alpha]_D$ -179.5.

Streith, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 1950 (*isol, struct*)
Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753 (*isol, cmr*)

9-Aromadendrene A-416



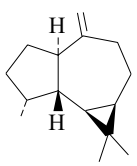
$C_{15}H_{24}$ 204.355

(1β,4α,5β,6α,7α)-*form* [112421-20-2]

Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ -78 (c, 0.6 in pentane).

Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753

10(14)-Aromadendrene A-417



(1α,4α,5β,6α,7α)-*form*

$C_{15}H_{24}$ 204.355

(1α,4α,5β,6α,7α)-*form* [14682-34-9]

[72747-25-2]

(-)-Aromadendrene. *β-Diploalbicene*

Constit. of *Bixa orellana* (annatto). Oil. $[\alpha]_D$ -11 (EtOH).

10β,14-Epoxide: [85710-39-0] *10,14-Epoxyaromadendrane.* ***Aromadendrene epoxide***

$C_{15}H_{24}O$ 220.354

Constit. of hops.

(1β,4α,5β,6β,7β)-*form* [25246-27-9]

[72747-25-2]

Alloaromadendrene. *α-Aromadendrene*

Constit. of essential oils of *Eucalyptus globulus* (Tasmanian blue gum). Oil. Bp_2 96°. $[\alpha]_D^{20}$ -21.6. n_D^{18} 1.5010.

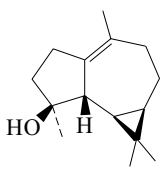
10β,14-Epoxide: [85760-81-2] ***Alloaromadendrene epoxide***
$C_{15}H_{24}O$ 220.354

(1β,4β,5α,6β,7β)-*form* [489-39-4]

[72747-25-2]
(+)-Aromadendrene
Oil. Bp 260-265°. $[\alpha]_D$ +24.5.

Dolejš, L. *et al., Coll. Czech. Chem. Comm.*, 1960, **25**, 1483 (*isol*)
Büchi, G. *et al., J.A.C.S.*, 1969, **91**, 6473 (*synth, abs config, bibl*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1983, **31**, 892 (*Aromadendrene epoxide*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 1950 (*Alloaromadendrene epoxide*)
Zafra-Polo, M.C. *et al., J. Chromatogr.*, 1990, **518**, 230 (*Aromadendrene epoxide*)
Williams, H.J. *et al., Phytochemistry*, 1995, **40**, 1633 (*pmr, cmr, ms*)
Tanaka, T. *et al., Tetrahedron*, 1996, **52**, 4257 (*synth*)

1(10)-Aromadendren-4-ol A-418



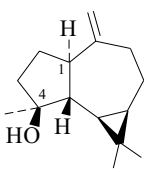
$C_{15}H_{24}O$ 220.354

(4β,5α,6α,7α)-*form* [88395-46-4]
Isospathulenol
Constit. of Clary sage oil (*Salvia sclarea*). Cryst. Mp 69-70.5°. $[\alpha]_D$ +99 (c, 0.6 in $CHCl_3$).

Maurer, B. *et al., Helv. Chim. Acta*, 1983, **66**, 2223

10(14)-Aromadendren-4-ol A-419

[72203-24-8]



(1α,4β,5β,6α,7α)-*form*

$C_{15}H_{24}O$ 220.354

(1α,4β,5β,6α,7α)-*form* [6750-60-3]
Spathulenol†
Constit. of *Salvia sclarea* (clary sage). Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. $[\alpha]_D$ +56.

3,5-Dinitrobenzoyl:
Cryst. Mp 148°.

(1β,4α,5β,6β,7β)-*form* ***Epispathulenol***
Cryst. Mp 102-103°. $[\alpha]_D$ +2 (c, 0.7 in Me_2CO).

(1β,4α,5α,6β,7β)-*form* [77171-55-2] **ent-*Spathulenol***
$[\alpha]_D$ -20 (c, 1 in $CHCl_3$).

Bowyer, R.C. *et al., Chem. Ind. (London)*, 1963, 1245 (*isol, struct*)
Juell, S. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 458 (*pmr*)
Asakawa, Y. *et al., Phytochemistry*, 1980, **19**, 2141 (*ent-Spathulenol*)
Surburg, H. *et al., Chem. Ber.*, 1981, **114**, 118 (*synth*)
Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 971 (*isol, pmr, cmr*)
Tringali, C. *et al., Phytochemistry*, 1995, **40**, 827 (*Epispathulenol*)
Toyota, M. *et al., Phytochemistry*, 1996, **41**, 1347 (*ent-Spathulenol*)

Arsenobetaine A-420

[64436-13-1]
(Carboxymethyl)trimethylarsonium hydroxide inner salt, 9CI
$Me_3As^{\oplus}CH_2COO^{\ominus}$

$C_5H_{11}AsO_2$ 178.062
Found in algae, lobsters, sharks, etc.. Deliquescent cryst. (Me_2CO/MeOH). Mp 204-210° dec. Low mammalian toxicity, excreted unchanged e.g. from seafood sources..

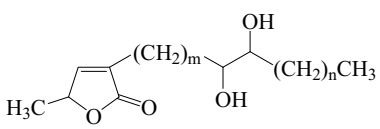
► LD_{50} (mus, orl) 10000 mg/kg. CH9750000

Hydrobromide: [71642-15-4]
$C_5H_{12}AsBrO_2$ 258.974
Non-hygroscopic white shiny cryst. (EtOH at 5°).

Edmonds, J.S. *et al., Tet. Lett.*, 1977, 1543 (*synth, pmr, cryst struct*)
Cannon, J.R. *et al., Aust. J. Chem.*, 1981, **34**, 787 (*isol, synth*)
Edmonds, J.S. *et al., Chemosphere*, 1981, **10**, 1041 (*isol, ir, pmr*)
Norin, H. *et al., Chemosphere*, 1982, **11**, 287 (*isol, ms, pmr, reaction*)
Luten, J.B. *et al., Chemosphere*, 1983, **12**, 131 (*isol, ms, reaction*)
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375 (*pmr, cmr*)
Edmonds, J.S. *et al., Appl. Organomet. Chem.*, 1988, **2**, 297 (*biosynth, occur, uv*)
Hanaoka, K. *et al., Appl. Organomet. Chem.*, 1988, **2**, 371 (*occur, metab*)
Ismail, H. *et al., Pertanika J. Trop. Agric. Sci.*, 1988, **11**, 437; *CA*, **112**, 7249 (*synth, cmr*)
Siu, K.W.M. *et al., Rapid Commun. Mass Spectrom.*, 1988, **2**, 69 (*ms*)
Beauchemin, D. *et al., J. Anal. At. Spectrom.*, 1989, **4**, 285 (*hplc, ms*)
Arsenic Environ., Part II:, (ed. Nriagu, J.O.), J. Wiley, 1994, (*rev, props*)
Minhas, R. *et al., Appl. Organomet. Chem.*, 1998, **12**, 635-641 (*synth, pmr, cmr, ms*)

Artemoin A A-421

3-(19,20-Dihydroxytriacontyl)-5-methyl-2(5H)-furanone



m = 18, n = 19

$C_{35}H_{66}O_4$ 550.904
Constit. of the seeds of *Annona atemoya* (custard apple). Isol. as a mixture with other Artemoins.

Chang, F.-R. *et al., Phytochemistry*, 1999, **51**, 883-889 (*isol, ir, pmr, cmr, ms*)

Artemoin B A-422

3-(17,18-Dihydroxytriacontyl)-5-methyl-2(5H)-furanone
As Artemoin A, A-421 with m = 16, n = 11

$C_{35}H_{66}O_4$ 550.904
Constit. of the seeds of *Annona atemoya* (custard apple). Isol. as a mixture with other Artemoins.

Chang, F.-R. *et al., Phytochemistry*, 1999, **51**, 883-889 (*isol, ir, pmr, cmr*)

Artemoin C A-423

3-(15,16-Dihydroxytriacontyl)-5-methyl-2(5H)-furanone
As Artemoin A, A-421 with m = 14, n = 13

$C_{35}H_{66}O_4$ 550.904
Constit. of the seeds of *Annona atemoya* (custard apple). Isol. as a mixture with other Artemoins.

Chang, F.-R. *et al., Phytochemistry*, 1999, **51**, 883-889 (*isol, ir, pmr, cmr, ms*)

Artemoin D A-424

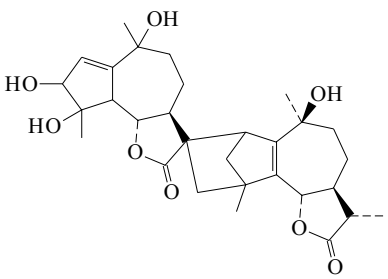
3-(13,14-Dihydroxytriacontyl)-5-methyl-2(5H)-furanone
As Artemoin A, A-421 with m = 12, n = 15

$C_{35}H_{66}O_4$ 550.904
Constit. of the seeds of *Annona atemoya* (custard apple). Isol. as a mixt. with other Artemoins.

Chang, F.-R. *et al., Phytochemistry*, 1999, **51**, 883-889 (*isol, ir, pmr, cmr, ms*)

Artenolide A-425

[113807-34-4]



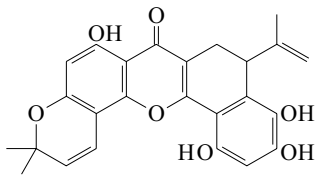
$C_{30}H_{40}O_8$ 528.641
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOH). Mp 163-174°.

Ovezdurdyev, A. *et al., Khim. Prir. Soedin.*, 1987, **23**, 667; *Chem. Nat. Compd. (Engl. Transl.)*, 553 (*isol, pmr, cmr*)

Artobiloxanthone A-426

[121748-25-2]

[133813-53-3]
*8,9-Dihydro-6,10,11,13-tetrahydroxy-3,3-dimethyl-9-(1-methylethenyl)-3*H,7H-*benzo[c]pyrano[3,2-*h*]xanthen-7-one, 9CI. KB 1*

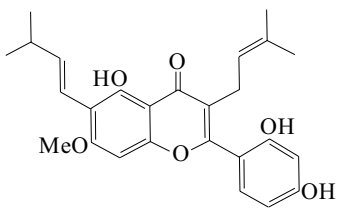


$C_{25}H_{22}O_7$ 434.445
Constit. of *Artocarpus communis* (breadfruit). Yellow solid. Mp 162-164°.

Sultanbawa, M.U.S. *et al., Phytochemistry*, 1989, **28**, 599
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1787-1789

Artocarpin **A-427**

[7608-44-8]
*2-(2,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-6-(3-methyl-1-butenyl)-3-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI*

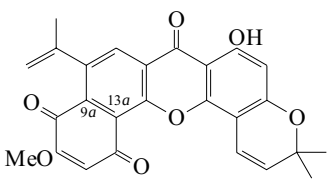


$C_{26}H_{28}O_6$ 436.504
Isol. from *Artocarpus heterophyllus* (jackfruit). Yellow needles (Me_2CO, C_6H_6 or MeOH). Mp 250° Mp 174-175°.

Dave, K.G. *et al., J. Sci. Ind. Res., Sect. B*, 1956, **15**, 1961; 1961 (*isol, struct*)
Rao, A.V.R. *et al., Indian J. Chem.*, 1972, **10**, 989 (*ms*)
Nomura, T. *et al., Heterocycles*, 1979, **12**, 1289 (*struct*)
Mereyala, H.B. *et al., Indian J. Chem., Sect. B*, 1988, **27**, 945 (*cmr*)

Artomunoxanthentrione **A-428**

[139921-73-6]



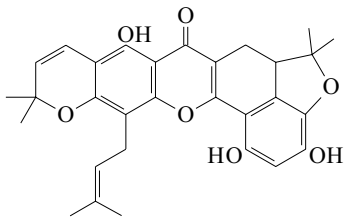
$C_{26}H_{20}O_7$ 444.44
Constit. of *Artocarpus communis* (breadfruit). Red cryst. (EtOAc). Mp 230-232°.

*9*a,*13*a-*Epoxide:* [143522-33-2] *Artomunoxanthentrione epoxide*
$C_{26}H_{22}O_8$ 462.455
Isol. from the root bark of *Artocarpus communis* (breadfruit). Orange needles (EtOAc). Mp 248-251°. CA numbering.

Shieh, W.-L. *et al., Phytochemistry*, 1992, **31**, 364 (*isol, pmr, cmr*)
Lin, C.-N. *et al., Phytochemistry*, 1992, **31**, 2563 (*epoxide*)

Artonin A **A-429**

[124721-15-9]

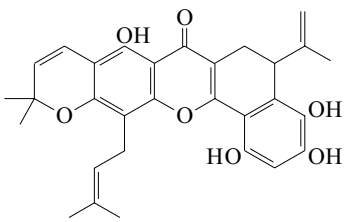


$C_{30}H_{30}O_7$ 502.563
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (MeOH). Mp 239-240°.

Hano, Y. *et al., Heterocycles*, 1989, **29**, 1447 (*isol, pmr, cmr, ms, cryst struct*)

Artonin B **A-430**

[124693-70-5]

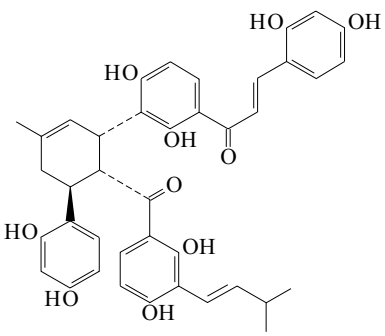


$C_{30}H_{30}O_7$ 502.563
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow needles (C_6H_6). Mp 219-222°.

Hano, Y. *et al., Heterocycles*, 1989, **29**, 1447 (*isol, pmr, cmr, ms*)

Artonin C **A-431**

[128553-97-9]

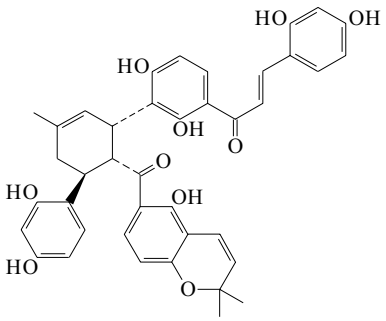


$C_{40}H_{38}O_{10}$ 678.734
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow powder. Mp 169-171°. $[\alpha]_D^{22}$ +20 (c, 0.09 in MeOH).

Hano, Y. *et al., J. Nat. Prod.*, 1990, **53**, 391 (*isol, pmr, cmr, ir, uv, ms*)

Artonin D **A-432**

[128532-95-6]

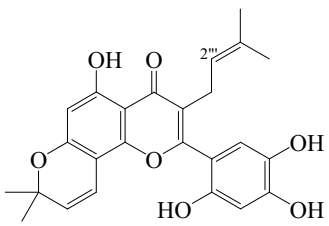


$C_{40}H_{36}O_{10}$ 676.718
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow powder. Mp 140-143°. $[\alpha]_D$ +77 (c, 0.172 in MeOH).

Hano, Y. *et al., J. Nat. Prod.*, 1990, **53**, 391 (*isol, pmr, cmr, ir, uv, ms*)

Artonin E **A-433**

[129683-93-8]
KB 3



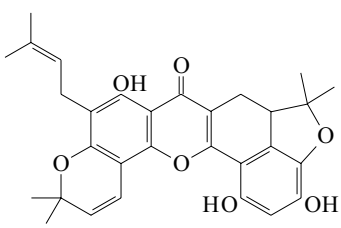
$C_{25}H_{24}O_7$ 436.46
Constit. of *Artocarpus communis* (breadfruit). Yellow needles (C_6H_6/Me_2CO). Mp 244-248°.

2‴,3‴-Dihydro, 3‴-hydroxy: [133740-64-4] ***KB 2***
$C_{25}H_{26}O_8$ 454.476
Constit. of *Artocarpus communis* (breadfruit). Mp 166-168°.

Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1787-1789 (*isol, deriv*)
Hano, Y. *et al., Heterocycles*, 1990, **31**, 877 (*isol, pmr, cmr*)

Artonin F **A-434**

[129683-94-9]



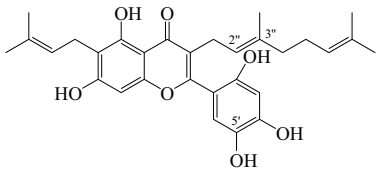
$C_{30}H_{30}O_7$ 502.563
Constit. of *Artocarpus communis* (breadfruit). Yellow needles (C_6H_6/Me_2CO). Mp 248°.

Hano, Y. *et al., Heterocycles*, 1990, **31**, 877 (*isol, pmr, cmr*)

Artonin H A-435

[133866-94-1]

3-Geranyl-2′,4′,5,5′,7-pentahydroxy-6-prenylflavone



$C_{30}H_{34}O_7$ 506.594
Amorph powder. λ_{max} 206 (ϵ 48980); 258 (ϵ 27540); 302 (ϵ 11220) (MeOH) (Berdy).

5′-Deoxy: [54835-67-5] ***Rubraflavone C***
$C_{30}H_{34}O_6$ 490.595
Constit. of *Morus rubra* (red mulberry). Yellow solid.

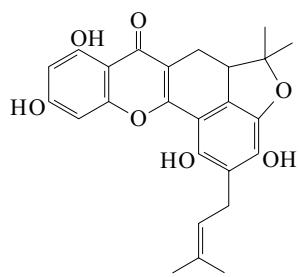
5′-Deoxy, 2′′,3′′-dihydroxy, 2′′,3′′-dihydro: [459155-95-4] ***Artocarpol H***
$C_{30}H_{36}O_8$ 524.61
Yellow needles (Me_2CO). Mp 199-200°. $[\alpha]_D^{27}$ -13.5 (c, 0.1 in Me_2CO). λ_{max} 215 (log ϵ 3.53); 291 (log ϵ 3.16) (MeOH).

Hano, Y. *et al., Heterocycles*, 1990, **31**, 2173 (*isol, struct*)

Lu, Y.-H. *et al., Helv. Chim. Acta*, 2002, **85**, 1626-1632 (*Artocarpol H, Rubraflavone C*)

Artonin J A-436

[148719-51-1]



$C_{25}H_{24}O_7$ 436.46
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (MeOH). Mp 281-282°. Racemic.

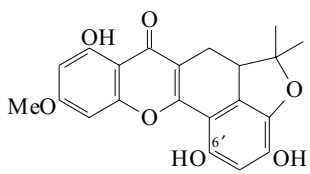
7-Me ether: [161017-03-4] ***Artonin T***
$C_{26}H_{26}O_7$ 450.487
Constit. of the bark of *Artocarpus heterophyllus* (jackfruit). Yellow needles (Me_2CO). Mp 252°. Racemic.

Aida, M. *et al., Heterocycles*, 1993, **36**, 575 (*isol, pmr, cmr*)

Aida, M. *et al., Heterocycles*, 1994, **39**, 847 (*Artonin T*)

Artonin K A-437

[148719-61-3]



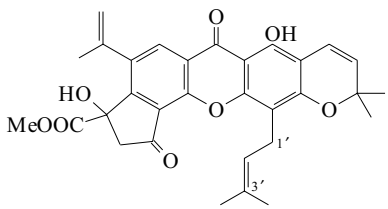
$C_{21}H_{18}O_7$ 382.369
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (Me_2CO). Mp 312-314°. Racemic.

6′-Me ether: [148719-52-2] ***Artonin L***
$C_{22}H_{20}O_7$ 396.396
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (MeOH). Mp 249-250°. Racemic.

Aida, M. *et al., Heterocycles*, 1993, **36**, 575 (*isol, pmr, cmr*)

Artonin Q A-438

[161017-00-1]



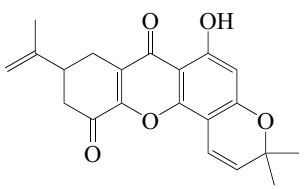
$C_{31}H_{30}O_8$ 530.573
Constit. of the bark of *Artocarpus heterophyllus* (jackfruit). Yellow cryst. (hexane/Et_2O). Mp 57-59°. Racemic λ_{max} 205 (ϵ 30900); 225 (ϵ 25120); 250 (sh) (ϵ 26300); 302 (ϵ 27540); 350 (ϵ 8910); 390 (ϵ 4070) (MeOH).

$\Delta^{1'}$-Isomer, 3′-hydroperoxy: [161017-01-2] ***Artonin R***
$C_{31}H_{30}O_{10}$ 562.572
Isol. from *Artocarpus heterophyllus* (jackfruit). Yellow cryst. (hexane/Et_2O). Mp 173°. λ_{max} 202 (ϵ 7940); 226 (ϵ 7410); 298 (ϵ 6310); 350 (ϵ 2090); 400 (ϵ 830) (MeOH).

Aida, M. *et al., Heterocycles*, 1994, **39**, 847 (*isol, uv, ir, ms, pmr, cmr*)

Artonol A A-439

[186824-57-7]

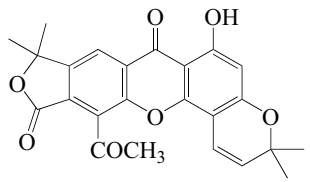


$C_{21}H_{20}O_5$ 352.386
Constit. of the bark of *Artocarpus communis* (breadfruit). Orange prisms (Me_2CO). Mp 189-196°. Racemic λ_{max} 236 (log ϵ 4.45); 279 (log ϵ 4.31); 337 (log ϵ 3.57) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175 (*isol, uv, ir, pmr, cmr*)

Artonol B A-440

[186824-58-8]

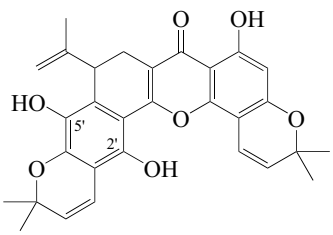


$C_{24}H_{20}O_7$ 420.418
Constit. of the bark of *Artocarpus communis* (breadfruit). Orange needles (C_6H_6). Mp 267-273°. λ_{max} 246 (log ϵ 4.1); 284 (log ϵ 3.99); 338 (log ϵ 3.5); 405 (log ϵ 3.1) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175 (*isol, uv, ir, pmr, cmr*)

Artonol C A-441

[186824-59-9]



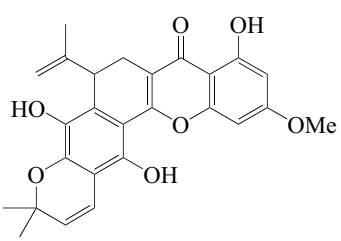
$C_{30}H_{28}O_7$ 500.547
Constit. of the bark of *Artocarpus communis* (breadfruit). Yellow needles (MeOH/C_6H_6). Mp 182-184°. Racemic λ_{max} 237 (log ϵ 4.36); 281 (log ϵ 4.44); 345 (log ϵ 3.9); 386 (log ϵ 4.11) (MeOH).

2′,5′-Quinone: [186824-60-2] ***Artonol D***
$C_{30}H_{26}O_7$ 498.531
Constit. of the bark of *Artocarpus communis* (breadfruit). Reddish needles (Me_2CO). Mp 130°. λ_{max} 235 (log ϵ 4.33); 265 (log ϵ 4.43); 337 (log ϵ 3.84) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175 (*isol, uv, ir, pmr, cmr*)

Artonol E A-442

[186824-61-3]



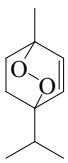
$C_{26}H_{24}O_7$ 448.471
Constit. of the bark of *Artocarpus communis* (breadfruit). Yellow needles (EtOAc). Mp 224-227°. λ_{max} 211 (log ϵ 4.31); 271 (log ϵ 4.26); 377 (log ϵ 4.09) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175

(*isol, uv, ir, pmr, cmr*)

Ascaridole A-443

[512-85-6]
*1-Methyl-4-(1-methylethyl)-2,3-dioxabicyclo[2.2.2]oct-5-ene, 9CI. 1-Isopropyl-4-methyl-7-oxabicyclo[2.2.1]hept-2-ene. 1,4-Epidioxy-*p*-menth-2-ene. Kebal II. Uncinacina. Ascapurin. Ascarisin*



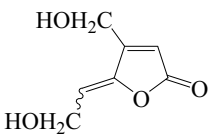
$C_{10}H_{16}O_2$ 168.235
Said to be the major constit. of oil of *Peumus boldus* (boldo). Oil. d_4^{20} 1.01. Mp 3.3°. Bp_{15} 115° $Bp_{0.2}$ 39-40°. Log P 1.34 (uncertain value) (calc). Unstable.

▶ Explodes on heating or on treatment with acids. LD_{50} (rat, orl) 200 mg/kg. Shows neoplastic activity. OT0175000

Schenk, G.O. *et al., Angew. Chem.*, 1952, **64**, 12 (*synth*)
Beckett, A.H. *et al., J. Pharm. Pharmacol.*, 1955, **7**, 55 (*purifn*)
Swern, D. *et al., Anal. Chem.*, 1969, **41**, 412 (*pmr*)
Bernhard, R.A. *et al., Phytochemistry*, 1971, **10**, 177 (*isol*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Haynes, R.K. *et al., Aust. J. Chem.*, 1978, **31**, 131 (*synth*)
Masilamani, D. *et al., J.O.C.*, 1983, **48**, 4918 (*synth*)
Zagorski, M.G. *et al., J.O.C.*, 1985, **50**, 4484 (*cmr, O-17 nmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 40
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARM500

Ascladiol A-444

[32013-85-7]
*5-(2-Hydroxyethylidene)-4-(hydroxymethyl)-2(5*H*)-furanone, 9CI*



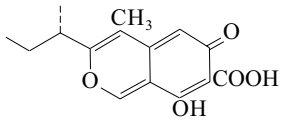
$C_7H_8O_4$ 156.138
Toxin from *Aspergillus clavatus* in wheat flour. Cryst. ($Me_2CO/CHCl_3$). Mp 65-66°. V. hygroscopic λ_{max} 271 (MeOH) (Berdy).

▶ Toxic.

Suzuki, T. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1786 (*isol, struct*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 517

Ascochitine A-445

[3615-05-2]
Ascochytin



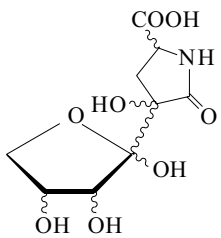
$C_{15}H_{16}O_5$ 276.288
Tautomerism possible. Causes brown rot in broad beans. Yellow cryst. Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 196-198°. $[\alpha]_D^{25}$ -86 ($CHCl_3$). λ_{max} 220 (ε); 286 (ε); 415 (ε) (EtOH) (Derep). λ_{max} 220 (ε 20617); 286 (ε 17550); 415 (ε 5700) (EtOH) (Berdy).

▶ Toxic.

Oku, H. *et al., Phytopathology*, 1963, **53**, 1321
Mishima, H. *et al., Sankyo Kenkyusho Nenpo*, 1970, **22**, 67; *CA*, **75**, 48824x (*struct*)
Galbraith, M.N. *et al., J.C.S.(C)*, 1971, 3557 (*synth*)
Colombo, L. *et al., J.C.S. Perkin 1*, 1980, 675; 2549 (*biosynth, cmr, struct*)
Beed, F.D. *et al., Mycol. Res.*, 1994, **98**, 1069 (*manuf*)

Ascorbalamic acid, 9CI A-446

[41679-87-2]

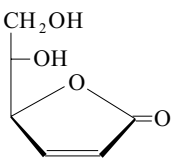


$C_9H_{13}NO_8$ 263.204
Constit. of cabbage (*Brassica oleracea*). $[\alpha]_D^{26}$ +24 (c, 1.25 in H_2O). pK_a 1.

Couchman, R. *et al., Phytochemistry*, 1973, **12**, 707 (*isol*)

Ascorbic acid, BAN, INN, USAN A-447

threo-*Hex-2-enonic acid γ-lactone, 9CI, 8CI.* threo-*Hexulosono-1,4-lactone-2,3-enediol. Hexuronic acid. Lyxoascorbic acid. Xyloascorbic acid*



L-*form*

$C_6H_8O_6$ 176.126Log P -2.21 (calc).

L-***form*** [50-81-7]
Vitamin C*. Vitamin C*[3]*. Ascorbicap. Cebione. Celaskon. Cenolate. Cevalin. Cevital. Citrovit. Roscorbic. Vitacimin. Vitascorbol. E300*
Occurs widely in animals and plants. Good sources are citrus fruits and hip berries. Isol. from ox adrenal cortex, lemons and paprika. Prod. industrially on a large scale from glucose. Vitamin (antiscorbutic), antioxidant, nutrient, preservative consistency enhancer. Used to reduce discoloration, mainly browning caused by polyphenol oxidase, in fruit and vegetable products. Used to enhance colour formn. and to reduced the formn. of nitrosamines in meat products. Used synergistically with Sulfur dioxide, S-277 in wine and beer as a preservative. Assists formn. of the gluten network in bread making, thus enhancing bread volume. Mp 190-192°. $[\alpha]_D^{25}$ +24 (c, 1 in H_2O). $[\alpha]_D^{18}$ +49 (MeOH). pK_{a2} 11.34 (25°, 0.1*M* KNO_3). Component of numerous preparations.

▶ Human systemic effects when administered intravenously. Exp. reprod. and teratogenic effects (v. large doses). LD_{50} (rat, orl) 11900 mg/kg. CI7650000

Na salt: [134-03-2] ***Sodium ascorbate, INN****. E301*
Antioxidant. $[\alpha]_D$ +24 (c, 3 in H_2O).

▶ CI7671000

Ca salt (2:1): [5743-27-1] *Calcium ascorbate. E302*
Antioxidant. $[\alpha]_D^{10}$ +91 (c, 0.3 in H_2O).

*Fe(*II*) salt:* [24808-52-4] *Ferrous ascorbate*
Dietary supplement.

6-Hexadecanoyl: [137-66-6] ***Ascorbyl palmitate, USAN****. E304*
$C_{22}H_{38}O_7$ 414.538
Antioxidant. Mp 107-117°. $[\alpha]_D^{20}$ +22.9 (c, 2 in MeOH).

▶ CI7671040

6-Octadecanoyl: [10605-09-1]

[25395-66-8] ***Ascorbyl stearate***
$C_{24}H_{42}O_7$ 442.592
Preservative for margarine.

[299-36-5, 5743-28-2, 6485-44-5, 6730-29-6, 25395-66-8, 124928-57-0]

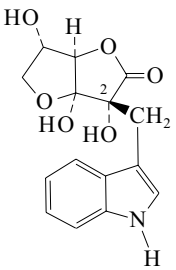
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 702B (*ir*)
Aldrich Library of ^{13}C *and* ^{1}H *FT NMR Spectra*, 1992, **1**, 1149C; 1150C; 1151A; 1151B (*nmr*)
Herbert, R.W. *et al., J.C.S.*, 1933, 1270 (*struct*)
Reichstein, T. *et al., Helv. Chim. Acta*, 1934, **17**, 311 (*synth*)
Hirst, E.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1939, **2**, 132
Sawyer, D.T. *et al., Anal. Chem.*, 1966, **38**, 192 (*pmr*)
Pilipenko, A.T. *et al., Zavod. Lab.*, 1966, **32**, 3 (*rev, use*)
Hvoslef, J. *et al., Acta Cryst. B*, 1969, **25**, 2214 (*cryst struct*)
Berger, S. *et al., Tetrahedron*, 1977, **33**, 1587 (*cmr*)
Crawford, T.C. *et al., Adv. Carbohydr. Chem.*, 1980, **37**, 7 (*rev*)
Sieb, P.A. *et al., Adv. Chem. Ser.*, 1982, **200**, 1-585 (*rev*)
Ascorbic acid: Chemistry, Metabolism and Uses (Adv. Chem. Ser. no. 200), ACS, 1982, (*book*)
Eur. Pat., 1985, 146 121, (*Takeda*); *CA*, **104**, 33286s (*CV 3611, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN000
Davies, M.B. *et al., Vitamin C: its Chemistry and Biochemistry*, RSC, 1991,

Parviainen, M.T. *et al., Chromatogr. Sci*, 1992, **60**, 235 (*rev, chromatog*)
Barili, P.L. *et al., Tetrahedron*, 1992, **48**, 6273 (*synth*)
Csiba, M. *et al., J.O.C.*, 1993, **58**, 7281 (*synth*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 15-18; 19-20; 431-432
Ruchmann, A. *et al., Magn. Reson. Chem.*, 1996, **34**, 116 (*O-17 nmr*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1387
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 205; 212; 213; 369-370; 1106-1107; 2526-2527 (*salts, rev*)
Loewus, F.A. *et al., Phytochemistry*, 1999, **52**, 193-210 (*rev, biosynth, metab*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN000; ARN125; CAM600

Ascorbigen A-448

[8075-98-7]

2-C-*(1*H-*Indol-3-ylmethyl)-3-hexulofuranosonic acid γ-lactone, 9CI*



(2*R*)-*form*

$C_{15}H_{15}NO_6$ 305.287

Present in plants, esp. cabbage and other crucifers.

(2*R*)-*form* [26548-49-2]
β-*L*-lyxo-*form*. ***Ascorbigen B***
Light yellow amorph. powder. Mp 70° (sinters). $[\alpha]_D^{25}$ +12.5 (c, 1.0 in MeOH).

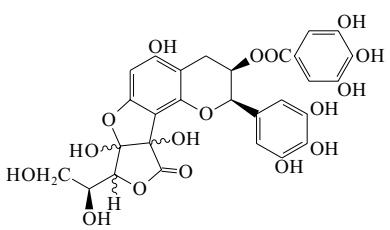
(2*S*)-*form* [26676-89-1]
β-*L*-xylo-*form*. ***Ascorbigen A***
Amorph. powder. Mp *ca.* 65° (sinters). $[\alpha]_D^{25}$ +11 (c, 2.0 in EtOH).

[29400-26-8]

Piironen, E. *et al., Acta Chem. Scand.*, 1962, **16**, 1286 (*synth, bibl*)
Kiss, G. *et al., Helv. Chim. Acta*, 1966, **49**, 989 (*synth, ir, uv, pmr, struct*)
Korolev, A.M. *et al., Bioorg. Khim.*, 1991, **17**, 981

8-*C*-Ascorbylepigallocatechin 3-*O*-gallate A-449

[126715-87-5]



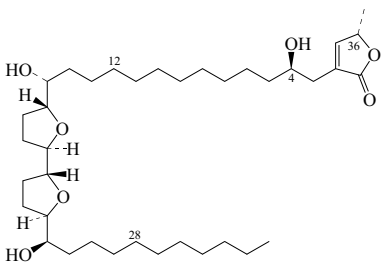
$C_{28}H_{24}O_{17}$ 632.487

Constit. of commercial oolong tea (*Camellia sinensis* var. *viridis*). Off-white amorph. powder + ½H_2O. $[\alpha]_D^{21}$ -215.1 (c, 1.0 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3255 (*struct, ir, pmr, cmr*)

Asimicin A-450

*3-[2,13-Dihydroxy-13-[octahydro-5′-(1-hydroxyundecyl)[2,2′-bifuran]-5-yl]tridecyl]-5-methyl-2(5*H*)-furanone, 9CI. Annonastatin. Squamocin H. Annonareticulin*



$C_{37}H_{66}O_7$ 622.924

Absolute configs. are not yet fully established and the identities of various isolates apparently having the same struct. are not all certain. Isol. from *Asimina triloba* (pawpaw), *Annona squamosa* (sugar apple), *Annona purpurea* (soncoya) and *Rollinia mucosa* (biriba). Cryst. Mp 70-72°. $[\alpha]_D$ +21.8 (c, 0.6 in MeOH). λ_{max} 208 (ε 14300) (MeOH).

20-Epimer: [140224-67-5] ***Trilobacin***
$C_{37}H_{66}O_7$ 622.924
Constit. of the bark of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D^{22}$ +10 (c, 0.0005 in $CHCl_3$). λ_{max} 223 (ε 2653) (EtOH) (Berdy).

24-Epimer: [123123-32-0]

[121917-13-3, 129212-94-8] ***Bullatacin***. *Rolliniastatin 2*. *Annonin VI*. *Squamocin G*
$C_{37}H_{66}O_7$ 622.924
Isol. from *Rollinia mucosa* (biriba), *Annona squamosa* (sugar apple) and *Annona reticulata* (custard apple). Cryst. (EtOAc). Mp 69-70°. $[\alpha]_D^{23}$ +13 (c, 0.004 in $CHCl_3$). $[\alpha]_D$ +15.3 (c, 0.4 in CH_2Cl_2). λ_{max} 208 (ε 14300) (MeOH) (Derep).

*24-Epimer, 27*S*-hydroxy:* ***27-Hydroxybullatacin***
$C_{37}H_{66}O_8$ 638.924
Constit. of *Annona glabra* (pond apple). Waxy solid. $[\alpha]_D^{25}$ +11 ($CHCl_3$).

24-Epimer, 28-hydroxy: [148057-45-8] ***Rioclarin***
$C_{37}H_{66}O_8$ 638.924
$[\alpha]_D$ +20 (c, 0.4 in MeOH).

24-Epimer, 30-hydroxy: [169390-19-6] ***30-Hydroxybullatacin***
$C_{37}H_{66}O_8$ 638.924
Powder. $[\alpha]_D$ +14 (c, 0.5 in $CHCl_3$). Isol. as a 4:1 mixt. of 30*S*- and 30*R*-epimers respectively.

*24-Epimer, 31*S*-hydroxy:* [169390-18-5] ***31-Hydroxybullatacin***
$C_{37}H_{66}O_8$ 638.924
Powder. $[\alpha]_D$ +19 (c, 0.08 in $CHCl_3$).

*24-Epimer, 32*S*-hydroxy:* [169390-17-4] ***32-Hydroxybullatacin***
$C_{37}H_{66}O_8$ 638.924
Powder. $[\alpha]_D$ +19 (c, 0.08 in $CHCl_3$).

19,20,24-Triepimer: [111056-97-4] ***Rolliniastatin 1***. *4-Hydroxy-25-desoxyneorollinicin*
$C_{37}H_{66}O_7$ 622.924
Isol. from *Rollinia mucosa* (biriba). Wax (Me_2CO). Mp 81-83°. $[\alpha]_D$ +25.2 (c, 1.03 in CH_2Cl_2). Relative config. only determined λ_{max} 208 (ε 14300) (MeOH) (Derep).

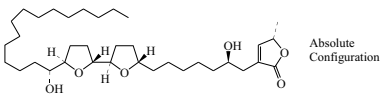
[123805-39-0, 129138-51-8, 130851-93-3]

Rupprecht, J.K. *et al., Heterocycles*, 1986, **24**, 1197 (*Asimicin*)
Pettit, G.R. *et al., Can. J. Chem.*, 1987, **65**, 1433 (*Rolliniastatin 1*)
Hoye, T.R. *et al., J.O.C.*, 1988, **53**, 5578 (*pmr, struct*)
Pettit, G.R. *et al., Heterocycles*, 1989, **28**, 213 (*Rolliniastatin 2*)
Hui, Y.H. *et al., J. Nat. Prod.*, 1989, **52**, 463; 1990, **53**, 81 (*isol, pmr, cmr, Bullatacin*)
Abreo, M.J. *et al., J. Nat. Prod.*, 1989, **52**, 822 (*4-Hydroxy-25-desoxyneorollinicin*)
Li, X.H. *et al., J. Nat. Prod.*, 1990, **53**, 81 (*Bullatacin*)
Rupprecht, J.K. *et al., J. Nat. Prod.*, 1990, **53**, 237 (*rev*)
Nonfon, M. *et al., Phytochemistry*, 1990, **29**, 2951 (*Annonin VI*)
Born, L. *et al., Planta Med.*, 1990, **56**, 312 (*Annonin VI*)
Lieb, F. *et al., Planta Med.*, 1990, **56**, 317-319 (*Annonastatin*)
Cortes, D. *et al., Tetrahedron*, 1991, **47**, 8195 (*Rolliniastatin 2*)
Zhao, G. *et al., J. Nat. Prod.*, 1992, **55**, 347-356 (*Trilobacin*)
Rieser, M.J. *et al., J.A.C.S.*, 1992, **114**, 10203 (*abs config*)
Laprévote, O. *et al., Tet. Lett.*, 1992, **33**, 5237 (*ms*)
Maillard, M.P. *et al., J. Chromatogr.*, 1993, **647**, 147 (*hplc*)
Ahammadsahib, K.I. *et al., Life Sci.*, 1993, **53**, 1113 (*Bullatacin, pharmacol*)
Cortes, D. *et al., Phytochemistry*, 1993, **32**, 1467; 1475 (*rev*)
Hoye, T.R. *et al., Tet. Lett.*, 1993, **34**, 5043; 1995, **36**, 1981-1984 (*(-)-Bullatacin, synth*)
Degli-Esposti, M. *et al., Biochem. J.*, 1994, **301**, 161 (*activity*)
Holschneider, C.H. *et al., Cancer Chemother. Pharmacol.*, 1994, **34**, 166 (*Bullatacin, pharmacol*)
Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*Squamocins*)
Koert, U. *et al., Tet. Lett.*, 1994, **35**, 2517 (*synth, Rolliniastatin 1*)
Laprevote, O. *et al., Tetrahedron*, 1994, **50**, 8479 (*ms, struct*)
Naito, H. *et al., J.O.C.*, 1995, **60**, 4419 (*Bullatacin, synth, ir, pmr*)
Morré, D.J. *et al., Life Sci.*, 1995, **56**, 343 (*Bullatacin*)
Gu, Z.-M. *et al., Phytochemistry*, 1995, **40**, 467-477 (*Hydroxybullatacins*)
Sinha, S.C. *et al., Tet. Lett.*, 1995, **36**, 9257-9260 (*synth*)
Sinha, S.C. *et al., J.O.C.*, 1996, **61**, 7640-7641 (*synth, Trilobacin*)
Zeng, L. *et al., Nat. Prod. Rep.*, 1996, **13**, 275-306 (*rev*)
Marshall, J.A. *et al., J.O.C.*, 1997, **62**, 5989-5995 (*synth*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)

Duret, P. *et al., J.O.C.*, 1998, **63**, 4717-4720 (*abs config*)
Martin, J.M. *et al., J. Nat. Prod.*, 1999, **62**, 2-4 (*activity*)
Liu, X.-X. *et al., J. Nat. Prod.*, 1999, **62**, 848-852 (*27-Hydroxybullatacin*)
Ruan, Z. *et al., Tet. Lett.*, 1999, **40**, 49-52 (*synth, Asimicin, Trilobacin*)
Avedissian, H. *et al., J.O.C.*, 2000, **65**, 6035-6051 (*synth*)
Marshall, J.A. *et al., J.O.C.*, 2003, **68**, 1771-1779; 1780-1785 (*synth*)

Asimilobin A-451

[168075-15-8]



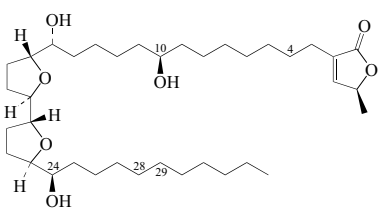
$C_{35}H_{62}O_6$ 578.871

Abs. config. revised in 1999. Constit. of the seeds of *Asimina triloba* (pawpaw). Needles. Sol. MeOH, hexane; poorly sol. H_2O. Mp 56-57°. $[\alpha]_D$ +11.3 (c, 1 in CH_2Cl_2). $[\alpha]_D$ +6 (c, 0.05 in $CHCl_3$). λ_{max} 228 (log ϵ 2.98) (EtOH). λ_{max} 228 (ϵ 955) (MeOH) (Berdy). λ_{max} 209 (ϵ 1000) (EtOH) (Berdy).

Zhang, Y. *et al., Heterocycles*, 1995, **41**, 1743-1755 (*isol*)
Woo, M.H. *et al., J. Nat. Prod.*, 1995, **58**, 1533 (*isol*)
Wang, Z.-M. *et al., Eur. J. Org. Chem.*, 2000, 349-356 (*synth, abs config*)

Asimin A-452

[156162-01-5]



$C_{37}H_{66}O_7$ 622.924

Constit. of the stem bark of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D$ +26 ($CHCl_3$). λ_{max} 215 (MeOH).

20-Epimer: [165525-53-1] ***Trilobin***
$C_{37}H_{66}O_7$ 622.924
Constit. of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D$ +33.3 (c, 0.1 in MeOH). λ_{max} 225 (ϵ 2695) (EtOH) (Berdy).

24-Epimer, 10-ketone: [212616-61-0]

[212575-88-7] ***Guanacone***
$C_{37}H_{64}O_7$ 620.908
Wax. $[\alpha]_D$ +22 (c, 1 in EtOH). λ_{max} 208 (log ϵ 3.83) (MeOH).

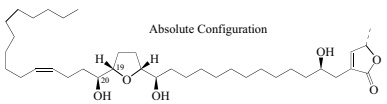
24-Epimer, 10-ketone, oxime:10-Oxime-guanacone
$C_{37}H_{65}NO_7$ 635.923

10,24-Diepimer: [158515-36-7] ***Bullatin***
$C_{37}H_{66}O_7$ 622.924
Constit. of *Asimina triloba* (pawpaw). $[\alpha]_D$ +7.5 (c, 0.04 in EtOH).

Zhao, G.-X. *et al., Heterocycles*, 1994, **38**, 1897-1908 (*Bullatin*)
Zhao, G.-X. *et al., J. Med. Chem.*, 1994, **37**, 1971-1976 (*isol, uv, ir, pmr, cmr, ms, props*)
Zhao, G. *et al., Tetrahedron*, 1995, **51**, 7149-7160 (*Trilobin*)
Zeng, L. *et al., Nat. Prod. Rep.*, 1996, **13**, 275-306 (*rev*)
Gallardo, T. *et al., J. Nat. Prod.*, 1998, **61**, 1001-1005 (*Guanacone*)
Marshall, J.A. *et al., J. Nat. Prod.*, 1999, **62**, 1123-1127 (*Trilobin, synth, abs config*)
Marshall, J.A. *et al., J.O.C.*, 1999, **64**, 971-975 (*Trilobin, synth*)
Sinha, A. *et al., J.O.C.*, 1999, **64**, 2381-2386 (*Trilobin, synth*)
Marshall, J.A. *et al., J.O.C.*, 2003, **68**, 1771-1779 (*synth*)

Asiminenin A A-453

[168075-11-4]



$C_{37}H_{66}O_6$ 606.925

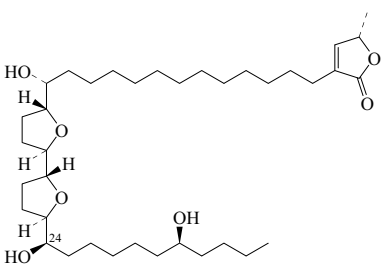
Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. Sol. MeOH, hexane; poorly sol. H_2O. Mp 58-59°. $[\alpha]_D$ +10 (c, 0.1 in CH_2Cl_2). λ_{max} 228 (log ϵ 3.55) (MeOH).

19,20-Diepimer: [168113-65-3] ***Asiminenin B***
$C_{37}H_{66}O_6$ 606.925
Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. Sol. MeOH, hexane; poorly sol. H_2O. Mp 54-55°. $[\alpha]_D$ +17 (c, 0.1 in CH_2Cl_2). λ_{max} 230 (log ϵ 2.93) (MeOH).

Woo, M.H. *et al., Heterocycles*, 1995, **41**, 1731-1742 (*isol, uv, ir, pmr, cmr, ms*)

Asiminocin A-454

[174693-31-3]



$C_{37}H_{66}O_7$ 622.924

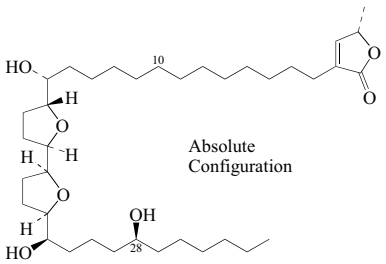
Constit. of *Annona triloba* (pawpaw). Wax. $[\alpha]_D$ +26 (c, 1 in $CHCl_3$).

24-Epimer: [158446-27-6] ***Bullanin***
$C_{37}H_{66}O_7$ 622.924
Constit. of the stem bark of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D$ +28 (EtOH). Both C-30 epimers are known λ_{max} 213 (ϵ 220) (EtOH). λ_{max} 220 (ϵ 263) (EtOH) (Berdy).

Zhao, G.X. *et al., Heterocycles*, 1994, **38**, 1897-1909 (*Bullanin*)
Zhao, G.X. *et al., Bioorg. Med. Chem.*, 1996, **4**, 25-32 (*Asiminocin*)
Marshall, J.A. *et al., J.O.C.*, 1997, **62**, 5996-6000; 2003, **68**, 1771-1779 (*synth*)

Asitribin A-455

[168113-64-2]



$C_{37}H_{66}O_7$ 622.924

Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. Sol. MeOH, hexane; poorly sol. H_2O. Mp 71-72°. $[\alpha]_D$ +15 (c, 0.1 in CH_2Cl_2). λ_{max} 234 (ϵ 3550) (MeOH) (Berdy).

20-Epimer: [156199-51-8] ***Asiminacin***. *Squamocin D*
$C_{37}H_{66}O_7$ 622.924
Constit. of *Asimina triloba* (pawpaw) and *Annona squamosa* (sugar apple). Wax. $[\alpha]_D$ +21.1 ($CHCl_3$). λ_{max} 215 (MeOH).

19,24-Diepimer: [240486-97-9] ***Ophrypetalin***
$C_{37}H_{66}O_7$ 622.924
Wax. $[\alpha]_D$ +21.3 (c, 0.9 in MeOH). λ_{max} 208 (log ϵ 4.26) (MeOH).

20,24-Diepimer: [120298-30-8]

[93303-16-3, 168609-25-4, 183507-41-7] ***Squamocin***. *Rollinicin*. *Squamocin A*. ***Annonin I***
$C_{37}H_{66}O_7$ 622.924
Constit. of various *Annona* spp.. Mp 30-32° (< 30°). $[\alpha]_D$ +21.2 (c, 0.4 in $CHCl_3$). $[\alpha]_D$ +16.2 (c, 1 in $CHCl_3$). λ_{max} 215 (ϵ 3160) (MeOH) (Derep).

20,24-Diepimer, 28-ketone: [133594-24-8] ***Squamocinone***. *Squamocin-28-one*
$C_{37}H_{64}O_7$ 620.908
Oil.

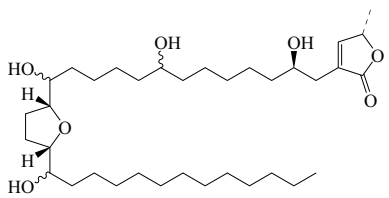
20,23,28-Triepimer: [201167-31-9] ***Carolin A***
$C_{37}H_{66}O_7$ 622.924
Oil. $[\alpha]_D^{20}$ +22 (c, 1 in $CHCl_3$). λ_{max} 208 (log ϵ 4.6) (EtOH).

Stereoisomer: [93236-32-9] ***Isorollinicin***
$C_{37}H_{66}O_7$ 622.924
Amorph. Sol. EtOH, $CHCl_3$, C_6H_6; poorly sol. H_2O. Mp 66-68°. λ_{max} 215 (ϵ 3160) (MeOH) (Derep). λ_{max} 231 (ϵ 20100) (CH_2Cl_2) (Berdy).

Dabrah, T.T. *et al., Phytochemistry*, 1984, **23**, 2013-2016 (*Rollinicin, Isorollinicin*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4802-4806 (*Squamocin*)
Nonfon, M.F. *et al., Phytochemistry*, 1990, **29**, 1951-1954 (*Squamocin*)
Born, L. *et al., Planta Med.*, 1990, **56**, 312-316 (*Annonin I*)
Hisham, A. *et al., Phytochemistry*, 1991, **30**, 545-548 (*Squamocinone*)
Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*Squamocin A*)
Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163 (*Squamocin D*)
Gu, Z. *et al., J.O.C.*, 1994, **59**, 5162-5172 (*Squamocin, abs config*)

Woo, M.H. *et al., Heterocycles*, 1995, **41**, 1731 (*Asitribin*)
Gypser, A. *et al., Tetrahedron*, 1995, **51**, 1921-1930 (*Annonin I, abs config*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)
Queiroz, E.F. *et al., J. Nat. Prod.*, 1998, **61**, 34 (*Carolin A*)
Duret, P. *et al., J.O.C.*, 1998, **63**, 4717-4720 (*abs config*)
Marshall, J.A. *et al., J.O.C.*, 1999, **64**, 971-975 (*synth, Trilobin*)
Sinha, A. *et al., J.O.C.*, 1999, **64**, 2381-2386 (*synth, Trilobin*)
Sung'Hwa, F. *et al., Nat. Prod. Lett.*, 1999, **13**, 195-202 (*Ophrypetalin*)
Emde, U. *et al., Eur. J. Org. Chem.*, 2000, 1889-1904 (*synth*)
Queiroz, E.F. *et al., J. Med. Chem.*, 2000, **43**, 1604-1610 (*Squamocin*)

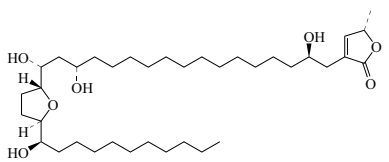
Asitrilobin B A-456



$C_{35}H_{64}O_7$ 596.886
Constit. of the seeds of *Asimina triloba* (pawpaw). Amorph. powder. Mp 65.3-68.4°. $[\alpha]_D^{22}$ +23.3 (c, 0.03 in CH_2Cl_2). λ_{max} 226 (log ε 4.1) (MeOH).

Woo, M.-H. *et al., Phytochemistry*, 1999, **50**, 1033-1040 (*isol, uv, ir, pmr, cmr, ms*)

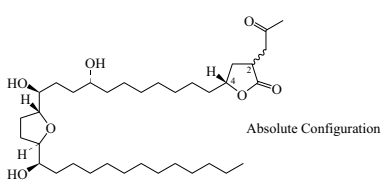
Asitrilobin D A-457



$C_{37}H_{68}O_7$ 624.94
Constit. of *Asimina triloba* (pawpaw). Powder. Mp 87.2-88.1°. $[\alpha]_D^{20}$ -4 (c, 0.005 in CH_2Cl_2). λ_{max} 226 (log ε 3.7) (MeOH).

Woo, M.-H. *et al., Bioorg. Med. Chem.*, 2000, **8**, 285-290

Asitrocinone A-458

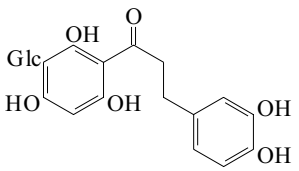


$C_{35}H_{64}O_7$ 596.886
Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. $[\alpha]_D^{23}$ +13.2 (c, 0.005 in CH_2Cl_2). Mixt. of 2,4-*cis*-and *trans*-isomers λ_{max} 205 (log ε 3.6) (MeOH).

Kim, E.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1503-1506

Aspalathin A-459

1-(3-C-β-D-Glucopyranosyl-2,4,6-trihydroxyphenyl)-3-(3,4-dihydroxyphenyl)-1-propanone. 3′-Glucosyl-2′,3,4,4′,6′-pentahydroxydihydrochalcone



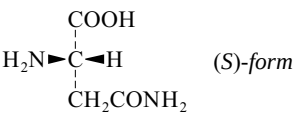
$C_{21}H_{24}O_{11}$ 452.414
Constit. of *Aspalathus linearis* (rooibos). Amorph. Sol. H_2O. $[\alpha]_D^{20}$ +34.7 (c, 2.14 in EtOH). $[\alpha]_D$ +58.4 (c, 2.21 in Me_2CO).

Nona-Ac:
Fine needles (EtOH). Mp 153-154°. $[\alpha]_D^{25}$ -35.8 (c, 2.16 in Me_2CO).

Koeppen, B.H. *et al., Tet. Lett.*, 1965, 3497; *Biochem. J.*, 1966, **99**, 604 (*isol, struct*)

Asparagine, 9CI A-460

[7006-34-0]
2,4-Diamino-4-oxobutanoic acid. Aspartic acid β-monoamide. β-Asparagine. Asparamide. Altheine. Asn



$C_4H_8N_2O_3$ 132.119
Derivs. labelled *N* (here and in 9CI) refer to those subst. on the amide (or N^4) nitrogen; N^2 refers to subst. on amino group.

(R)-form [2058-58-4]

[5794-24-1]
D-form
Cryst. + $1H_2O$. Mp 234-235°. $[\alpha]_D^{15}$ +5.4 (H_2O).

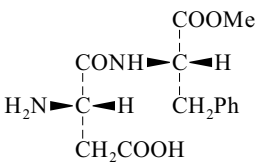
(S)-form [70-47-3]
L-form
One of the nonessential amino acids. Dietary supplement, nutrient. Widely distributed in the plant kingdom. Isol. from asparagus, beetroot, peas, beans, etc.. Rhombic hemihedral cryst. + $1H_2O$ (H_2O). Mod. sol. H_2O (3.1g/100g at 25°). Mp 234-235° (rapid heat) Mp 226-227° dec. (slow heat). $[\alpha]_D^{25}$ -7.4 (c, 2 in H_2O). $[\alpha]_D$ +33.2 (3*M* HCl). pK_{a2} 8.6 (NH_2). Isoelectric point 5.41. Bitter taste.

(±)-form [3130-87-8]
Cryst. + $1H_2O$ (EtOH/HCl aq.). Loses H_2O at 210°, dec. at 280-5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 782A; 782B; 782C; **2**, 263A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1277C; 1278A (*nmr*)
Aldrich Library of NMR Spectra, **3**, 10A; 121C (*pmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **2**, 1257; **3**, 1856 (*occur, isol, synth*)
Gray, D.O. *et al., Nature (London)*, 1961, **189**, 401 (*isol, deriv*)
Biochem. Prep., 1963, **10**, 10
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Ramanadham, M. *et al., Acta Cryst. B*, 1972, **28**, 3000 (*cryst struct*)
Verbis, J.J. *et al., Acta Cryst. B*, 1972, **28**, 3006 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2370 (*occur*)
Toi, K. *et al., Synth. Prod. Util. Amino Acids*, 1974, 75 (*rev*)
Tome, D. *et al., Int. J. Pept. Protein Res.*, 1981, **17**, 501 (*cmr*)
Yoshifuji, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2994 (*synth*)
Sieciechowicz, K.A. *et al., Phytochemistry*, 1988, **27**, 663 (*rev, metab*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN810
Casado, J. *et al., J. Mol. Struct.*, 1995, **349**, 57 (*ir, Raman*)
Casado, J. *et al., J. Raman Spectrosc.*, 1995, **26**, 1003 (*ir, Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 213-214
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN810

Aspartame, BAN, USAN A-461

[22839-47-0]
N-α-*Aspartyl-L-phenylalanine 1-methyl ester, 9CI. Methyl aspartylphenylalanine. Nutrasweet. Canderel. α-APM. SC-18862. E951*



$C_{14}H_{18}N_2O_5$ 294.307
Compd. with 100 times the sweetness of sucrose. Artificial sweetener permitted in foods in EU at 300-5500 ppm. Also permitted in USA. Widely used in foods, beverages and pharmaceutical formulations. Cryst. (EtOH aq. or H_2O). Mp 190° Mp 245-247° (double Mp) (235-236° dec.). $[\alpha]_D$ 0 (H_2O). $[\alpha]_D^{22}$ +32 (c, 1 in AcOH). Log P -2.16 (calc).

▶ WM3407000

Hydrochloride: [5910-52-1]
Mp 127-128° dec. (partly melts at 103°). $[\alpha]_D^{25}$ +1.3 (c, 2 in H_2O).

Hydrobromide: [36771-92-3]
Mp 155° dec. $[\alpha]_D^{25}$ +1 (c, 2 in H_2O).

3-N-tert-*Butyloxycarbonyl:* [40944-73-8]
$C_{19}H_{26}N_2O_7$ 394.424
Cryst. (EtOAc/Et_2O). Mp 164-166° (149-151°). $[\alpha]_D^{18}$ -34.5 (c, 0.5 in DMF).

3-N-*Benzyloxycarbonyl:* [33605-72-0]
$C_{22}H_{24}N_2O_7$ 428.441
Cryst. Mp 120-124°. $[\alpha]_D^{25}$ -14.4 (c, 1 in MeOH).

[53906-69-7]

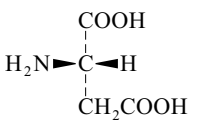
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 267D (*ir*)
Neuman, M. *et al., Drugs of Today (Barcelona)*, 1980, **16**, 63-67 (*rev*)

Shvachkin, Y.P. *et al., Zh. Obshch. Khim.*, 1982, **52**, 2791-2792; *CA*, **98**, 107764c (*synth*)
Fujii, N. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3503-3514 (*tert-butyloxycarbonyl*)
Steginк, L.D. *et al., Food Sci. Technol.*, Aspartame: Physiol. Biochem., Dekker, N.Y., 1984, **12**, (*book*)
Renwick, A.G. *et al., Food Chem.*, 1985, **16**, 281-301 (*metab*)
Hatada, M. *et al., J.A.C.S.*, 1985, **107**, 4279-4282 (*cryst struct*)
Tou, J.S. *et al., J.O.C.*, 1985, **50**, 4982-4984 (*synth*)
Fuganti, C. *et al., J.O.C.*, 1986, **51**, 1126-1128 (*synth*)
Görbitz, C.H. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 87-92 (*hydrochloride, cryst struct*)
Nakanishi, K. *et al., Food Biotechnol.*, 1988, **2**, 219-249 (*rev, synth*)
Chen, S.T. *et al., J.O.C.*, 1988, **53**, 4589-4590 (*tert-butyloxycarbonyl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN825
Keirs, D. *et al., Heterocycles*, 1989, **28**, 841-848 (*synth*)
Kuhl, P. *et al., Pharmazie*, 1990, **45**, 881-887 (*rev, synth*)
Homler, B.E. *et al., Food Sci. Technol.*, 1991, **48**, 39-69 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 21-23
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1354
Ager, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*degradn, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN825

Aspartic acid, INN, USAN A-462

[6899-03-2]

Aminobutanedioic acid, 9CI. Aminosuccinic acid. Asparagic acid. Asparaginic acid. Asp



(*S*)-*form*

$C_4H_7NO_4$ 133.104

(*S*)-*form* [56-84-8]

L-form. FEMA 3656

Found in sugar cane and sugar beet molasses and proteins/peptides. Dietary supplement, nutrient. Leaflets (H_2O). Spar. sol. H_2O (0.5g/100g at 25°). Mp 269-271° dec. $[\alpha]_D^{25}$ +5.05 (c, 1 in H_2O). $[\alpha]_D$ +25.4 (c, 1 in 5*M* HCl). pK_{a3} 9.82-0 (25°,1-COOH). Isoelectric point 2.77. Bitter taste.

▶ LD_{50} (mus, ipr) 6000 mg/kg. CI9098500

N-*Benzoyl:* [4631-12-3]
Constit. of pea (*Pisum sativum*). Mp 171-173°. $[\alpha]_D^{20}$ +37 (c, 10 in 1*M* NaOH).

N-*(2-Hydroxybenzoyl):* [56145-94-9] **N-*Salicyloylaspartic acid***
$C_{11}H_{11}NO_6$ 253.211
Constit. of kidney beans (*Phaseolus vulgaris*) and grape (*Vitis* spp.). λ_{max} 238 ; 305 (MeOH) (Berdy).

▶ CI9455500

N-*(4-Hydroxy-3-methoxycinnamoyl):* [135068-96-1] **N-*Feruloylaspartic acid***
$C_{14}H_{15}NO_7$ 309.275
Constit. of beet (*Beta vulgaris*).

N-*Phenylacetyl:* [2752-32-1] N-*Phenylacetylaspartic acid*
$C_{12}H_{13}NO_5$ 251.238
Constit. of pea (*Pisum sativum*). Mp 136°.

[1115-63-5, 3792-50-5, 14007-45-5, 17090-93-6, 17833-53-3]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 496C; 496D; 497A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 588D; 589A; 589B (*ir*)
Vickery, H.B. *et al., Biochem. Prep.*, 1952, **2**, 71 (*synth*)
Wood, J.W. *et al., J.O.C.*, 1952, **17**, 891
Katchalsky, A. *et al., J.A.C.S.*, 1954, **76**, 6042 (*synth*)
Block, S. *et al., J. Biol. Chem.*, 1955, **213**, 27 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1856; 2759 (*rev*)
Org. Synth., Coll. Vol., 4, 1963, 55 (*synth*)
Fujiwara, S. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 344 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Young, D.P. *et al., Chem. Ind. (London)*, 1967, 1251
Zintel, J.A. *et al., Can. J. Chem.*, 1969, **47**, 411 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2369 (*occur*)
Rao, S.T. *et al., Acta Cryst. B*, 1973, **29**, 1718 (*cryst struct*)
Sergeev, G.M. *et al., CA*, 1977, **89**, 208521r (*use*)
Gianfagna, T.J. *et al., Phytochemistry*, 1980, **19**, 959 (*isol, N-benzoyl, N-phenylacetyl*)
Hardin, E.D. *et al., Anal. Chem.*, 1981, **53**, 1492 (*ms*)
Harada, K. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 653 (*resoln*)
Zahradnik, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 2122 (*manuf*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN830; ARN850
Bokern, M. *et al., Phytochemistry*, 1991, **30**, 3261 (*N-Feruloylaspartic acid*)
Bourne, D.J. *et al., Phytochemistry*, 1991, **30**, 4041 (*N-Salicyloylaspartic acid*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1036
Castro, J.L. *et al., J. Mol. Struct.*, 1995, **349**, 113 (*ir, Raman*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN830; ARN850

N^{β}-Aspartylglycine, 9CI A-463

$HOOCCH(NH_2)CH_2CONHCH_2COOH$

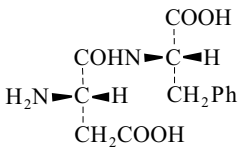
$C_6H_{10}N_2O_5$ 190.155

D-*form* [67176-36-7]
Mp 210-228°. $[\alpha]_D^{28}$ -8.9 (c, 1 in 50% AcOH).

L-*form* [3790-52-1]
Cryst. (H_2O). Mp 160-168°. $[\alpha]_D^{28}$ +18.1 (c, 1 in 1*M* HCl).

Takashi, A. *et al., Biochem. Biophys. Res. Commun.*, 1978, **82**, 707
Welling, G.W. *et al., Biochem. J.*, 1978, **175**, 807
Welling, G.W. *et al., J. Chromatogr.*, 1982, **232**, 55 (*anal*)

N^{α}-Aspartylphenylalanine A-464



$C_{13}H_{16}N_2O_5$ 280.28

L-L-*form* [13433-09-5]
Degradn. product of Aspartame, A-461. Mp 232-235°. $[\alpha]_D$ +16 (c, 1 in DMF).

Me ester: Aspartame, A-461

N-*(3,3-Dimethylbutyl), Me ester:* [165450-17-9] *Neotame*
$C_{20}H_{30}N_2O_5$ 378.467
Submitted to FDA (1999) for approval as food sweetener
Potential high-intensity sweetener, sweetness variously stated to be 40 x sucrose and 7000-13000 x sucrose. Cryst. + $1H_2O$ (EtOAc/hexane). Mp 80-83° (monohydrate). $[\alpha]_D$ -54.84 (c, 1 in MeOH). Other diastereomers do not exhibit sweetening power.

Davey, J.M. *et al., J.C.S.(C)*, 1966, 555 (*deriv*)
Mazur, R.H. *et al., J.A.C.S.*, 1969, **91**, 2684 (*synth*)
Roberts, G.C.K. *et al., Biochem. J.*, 1971, **125**, 88P (*pmr*)
Yasutake, A. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 2413 (*deriv*)
U.S. Pat., 1996, 5 510 508; *CA*, **124**, 203104p (*Neotame*)
Wink, D.J. *et al., Acta Cryst. C*, 1999, **55**, 1365-1368 (*Neotame, synth, pmr, cryst struct*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261

Aspergillomarasmine A A-465

[3484-65-9]

N-*[2-(2-Amino-2-carboxyethyl)amino]-2-carboxyaspartic acid, 9CI. Toxin C*

$HOOCCH_2CH(COOH)NHCH_2CH(COOH)NHCH_2CH(NH_2)COOH$

$C_{10}H_{17}N_3O_8$ 307.26

Metab. of the cereal fungus (*Aspergillus flavus*), found only in young cultures. Sol. acids, bases; poorly sol. H_2O, butanol, hexane. Mp 230-236° dec. $[\alpha]_D^{20}$ -48 (phosphate buffer, pH 7).

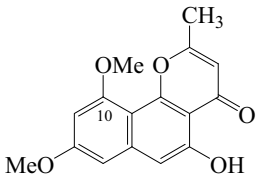
▶ LD_{50} (mus, ivn) 250 mg/kg. CI9098825

Barter, M. *et al., Bull. Soc. Chim. Fr.*, 1962, 187
Bogdanovsky, O. *et al., Bull. Soc. Chim. Fr.*, 1965, 832 (*synth*)
Haenni, A.L. *et al., Helv. Chim. Acta*, 1965, **48**, 729 (*struct*)
Mikami, Y. *et al., Agric. Biol. Chem.*, 1983, **47**, 2693

Asperxanthone A-466

[3566-99-2]

5-Hydroxy-8,10-dimethoxy-2-methyl-4H-naphtho[1,2-b]pyran-4-one, 9CI. Flavasperone. Antibiotic TMC 256C2. TMC 256C2



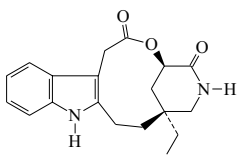
$C_{16}H_{14}O_5$ 286.284
Constit. of *Aspergillus niger*, *Aspergillus awamori* and *Aspergillus fonsecaeus*. Isol. from *A. niger* infected mango fruits and peanuts. Yellow needles ($CHCl_3$/EtOH). Mp 203°. λ_{max} 282 (ϵ 22400); 370 (ϵ 46400) (MeOH) (Berdy). λ_{max} 241 (ϵ 38400) (EtOH) (Berdy).

*10-*O*-De-Me, 10-*O*-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [200127-93-1] *10-*O*-Demethylflavasperone 10-gentiobioside. Isorubrofusarin 10-gentiobioside*
$C_{27}H_{32}O_{15}$ 596.541
Constit. of the seeds of *Cassia tora* (charota). Yellow powder. $[\alpha]_D$ -14 (c, 0.1 in Py). λ_{max} 240 (log ϵ 4.49); 248 (sh) (log ϵ 4.39); 279 (log ϵ 4.35); 313 (sh) (log ϵ 3.84); 367 (log ϵ 3.5) (MeOH).

Lund, N.A. *et al., J.C.S.*, 1953, 2434 (*isol*)
Bycroft, B.W. *et al., J.C.S.*, 1962, 40; 1963, 4868 (*struct, synth*)
Tanaka, H. *et al., Agric. Biol. Chem.*, 1966, **30**, 107 (*isol*)
Ghosal, S. *et al., J. Agric. Food Chem.*, 1979, **27**, 1347 (*isol, props*)
Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1980, 2474 (*isol, uv, ir, pmr, cmr*)
Lee, H.J. *et al., Arch. Pharmacal Res.*, 1997, **20**, 513-515 (*Isorubrofusarin gentiobioside*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1121-1127 (*isorubrofusarin 10-gentiobioside*)

Aspidochibine A-467

[139955-86-5]
Alkaloid AQC2



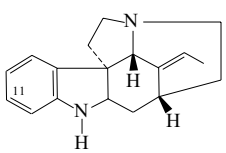
Relative configuration

$C_{19}H_{22}N_2O_3$ 326.394
New structural class of the quebrachamine series. Alkaloid from cell cultures of *Aspidosperma quebracho-blanco* (quebracho). Amorph.

Aimi, N. *et al., Tet. Lett.*, 1991, **32**, 4949 (*isol, pmr, cmr, struct*)

Aspidospermatidine A-468

[3890-05-9]
14,19-Didehydrocondyfolan, 9CI



Absolute configuration

$C_{18}H_{22}N_2$ 266.385
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Cryst. (Et_2O/hexane). Mp 168-170° Mp 184-186°.

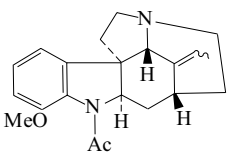
N-*Ac:***N-*Acetylaspidospermatidine***
$C_{20}H_{24}N_2O$ 308.422
Noncryst. $[\alpha]_D$ -28 (EtOH).

N-*Me:***N-*Methylaspidospermatidine***
$C_{19}H_{24}N_2$ 280.412
Alkaloid in *Aspidosperma quebracho-blanco* (quebracho). Amorph.

11-Hydroxy, N-*Ac:***N-*Acetyl-11-hydroxyaspidospermatidine***
$C_{20}H_{24}N_2O_2$ 324.422
Noncryst.

Biemann, K. *et al., J.A.C.S.*, 1963, **85**, 631 (*isol, uv, ms, struct*)
Walser, A. *et al., Helv. Chim. Acta*, 1965, **48**, 391 (N-*Acetylaspidospermatidine*)
Gilbert, B. *et al., Tetrahedron*, 1965, **21**, 1141 (N-*Acetyl-11-hydroxyaspidospermatidine*)

Aspidospermatine A-469



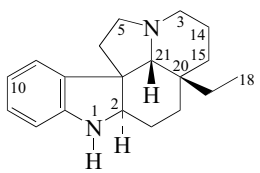
Absolute configuration

$C_{21}H_{26}N_2O_2$ 338.449
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 162° (157-159°). $[\alpha]_D$ -73 (EtOH).

14,19-Dihydro: ***Dihydroaspidospermatine***
$C_{21}H_{28}N_2O_2$ 340.464
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Noncryst.

Biemann, K. *et al., J.A.C.S.*, 1963, **85**, 631 (*isol, uv, ir, pmr, ms, struct*)

Aspidospermidine A-470



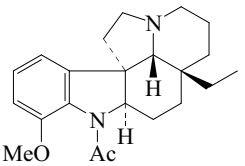
(+)-*form*

$C_{19}H_{26}N_2$ 282.428
(+)-*form* [2912-09-6]
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 119.5-121°. $[\alpha]_D^{23}$ +21 (EtOH).

Biemann, K. *et al., J.A.C.S.*, 1963, **85**, 631 (*ms*)
Smith, G.F. *et al., J.C.S.*, 1963, 4002 (*synth, uv*)
Klyne, W. *et al., Helv. Chim. Acta*, 1968, **51**, 1169 (*ord*)
Laronze, J.-Y. *et al., Tet. Lett.*, 1974, 491 (*synth*)
Seki, K. *et al., Tet. Lett.*, 1975, 723 (*synth*)
Paccioni, J.P. *et al., Phytochemistry*, 1978, **17**, 2146
Gallagher, T. *et al., J.A.C.S.*, 1983, **105**, 4750 (*synth*)
Mandal, S.B. *et al., J.O.C.*, 1988, **53**, 4236 (*synth*)
Node, M. *et al., J.O.C.*, 1990, **55**, 517 (*synth*)
Le Ménez, P. *et al., J.O.C.*, 1991, **56**, 2915 (*synth*)
Desmaële, D. *et al., J.O.C.*, 1994, **59**, 2292 (*synth*)
Wenkert, E. *et al., J.O.C.*, 1994, **59**, 7677 (*synth*)
Forns, P. *et al., J.O.C.*, 1996, **61**, 7882 (*synth*)
Schultz, A.G. *et al., J.O.C.*, 1997, **62**, 6855-6861 (*synth*)
Callaghan, O. *et al., J.C.S. Perkin 1*, 1999, 995-1001 (*synth*)
Callaghan, O. *et al., Tet. Lett.*, 1999, **40**, 161-164; 2225 (*synth, bibl*)
Toczko, M.A. *et al., J.O.C.*, 2000, **65**, 2642-2645 (*synth*)
Iyengar, R. *et al., Org. Lett.*, 2000, **2**, 1625-1627 (*synth*)
Kozmin, S.A. *et al., J.A.C.S.*, 2002, **124**, 4628-4641 (*synth*)

Aspidospermine A-471

1-Acetyl-17-methoxyaspidospermidine, 9CI



(-)-*form*

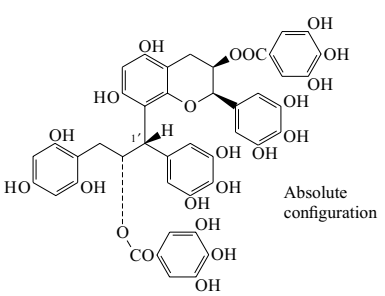
$C_{22}H_{30}N_2O_2$ 354.491
λ_{max} 218 (ϵ 37500); 255 (ϵ 11000); 285 (ϵ 3400) (MeOH) (Berdy).

(-)-*form* [466-49-9]
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 208-209°. $[\alpha]_D^{15}$ -100 (EtOH). pK_a 7.63 (25°).
▶ LD_{50} (mus, ipr) 40 mg/kg. CJ0175000
O-*De-Me:* See Demethylaspidospermine in *The Combined Chemical Dictionary.*
(±)-*form* [23360-86-3]
Mp 195-195.5°.

Chalmers, J.R. *et al., J.C.S.*, 1957, 1115 (*uv*)
Conroy, H. *et al., J.A.C.S.*, 1958, **80**, 5178 (*ir, pmr*)
Biemann, K. *et al., Tet. Lett.*, 1961, 485 (*ms*)
Craven, B.M. *et al., Experientia*, 1968, **24**, 770 (*cryst struct, abs config*)
Stevens, R.V. *et al., Chem. Comm.*, 1971, 857 (*synth*)
Meyers, A.I. *et al., J.O.C.*, 1989, **54**, 4673 (*synth*)
Campbell, W.E. *et al., Spectrosc. Lett.*, 1993, **26**, 707 (*pmr, cmr*)
fukuda, Y.-I. *et al., Org. Lett.*, 2003, **5**, 749-751 (*synth*)

Assamicain A A-472

[121795-66-2]



Absolute configuration

$C_{44}H_{36}O_{22}$ 916.755
Isol. from the leaves of *Camellia sinensis* var. *assamica* (Assam tea). Off-white amorph. powder + $3H_2O$. $[\alpha]_D^{17}$ -120 (c, 1.0 in Me_2CO).

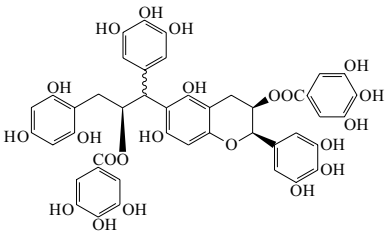
1′-Epimer: [121844-27-7] ***Assamicain B***

$C_{44}H_{36}O_{22}$ 916.755
Isol. from leaves of *Camellia sinensis* var. *assamica* (Assam tea). Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{17}$ -54.3 (c, 1.0 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 77 (*isol, pmr, cmr*)

Assamicain C A-473

[121795-67-3]

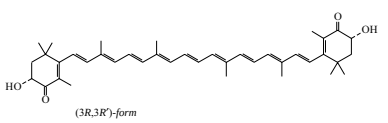


$C_{44}H_{36}O_{22}$ 916.755
Derived from the leaves of *Camellia sinensis* var. *assamica* (Assam tea). Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{17}$ +60.5 (c, 1.3 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 77 (*isol, pmr, cmr, synth*)

Astaxanthin A-474

[7542-45-2]
3,3′-Dihydroxy-β,β-carotene-4,4′-dione. 3,3′-Dihydroxycanthaxanthin. 3,3′-Dihydroxy-4,4′-diketo-β-carotene. Ovoester



$C_{40}H_{52}O_4$ 596.848

(3R,3′R)-form [60760-95-4]
Mp 222-223°. CD:$\Delta\epsilon_{385}$ -6.2, $\Delta\epsilon_{324}$ +24.0 λ_{max} 492 ($CHCl_3$).

(3S,3′S)-form [472-61-7]
Mp 223-225°. λ_{max} 472 (MeOH) (Berdy). λ_{max} 466 (hexane) (Berdy). λ_{max} 485 ($CHCl_3$) (Berdy). λ_{max} 492 ($CHCl_3$).

3-O-β-D-Glucopyranoside:
$C_{46}H_{62}O_9$ 758.99
λ_{max} 487 (C_6H_6).

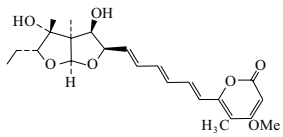
(3′RS,3′SR)-form [71772-51-5]
Used in fish farming to induce trout flesh colouring. Red food dye. Mp 216-219°. Meso-isomer.

[74601-68-6]

Andrewes, A.G. *et al., Phytochemistry*, 1976, **15**, 1009 (*isol*)
Muller, R.K. *et al., Helv. Chim. Acta*, 1980, **63**, 1654 (*hplc, isol, isom*)
Zell, R. *et al., Helv. Chim. Acta*, 1981, **64**, 2447 (*synth*)
Renstrom, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 249 (*isol, isomers*)
Berger, H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 253 (*isol*)
Yokoyama, A. *et al., J. Nat. Prod.*, 1995, **58**, 1929 (*glucoside*)

Asteltoxin A-475

[79663-49-3]



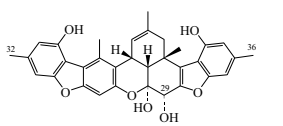
$C_{23}H_{30}O_7$ 418.486
Mycotoxin of *Aspergillus stellatus* and *Emericella varicolor*. Small pale-yellow needles. Mp 130-132°. $[\alpha]_D^{23}$ +20 (c, 1.15 in MeOH). λ_{max} 267 (ϵ 29300); 273 (ϵ 29400); 367 (ϵ 32800) (MeOH) (Derep).

▶ UQ0860000

Kruger, G.J. *et al., Chem. Comm.*, 1979, 441 (*isol, spectra, cryst struct*)
Schreiber, S.L. *et al., J.A.C.S.*, 1983, **105**, 6723; 1984, **106**, 4186 (*synth*)
Steyn, P.S. *et al., Chem. Comm.*, 1984, 977 (*biosynth*)
De Jesus, A.E. *et al., Chem. Comm.*, 1985, 1633 (*biosynth, cmr*)
Schreiber, S.L. *et al., Tet. Lett.*, 1986, **27**, 2575 (*abs config*)
Tadano, K. *et al., Tetrahedron*, 1990, **46**, 2353 (*synth*)
Raman, J.V. *et al., Tet. Lett.*, 1995, **36**, 3095 (*synth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 317 (*bibl, synth*)

Asticolorin A A-476

[93376-70-6]



$C_{33}H_{30}O_7$ 538.596
Mycotoxin prod. by *Aspergillus multicolor*. Cryst. (Me_2CO). Sol. MeOH, EtOAc. Mp 320°. $[\alpha]_D^{20}$ -120.5 (c, 0.2 in Me_2CO). λ_{max} 225 (ϵ 81400); 263 (ϵ 28100); 290 (ϵ 13300); 304 (ϵ 12700); 316 (ϵ 20500) (MeOH) (Derep).

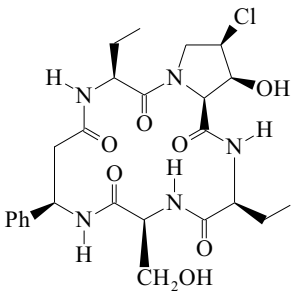
29-Ketone: [93376-71-7] ***Asticolorin B***
$C_{33}H_{28}O_7$ 536.58
Mycotoxin from *Aspergillus multicolor*. Cryst. Sol. MeOH, EtOAc. Mp 320°. λ_{max} 225 (ϵ 81400); 263 (ϵ 28100); 290 (ϵ 13300); 304 (ϵ 12700); 316 (ϵ 20500) (MeOH) (Derep).

32,36-Dihydroxy, 29-ketone: [93395-44-9] ***Asticolorin C***
$C_{33}H_{28}O_9$ 568.579
Mycotoxin of *Aspergillus multicolor*. Cryst. Sol. MeOH, EtOAc. Mp 320°. λ_{max} 225 (ϵ 81400); 263 (ϵ 28100); 290 (ϵ 23300); 304 (ϵ 12700); 316 (ϵ 20500) (EtOH) (Derep).

Rabie, C.J. *et al., Chem. Comm.*, 1984, 764-765 (*isol, struct*)
Steyn, P.S. *et al., Chem. Comm.*, 1984, 765-767 (*nmr, biosynth*)

Astin I A-477

[161162-22-7]

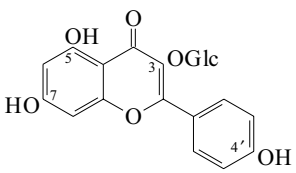


$C_{25}H_{34}ClN_5O_7$ 552.026
Cyclic peptide antibiotic. Constit. of *Actinidia kolomikta* (kiwi fruit). Mp 174.1-176.5°. $[\alpha]_D$ -78.8 (c, 0.1 in MeOH).

Morita, H. *et al., Chem. Lett.*, 1994, 2009 (*isol, pmr, cmr*)
Wang, Y. *et al., CA*, 1995, **122**, 156308e (*isol*)

Astragalin A-478

[480-10-4]
3-O-β-D-Glucopyranosyloxy-4′,5,7-trihydroxyflavone. Kaempferol 3-glucoside



$C_{21}H_{20}O_{11}$ 448.382
Present in red wine. Isol. from many plant spp.. Yellow needles. Mp 178°. $[\alpha]_D^{18}$ +16.9 (c, 0.62 in MeOH). Log P -2.32 (calc).

▶ DJ3080000

2″-O-β-D-Apiofuranosyl: [99816-59-8]
$C_{26}H_{28}O_{15}$ 580.498
Possibly isol. from the leaves of *Cicer arietinum* (chickpea). Yellowish powder. Mp 165-170°. The *Cicer arietinum* isolate was not fully characterised structurally and had no phys. props. reported.

2″-O-β-D-Xylopyranosyl, 6″-O-α-L-rhamnopyranosyl: [131573-90-5] ***Camelliaside B***. *Astragalin 2″-xyloside 6″-rhamnoside*
$C_{32}H_{38}O_{19}$ 726.641
Isol. from China tea (*Camellia sinensis*) seeds. Yellow solid. Mp 194-196°. $[\alpha]_D$ -57.4 (c, 0.36 in MeOH).

O″-Xylosyl:
$C_{26}H_{28}O_{15}$ 580.498
Isol. from French beans.

2″-O-β-D-Galactopyranosyl: [152390-63-1] ***Camelliaside C***
$C_{27}H_{30}O_{16}$ 610.524
Constit. of China tea (*Camellia sinensis*) seeds. Yellow solid. Mp 200-202°. $[\alpha]_D$ -45.9 (c, 0.025 in MeOH). May be identical with the prev. isolated *Heuchera* galactoside above.

2″-O-β-D-Galactopyranosyl, 6″-O-α-L-

rhamnopyranosyl: [135095-52-2] ***Camelliaside A***. *Astragalin 2″-galactoside 6″-rhamnoside*
$C_{33}H_{40}O_{20}$ 756.667
Isol. from China tea (*Camellia sinensis*) seeds. Yellow solid. Mp 203-205°. $[\alpha]_D$ -39.6 (c, 0.35 in MeOH).

2″-O-β-D-Glucopyranosyl, 6″-O-α-L-rhamnopyranosyl: [55696-58-7] *Astragalin 2″-glucoside 6″-rhamnoside. Kaempferol 3-(2″-glucosylrutinoside). Kaempferol 3-(6″-rhamnosylsophoroside)*
$C_{33}H_{40}O_{20}$ 756.667
Isol. from *Solanum* spp. and soya beans.

2″-O-β-D-Glucopyranosyl, 7-O-[4-hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucopyranoside]: [87891-34-7] *Kaempferol 3-sophoroside 7-(2-feruloylglucoside)*
$C_{43}H_{48}O_{24}$ 948.838
Isol. from Chinese chives (*Allium tuberosum*). Yellow powder + $1H_2O$ (EtOH aq.). Mp 212-215°. $[\alpha]_D^{22}$ -84.9 (c, 1 in Py).

2″-O-β-D-Glucopyranosyl, 7-O-β-D-glucuronopyranoside: [140163-56-0] *Kaempferol 3-sophoroside 7-glucuronide*
$C_{33}H_{38}O_{22}$ 786.65
Isol. from alliums incl. onion (*Allium cepa*) epidermis. Yellow-green powder.

2″-O-(6-O-Acetyl-β-D-glucopyranosyl): [133763-02-7]
$C_{29}H_{32}O_{17}$ 652.562
Constit. of the flower petals of saffron (*Crocus sativus*).

*2″-O-[4-Hydroxy-*E*-cinnamoyl-(→2)-β-D-glucopyranosyl], 7-O-β-D-glucopyranoside:* [151649-64-8] *Kaempferol 3-(2-*p*-coumaroylsophoroside) 7-glucoside*
$C_{42}H_{46}O_{23}$ 918.812
Constit. of *Brassica oleracea* (cabbage) leaves.

*2″-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucopyranosyl], 7-O-β-D-glucopyranoside:* [151649-63-7] *Kaempferol 3-(2-feruloylsophoroside) 7-glucoside*
$C_{43}H_{48}O_{24}$ 948.838
Constit. of *Brassica oleracea* (cabbage) leaves.

2″-O-[4-Hydroxy-3,5-dimethoxycinnamoyl-(→2)-β-D-glucopyranosyl], 7-O-β-D-glucopyranoside: [112294-86-7] *Kaempferol 3-(2-sinapoylsophoroside) 7-glucoside*
$C_{44}H_{50}O_{25}$ 978.864
Isol. from rape seeds (*Brassica napus*).

4′-O-β-D-Glucopyranoside: [71939-16-7] ***Allivicin***. *Kaempferol 3,4′-diglucoside*
$C_{27}H_{30}O_{16}$ 610.524
Isol. from caucas (*Allium victorialis*) and *Prunus* spp..

4′-O-β-D-Glucopyranoside, 7-O-[4-hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucopyranoside]: [108887-46-3] *Kaempferol 3,4′-diglucoside 7-(2-feruloylglucoside)*
$C_{43}H_{48}O_{24}$ 948.838
Isol. from Chinese chives (*Allium tuberosum*) leaf. Pale yellow powder + $2H_2O$ (EtOH aq.). Mp 214-217°. $[\alpha]_D^{22}$ -39.9 (c, 0.26 in Py).

6″-O-[α-L-Rhamnopyranosyl-(1→2)-α-L-rhamnopyranosyl]: [32602-83-8]
$C_{33}H_{40}O_{19}$ 740.668
Isol. from hop flowers *Humulus lupulus*.

6″-O-[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranosyl]: [136449-09-7] *Kaempferol 3-(3^R-glucosylrutinoside)*
$C_{33}H_{40}O_{20}$ 756.667
Isol. from black tea (*Camellia sinensis*).

2″-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl]: [197250-98-9]
$C_{33}H_{40}O_{21}$ 772.666
Constit. of the seeds of black cumin (*Nigella sativa*). λ_{max} 265 ; 300 (sh) ; 348 (MeOH).

Mono-Ac: [36310-43-7] ***Acetylastragalin***
$C_{23}H_{22}O_{12}$ 490.42
Isol. from liquorice (*Glycyrrhiza glabra*). Full struct. not determined. May be identical with the 6″-Ac above.

6″-O-Malonoyl: [81149-02-2] *6″-Malonylastragalin*
$C_{24}H_{22}O_{14}$ 534.429
Constit. of *Cicer* sp. and pears.

3″-O-β-Apiofuranosyl, 6″-O-malonyl: [119067-83-3]
$C_{29}H_{30}O_{18}$ 666.545
Isol. from *Cicer arietinum* (chickpea) leaves and stems.

6″-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl): [157407-84-6] *Kaempferol 3-[6-O-(3-hydroxy-3-methylglutaroyl)glucoside]*
$C_{27}H_{28}O_{15}$ 592.509
Constit. of aged callus cultures of lime (*Citrus aurantifolia*). Yellow powder (MeOH). Mp 210-213°.

6″-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl), 7-O-β-D-glucopyranoside: [157407-85-7]
$C_{33}H_{38}O_{20}$ 754.651
Constit. of 10 year old callus cultures of lime (*Citrus aurantifolia*).

*2″-O-(*E*-4-Hydroxycinnamoyl):* [137018-32-7]

[189098-16-6] *Kaempferol 3-(*E*-p-coumarylglucoside)*
$C_{30}H_{26}O_{13}$ 594.528
Isol. from *Lithocarpus polystachya* tea. The *Z*-isomer was isol. in admixture with the *E*-isomer from *Eryngium campestre*.

6″-O-(4-Hydroxycinnamoyl), 4′-O-β-D-glucopyranoside: [87339-51-3]
$C_{36}H_{36}O_{18}$ 756.67
Isol. from Tartar bread plant (*Crambe tatarica*).

7-O-(4-Hydroxycinnamoyl): [51795-36-9]
$C_{30}H_{26}O_{13}$ 594.528
Constit. of *Elaeagnus angustifolia* (Russian olive).

2″,4″-Bis-O-(4-hydroxycinnamoyl): [85122-24-3]
$C_{39}H_{32}O_{15}$ 740.673
Isol. from *Quercus ilex* (holly oak). Needles (MeOH aq.). Dec. above 280°.

2″,6″-Bis-O-(4-hydroxycinnamoyl): [94474-74-5]
$C_{39}H_{32}O_{15}$ 740.673
Isol. from *Quercus ilex* (holly oak). Amorph.

*6″-O-(3,4-Dihydroxy-*E*-cinnamoyl):* [190328-43-9] *6″-O-Caffeoylastragalin*
$C_{30}H_{26}O_{14}$ 610.527
Constit. of young bracken fronds (*Pteridium aquilinium*).

2″-O-(4-Hydroxy-3-methoxycinnamoyl), 4′,7-di-O-β-D-glucopyranoside: [108887-47-4] *Kaempferol 3-(2-feruloylglucoside) 4′,7-diglucoside*
$C_{43}H_{48}O_{24}$ 948.838
Isol. from Chinese chives (*Allium tuberosum*). Amorph. solid + $1H_2O$ (H_2O). Mp 235-238°. $[\alpha]_D^{22}$ -206 (c, 0.22 in Py).

2″-O-(4-Hydroxy-3,5-dimethoxycinnamoyl), 7-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]: [112208-89-6] *Kaempferol 3-(sinapoylglucoside) 7-sophoroside*
$C_{44}H_{50}O_{25}$ 978.864
Isol. from rapeseed (*Brassica napus*).

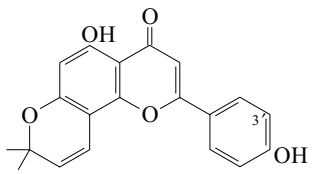
[85899-03-2, 94535-60-1]

Vancraenenbroeck, R. *et al., CA*, 1971, **74**, 110377p (*hop rhamnopyranosides*)
Markham, K.R. *et al., Tetrahedron*, 1978, **34**, 1389-1397 (*cmr*)
Ishikura, N. *et al., Agric. Biol. Chem.*, 1979, **43**, 1923-1926 (*4′-glucoside*)
Imperato, F. *et al., Chem. Ind. (London)*, 1981, 695-696 (*6″-malonate*)
Aguinagalde, I. *et al., Phytochemistry*, 1982, **21**, 2875-2878 (*4′-glucosides*)
Hamburger, M. *et al., Phytochemistry*, 1985, **24**, 2689-2692 (*2″-apiosyl*)
Piegay, I. *et al., Pharmazie*, 1986, **41**, 524-525 (*mono-Ac*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 97-107 (*Allium tuberosum constits*)
Tantawy, B. *et al., CA*, 1988, **108**, 34772s (*rape seed acyl glycosides*)
Merfort, I. *et al., Phytochemistry*, 1988, **27**, 3281-3284 (*6″-O-Acetylastragalin*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Budzianowski, J. *et al., Phytochemistry*, 1990, **29**, 3643-3647; 1991, **30**, 1679-1682 (*derivs*)
Markham, K.R. *et al., Phytochemistry*, 1990, **29**, 3919-3920 (*Kaempferol 3-sophoroside 7-arabinoside*)
Romussi, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1991, **324**, 519-524 (*diacetyldicoumarates*)
Yang, D. *et al., CA*, 1991, **115**, 228326q (*4-hydroxycinnamoyl esters*)
Finger, A. *et al., J. Sci. Food Agric.*, 1991, **55**, 313-321 (*3R-glucosylrutinoside*)
Sekine, T. *et al., Phytochemistry*, 1991, **30**, 991-995 (*Camelliasides*)
Urushibara, S. *et al., Tet. Lett.*, 1992, **33**, 1213-1216 (*2″-glucosyl 7-glucuronide*)
Sekine, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1185-1187 (*Camelliaside C*)
Neilsen, J.K. *et al., Phytochemistry*, 1993, **34**, 539-544 (*3-acylsophoroside 7-glucosides*)
Berkow, M.A. *et al., Phytochemistry*, 1994, **36**, 1225-1227 (*3-hydroxy-3-methylglutarates*)
Catalano, S. *et al., Phytochemistry*, 1994, **36**, 1777 (*3-feruloylglucoside*)
Imperato, F. *et al., Phytochemistry*, 1997, **45**, 199-200 (*6″-Caffeoylastragalin*)
Merfort, I. *et al., Phytochemistry*, 1997, **46**, 359-363 (*2"-glucosylgalactosyl*)
Bloor, S.J. *et al., Phytochemistry*, 1998, **49**, 1427-1430 (*2″-feruloylglucosyl-6″-malonyl*)

Afifi, M.S. *et al., Bull. Fac. Pharm. (Cairo Univ.)*, 1999, **37**, 119-124; *CA*, **132**, 163461 (*isol, activity*)
Liu, H. *et al., J. Nat. Prod.*, 1999, **62**, 70-75 (*Stenopalustrosides*)

Atalantoflavone A-479

[119309-02-3]
*5-Hydroxy-2-(4-hydroxyphenyl)-8,8-dimethyl-4*H,*8*H-*benzo[1,2*-b:*3,4*-b′*]dipyran-4-one, 9CI. Limonianin*



$C_{20}H_{16}O_5$ 336.343
Isol. from rootbark of lemon trees. Yellow needles (Me_2CO/hexane). Mp 289-290° (275-277°). Physical data varies between Atalantoflavone and Limonianin.

Di-Ac:
Needles (Me_2CO/petrol). Mp 230-232° (221-223°).

Di-Me ether:
Pale yellow cryst. (Me_2CO/hexane). Mp 207-209° (185-188°).

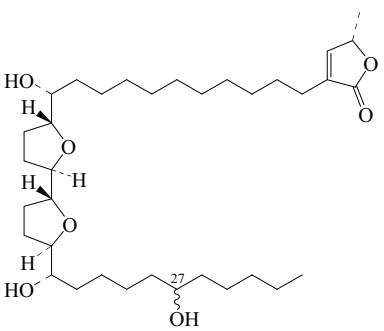
3″,4″-Dihydroxy, 3″,4″-dihydro:
$C_{20}H_{18}O_7$ 370.358
λ_{max} 270 ; 317 (sh) ; 339 (MeOH).

3′-Methoxy: [106055-12-3] ***Racemoflavone***
$C_{21}H_{18}O_6$ 366.37
Yellow cryst. (Me_2CO/hexane). Mp 236-237°.

Banerji, A. *et al., Phytochemistry*, 1988, **27**, 3637 (*isol, struct, synth*)
Chang, S.-H. *et al., Phytochemistry*, 1990, **29**, 351 (*Limonianin*)
Subramanian, M. *et al., J. Nat. Prod.*, 1992, **55**, 1213 (*synth*)
Vijayalakshmi, C.S. *et al., Z. Naturforsch., B*, 1992, **47**, 1021 (*synth*)
Prasad, K.J.R. *et al., J. Nat. Prod.*, 1993, **56**, 208 (*synth*)
Kassem, M. *et al., Fitoterapia*, 2000, **71**, 649-654 (*3″,4″-dihydrodihydroxy deriv*)

Atemoyacin B A-480

[164991-85-9]



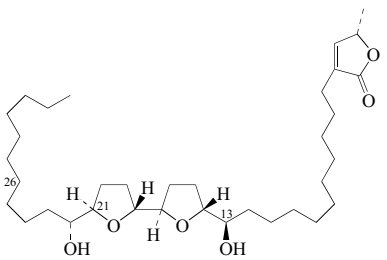
$C_{35}H_{62}O_7$ 594.871
Constit. of the seeds of *Annona atemoya* (custard apple). Cytotoxic. Wax. $[\alpha]_D$ +12.9 (c, 0.02 in MeOH). λ_{max} 210 (ε 7150) (MeOH).

Chen, W.-S. *et al., Huaxue Xuebao*, 1995, **53**, 516; *CA*, **123**, 79506j

Atemoyin A-481

[161169-70-6]

[159993-38-1]
Squamocin K



$C_{35}H_{62}O_6$ 578.871
Constit. of *Annona squamosa* (sugar apple) and the seeds of *Annona atemoya* (custard apple). Wax. $[\alpha]_D^{25}$ +20.5 (c, 0.5 in MeOH).

13-Epimer: [159993-37-0] *Squamocin I*
$C_{35}H_{62}O_6$ 578.871
Constit. of *Annona squamosa* (sugar apple). Needles (MeOH aq.). Mp 68.5-71°. $[\alpha]_D^{24}$ +22.2 (c, 0.5 in MeOH).

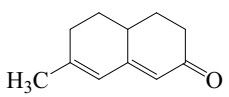
21-Epimer, 26ξ-hydroxy: ***Carolin C***
$C_{35}H_{62}O_7$ 594.871
Oil. $[\alpha]_D^{20}$ +8 (c, 0.5 in $CHCl_3$). λ_{max} 205 (log ε 4) (EtOH). λ_{max} 208 (ε 10000) (MeOH) (Berdy).

[161025-06-5]

Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*Squamocins*)
Duret, P. *et al., Nat. Prod. Lett.*, 1995, **5**, 295-302 (*isol, uv, pmr, cmr, ms*)
Queiroz, E.F. *et al., J. Nat. Prod.*, 1998, **61**, 34-39 (*Carolin C*)

4,4a,5,6-Tetrahydro-7-methyl-2(3*H*)-naphthalenone, 9CI A-482

[34545-88-5]
FEMA 3715

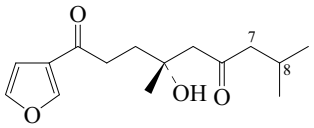


$C_{11}H_{14}O$ 162.231
(±)-*form*
Flavouring ingredient for foods and chewing gum. Cryst. (MeOH) with a sweet coumarin-like odour. Mp 36.6° (31-33°). Bp_2 138°.

Pfau, M. *et al., Bull. Soc. Chim. Fr.*, Part II, 1979, 627-632 (*synth, uv, pmr, cmr*)
U.S. Pat., 1983, 4 385 073; *CA*, **99**, 138408q (*synth, ms, ir, pmr, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1225-1226 (*use, props*)

Athanagrandione A-483

1-(3-Furanyl)-4-hydroxy-4,8-dimethyl-1,6-nonanedione, 9CI. 4-Hydroxymyoporone



$C_{15}H_{22}O_4$ 266.336
(*R*)-*form* [69926-93-8]
Prod.by sweet potato tubers (*Ipomoea batatas*) infected by *Fusarium solani*. Oil.

7,8-Didehydro: [72896-64-1]

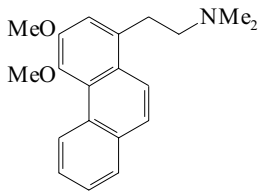
[63955-86-2, 135029-99-1] *4-Hydroxydehydromyoporone, 9CI. Furopinnatin*
Prod.by sweet potatoes infected by *Fusarium solani*. Oil. The abs. config. of Furopinnatin was not determined, and no opt. rotn. was reported for it.

Burka, L.T. *et al., Tet. Lett.*, 1974, 4017 (*struct*)
Inoue, H. *et al., Phytochemistry*, 1977, **16**, 1063-1065 (*4-Hydroxydihydromyoporone*)
Burka, L.T. *et al., Phytochemistry*, 1977, **16**, 2022 (*biosynth*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1595 (*isol, struct*)
Oba, K. *et al., Plant Cell Physiol.*, 1979, **20**, 819 (*biosynth*)
Dimitriadis, E. *et al., Phytochemistry*, 1984, **23**, 1325 (*abs config*)
Zdero, C. *et al., Phytochemistry*, 1991, **30**, 1161 (*Furopinnatin*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 736

Atherosperminine A-484

[5531-98-6]

[98900-05-1]
3,4-Dimethoxy-N,N-*dimethyl-1-phenanthreneethanamine, 9CI. 1-Dimethylaminoethyl-3,4-dimethoxyphenanthrene*



$C_{20}H_{23}NO_2$ 309.407
Alkaloid from the stem bark of *Annona muricata* (soursop). Needles (Me_2CO/petrol). Mp 199-200°.

Hydrochloride: [54749-97-2]
Mp 234-235° dec.

Picrate: [5531-99-7]
Yellow needles (Me_2CO/MeOH). Mp 189-190°.

N-*Oxide:* [91174-15-1] ***Atherosperminine* N-*oxide***
$C_{20}H_{23}NO_3$ 325.407
Noncryst.

N-*Me:* [98900-03-9]

[5532-00-3, 98900-04-0] **N-*Methylatherosperminium***

$C_{21}H_{26}NO_2^{\oplus}$ 324.442
Needles (EtOH)(as iodide). Mp 282-284° (iodide).

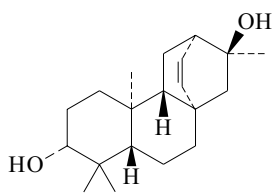
N-*De-Me:* [74606-53-4] ***Noratherosperminine***
$C_{19}H_{21}NO_2$ 295.38
Mp 180°.

O^2-*De-Me:* [16625-57-3] *1-[2-(Dimethylamino)ethyl]-4-methoxy-3-phenanthrenol. 1-(2-Dimethylaminoethyl)-3-hydroxy-4-methoxyphenanthrene.* ***Argentinine***
$C_{19}H_{21}NO_2$ 295.38
Oil.

O^2-*De-Me,* N-*Oxide:* [138690-45-6] ***Argentinine* N-*oxide***
$C_{19}H_{21}NO_3$ 311.38
Oil. Possible artifact.

Cooke, R.G. *et al., Aust. J. Chem.*, 1954, **7**, 99 (*isol, uv*)
Bick, I.R.C. *et al., Aust. J. Chem.*, 1956, **9**, 111; 1965, **18**, 1997 (*isol, pmr, uv*)
Priestap, H.A. *et al., Chem. Comm.*, 1967, 754 (*Argentinine, Atherosperminine*)
Aguilar-Santos, G. *et al., Philipp. J. Sci.*, 1967, **96**, 399; *CA*, **74**, 1066r (*isol*)
Priestap, H.A. *et al., An. Asoc. Quim. Argent.*, 1972, **60**, 309; *CA*, **77**, 164898q (*Argentinine, Atherosperminine*)
Roblot, F. *et al., Plant. Med. Phytother.*, 1978, **12**, 259
Guinaudeau, H. *et al., J. Nat. Prod.*, 1979, **42**, 325 (*Noratherosperminine*)
Leboeuf, M. *et al., Planta Med.*, 1980, **38**, 33; 1981, **42**, 37
Castedo, L. *et al., Heterocycles*, 1982, **19**, 209 (*Noratherosperminine, synth*)
Hocquemiller, R. *et al., J. Nat. Prod.*, 1984, **47**, 353 (*Atherosperminine N-oxide*)
Lu, S.T. *et al., Phytochemistry*, 1985, **24**, 1829 (*N-Methylatherosperminium*)
Achenbach, H. *et al., J. Nat. Prod.*, 1991, **54**, 1331 (*Argentinine N-oxide*)
Chen, K.-S. *et al., J. Nat. Prod.*, 1996, **59**, 531-534 (*activity*)
Lopez-Martin, J. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1613-1615 (*Argentinine, isol, pmr, cmr*)

13-Atisene-3,16-diol A-485



$C_{20}H_{32}O_2$ 304.472

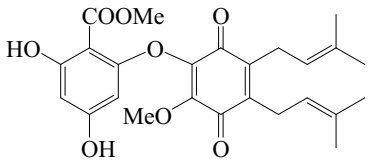
(*ent*-3β,16α)-*form*
Cryst. (diisopropyl ether/EtOAc). Mp 192-193°.

3-Ketone: [119642-81-8] ent-*16α-Hydroxy-13-atisen-3-one.* ***Yucalexin A16***
$C_{20}H_{30}O_2$ 302.456
Gum. Stress metab. of cassava root (*Manihot esculenta*).

13,14-Dihydro: [87013-77-2] **ent-*3β,16α-Atisanediol***
$C_{20}H_{34}O_2$ 306.487
Cryst. (C_6H_6). Mp 205-206°. $[\alpha]_D$ -28 (c, 0.22 in $CHCl_3$).

Schmitz, F.J. *et al., J.O.C.*, 1983, **48**, 3941
Delgado, G. *et al., Phytochemistry*, 1984, **23**, 2285
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769 (*Yucalexin A16*)
De Heluani, C.S. *et al., Magn. Reson. Chem.*, 1998, **36**, 947-950 (*Yucalexin A16, pmr, cmr*)

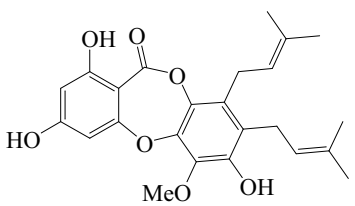
Atrovirinone A-486



$C_{25}H_{28}O_8$ 456.491
Constit. of the roots of *Garcinia atroviridis* (gelugor). Red needles ($CHCl_3$/hexane). Mp 124-125°. λ_{max} 204 (log ϵ 5.14); 221 (log ϵ 5.1); 273 (log ϵ 5.04) (EtOH).

Permana, D. *et al., J. Nat. Prod.*, 2001, **64**, 976-979

Atrovirisidone A-487

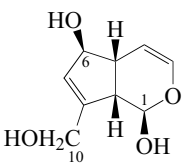


$C_{24}H_{26}O_7$ 426.465
Constit. of the roots of *Garcinia atroviridis* (gelugor). Cryst. ($CHCl_3$/hexane). Mp 75-76°. λ_{max} 207 (log ϵ 4.93); 269 (log ϵ 4.36) (EtOH).

Permana, D. *et al., J. Nat. Prod.*, 2001, **64**, 976-979

Aucubigenin A-488

[64274-28-8]
Rhinanthogenin



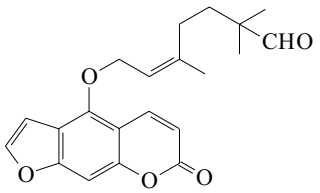
$C_9H_{12}O_4$ 184.191
Oil. Unstable λ_{max} 204 (ϵ 1300) (MeOH) (Berdy).

*10-*O*-(4-Hydroxybenzoyl), 1-*O*-β-D-glucopyranoside:* [11027-63-7] ***Agnuside.*** *Agnoside*
$C_{22}H_{26}O_{11}$ 466.441
Isol. from *Vitex agnus-castus* (agnus castus). Cryst. (H_2O). Mp 146°. $[\alpha]_D^{20}$ -91.5 (EtOH).

Hänsel, R. *et al., Phytochemistry*, 1965, **4**, 19 (*Agnuside*)

Aurantiumal A-489

5-[(3,6-Dimethyl-6-formyl-2-heptenyl)oxy]psoralen

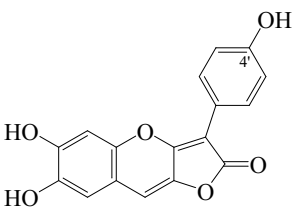


$C_{21}H_{22}O_5$ 354.402
Isol. from oil of grapefruit peel (*Citrus paradisi*). Cryst. (EtOAc/EtOH). Mp 134-136°. Prob. artifact.

Fisher, J.F. *et al., Tetrahedron*, 1966, **22**, 1489 (*isol*)
Fisher, J.F. *et al., J. Agric. Food Chem.*, 1979, **27**, 1334

Aurantricholide B A-490

[264923-56-0]
*6,7-Dihydroxy-3-(4-hydroxyphenyl)-2*H*-furo[3,2-*b*][1]benzopyran-2-one, 9CI*



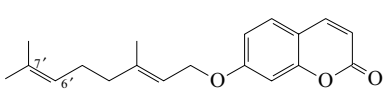
$C_{17}H_{10}O_6$ 310.262
Pigment isol. from the mushroom *Suillus grevillei* (larch bolete). Unstable orange solid. Mp 320° dec. λ_{max} 204 (log ϵ 4.54); 267 (log ϵ 4.19); 416 (log ϵ 4.32) (MeOH).

4′-Deoxy: [264923-55-9] ***Aurantricholide A***
$C_{17}H_{10}O_5$ 294.263
Unstable orange solid. Mp 272° dec. λ_{max} 270 ; 412 ; 482 (MeOH).

Klostermeyer, D. *et al., Eur. J. Org. Chem.*, 2000, 603-609 (*isol, synth, pmr, cmr*)

Auraptene A-491

[495-02-3]
*7-(3,7-Dimethyl-2,6-octadienyl)oxy-2*H*-1-benzopyran-2-one, 9CI.* O-*Geranylumbelliferone. Feronialactone. 7-Geranyloxycoumarin*



$C_{19}H_{22}O_3$ 298.381
Not to be confused with Meranzin, M-195. Isol. from *Citrus aurantium* (Seville orange) and bael fruit (*Aegle marmelos*). Prisms (EtOH). Mp 68°. λ_{max} 252 ; 329 (MeOH) (Berdy).

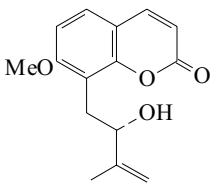
*Δ$^{7'}$-Isomer, 6′*R*-hydroxy:* [118584-19-3] *7-[(6-Hydroxy-3,7-dimethyl-2,7-octadienyl)oxy]-2*H*-1-benzopyran-2-one*
$C_{19}H_{22}O_4$ 314.38
Isol. from *Citrus hassaku* juice oil. Cryst. Mp 75°. $[\alpha]_D^{26}$ +10 (c, 1.0 in

EtOH).

Kariyone, T. *et al., Chem. Pharm. Bull.*, 1959, **1**, 119 (*struct, synth, bibl*)
Coates, R.M. *et al., Tetrahedron*, 1970, **26**, 5699 (*synth*)
Yamada, S. *et al., Tet. Lett.*, 1976, **29**, 2557 (*synth, abs config, deriv*)
Masuda, T. *et al., Phytochemistry*, 1992, **31**, 1363-1366 (*6′-hydroxy*)

Auraptenol A-492

*8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, 9CI. 8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxycoumarin*



(*S*)-*form*

$C_{15}H_{16}O_4$ 260.289

(S)-form [1221-43-8]
Constit. of Seville bitter orange (*Citrus aurantium* ssp. *amara*) oil. Needles (EtOH). Mp 109-110°. $[\alpha]_D^{26}$ +14 (c, 1 in EtOH).

2′-Deoxy, 2′-hydroperoxy: [109741-39-1] ***Peroxyauraptenol***
$C_{15}H_{16}O_5$ 276.288
Prisms. Mp 114-116°. $[\alpha]_D$ +3.53 ($CHCl_3$).

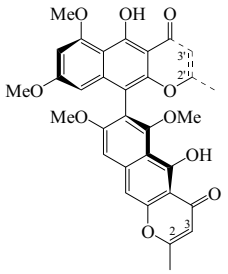
2′-Ketone: [19668-69-0] *7-Methoxy-8-(3-methyl-2-oxo-3-butenyl)-2*H*-1-benzopyran-2-one, 9CI.* ***Murrayone****. Prangone*
$C_{15}H_{14}O_4$ 258.273
Mp 130°.

(±)-form [61235-25-4]
Cryst. (C_6H_6/hexane). Mp 109-110°.

Stanley, W.L. *et al., Tetrahedron*, 1965, **21**, 89 (*isol, struct*)
Lakshmi, M.V. *et al., Indian J. Chem.*, 1972, **10**, 564 (*Murrayone*)
Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1974, **10**, 568; *Chem. Nat. Compd. (Engl. Transl.)*, 581 (*Murrayone*)
Raj, K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 332 (*synth*)
Barik, B.R. *et al., Phytochemistry*, 1983, **22**, 792 (*abs config*)
Yamahara, J. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1676 (*isol*)
Ito, C. *et al., Heterocycles*, 1987, **26**, 1731 (*Peroxyauraptenol*)

Aurasperone A A-493

[15085-74-2]
*5,5′-Dihydroxy-6,6′,8,8′-tetramethoxy-2,2′-dimethyl-7,10′-bi-4*H*-naphtho[2,3-*b*]pyran-4,4′-dione, 9CI*



Absolute Configuration

$C_{32}H_{26}O_{10}$ 570.551
Metab. of *Aspergillus niger, Aspergillus awamori* and *Aspergillus fonsecaeus*. Isol. from *Aspergillus niger* infected mango fruits. Yellow plates ($CHCl_3$/propanol); needles (EtOH). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 207° (prisms), 290-291° (270°) (needles). $[\alpha]_D^{25}$ -242 (c, 1.0 in $CHCl_3$). λ_{max} 225 (ϵ 51286); 258 (ϵ 53700); 280 (ϵ 100000); 325 (ϵ 8700); 405 (ϵ 12900) (EtOH) (Berdy).

Di-Ac:
Pale yellow needles (EtOH aq.). Mp 320° dec. $[\alpha]_D^{25}$ -242 (c, 1.0 in $CHCl_3$).

$O^{6′}$*-De-Me:* [67924-64-5] ***Aurasperone D***
$C_{31}H_{24}O_{10}$ 556.525
Mycotoxin from *Aspergillus niger* infected mango fruits. Microcryst. yellow solid. Mp 115°. Abs. config. not certain.
► DU3122000

O^{6},$O^{6′}$*-Di-de-Me,* O^{5},$O^{5′}$*-di-Me:* [71695-22-2] ***Isoaurasperone A****. Isoaurasperone*
$C_{32}H_{26}O_{10}$ 570.551
Mycotoxin from *Aspergillus niger* infected mango fruits. Pale yellow solid. Mp 198-203°. Abs. config. not certain.

O^{6},$O^{6′}$*-Di-de-Me,* O^{5},$O^{5′}$*-di-Me, di-Ac:*
Mp 148-151°.

2,3-Dihydro, 2ξ-hydroxy: [95272-15-4]

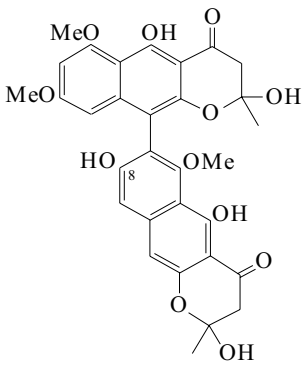
[71722-01-5] ***Fonsecinone D****. Aurasperone E*
$C_{32}H_{28}O_{11}$ 588.567
Mycotoxin prod. by *Aspergillus fonsecaeus* and *Aspergillus niger*. Isol. from *Aspergillus niger* infected mango fruits. Solid. Mp 166-170°. Abs. config. not certain λ_{max} 229 (ϵ 38900); 255 (sh) (ϵ 41700); 280 (ϵ 70800); 320 (ϵ 14100); 328 (sh) (ϵ 14100); 403 (ϵ 9120) (95% EtOH) (Derep).

2′,3′-Dihydro, 2′ξ-hydroxy: [95152-76-4] ***Fonsecinone B***
$C_{32}H_{28}O_{11}$ 588.567
Mycotoxin prod. by *Aspergillus fonsecaeus*. Isol. from infected mango fruits. Amorph. Mp 172-173°. Abs. config. not certain λ_{max} 229 (ϵ 38900); 255 (sh) (ϵ 41700); 280 (ϵ 70800); 320 (ϵ 14100); 328 (sh) (ϵ 14100); 403 (ϵ 9120) (95% EtOH) (Derep).

Wang, P. *et al., Agric. Biol. Chem.*, 1966, **30**, 683-687 (*struct*)
Ghosal, S. *et al., Phytochemistry*, 1978, **17**, 689-694 (*Aurasperone D*)
Ghosal, S. *et al., J. Agric. Food Chem.*, 1979, **27**, 1347-1351 (*Aurasperone A, Aurasperone D, Isoaurasperone A*)
Priestap, H. *et al., Tetrahedron*, 1984, **40**, 3617-3624 (*Fonsecinones*)
Koyama, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4049-4055 (*abs config*)

Aurasperone C A-494

[41689-66-1]
*2,2′,3,3′-Tetrahydro-2,2′,5,5′,8-pentahydroxy-6,6′,8′-trimethoxy-2,2′-dimethyl-7,10′-bi-4*H*-naphtho[2,3-*b*]pyran-4,4′-dione, 9CI*



$C_{31}H_{28}O_{12}$ 592.555
Mycotoxin pigment from *Aspergillus niger* and *Aspergillus awamori*. Yellow. Mp 185° dec. Similar to Fonsecinones.

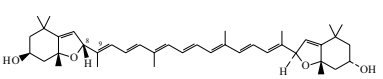
8-Me ether: [41689-67-2] ***Aurasperone B***
$C_{32}H_{30}O_{12}$ 606.582
Mycotoxin from *Aspergillus niger, Aspergillus awamori* and *Aspergillus fonsecaeus*. Yellow. Mp 186° dec. $[\alpha]_D^{25}$ +46.3 (c, 1.4 in $CHCl_3$). λ_{max} 233 ; 280 ; 315 ; 331 ; 404 (MeOH) (Berdy).

2,2′-Dideoxy, 2,2′,3,3′-tetradehydro: [92280-05-2] ***Dianhydroaurasperone C***
$C_{31}H_{24}O_{10}$ 556.525
Prod. by *Aspergillus niger*. λ_{max} 225 (ϵ 23000); 255 (ϵ 27000); 280 (ϵ 85000); 325 (ϵ 3700); 405 (ϵ 5800) (MeOH) (Berdy).

Tamura, T. *et al., Agric. Biol. Chem.*, 1966, **30**, 107; 683 (*isol*)
Namiki, N. *et al., Agric. Biol. Chem.*, 1972, **36**, 2511 (*struct*)
Ehrlich, K.C. *et al., Appl. Environ. Microbiol.*, 1984, **48**, 1-4 (*Dianhydroaurasperone C*)
Priestap, H.A. *et al., Tetrahedron*, 1984, **40**, 3617 (*deriv*)

Auroxanthin A-495

[27785-15-5]
5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-carotene-3,3′-diol



(*8R,8′R*)-*form*

$C_{40}H_{56}O_4$ 600.88
Isol. from *Viola tricolor, Lonicera japonica, Delonix regia* and other plants. Yellow cryst. (EtOH). Mp 203°. A *cis*-isomer was reported from *D. regia*.

3,3′-Dideoxy: [6821-09-6] *5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-carotene.* ***Aurochrome***
$C_{40}H_{56}O_2$ 568.881
Widespread carotenoid. Cryst.(C_6H_6/MeOH). Mp 185°.

3′-Deoxy: [73745-06-9] *5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-caroten-3-ol.*

Cryptochrome
$C_{40}H_{56}O_3$ 584.881
Isol. from *Prunus persica* (peach) and fruits of *Averrhoa carambola*. Isol. only in trace amounts λ_{max} 424 ; 456 (CS_2). λ_{max} 399 ; 424 (EtOH).

(8R,8′R)-form [95034-12-1]
λ_{max} 378 ; 398 ; 423 (no solvent reported).

(8R,8′S)-form [51921-06-3]
λ_{max} 378 ; 398 ; 423 (no solvent reported).

(8S,8′S)-form [51921-05-2]
λ_{max} 378 ; 398 ; 423 (no solvent reported).

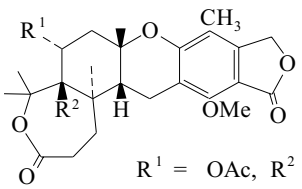
(8R,8′R,9Z)-form [95119-78-1]
λ_{max} 378 ; 398 ; 423 (no solvent reported).

[22350-65-8]

Karrer, P. *et al., Helv. Chim. Acta*, 1944, **27**, 1684; 1945, **28**, 427 (*struct*)
Goodwin, T.W. *et al., Biochem. J.*, 1956, **62**, 346 (*isol*)
Jungalwala, F.B. *et al., Biochem. J.*, 1962, **85**, 1 (*isol*)
Stobart, A.K. *et al., Phytochemistry*, 1967, **6**, 1467 (*isol*)
Gross, J. *et al., Phytochemistry*, 1983, **22**, 1479 (*Cryptochrome*)
Acemoglu, M. *et al., Helv. Chim. Acta*, 1984, **67**, 471 (*synth, uv, pmr, cmr*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1984, **67**, 2143 (*isol*)

Austalide I A-496

[96817-08-2]



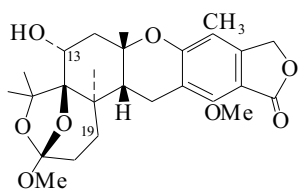
R^1 = OAc, R^2 = H

$C_{27}H_{34}O_8$ 486.561
Terpenoid antibiotic. Mycotoxin from the food storage mould (*Aspergillus ustus*). Cryst. Mp 236-238°. $[\alpha]_D^{24}$ -132.6 (c, 1 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

Horak, R.M. *et al., J.C.S. Perkin 1*, 1985, 345; 363 (*isol, struct, nmr*)

Austalide B A-497

[81543-02-4]



$C_{26}H_{34}O_8$ 474.55
Terpenoid antibiotic. Mycotoxin of. of the food storage mould *Aspergillus ustus*. Cryst. (C_6H_6/hexane). Mp 243-245°. $[\alpha]_D$ -46.2 (c, 1 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

13-Ac: [81543-01-3] ***Austalide A***
$C_{28}H_{36}O_9$ 516.587
Metab. of *Aspergillus ustus*. Cryst. ($CHCl_3$/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 212-214°. $[\alpha]_D^{24}$ -84.4 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep). λ_{max} 207 (ϵ 17140); 222 (ϵ 35400) (MeOH) (Berdy).

19α-Hydroxy: [81543-06-8] ***Austalide F***
$C_{26}H_{34}O_9$ 490.549
Mycotoxin of *Aspergillus ustus*. Cryst. (Me_2CO). Mp 261-263°. $[\alpha]_D$ -57.7 (c, 1 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

19α-Hydroxy, 13-Ac: [81543-05-7] ***Austalide E***
$C_{28}H_{36}O_{10}$ 532.586
Metab. of *Aspergillus ustus*. Cryst. (Me_2CO). Mp 262-264°. $[\alpha]_D$ -123.6 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep).

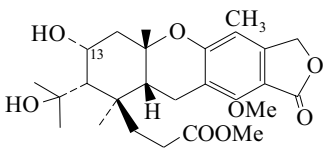
19α-Hydroxy, 19-Ac: [81543-04-6] ***Austalide D***
$C_{28}H_{36}O_{10}$ 532.586
Metab. of *Aspergillus ustus*. Cryst. (Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 259-261°. $[\alpha]_D$ -73.4 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep). λ_{max} 207 (ϵ 17140); 222 (ϵ 35400) (MeOH) (Berdy).

19α-Hydroxy, di-Ac: [81543-03-5] ***Austalide C***
$C_{30}H_{38}O_{11}$ 574.624
Metab. of *Aspergillus ustus*. Amorph. $[\alpha]_D$ -99 (c, 1 in $CHCl_3$).

Horak, R.M. *et al., J.C.S. Perkin 1*, 1985, 345; 347 (*isol, struct, pmr*)
De Jesus, A.E. *et al., J.C.S. Perkin 1*, 1987, 2253 (*biosynth*)
Dillen, J.L.M. *et al., Chem. Comm.*, 1989, 393 (*biosynth, abs config*)
Paquette, L.A. *et al., J.A.C.S.*, 1994, **116**, 11323 (*synth*)

Austalide H A-498

[96817-10-6]



$C_{26}H_{36}O_8$ 476.566
Terpenoid antibiotic. Mycotoxin of the food storage mould (*Aspergillus ustus*). Glass. $[\alpha]_D^{24}$ -19.5 (c, 1.0 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

13-Ac: [96817-09-3] ***Austalide G***
$C_{28}H_{38}O_9$ 518.603
Mycotoxin prod. by *Aspergillus ustus*. Glass. $[\alpha]_D^{24}$ -100.2 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep).

Horak, R.M. *et al., J.C.S. Perkin 1*, 1985, 345; 363 (*isol, struct, nmr*)

Austalide J A-499

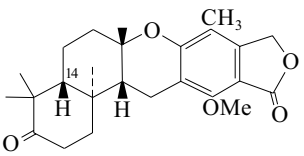
[87833-51-0]
As Austalide I, A-496 with
R^1 = H, R^2 = OH

$C_{25}H_{32}O_7$ 444.524
Terpenoid antibiotic. Mycotoxin of the food storage mould (*Aspergillus ustus*). Cryst. (MeOH). Mp 284-286°. $[\alpha]_D^{24}$ -42.1 (c 1.0 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

Horak, R.M. *et al., J.C.S. Perkin 1*, 1985, 345; 363 (*isol, struct, nmr*)

Austalide K A-500

[87833-53-2]



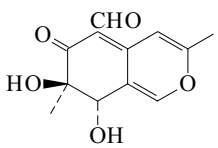
$C_{25}H_{32}O_5$ 412.525
Terpenoid antibiotic. Mycotoxin of the food storage mould (*Aspergillus ustus*). Glass. $[\alpha]_D^{24}$ -75.9 (c, 1.00 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

14β-Hydroxy: [87833-52-1] ***Austalide L***
$C_{25}H_{32}O_6$ 428.524
Mycotoxin prod. by *Aspergillus ustus*. Cryst. (C_6H_6/hexane). Mp 207-208°. $[\alpha]_D^{24}$ -71 (c, 1.00 in $CHCl_3$). λ_{max} 223 (ϵ 31200); 269 (ϵ 16600) (MeOH) (Derep).

Horak, R.M. *et al., J.C.S. Perkin 1*, 1985, 345; 363 (*isol, struct, nmr*)

Austdiol A-501

[53043-28-0]
*7,8-Dihydro-7,8-dihydroxy-3,7-dimethyl-6-oxo-6*H*-2-benzopyran-5-carboxaldehyde, 9CI*



Absolute configuration

$C_{12}H_{12}O_5$ 236.224
Toxic metab. of the food storage mould *Aspergillus ustus*. Yellow needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 255° dec. $[\alpha]_D^{26}$ +160.3 (c, 1.25 in Py). λ_{max} 256 (ϵ 15135); 376 (ϵ 23990) (EtOH) (Berdy).

▶ Mutagenic activity (without metabolic activation). DJ2232000

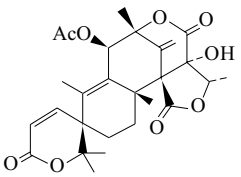
Di-Ac:
Needles (C_6H_6/hexane). Mp 238-239° dec.

Nagel, D.W. *et al., J.C.S. Perkin 1*, 1974, 45 (*isol, struct*)
Engel, D.W. *et al., Acta Cryst. B*, 1976, **32**, 2545 (*cryst struct*)
Wehner, F.C. *et al., Mutat. Res.*, 1978, **58**, 193
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Colombo, L. *et al., J.C.S. Perkin 1*, 1983, 2745 (*biosynth*)

Lo Presti, L. *et al., Acta Cryst. C*, 2003, **59**, o199-o201 (*cryst struct*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 790

Austin, 9CI A-502

[61103-89-7]



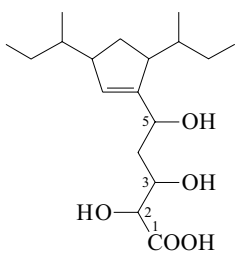
Absolute configuration

$C_{27}H_{32}O_9$ 500.544
Mycotoxin prod. by the food storage mould (*Aspergillus ustus*). Cryst. ($CHCl_3$/MeOH). Mp 298-300°. λ_{max} 243 (ϵ 11900) (EtOH) (Berdy).

O-*De-Ac:* [72040-27-8] ***Austinol***
$C_{25}H_{30}O_8$ 458.507
Metab. of *Emericella nidulans, Emericella dentata, Aspergillus variecolor* and *Aspergillus ustus*. Amorph.

Chexal, K.K. *et al., J.A.C.S.*, 1976, **98**, 6748 (*cryst struct*)
Fukuyama, K. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2270 (*cryst struct*)
Simpson, T.J. *et al., Chem. Comm.*, 1981, 1042 (*biosynth*)
Maebayashi, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1911 (*abs config*)
McIntyre, C.R. *et al., Chem. Comm.*, 1982, 781 (*biosynth*)
Simpson, T.J. *et al., J.C.S. Perkin 1*, 1982, 2687 (*cmr*)
Simpson, T.J. *et al., Chem. Comm.*, 1984, 1242 (*biosynth*)
Ahmed, S.A. *et al., J.C.S. Perkin 1*, 1989, 807 (*biosynth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 802

Auxin a A-503



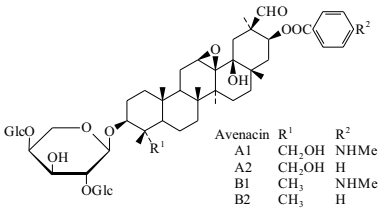
$C_{18}H_{32}O_5$ 328.448
Fraudulent work. Claimed to have been isolated from peanut oil and corn oil. Mp 196°. Almost certainly Cholic acid.

1,5-Lactone:Auxin a lactone
$C_{18}H_{30}O_4$ 310.433
Mp 173°. Almost certainly 1,4-Benzenediol, B-21.

2-Deoxy, 3-ketone:Auxin b
$C_{18}H_{30}O_4$ 310.433
Claimed isoln. from peanut and corn oils. Mp 183°. Almost certainly Thiosemicarbazide.

Kögl, F. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1933, **214**, 241; 1934, **225**, 215
Mori, K. *et al., Annalen*, 1991, 775 (*bibl*)

Avenacin A-504



Avenacin	R^1	R^2
A1	CH_2OH	NHMe
A2	CH_2OH	H
B1	CH_3	NHMe
B2	CH_3	H

Isol. from oat root.

Avenacin A1 [90547-90-3]
$C_{55}H_{83}NO_{21}$ 1094.255
Cryst. Sol. MeOH, EtOH; poorly sol. H_2O, Et_2O. Mp 228-233°. λ_{max} 223 (ϵ 25300); 255 (ϵ 7900); 357 (ϵ 5500) (EtOH) (Derep). λ_{max} 253 (E1%/1cm 80); 255 (ϵ 7900) (MeOH) (Berdy). λ_{max} 222 (ϵ 26013); 255 (ϵ 8088); 356 (ϵ 5902) (EtOH) (Berdy).
► LD_{50} (mus, ivn) 4 - 10 mg/kg.

Avenacin A2 [90547-91-4]
$C_{54}H_{80}O_{21}$ 1065.213
Cryst. Sol. MeOH, butanol; fairly sol. H_2O; poorly sol. hexane. Mp 237-239°. λ_{max} 230 (ϵ 14700); 274 (ϵ 1200); 281 (ϵ 1100) (EtOH) (Derep). λ_{max} 230 (ϵ 14700); 274 (ϵ 1200); 281 (ϵ 1100) (EtOH) (Berdy).

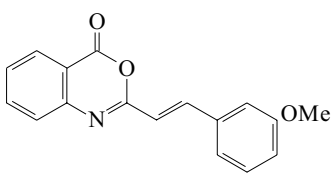
Avenacin B1 [90547-92-5]
$C_{55}H_{83}NO_{20}$ 1078.255
Glass. λ_{max} 223 (ϵ 25300); 255 (ϵ 7900); 357 (ϵ 5500) (EtOH) (Derep).

Avenacin B2 [90547-93-6]
$C_{54}H_{80}O_{20}$ 1049.214
Glass. λ_{max} 230 (ϵ 14700); 274 (ϵ 1200); 281 (ϵ 1100) (EtOH) (Derep).

Begley, M.J. *et al., J.C.S. Perkin 1*, 1986, 1905; 1917 (*isol, struct*)
Crombie, W.M.L. *et al., Phytochemistry*, 1986, **25**, 2069; 2075 (*isol*)
Trojanowska, M.R. *et al., Phytochemistry*, 2000, **54**, 153-164 (*biosynth*)

Avenalumin II A-505

[78214-14-9]
*2-[2-(3-Methoxyphenyl)ethenyl]-4*H*-3,1-benzoxazin-4-one, 9CI. 2-(3-Methoxycinnamoyl)-4*H*-3,1-benzoxazin-4-one*

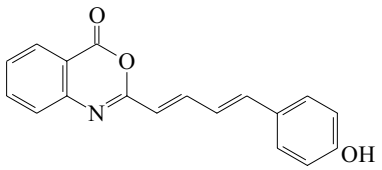


$C_{17}H_{13}NO_3$ 279.295
The proposed struct. illus. has been questioned (see Crombie *et al*). Phytoalexin from oat (*Avena sativa*) infected with rust fungus *Puccinia coronata*. Poorly sol. hexane. λ_{max} 317 ; 336 (MeOH) (Berdy).

Mayama, S. *et al., Physiol. Plant Pathol.*, 1981, **19**, 217 (*isol*)
Collins, F.W. *et al., Spectroscopy (Ottawa)*, 1985, **4**, 171 (*synth, ms*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth*)

Avenalumin III A-506

[78214-15-0]
*2-[4-(4-Hydroxyphenyl)-1,3-butadienyl]-4*H*-3,1-benzoxazin-4-one, 9CI*

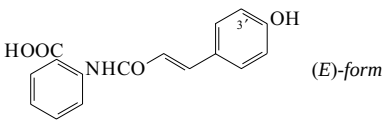


$C_{18}H_{13}NO_3$ 291.306
The proposed struct. illus. has been questioned (see Crombie *et al*). Phytoalexin isol. from oat (*Avena sativa*) infected with rust fungus (*Puccinia coronata*). Poorly sol. hexane.

Mayama, S. *et al., Physiol. Plant Pathol.*, 1981, **19**, 217 (*isol*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth*)

Avenanthramide D A-507

[115610-36-1]
N-p-*Hydroxycinnamoylanthranilic acid. Dianthramide P*



(*E*)-*form*

$C_{16}H_{13}NO_4$ 283.283
Sol. EtOAc, Et_2O, H_2O-Me_2CO; poorly sol. $CHCl_3$, H_2O, C_6H_6. λ_{max} 218 (ϵ 19950); 329 (ϵ 29500) (MeOH) (Berdy). λ_{max} 213 (ϵ 26900); 314 (ϵ 12020); 371 (ϵ 32360) (MeOH-NaOH) (Berdy).

(E)-form
Isol. from the oat *Avena sativa*. Rods (Me_2CO aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 219°. λ_{max} 300 ; 329 (MeOH) (Berdy).

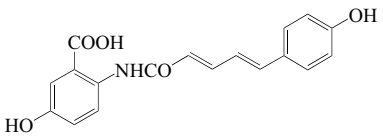
3′-Methoxy: [93755-77-2] ***Avenanthramide E***. N-*Feruloylanthranilic acid*
$C_{17}H_{15}NO_5$ 313.309
Isol. from the oat *Avena sativa*. Pale yellow needles (Me_2CO aq.). Sol. EtOAc, Et_2O, H_2O-Me_2CO; poorly sol. $CHCl_3$, H_2O, C_6H_6. Mp 235°. λ_{max} 211 ; 338 (MeOH) (Berdy). λ_{max} 219 ; 385 (MeOH-NaOH) (Berdy).

(Z)-form
3′-Methoxy: [116764-24-0] Z-*Avenanthramide E*
$C_{17}H_{15}NO_5$ 313.309
Isol. from oat.

Collins, F.W. *et al., J. Chromatogr.*, 1988, **445**, 363 (*hplc*)
Ponchet, M. *et al., Phytochemistry*, 1988, **27**, 725
Collins, F.W. *et al., J. Agric. Food Chem.*, 1989, **37**, 60 (*isol, pmr, cmr, uv, ms*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth*)
Ishihara, A. *et al., Phytochemistry*, 1999, **50**, 237-242 (*biosynth*)

Avenanthramide L A-508

[172549-38-1]



$C_{18}H_{15}NO_5$ 325.32

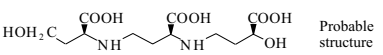
Isol. from oat, *Avena sativa*, inoculated with *Puccinia coronata* f.sp. *avenae*. Yellow cryst. Mp 267-269°. λ_{max} 355 (log ϵ 4.8) (MeOH).

Miyagawa, H. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2305-2306 (*isol, uv, pmr*)
Ishihara, A. *et al., Phytochemistry*, 1999, **50**, 237-242 (*biosynth*)

Avenic acid A A-509

[76224-57-2]

N-*[3-(3-Hydroxy-3-carboxypropylamino)-3-carboxypropyl]homoserine, 9CI*



$C_{12}H_{22}N_2O_8$ 322.314

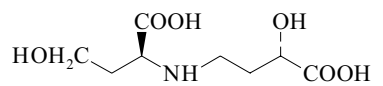
Isol. from root washings of *Avena sativa* (oats). Mp 300°. $[\alpha]_D$ +16.4 (c, 0.11 in 2N HCl).

Fushiya, S. *et al., Tet. Lett.*, 1980, 3071 (*isol, struct*)
Fushiya, S. *et al., Chem. Lett.*, 1981, 909 (*synth*)

Avenic acid B A-510

[76224-58-3]

N-*(3-Carboxy-3-hydroxypropyl)-L-homoserine, 9CI*



$C_8H_{15}NO_6$ 221.21

Constit. of the roots of *Avena sativa* (oats). Amorph. solid.

Fushiya, S. *et al., Chem. Lett.*, 1980, 1215 (*isol, pmr, cmr, synth*)
Ripperger, H. *et al., Heterocycles*, 1982, **17**, 447 (*rev*)

Avenothionin A-511

Peptides. Analogs of purothionins. Two avenothionins (α- and β-) have been characterized. They contain 45 AA residues including 8 cysteines. Isol. from oat (*Avena sativa*).

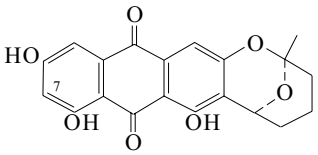
[79468-42-1, 79468-43-2]

Bekes, F. *et al., Cereal Chem.*, 1981, **58**, 360 (*isol*)

Averufin A-512

[14016-29-6]

*3,4,5,6-Tetrahydro-7,9,11-trihydroxy-2-methyl-2,6-epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 9CI*



$C_{20}H_{16}O_7$ 368.342

Bright orange-red laths (Me_2CO). Sol. MeOH, C_6H_6, bases; poorly sol. H_2O. Mp 280-282° dec. $[\alpha]_D$ 0. λ_{max} 223 (ϵ 34673); 266 (ϵ 18200); 294 (ϵ 33100); 324 (ϵ 9550); 453 (ϵ 10715) (EtOH) (Berdy).

▶ Shows mutagenic activity. KC4150000

Tri-Ac: [74810-25-6]
$C_{26}H_{22}O_{10}$ 494.454
Yellow needles (EtOH). Mp 210-214°. $[\alpha]_D$ -14.9 (c, 0.424 in $CHCl_3$).

6,8-Di-Me ether: [61470-56-2]

[79896-27-8] *6,8-Di-O-methylaverufin. Antibiotic SIPI 8917-I. SIPI 8917-I*
$C_{22}H_{20}O_7$ 396.396
Prod. by rice inoculated with *Emericella foeniculicola* and from a fungal isolate SIPI-8917. Cryst. (Me_2CO). Mp 208-209°. λ_{max} 225 ; 250 ; 287 ; 313 ; 439 (MeOH).

Tri-Me ether: [15894-83-4]
$C_{23}H_{22}O_7$ 410.423
Yellow prisms. Mp 190-191°.

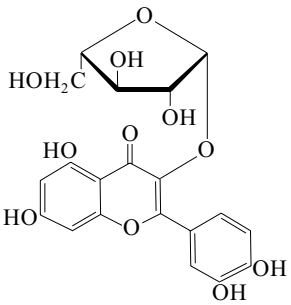
7-Methoxy: [95963-94-3] ***7-Methoxyaverufin***
$C_{21}H_{18}O_8$ 398.368
Yellow cryst. (Me_2CO). Mp 198-200° dec.

Pusey, D.F.G. *et al., J.C.S.*, 1963, 3542 (*isol*)
Knight, J.A. *et al., J.C.S.(C)*, 1967, 2328 (*struct*)
Ando, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2091 (*cryst struct*)
Fitzell, D.C. *et al., J. Agric. Food Chem.*, 1975, **23**, 442 (*biosynth*)
Castonguay, A. *et al., Can. J. Chem.*, 1977, **55**, 1324 (*synth*)
Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1977, 2181 (*cmr, biosynth*)
Steyn, P.S. *et al., J.C.S. Perkin 1*, 1979, 451-459 (*pmr, deriv*)
Townsend, C.A. *et al., J.A.C.S.*, 1981, **103**, 6885; 1985, **107**, 270 (*synth, abs config*)
Simpson, T.J. *et al., Chem. Comm.*, 1982, 631; 632 (*biosynth*)
Sankawa, U. *et al., Heterocycles*, 1982, **19**, 1053 (*biosynth*)
Kachholz, T. *et al., J. Nat. Prod.*, 1983, **46**, 499 (*biosynth*)
Koreeda, M. *et al., J.O.C.*, 1985, **50**, 5426 (*synth, abs config*)
O'Malley, G.J. *et al., J.O.C.*, 1985, **50**, 5533 (*synth*)
Maebayashi, Y. *et al., Mycotoxins (Tokyo)*, 1985, **21**, 36-37 (*Di-O-methylaverufin*)
Ahmad, V.U. *et al., Z. Naturforsch., B*, 1985, **40**, 319 (*isol, uv, ir, pmr, ms, deriv*)
Chandler, I.M. *et al., Chem. Comm.*, 1987, 17 (*biosynth*)
Townsend, C.A. *et al., J.C.S. Perkin 1*, 1988, 839 (*synth, bibl*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 107

Avicularin A-513

[572-30-5]

*3-(α-L-Arabinofuranosyloxy)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. Quercetin 3-α-L-arabofuranoside. Aviculariside. Fenicularin*



$C_{20}H_{18}O_{11}$ 434.356

Constit. of *Vaccinium myrtillus* (bilberry) and *Juglans regia* (walnut). Yellow needles + H_2O (EtOH aq.). Sol. EtOH, bases; fairly sol. Et_2O; poorly sol. H_2O, hexane. Mp 217° (anhyd. 222°). $[\alpha]_D$ -241 (c, 0.138 in MeOH) → -116 (24 hr). Identity of Fenicularin from *Foeniculum vulgare* with Avicularin not fully establ. (same struct. assigned but higher Mp (256°) given) λ_{max} 260 (ϵ 20900); 360 (ϵ 17400) (EtOH) (Berdy).

Hepta-Ac:
Needles ($CHCl_3$/petrol). Mp 187°. $[\alpha]_D$ -136 (c, 1.22 in $CHCl_3$).

[119786-64-0]

Ohta, T. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1940, **263**, 221 (*isol, struct*)
El Khadem, H. *et al., J.C.S.*, 1958, 3320 (*isol*)
Ohta, T. *et al., Yakugaku Zasshi*, 1959, **79**, 986; *CA*, **53**, 20695 (*Fenicularin*)
Mabry, T.J. *et al., Tetrahedron*, 1978, **34**, 1389 (*cmr*)

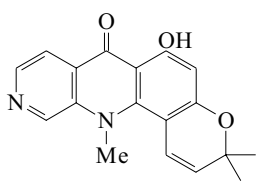
AX Peptides A-514

Peptides consisting of 46 amino acid residues including 8 cysteines. Isol. from leaves of *Beta vulgaris* infected with *Cercospora beticola*.
[159075-61-3]

Eur. Pat., 1994, 612 847; *CA*, **121**, 297401w (*isol*)
Kragh, K.M. *et al., Mol. Plant-Microbe Interact.*, 1995, **8**, 424-434 (*isol*)

Azaacridone A A-515

[150050-14-9]



$C_{18}H_{16}N_2O_3$ 308.336

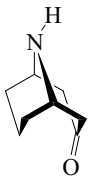
First naturally occurring azaacridone alkaloid. Alkaloid from roots of *Citrus paradisi* (grapefruit). Light brown oil.

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1993,

41, 789 (*isol, uv, ir, pmr, struct*)

9-Azabicyclo[3.3.1]nonan-3-one, 9CI A-516

[4390-39-0]
Granatonine. Norgranatan-3-one. Norpseudopelletierine



$C_8H_{13}NO$ 139.197
Found in pomegranate (*Punica granatum*) bark. Mp 123°.

▶ CL5593500

Picrate:
Cryst. (MeOH). Mp 216°.

N-*(Trifluoroacetyl):* [180406-55-7]
$C_{10}H_{12}F_3NO_2$ 235.206
Cryst. (Et_2O/hexane). Mp 70-73°.

N-*Benzoyl:* [36146-90-4]
$C_{15}H_{17}NO_2$ 243.305
Oil.

N-*(4-Methylbenzenesulfonyl):* [180406-57-9]
$C_{15}H_{19}NO_3S$ 293.386
Cryst. (EtOH). Mp 149-151°.

N-*Me:* [552-70-5] *9-Methyl-9-azabicyclo[3.3.1]nonan-3-one, 9CI. Granatan-3-one.* N-*Methylgranatonine. Pseudopelletierine. Ψ-Pelletierine*
$C_9H_{15}NO$ 153.224
Found in bark of pomegranate (*Punica granatum*). Prismatic plates (petrol). V. sol. H_2O. Mp 62-64°. Bp 246°. Strong base.

N-*Me, oxime:* [6164-67-6]
$C_9H_{16}N_2O$ 168.238
Plates (Et_2O). Mp 128-129°.

N-*Me,* N-*oxide:*
$C_9H_{15}NO_2$ 169.223
Mp 160-162°.

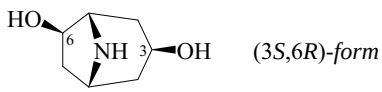
N-*Me,* N-*oxide; hydrochloride:*
Mp 224°.

N-*Benzyl:*
$C_{15}H_{19}NO$ 229.321
Mp 72°. $Bp_{0.005}$ 115-120°.

Org. Synth., Coll. Vol., 4, 1963, 816 (*synth, bibl*)
Chen, C.-Y. *et al., J.C.S.(B)*, 1966, 539 (*conformn*)
Guthrie, R.D. *et al., J.C.S.(C)*, 1966, 1207 (*ms, N-Me*)
Wiseman, J.R. *et al., J.O.C.*, 1977, **42**, 629 (*synth, N-Me*)
Dupeyre, R.M. *et al., Bull. Soc. Chim. Fr.*, Part II, 1978, 612-620 (*synth, pmr, N-benzyl*)
Hill, R.K. *et al., Tetrahedron*, 1982, **38**, 1959 (*synth, N-Me*)
Neuhoefer, H. *et al., Pharmazie*, 1993, **48**, 389-391 (*isol*)
Momose, T. *et al., J.C.S. Perkin 1*, 1997, 1307-1313 (*N-benzyl*)
Kirihara, M. *et al., Tetrahedron*, 1999, **55**, 2911-2926 (*derivs*)

8-Azabicyclo[3.2.1]octane-3,6-diol A-517

3,6-Dihydroxynortropane. 3,6-Nortropanediol



(3*S*,6*R*)-*form*

$C_7H_{13}NO_2$ 143.185

(3*S*,6*R*)-*form*
Alkaloid from the fruit of *Morus alba* (white mulberry). Powder. $[\alpha]_D$ -1.3 (c, 0.6 in H_2O).

(3*R,6*R**)-*form***
N-*Me:* See 8-Methyl-8-azabicyclo[3.2.1]octane-3,6-diol in *The Combined Chemical Dictionary.*

O^3-*Tigloyl:* [65636-83-1]

[65636-84-2] ***3-Tigloyloxynortropan-6-ol***
$C_{12}H_{19}NO_3$ 225.287
Plates (EtOH) (as hydrochloride). Mp 289-290° (hydrochloride). Opt. rotn. not measured.

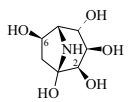
O^3-*Benzoyl:****3-Benzoyloxynortropan-6-ol***
$C_{14}H_{17}NO_3$ 247.293
Mp 225° (as picrate).

O^3-*(3,4,5-Trimethoxybenzoyl):****3-(3,4,5-Trimethoxybenzoyloxy)nortropan-6-ol***
$C_{17}H_{23}NO_6$ 337.372
Prisms (EtOH aq.) (as picrate). Mp 201° (picrate).

(3*R*,6*S*)-*form* *3β,6β-Dihydroxynortropane*
Alkaloid from the fruit of *Morus alba* (white mulberry). $[\alpha]_D$ -8.2 (c, 0.34 in H_2O).
Evans, W.C. *et al., Phytochemistry*, 1978, **17**, 171 (*isol, pmr, struct*)
Al-Said, M.S. *et al., Phytochemistry*, 1986, **25**, 851 (*isol, ir, pmr, ms, struct*)
El-Iman, Y.M.A. *et al., Phytochemistry*, 1987, **26**, 2385 (*deriv*)
Asano, N. *et al., J. Agric. Food Chem.*, 2001, **49**, 4208-4213 (*3β,6β-form*)
Kusano, G. *et al., Chem. Pharm. Bull.*, 2002, **50**, 185-192 (*Morus alba isolate*)

8-Azabicyclo[3.2.1]octane-1,2,3,4,6-pentol A-518

1,2,3,4,6-Pentahydroxynortropane



(1*R**,2*R**,3*R**,4*S**,6*R**)-*form*

$C_7H_{13}NO_5$ 191.183

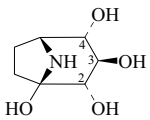
(1*R*,2*R*,3*R*,4*S*,6*R*)-*form* [190957-44-9]
Calystegine C₂
Alkaloid from *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ -40.6 (c, 0.32 in H_2O).

(1*R*,2*S*,3*R*,4*S*,6*R*)-*form* [156705-04-3]
Calystegine C₁
Alkaloid from *Morus alba* (white mulberry) and *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D$ +23.1 (c, 0.8 in H_2O).

N-*Me:* [197449-07-3] **N-*Methylcalystegine C₁***
$C_8H_{15}NO_5$ 205.21
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ +27.6 (c, 0.3 in H_2O).
Asano, N. *et al., Eur. J. Biochem.*, 1995, **229**, 369-376; 1997, **248**, 296-303 (*isol, pmr, cmr*)
Kato, A. *et al., Phytochemistry*, 1997, **45**, 425-429 (*Calyctegine C_2*)
Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)
Watson, A.A. *et al., Phytochemistry*, 2001, **56**, 265-295 (*rev*)

8-Azabicyclo[3.2.1]octane-1,2,3,4-tetrol A-519

1,2,3,4-Tetrahydroxynortropane



(1*R*,2*S*,3*R*,4*S*)-*form*

$C_7H_{13}NO_4$ 175.184

(1*R*,2*S*,3*R*,4*S*)-*form* [127414-85-1]
Calystegine B₂. *Nortropanoline*
Alkaloid from *Solanum tuberosum* (potato), *Solanum melongena* (aubergine). $[\alpha]_D$ +2.9 (c, 0.2 in H_2O). $[\alpha]_D$ +17.1 (c, 0.41 in H_2O) (synthetic).

N-*Me:* [184045-65-6] **N-*Methylcalystegine B₂***
$C_8H_{15}NO_4$ 189.211
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ +22.2 (c, 0.22 in H_2O).

(1*S*,2*R*,3*S*,4*R*)-*form* [146275-92-5]
$[\alpha]_D$ -17.5 (c, 0.37 in H_2O).

*4-O-α-D-Galactopyranoside:****4-O-α-D-Galactopyranosylcalystegine B₂***
$C_{13}H_{23}NO_9$ 337.326
Alkaloid from the fruit of *Morus alba* (white mulberry). $[\alpha]_D$ +114.5 (c, 0.48 in H_2O).

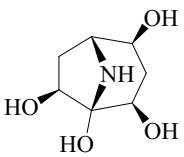
(1*R*,2*R*,3*R*,4*S*)-*form* [178231-95-3]
Calystegine B₃
Powder. $[\alpha]_D$ +82.8 (c, 0.5 in H_2O).

(1*R*,2*S*,3*R*,4*R*)-*form* [184046-85-3]
Calystegine B₄
Powder. $[\alpha]_D$ -63 (c, 0.65 in H_2O).
Goldmann, A. *et al., Phytochemistry*, 1990, **29**, 2125 (*isol*)
Ducrot, P.-H. *et al., Tet. Lett.*, 1990, **31**, 3879; 3883 (*pmr, cmr, struct, synth*)
Boyer, F.-D. *et al., Synlett*, 1992, 969 (*synth*)
Duclos, O. *et al., Tet. Lett.*, 1992, **33**, 8061 (*synth*)
Nash, R.J. *et al., Phytochemistry*, 1993, **34**, 1281 (*occur*)
Boyer, F.-D. *et al., Tetrahedron*, 1994, **50**, 10443 (*synth*)
Asano, N. *et al., Eur. J. Biochem.*, 1995, **229**, 369 (*Calystegine B_3*)
Asano, N. *et al., Carbohydr. Res.*, 1996, **284**, 169; **293**, 195 (*Calystegine B_3, Calystegine B_4*)
Goldmann, A. *et al., J. Nat. Prod.*, 1996, **59**, 1137
Soulié, J. *et al., Tetrahedron*, 1996, **52**, 15137 (*synth*)
Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*N-Methylcalystegine B_2*)
Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)
Asano, N. *et al., J. Agric. Food Chem.*, 2001, **49**, 4208-4213 (*4-Galactosylcalystegine B_2*)
Watson, A.A. *et al., Phytochemistry*, 2001, **56**, 265-295 (*rev*)

Bekkouche, K. *et al., Phytochemistry*, 2001, **58**, 455-462 (*occur*)
Boyer, F.-D. *et al., Tet. Lett.*, 2001, **42**, 1275-1277 (*Calystegine B_2, synth*)
Marco-Contelles, J. *et al., J.O.C.*, 2002, **67**, 3705-3717 (*Calystegine B_2, synth*)
Scholl, Y. *et al., Phytochemistry*, 2003, **62**, 325-332 (*biosynth*)

8-Azabicyclo[3.2.1]octane-1,2,4,7-tetrol A-520

1,2,4,7-Tetrahydroxynortropane. 1,2,4,7-Nortropanetetrol

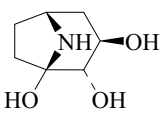


$C_7H_{13}NO_4$ 175.184

(1*R,2*R**,4*S**,7*S**)-*form*** [197565-91-6]
Calystegine B_5
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ +9.6 (c, 0.31 in H_2O).
Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*Calystegine B_5*)

8-Azabicyclo[3.2.1]octane-1,2,3-triol A-521

1,2,3-Trihydroxynortropane

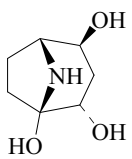


$C_7H_{13}NO_3$ 159.185

(1*R*,2*S*,3*R*)-*form* [131580-36-4]
Calystegin A_3
Alkaloid from *Solanum tuberosum* (potato). Powder. $[\alpha]_D$ -17.3 (c, 0.5 in H_2O).
Goldmann, A. *et al., Phytochemistry*, 1990, **29**, 2125 (*isol*)
Ducrot, P.-H. *et al., Tet. Lett.*, 1990, **31**, 3879; 3883 (*pmr, cmr, struct, synth*)
Boyer, F.-D. *et al., Synlett*, 1992, 357 (*synth*)
Nash, R.J. *et al., Phytochemistry*, 1993, **34**, 1281 (*occur*)
Asano, N. *et al., Eur. J. Biochem.*, 1995, **229**, 369 (*isol, pmr, cmr*)
Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)
Bekkouche, K. *et al., Phytochemistry*, 2001, **58**, 455-462 (*occur*)

8-Azabicyclo[3.2.1]octane-1,2,4-triol A-522

1,2,4-Trihydroxynortropane. 1,2,4-Nortropanetriol

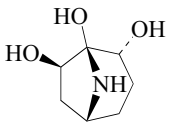


$C_7H_{13}NO_3$ 159.185

(1*R,2*S**,4*S**)-*form*** [197565-90-5]
Calystegine A_7
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ -10.8 (c, 0.27 in H_2O).
Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*Calystegine A_7*)

8-Azabicyclo[3.2.1]octane-1,2,7-triol A-523

1,2,7-Trihydroxynortropane

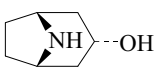


$C_7H_{13}NO_3$ 159.185

(1*R,2*R**,7*R**)-*form*** [177794-04-6]
Calystegine A_6
Alkaloid from and *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ -27.6 (c, 0.4 in H_2O).
Asano, N. *et al., Carbohydr. Res.*, 1996, **284**, 169-178 (*isol, pmr, cmr*)
Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*isol*)
Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)

8-Azabicyclo[3.2.1]octan-3-ol, 9CI A-524

3-Nortropanol



(1*RS*,3*RS*,5*SR*)-*form*

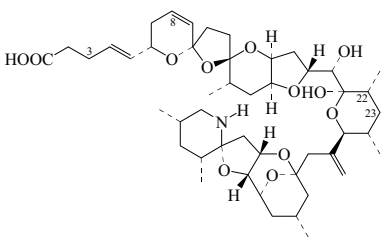
$C_7H_{13}NO$ 127.186

(1*RS*,3*SR*,5*SR*)-*form* [501-33-7]
exo-*form*. ***Nor-ψ-tropine***. *Norpseudotropine*
Alkaloid from the fruit of *Morus alba* (white mulberry). Cryst. (C_6H_6/pentane). Mp 134.5-135° (129-130°).
► LD_{50} (mus, orl) 227 mg/kg. RD0875000
Hydrochloride: [14383-51-8]
Cryst. Mp 280-282° dec.
► RD0600000
N-*Benzoyl:* [18470-33-2] ***Nortropacocaine***
$C_{14}H_{17}NO_2$ 231.294
Feathery cryst. (synthetic, as picrate). Mp 234° (picrate).
N-*Me:* See 8-Methyl-8-azabicyclo[3.2.1]octan-3-ol in *The Combined Chemical Dictionary.*

(1*RS*,3*RS*,5*SR*)-*form* [538-09-0]
endo-*form*. *Nortropeine. Tropigenin. Nortropenol. Nortropine*
► LD_{50} (mus, orl) 1420 mg/kg. RD0700000
Hydrochloride: [17366-48-2]
Cryst. Mp 200°.
O-*(2-Methylbutanoyl):* [537-28-0] ***Isoporoidine***
$C_{12}H_{21}NO_2$ 211.303
O-*(3-Methylbutanoyl):* [500-58-3] ***Poroidine***
$C_{12}H_{21}NO_2$ 211.303Co-isol. with Isoporoidine, difficult to separate.
O-*Benzoyl:****3α-Benzoyloxynortropane***
$C_{14}H_{17}NO_2$ 231.294
Mp 232° (as picrate).
O-*Phenylacetyl:****Nortropan-3-yl phenylacetate***
$C_{15}H_{19}NO_2$ 245.321
O-*Cinnamoyl (*E-*):* [126394-79-4] ***Nortropinyl cinnamate***
$C_{16}H_{19}NO_2$ 257.332
Yellow gum.
O-*Cinnamoyl,* N-*Ac:* [136945-63-6]
Needles (CH_2Cl_2/petrol). Mp 143°.
N-*Me:* See 8-Methyl-8-azabicyclo[3.2.1]octan-3-ol in *The Combined Chemical Dictionary.*
Barger, G. *et al., J.C.S.*, 1937, 1820 (*Poroidine, Isoporoidine*)
Werner, G. *et al., Annalen*, 1967, **708**, 210 (*synth*)
Kraiss, G. *et al., Tet. Lett.*, 1971, 57 (*synth*)
Chappell, G.S. *et al., J. Pharm. Sci.*, 1973, **62**, 414 (*nmr*)
Tufariello, J.J. *et al., J.A.C.S.*, 1979, **101**, 2435 (*synth*)
Al-Yahya, M.A.I. *et al., J.C.S. Perkin 1*, 1979, 2130 (*isol, Poroidine, Isoporoidine*)
El-Imam, Y.M.A. *et al., Phytochemistry*, 1985, **24**, 2285-2289 (*Nortropacocaine*)
Al-Said, M.S. *et al., J.C.S. Perkin 1*, 1986, 957 (*Phenylacetate*)
Al-Said, M.S. *et al., Phytochemistry*, 1986, **25**, 851-853 (*isol, ir, pmr, ms, struct, deriv*)
Arbain, D. *et al., Aust. J. Chem.*, 1991, **44**, 1013 (*Nortropinyl cinnamate*)
Kusano, G. *et al., Chem. Pharm. Bull.*, 2002, **50**, 185-192 (*isol, pmr, cmr*)

Azaspiracid A-525

[214899-21-5]



$C_{47}H_{71}NO_{12}$ 842.077
Alkaloid from *Mytilus edulis* (blue mussel). Shellfish toxin. Amorph. solid. $[\alpha]_D^{20}$ -21 (c, 0.1 in MeOH).

8-Methyl: [265996-92-7] ***Azaspiracid 2***
$C_{48}H_{73}NO_{12}$ 856.104
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl: [265996-93-8] ***Azaspiracid 3***
$C_{46}H_{69}NO_{12}$ 828.051
Alkaloid from *Mytilus edulis* (blue mussel).

*22-Demethyl, 3*R*-hydroxy:****Azaspiracid 4***
$C_{46}H_{69}NO_{13}$ 844.05
Alkaloid from *Mytilus edulis* (blue mussel).

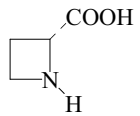
*22-Demethyl, 23*S*-hydroxy:****Azaspiracid 5***
$C_{46}H_{69}NO_{13}$ 844.05
Alkaloid from *Mytilus edulis* (blue mussel).

Satake, M. *et al., J.A.C.S.*, 1998, **120**, 9967-9968

(*Azaspiracid*)
Ofuji, K. *et al., Nat. Toxins*, 1999, **7**, 99-102 (*Azaspiracids 2,3*)
Ofuji, K. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 740-742 (*Azaspiracids 4,5*)

2-Azetidinecarboxylic acid, 9CI A-526

[2517-04-6]



(*R*)-*form*

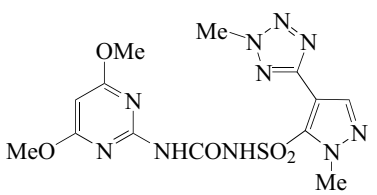
$C_4H_7NO_2$ 101.105

(*S*)-*form* [2133-34-8]
Present in roots and leaves of *Convallaria majalis* (lily-of-the-valley). *Convallaria majalis* is banned by the FDA from food use in the USA. Cryst. (MeOH). Sol. H_2O. $[\alpha]_D^{20}$ -108 (c, 3.6 in H_2O). Unstable in mineral acids. Does not melt but darkens at 270°.
▶ Exp. reprod. and teratogenic effects. LD_{50} (mus, scu) 1000 mg/kg. CM4310500

N-*(3-Hydroxypropyl):* [91106-30-8] ***Medicanine***
$C_7H_{13}NO_3$ 159.185
Amino acid from seeds of *Medicago sativa* (alfalfa). Hygroscopic cryst. Mp 124-126° (synthetic). $[\alpha]_D$ -92.2 (c, 0.13 in H_2O) (natural). $[\alpha]_D$ -100.5 (c, 0.45 in H_2O) (synthetic).
Fushiya, S. *et al., Heterocycles*, 1984, **22**, 1039-1040 (*Medicanine*)

Azimsulfuron, ANSI, BSI A-527

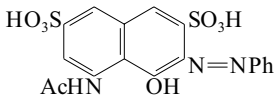
[120162-55-2]
N-*[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]-1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)-1*H*-pyrazole-5-sulfonamide, 9CI. 1-(4,6-Dimethoxy-2-pyrimidinyl)-3-[[1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)-pyrazol-5-yl]sulfonyl]urea. Gulliver. IN-A8947. A 8947*



$C_{13}H_{16}N_{10}O_5S$ 424.399
Acetolactate synthase inhibitor. Post-emergence herbicide for control of *Echinochloa* spp., used esp. on rice. Solid. Mp 170°. pK_a 3.6.
▶ LD_{50} (rat, orl) >5000 mg/kg.
U.S. Pat., 1988, 4 746 353, (*du Pont de Nemours*); *CA*, **110**, 173240w (*synth, activity*)
Marquez, T. *et al., Brighton Crop Prot. Conf. - Weeds*, 1995, 65-72 (*activity*)
Barefoot, A.C. *et al., Brighton Crop Prot. Conf. - Weeds*, 1995, 713-718 (*metab*)
Pesticide Manual, 11th edn., 1997, 39; 63-65
Powley, C.R. *et al., J. Agric. Food Chem.*, 1998, **46**, 514-519 (*anal, hplc*)

Azorhodine 2G A-528

5-(Acetylamino)-4-hydroxy-3-(phenylazo)-2,7-naphthalenedisulfonic acid, 9CI. C.I. Acid red 1. C.I. Food red 10. C.I. 18050. Brilliant acid red G. Fast crimson GR. Naphthazine rose 2G. Red 2G. Solar fast red 3G. Vopsider red ASTR G. E128. Many other names

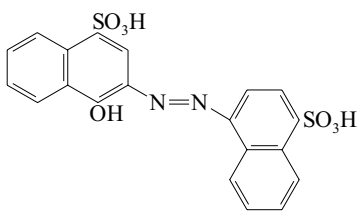


$C_{18}H_{15}N_3O_8S_2$ 465.464
Strictly, the name Azorhodine 2G applies to the disodium salt. Colourant additive for food.
▶ QJ6030000

Di-Na salt: [3734-67-6]
$C_{18}H_{13}N_3O_8S_2$ 463.448
Dark red cryst. Sol. H_2O; sl. sol. EtOH; insol. Et_2O.
▶ QJ6030000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 984B (*ir*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 29
Popa, G. *et al., Zh. Anal. Khim.*, 1959, **14**, 322 (*detn, Pd*)
Mathur, J.N. *et al., Indian J. Appl. Chem.*, 1970, **33**, 209
Colour Index, *3rd Edn*, 1971, **4**, 4116 (*synth*)
Nemodruk, A.A. *et al., Zh. Anal. Khim.*, 1972, **27**, 326 (*detn, Fe*)

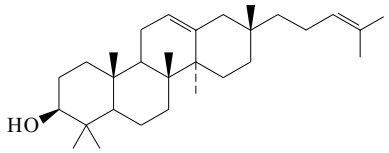
Azorubine A-529

[3567-69-9]
4-Hydroxy-3-[(4-sulfo-1-naphthalenyl)azo]-1-naphthalenesulfonic acid, 9CI. Brilliant carmoisine. Carmoisine. Chromotrope FB. C.I. Chromotrope FB. Lissamine red W. Nacarat. C.I. Acid red 14. C.I. Food red 3. C.I. Mordant blue 79. E122. Many other names



$C_{20}H_{14}N_2O_7S_2$ 458.472
Strictly, the name Azorubine applies to the disodium salt. Food dye. Dark red cryst. powder (as Na salt). Na salt sol. H_2O; mod. sol. EtOH; insol. Me_2CO. CAS no. refers to Na salt.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 988C (*ir*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 204
Colour Index, *3rd Edn*, 1971, **4**, 4068 (*synth*)
Bosch Serrat, F. *et al., An. Quim.*, 1972, **68**, 155; *CA*, **77**, 42752s (*detn, Mg*)
Bosch Serrat, F. *et al., Inf. Quim. Anal.*, 1973, **27**, 14; *CA*, **79**, 111414p (*detn, Pd*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HJF500

12,21-Baccharadien-3-ol B-1



$C_{30}H_{50}O$ 426.724

3β-*form* [160598-94-7]
Constit. of *Glycine max* (soybean). Cryst. Mp 133-135°.

Akihisa, T. *et al., Phytochemistry*, 1994, **37**, 1413 (*isol, pmr, cmr*)

Bacillolysin B-2

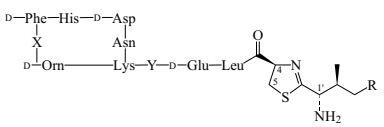
[76774-43-1]
Bacillus metalloendopeptidase. Bacillus subtilis neutral proteinase. E.C. 3.4.24.28

Enzyme, a peptidase of the thermolysin family with Zn and Ca as cofactors. Used for lactose redn. and flavour modification in dairy processing, for fortifying brewing malt proteins and for softening wheat gluten in baking.

Feder, J. *et al., Biochim. Biophys. Acta*, 1971, **251**, 74-78 (*isol*)
Pauptit, R.A. *et al., J. Mol. Biol.*, 1988, **199**, 525-537 (*cryst struct*)

Bacitracin, BAN, INN, JAN, USAN B-3

Bacilliquin



Bacitracin A X = Y = Ile, R = CH_3
B_1 X = Y = Ile, R = H
B_2 X = Val, Y = Ile, R = CH_3
B_3 X = Ile, Y = Val, R = CH_3
D_1 X = Val, Y = Ile, R = H
D_2 X = Ile, Y = Val, R = H
D_3 X = Y = Val, R = CH_3
E X = Y = Val, R = H

Cyclic peptide antibiotic. Permitted food additive for animal and human consumption. Sol. H_2O, $HCONH_2$, 2-propanol, Py, EtOH, MeOH; fairly sol. Me_2CO, butanol, dioxan; poorly sol. EtOAc, hexane. Non toxic in human fibroblast cells. Coml. prod. contains small quantities of other components. Nomenclature for minor components was revised in 1995 λ_{max} 270 (ϵ) (12*M* HCl) (Derep). λ_{max} 252 (ϵ 3550) (EtOH) (Derep). λ_{max} 254 (E1%/1cm 21.4) (H_2O) (Berdy).

► Nephrotoxic effects and hypersensitivity reactions reported from therapuetic use (intramuscular administration). LD_{50} (rat, ipr) 190 mg/kg. LD_{50} (gpg, orl) 2000 mg/kg (Bacitracin) ; LD_{50} (mus, ivn) 360 mg/kg , LD_{50} (mus, ipr) 200-640 mg/kg , LD_{50} (mus, scu) 1300-2500 mg/kg. CP0350000

Bacitracin A [22601-59-8]
$C_{66}H_{103}N_{17}O_{16}S$ 1422.71
Permitted food additive for animal and human consumption. Hygroscopic amorph. powder. $[\alpha]_D^{23}$ +5 (c, 0.1 in 0.02*M* HCl).

1′-Deamino, 1′-oxo, 4,5-didehydro: [22601-63-4] ***Bacitracin F***
$C_{66}H_{98}N_{16}O_{17}S$ 1419.663
λ_{max} 288 (ϵ 3980) (EtOH) (Derep). λ_{max} 289 (ϵ 4830) (MeOH).

Bacitracin B_1 [57762-79-5]
$C_{65}H_{101}N_{17}O_{16}S$ 1408.683

1′-Deamino, 1′-oxo, 4,5-didehydro: [167289-64-7] ***Bacitracin H_1***
$C_{65}H_{96}N_{16}O_{17}S$ 1405.636

Bacitracin B_2 [57762-78-4]
$C_{65}H_{101}N_{17}O_{16}S$ 1408.683

1′-Deamino, 1′-oxo, 4,5-didehydro: [144572-54-3] ***Bacitracin H_2***
$C_{65}H_{96}N_{16}O_{17}S$ 1405.636

Bacitracin B_3 [149146-32-7]
$C_{65}H_{101}N_{17}O_{16}S$ 1408.683

1′-Deamino, 1′-oxo, 4,5-didehydro: [144572-55-4] ***Bacitracin H_3***
$C_{65}H_{96}N_{16}O_{17}S$ 1405.636

Bacitracin D_1
$C_{64}H_{99}N_{17}O_{16}S$ 1394.656

1′-Deamino, 1′-oxo, 4,5-didehydro: [167289-62-5] ***Bacitracin I_1***
$C_{64}H_{94}N_{16}O_{17}S$ 1391.61

Bacitracin D_2
$C_{64}H_{99}N_{17}O_{16}S$ 1394.656

1′-Deamino, 1′-oxo, 4,5-didehydro: [167289-63-6] ***Bacitracin I_2***
$C_{64}H_{94}N_{16}O_{17}S$ 1391.61

Bacitracin D_3 [144572-46-3]
$C_{64}H_{99}N_{17}O_{16}S$ 1394.656

1′-Deamino, 1′-oxo, 4,5-didehydro: [144572-52-1] ***Bacitracin I_3***
$C_{64}H_{94}N_{16}O_{17}S$ 1391.61

Bacitracin E
$C_{63}H_{97}N_{17}O_{16}S$ 1380.63

[1405-87-4, 1405-89-6]

Newton, G.G.F. *et al., Biochem. J.*, 1950, **47**, 257
Lockhart, I.M. *et al., Biochem. J.*, 1955, **61**, 534 (*struct*)
Weisiger, J.R. *et al., J.A.C.S.*, 1955, **77**, 731; 3123 (*struct*)
Konigsberg, W. *et al., J.O.C.*, 1962, **27**, 934 (*Bacitracin F, synth*)
Nussbaumer, P.A. *et al., Pharm. Acta Helv.*, 1965, **40**, 210 (*Bacitracin F, chromatog*)
Ressler, C. *et al., J.A.C.S.*, 1966, **88**, 2025 (*struct*)
Galardy, R.E. *et al., Biochemistry*, 1971, **10**, 2429 (*conformn*)
Tsuji, K. *et al., J. Chromatogr.*, 1975, **112**, 663 (*chromatog*)
Hirotsu, Y. *et al., Pept. Chem.*, 1978, **16**, 171 (*Bacitracin F, synth*)
Storm, D.R. *et al., Antibiotics (N.Y.)*, 1979, **5**, 1 (*rev*)
Brewer, G.A. *et al., Anal. Profiles Drug Subst.*, 1980, **9**, 1 (*rev*)
Toscano, W.A. *et al., Pharmacol. Ther.*, 1982, **16**, 199 (*pharmacol, rev*)
Froeyshov, O. *et al., Drugs Pharm. Sci.*, 1984, **22**, 665 (*isol, props, rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 8368
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BAC 250
Pfeffer, S. *et al., FEBS Lett.*, 1991, **285**, 115 (*cryst struct*)
Ikai, Y. *et al., J. Antibiot.*, 1992, **45**, 1325 (*ms, struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 121
Ikai, Y. *et al., J. Antibiot.*, 1995, **48**, 233-242 (*isol, struct, abs config*)
Lee, J. *et al., J.O.C.*, 1996, **61**, 3983 (*synth, pmr*)
Kimura, K. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1754-1756 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAC250

Bacteriocin 28b B-4

[148466-49-3]

[173432-00-3]

Peptide. Bacteriocin prod. by *Serratia marcescens* N28b.

Viejo, M.B. *et al., J. Gen. Microbiol.*, 1992, **138**, 1737-1743

Bacteriocin Bc48 B-5

[138635-52-6]

Protein; MW 80 kDa. Bacteriocin prod. by *Enterococcus faecalis* ssp. *liquefaciens* S-48 and its mutant strain B-48-28.

Lopez-Lara, I. *et al., Can. J. Microbiol.*, 1991, **37**, 769-774 (*isol*)

Bacteriocin J46 B-6

[173584-72-0]

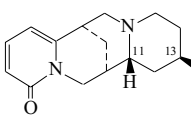
[181232-45-1]

Polypeptide. Prod. by *Lactococcus lactis* ssp. *cremoris* J46, isol. from fermented milk. Bacteriocin.

Huot, E. *et al., Anaerobe*, 1996, **2**, 137-145 (*isol*)

Baptifoline B-7

[732-50-3]
13-Hydroxyanagyrine. Alkaloid P3†



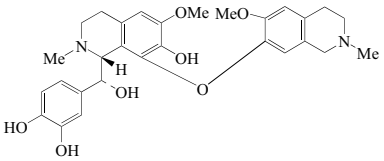
Absolute configuration

$C_{15}H_{20}N_2O_2$ 260.335
Alkaloid from *Caulophyllum thalictroides* (blue cohosh). Hexagonal or triangular plates (MeOH), needles (Me_2CO). Mp 210°. $[\alpha]_D$ -147.7 (-140) (EtOH). $[\alpha]_D^{16}$ -89.05 (c, 1.415 in H_2O).

Marion, L. *et al., J.A.C.S.*, 1948, **70**, 3253; 3472 (*isol*)
Martin-Smith, M. *et al., Can. J. Chem.*, 1957, **35**, 37 (*struct*)
Bohlmann, F. *et al., Chem. Ber.*, 1958, **91**, 2189; 2194; 1962, **95**, 944 (*isol, struct, synth*)
Flom, M.S. *et al., J. Pharm. Sci.*, 1967, **56**, 1515 (*isol*)
Monakhova, T.E. *et al., Khim. Prir. Soedin.*, 1973, **9**, 59; *Chem. Nat. Compd. (Engl. Transl.)*, 52 (*isol*)
Ohmiya, S. *et al., Phytochemistry*, 1974, **13**, 1016 (*isol*)
Kennelly, E.J. *et al., J. Nat. Prod.*, 1999, **62**, 1385-1389 (*isol, pmr, cmr*)

Bargustanine B-8

[169626-12-4]



$C_{29}H_{34}N_2O_7$ 522.597

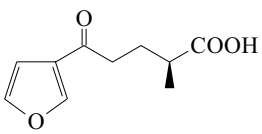
Alkaloid from roots of *Berberis vulgaris* (barberry). Cryst. (MeOH). Mp 193-194°. $[\alpha]_D^{20}$ +114.2 (c, 0.3 in MeOH). λ_{max} 218 (sh) (log ϵ 4.85); 286 (log ϵ 3.98) (EtOH).

Karimov, A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 44-47; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 35-38

Batatic acid B-9

[496-07-1]

α-Methyl-δ-oxo-3-furanpentanoic acid, 9CI. 5-(3-Furanyl)-2-methyl-5-oxopentanoic acid



(*S*)-*form*

$C_{10}H_{12}O_4$ 196.202

(*S*)-*form*

Obt. from sweet potato infected with *Ceratostomella fimbriata*. Poorly sol. hexane. Mp 88.5-89.5°. $[\alpha]_D^{10}$ +17.5 (EtOH).

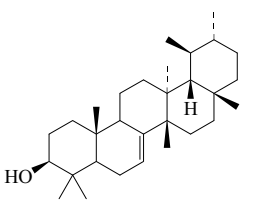
2,4-Dinitrophenylhydrazone: Mp 154.5-155.5°.

(±)-*form*

Mp 106-107°.

Kubota, T. *et al., Tetrahedron*, 1958, **4**, 68

7-Baueren-3-ol B-10



3β-*form*

$C_{30}H_{50}O$ 426.724

3β-*form* [6466-94-0]

Ilexol. *Baurenol*. *Bauerenol*

Cryst. (Me_2CO). Mp 207-208°. $[\alpha]_D^{19}$ -20.7 (c, 0.7 in $CHCl_3$).

Ac: [17020-04-1]

$C_{32}H_{52}O_2$ 468.762

Constit. of the famine food *Adansonia digitata* (baobab). Cryst. ($CHCl_3$/hexane). Mp 290-292°. $[\alpha]_D^{24}$ -1.1 (c, 1 in $CHCl_3$).

Me ether: [11008-41-6]

$C_{31}H_{52}O$ 440.751

Constit. of *Saccharum officinarum* (sugar cane). Cryst. (EtOAc). Mp 212-215°. $[\alpha]_D$ -32 (c, 1.2 in $CHCl_3$).

3-Ketone: [6895-55-2] ***7-Bauren-3-one***. *Bauerenone*

$C_{30}H_{48}O$ 424.709

Cryst. (EtOAc). Mp 240°. $[\alpha]_D^{25}$ -47.5 (c, 1 in $CHCl_3$).

(3β,13β)-*form*

Ac: [309724-35-4] ***Mongolenin***

$C_{32}H_{52}O_2$ 468.762

Cryst. ($CHCl_3$). Mp 283-284°. $[\alpha]_D^{12}$ -33 (c, 0.2 in $CHCl_3$).

Bryce, T.A. *et al., Tetrahedron*, 1967, **23**, 1283 (*Me ether*)

Buckley, D.G. *et al., Chem. Ind. (London)*, 1971, 298 (*pmr*)

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 974 (*isol, struct*)

Campello, J. de P. *et al., Phytochemistry*, 1975, **14**, 2300 (*ketone*)

Khan, M.R. *et al., Pak. J. Sci. Ind. Res.*, 1979, **22**, 301 (*cmr*)

Tinant, B. *et al., Bull. Soc. Chim. Belg.*, 1982, **91**, 117 (*cryst struct*)

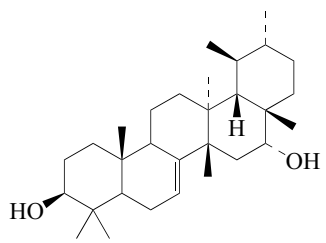
Chakravarty, A.K. *et al., Tetrahedron*, 1991, **47**, 2337 (*cmr*)

Shin, S.C. *et al., CA*, 1993, **119**, 266455w (*Ac*)

Yaoita, Y *et al., Nat. Med. (Tokyo)*, 1998, **52**, 273-275 (*pmr*)

Hu, J.-F. *et al., Nat. Prod. Lett.*, 2000, **14**, 211-215 (*Mongolenin*)

7-Baurene-3,16-diol B-11



$C_{30}H_{50}O_2$ 442.724

(3β,16α)-*form* [214351-30-1]

Constit. of *Tussilago farfara* (coltsfoot). Needles. Mp 282-285°. $[\alpha]_D^{28}$ -25.6 (c, 0.2 in Py).

Yaoita, Y. *et al., Nat. Med. (Tokyo)*, 1998, **52**, 273-275; *CA*, **129**, 287778a (*isol, pmr, cmr*)

Bavaricins B-12

Peptides. Prod. by *Lactobacillus bavaricus*. Bacteriocins with potential food uses.

Bavaricin A [154213-77-1]

Prod. by *Lactobacillus bavaricus* MI401. MW 3500-4000; partial struct. reported.

Bavaricin MN [144376-92-1]

Prod. by *Lactobacillus bavaricus* MN. Struct. comprises 42 aminoacid residues, MW 4769.

Larsen, A.G. *et al., J. Appl. Bacteriol.*, 1993, **75**, 113-122 (*Bavaricin A*)

Kaiser, A.L. *et al., J. Appl. Bacteriol.*, 1993, **75**, 536-540 (*Bavaricin MN*)

Kaiser, A.L. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 4529-4535 (*Bavaricin MN*)

Beijeran B-13

[→3)-α-D-Gal A-(1→3)-β-L-Rha-(1→3)-α-D-Glc-6-Ac-(1→]

Exopolysaccharide prod. by *Azotobacter beijerinckii* YNM1. Proposed for use in food industries.

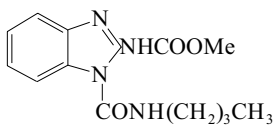
Ogawa, K. *et al., Carbohydr. Res.*, 1997, **300**, 41-45

Yui, T. *et al., Carbohydr. Res.*, 1997, **304**, 341-345 (*struct*)

Benomyl, ANSI, BSI, ISO, JMAF B-14

[17804-35-2]

Methyl 1-[(butylamino)carbonyl]-1H-benzimidazol-2-ylcarbamate, 9CI. Methyl 1-(butylcarbamoyl)benzimidazol-2-ylcarbamate. Benlate. Fungochrom. Agrocit. Fundazol



$C_{14}H_{18}N_4O_3$ 290.321

Agricultural and horticultural systemic fungicide mainly used on rice and soybean. V. spar. sol. H_2O; sol. $CHCl_3$; less sol. other org. solvs. Dec. before melting.

▶ Toxic to freshwater fish and aquatic invertebrates. OES: long-term 10 mg m^{-3}; short-term 15 mg m^{-3}. Skin irritant. Can cause contact dermatitis. Exp. reprod. and teratogenic effects. DD6475000

[8068-35-7]

U.S. Pat., 1966, 3 631 176; *CA*, **72**, 21692d

Tolkmith, H. *et al., Residue Rev.*, 1974, **53**, 99 (*rev*)

Bleidner, W.E. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1978, **10**, 157 (*rev, props, detn*)

Kirino, O. *et al., Agric. Biol. Chem.*, 1980, **44**, 35 (*activity*)

Cairns, T. *et al., Biomed. Mass Spectrom.*, 1983, **10**, 24 (*ms*)

Dangerous Prop. Ind. Mater. Rep., 1988, **8**, 45 (*rev*)

Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A31

Hanson, D.J. *et al., Chem. Eng. News*, Apr. 6, 1992, 15; Nov. 16, 4 (*rev, tox*)

Pharmaceutical Manufacturing Encyclopaedia, 1997, No. 60

Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1452

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAV575

Bentonite B-15

[1302-78-9]

E558

$Na_{0.33}[Al_{1.67}Mg_{0.33}Si_4O_{10}(OH)_2]$

$[Al_{1.67}H_2Mg_{0.33}Na_{0.33}O_{12}Si_4]$ 367.017

Rock containing Montmorillonite, M-748 and various other clay minerals. Widely distributed mineral. Used in foods as a colourant, pigment and stabiliser.

▶ CT9450000

van Olpen, H. *et al., Clay Colloid Chemistry*, 2nd Edn., Wiley, N. Y., 1977,

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 238; 241; **6**, 193; 200 (*rev*)

Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American

Pharmaceutical Association/Pharmaceutical Press, 1994, 24-26
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1536
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 242-243
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAV750

Benzaldehyde, USAN B-16

[100-52-7]
Benzenecarboxaldehyde. Formylbenzene. FEMA 2127

PhCHO

C_7H_6O 106.124

Found in plants, esp. in almond kernels. Also present in strawberry jam, leek, crispbread, cheese, black tea and several essential oils. Parent and derivs. (e.g. glyceryl acetal) are used as flavourings. Liq. with characteristic almond-type odour. V. spar. sol. H_2O; misc. org. solvs. d_4^{15} 1.05. Mp -26° Fp -56.9. Bp 178-179° Bp_{10} 62°. pK_a 14.9 (25°,hydrate, 1% EtOH). pK_a -6.9 (as base). Log P 1.5 (calc). Steam-volatile. Forms bisulfite compd. Slowly oxid. in air. Reduces $AgNO_3.NH_2$ but not Fehling's soln. λ_{max} 244 ; 280 (MeOH) (Berdy).

► Fl. p. 63°, autoignition temp. 190°. Violently oxid. by 90% HCOOOH. Skin irritant. May cause dermatitis. CNS depressant. LD_{50} (rat, orl) 1300 mg/kg. CU4375000

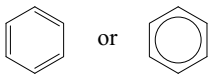
Di-Me acetal: [1125-88-8] *(Dimethoxymethyl)benzene. Dimethoxyphenylmethane. FEMA 2128*
$C_9H_{12}O_2$ 152.193
Constit. of rhubarb and potato. Used in perfumery and food flavouring. Moisture-sensitive liq. $d_4^{15.5}$ 1.03. Bp 198° Bp_{18} 87-89°. n_D^{20} 1.4930.

[932-90-1, 3592-47-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 104A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 932B; **3**, 492A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1283B; 1578B (*ir*)
Briner, E. *et al., Helv. Chim. Acta*, 1937, **20**, 293
Braude, E.A. *et al., J.C.S.*, 1955, 3754 (*uv*)
Natalis, P. *et al., J. Phys. Chem.*, 1965, **69**, 2943 (*ms*)
Org. Synth., 1971, **51**, 11; 20; 31; 1974, **54**, 42; 1977, **56**, 36 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 693 (*rev, tox*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 26; 1979, **7**, 6 (*use*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 64 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1340
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 244; 245 (*use, occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2561; 2583
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 106
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAY500

Benzene B-17

[71-43-2]
Cyclohexatriene. [6]Annulene



C_6H_6 78.113

Used in processing of modified hop extract. Liq. V. spar. sol. H_2O; misc. most org. solvs. d_4^{20} 0.88. Mp 5.53°. Bp 80.8° (80.103°, 80.12°, 80.36°, 80.49°). n_D^{20} 1.5014. The name Benzene should not be confused with Benzol(e) (coml. products consisting mainly of benzene) or with Benzin(e) (obsolescent name for low-boiling petroleum spirit). The German name for Benzene is however Benzol. First isol. by Faraday in 1825.

► Highly flammable, fl. p. -11°. Human carcinogen. Direct skin contact with liq. causes erythema and vesiculation; prolonged contact can cause dermatitis. Acute exposure by ingestion or inhalation produces the symptoms of CNS depression, and depression of haematopoietic system. Prolonged or repeated exposure injures the bone marrow (often irreversibly) and depletes erythrocytes, leukocytes or platelets producing headache, fatigue, anorexia. More severe exposure is associated with development of pancytopenia and aplastic anaemia. Various forms of leukaemia are implicated in occup. exposures. MEL: long-term 5 ppm. CY1400000

Picrate:
Mp 82-84°. Readily dissociates on exp. to air.

[1076-43-3, 1120-89-4, 34504-50-2]

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Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 247-248
Snyder, C.A. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 3 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2149
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Benzenecarbothioic acid, 9CI B-18

[98-91-9]
Thiobenzoic acid, 8CI. Monothiobenzoic acid

PhCOSH⇔PhC(S)OH

C_7H_6OS 138.19

Yellow oil cryst. on chilling in ice. Mp 15-18° Mp 24°. pK_a 2.66 (H_2O).

► LD_{50} (rat, ipr) 350 mg/kg. DH6839000

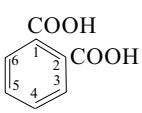
SH-form

Me ester: [5925-68-8] S-*Methyl benzenecarbothioate.* S-*Methyl thiobenzoate.* S-*Methyl benzothioate*
C_8H_8OS 152.217
Flavouring agent for foods. Yellow liq. Bp 210-212°.

Garcia, J. *et al., Synthesis*, 1989, 305 (*S-alkyl esters*)
Katritzky, A.R. *et al., Org. Prep. Proced. Int.*, 1995, **27**, 361 (*synth, Me ester, benzyl ester, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1073 (*S-Me ester*)

1,2-Benzenedicarboxylic acid, 9CI B-19

[88-99-3]
Phthalic acid, 8CI. Alizarinic acid. Naphthalinic acid†. Phthalinic acid



$C_8H_6O_4$ 166.133

Plates (H_2O). Sol. hot H_2O, alkalis; mod. sol. H_2O, EtOH; spar. sol. Et_2O. Mp 210° dec Mp 234°. pK_{a1} 2.95; pK_{a2} 5.41 (25°,H_2O). Forms anhydride at Mp. Frequent reports of the isol. of phthalate esters as nat. prods. are in prob. all cases

erroneous because of their ubiquitous presence in solvs., laboratory plastics, etc. as plasticisers.

► Fl. p. 168°. Violent reaction on heating with $NaNO_2$. Skin and mucous membrane irritant. Low acute mammalian toxicity. TH9625000

Mono-K salt: [877-24-7]
Mp 295-300° dec.

Mono-Me ester: [4376-18-5] *Monomethyl phthalate*
$C_9H_8O_4$ 180.16
Needles (C_6H_6). Mp 85°.

Di-Me ester: [131-11-3] *Dimethyl phthalate, BSI, ISO. DMP*
$C_{10}H_{10}O_4$ 194.187
Liq. Insol. H_2O; misc. EtOH, Et_2O. d_{25}^{25} 1.19. Mp 0°. Bp 282.4° Bp_2 116-116.5°. n_D^{25} 1.5138. Vp < 0.1 mmHg (20°).

► Fl. p. 146°, autoignition temp. 490/555°. Eye irritant. Lacks biological effects associated with long-chain analogues. OES: long-term 5 mg m^{-3}; short-term 10 mg m^{-3}. TI1575000

Mono-Et ester: [2306-33-4] *Monoethyl phthalate*
$C_{10}H_{10}O_4$ 194.187
Cryst. (CS_2). Mp 47-48°.

► TI2495000

Di-Et ester: [84-66-2] *Diethyl phthalate. DEP*
$C_{12}H_{14}O_4$ 222.24
Insol. H_2O; misc. most org. solvs. Mp -0.3°. Bp 298° Bp_{10} 157°. n_D^{25} 1.5002.

► Irritant, fl. p. 117°, autoignition temp. 457°. OES long-term 5 mg m^{-3}; short-term 10 mg m^{-3}. TI1050000

Monopropyl ester: [4376-19-6] *Monopropyl phthalate*
$C_{11}H_{12}O_4$ 208.213
Cryst. ($CHCl_3$/Et_2O). Mp 54-55°.

Dipropyl ester: [131-16-8] *Dipropyl phthalate*
$C_{14}H_{18}O_4$ 250.294
d^{25} 1.07. Bp 317.5° (304-305°). n_D^{20} 1.4170.

► TI1940000

Diisopropyl ester: [605-45-8] *Diisopropyl phthalate*
$C_{14}H_{18}O_4$ 250.294
Liq. $d^{15.6}$ 1.06. Bp_{10} 152-155°. n_D^{20} 1.4900.

Bis(2-methylpropyl) ester: [84-69-5] *Diisobutyl phthalate. DIBP*
$C_{16}H_{22}O_4$ 278.347
Liq. d_{20}^{20} 1.04. Bp 327°. n_D^{20} 1.4900.

Di(2-propenyl) ester: [131-17-9] *Diallyl phthalate*
$C_{14}H_{14}O_4$ 246.262
Insol. H_2O. Mp -70°. Bp_5 165-167°. n_D^{20} 1.5190. Polym. if not inhibited.

► Lachrymator. OES: long-term 5 mg m^{-3}. CZ4200000

Monobutyl ester: [131-70-4] *Monobutyl phthalate*
$C_{12}H_{14}O_4$ 222.24
Leaflets (EtOH). Mp 73-74°.

► TI2475000

Dibutyl ester: [84-74-2] *Dibutyl phthalate*
$C_{16}H_{22}O_4$ 278.347
Insol. H_2O; misc. common org. solvs. d_{20}^{20} 1.05. Mp -35°. Bp 340°. n_D^{25} 1.4915.

► Toxic, fl. p. 157°, autoignition temp. 400°. OES: long-term 5 mg m^{-3}; short-term 10 mg m^{-3}. TI0875000

Butyl 2-ethylbutyl ester: [26227-08-7] *Butyl 2-ethylbutyl phthalate*
$C_{18}H_{26}O_4$ 306.401Claimed isolations of phthalate esters are suspect.

Dipentyl ester: [131-18-0] *Dipentyl phthalate. Diamyl phthalate*
$C_{18}H_{26}O_4$ 306.401
Oily liq. d^{20} 1.02. Mp -55°. Bp 342° Bp_{11} 204-206°. n_D^{20} 1.4880.

Dihexyl ester: [84-75-3] *Dihexyl phthalate*
$C_{20}H_{30}O_4$ 334.455
Mp -40°. Bp 333°.

Mono(2-ethylhexyl) ester: [4376-20-9] *Mono(2-ethylhexyl) phthalate*
$C_{16}H_{22}O_4$ 278.347

► Potent eye irritant. Exp. hepatic and testicular effects. TI2500000

Bis(2-ethylhexyl) ester: [117-81-7] *Bis(2-ethylhexyl) phthalate. Diethylhexyl phthalate. Octoil. Palatinol. Eviplast 80. Eviplast 81. Kodaflex DOP. Vestinol AH. Vinizer 80. DEHP. DOP*
$C_{24}H_{38}O_4$ 390.562
Liq. Insol. H_2O. d^{20} 0.99. Mp -46°. Bp_5 231°. λ_{max} 250 (ϵ); 283 (sh) (ϵ) (hexane) (Derep). λ_{max} 275 (ϵ 1330) (isopropanol) (Derep).

► Mod. skin irritant. Low acute mammalian toxicity. Exp. hepatocarcinogen. Exp. reprod. and teratogenic effects. A non-genotoxic (exp.) carcinogen with weak peroxisome proliferating props.. TI0350000

Bis(2,5-dimethylhexyl) ester: [104719-70-2] *Bis(2,5-dimethylhexyl) phthalate. Phyllester*
$C_{24}H_{38}O_4$ 390.562
Mp 40°.

Bis(3,5,5-trimethylhexyl) ester: [14103-61-8]
$C_{26}H_{42}O_4$ 418.615
Bp_2 202°. n_D^{25} 1.4802.

Dicyclohexyl ester: [84-61-7] *Dicyclohexyl phthalate*
$C_{20}H_{26}O_4$ 330.423
Cryst. Insol. H_2O; sol. most org. solvs. d_{20}^{20} 1.2. Mp 64-66°. Bp_{10} 245-246°.

► TI0889000

Diheptyl ester: [3648-21-3] *Diheptyl phthalate*
$C_{22}H_{34}O_4$ 362.508
d_4^{20} 0.99. Bp_{26} 264°. n_D^{20} 1.4867.

Heptyl hydroxynonyl ester: [160525-14-4] *Heptyl hydroxynonyl phthalate. Phthalomycin*
$C_{24}H_{24}O_5$ 392.451
Sol. H_2O, MeOH; poorly sol. $CHCl_3$, hexane. Mp 320°. Struct. not fully assigned.

Dioctyl ester: [117-84-0] *Dioctyl phthalate*
$C_{24}H_{38}O_4$ 390.562
Liq. d_{20}^{20} 0.98. Mp -25°. Bp_1 185° $Bp_{0.1}$ 165°. n_D^{25} 1.4848. Almost certainly a contaminant.

Diisooctyl ester: [27554-26-3] *Diisooctyl phthalate. DIOP*
$C_{24}H_{38}O_4$ 390.562
Liq. Insol. H_2O. d_{20}^{20} 0.99. Mp -50°. Bp 37°. Mixt. of isomers obtained from phthalic anhydride and the mixed octyl esters made by the oxo process. See also the bis(2-ethylhexyl) component above.

Dinonyl ester: [84-76-4] *Dinonyl phthalate. DNP*
$C_{26}H_{42}O_4$ 418.615
Oil. Insol. H_2O. d^{25} 0.98. Bp_1 205-220°. n_D^{20} 1.4871.

► Fl. p. 141°. TI1800000

Bis(2-ethylnonyl) ester:Bis(2-ethylnonyl) phthalate
$C_{30}H_{50}O_4$ 474.723

Decyl octyl ester: [119-07-3] *Decyl octyl phthalate*
$C_{26}H_{42}O_4$ 418.615
Liq. Mp -28°. Bp_5 250°.

Didecyl ester: [84-77-5] *Didecyl phthalate. DDP*
$C_{28}H_{46}O_4$ 446.669
Liq. Insol. H_2O. d_{20}^{20} 0.97. Mp 2-4°. Bp_5 261°.

Diisodecyl ester: [26761-40-0] *Diisodecyl phthalate. DIDP*
$C_{28}H_{46}O_4$ 446.669
Involatile liq. Insol. H_2O; sol. most org. solvs. d_{20}^{20} 0.97. Mp -50°. Bp_4 250-257°. n_D^{20} 1.4830.

Diundecyl ester: [3648-20-2] *Diundecyl phthalate*
$C_{30}H_{50}O_4$ 474.723
Cryst. (EtOH). Mp 35.5°.

Didodecyl ester: [2432-90-8] *Didodecyl phthalate*
$C_{32}H_{54}O_4$ 502.776
d^{30} 0.94. Mp 21-23°. Bp_1 256-257°. n_D^{30} 1.4778.

Ditridecyl ester: [119-06-2] *Ditridecyl phthalate. DTDP*
$C_{34}H_{58}O_4$ 530.83
Liq. d^{25} 0.95. $Bp_{3.5}$ 285°. n_D^{24} 1.4840.

Benzyl butyl ester: [85-68-7] *Benzyl butyl phthalate. BBP. Santicizer 160. Unimoll BB*
$C_{19}H_{20}O_4$ 312.365
Liq. Insol. H_2O. d^{25} 1.12. Bp 370° Bp_{10} 235-255°. n_D^{25} 1.5380.

Dibenzyl ester: [523-31-9] *Dibenzyl phthalate*
$C_{22}H_{18}O_4$ 346.382
Prisms (EtOH). Mp 44.5-45.5°. Bp_{15} 277°.

Mono-Ph ester: [6139-63-5] *Monophenyl phthalate*
$C_{14}H_{10}O_4$ 242.231
Cryst. (C_6H_6/petrol). Mp 94-96°.

Di-Ph ester: [84-62-8] *Diphenyl phthalate*
$C_{20}H_{14}O_4$ 318.328
Cryst. Insol. H_2O. Mp 74-76°. Bp 405°.

► Fl. p. 224°. TI1935000

Bis(2-methoxyethyl) ester: [117-82-8] *Bis(2-methoxyethyl) phthalate. Dimethyl glycol phthalate. DMEP. DMGP. DMOP*
$C_{14}H_{18}O_6$ 282.293
Liq. Insol. H_2O. d_{20}^{20} 1.17. Mp -60° Mp -45°. Bp 340° Bp_{12} 214°. n_D^{20} 1.5025.

Bis(2-butoxyethyl) ester: [117-83-9] *Bis(2-butoxyethyl) phthalate. Dibutylglycol phthalate. DBOEP*
$C_{20}H_{30}O_6$ 366.453
Involatile liq. Insol. H_2O. d^{20} 1.17. Mp -

40°. Bp_4 210-233°. n_D^{25} 1.5020.

(Ethoxycarbonyl)methyl methyl ester: [85-71-2] *2-Ethoxy-2-oxoethyl methyl phthalate*
$C_{13}H_{14}O_6$ 266.25
Insol. H_2O. d_4^{25} 1.22. Bp_5 189°. n_D^{25} 1.5049.

(Butoxycarbonyl)methyl butyl ester: [85-70-1] *2-Butoxy-2-oxoethyl butyl phthalate. Santicizer B 16*
$C_{18}H_{24}O_6$ 336.384
Liq. Insol. H_2O. d_4^{25} 1.1. Bp_5 219°. n_D^{25} 1.4897.

Difluoride: [445-69-2]
$C_8H_4F_2O_2$ 170.115
Prisms (petrol). Mp 42-43°. Bp 224-226° Bp_{54} 135°.

Dichloride: [88-95-9]
$C_8H_4Cl_2O_2$ 203.024
Sol. Et_2O. Mp 15-16°. Bp 281° Bp_{22} 153.3°. n_D^{20} 1.5680. Hydrol. by H_2O and alcohols.

Monoamide: [88-97-1] *Phthalamic acid*
$C_8H_7NO_3$ 165.148
Prisms (MeOH). Mp 149°. pK_a 3.76 (25°).

Diamide: [88-96-0] *Phthalamide*
$C_8H_8N_2O_2$ 164.163
Mp 222° dec.
▶ CZ2200000

Bis(diethylamide): [83-81-8] *Phthalethamide*
$C_{16}H_{24}N_2O_2$ 276.378
Mp 36°. Bp_{16} 204° $Bp_{0.01}$ 118-120°.
▶ TH7400000

Monoanilide: [4727-29-1] *2-[(Phenylamino)carbonyl]benzoic acid, 9CI. Phthalanilic acid. Nevirol*
$C_{14}H_{11}NO_3$ 241.246
Needles (EtOH). Mp 170° dec. Also used as salts.
▶ DH6298150

Dianilide: [16497-41-9]
$C_{20}H_{16}N_2O_2$ 316.359
Cryst. (THF). Mp 240°.

3-Methylanilide: [85-72-3] *2-[[(3-Methylphenyl)amino]carbonyl]benzoic acid, 9CI. 3′-Methylphthanilic acid.* N-m-*Tolylphthalamic acid. 2-Carboxy-3′-methylbenzanilide*
$C_{15}H_{13}NO_3$ 255.273
Needles (C_6H_6). Mp 159-161°.
▶ LD_{50} (rat, orl) >5000 mg/kg.

Mononitrile: See 2-Cyanobenzoic acid in *The Combined Chemical Dictionary.*

Dinitrile: See 1,2-Benzenedicarbonitrile in *The Combined Chemical Dictionary.*

Anhydride: See Phthalic anhydride in *The Combined Chemical Dictionary.*

Imide: See Phthalimide in *The Combined Chemical Dictionary.*

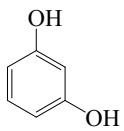
[131-15-7, 523-24-0, 3198-29-6, 4409-98-7, 10197-71-4, 15968-01-1, 28553-12-0, 79723-02-7, 102904-15-4]

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Ger. Pat., 1925, 516 135; *CA*, **25**, 1840[7] (*diisobutyl ester*)
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DeSilva, S.O. *et al., Tetrahedron*, 1992, **48**, 4863 (*synth, ir, pmr, cmr, ms, ethylamide*)
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Satyan, K.S. *et al., Planta Med.*, 1995, **61**, 293 (*Phyllester*)
Pesticide Manual, 11th edn., 1997, No. 716
Wahidulla, S. *et al., Phytochemistry*, 1998, **48**, 1203-1206 (*isol, bis-2-ethylnonyl ester*)
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1,3-Benzenediol, 9CI B-20

[108-46-3]

[12385-08-9]
Resorcinol, 8CI. 1,3-Dihydroxybenzene. Astriderm. Resorcin. Rezacuid. FEMA 3589



$C_6H_6O_2$ 110.112
Present in roasted barley, cane molasses, coffee, beer and wine. Flavouring ingredient. Platelets (EtOH). Sol. Et_2O, H_2O, EtOH, C_6H_6; sl. sol. $CHCl_3$. Mp 111°. Bp 280°. pK_{a1} 9.3; pK_{a2} 11.06 (20°). Log P 0.81 (calc).
▶ Fl. p. 127°, autoignition temp. 608°. Skin and eye irritant. Possible skin sensitiser. Can cause restlessness, methaemoglobinaemia, convulsions and other systemic effects by skin absorption and ingestion. LD_{50} (rat, orl) 301 mg/kg. OES: long-term 10 ppm; short-term 20 ppm. VG9625000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1057B; 1104C; **2**, 300A; 312D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 212B; 300A; 1289A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 988B; 1039B; 1380B; 1380C (*ir*)
Registry of Mass Spectral Data, Wiley, 128 (*ms*)
Sadtler Standard C-13 NMR Spectra, 4428 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 2572 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **13**, 996 (*rev*)
Resorcinol: Its uses and derivatives, (ed. Dressler, H.), Plenum Press, New York, 1994, (***book***)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 715
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996,
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2420-2421
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 501
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1092
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HNH500; REA000; REF050; REA100; RDZ900

1,4-Benzenediol, 9CI B-21

[123-31-9]
Hydroquinone, 8CI, USAN. *Hydroquinol. 1,4-Dihydroxybenzene. Quinol. Arctuvin. Eldopaque. Eldoquin. Pyrogentisinic acid. Pyrogentisic acid*

$C_6H_6O_2$ 110.112
Needles (H_2O). Sol. MeOH. Mp 172°. Bp_{730} 285°. pK_{a1} 9.91; pK_{a2} 11.56 (20°). Log P 0.81 (calc). Component of Artra and Solaquin λ_{max} 227 ; 295 (MeOH) (Berdy). λ_{max} 250 (ϵ 204) ($CHCl_3$) (Berdy).

▶ Fl. p. 165°, autoignition temp. 515°. Eye irritant. Prolonged or repeated exposure can cause corneal pigmentation and other damage to the eyes. Repeated skin contact produces irritation; sensitisation, dermatitis, and depigmentation. LD_{50} (rat, orl) 320 mg/kg. OES: long-term 2 mg m^{-3}; short-term 4 mg m^{-3}. Exp. carcinogen.
MX3500000

Mono-Et ether: [622-62-8] *4-Ethoxyphenol. FEMA 3695*
$C_8H_{10}O_2$ 138.166
Isol. from Chinese star anise oil (*Illicium verum*). Food flavourant. Leaflets (H_2O) with sweet herbaceous odour. Sl. sol. H_2O; sol. C_6H_6, Me_2CO, EtOAc, EtOH. Mp 66-67°. Bp 246° Bp 246-247°. pK_{a1} 10.13 (25°).

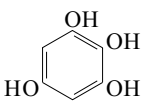
▶ SL3790000

[1122-95-8, 3225-30-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1079A; 1079B; 1079D; 1107D; 1169B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 254B; 255A; 255C; 304C; 411C; 1289B (*nmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 203; 205; 208
Tashiro, M. *et al., Synthesis*, 1979, 988-989 (*monoethers, synth, ir*)

1,2,3,5-Benzenetetrol, 9CI, 8CI B-22

[634-94-6]
1,2,3,5-Tetrahydroxybenzene



$C_6H_6O_4$ 142.111
Needles (H_2O). Mp 168-170° (165°).

1,3-Di-Me ether, 2-O-β-D-glucopyranoside: [121748-12-7] *4-Hydroxy-2,6-dimethoxyphenyl glucoside.* ***Leonuriside A***
$C_{14}H_{20}O_9$ 332.307
Constit. of *Coix lachryma-jobi* (Job's tears) and *Prunus* sp.. Needles (Me_2CO aq.). Mp 232-234°. $[\alpha]_D^{25}$ -44.4 (c, 0.2 in Me_2CO/MeOH).

1,2,3-Tri-Me ether, 5-O-β-D-glucopyranoside: [41514-64-1]
$C_{15}H_{22}O_9$ 346.333
Constit. of *Quillaja saponaria* (soapbark tree). Needles (Et_2O/MeOH). Mp 201-203°. $[\alpha]_D^{20}$ -22.3 (c, 0.38 in MeOH).

1,2,3-Tri-Me ether, 5-O-[2,6-bis(3,4,5-trihydroxybenzoyl)-β-D-glucopyranoside]: [125288-23-5] *3,4,5-Trimethoxyphenyl 2,6-digalloylglucoside*
$C_{29}H_{30}O_{17}$ 650.546
Isol. from *Psidium guajava* (guava). Needles + $3H_2O$ (H_2O). Mp 269-271°. $[\alpha]_D^{26}$ -33.5 (c, 0.5 in Me_2CO).

1,2,3-Tri-Me ether, 5-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [87562-76-3] ***Kelampayoside A***
$C_{20}H_{30}O_{13}$ 478.449
Isol. from *Cinnamomum cassia* (Chinese cinnamon). Amorph. powder; needles (as hexa-Ac). Mp 132-134° (hexa-Ac). $[\alpha]_D^{25}$ -99.8 (c, 0.5 in MeOH) (-81.7). λ_{max} 205 (ϵ 42660); 225 (ϵ 12300); 275 (ϵ 3800) (MeOH).

1,2,3-Tri-Me ether, 5-Ac: [17742-46-0]
$C_{11}H_{14}O_5$ 226.229
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. (MeOH aq.). Mp 74°.

1,3,5-Tri-Me ether, Ac: [30225-90-2]
$C_{11}H_{14}O_5$ 226.229
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. (EtOH aq.). Mp 100°.

[67173-66-4, 68944-24-1, 87562-77-4, 108543-42-6]

Hattori, S. *et al., Acta Phytochim.*, 1931, **5**, 219; *CA*, **26**, 1282 (*deriv*)
Hue, R. *et al., Bull. Soc. Chim. Fr.*, 1970, 3617 (*synth, derivs*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2061 (*Trimethoxyphenyl galloylglucoside*)
Sargent, M.V. *et al., J.C.S. Perkin 1*, 1982, 403 (*synth, 1,3,5-tri-Me*)
Miyamura, M. *et al., Phytochemistry*, 1983, **22**, 215 (*Trimethoxyphenyl apiofuranosylglucoside*)
Shimomura, H. *et al., Phytochemistry*, 1988, **27**, 644 (*isol, pmr, cmr*)
Otsuka, H. *et al., Phytochemistry*, 1989, **28**, 883; 1990, **29**, 3823 (*Leonuriside A*)
Fuchino, H. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1937 (*tri-Me apiosylglucoside*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1162-1167 (*Kelampayosides*)
Santos, G.G. *et al., Phytochemistry*, 1997, **44**, 1309 (*isol, derivs*)
Sugaya, K. *et al., CA*, 1999, **130**, 279238e (*Leonuriside A*)
Duynstee, H.I. *et al., Tetrahedron*, 1999, **55**, 9881-9898 (*Kelampayosides, synth*)

Benzenethiol, 9CI B-23

[108-98-5]
Thiophenol. Phenyl mercaptan. Mercaptobenzene. FEMA 3616
PhSH
C_6H_6S 110.179
Flavouring agent. Liq. with penetrating odour. d_4^{20} 1.08 d_4^{25} 1.97. Fp -14.8. Bp 169.5° Bp_{30} 77°. n_D^{20} 1.5893.

▶ Violent explosion has resulted during prep. from benzenediazonium chloride. Flammable, fl. p. < 21°. Severe eye irritant . Can cause dermatitis. Inhalation may cause headache and dizziness. LD_{50} (rat, orl) 46 mg/kg. LD_{50} (rat, skn) 300 mg/kg. LC_{50} (rat, ihl) 33 ppm (4h exposure). OES: long-term 0.5 ppm.
DC0525000

S-*Me:* Methyl phenyl sulfide, M-291

S-*Et:* See Ethyl phenyl sulfide in *The Combined Chemical Dictionary.*

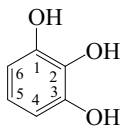
S-tert-*Butyl:* See *tert*-Butyl phenyl sulfide in *The Combined Chemical Dictionary.*

[930-69-8, 3111-52-2, 13133-62-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1173A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 415A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1089A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 504 (*synth, bibl*)
Adv. Chem. Ser., 1955, **15**, 325 (***props***)
Lawesson, S.-O. *et al., Acta Chem. Scand.*, 1966, **20**, 2325 (*ms*)
Wagner, A.W. *et al., Chem. Ber.*, 1966, **99**, 375 (*synth*)
Jenden, D.L. *et al., Anal. Chem.*, 1968, **40**, 125; 1972, **44**, 1879 (*use*)
Jones, I.W. *et al., J.C.S. Perkin 2*, 1973, 1125 (*uv*)
Overman, L.E. *et al., Synthesis*, 1974, 59 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 585; 1984, **11**, 57; 1982, **10**, 281; 1988, **13**, 297; 1981, **9**, 312; 1988, **13**, 312; 1992, **16**, 327; 1979, **7**, 367; 1982, **10**, 399; 1980, **8**, 420; 1981, **9**, 447; 465; 1986, **12**, 485; 505; 545 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 53
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 248-249
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2200
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 110
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PFL850

1,2,3-Benzenetriol, 9CI B-24

[87-66-1]
Pyrogallol, 8CI. 1,2,3-Trihydroxybenzene. Pyrogallic acid



$C_6H_6O_3$ 126.112
Plates or needles. V. sol. H_2O, EtOH, Et_2O; sl. sol. $CHCl_3$, C_6H_6. Mp 133-134°. Bp 309° Bp_{12} 171.5°. pK_{a1} 9.28; pK_{a2} 11.34 (20°, μ = 0.1). Bitter taste. Readily absorbs O_2 λ_{max} 244 ; 267 ; 275 (MeOH) (Berdy).

▶ Stains skin and hair black. Skin and eye irritant. Skin absorption can cause methaemoglobinaemia, haemolysis and kidney damage. LD_{50} (mus, orl) 300 mg/kg. Exp. reprod. and teratogenic effects.
UX2800000

1,3-Di-Me ether: [91-10-1] *2,6-Dimethoxyphenol. Syringol. FEMA 3137*
$C_8H_{10}O_3$ 154.165
Isol. from maople syrup. Flavouring ingredient. Spar. sol. H_2O; sol. EtOH, Et_2O. Mp 55-56°. Bp 262-267°.

▶ SL0900000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1046D; 1081C; 1083D; 1101C; 1103D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 193A; 258A; 261C; 295C; 299A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 975C; 1014A; 1017A; 1037D; 1038D (*ir*)
Shipchandler, M.T. *et al., J.C.S. Perkin 1*, 1975, 1400 (*synth*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **18**, 670 (*rev*)
Ollis, W.D. *et al., Phytochemistry*, 1978, **17**, 1383; 1401 (*isol, 3-Methoxy-1,2-benzenediol, 2,3-Dimethoxyphenol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 171 (*2,3-di-Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 842-843 (*2,3-di-Me ether*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1088
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOJ200; PPQ500

1,3,5-Benzenetriol, 9CI B-25

[108-73-6]
1,3,5-Trihydroxybenzene. ***Phloroglucinol****. Phloroglucin. Dilospan S. Spasfon-Lyoc*

$C_6H_6O_3$ 126.112
Leaflets or plates + $2H_2O$ (H_2O). Mod. sol. H_2O; sol. EtOH, Et_2O, Py, Me_2CO. Mp 117° (dihydrate) Mp 217-219° (anhyd.) (rapid heat) Mp 200-209° (slow heat). pK_{a1} 7.97; pK_{a2} 9.23 (20°). Log P 0.14 (calc). Forms polymers with aldehydes and with diamines; no coml. importance.

▶ Skin and eye irritant. LD_{50} (rat, orl) 5200 mg/kg. Exp. reprod. effects. SY1050000

O-*β-D-Glucopyranoside:* [28217-60-9]
Phlorin
$C_{12}H_{16}O_8$ 288.254
Isol. from thyme (*Thymus vulgaris*) and from citrus fruit. Proposed marker for adulteration of orange juice with peel. Cryst. Mp 231-233°. $[\alpha]_D^{22}$ -74.58.

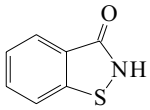
O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:* [94356-21-5] *3,5-Dihydroxyphenyl 1*-O-*(6*-O*-galloyl-β-D-glucopyranoside)*
$C_{19}H_{20}O_{12}$ 440.36
Isol. from commercial rhubarb (*Rheum* spp.). Needles + $1H_2O$ (H_2O). Mp 168-169°. $[\alpha]_D^{25}$ -41.2 (c, 0.59 in MeOH).

[6099-90-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1050B; 1085C; 1106D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 202B; 264A; 303B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 982A; 1018D; 1040D (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 455 (*synth*)
Arison, B.H. *et al., J.A.C.S.*, 1963, **85**, 627 (*pmr, derivs*)
McKillop, A. *et al., Synth. Commun.*, 1974, **4**, 35 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **18**, 684 (*rev, props, tox*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461 (*6-galloylglucoside*)
Highet, R.J. *et al., J.O.C.*, 1988, **53**, 2843 (*tautom, props*)
Laurence, M.-M. *et al., J. Agric. Food Chem.*, 1998, **46**, 4193-4197 (*Phlorin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PGR000; TKY250

1,2-Benzisothiazol-3(2*H*)-one, 9CI B-26

[2634-33-5]
1,2-Benzisothiazolinone. 2-Thiobenzimide. Proxel



C_7H_5NOS 151.189
Industrial biocide. Present in can-end cements. Needles (EtOH aq.). Mp 157-158°.

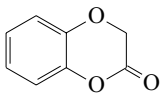
▶ DE4620000

S-*Oxide:* [14599-38-3]
$C_7H_5NO_2S$ 167.188
Cryst. (Me_2CO). Mp 157-158°.

S,S-*Dioxide:* Saccharin, S-2

McKibben, M. *et al., J.C.S.*, 1923, 170 (*synth*)
Reissert, A. *et al., Ber.*, 1928, **61**, 1680 (*props*)
Cavalca, L. *et al., Gazz. Chim. Ital.*, 1970, **100**, 629 (*cryst struct*)
Feichtinger, H. *et al., Chem. Ber.*, 1971, **104**, 1697 (*synth*)
Davis, M. *et al., Adv. Heterocycl. Chem.*, 1972, **14**, 43 (*rev*)
Japan. Pat., 1978, 78 37 862; *CA*, **90**, 121580 (*synth*)
Szabó, J. *et al., Tetrahedron*, 1988, **44**, 2985 (*oxide, synth, cmr, pmr, ir*)

1,4-Benzodioxin-2(3*H*)-one B-27

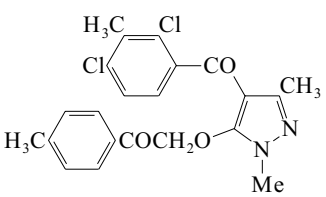


$C_8H_6O_3$ 150.134
Patented as food aroma and flavour enhancer. Yellow-white solid. Mp 55°. A synthesis giving a Mp of 135° was erroneous.

Sampson, P. *et al., J. Het. Chem.*, 1994, **31**, 1011 (*synth, pmr, cmr, bibl*)

Benzofenap, BSI B-28

[82692-44-2]
*4-(2,4-Dichloro-3-methylbenzoyl)-1,3-dimethyl-5-[(4-methylbenzoyl)methoxy]-1*H*-pyrazole. 2-[4-(2,4-Dichloro-*m*-toluoyl)-1,3-dimethylpyrazol-5-yloxy]-4′-methylacetophenone. Yukawide. MY 71*

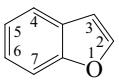


$C_{22}H_{20}Cl_2N_2O_3$ 431.317
Herbicide used on rice. Solid. Mp 133.1-133.5°.

Japan. Pat., 1986, 61 103 872, (*Mitsubishi*); *CA*, **105**, 226552 (*synth*)
Ikeda, K. *et al., Jpn. Pestic. Inf.*, 1991, **59**, 16 (*props*)
Pesticide Manual, 11th edn., 1997, No. 66 (*use*)

Benzofuran, 9CI B-29

[271-89-6]
Coumarone. Benzo[b]furan. Benzofurfuran. 1-Oxaindene. 1-Oxindene



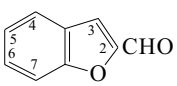
C_8H_6O 118.135
Maillard prod. present in roasted coffee aroma. Constit. of *Coix lachryma-jobi* (Job's tears) and *Gentiana lutea* (yellow gentian). Oil. d_{15}^{15} 1.08. Bp_{735} 166.5-168° Bp_{80} 97.5-99°. Steam-volatile. Stable to alkalis, polymerised by H_2SO_4.

▶ LD_{50} (mus, ipr) 500 mg/kg. DF6423800

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 683B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 168C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1505A (*ir*)
Badger, G.M. *et al., J.C.S.*, 1956, 3438 (*uv*)
Black, P.J. *et al., Aust. J. Chem.*, 1965, **18**, 353 (*pmr*)
Org. Synth., 1966, **46**, 28 (*synth, uv*)
Appleton, R.A. *et al., Phytochemistry*, 1971, **10**, 447-449 (*isol*)
Platzer, N. *et al., Bull. Soc. Chim. Fr.*, 1974, 905 (*cmr*)
Cagniant, P. *et al., Adv. Heterocycl. Chem.*, 1975, **18**, 337 (*rev*)
Kuster, T. *et al., Helv. Chim. Acta*, 1978, **61**, 1017 (*ms*)
Audit, M. *et al., Org. Magn. Reson.*, 1983, **21**, 698 (*pmr*)
Fraser, R.R. *et al., Can. J. Chem.*, 1985, **63**, 3505 (*cmr*)
Kreher, R.P. *et al., Chem. Ber.*, 1991, **124**, 645 (*bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCK250

2-Benzofurancarboxaldehyde, 9CI B-30

[4265-16-1]
2-Formylbenzofuran. FEMA 3128



$C_9H_6O_2$ 146.145
Flavouring ingredient. Bp_1 135-145°.

Robba, M. *et al., Bull. Soc. Chim. Fr.*, 1977, 142 (*synth, pmr*)
Shiotani, S. *et al., J. Het. Chem.*, 1991, **28**, 1469 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 280
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 249

Benzoic acid, 9CI, USAN B-31

[65-85-0]
Benzenecarboxylic acid. E210. FEMA 2131

PhCOOH

$C_7H_6O_2$ 122.123

For salts see Benzoic acid salts, B-32. Widespread in plants esp. in essential

oils and fruits, mostly in esterified form. Also present in butter, cooked meats, pork fat, white wine, black and green tea, mushroom and Bourbon vanilla. Used in foodstuffs as antimicrobial and flavouring agent and as preservative. In practical food preservation, the Na salt of benzoic acid is the most widely used form (see, Na salt). The antimicrobial activity comprises a wide range of microorganisms, particularly yeasts and moulds. Undissociated benzoic acid is more effective than dissociated, thus the preservative action is more efficient in acidic foodstuffs. Typical usage levels are 500-2000 ppm. Leaflets or needles (H_2O). Sol. MeOH, C_6H_6; fairly sol. hexane; v. spar. sol. H_2O. Mp 122°. Bp 249° Bp_{10} 133°. Log P 1.88 (calc). Steam-volatile λ_{max} 228 (E1%/1cm 728); 273 (E1%/1cm 93.2); 300 (E1%/1cm 46.8) (MeOH) (Berdy).

▶ Fl. p. 121°, autoignition temp. 570°. Eye, skin and mucous membrane irritant. Hypersensitivity reactions reported. Low systemic toxicity. Detoxification in humans occurs by conjugation with amino acids (mainly glycine resulting in hippuric acid). DG0875000

Me ester: [93-58-3] *Methyl benzoate. FEMA 2683*
$C_8H_8O_2$ 136.15
Present in various flower oils, banana, cherry, pimento berry, ceriman (*Monstera deliciosa*), clove bud and stem, mustard, coffee, black tea, dill, starfruit and cherimoya (*Annona cherimola*). Used in flavourings. Liq. with fruity odour. d_{25}^{25} 1.09. Fp -12.3. Bp 199.6° Bp_{24} 96-98°.

▶ Fl. p. 83°. Skin and eye irritant. LD_{50} (rat, orl) 1350 mg/kg. DH3850000

Et ester: [93-89-0] *Ethyl benzoate. FEMA 2422*
$C_9H_{10}O_2$ 150.177
Found in various fruits, e.g. apple, banana, sweet cherry. Also present in milk, butter, wines, black tea, bourbon vanilla and fruit brandies. Flavouring agent. Liq. with aromatic/fruity odour. d_4^{25} 1.04. Fp -34. Bp 212.9° Bp_{10} 87.2°. n_D^{20} 1.5045.

▶ Fl. p. 88°, autoignition temp. 490°. Skin and eye irritant. LD_{50} (rat, orl) 2100 mg/kg. DH0200000

Propyl ester: [2315-68-6] *Propyl benzoate. FEMA 2931*
$C_{10}H_{12}O_2$ 164.204
Present in cherry and clove stem, also in butter. Flavouring ingredient. Liq. with balsamic, nutty odour and sweet fruity-nutty flavour. d_{15}^{15} 1.03. Fp -51–52. Bp 230°. n_D^{20} 1.5100.

Isopropyl ester: [939-48-0] *Isopropyl benzoate. FEMA 2932*
$C_{10}H_{12}O_2$ 164.204
Present in feijoa fruit (*Feijoa sellowiana*), apple, pear, cocoa and honey. Flavouring ingredient. d_{15}^{15} 1.02. Bp 218-219°.

▶ Fl. p. 89/99°. Skin and eye irritant. LD_{50} (rat, orl) 3730 mg/kg. DH3150000

2-Propenyl ester: 2-Propen-1-ol, P-488

Benzyl ester: [120-51-4] ***Benzyl benzoate, USAN.*** *Ascabin. Benylate. Vanzoate. FEMA 2138. Many other names*
$C_{14}H_{12}O_2$ 212.248
Contained in Peru balsam and Tolu balsam. Isol. from other plants e.g. *Jasminum* spp., ylang-ylang oil. Used in food flavouring. Leaflets with balsamic/almond flavour and sharp, pungent flavour. d^{18} 1.11. Mp 21° (19.5°). Bp 323-324° (316-317°) $Bp_{0.1}$ 80-82°. Log P 3.88 (uncertain value) (calc). Spar. steam-volatile.

▶ Fl. p. 148°, autoignition temp. 480°. Eye, mucous membrane, and possible skin irritant. Hypersensitivity reactions reported. LD_{50} (rat, orl) 500 mg/kg. DG4200000

[766-76-7, 1079-02-3, 8000-95-1, 43019-90-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 186A; 271B; 291B; 291C; 292D; 340A; 340B; 340C; 380D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1063B; 1199A; 1240A; 1240B; 1241A; 1241B; 1244A; 1337C; 1411A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 181D; 1322C; 1357D; 1358A; 1358B; 1358C; 1360A; 1389D; 1390A; 1390B (*ir*)
Jesson, J.P. *et al., Proc. R. Soc. London, A*, 1962, **268**, 68-78 (*Raman*)
Beynon, J.H. *et al., Z. Naturforsch., A*, 1965, **20**, 883-887 (*ms*)
Evans, H.B. *et al., J. Phys. Chem.*, 1968, **72**, 2552-2562 (*pmr*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037-1064 (*Me ester, Et ester, ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 715-722 (*rev, tox*)
Ullmann's Encycl. Ind. Chem., 5th Ed, VCH, Weinheim, 1985, **A3**, 555 (*rev*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493-1518 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BCL750; BCM000; EGR000; MHA500
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 103 (*rev*)
Tremblay, G.C. *et al., Pharmacol. Ther.*, 1993, **60**, 63-90 (*rev, pharmacol, tox*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 32-34; 38-39; 433-435
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1118; 1431
Merck Index, 12th edn., 1996, No. 1122; No. 1123; No. 1162; No. 3814; No. 6104 (*derivs*)
Lúck, E. *et al., Antimicrobial Food Additives: Characteristics, Uses, Effects*, 2nd edn., Springer-Verlag, 1997, 174 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 249; 263; 951; 1485; 1718; 2281; 2340; 2527 (*occur, props, esters*)
Indrayanto, G. *et al., Anal. Profiles Drug Subst.*, 1999, **26**, 1-46 (*rev*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2511
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 107
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 117
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Benzoic acid salts B-32

Benzoates
Salts of Benzoic acid, B-31.

Na salt: [532-32-1] *Sodium benzoate. E211. FEMA 3025*
$C_7H_5NaO_2$ 144.105
Antimicrobial preservative in foods, e.g. margarine and artificially sweetened fruit preserves. Flavouring agent and adjuvant. Powder or flakes.

▶ DH6650000

K salt: [582-25-2] *Potassium benzoate. E212*
$C_7H_5KO_2$ 160.214
Preservative for margarines and wines. Cryst. $+3H_2O$.

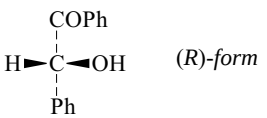
NH_4 salt: [1863-63-4] *Ammonium benzoate. Vulnoc AB*
$C_7H_9NO_2$ 139.154
Preservative. d 1.26. Mp 198°. Undergoes conversion to ammonium hydrogen benzoate on crystallisation from hot H_2O or on prolonged storage in the solid state.

Ca(II) salt: [2090-05-3] *Calcium benzoate. E213*
$C_{14}H_{10}CaO_4$ 282.309
Preservative, used in margarine.

U.S. Pat., 1929, 1 704 636; *CA*, **23**, 1909^6 (*NH_4 salt, synth*)
Kirk-Othmer Encycl. Chem. Technol., 2nd edn., Wiley, 1963, **3**, 433 (*NH_4 salt, use, props*)
Adams, S.K. *et al., Inorg. Chim. Acta*, 1975, **12**, 163-166 (*ms, ir*)
Oxton, I.A. *et al., Can. J. Chem.*, 1977, **55**, 3831-3837 (*NH_4 salt, pmr, stability*)
Czech. Pat., 1982, 225 768; *CA*, **104**, 68601t (*Ca salt, synth*)
Lewandowski, W. *et al., Can. J. Spectrosc.*, 1987, **32**, 41-45 (*synth, ir*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, 107 (*Ca salt, use, props*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 727 (*Na salt*)
Merck Index, 12th edn., 1996, No. 521 (*NH_4 salt, props, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 370-371; 2281-2282; 2527-2529 (*salts*)

Benzoin, 8CI B-33

[119-53-9]
2-Hydroxy-1,2-diphenylethanone, 9CI. α-Hydroxybenzyl phenyl ketone. Benzoylphenylcarbinol. 2-Hydroxy-2-phenylacetophenone. FEMA 2132



(*R*)-*form*

$C_{14}H_{12}O_2$ 212.248
For enol form see 1,2-Diphenyl-1,2-ethenediol in The Combined Chemical Dictionary.

► LD_{50} (rat, orl) 10,000 mg/kg. DI1590000

(R)-form [5928-66-5]
Needles. Mp 131-132.5°. $[\alpha]_D^{12}$ -117.5 (Me_2CO).

(S)-form [5928-67-6]
Needles. Mp 131-132.5°. $[\alpha]_D^{25}$ +118.4 (Me_2CO).

(±)-form [579-44-2]
Flavouring ingredient. Prisms (EtOH) with vanilla taste. Insol. H_2O; sol. Me_2CO, hot EtOH. Mp 133-134°. Bp_{768} 344° Bp_{12} 194°.

[441-38-3, 574-06-1, 1459-20-7, 8050-35-9, 57794-28-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 37B; 37C; 38B; 38C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 852C; 853A; 853C; 854A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1257C (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 94 (*synth*)
Watson, M.B. *et al., Chem. Ind. (London)*, 1954, 658 (*abs config*)
Kenyon, J. *et al., J.C.S.*, 1965, 435 (*resoln*)
Kreiser, W. *et al., Annalen*, 1971, **745**, 164 (*synth*)
Couvert, O. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1972, **274**, 296 (*pmr*)
Ohgo, Y. *et al., Chem. Lett.*, 1974, 1327 (*synth*)
Kudo, T. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2969
Hakimelahi, G.H. *et al., Helv. Chim. Acta*, 1977, **60**, 342 (*synth*)
Haisa, M. *et al., Acta Cryst. B*, 1980, **36**, 2832 (*cryst struct*)
Merck Index, 11th edn., 1989, 1103
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 54
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Benzophenone, 8CI B-34

[119-61-9]
Diphenylmethanone, 9CI. Diphenyl ketone. Phenyl ketone. FEMA 2134

PhCOPh

$C_{13}H_{10}O$ 182.221
Present in grapes. Flavouring agent. Rhombic prisms (stable form), monoclinic prisms (labile form). Insol. H_2O. d_4^{18} 1.11. Mp 48.5-49° (stable form) Mp 26° (labile form). Bp_{100} 224° Bp_{10} 157.6°.

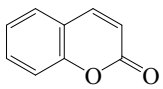
► LD_{50} (mus, orl) 2895 mg/kg. DI9950000

[16592-08-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1264D; **2**, 58A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 884C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1265B (*ir*)
Adv. Chem. Ser., 1955, **15**, 354 (***props***)
Natlis, P. *et al., J. Phys. Chem.*, 1965, **69**, 2943 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 873 (*rev, tox*)
Grimaud, M. *et al., Bull. Soc. Chim. Fr.*, 1974, 1935 (*uv*)
Loletta, M. *et al., Inorg. Chim. Acta*, 1977, **24**, 195 (*pmr, cmr*)
Abraham, R.J. *et al., J.C.S. Perkin 2*, 1988, 1429 (*conformn*)
Zadel, G. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1035 (*synth*)
Zhao, D. *et al., Synthesis*, 1994, 915 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 54
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 254-255
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCS250

2*H*-1-Benzopyran-2-one, 9CI B-35

[91-64-5]
Coumarin. Coumarinic anhydride. α-Benzopyrone. Cumarin



$C_9H_6O_2$ 146.145
Occurs in sweet clover. Banned by FDA for use in food. Rhombic cryst. Sol. EtOH, MeOH, Et_2O; poorly sol. H_2O. Mp 70°. Bp 291°. Log P 1.41 (calc). Hydrol. by hot conc. alkalis λ_{max} 273 (ϵ 10960); 307 (ϵ 5623) (MeOH) (Berdy).

► LD_{50} (rat, orl) 293 kg/kg. Exp. hepatotoxic with species differences between rodent/primate. Exp. teratogen. GN4200000

Hydrazone: [5841-34-9]
Yellow cryst. (MeOH). Mp 85-86°.

Semicarbazone:
Light yellow cryst. (EtOH aq.). Mp 218-220°.

Di-Et acetal: [33871-81-7] *2,2-Diethoxy-2*H*-1-benzopyran*
$C_{13}H_{16}O_3$ 220.268
Liq. Bp_{10} 134-136° $Bp_{0.5}$ 104°. Hydrol. to 2*H*-1-Benzopyran-2-one, B-35.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 322B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1311B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1386C (*ir*)
May, P. *et al., Perfum. Essent. Oil Res.*, 1925, **16**, 45; *CA*, **19**, 1471 (*synth*)
Dean, F.M. *et al., Prog. Chem. Org. Nat. Prod.*, 1952, **9**, 225 (*rev*)
Stoker, J.R. *et al., J. Biol. Chem.*, 1962, **237**, 2303 (*biosynth*)
Barnes, C.S. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
Sheinker, Yu.N. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 1352 (*pmr*)
Abernethy, J.L. *et al., J. Chem. Educ.*, 1969, **46**, 561 (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1318 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 385 (*rev, tox*)
Subbotin, O.A. *et al., Khim. Prir. Soedin.*, 1975, **11**, 458; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 476 (*cmr*)
IARC Monog., 1976, **10**, 113; *Suppl.*, **7**, 61 (*rev, tox*)
Chan, K.K. *et al., Tetrahedron*, 1977, **33**, 899 (*nmr*)
Duddeck, H. *et al., Org. Magn. Reson.*, 1982, **20**, 55 (*cmr*)
Abu-Eittah, R.H. *et al., Can. J. Chem.*, 1985, **63**, 1173 (*uv*)
Ziegler, T. *et al., Chem. Ber.*, 1987, **120**, 373 (*synth*)
Sato, K. *et al., J.C.S. Perkin 1*, 1987, 1753 (*synth*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1988, **A11**, 208 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CNV000
Nyquist, R.A. *et al., Appl. Spectrosc.*, 1990, **44**, 791 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **7**, 647 (*rev*)
Zhou, C. *et al., Yingyong Huaxue*, 1992, **9**, 79; *CA*, **117**, 131020 (***synth***)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1358
Sigma-Aldrich Library of Stains, Dyes and Indicators, 224
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNV000

4*H*-1-Benzopyran-4-one, 9CI B-36

[491-38-3]
Chromone. Benz-γ-pyrone. Benzopyrone

$C_9H_6O_2$ 146.145
Isol from Ye Hao (*Carum carvi*). Needles (H_2O or petrol). Mp 59°. Sublimes. Steam-volatile.

► LD_{50} (mus, ipr) 91 mg/kg. GB7887000

Hydrochloride:
Mp 101-102°.

Hydrobromide:
Mp 175° (sinters at 169°).

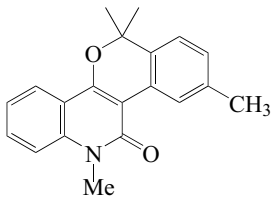
Oxime: [61348-46-7]
$C_9H_7NO_2$ 161.16
Cryst. Mp 130° (127°).

Phenylhydrazone: [34810-68-9]
Pale yellow cryst. (MeOH). Mp 112° (108-109°).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 95D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 93C (*ir*)
Schönberg, A. *et al., J.A.C.S.*, 1950, **72**, 3396-3399 (*synth*)
Badawi, M.M. *et al., Chem. Ind. (London)*, 1966, 498-499 (*ms*)
Badawi, M.M. *et al., Indian J. Chem.*, 1967, **5**, 93-96 (*nmr*)
Kostka, K. *et al., Chem. Anal. (Warsaw)*, 1969, **14**, 1145; *CA*, **72**, 128486n (*use*)
Griffiths, P.J.F. *et al., Spectrochim. Acta A*, 1972, **28**, 707-713 (*uv*)
Ellis, G.P. *et al., J.C.S. Perkin 1*, 1981, 2557-2560 (*cmr*)
Shanker, Ch.G. *et al., Synthesis*, 1983, 310-311 (*synth*)
Szabó, V. *et al., Tetrahedron*, 1986, **42**, 4215-4222 (*oxime*)
Baba, K. *et al., Shokubutsugaku Zasshi*, 1989, 216-221; *CA*, **112**, 240358 (*occur*)
Aléman, C. *et al., J.O.C.*, 1999, **64**, 1768-1769 (*struct*)

Benzosimuline B-37

[198336-58-2]



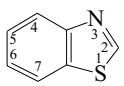
$C_{20}H_{19}NO_2$ 305.376

Alkaloid from the bark of *Zanthoxylum simulans* (Szechuan pepper). Oil. λ_{max} 210 (log ϵ 4.19); 233 (log ϵ 4.42); 250 (sh) (log ϵ 4.05); 268 (log ϵ 3.95); 310 (sh) (log ϵ 3.74); 320 (sh) (log ϵ 3.79); 331 (log ϵ 3.86); 346 (log ϵ 3.94); 365 (log ϵ 3.81) (EtOH).

Chen, I.-S. *et al., Phytochemistry*, 1997, **46**, 525-529 (*isol, uv, ir, pmr, cmr*)

Benzothiazole, 9CI B-38

[95-16-9]



C_7H_5NS 135.189

Isol. from cranberries. Sol. EtOH, CS_2, v. spar. sol. H_2O. Bp 223-225° Bp_{25} 119-120°. pK_a 1.2 (H_2O). Steam-volatile.

▶ Fl. p. 112°. LD_{50} (rat, orl) 466 mg/kg; LD_{50} (mus, orl) 900 mg/kg. DL0875000

Picrate:
Mp 176°.

N-*Oxide:* [27655-38-5]
C_7H_5NOS 151.189
Prisms + $1H_2O$ (MeOAc or Et_2O). Mp 45-48°.

Methiodide: [2786-31-4]
Needles. Mp 210°.

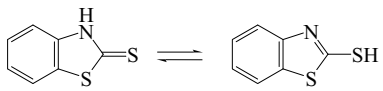
N-*Et:* See 3-Ethylbenzothiazolium(1+) in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 699C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 200A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1511A (*ir*)
Reid, W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1962, **295**, 143 (*synth*)
Ellis, B. *et al., Spectrochim. Acta*, 1965, **21**, 1881 (*uv*)
Anjou, K. *et al., Acta Chem. Scand.*, 1967, **21**, 2076-2082 (*isol*)
Takahashi, S. *et al., Chem. Pharm. Bull.*, 1970, **18**, 1176 (*oxide*)
Witanowski, M. *et al., Tetrahedron*, 1972, **28**, 637 (*nmr*)
Selva, A. *et al., Org. Mass Spectrom.*, 1974, **9**, 1161 (*ms*)
Diehl, P. *et al., Org. Magn. Reson.*, 1976, **8**, 155 (*pmr*)
Faure, R. *et al., Can. J. Chem.*, 1978, **56**, 46 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 274; **15**, 20 (*use*)
Angelelli, J.M. *et al., Spectrosc. Lett.*, 1980, **13**, 741 (*ir*)
Bakke, J.M. *et al., J. Chem. Ecol.*, 1983, **9**, 513
Bieräugel, H. *et al., Tetrahedron*, 1983, **39**, 3971 (*synth*)
Bordwell, F.G. *et al., J.A.C.S.*, 1991, **113**, 985 (*deriv, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDE500

2(3*H*)-Benzothiazolethione, 9CI B-39

[149-30-4]

2-Benzothiazolethiol. 2-Mercaptobenzothiazole. 2-Benzothiazolinethione. Accelerator M. Accel M. Pneumax MBT. Thiotax



$C_7H_5NS_2$ 167.255

NH-form predominates. Constit. of cranberries. Needles (MeOH aq.). Spar. sol. EtOH, Et_2O, AcOH; insol. H_2O; sol. alkalis. Mp 177-179°. Readily oxidised to the disulfide.

▶ LD_{50} (rat, orl) 100 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects. DL6475000

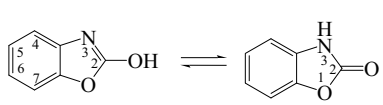
[155-04-4, 2492-26-4, 37437-20-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 701D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 204B; 204C (*nmr*)
Jacobson, P. *et al., Ber.*, 1891, **24**, 1403
Rassow, B. *et al., Chem. Zentralbl.*, 1916, **2**, 394
Welcher, J.F. *et al., Organic Analytical Reagents*, Van Nostrand, N.Y., 1948, **4**, 109 (*use*)
Morgan, K.I. *et al., J.C.S.*, 1958, 854-858 (*uv*)
Chesick, J.P. *et al., Acta Cryst. B*, 1971, **27**, 1441 (*cryst struct*)
DeJongh, D.C. *et al., Adv. Mass Spectrom.*, 1974, **6**, 99 (*ms*)
Fries, J. *et al., Organic Reagents for Trace Analysis*, E. Merck, Darmstadt, 1977, 302 (*use*)
Uher, M. *et al., Chem. Zvesti*, 1978, **32**, 486; *CA*, **90**, 167746 (*tautom*)
Faure, R. *et al., Org. Magn. Reson.*, 1978, **11**, 617 (*cmr, tautom*)
Cristiani, F. *et al., Phosphorus Sulfur Relat. Elem.*, 1984, **20**, 231 (*ir*)
Radha, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1985, **171**, 225 (*cryst struct*)
Stierle, A.A. *et al., Tet. Lett.*, 1991, **32**, 4847-4848 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDF000; SIG500; BHA750

2-Benzoxazolol B-40

[59-49-4]

2(3H)-Benzoxazolone, 9CI. 2-Benzoxazolinone, 8CI. 2-Hydroxybenzoxazole. BOA



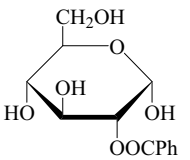
$C_7H_5NO_2$ 135.122

Tautomeric. *NH*-form predominates. Found in rye seedlings. Sol. bases, Et_2O; fairly sol. H_2O; poorly sol. hexane. Mp 141-142°. pK_{a1} 8.9 (23°). λ_{max} 270 (H_2O) (Berdy). λ_{max} 275 (EtOH) (Berdy).

▶ LD_{50} (rat, orl) 700 mg/kg. LD_{50} (mus, orl) 554 mg/kg. DM4905000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 698A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 198A (*nmr*)
Sandmeyer, T. *et al., Ber.*, 1886, **19**, 564 (*synth*)
Williams, R.T. *et al., Biochem. J.*, 1947, **41**, 1 (*synth*)
Hutchins, J.E.C. *et al., J.A.C.S.*, 1973, **95**, 2282 (*uv*)
Llinares, J. *et al., Can. J. Chem.*, 1979, **57**, 937 (*cmr, tautom*)
Maleski, R.J. *et al., J. Het. Chem.*, 1991, **28**, 1937 (***synth***)
Press, J.B. *et al., J.O.C.*, 1992, **57**, 6335 (*synth*)
Patonay, T. *et al., Synth. Commun.*, 1994, **24**, 2507 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDJ000

2-*O*-Benzoylglucose B-41



α-D-Pyranose-*form*

$C_{13}H_{16}O_7$ 284.265

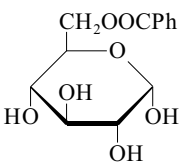
D-*form* [63029-01-6]
Constit. of *Vaccinium vitis-idaea* (cowberry) and *Vaccinium macrocarpon* (cranberry).

α-D-Pyranose-*form* [80358-04-9]

Chaudhuri, R.K. *et al., Helv. Chim. Acta*, 1981, **64**, 2401-2404 (*isol, pmr, cmr*)
Heimhuber, B. *et al., Phytochemistry*, 1990, **29**, 2726-2727 (*isol, synth, nmr*)

6-*O*-Benzoylglucose B-42

*Glucose 6-benzoate, 9CI. **Vacciniin***



α-D-Pyranose-*form*

$C_{13}H_{16}O_7$ 284.265

D-*form* [14200-76-1]
Isol. from *Vaccinium* sp. (red whortleberries and cranberries). Amorph., cryst. hydrate (Me_2CO). Mp 104-106°. $[\alpha]_D$ +48 (EtOH).

[90-75-5, 130323-07-8]

Brigl, P. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1934, **229**, 117 (*isol, struct*)
Heimhuber, B. *et al., Phytochemistry*, 1990, **29**, 2726 (*isol, synth, pmr*)

Benzyl acetate B-43

[140-11-4]
FEMA 2135

$H_3CCOOCH_2Ph$

$C_9H_{10}O_2$ 150.177

Occurs in jasmine, apple, cherry, guava fruit and peel, wine grape, white wine, tea,

plum, cooked rice, Bourbon vanilla, naranjilea fruit (*Solanum quitoense*), Chinese cabbage and quince. Flavouring agent. Liq. with jasmine odour and bitter, pungent taste. d_{25}^{25} 1.05. Bp 215.5-216° Bp_{102} 134°. n_D^{25} 1.4994.

▶ Skin irritant. LD_{50} (rat, orl) 2490 mg/kg. AF5075000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 277A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1201B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1335C (*ir*)
Merker, R.L. *et al., J.O.C.*, 1961, **26**, 5180 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 875 (*rev, tox*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1981, **9**, 82 (*use*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BDX000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 259-260 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Benzyl alcohol, BAN, INN, USAN B-44

[100-51-6]
Benzenemethanol, 9CI. Benzenecarbinol. Hydroxymethylbenzene. α-Hydroxytoluene. Phenylcarbinol. Phenylmethanol. Peruvin†. FEMA 2137

$PhCH_2OH$

C_7H_8O 108.14
Constit. of jasmine and other ethereal oils, both free and as esters. Also present in cherry, orange juice, mandarin peel oil, guava fruit, feijoa fruit, pineapple, leek, cinnamon, cloves, mustard, fermented tea, basil and red sage. Flavouring ingredient. Liq. Mod. sol. H_2O. d^{20} 1.05 d_{15}^{15} 1.05. Fp -15.2. Bp 205.3° Bp_{10} 93°. n_D^{20} 1.5396. pK_a 15.4 (25°).

▶ Fl. p. 93/96/101°, autoignition temp. 436°. Mixt. with 58% H_2SO_4 dec. explosively at 180°. Eye and skin irritant. Ingestion or inhalation can cause adverse gastrointestinal and CNS effects. LD_{50} (rat, orl) 1230 mg/kg. DN3150000

O-*Sulfate:* ***Benzyl sulfate***
$C_7H_8O_4S$ 188.204
Constit. of various plant spp.. Flavour component.

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [88510-11-6]
$C_{18}H_{26}O_{10}$ 402.397
Isol. from wine grapes (*Vitis vinifera*).

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{18}H_{26}O_{10}$ 402.397
Constit. of tomato cell cultures (*Lycopersicon esculentum* Solanaceae). $[\alpha]_D$ -39 (c, 0.02 in H_2O).

O-*[β-D-Xylopyranosyl-(1→6)-D-glucopyranoside]:* [130622-31-0] *Benzyl β-primeveroside*
$C_{18}H_{26}O_{10}$ 402.397
Aroma precursor from Oolong tea leaves (*Camellia sinensis*). Cryst. (EtOH). Mp 188-189°. $[\alpha]_D^{20}$ -71.2 (c, 1 in H_2O).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [56775-64-5] *Benzyl gentiobioside*
$C_{19}H_{28}O_{11}$ 432.424
Constit. of tomato cell cultures (*Lycopersicon esculentum* Solanaceae). $[\alpha]_D$ -76.2 (c, 0.01 in H_2O).

O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]:* [81417-79-0] ***Zizybeoside II***
$C_{25}H_{38}O_{16}$ 594.566
Constit. of dried fruits of Chinese jujube (*Zizyphus jujuba*). Needles (MeOH aq.). Mp 237-238°. $[\alpha]_D^{26}$ -39 (c, 1.00 in H_2O).

[20194-18-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1121D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 326B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1046D (*ir*)
Truett, W.L. *et al., J.A.C.S.*, 1951, **73**, 5913 (*synth*)
Adv. Chem. Ser., 1955, **15**, 347 (***props***)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1045
Brownlee, R.T.C. *et al., J.A.C.S.*, 1968, **90**, 1757 (*ir*)
Aplin, R.T. *et al., Can. J. Chem.*, 1969, **47**, 1599 (*ms*)
Walling, C. *et al., J.A.C.S.*, 1972, **94**, 2007 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 248 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1011 (*rev, tox*)
Shapiro, M.J. *et al., J.O.C.*, 1976, **41**, 3197 (*cmr*)
Bastaert, G. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1980, **290**, 193 (*uv*)
Okamura, N. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3507 (*Zizybeoside*)
Williams, P.J. *et al., Phytochemistry*, 1983, **22**, 2039 (*6-arabinofuranosylglucoside*)
Schaefer, T. *et al., Can. J. Chem.*, 1989, **67**, 1015 (*pmr, conformn*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BDX000; BDX500
Guo, W. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1532 (*primeveroside*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1119
De Rosa, S. *et al., Phytochemistry*, 1996, **42**, 1031 (*6-arabinopyranosylglucoside*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 261-262 (*occur, props*)
Boss, B. *et al., Phytochemistry*, 1999, **50**, 219-225 (*Benzyl sulfate*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2625
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 120; 121
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDX500

Benzyl butyl ether B-45

[588-67-0]
(Butoxymethyl)benzene, 9CI. 1-Benzyloxybutane. α-Butoxytoluene. FEMA 2139

$PhCH_2OCH_2CH_2CH_2CH_3$

$C_{11}H_{16}O$ 164.247
Constit. of the aroma of roasted cashew and some edible mushrooms. Flavouring agent. d_4^{20} 0.92. Bp_{15} 95-97° Bp_{10} 92°. n_D^{20} 1.4833.

Barluenga, J. *et al., Synthesis*, 1983, 53 (*synth, pmr, cmr*)
Li, J. *et al., CA*, 1987, **107**, 115303w (*synth*)
Jayalekshmy, A. *et al., ACS Symp. Ser.*, 1988, **409**, 355 (*occur*)
Motoi, M. *et al., Polym. J. (Tokyo)*, 1989, **21**, 987 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 264 (*use, occur*)

Benzyl ethyl ether B-46

[539-30-0]
(Ethoxymethyl)benzene, 9CI. Ethyl benzyl ether. FEMA 2144

$PhCH_2OEt$

$C_9H_{12}O$ 136.193
Present in cocoa. Flavouring agent. Liq. with powerful fruity odour. d^{20} 0.95. Bp 189° Bp_{18} 78°. n_D^{20} 1.4955.

McKillop, A. *et al., Tetrahedron*, 1974, **30**, 2467 (*synth*)
Adcock, W. *et al., J.O.C.*, 1976, **41**, 1498 (*cmr*)
Grandi, R. *et al., J.O.C.*, 1976, **41**, 1755 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 60
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 267-268
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 411

Benzyl formate B-47

[104-57-4]
Phenylmethyl formate. FEMA 2145

$HCOOCH_2Ph$

$C_8H_8O_2$ 136.15
Occurs in essential oils. Present in sour cherry, crowberry, *Vaccinium spp.* fruits, coffee, black tea, yellow passion fruit, *Ocimum basilicum* varieties and other foods. Used in perfumery and food flavouring. Liq. with fruity odour. Bp 203° Bp_{10} 83-84°. n_D^{20} 1.5404.

Be'hal, M.A. *et al., Ann. Chim. (Paris)*, 1900, **20**, 411 (*props*)
Bredereck, H. *et al., Chem. Ber.*, 1954, **87**, 726 (*synth*)
Suezawa, H. *et al., J. Phys. Org. Chem.*, 1993, **6**, 399 (*conformn*)
Suri, S.C. *et al., Synth. Commun.*, 1996, **26**, 1031 (*synth, ir, pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 268-269 (*props, occur*)

Benzyl glucosinolate B-48

[499-26-3]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)benzenethanimidate], 9CI. ***Glucotropaeolin****. Phenylmethyl glucosinolate*

$PhCH_2C(SGlc){=}NOSO_3H$

$C_{14}H_{19}NO_9S_2$ 409.437
Isol. from seeds of *Tropaeolum majus* (garden nasturtium), *Lepidium sativum* (garden cress) and other crucifers.

K salt: [5115-71-9]

Amorph. powder.

Me_4N salt:
Cryst. Mp 188-189°. $[\alpha]_D^{28}$ -16.7 (H_2O).

Tetra-Ac:
Cryst. +1H_2O (EtOH aq.) (as K salt). Mp 197-199° dec. (K salt). $[\alpha]_D^{25}$ -19 (c, 0.5 in H_2O).

[92761-40-5, 117489-68-6]

Schultz, O.E. *et al., Z. Naturforsch., B*, 1952, **7**, 500; 1953, **8**, 151 (*isol*)
Schultz, O.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1955, **288**, 525 (*isol*)
Ettlinger, M.G. *et al., J.A.C.S.*, 1957, **79**, 1764 (*synth*)
Benn, M.H. *et al., Can. J. Chem.*, 1963, **41**, 2836 (*synth*)
Underhill, E.W. *et al., Biochem. Biophys. Res. Commun.*, 1964, **14**, 425 (*biosynth*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Hanley, A.B. *et al., J. Sci. Food Agric.*, 1983, **34**, 869 (*isol*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*pmr, cmr*)

Benzyl isothiocyanate B-49

[622-78-6]
(Isothiocyanatomethyl)benzene, 9CI. Phenylmethyl isothiocyanate. Benzyl mustard oil. Tromocaps. Tromalyt active substance. Urogran

$PhCH_2NCS$

C_8H_7NS 149.216
Isol. from *Tropaeolum majus* (garden nasturtium) and *Lepidium sativum* (garden cress), also in other plants esp. in the Cruciferae. Potential nutriceutical. Pale yellow oil or orange-red cryst. Mp 41°. Bp 243° Bp_{12} 125-126°. Log P 3.2 (calc).

▶ Severe irritant. LD_{50} (mus, scu) 150 mg/kg ; LD_{50} (mus, scu) 150 mg/kg. NX8250000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1552C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 465D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1422D (*ir*)
Hofmann, A.W. *et al., Ber.*, 1868, **1**, 201 (*synth*)
McKay, A.F. *et al., J.A.C.S.*, 1959, **81**, 4328 (*synth, props*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Tahahashi, K. *et al., Bull. Chem. Soc. Jpn.*, 1963, **36**, 108 (*pmr*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)
Martin, D. *et al., Angew. Chem., Int. Ed.*, 1967, **6**, 168
Jochims, J.C. *et al., Angew. Chem., Int. Ed.*, 1967, **6**, 174 (*synth*)
Weuffen, W. *et al., Pharmazie*, 1967, **22**, 506; 510; 1968, **23**, 579 (*props*)
Lien, E.J. *et al., J. Med. Chem.*, 1968, **11**, 430 (*props*)
Molina, P. *et al., Synthesis*, 1982, 596 (*synth*)
Goerler, K. *et al., Xenobiotica*, 1982, **12**, 535 (*metab*)
Kim, S. *et al., J.O.C.*, 1986, **51**, 2613 (*synth*)
Muthusamy, S. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 228 (*synth*)
Pintao, A.M. *et al., Planta Med.*, 1995, **61**, 233 (*pharmacol*)
Hecht, S.S. *et al., Adv. Exp. Med. Biol.*, 1996, **401**, 1; 13 (*pharmacol, rev*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1678
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEU250

Benzyl methyl disulfide B-50

[699-10-5]
Methyl phenylmethyl disulfide, 9CI. FEMA 3504

$PhCH_2$-S-SMe

$C_8H_{10}S_2$ 170.299
Present in cocoa and roasted peanut. Flavouring ingredient. Liq. $Bp_{0.2}$ 66°. n_D^{24} 1.5996.

▶ JO0400000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 432A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1103C (*ir*)
Armitage, D.A. *et al., J.C.S. Perkin 1*, 1972, 680 (*synth*)
Harpp, D.N. *et al., J.O.C.*, 1979, **44**, 4140 (*synth*)
Masui, M. *et al., Chem. Comm.*, 1984, 843 (*synth*)
Graber, D.R. *et al., J.O.C.*, 1987, **52**, 4620 (*synth*)
Metzner, P. *et al., Synthesis*, 1994, 761 (*synth, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 474
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1723-1724

Benzyl methyl sulfide, 8CI B-51

[766-92-7]
[(Methylthio)methyl]benzene, 9CI. FEMA 3597

$PhCH_2SMe$

$C_8H_{10}S$ 138.233
Flavouring agent. Present in cooked pork. Liq. with powerful horseradish odour. d^{20} 1.03. Bp 199-201° Bp_{25} 80° Bp_4 70-72°. n_D^{20} 1.5632.

S-*Oxide:* [824-86-2] *[(Methylsulfinyl)-methyl]benzene, 9CI. Benzyl methyl sulfoxide*
$C_8H_{10}OS$ 154.232
Cryst. (petrol). Mod. sol. H_2O, Et_2O, petrol, sol. EtOH, AcOH. Mp 54°. Opt. active forms known.

S,S-*Dioxide:* [3112-90-1] *[(Methylsulfonyl)methyl]benzene. Benzyl methyl sulfone. DMIT*
$C_8H_{10}O_2S$ 170.232
Sol. H_2O. Mp 127°.

Thomson, T. *et al., J.C.S.*, 1932, 69 (*synth, dioxide*)
Hünig, S. *et al., Annalen*, 1953, **579**, 23 (*oxide*)
Doerftel, K. *et al., J. Prakt. Chem.*, 1970, **312**, 701 (*ir*)
Russell, G.A. *et al., J.O.C.*, 1979, **44**, 3990 (*synth*)
Youm, J.R. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2140 (*cmr*)
Luzzio, F.A. *et al., Synth. Commun.*, 1984, **14**, 209 (*synth*)
Fujisaki, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 2429 (*synth*)
Langler, R.F. *et al., Can. J. Chem.*, 1987, **65**, 2385 (*synth*)
Comasseto, J.V. *et al., J. Organomet. Chem.*, 1987, **334**, 329 (*synth, pmr*)
Lu, X. *et al., Synthesis*, 1987, 66 (*synth*)
Christophersen, C. *et al., Biochem. Syst. Ecol.*, 1989, **17**, 459 (*occur*)
Torisawa, Y. *et al., Tet. Lett.*, 1990, **29**, 1729 (*synth*)
Olah, G.A. *et al., Synthesis*, 1994, 277 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 63
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 274

Benzyl thiocyanate B-52

[3012-37-1]
Phenylmethyl thiocyanate, 9CI. Benzyl rhodanide

$PhCH_2SCN$

C_8H_7NS 149.216
Isol. from *Lepidium sativum* (garden cress) as a benzyl glucosinolate (see Benzyl glucosinolate, B-48) degradation prod.. Cryst. (petrol). Mp 41-42°.

▶ LD_{50} (mus, scu) 100 mg/kg. XK8155000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 465A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1550C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1422B (*ir*)
Footner, H.B. *et al., J.C.S.*, 1925, **127**, 2887 (*synth*)
Gmelin, R. *et al., Acta Chem. Scand.*, 1959, **13**, 1474 (*isol*)
Bacon, R.G.R. *et al., J.C.S.*, 1964, 5594 (*synth*)
Mravec, D. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 3274 (*synth*)
Harpp, D.N. *et al., Synthesis*, 1979, 181 (*synth*)
Hasapis, H. *et al., Phytochemistry*, 1982, **21**, 1009 (*isol*)
Renwick, G.R. *et al., Crit. Rev. Food Sci. Nutr.*, 1983, **18**, 123 (*glucosinolates, rev*)
Kagabu, S. *et al., Chem. Pharm. Bull.*, 1991, **39**, 784 (*synth*)
Fujiki, K. *et al., Synth. Commun.*, 1999, **29**, 3289-3294 (*synth, ms*)
Renard, P.Y. *et al., Chem. Eur. J.*, 2002, **8**, 2910-2918 (*synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BFL000

Benzylamine, 8CI B-53

[100-46-9]
Benzenemethanamine, 9CI. α-Aminotoluene. Moringine

$PhCH_2NH_2$

C_7H_9N 107.155
Alkaloid from *Moringa oleifera* (horseradish tree). d_4^{19} 0.98. Bp 185° Bp_{12} 90°. n_D^{20} 1.5401. pK_a 8.82 (20°, 60% dioxan aq.). Absorbs CO_2 from air.

▶ Fl. p. 63°. Reacts violently with *N*-haloimides. Corrosive and irritating to all tissues. DP1488500

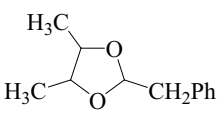
N-*Hexadecanoyl:* [74058-71-2] N-*Benzylhexadecanamide.* ***Macamide B***
$C_{23}H_{39}NO$ 345.567
Alkaloid from the tubers of *Lepidium meyenii* (maca). Amorph. solid. λ_{max} 208 (log ε 4.03) (MeOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1266B; 1266C; 1274A; 1274C; 1274D; 1275A; 1279B; **2**, 366B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 565B; 565C; 581B; 582A; 582B; 582C; 589A; 1385A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1163A; 1165D; 1166B; 1166C; 1167D (*ir*)
Chen, A.L. *et al., J. Am. Pharm. Assoc.*, 1931, **20**, 339 (*isol, derivs*)
Chakravarti, R.N. *et al., CA*, 1955, **50**, 16891f (*isol*)
Leyson, R. *et al., Spectrochim. Acta*, 1963, **19**, 243 (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 51; 1975, **5**, 479; 1980, **8**, 70; 1982, **10**, 26 (*use*)
Witanowski, M. *et al., Can. J. Chem.*, 1969, **47**, 1321 (*N-15 nmr*)
Egli, R.A. *et al., Helv. Chim. Acta*, 1970, **53**, 47 (*synth*)
Aihara, A. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1942 (*pmr*)
Lichter, R.L. *et al., J.A.C.S.*, 1972, **94**, 2495 (*N-15 nmr*)
Shapiro, M.J. *et al., J.O.C.*, 1976, **41**, 3197 (*cmr*)
Kostyanovsky, R.G. *et al., Org. Mass Spectrom.*, 1976, **11**, 237 (*ms*)
Knights, R.J. *et al., Anal. Biochem.*, 1977, **77**, 106 (*use*)
Bastaert, G. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1980, **290**, 193 (*uv*)
Bradamante, S. *et al., J.O.C.*, 1980, **45**, 105 (*cmr*)
Elmore, D.T. *et al., Acta Cryst. C*, 1992, **48**, 1331 (*cryst struct*)
Muhammad, I. *et al., Phytochemistry*, 2002, **59**, 105-110 (*Macamide B*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2631
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 122
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDY000; DQQ000; DQP800

2-Benzyl-4,5-dimethyl-1,3-dioxolane B-54

[5468-06-4]
Phenylacetaldehyde 2,3-butylene glycol acetal. FEMA 2875

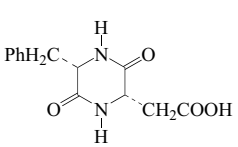


$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient for baked goods, puddings, candies and nonalcoholic beverages. Viscous liq. with floral-earthy odour and fruity flavour.

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1456-1457 (*use*)

5-Benzyl-3,6-dioxo-2-piperazineacetic acid B-55

[55102-13-1]
3,6-Dioxo-5-(phenylmethyl)-2-piperazineacetic acid, 9CI. 5-Benzyldiketopiperazine-2-acetic acid. Cyclo(aspartylphenylalanyl). Cyclo(phenylalanylaspartyl)



(2*S*,5*S*)-*form*
$C_{13}H_{14}N_2O_4$ 262.265

(2*S*,5*S*)-*form* [5262-10-2]
L-cis-*form*
Degradn. product of Aspartame, A-461. Gelatinous needles (AcOH). Mp 256-258°.

[108147-50-8, 109062-52-4, 130856-96-1, 130856-97-2, 156769-20-9]

Davey, J.M. *et al., J.C.S.(C)*, 1966, 555-566 (*synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*formn*)

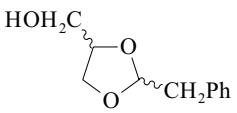
3-Benzyl-4-heptanone B-56

[7492-37-7]
3-(Phenylmethyl)-4-heptanone, 9CI. Benzyl dipropyl ketone (incorr.). Morellone. FEMA 2146
$H_3CCH_2CH(CH_2Ph)COCH_2CH_2CH_3$
$C_{14}H_{20}O$ 204.311
Used in food flavouring (plum/peach). No phys. props. reported.

Eur. Pat., 1989, 373 993; *CA*, **114**, 61550y (*synth*)

2-Benzyl-5-hydroxymethyl-1,3-dioxolane B-57

[5694-72-4]
Phenylacetaldehyde glyceryl acetal. Acetal CD. FEMA 2877



$C_{11}H_{14}O_3$ 194.23
Mixt. with 5-Hydroxy-2-benzyl-1,3-dioxane, H-362 is used as a flavouring ingredient. No phys. props. reported.

[29895-73-6]

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 829
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2180-2181

2-Benzylidene-1-heptanol B-58

[101-85-9]

[184900-07-0]
2-(Phenylmethylene)-1-heptanol, 9CI. 2-Pentyl-3-phenyl-2-propen-1-ol. α-Pentylcinnamyl alcohol. α-Amylcinnamyl alcohol. FEMA 2065
$PhCH{=}C(CH_2OH)(CH_2)_4CH_3$
$C_{14}H_{20}O$ 204.311
Flavouring ingredient. Liq. with light floral odour. Bp_{12} 162° Bp_5 141-143°. *E*/*Z*-form unspecified.

Phenylurethane:
Bp 61-62°.

Formyl: [7493-79-0] *α-Amylcinnamyl formate. FEMA 2066*
$C_{15}H_{20}O_2$ 232.322
Flavouring ingredient. Liq. with sweet, herbaceous somewhat green odour.

Ac: [7493-78-9] *α-Amylcinnamyl acetate. FEMA 2064*
$C_{16}H_{22}O_2$ 246.349
Flavouring ingredient. Liq. with somewhat fruity flavour. d_4^{20} 1. Bp_2 125-128°. n_D^{20} 1.5356.

3-Methylbutanoyl: [7493-80-3] *α-Amylcinnamyl isovalerate. FEMA 2067*
$C_{19}H_{28}O_2$ 288.429
Flavouring ingredient. Liq. with mild fruity, somewhat spicy flavour.

Bogert, M.T. *et al., J.A.C.S.*, 1931, **53**, 1605-1609 (*synth*)
Mastagli, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1937, **204**, 1656-1658 (*synth*)
Mastagli, P. *et al., Annalen*, 1938, **10**, 281-377 (*synth*)
Pansevich-Kolyada, V.I. *et al., CA*, 1967, **68**, 2746a; 1968, **71**, 12892w (*Ac, synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 817; 1976, **14**, 677 (*tox, use, Ac*)
Dallacker, F. *et al., Chem.-Ztg.*, 1990, **114**, 1-5 (*synth*)
Konings, A.W.T. *et al., Chem.-Ztg.*, 1990, **114**, 1-5 (*synth*)
Choi, J. *et al., Tet. Lett.*, 1996, **37**, 1057-1060 (*Z-form, synth*)
Lutz, C. *et al., J.O.C.*, 1997, **62**, 7895-7898 (*E,S-form, synth, pmr, cmr*)
Mosciano, G. *et al., Perfum. Flavor.*, 1997, **22**, 47-50 (*Ac, use, props*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 76-78 (*esters, props, use*)

2-Benzyl-3-oxobutanoic acid B-59

[2382-58-3]
2-Benzylacetoacetic acid. 2-Acetyl-3-phenylpropanoic acid
$H_3CCOCH(COOH)CH_2Ph$
$C_{11}H_{12}O_3$ 192.214

(±)-*form*
Oil with aromatic smell. Spar. sol. H_2O. Bp_{13} 156-162°. Decarboxylates on warming.

Me ester: [3666-82-8]
$C_{12}H_{14}O_3$ 206.241
Bp_5 145°.

Et ester: [620-79-1] *FEMA 2416*
$C_{13}H_{16}O_3$ 220.268
Flavouring ingredient. Insol. H_2O, misc. EtOH, Et_2O. d^{25} 1.06. Bp 276°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 280A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1216B (*nmr*)
Ceresole, M. *et al., Ber.*, 1882, **15**, 1871 (*synth*)
Rupe, H. *et al., Annalen*, 1920, **426**, 33 (*resoln*)
Kabachnik, M.I. *et al., Tetrahedron*, 1961, **12**, 76 (*ester*)
Kazankova, M.A. *et al., Zh. Obshch. Khim.*, 1965, **35**, 1447 (*ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 214 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 943 (*Et ester*)

1-Benzyloxy-1-(2-methoxyethoxy)ethane B-60

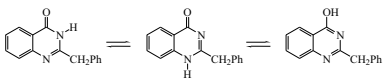
[7492-39-9]
Benzyl methoxyethyl acetal. Acetaldehyde benzyl β-methoxyethyl acetal. FEMA 2148
$MeOCH_2CH_2OCH(CH_3)OCH_2Ph$
$C_{12}H_{18}O_3$ 210.272
Flavouring ingredient. Liq. with sweet, green, fruity odour.

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 63 (*props, use*)

2-Benzyl-4(3*H*)-quinazolinone B-61

[4765-56-4]

*2-(Phenylmethyl)-4(3*H*)-quinazolinone, 9CI. **Glycosminine**. Glycophymine. 2-Benzyl-4-hydroxyquinazoline. 2-(Phenylmethyl)-4-quinoxalinol*



$C_{15}H_{12}N_2O$ 236.273

Specific inhibitor of serine protease and human leucocyte elastase. Cryst. (MeOH, EtOH, $CHCl_3$ or C_6H_6). Mp 254-256° (248-249°).

OH-form

Me ether: [72361-61-6] *4-Methoxy-2-(phenylmethyl)quinazoline. 2-Benzyl-4-methoxyquinazoline.* ***Glycophymoline***

$C_{16}H_{14}N_2O$ 250.299

Cryst. (C_6H_6/MeOH). Mp 165°.

1H-form

N-*Me:* [6873-15-0] *1-Methyl-2-(phenylmethyl)-4(1*H*)-quinazolinone. 2-Benzyl-1-methyl-4(1*H*)-quinazolinone.* ***Arborine***. *Glycosine*

$C_{16}H_{14}N_2O$ 250.299

Major alkaloid from *Ruta graveolens* (rue). Cryst. (MeOH/$CHCl_3$). Mp 161-162° (155-156°).

N-*Me, hydrochloride:*

Cryst. + $2H_2O$ (H_2O). Mp 215° dec. (partial melting at 106-108°).

N-*Me, picrate:*

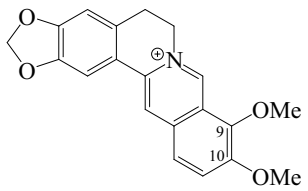
Yellow needles (EtOH). Mp 172-173°.

Chakravarti, D. *et al., Tetrahedron*, 1961, **16**, 224-250 (*Arborine, uv, ir, pmr, struct*)
Pakrashi, S.C. *et al., Tetrahedron*, 1963, **19**, 1011 (*uv, ir, pmr, ms, struct, synth*)
Pakrashi, S.C. *et al., Indian J. Chem.*, 1968, **6**, 472 (*synth*)
O'Donovan, D.G. *et al., J.C.S.(C)*, 1970, 2466-2470 (*biosynth*)
Patel, V.S. *et al., J. Indian Chem. Soc.*, 1972, **49**, 59 (*uv*)
Kametani, T. *et al., J.A.C.S.*, 1977, **99**, 2306-2309 (*synth, ir, pmr*)
Rhee, R.P. *et al., J.O.C.*, 1977, **42**, 3650 (*synth, ir, pmr*)
Sarkar, M. *et al., Phytochemistry*, 1977, **16**, 2007 (*isol, uv, ir, ms, synth*)
Kametani, T. *et al., Heterocycles*, 1978, **9**, 1585 (*synth*)
Bhattacharyya, J. *et al., Heterocycles*, 1979, **12**, 929; 1980, **14**, 1469 (*uv, ir, pmr, cmr*)
Naik, N.R. *et al., J. Indian Chem. Soc.*, 1979, **56**, 708-711 (*synth, uv, ir*)
Sarkar, M. *et al., Phytochemistry*, 1979, **18**, 694 (*Glycophymoline*)
Yamato, M. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3124 (*synth*)
Chakraborty, D.P. *et al., Synthesis*, 1981, 977-979 (*synth*)
Teshima, T. *et al., J. Biol. Chem.*, 1982, **257**, 5085 (*pharmacol*)
Ganjian, I. *et al., Synth. Commun.*, 1984, **14**, 33 (*synth, pmr*)
Johne, S. *et al., Alkaloids (N.Y.)*, 1986, **29**, 129-140 (*Arborine, rev, pharmacol*)
Uozumi, Y. *et al., J.A.C.S.*, 1989, **111**, 3725 (*synth, ir, pmr, ms*)
Muthukrishnan, J. *et al., Phytochemistry*, 1999, **50**, 249-254 (*Arborine, isol, pmr, cmr*)

Berberine B-62

[2086-83-1]

5,6-Dihydro-9,10-dimethoxybenzo[g]-1,3-benzodioxolo[5,6-a]quinolizinium(1+), 9CI. Umbellatine. Berbericine. Natural yellow 18. C.I. 75160. Majarine



$C_{20}H_{18}NO_4^{\oplus}$ 336.366

Log P -0.4 (uncertain value) (calc).

▶ Adverse human effects including reduced body temperature. Can cause death by central paralysis. LD_{50} (mus, orl) 329 mg/kg. DR9870000

O^9-*De-Me:* [17388-19-1] ***Berberrubine***. *Chileninone*

$C_{19}H_{16}NO_4^{\oplus}$ 322.34

Alkaloid from *Berberis vulgaris* (barberry). Deep red amorph. solid (as chloride).

[79236-58-1]

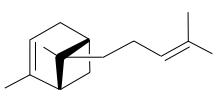
Späth, E. *et al., Monatsh. Chem.*, 1929, **52**, 117 (*Berberrubine, isol*)
Ghabro, S.A. *et al., J. Nat. Prod.*, 1973, **36**, 349-351 (*Berberrubine, activity*)
Siwon, J. *et al., Planta Med.*, 1981, **41**, 65 (*Berberrubine, occur*)
Valencia, E. *et al., Tetrahedron*, 1984, **40**, 3957 (*Berberrubine, isol, uv, ir, pmr, ms*)
Shamma, M. *et al., J. Nat. Prod.*, 1986, **49**, 398 (*Berberrubine, struct*)

α-Bergamotene B-63

[13474-59-4]

[17699-05-7]

Bergamotene

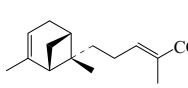


$C_{15}H_{24}$ 204.355

Constit. of oils of carrot (*Daucus carota*), bergamot (*Citrus bergamia*), also lime (*Citrus aurantifolia*), citron (*Citrus medica*) and cottonseed oil (*Gossypium hirsutum*). Oil. d^{20} 0.86. $[\alpha]_D^{20}$ -44.1 ($CHCl_3$). n_D^{20} 1.4904.

Kováts, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2705 (*pmr, ms, struct*)
Larsen, S.D. *et al., J.A.C.S.*, 1977, **99**, 8015
Kulkarni, Y.S. *et al., J.O.C.*, 1985, **50**, 2809 (*synth*)
Snider, B.B. *et al., J.O.C.*, 1988, **53**, 4508 (*synth*)

α-Bergamotenoic acid B-64



(*E*)-*form*

$C_{15}H_{22}O_2$ 234.338

(***E*)-*form*** [114248-38-3]

Cryst. (pentane). Mp 59-60°. $[\alpha]_D^{23}$ -46.3 (c, 1.3 in $CHCl_3$).

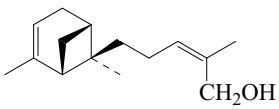
(***Z*)-*form*** [124439-27-6]

Flavouring ingredient. Constit. of East Indian sandalwood oil. Oil.

Coates, R.M. *et al., J.O.C.*, 1988, **53**, 2186-2192 (*isol*)
Nikiforov, A. *et al., Annalen*, 1990, 119-121 (*isol, pmr*)
Mori, K. *et al., Synthesis*, 1994, 417-421 (*synth*)

α-Bergamotenol B-65

[88034-74-6]



$C_{15}H_{24}O$ 220.354

Constit. of the famine food *Santalum album* (sandalwood). Flavouring ingredient. Oil. $[\alpha]_D$ -55.6 (c, 0.39 in $CHCl_3$).

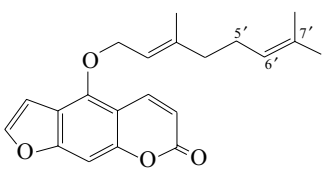
[65336-63-2, 176777-61-0]

Brunke, E.J. *et al., Dev. Food Sci.*, 1988, **18**, 819-831 (*rev*)
Pant, A.K. *et al., J. Essent. Oil Res.*, 1992, **4**, 9-13 (*isol*)
Yu, J.G. *et al., Yaoxue Xuebao*, 1993, **28**, 840-844 (*isol*)

Bergamottin B-66

[7380-40-7]

*4-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-g][1]benzopyran-7-one, 9CI. Bergaptol geranyl ether. 5-Geranyloxypsoralen. Bergaptin*



$C_{21}H_{22}O_4$ 338.402

Constit. of bergamot oil. Also from lemon oil and oils of other *Citrus* spp. and carrot (*Daucus carota*). Cryst. (Et_2O/petrol). Mp 59-61° (54°).

6′R,7′-Epoxide: [105866-30-6]

$C_{21}H_{22}O_5$ 354.402

Constit. of grapefruit (*Citrus paradisi*) peel oil. Cryst. (EtOAc/hexane). Mp 82.5-83.5°.

6′,7′-Dihydro, 6′R,7′-dihydroxy: [71339-34-9]

[51956-35-5] *4-[(6,7-Dihydroxy-3,7-dimethyl-2-octenyl)oxy]-7*H*-furo[3,2-g][1]benzopyran-7-one.* ***6′,7′-Dihydroxybergamottin***

$C_{21}H_{24}O_6$ 372.417

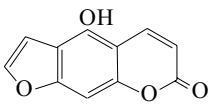
Isol. from *Citrus macroptera* whole fruits, a non-commercial sp. of the South Pacific. Cryst. Mp 104-106°. $[\alpha]_D$ +12.7 ($CHCl_3$). Config. not detd..

Kainrath, P. *et al., Ber.*, 1937, **70**, 2272 (*6′,7′-*

epoxide)
Chatterjee, A. *et al., J.C.S.*, 1961, 2246 (*synth*)
Bates, R.B. *et al., Tet. Lett.*, 1963, 1683 (*config*)
Dreyer, D.L. *et al., Phytochemistry*, 1973, **12**, 3011 (*6′,7′-dihydro-6′,7-dihydroxy*)
Bohlmann, F. *et al., Chem. Ber.*, 1975, **108**, 2955 (*isol, uv*)
Tatum, J.H. *et al., Phytochemistry*, 1979, **18**, 500 (*6′,7′-epoxide*)
Bellevue, F.H. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 2593-2598 (*synth, 6′,7′-dihydroxy*)

Bergaptol B-67

[486-60-2]
*4-Hydroxy-7*H-*furo[3,2-*g*][1]benzopyran-7-one, 9CI. 4-Hydroxypsoralen*



$C_{11}H_6O_4$ 202.166
Present in various citrus spp.. Needles (EtOAc). Mp 277-278°.

O-*β-D-Glucopyranoside:*
$C_{17}H_{16}O_9$ 364.308
Needles (MeOH). Mp 254-256°.

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: Bergaptol rutinoside*
$C_{23}H_{26}O_{13}$ 510.451
Mp 240-242°. $[\alpha]_D^{25}$ +150 (c, 0.5 in MeOH). λ_{max} 222 ; 251 ; 258 ; 266 ; 308 (MeOH).

Me ether: [484-20-8] *4-Methoxy-7*H-*furo[3,2-*g*]benzopyran-7-one.* ***Bergapten****. Heraclin. Majudin. 5-Methoxypsoralen (obsol.)*
$C_{12}H_8O_4$ 216.193
Major constit. of bergamot oil (*Citrus bergamia*). Present in celery, esp. the outer leaves, and other common grocery vegetables. Implicated in photodermatitis among grocery workers. Needles (EtOH). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 188°. Log P 2.3 (calc). Pastinacin was impure Bergapten. λ_{max} 222 (ϵ 22600); 250 (ϵ 16500); 310 (ϵ 13600) (MeOH) (Berdy). λ_{max} 220 (ϵ 14100); 242 (ϵ 8000); 268 (ϵ 10700); 310 (ϵ 9100) (EtOH) (Berdy).

▶ Skin photosensitiser. Probable human carcinogen. LD_{50} (mus, orl) 8100 mg/kg. LV1300000

O-*(3-Methyl-2-butenyl):* See Isoimperatorin in *The Combined Chemical Dictionary.*

O-*(2,3-Epoxy-3-methylbutyl):* Oxypeucedanin, O-260

O-*(2,3-Dihydroxy-3-methylbutyl):* See Aviprin in *The Combined Chemical Dictionary.*

O-*(2-Hydroxy-3-methyl-3-butenyl):* Pabulenol, P-1

O-*(3,6,6-Trimethyl-7-oxo-2-heptenyl):* Aurantiumal, A-489

O-*(3,7-Dimethyl-2,6-octadienyl):* Bergamottin, B-66

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1321A (*nmr*)
Baetcke, E. *et al., Ber.*, 1912, **45**, 3705 (*struct*)
Glatfelder, A. *et al., Helv. Chim. Acta*, 1920, **3**, 541; 1921, **4**, 718 (*synth*)
Socias, L. *et al., Ber.*, 1934, **67**, 59 (*isol*)
Kubiczek, G. *et al., Ber.*, 1937, **70**, 1253 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1369 (*occur, deriv*)
Austin, D.J. *et al., Phytochemistry*, 1973, **12**, 1657 (*biosynth*)
Boyd, R.K. *et al., Can. J. Chem.*, 1979, **57**, 1995 (*ms*)
Duddeck, H. *et al., Phytochemistry*, 1979, **18**, 139 (*cmr*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, 291 (*furanocoumarins, biol, prop*)
IARC Monog., 1986, **40**, 327 (*tox, rev*)
Gu, Z. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2498 (*deriv*)
Ginderow, D. *et al., Acta Cryst. C*, 1991, **47**, 2144 (*cryst struct*)
Diawara, M.M. *et al., J. Agric. Food Chem.*, 1995, **43**, 723-727 (*occur*)
McNeely, W. *et al., Drugs*, 1998, **56**, 667-690 (*rev, Me ether*)
Masuda, T. *et al., Phytochemistry*, 1998, **47**, 13-16 (*Bergapten, isol, pmr, cmr*)
Kawaii, S. *et al., J. Agric. Food Chem.*, 1999, **47**, 4073 (*activity*)
Oliva, A. *et al., J. Chem. Ecol.*, 1999, **25**, 519-526 (*activity*)
Caceres, A. *et al., Fitoterapia*, 2001, **72**, 376-381 (*rutinoside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFN275

Bervulcine B-68

$C_{18}H_{19}NO_3$ 297.353
Struct. unknown. Alkaloid from *Berberis vulgaris* (barberry). Mp 125-126° dec. $[\alpha]_D^{24}$ -185 (c, 0.2 in $CHCl_3$).

Hydroiodide:
Prisms (H_2O). Mp 236° dec.

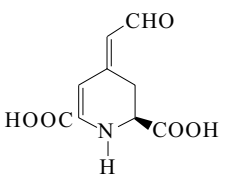
Methiodide:
Cryst. (H_2O). Mp 269° dec.

Picrate:
Fine needles (MeOH). Mp 188-190° dec.

Döpke, W. *et al., Naturwissenschaften*, 1963, **50**, 595

Betalamic acid B-69

[18766-66-0]
1,2,3,4-Tetrahydro-4-(oxoethylidene)-2,6-pyridinedicarboxylic acid



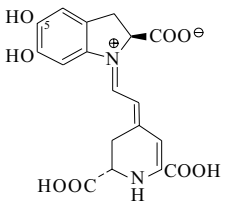
Absolute configuration

$C_9H_9NO_5$ 211.174
Precursor of betalain pigments in plants of the Centrospermae. Detected in *Beta vulgaris* (beetroot). Yellow soln. in H_2O at pH 9, or amorph. green residue. Sensitive to air, acids and strong alkali. Various protected derivs. known λ_{max} 430 (no solvent reported).

Kimler, L. *et al., Chem. Comm.*, 1971, 1329 (*isol, synth, struct*)
Döpp, H. *et al., Chem. Ber.*, 1973, **106**, 3473 (*synth, uv*)
Büchi, G. *et al., J.O.C.*, 1977, **42**, 2192 (*synth*)
Hilpert, H. *et al., Helv. Chim. Acta*, 1984, **67**, 1547 (*synth*)

Betanidin B-70

[2181-76-2]
*2-Carboxy-1-[(2,6-dicarboxy-2,3-dihydro-4(1*H*)-pyridinylidene)ethylidene]-2,3-dihydro-5,6-dihydroxy-1*H*-indolium hydroxide inner salt*



Absolute configuration

$C_{18}H_{16}N_2O_8$ 388.333
Cryst. (as hydrochloride). Forms cryst. K and NH_4 salts. Shows rapid *E/Z* isom. in soln. λ_{max} 271 (ϵ 8530); 295 (sh) (ϵ 7170); 544 (ϵ 51000) (no solvent reported) (hydrochloride).

5-O-β-D-Glucopyranoside: [7659-95-2] ***Betanin****. Phytolaccanin. E162*
$C_{24}H_{26}N_2O_{13}$ 550.475
Red pigment from beetroot, *Beta vulgaris* var. *rubra* and other Centrospermae. Used as a food dye.

▶ US7968100

5-O-(6-O-Sulfo-β-D-glucopyranoside): [13798-16-8] ***Prebetanin***
$C_{24}H_{26}N_2O_{16}S$ 630.539
Pigment from beetroot *Beta vulgaris*.

*6-O-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranoside]:* [143022-02-0] ***Gomphrenin II***
$C_{33}H_{32}N_2O_{15}$ 696.62
Pigment from the fruits of *Basella rubra* (Malabar spinach).

*5-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [290313-64-3]

[178885-00-2]
$C_{39}H_{42}N_2O_{20}$ 858.762
Pigment from *Phytolacca americana* (pokeberry).

5-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucopyranoside]: [15167-84-7]

[11033-33-3] ***Amaranthin****. Amarantin*
$C_{30}H_{34}N_2O_{19}$ 726.601
Pigment from *Amaranthus caudatus* (lovelies-bleeding) and *Amaranthus tricolor* (Chinese spinach).

14,15-Didehydro, 5-O-β-D-glucopyranoside: [71199-29-6] ***Neobetanin***
$C_{24}H_{24}N_2O_{13}$ 548.459
Present in roots of red beet (*Beta vulgaris* ssp. *vulgaris* var. *conditiva*). Also in flowers of Barbary fig (*Opuntia ficus-indica*). Prob. artifact λ_{max} 267 ; 306 ; 470 (no solvent reported). λ_{max} 298 ; 365 (H_2O).

15-Epimer: [4934-32-1] ***Isobetanidin***

$C_{18}H_{16}N_2O_8$ 388.333
Minor congener of Betanidin. Epimeric at the piperidine COOH group.

*15-Epimer, 5-*O*-β-D-glucopyranoside:* [15121-53-6] ***Isobetanin***
$C_{24}H_{26}N_2O_{13}$ 550.475
Minor congener of Betanin, e.g. from beetroot and *Amaranthus* spp..

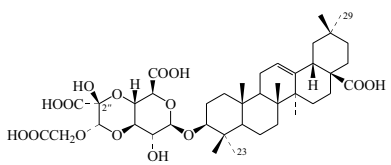
*15-Epimer, 6-*O*-[4-hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranoside]:* [143062-65-1] ***Isogomphrenin II***
$C_{33}H_{32}N_2O_{15}$ 696.62
Pigment from the fruits of *Basella rubra* (Malabar spinach).

*15-Epimer, 5-*O*-[4-hydroxy-3-methoxy-*E*-cinnamoyl-(→3)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{39}H_{42}N_2O_{20}$ 858.762
Pigment from *Phytolacca americana* (pokeberry).

Piattelli, M. *et al., Ann. Chim. (Rome)*, 1966, **56**, 1060; *CA*, **66**, 65805y (*Amaranthin*)
Wyler, H. *et al., Helv. Chim. Acta*, 1967, **50**, 545-560; 1984, **67**, 1793-1800 (*Prebetanin*)
Hilpert, H. *et al., Helv. Chim. Acta*, 1984, **67**, 1547-1561 (*synth*)
Alard, D. *et al., Phytochemistry*, 1985, **24**, 2383-2385 (*Neobetanin*)
Schliemann, W. *et al., Phytochemistry*, 1996, **42**, 1039-1046 (*Phytolacca americana constits*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 241 (*Betanin, use*)
Cai, Y. *et al., J. Agric. Food Chem.*, 2001, **49**, 1971 (*bibl, Gomphrenin II, Celosianin I, IsocelosianinsI, Isogomphrenin II*)

Betavulgaroside II B-71

[168010-05-7]



$C_{41}H_{60}O_{15}$ 792.916

Complex glycoside of 3-Hydroxy-12-oleanen-28-oic acid, H-663. Constit. of *Beta vulgaris* (sugar beet). Cryst. Mp 173-174°. $[\alpha]_D$ +70.1 (MeOH).

*28-*O*-β-D-Glucopyranosyl ester:* [158511-55-8] ***Betavulgaroside I***. *Achyranthoside B*
$C_{47}H_{70}O_{20}$ 955.058
Constit. of *Beta vulgaris* (sugar beet). Cryst. Mp 215-217°. $[\alpha]_D$ +49.5 (MeOH).

*2′′-Me ether, 28-*O*-β-D-glucopyranosyl ester:* [158511-54-7] ***Achyranthoside A***
$C_{48}H_{72}O_{20}$ 969.085
$[\alpha]_D$ +64.3 (MeOH) (as tri-Me ester).

*23-Hydroxy, 28-*O*-β-D-glucopyranosyl ester:* [354552-00-4] ***Basellasaponin A***
$C_{47}H_{70}O_{21}$ 971.057
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 228-230°. $[\alpha]_D^{24}$ +30.1 (c, 0.1 in MeOH). Complex glycoside of D-582.

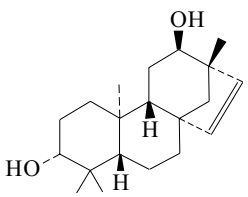
*23-Aldehyde, 28-*O*-β-D-glucopyranosyl ester:* [354552-02-6] ***Basellasaponin B***
$C_{47}H_{68}O_{21}$ 969.042
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 226-228°. $[\alpha]_D^{26}$ +57.4 (c, 0.1 in MeOH). Complex glycoside of H-695.

*23-Carboxylic acid, 28-*O*-β-D-glucopyranosyl ester:* [354552-04-8] ***Basellasaponin C***
$C_{47}H_{68}O_{22}$ 985.041
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 230-232°. $[\alpha]_D^{25}$ +42.1 (c, 0.1 in MeOH). Complex glycoside of H-661.

*29-Carboxylic acid, 28-*O*-β-D-glucopyranosyl ester:* [354552-06-0] ***Basellasaponin D***
$C_{47}H_{68}O_{22}$ 985.041
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 215-217°. $[\alpha]_D^{27}$ +24 (c, 0.1 in MeOH).

Ida, Y. *et al., Tet. Lett.*, 1994, **35**, 6887 (*Achyranthosides, isol, pmr, cmr, cryst struct*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1212-1217 (*Betavulgarosides*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1717-1724 (*abs config*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 776-779 (*Basellasaponins*)

15-Beyerene-3,12-diol B-72



$C_{20}H_{32}O_2$ 304.472

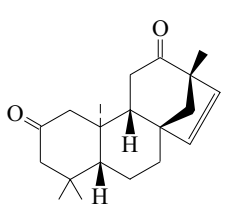
(ent*-3β,12α)-*form [88047-95-4] ***15-Stachene-3α,12β-diol***
Cryst. Mp 204-205°. $[\alpha]_D^{25}$ +8.73 (c, 0.126 in MeOH).

12-Ketone: [119626-51-6] ent-*3β-Hydroxy-15-beyeren-12-one.* ***Yucalexin B14***
$C_{20}H_{30}O_2$ 302.456
Constit. of *Manihot esculenta* (cassava).

3,12-Diketone: [88048-00-4] ent-*15-Beyerene-3,12-dione.* ***Yucalexin B16***
$C_{20}H_{28}O_2$ 300.44
Constit. of *Manihot esculenta* (cassava). Cryst. Mp 70-73°.

Delgado, G. *et al., Phytochemistry*, 1983, **22**, 1227 (*isol, cryst struct*)
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769 (*Yucalexins*)
De Heluani, C.S. *et al., Magn. Reson. Chem.*, 1998, **36**, 947-950 (*Yucalexin B16, pmr, cmr*)

15-Beyerene-2,12-dione B-73

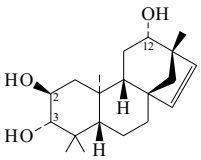


$C_{20}H_{28}O_2$ 300.44

ent*-form** [64657-12-1] ***Yucalexin B7
Constit. of cassava roots (*Manihot esculenta*).

Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769

15-Beyerene-2,3,12-triol B-74



(*ent*-2α,3β,12β)-*form*

$C_{20}H_{32}O_3$ 320.471

(ent*-2α,3β,12β)-*form
Needles (EtOH aq.). Mp 218-221.5°. $[\alpha]_D$ -11 (c, 1.86 in $CHCl_3$).

2-Ketone: [119626-53-8] ent-*3β,12β-Dihydroxy-15-beyeren-2-one.* ***Yucalexin B18***
$C_{20}H_{30}O_3$ 318.455
Constit. of *Manihot esculenta* (cassava root). $[\alpha]_D^{26}$ -9.4 (c, 0.17 in $CHCl_3$).

12-Ketone: [119626-55-0] ent-*2α,3β-Dihydroxy-15-beyeren-12-one.* ***Yucalexin B22***
$C_{20}H_{30}O_3$ 318.455
Constit. of cassava roots (*Manihot esculenta*).

2,12-Diketone: [35470-61-2] ent-*3β-Hydroxy-15-beyerene-2,12-dione.* ***Yucalexin B9***
$C_{20}H_{28}O_3$ 316.439
Constit. of cassava root *Manihot esculenta*. Mp 163-165.5°. $[\alpha]_D$ -329 ($CHCl_3$). $[\alpha]_D^{23}$ -73.9 (c, 0.83 in $CHCl_3$). Bitter taste. Large discrepancy in opt. rotn. of the two isolates.

Triketone: [50719-31-8] ent-*15-Beyerene-2,3,12-trione.* ent-*2-Hydroxy-1,15-beyeradiene-3,12-dione.* ***Yucalexin B5***
$C_{20}H_{26}O_3$ 314.424
Constit. of cassava roots *Manihot esculenta*. Prisms. Mp 170-173°. $[\alpha]_D$ -374 (c, 2.3 in $CHCl_3$). Exists as an enol form.

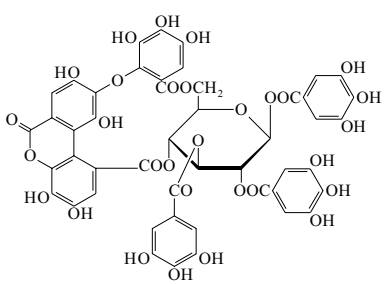
(ent*-3β,12α)-*form

2-Ketone: [119679-04-8] ent-*3β,12α-Dihydroxy-15-beyeren-2-one.* ***Yucalexin B20***
$C_{20}H_{30}O_3$ 318.455
Constit. of cassava *Manihot esculenta*.

Piacenza, L.P.L. *et al., J.C.S. Perkin 1*, 1979, 1004-1012 (*Androstachys johnsonii constit*)
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769-3779 (*Manihot esculenta constits*)

Bicornin B-75

[124854-12-2]



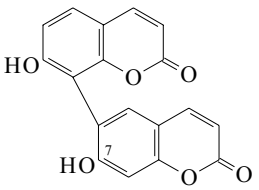
$C_{48}H_{32}O_{30}$ 1088.763

Constit. of *Trapa bicornis* (horn nut). Amorph. powder. $[\alpha]_D$ +4.7 (MeOH).

Yoshida, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2655 (*struct, pmr, cmr*)

Bicoumol B-76

[15575-52-7]
*7,7′-Dihydroxy[6,8′-bi-2*H*-1-benzopyran]-2,2′-dione. 7,7′-Dihydroxy-6,8′-bicoumarin*



$C_{18}H_{10}O_6$ 322.273
Struct. in 9CI and 8CI is incorrect. Isol. from white clover (*Trifolium repens*). Cryst. (EtOH/Me_2CO). Mp 293-294°. λ_{max} 211 (log ϵ 4.08); 258 (log ϵ 3.54); 327 (log ϵ 4.01) (MeOH).

Di-Ac: [18304-03-5]
Cryst. (Me_2CO aq.). Mp 228.5-229.5°.

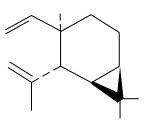
7-Me ether: [89320-82-1] ***Bhubaneswin***
$C_{19}H_{12}O_6$ 336.3
Cryst. ($Me_2CO/CHCl_3$). Mp 320°.

Di-Me ether: [3153-73-9] *7,7′-Dimethoxy-[6,8′-bi-2*H*-benzopyran]-2,2′-dione. 7,7′-Dimethoxy-6,8′-bicoumarin*. ***Matsukaze lactone***
$C_{20}H_{14}O_6$ 350.327
Platelets (MeOH). Mp 266.5-267.5°.

Miyazaki, T. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1236 (*isol*)
Spencer, R.R. *et al., J. Agric. Food Chem.*, 1967, **15**, 536 (*isol, struct*)
Kozawa, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2746 (*isol*)
Gonzalez, A.G. *et al., An. Quim.*, 1977, **73**, 1015 (*isol*)
Basa, S.C. *et al., Heterocycles*, 1984, **22**, 333 (*isol, cmr, pmr*)
Basa, S.C. *et al., Phytochemistry*, 1988, **27**, 1933 (*rev*)
Su, B.-N. *et al., J. Nat. Prod.*, 2002, **65**, 1278-1282 (*isol, pmr, cmr, ms*)

Bicycloelemene B-77

[32531-56-9]
3-Ethenyl-3,7,7-trimethyl-2-(1-methylethenyl)bicyclo[4.1.0]heptane, 9CI. 2-Isopropenyl-3-methyl-3-vinylbicyclo[4.1.0]heptane

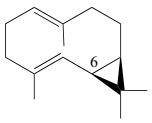


$C_{15}H_{24}$ 204.355
Constit. of peppermint oil. Oil. $[\alpha]_D^{20}$ -34.

Ulahov, R. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 808 (*isol*)
Takeda, K. *et al., Chem. Comm.*, 1971, 308 (*struct*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 852 (*synth*)

Bicyclogermacrene B-78

[24703-35-3]



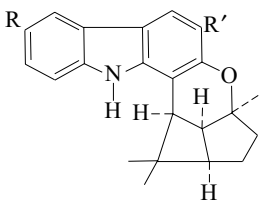
$C_{15}H_{24}$ 204.355
Constit. of the peel oil of *Citrus junos* (yuzu). Oil. $[\alpha]_D$ +61 ($CHCl_3$).

6-Epimer: [169276-07-7] ***Isolepidozene***
$C_{15}H_{24}$ 204.355
Oil. $[\alpha]_D$ -50 (c, 0.05 in $CHCl_3$).

Nishimura, K. *et al., Tetrahedron*, 1973, **29**, 271 (*isol, struct*)
McMurry, J.E. *et al., J.O.C.*, 1987, **52**, 4885 (*synth*)
Ihara, M. *et al., J.O.C.*, 1994, **59**, 8092 (*synth*)
Hardt, I.H. *et al., Phytochemistry*, 1995, **40**, 605 (*Isolepidozene*)

Bicyclomahanimbicine B-79

[28613-80-1]
*1,2,2*a*,10,10*c*,11,11*a*,11*b*-Octahydro-2*a*,7,11,11-tetramethyl-3-oxa-10-azacyclobut[3,4]indeno[5,6-*a*]fluorene, 9CI*



R = Me, R′ = H

$C_{23}H_{25}NO$ 331.457
Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Mp 218° dec. Probably an artifact. Also obt. by shaking a sol. of Mahanimbicine, M-30 with ion-exchange resin (H^+).

Kureel, S.P. *et al., Chem. Ind. (London)*, 1970, 958 (*uv, ir, pmr, struct, synth*)

Bicyclomahanimbine B-80

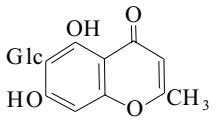
[31077-94-8]
*1,2,2*a*,10,10*c*,11,11*a*,11*b*-Octahydro-2*a*,4,11,11-tetramethyl-3-oxa-10-azacyclobut[3,4]indeno[5,6-*a*]fluorene, 9CI*
As Bicyclomahanimbicine, B-79 with
R = H, R′ = Me
$C_{23}H_{25}NO$ 331.457
Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Mp 145°. $[\alpha]_D^{23}$ -1.23 ($CHCl_3$). Probably an artifact. Also obt. readily from Mahanimbine, M-32.

N-*Me:*
Mp 156°.

Kureel, S.P. *et al., Tet. Lett.*, 1969, 3857 (*uv, ir, pmr, ms*)
Bandaranayake, W.M. *et al., J.C.S. Perkin 1*, 1974, 998 (*struct*)

Biflorin B-81

[89701-85-9]
*6-β-D-Glucopyranosyl-5,7-dihydroxy-2-methyl-4*H*-1-benzopyran-4-one, 9CI*

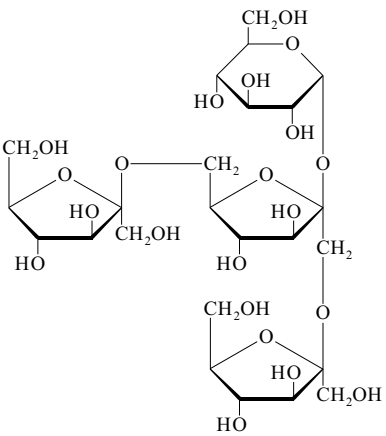


$C_{16}H_{18}O_9$ 354.313
Constit. of *Eugenia caryophyllata* (clove). Cryst. Mp 300-303° dec. $[\alpha]_D^{28}$ +24.4 (c, 0.34 in Py).

Ghosal, S. *et al., Phytochemistry*, 1983, **22**, 2591
Zhang, Y. *et al., Phytochemistry*, 1997, **45**, 401 (*isol, pmr, cmr*)

Bifurcose B-82

[3568-31-8]
1-β-D-Fructofuranosyl(2→1)-[β-D-fructofuranosyl(2→6)]-β-D-fructofuranosyl α-D-glucopyranoside. 1,6-Kestotetraose

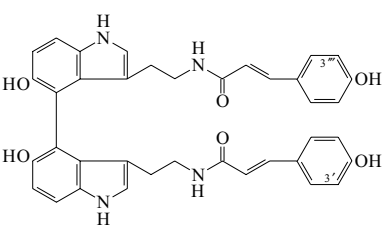


$C_{24}H_{42}O_{21}$ 666.583
A fructan. Isol. from barley (*Hordeum vulgare*) and *Panicum miliaceum* (proso millet). Cryst. Mp 156°. $[\alpha]_D^{20}$ +8.8 (H_2O).

Schlubach, H.H. *et al., Annalen*, 1958, **614**, 126; 1963, **665**, 191; 1964, **677**, 165 (*isol*)

4,4′′-Bi(*N*-4-hydroxycinnamoylserotonin) B-83

*4,4′′-Bis(*N-p-*coumaroylserotonin)*



$C_{38}H_{34}N_4O_6$ 642.71
(E,E)-form [175702-01-9]
Isol. from safflower (*Carthamus tinctorius*) oil cake. Powder. Mp 180-182°. λ_{max} 221 (ϵ 43000); 294 (ϵ 35000); 305 (ϵ 34700) (MeOH).

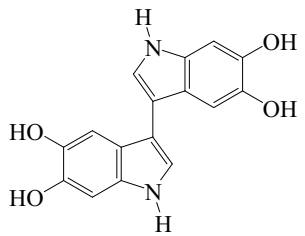
3′-Methoxy: [175702-02-0] ***4-[*N*-(*p*-Coumaroyl)serotonin-4″-yl]-*N*-feruloylserotonin***
$C_{39}H_{36}N_4O_7$ 672.736
From *Carthamus tinctorius* oil cake. Powder. Mp 179-181°. λ_{max} 221 (ϵ 70500); 292 (ϵ 51000); 309 (ϵ 52700) (MeOH).

3′,3‴-Dimethoxy: [175702-03-1] *4,4″-Bis(*N*-feruloyl)serotonin. 4,4″-Bi[*N*-(4-hydroxy-3-methoxycinnamoyl)serotonin]*
$C_{40}H_{38}N_4O_8$ 702.762
From *Carthamus tinctorius* oil cake. Mp 158-160°. λ_{max} 289 (ϵ 35400); 317 (ϵ 38800) (MeOH).

Zhang, H.-L. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1910-1914 (*isol, uv, ir, pmr, cmr*)

3,3′-Bi-1*H*-indole-5,5′,6,6′-tetrol B-84

*5,5′,6,6′-Tetrahydroxy-3,3′-bi-1*H*-indole*

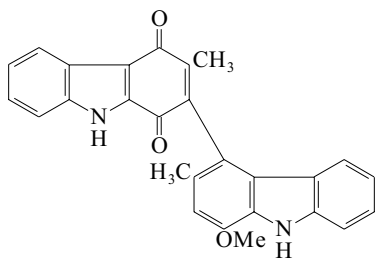


$C_{16}H_{12}N_2O_4$ 296.282
Constit. of beetroot peel, *Beta vulgaris*.

Kujala, T. *et al., Z. Naturforsch., C*, 2001, **56**, 714-718 (*isol, pmr, cmr, ms*)

Bikoeniquinone A B-85

[155519-84-9]
*1′-Methoxy-3,3′-dimethyl-[2,4′-bi-9*H*-carbazole]-1,4-dione, 9CI*

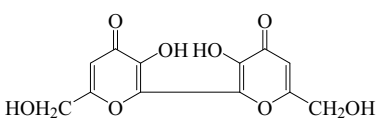


$C_{27}H_{20}N_2O_3$ 420.467
Alkaloid from roots of *Murraya koenigii* (curryleaf tree) (Rutaceae). Orange oil.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)

Bikojic acid B-86

*6,6′-Bis(5-hydroxy-2-hydroxymethyl-4*H*-pyran-4-one). BGY-F*

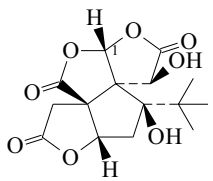


$C_{12}H_{10}O_8$ 282.206
Dimer of 5-Hydroxy-2-(hydroxymethyl)-4*H*-pyran-4-one, H-500. Found in cotton lint associated with aflatoxin contamination in cotton seed *Gossypium hirsutum*. Bright greenish-yellow fluorescent compd.

Zeringue, H.J. *et al., Phytochemistry*, 1999, **52**, 1391-1397

Bilobalide A B-87

[33570-04-6]
Bilobalide

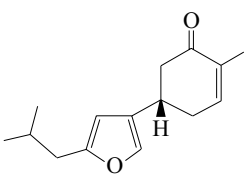


$C_{15}H_{18}O_8$ 326.302
Constit. of leaves of *Ginkgo biloba* (ginkgo). Cryst. (H_2O). Mp 300°. $[\alpha]_D^{20}$ -66.6. Log P -3.25 (uncertain value) (calc). Component of commercially available *Ginkgo biloba* extract (GBE).

Weinges, K. *et al., Annalen*, 1969, **724**, 214; 1972, **759**, 158 (*isol, pmr*)
Nakanishi, K. *et al., J.A.C.S.*, 1971, **93**, 3544 (*isol, struct*)
Corey, E.J. *et al., J.A.C.S.*, 1987, **109**, 7534 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 1988, **29**, 3423 (*synth*)
Crimmins, M.T. *et al., J.A.C.S.*, 1992, **114**, 5445; 1993, **115**, 3146 (*synth*)
Atzori, C. *et al., Antimicrob. Agents Chemother.*, 1993, **37**, 1492 (*activity*)
Bruno, C. *et al., Planta Med.*, 1993, **59**, 302 (*pharmacol*)
Van Beek, T. *et al., J. Nat. Prod.*, 1997, **60**, 735-738 (*isol*)
Song, W. *et al., Acta Pharm. Sin.*, 2000, **21**, 415-420 (*activity*)

Bilobanone B-88

2-Methyl-5-[5-(2-methylpropyl)-3-furanyl]-2-cyclohexen-1-one, 9CI



$C_{15}H_{20}O_2$ 232.322
(S)-form [17015-33-7]
Constit. of *Ginkgo biloba* (ginkgo). Oil. $Bp_{0.09}$ 118-122° (bath). $[\alpha]_D$ +6.7.

Oxime:
Mp 64-65°.

Semicarbazone:
Mp 142-144°.

1ξ-Alcohol: ***Bilobanol***
$C_{15}H_{22}O_2$ 234.338

Irie, H. *et al., Chem. Comm.*, 1967, 678 (*struct*)
Büchi, G. *et al., J.O.C.*, 1969, **34**, 857 (*synth*)
Hegde, S.E. *et al., J.O.C.*, 1982, **47**, 3148 (*synth*)

Traditional Chinese Medicines, (ed. Milne, G.A.), Ashgate, 1999, 651 (*Bilobanol*)

Biochanin C B-89

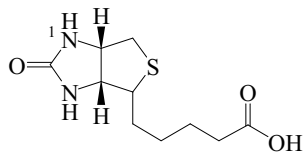
$C_{16}H_{13}N_3O_4$ 311.296
Struct. unknown. Presumably an alkaloid. Isol. from seeds of *Cicer arietinum* (chickpea). Large prisms (EtOH or H_2O). Sol. H_2O. Mp 315°. Conts. one OMe group, unsatd. to Br_2.

Siddiqui, S. *et al., J. Sci. Ind. Res.*, 1945, **4**, 68; *CA*, **40**, 1502
Warsi, S.A. *et al., Pak. J. Sci. Res.*, 1951, **3**, 85; *CA*, **47**, 3305f

Biotin, INN, USAN B-90

[58-85-5]

[22879-79-4]
*Hexahydro-2-oxo-1*H*-thieno[3,4-d]imidazole-4-pentanoic acid, 9CI. Vitamin H. Coenzyme R. Vitamin B_7. Factor S*†



$C_{10}H_{16}N_2O_3S$ 244.314
Present in many foods; particularly rich sources include yeast, eggs, liver, certain fish (e.g. mackerel, salmon, sardines), soybeans, cauliflower and cow peas. Dietary supplement. Isol. from various higher plant sources, e.g. sweet corn seedlings and radish leaves. Fine needles (H_2O). Sol. H_2O. Mp 232-233°. $[\alpha]_D^{20}$ +91 (c, 1 in 0.1*M* NaOH). Log P -0.18 (calc).

▶ Shows exp. reproductive effects.

S-Oxide: [3376-83-8] *Biotin sulfoxide*
$C_{10}H_{16}N_2O_4S$ 260.313
Polymorphic plates (H_2O). Mp 238° part. dec. $[\alpha]_D^{20}$ -39.5 (c, 1.01 in 0.1*M* NaOH).

Me ester: [608-16-2]
$C_{11}H_{18}N_2O_3S$ 258.341
Cryst. Mp 166.5°. $[\alpha]_D^{15}$ +82 (c, 0.45 in MeOH).

Succinimidoyl ester: [35013-72-0]
$C_{14}H_{19}N_3O_5S$ 341.387
Cryst. (2-propanol). Mp 196-198°.

Amide: [6929-42-6] *Biotinamide*
$C_{10}H_{17}N_3O_2S$ 243.329
Rosettes (MeOH or H_2O). Mp 242-244°. $[\alpha]_D^{23}$ +80 (c, 2.5 in EtOH).

N^1*-Benzyl:*N*-Benzylbiotin. γ-Biotin*
$C_{17}H_{22}N_2O_3S$ 334.438
Needles (MeOH aq.). Mp 183-184°. Originally descr. as a natural vitamin under the name γ-biotin and descr. as *N*-phenylbiotin. Later shown to be an artifact with no vitamin activity.

[10406-89-0]

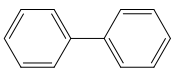
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 809C (*ir*)
Aldrich Library of ^{13}C *and* ^1H *FT NMR Spectra*, 1992, **1**, 1317C (*nmr*)
Harris, S.A. *et al., J.A.C.S.*, 1944, **66**, 1756 (*synth, resoln*)

Wolf, D.E. *et al., J.A.C.S.*, 1951, **73**, 4142 (*amide*)
Jansen, A.B.A. *et al., J.C.S.*, 1962, 4909; 1964, 1530 (*γ-Biotin*)
Trotter, J. *et al., Biochemistry*, 1966, **5**, 713 (*cryst struct, abs config*)
Green, N.M. *et al., J.C.S.(C)*, 1970, 1330 (*cd, ord*)
De Titta, G.T. *et al., J.A.C.S.*, 1976, **98**, 1920 (*cryst struct*)
Marx, M. *et al., J.A.C.S.*, 1977, **99**, 6754 (*synth, bibl*)
Ohrui, H. *et al., Agric. Biol. Chem.*, 1978, **42**, 865 (*synth*)
Vasilevskis, J. *et al., J.A.C.S.*, 1978, **100**, 7423 (*synth, bibl*)
Uskokovic, M.R. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **24**, 41 (*rev*)
Baggiolini, E.G. *et al., J.A.C.S.*, 1982, **104**, 6460 (*synth*)
Whitney, R.A. *et al., Can. J. Chem.*, 1983, **61**, 1158 (*synth*)
Bonjour, J.-P. *et al., Handbook of Vitamins*, (ed. Machlin, L.J.), M. Dekker, New York, 1984, 403 (*rev*)
Dakshinamurti, K. *et al., Ann. N.Y. Acad. Sci.*, (Eds.), 1985, **447**, (*book*)
Bentley, R. *et al., Trends Biochem. Sci.*, 1985, **10**, 51 (*rev, abs config*)
Al-Hakim, A.H. *et al., Nucleic Acids Res.*, 1986, **14**, 9965-9976 (*succinimidoyl ester*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1715
Lee, H.L. *et al., Tetrahedron*, 1987, **43**, 4887 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 1988, **29**, 57 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BGD100
Senuma, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 882 (*rev, synth*)
Parameswaran, K.N. *et al., Org. Prep. Proced. Int.*, 1990, **22**, 119 (*amide*)
Alcázar, V. *et al., Tetrahedron*, 1990, **46**, 1057 (*synth*)
Bihovsky, R. *et al., Tetrahedron*, 1990, **46**, 7667 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1037
De Titta, G.T. *et al., J.A.C.S.*, 1994, **116**, 6485 (*cryst struct, nmr*)
Moolenaar, M.J. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 2391 (*synth*)
Deroose, F.D. *et al., J.O.C.*, 1995, **60**, 321 (*synth, bibl*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 285 (*bibl, synth*)
De Clercq, P.J. *et al., Chem. Rev.*, 1997, **97**, 1755-1792 (*rev, synth*)
Chen, F.-E. *et al., Synthesis*, 2000, 2004-2008 (*synth, ir, pmr, ms*)
Chavan, S.P. *et al., J.O.C.*, 2001, **66**, 6197-6201 (*synth*)
Mori, Y. *et al., Heterocycles*, 2002, **58**, 125-127 (*synth*)
Seki, M. *et al., J.O.C.*, 2002, **67**, 5527-5536 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSU100

Biphenyl, 8CI, BSI, ISO B-91

[92-52-4]

1,1′-Biphenyl, 9CI. Phenylbenzene. Diphenyl. Bibenzene. E230. FEMA 3129



$C_{12}H_{10}$ 154.211

Fungistat, esp. for citrus fruits. Used as food preservative and flavouring agent. Detected in bilberry, wine grape, carrot, peas, rum, potato, bell pepper, tomato, butter, milk, smoked fatty fish, cocoa, coffee, roast peanuts, olive, buckwheat and tamarind. Generally, the fruit packaging is impregnated with biphenyl, which evaporates into the air space surrounding the fruit. Some biphenyl is absorbed by the fruit skins. Monoclinic cryst. with faint pleasant odour. Mp 71°. Bp 254-255° Bp_{22} 145° $Bp_{0.2}$ 70-78°. Planar in the cryst. state at -233°, dihedral angle 10° in cryst. state >-233°, 25° in molten state, 32° in soln., 42° in gas phase.

▶ Fl. p. 113°, autoignition temp. 540°. Eye and mucous membrane irritant. Prolonged or repeated skin contact may cause sensitisation and dermatitis. Occup. exposure causes changes to central and peripheral nervous systems, and gastrointestinal disturbances. LD_{50} (rat, orl) 3280 mg/kg. OES: long-term 0.2 ppm; short-term 0.6 ppm. DU8050000

[8004-13-5]

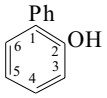
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 948A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 28C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 871B (*ir*)
Forrest, J. *et al., J.C.S.*, 1960, 574 (*synth*)
Brownlee, R.T.C. *et al., J.A.C.S.*, 1968, **90**, 1757 (*ir*)
Laseter, J.L. *et al., Org. Mass Spectrom.*, 1970, **4**, 599 (*ms*)
Nordén, B. *et al., Acta Chem. Scand.*, 1972, **26**, 429 (*uv*)
Kamezawa, N. *et al., J. Magn. Reson.*, 1973, **11**, 88 (*pmr*)
Schulman, E.M. *et al., J.O.C.*, 1974, **39**, 2686 (*cmr*)
Charbonneau, G.P. *et al., Acta Cryst. B*, 1976, **32**, 1420; 1977, **33**, 1586 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 782 (*rev*)
Takagi, K. *et al., Chem. Lett.*, 1979, 917 (*synth*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Pesticide Manual, 9th edn., 1991, 1010
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A166
Bock, H. *et al., Chem. Eur. J.*, 1995, **1**, 557 (*bibl, conformn*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 156-157 (*use, props, occur*)
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 113
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 134
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BGE000

2-Biphenylol, 8CI B-92

[90-43-7]

[1322-20-9]

2-Hydroxybiphenyl. 2-Phenylphenol, BSI, ISO. o-Xenol. Orthophenylphenol. Orthoxenol. Dowicide 1. Manusept. Nipacide OPP. Rotoline. Stellisept. Torsite. E231. FEMA 3959



$C_{12}H_{10}O$ 170.21

Antifungal agent, preservative. Used for post-harvest control of storage disease in apples, citrus fruit, stone fruit, tomatoes, cucumber and peppers through the use of impregnated wrapping materials or by direct application in a wax. Used in food seasonings. Inhibitory to a wider range of moulds than Biphenyl, B-91. The practical way of treatment is to immerse citrus fruit in an alkaline aq. soln. of the parent compd. or its Na salt. Needles (petrol). Mp 56°. Bp 275° Bp_{14} 145°. pK_{a1} 10.01 (20°).

▶ Eye and skin irritant. LD_{50} (mus, orl) 1050 mg/kg. Exp. carcinogen. Exp. teratogenic effects. Fl. p. 107°.. DV5775000

Na salt: [132-27-4] *Dowicide A. Natriphene. E232*
Agricultural fungicide, disinfectant, food preservative, mould inhibitor for apples. Tetrahydrate. Sol. H_2O.

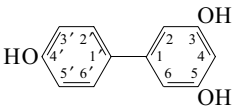
▶ DV7700000

[132-27-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1057A; 1059D; 1115D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 212A; 215C; 317A (*nmr*)
Hirsch, R. *et al., Ber.*, 1890, **23**, 3705 (*synth*)
Musso, H. *et al., Chem. Ber.*, 1959, **92**, 3101 (*ir*)
Trible, M.T. *et al., J.A.C.S.*, 1969, **91**, 379 (*pmr*)
Drapala, T. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1974, **48**, 965 (*ir, uv*)
Asabe, Y. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1975, **24**, 160; *CA*, **83**, 22035f (*use*)
Robbiani, R. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 120 (*ms*)
Lotjonen, S. *et al., Finn. Chem. Lett.*, 1978, 260; *CA*, **90**, 120562q (*cmr*)
Reitz, R.H. *et al., Chem. Biol. Interact.*, 1983, **43**, 99 (*Na salt*)
IARC Monog., 1983, **30**, 329; *Suppl.* 7, 70 (*rev, tox*)
Perrin, M. *et al., Acta Cryst. C*, 1987, **43**, 980 (*cryst struct*)
Roshchina, E.N. *et al., Zh. Prikl. Khim. (Leningrad)*, 1989, **62**, 1295 (*synth*)
Nakagawa, Y. *et al., Biochem. Pharmacol.*, 1992, **43**, 159 (*tox*)
Lambert, A.C. *et al., Mutat. Res.*, 1994, **322**, 243 (*tox*)
Nakagawa, Y. *et al., Cancer Lett. (Shannon, Irel.)*, 1996, **101**, 227 (*tox*)
Pesticide Manual, 11th edn., 1997, No. 567
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1473 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BGJ250; PEG000; BGJ750

3,4′,5-Biphenyltriol B-93

[74276-54-3]
3,4′,5-Trihydroxybiphenyl

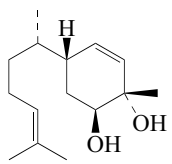


$C_{12}H_{10}O_3$ 202.209
Constit. of *Trifolium repens* (white clover). Characterised as the Tri-Me ether.

Tri-Me ether: [54960-97-3] *3,4′,5-Trimethoxybiphenyl*
$C_{15}H_{16}O_3$ 244.29
Plates (MeOH). Mp 61-62°.

Scheinmann, F. *et al., J.C.S. Perkin 1*, 1974, 2423 (*synth, deriv, uv, pmr*)
Ghosal, S. *et al., J. Chem. Res., Synop.*, 1988, 196 (*isol, uv, ir, pmr*)

1,10-Bisaboladiene-3,4-diol B-94

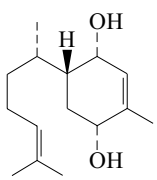


(3*S*,4*S*,6*R*,7*S*)-*form*

$C_{15}H_{26}O_2$ 238.369
(3*S*,4*S*,6*R*,7*S*)-*form* [129673-87-6]
Constit. of *Curcuma longa* (turmeric). Viscous oil. $[\alpha]_D$ -31.7 (c, 0.23 in MeOH).
(3*S*,4*S*,6*S*,7ξ)-*form*
Oil.

Zdero, C. *et al., Phytochemistry*, 1987, **26**, 1999-2006 (*isol, pmr*)
Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201-2205 (*isol, pmr, cmr*)
Sy, L.-K. *et al., Phytochemistry*, 1997, **45**, 537 (*isol, pmr, cmr*)

2,10-Bisaboladiene-1,4-diol B-95

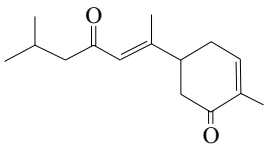


$C_{15}H_{26}O_2$ 238.369
Constit. of *Curcuma longa* (turmeric). Needles (hexane). Mp 126.5-129°. $[\alpha]_D$ +5 (MeOH).

Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201-2205 (*isol, pmr, cmr*)

3,7-Bisaboladiene-2,8-dione B-96

[57095-92-8]
10,11-Dihydro-6-oxoatlantone

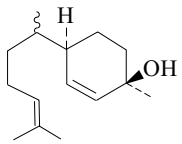


$C_{15}H_{22}O_2$ 234.338
Constit. of *Ginkgo biloba* (ginkgo).

Irie, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1892

1,10-Bisaboladien-3-ol B-97

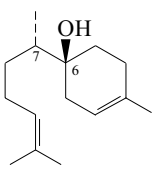
[58334-55-7]
Zingiberenol



$C_{15}H_{26}O$ 222.37
Constit. of *Zingiber officinale*, isol. by glc. Oil.

Terhune, S.J. *et al., Can. J. Chem.*, 1975, **53**, 3285 (*isol*)
Paquette, L.A. *et al., Tet. Lett.*, 1982, **23**, 131 (*synth*)

2,10-Bisaboladien-6-ol B-98



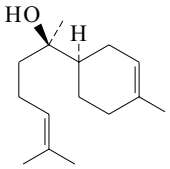
(6*S*,7*S*)-*form*

$C_{15}H_{26}O$ 222.37
(6*S*,7*S*)-*form* [15352-77-9]
β-Bisabolol
Constit. of *Gossypium hirsutum* (cotton) oil and other essential oils. Oil. Bp_2 121-122°. $[\alpha]_D^{20}$ +7.16 (c, 0.28 in $CHCl_3$). $[\alpha]_D^{20}$ +23.3 ($CHCl_3$).
(6*R*,7*S*)-*form*
6*-epi-*β-Bisabolol
Constit. of bergamot oil. $[\alpha]_D^{20}$ -57 (c, 0.1 in $CHCl_3$).

Minyard, J.P. *et al., J.O.C.*, 1968, **33**, 909 (*isol*)
Takaoka, D. *et al., Phytochemistry*, 1976, **15**, 425 (*isol*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1986, **69**, 698 (*abs config*)
Fráter, G. *et al., Helv. Chim. Acta*, 1989, **72**, 653 (*synth*)

2,10-Bisaboladien-7-ol B-99

6-Methyl-2-(4-methyl-3-cyclohexen-1-yl)-5-hepten-2-ol, 8CI



(6*R*,7*R*)-*form*

$C_{15}H_{26}O$ 222.37Log P 4.66 (calc).
(6*R*,7*R*)-*form* [23178-88-3]
(+)-α-Bisabolol. *Bisabolol*
Constit. of essential oil of *Populus balsamifera* (balsam poplar). Oil. Bp_{12} 154-156°. $[\alpha]_D^{23}$ +53.8 (c, 2.6 in $CHCl_3$).
► LD_{50} (rat, orl) 14850 mg/kg. MJ9685000
7-O-*β-D-Fucopyranoside:* [84847-68-7]
$C_{21}H_{36}O_5$ 368.512
Oil. $[\alpha]_D$ -20.6 (c, 1 in $CHCl_3$).
(6*R*,7*S*)-*form* [76738-75-5] ***6*-Epi-α-bisabolol***
Syrup. $[\alpha]_D^{23}$ +67.4 (MeOH).
(6*S*,7*R*)-*form* [78148-59-1] ***Anymol***. *7-Epi-α-Bisabolol*
Oil. Bp_1 114°. $[\alpha]_D$ -69 (c, 1.3 in EtOH).
p-*Phenylazophenylurethane:*
Orange needles (petrol). Mp 103-103.5°. $[\alpha]_D$ -7 (c, 1 in $CHCl_3$).
7-O-*Lyxopyranoside:* [258337-41-6]
$C_{20}H_{34}O_5$ 354.486
(6*S*,7*S*)-*form* [23089-26-1] ***(-)-α-Bisabolol***. *Levomenol, INN*
Isol. from essential oil of *Matricaria chamomilla* (German chamomile). Yellowish oil with sweetish odour. d_4^{20} 0.92. Bp_{12} 153°. $[\alpha]_D^{24}$ -68.4 (c, 1.16 in EtOH). n_D^{20} 1.4936. Log P 4.66 (calc).
► LD_{50} (rat) 0.014 mg/kg.
(6ξ,7ξ)-*form*
O-*(6-Deoxy-β-D-altropyranoside):* [79197-22-1]
$C_{21}H_{36}O_5$ 368.512
Gum. $[\alpha]_D^{24}$ -6.5 (c, 1 in $CHCl_3$). Config. unknown.

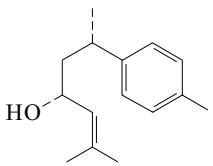
[515-69-5]

Šorm, F. *et al., Coll. Czech. Chem. Comm.*, 1951, **16**, 626 (*isol*)
O'Brien, K.G. *et al., Aust. J. Chem.*, 1953, **6**, 166; 1954, **7**, 298 (*Anymol*)
Yakovlev, V. *et al., Arzneim.-Forsch.*, 1969, **19**, 615 (*pharmacol, tox*)
Sampath, V. *et al., Indian J. Chem.*, 1969, **7**, 1060 (*isol*)
Kergomard, A. *et al., Tetrahedron*, 1977, **33**, 2215 (*synth*)
Schwartz, M.A. *et al., J.O.C.*, 1979, **44**, 953 (*synth, abs config*)
Rustaiyan, A. *et al., Phytochemistry*, 1981, **20**, 1429 (*deoxyaltroside*)
Babin, D. *et al., Tetrahedron, Suppl.*, No. 1, 1981, 1 (*synth, abs config*)
San Feliciano, A. *et al., Phytochemistry*, 1982, **21**, 2115-2116 (*fucoside*)
Khan, V.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 575; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 575 (*isol, cmr*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1986, **69**, 698 (*isol*)
Titova, T.F. *et al., Khim. Prir. Soedin.*, 1987, **23**, 460; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 386 (*isol*)
O'Donnell, G.W. *et al., Aust. J. Chem.*, 1989, **42**, 2021 (*bibl, isol, deriv*)

Carman, R.M. *et al., Aust. J. Chem.*, 1989, **42**, 2035; 2041 (*cryst struct, bibl, synth*)
Wu, C.-L. *et al., Phytochemistry*, 1992, **31**, 4213 (*pmr, cmr*)
Chen, X.-J. *et al., J.O.C.*, 1993, **58**, 5528 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1383
Nemoto, H. *et al., Tet. Lett.*, 1993, **34**, 4939 (*synth*)
Hashidoko, Y. *et al., Phytochemistry*, 1994, **35**, 325 (*6-Epi-α-bisabolol*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995,
Meng, J.C. *et al., Spectrosc. Lett.*, 1999, **32**, 1005-1012 (*lyxopyranoside*)
Hashidoko, Y. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 907-910 (*isol, pmr, cmr*)

1,3,5,10-Bisabolapentaen-9-ol B-100

[120710-98-7]
Bisacumol

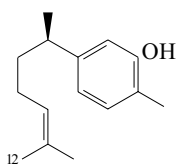


$C_{15}H_{22}O$ 218.338
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ +13.9 (c, 0.42 in EtOH).

Uehara, S. *et al., Chem. Pharm. Bull.*, 1989, **37**, 237 (*isol, pmr, cmr*)

1,3,5,10-Bisabolatetraen-2-ol B-101

[30199-26-9]
5-(1,5-Dimethyl-4-hexenyl)-2-methylphenol, 9CI. ***Xanthorrhizol***



$C_{15}H_{22}O$ 218.338
Constit. of rhizomes of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D^{20}$ -52.5. λ_{max} 275 (ϵ 1900) (EtOH) (Derep).

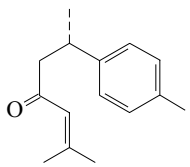
12-Acetoxy: ***12-Acetoxyxanthorrhizol****. 13-Acetoxyxanthorrhizol*
$C_{17}H_{24}O_3$ 276.375
Oil. $[\alpha]_D$ -76.5 (c, 0.52 in $CHCl_3$).

10,11-Epoxide: [364373-61-5] *10,11-Epoxy-1,3,5-bisabolatrien-2-ol.* ***10,11-Epoxyxanthorrhizol****. 12,13-Epoxyxanthorrhizol (incorr.)*
$C_{15}H_{22}O_2$ 234.338
Oil. $[\alpha]_D$ -0.13 (c, 0.54 in MeOH). Mixt. of 10-epimers λ_{max} 272 (ϵ 2317) (MeOH).

Rimpler, H. *et al., Z. Naturforsch., B*, 1970, **25**, 995 (*isol, struct*)
Mane, R.B. *et al., Indian J. Chem.*, 1974, **12**, 938 (*synth*)
John, T.K. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 35 (*synth*)
Rane, R.K. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 572 (*synth*)
Garcá, G.E. *et al., J. Nat. Prod.*, 1987, **50**, 1055 (*synth*)
Joseph-Nathan, P. *et al., J. Nat. Prod.*, 1988, **51**, 1116 (*cmr*)
Mendoza, G.V. *et al., J. Nat. Prod.*, 1993, **56**, 2073 (*12-Acetoxyxanthorrhizol*)
Aguilar, M.I. *et al., Phytochemistry*, 1993, **33**, 1161 (*cmr*)
Meyers, A.I. *et al., J.O.C.*, 1997, **62**, 5219-5221 (*synth*)
Pat. Coop. Treaty (WIPO), 2000, 00 67 711; *CA*, **133**, 355216
Hwang, J.-K. *et al., Planta Med.*, 2000, **66**, 196 (*Xanthorrhizol, isol, activity*)
Aguilar, M.I. *et al., Nat. Prod. Lett.*, 2001, **15**, 93-101 (*10,11-Epoxyxanthorrhizol*)

1,3,5,10-Bisabolatetraen-9-one B-102

2-Methyl-6-(4-methylphenyl)-2-hepten-4-one, 9CI. **ar-*Turmerone***. *Dehydroturmerone*



$C_{15}H_{20}O$ 216.322
(R)-form [532-65-0]
Constit. of essential oil from *Curcuma longa* (turmeric), *Curcuma amada* (mango-ginger). Pale yellow oil. Sol. C_6H_6, hexane. Bp_{10} 159-160°. $[\alpha]_D^{20}$ +82.21. Poss. artifact arising from aromatisation of 2,5,10-Bisabolatrien-9-one, B-113 λ_{max} 275 (ϵ 15700) (MeOH) (Berdy).

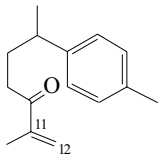
Semicarbazone:
Cryst. (C_6H_6). Mp 106°.

10,11-Dihydro: [4179-20-8] *2-Methyl-6-(4-methylphenyl)-4-heptanone. 1,3,5-Bisabolatrien-9-one. Dihydro-*ar*-turmerone*
$C_{15}H_{22}O$ 218.338
Oil. Bp_1 115°. $[\alpha]_D$ +31 (c, 7.2 in $CHCl_3$).

Rupe, H. *et al., Helv. Chim. Acta*, 1936, **19**, 569 (*isol*)
Honwad, V.K. *et al., Tetrahedron*, 1964, **20**, 2921; 1965, **21**, 2593 (*abs config, synth, pmr*)
Rao, G.S.K. *et al., Can. J. Chem.*, 1968, **46**, 1467 (*synth*)
Grieco, P.A. *et al., J.O.C.*, 1973, **38**, 2909 (*synth*)
Kashima, C. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 1735 (*synth, pmr*)
Gosselin, P. *et al., J.O.C.*, 1979, **44**, 2807 (*synth*)
Meyers, A.I. *et al., Tet. Lett.*, 1979, 2749 (*synth*)
Su, H.C.F. *et al., J. Agric. Food Chem.*, 1982, **30**, 290-292 (*isol*)
El Jazouli, M. *et al., Chem. Comm.*, 1985, 1598 (*synth*)
Motoyoshiya, J. *et al., J.O.C.*, 1985, **50**, 1326 (*synth*)
Gharpure, M.M. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 1214 (*synth*)
Strunz, G.M. *et al., Can. J. Chem.*, 1992, **70**, 1317 (*synth*)
Ferreira, L.A. *et al., Toxicon*, 1992, **30**, 1211-1218 (*pharmacol*)
Kitahara, T. *et al., Biosci., Biotechnol., Biochem.*, 1993, **53**, 1137 (*synth*)
Fuganti, C. *et al., J.C.S. Perkin 1*, 1999, 279-282 (*synth*)

1,3,5,11-Bisabolatetraen-10-one B-103

[76760-39-9]
2-Methyl-6-(4-methylphenyl)-1-hepten-3-one



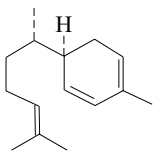
$C_{15}H_{20}O$ 216.322
Props. and registry nos. refer to racemates which were obt. synthetically. Constit. of oil of *Cinnamomum cassia* (Chinese cinnamon). Oil. $Bp_{0.01}$ 71-74°.

11,12-Dihydro: [76760-40-2] *1,3,5-Bisabolatrien-10-one. 2-Methyl-6-(4-methylphenyl)-3-heptanone*
$C_{15}H_{22}O$ 218.338
Constit. of oil of *Cinnamomum cassia* (Chinese cinnamon). Oil. $Bp_{0.01}$ 90°.

Thomas, A.F. *et al., Helv. Chim. Acta*, 1980, **63**, 1615 (*isol, struct, ms, synth*)

1,3,10-Bisabolatriene B-104

[495-60-3]
Zingiberene



Absolute configuration

$C_{15}H_{24}$ 204.355
Constit. of ginger oil. Also from wild thyme (*Thymus serpyllum*), long pepper (*Piper longum*) and kua (*Curcuma zedoaria*). Oil. Bp_{11} 128-130°. $[\alpha]_D^{27}$ -61.7 ($CHCl_3$).

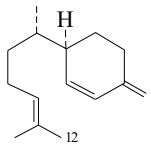
Nitrosochloride:
Cryst. Mp 93-94°.

7-Epimer: ***7-Epizingiberene***
$C_{15}H_{24}$ 204.355
Oil. $[\alpha]_D^{26}$ -76.1 ($CHCl_3$).

Eschenmoser, A. *et al., Helv. Chim. Acta*, 1950, **33**, 171 (*isol, struct*)
Arigoni, D. *et al., Helv. Chim. Acta*, 1954, **37**, 881 (*abs config*)
Joshi, G.D. *et al., Indian J. Chem.*, 1965, **3**, 91 (*synth*)
Soffer, M.D. *et al., Tet. Lett.*, 1985, **26**, 3543 (*cryst struct*)
Bhonsle, J.B. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 313 (*synth, bibl*)
Breedon, D.C. *et al., Tetrahedron*, 1994, **50**, 11123 (*isol, cmr, pmr*)
Millar, J.G. *et al., J. Nat. Prod.*, 1998, **61**, 1025-1026 (*isol*)

1,3(15),10-Bisabolatriene B-105

[20307-83-9]
3-(1,5-Dimethyl-4-hexenyl)-6-methylenecyclohexene, 9CI. ***β-Sesquiphellandrene***



$C_{15}H_{24}$ 204.355
Constit. of the oil of ginger (*Zingiber officinale*). Oil. Bp_1 90°. $[\alpha]_D^{20}$ -3.99 (neat).

Nitrosite:
Cryst. (Me_2CO). Mp 88-90° dec. $[\alpha]_D^{20}$ +29 (c, 1.5 in $CHCl_3$).

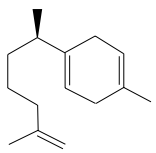
10ξ,11ξ-Epoxide: [80442-54-2] ***10,11-Epoxy-1,3(15)-bisaboladiene***. *10,11-Epoxy-β-sesquiphellandrene*
$C_{15}H_{24}O$ 220.354
Oil.

12-Oxo: [71939-69-0] *1,3(15),10-Bisabolatrien-12-al. 12-Oxo-β-sesquiphellandrene*
$C_{15}H_{22}O$ 218.338
Oil. $[\alpha]_D$ -9.3 (c, 0.15 in $CHCl_3$).

Connell, D.W. *et al., Aust. J. Chem.*, 1966, **19**, 283 (*β-Sesquiphellandrene*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 677 (*12-Oxo-β-sesquiphellandrene*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1887 (*Epoxybisaboladiene*)
Kreiser, W. *et al., Helv. Chim. Acta*, 1999, **82**, 1427-1433 (*synth*)

2,5,11-Bisabolatriene B-106

[451-56-9]
1-(1,5-Dimethyl-5-hexenyl)-4-methyl-1,4-cyclohexadiene, 9CI. ***β-Curcumene***



(*R*)-form

$C_{15}H_{24}$ 204.355

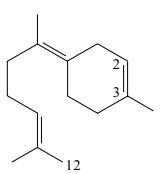
(R)-form [28976-67-2]
Constit. of the essential oil of *Curcuma amada* (mango-ginger) and *Curcuma xanthorrhiza* (Java turmeric). Liq. Bp_{19} 142°. $[\alpha]_D$ -48.2. The abs. config is as in CA but does not appear to be explicitly stated in the lit..

(S)-form
$Bp_{2.2}$ 98-100°. $[\alpha]_D^{20}$ +26.7.

Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1951, 987
Jain, M.K. *et al., Indian J. Chem.*, 1964, **2**, 39 (*isol*)

2,6,10-Bisabolatriene B-107

[495-62-5]
4-(1,5-Dimethyl-4-hexenylidene)-1-methylcyclohexene, 9CI. ***γ-Bisabolene***. *α-Bisabolene (obsol.)†. γ-Limene*



(*E*)-form

$C_{15}H_{24}$ 204.355
Flavouring ingredient used singly or as mixed isomers. Component of FEMA 3331. See also 2,7,10-Bisabolatriene, B-108.

(E)-form [53585-13-0]
Oil. $[\alpha]_D^{24}$ -18.8 (c, 1 in $CHCl_3$).

2,3-Epoxide: [75744-73-9] *2,3-Epoxy-6,10-bisaboladiene.* ***γ-Bisabolene-2,3-epoxide***
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D$ +37.3 (c, 2.2 in $CHCl_3$). Called γ-Bisabolene 8,9-epoxide in the reference.

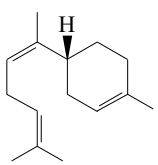
12-Hydroxy:2,6,10-Bisabolatrien-12-ol. ***12-Hydroxy-γ-bisabolene***
$C_{15}H_{24}O$ 220.354
Oil.

(Z)-form [13062-00-5]
Constit. of oil of myrrh and oil of lime. Oil.

Vig, O.P. *et al., Indian J. Chem.*, 1970, **8**, 955 (*synth*)
Giraudi, E. *et al., Recherches*, 1974, **19**, 205 (*synth*)
Overton, K.H. *et al., Chem. Comm.*, 1976, 105 (*biosynth*)
Wolinsky, J.E. *et al., J.O.C.*, 1976, **41**, 697 (*struct*)
Delay, F. *et al., Helv. Chim. Acta*, 1979, **62**, 369 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **80**, 1997 (*isol*)
Suzuki, T. *et al., Chem. Lett.*, 1980, 1267 (*epoxide*)
Buss, A.D. *et al., Tet. Lett.*, 1983, **24**, 111 (*synth*)
Anastasis, P. *et al., Can. J. Chem.*, 1984, **62**, 2079 (*biosynth, bibl*)
Look, S.A. *et al., Experientia*, 1984, **40**, 931 (*12-Hydroxy-γ-bisabolene*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 617 (*synth, deriv*)
Anastasia, L. *et al., Eur. J. Org. Chem.*, 2001, 3039-3043 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 159-160 (*FEMA 3331, use*)

2,7,10-Bisabolatriene B-108

[17627-44-0]
4-(1,5-Dimethyl-1,4-hexadienyl)-1-methylcyclohexene, 9CI. ***α-Bisabolene***†. *α-Limene. FEMA 3331*



(*R,E*)-form

$C_{15}H_{24}$ 204.355
Not the same as 2,6,10-Bisabolatriene, B-107 which has been renamed (formerly α-Bisabolene). The FEMA number refers to mixed bisabolenes including 2,7(14),10-Bisabolatriene, B-109 and 2,6,10-Bisabolatriene B-107. Flavouring ingredient isol. from bisabol myrrh and other natural sources, e.g. lemon, bergamot.

(R,E)-form [70286-31-6]
Oil. $[\alpha]_D^{20}$ +54.3 (c, 1 in EtOH).

(R,Z)-form [70286-33-8]
Oil. $[\alpha]_D^{20}$ -12 (c, 1 in EtOH).

(S,E)-form [70286-32-7]
Oil. $[\alpha]_D^{20}$ -38.9 (c, 1 in EtOH).

(S,Z)-form [58845-44-6]
Constit. of oil of Opoponax. Oil. Bp_{12} 155-157°. $[\alpha]_D^{20}$ +8 (c, 1 in EtOH).

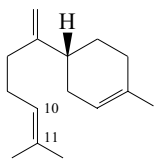
(ξ,E)-form
Oil. Abs. config. not detd., no opt. rotn. given.

[25532-79-0, 29837-07-8, 70286-16-7, 70332-15-9, 73465-96-0]

Delay, F. *et al., Helv. Chim. Acta*, 1979, **62**, 369 (*synth, bibl*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1987, **64**, 756 (*synth*)
Buss, A.D. *et al., J.C.S. Perkin 1*, 1987, 2569 (*synth*)
Zdero, C. *et al., Phytochemistry*, 1991, **30**, 1163 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 283-284 (*use, props*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 159-160 (*FEMA 3331, use*)

2,7(14),10-Bisabolatriene B-109

1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)cyclohexene, 9CI. ***β-Bisabolene***. *β-Limene*



(*R*)-form

$C_{15}H_{24}$ 204.355
Flavouring ingredient used singly or as mixed isomers. Component of FEMA 3331. See also 2,7,10-Bisabolatriene, B-108.

(R)-form
$[\alpha]_D$ +75. n_D^{20} 1.4879.

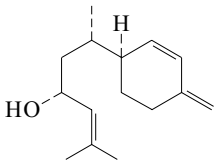
(S)-form [495-61-4]
Constit. of the essential oils of bergamot, lemon and wild carrot. Oil. $Bp_{10.5}$ 129-130°. $[\alpha]_D^{20}$ -84.4.

10ξ,11ξ-Epoxide: [88861-98-7] ***10,11-Epoxy-2,7(14)-bisaboladiene***
$C_{15}H_{24}O$ 220.354
Oil. $Bp_{0.1}$ 120°. $[\alpha]_D^{24}$ -89 (c, 11.1 in $CHCl_3$).

Pentegova, V.A. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1362 (*isol*)
Manjarrez, A. *et al., J.O.C.*, 1966, **31**, 348 (*synth*)
Andersen, N.H. *et al., Phytochemistry*, 1970, **9**, 1325 (*isol*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1971, **48**, 993 (*synth*)
Crawford, R.J. *et al., J.A.C.S.*, 1972, **94**, 4298 (*synth*)
Sakane, S. *et al., J.A.C.S.*, 1983, **105**, 6154 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1983, **22**, 2243 (*epoxide*)
Sakurai, H. *et al., Tetrahedron*, 1983, **39**, 883 (*synth*)
Nabeta, K. *et al., Agric. Biol. Chem.*, 1986, **50**, 2915 (*biosynth*)
Nabeta, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 792 (*biosynth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 159-160 (*FEMA 3331, use*)

1,3(15),10-Bisabolatrien-9-ol B-110

[120681-80-3]
Bisacurol



$C_{15}H_{24}O$ 220.354
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ -8.6 (c, 0.33 in MeOH).

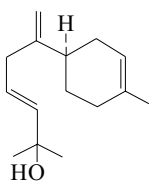
Ketone: [87440-60-6]

[82508-14-3] ***1,3(15),10-Bisabolatrien-9-one***. ***Curlone***. *β-Turmerone*
$C_{15}H_{22}O$ 218.338
Constit. of *Curcuma longa* (turmeric). Oil. $[\alpha]_D$ -0.03 (c, 2.16 in $CHCl_3$).

Golding, B.T. *et al., Chem. Comm.*, 1982, 363 (*β-Turmerone*)
Kiso, Y. *et al., Phytochemistry*, 1983, **22**, 596 (*Curlone*)
Uehara, S. *et al., Chem. Pharm. Bull.*, 1989, **37**, 237 (*isol, pmr, cmr*)
Golding, B.T. *et al., J.C.S. Perkin 1*, 1992, 1519 (*struct*)
Kreiser, W. *et al., Helv. Chim. Acta*, 1999, **82**, 1610-1639 (*synth, bibl*)

2,7(14),9-Bisabolatrien-11-ol B-111

Helianthol A

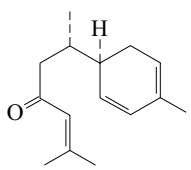


$C_{15}H_{24}O$ 220.354
(R)-form [72916-06-4]
Constit. of essential oil of *Helianthus tuberosus* (Jerusalem artichoke). Oil. $[\alpha]_D^{20}$ +61 (c, 0.3 in EtOH).

Miyazawa, M. *et al., Phytochemistry*, 1983, **22**, 1040

1,3,10-Bisabolatrien-9-one B-112

[82508-15-4]
2-Methyl-6-(4-methyl-2,4-cyclohexadien-1-yl)-2-hepten-4-one, 9CI. ***α-Turmerone***

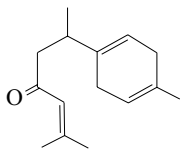


$C_{15}H_{22}O$ 218.338
Constit. of turmeric (*Curcuma longa*). Oil.

Golding, B.T. *et al., Chem. Comm.*, 1982, 363
Golding, B.T. *et al., J.C.S. Perkin 1*, 1992, 1519 (*struct*)

2,5,10-Bisabolatrien-9-one B-113

[56485-42-8]
Turmerone. *Tumerone*

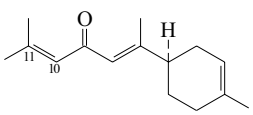


$C_{15}H_{22}O$ 218.338
Oil. Bp_{10} 125-126°. Unstable in air and light, dimerising and isomerising to B-112.

Mima, H. *et al., Yakugaku Zasshi*, 1959, **79**, 644 (*isol, struct, uv*)
Malingre, Th.M. *et al., Pharm. Weekbl.*, 1975, **110**, 601
Su, H.C.F. *et al., J. Agric. Food Chem.*, 1982, **30**, 290-292 (*isol*)

2,7,10-Bisabolatrien-9-one B-114

2-Methyl-6-(4-methyl-3-cyclohexen-1-yl)-2,5-heptadien-4-one, 9CI. ***Atlantone***. *α-Atlantone*



(*E*)-*form*

$C_{15}H_{22}O$ 218.338
(E)-form [26294-59-7]
Oil. Bp_1 142-145° (bath). $[\alpha]_D$ +1.2 (c, 0.83 in $CHCl_3$). n_D^{30} 1.5342.

10,11-Dihydro: [57130-01-5] *2,7-Bisaboladien-9-one*. ***10,11-Dihydroatlantone***
Isol. from heartwoods of *Ginkgo biloba* (ginkgo). Oil. Opt. inactive. Interconverts with the (*Z*)-form on standing.

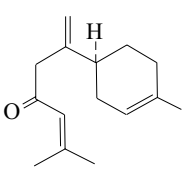
(Z)-form [56192-70-2]
Oil. n_D^{30} 1.5228.

10,11-Dihydro: [57130-00-4]
Found in *Ginkgo biloba* (ginkgo). Oil. Opt. inactive.

Pande, B.S. *et al., Tetrahedron*, 1971, **27**, 841 (*isol, struct*)
Babler, J.H. *et al., J.O.C.*, 1974, **39**, 1656 (*synth*)
Plattier, M. *et al., Recherches*, 1974, **19**, 131 (*Dihydroatlantone*)
Irie, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1892 (*Dihydroatlantone*)
Adams, D.R. *et al., J.C.S. Perkin 1*, 1975, 1741 (*synth*)
Motoyoshiya, J. *et al., J.O.C.*, 1985, **50**, 1326 (*synth*)
Manville, J.F. *et al., Phytochemistry*, 1989, **28**, 3073 (*pmr, cmr*)
Friesen, R.W. *et al., J.O.C.*, 1996, **61**, 7202 (*synth*)

2,7(14),10-Bisabolatrien-9-one B-115

[38331-79-2]
β-Atlantone

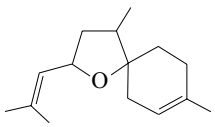


$C_{15}H_{22}O$ 218.338
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D^{26}$ -48.8 (c, 0.12 in EtOH). λ_{max} 242 (ϵ 10900) (EtOH) (Derep).

Crawford, R.J. *et al., J.A.C.S.*, 1972, **94**, 4298 (*synth*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3488 (*isol*)

Bisabolene oxide B-116

[38970-57-9]

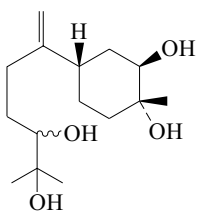


$C_{15}H_{24}O$ 220.354
Struct. shown to be incorrect by synth.. Constit. of *Gossypium hirsutum* (cotton). Oil.

Hedin, P.A. *et al., Phytochemistry*, 1972, **11**, 2118
Buchmann, B. *et al., Tetrahedron*, 1984, **40**, 3393 (*synth*)

7(14)-Bisabolene-2,3,10,11-tetrol B-117

[122470-42-2]

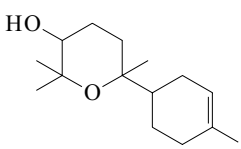


$C_{15}H_{28}O_4$ 272.384
Mycotoxin of *Fusarium sambucinum*. Glass.

Sanson, D.R. *et al., J.O.C.*, 1989, **54**, 4313 (*isol*)

α-Bisabolol oxide A B-118

[22567-36-8]

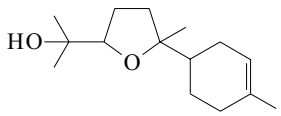


$C_{15}H_{26}O_2$ 238.369
Constit. of *Matricaria chamomilla* (German chamomile). Liq. Bp 156-158°. Log P 3.74 (calc).

Sampath, V. *et al., Indian J. Chem.*, 1969, **7**, 100 (*struct*)
Schilcher, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, 309 (*isol, struct*)
Adam, K.-P. *et al., Phytochemistry*, 1998, **48**, 953-959 (*biosynth*)

α-Bisabolol oxide B B-119

[26184-88-3]

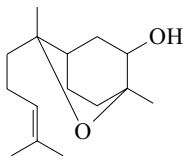


$C_{15}H_{26}O_2$ 238.369
Constit. of *Matricaria chamomilla* (German chamomile). Liq. Log P 3.6 (calc).

Schilcher, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, 309

α-Bisabolol oxide C B-120

[59861-08-4]

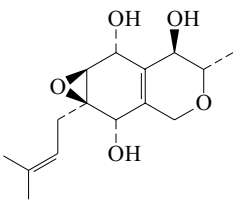


$C_{15}H_{26}O_2$ 238.369
Constit. of *Matricaria chamomilla* (German chamomile). Cryst. (EtOH). Mp 99-100°.

Schilcher, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 189

Bisbynin B-121

[163365-14-8]
1a,3,5,6,7,7a-Hexahydro-5-methyl-1a-(3-methyl-2-butenyl)-2H-oxireno[g][2]benzopyran-2,6,7-triol, 9CI



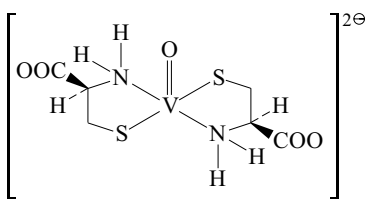
Relative configuration

$C_{15}H_{22}O_5$ 282.336
Isol. from seeds of *Oryza sativa* (rice). Cryst. (CH_2Cl_2/MeOH). Sol. MeOH. Mp 144°.

De Silva, L.B. *et al., Tet. Lett.*, 1995, **36**, 1997 (*isol, pmr, cryst struct*)

Bis[L-cysteinato(2-)-*N,S*]oxovanadate(*IV*)(2-), 11CI B-122

[78802-82-1]



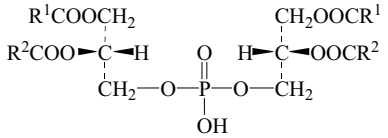
$C_6H_{10}N_2O_5S_2V^{2\ominus}$ 305.229
Prob. square pyramidal at V.
Di-H compd.: [90898-56-9] *Bis(L-cysteinato)oxovanadate(*IV*)*
Purple soln.

[85166-37-6]

Sakurai, H. *et al., Inorg. Chim. Acta*, 1981, **55**, L67 (*synth, epr, uv-vis*)
Gillard, R.D. *et al., Phytochemistry*, 1984, **23**, 179 (*epr*)

Bis(diacylglycero)phosphonic acids B-123

Bis(phosphatidic) acids. Bis(1,2-diacylglycero)-3-phosphate



An undefined mixt. has been isol. from soya bean.

Bis(ditetradecanoylglycero)phosphonic acid [105380-97-0]

[63988-25-0, 83818-31-9, 99759-77-0] *Phosphinicobis[oxy-3,1,2-propanetriyl] tetradecanoate, 9CI. Bis(1,2-ditetradecanoylglycero)-3-phosphate. Bis(dimyristoylglycero)phosphonic acid*

$C_{62}H_{119}O_{12}P$ 1087.589
Mp 49-50°. $[\alpha]_D^{22}$ +7.5 (c, 4 in C_6H_6).

Bis(dihexadecanoylglycero)phosphonic acid [84905-98-6]

[21289-05-4] *Phosphinicobis[oxy-3,1,2-propanetriyl] hexadecanoate, 9CI. Bis(1,2-dihexadecanoylglycero)-3-phosphate. Bis(dipalmitoylglycero)phosphonic acid*

$C_{70}H_{135}O_{12}P$ 1199.803
Cryst. (toluene/Me_2CO). Mp 62-63°. $[\alpha]_D^{23}$ +6.7 (c, 4 in C_6H_6).

Bis(dioctadecanoylglycero)phosphonic acid [105380-98-1]

[62438-23-7] *Phosphinicobis[oxy-3,1,2-propanetriyl] octadecanoate, 9CI. Bis(1,2-dioctadecanoylglycero)-3-phosphate. Bis(distearoylglycero)phosphonic acid*

$C_{78}H_{151}O_{12}P$ 1312.017
Cryst. (Me_2CO). Mp 69.5-70.5°. $[\alpha]_D^{24}$ +6.2 (c, 4 in C_6H_6).

Bis(9*Z*-octadecenoylglycero)phosphonic acid [17708-93-9]
Phosphinicobis[oxy-3,1,2-propanetriyl] 9-octadecenoate, 9CI. Olein 1,2-dihydrogen phosphate, 8CI. Bis(oleoylglycero)-phosphonic acid

$C_{78}H_{143}O_{12}P$ 1303.954
$[\alpha]_D$ +6.1 (c, 10 in $CHCl_3$).

Baer, E. *et al., J. Biol. Chem.*, 1952, **198**, 853-859 (*ditetradecanoyl, dihexadecanoyl, dioctadecanoyl*)
Baer, E. *et al., Arch. Biochem. Biophys.*, 1958, **78**, 294-305 (*dioctadecanoyl, dioleoyl*)
Baer, E. *et al., Prog. Chem. Fats Other Lipids*, 1963, **6**, 31-86 (*ditetradecanoyl, dihexadecanoyl, dioctadecanoyl, dioleoyl, synth, rev*)
Bioorg. Khim., 1977, **3**, 76-82; *CA*, **86**, 139333 (*dioctadecanoyl*)
Stearns, E.M. *et al., Lipids*, 1977, **12**, 451-454 (*isol*)
Ramirez, F. *et al., Tetrahedron*, 1977, **33**, 599-608 (*ditetradecanoyl, dihexadecanoyl, dioctadecanoyl*)
Dang Quoc Quan, *et al., Lipids*, 1982, **17**, 798-802 (*ditetradecanoyl*)
Dang Quoc Quan, *et al., Chem. Phys. Lipids*, 1983, **33**, 33-40 (*dihexadecanoyl, synth, nmr*)

1,2-Bis(3,4-dihydroxyphenyl)ethylene B-124

[133084-84-1]
4,4′-(1,2-Ethenediyl)bis[1,2-benzenediol], 9CI. 3,3′,4,4′-Stilbenetetrol. 3,3′,4,4′-Tetrahydroxystilbene

$C_{14}H_{12}O_4$ 244.246

(*E*)-*form* [136273-05-7]
Mp 241° dec.

3-O-β-D-Glucopyranoside: [113231-13-3]
$C_{20}H_{22}O_9$ 406.388

3,3′-Di-Me ether: [7329-69-3]

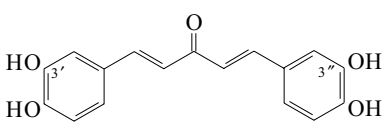
[4957-27-1, 137219-46-6] *1,2-Bis(4-hydroxy-3-methoxyphenyl)ethylene. 4,4′-Dihydroxy-3,3′-dimethoxystilbene*
$C_{16}H_{16}O_4$ 272.3
Constit. of the leaves of *Ginkgo biloba* (ginkgo). Cryst. (EtOH aq. or CH_2Cl_2/MeOH). Mp 212-215°. λ_{max} 224 ; 239 (sh) ; 309 (sh) ; 338 ; 350 (sh) (MeOH).

Bis(methylene)ether: [76306-40-6]
3,4:3′,4′-Bis(methylenedioxy)stilbene
$C_{16}H_{12}O_4$ 268.268
Prisms (CH_2Cl_2). Mp 214-215°.

[136273-06-8]

Talvitie, A. *et al., Finn. Chem. Lett.*, 1987, **14**, 43 (*isol, deriv*)
Gierer, J. *et al., J. Wood Chem. Technol.*, 1991, **11**, 171 (*synth*)
Thakkar, K. *et al., J. Med. Chem.*, 1993, **36**, 2950 (*synth, pmr*)
Chi, J. *et al., CA*, 1997, **127**, 231887b (*isol, 3,3′-di-Me ether*)
Hajdu, Z. *et al., J. Nat. Prod.*, 1998, **61**, 1298-1299 (*3,3′-di-Me ether*)
Wyatt, P. *et al., J.C.S. Perkin 1*, 2001, 279-297 (*bismethylene ether, pmr, cmr*)

1,5-Bis(3,4-dihydroxyphenyl)-1,4-pentadien-3-one B-125



$C_{17}H_{14}O_5$ 298.295

(*E,E*)-*form*

3′,3″-Di-Me ether: [131359-25-6] *1,5-Bis(4-hydroxy-3-methoxyphenyl)-1,4-pentadien-3-one, 9CI*
$C_{19}H_{18}O_5$ 326.348
Constit. of the rhizomes of *Curcuma domestica* (turmeric). Yellow powder ($CHCl_3$/hexane). Mp 82-83°.

Tetra-Me ether: [39777-59-8] *1,5-Bis(3,4-dimethoxyphenyl)-1,4-pentadien-3-one. Diveratrylideneacetone*
$C_{21}H_{22}O_5$ 354.402
Yellow needles. Mp 83-85° (84°).

Bis(methylene ether): [614-66-4] *1,5-Bis(1,3-benzodioxol-5-yl)-1,4-pentadien-3-one, 9CI. 1,5-Bis(3,4-methylenedioxyphenyl)-1,4-pentadien-3-one*
$C_{19}H_{14}O_5$ 322.317
Mp 198-200° (185°).

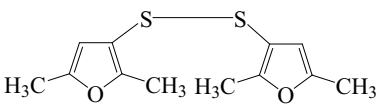
3′-Deoxy, 3′′-Me ether: [148625-88-1] *1-(4-Hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1,4-pentadien-3-one*
$C_{18}H_{16}O_4$ 296.322
Constit. of the rhizomes of *Curcuma domestica* (turmeric). Yellow powder ($CHCl_3$/hexane). Mp 161.5-162.5°.

[2150-50-7, 38552-39-5]

Wattanasin, S. *et al., Synthesis*, 1980, 647 (*synth*)
Masuda, T. *et al., Phytochemistry*, 1993, **32**, 1557-1560 (*isol, synth, pmr, cmr*)

Bis(2,5-dimethyl-3-furanyl) disulfide B-126

[28588-73-0]
3,3′-Dithiobis[2,5-dimethylfuran], 9CI, 8CI. FEMA 3476

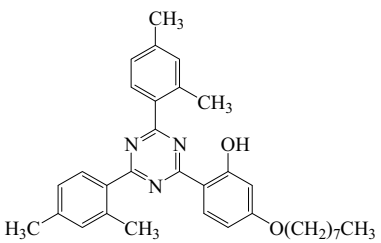


$C_{12}H_{14}O_2S_2$ 254.373
Synthetic meat flavouring agent. Yellow liq.

U.S. Pat., 1977, 4 020 175; *CA*, **87**, 13502024 (*synth, use*)
Huber, U.A. *et al., Helv. Chim. Acta*, 1993, **76**, 2528-2536 (*synth, pmr*)

2-[4,6-Bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl]-5-(octyloxy)-phenol, 9CI B-127

[2725-22-6]
2-[4,6-Di-(2,4-xylyl)-s-triazin-2-yl]-5-(octyloxy)phenol, 8CI. Cysorb UV-1164

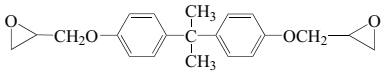


$C_{33}H_{39}N_3O_2$ 509.69
FDA permitted light stabiliser for food-contact olefinic polymers. Mp 83.5-84°.

Swiss Pat., 1969, 480 091; *CA*, **72**, 79 103d (*use, synth*)
Carrott, M.J. *et al., Analyst (London)*, 1998, **123**, 1827-1833 (*detn, ms*)
Fed. Regist., 2000, **65**, 26 746-26 747; *CA*, **133**, 149 473d (*use*)

2,2-Bis[4-(2,3-epoxypropoxy)-phenyl]propane, 8CI B-128

[1675-54-3]
2,2′-[(1-Methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane, 9CI. 2,2-[Bis(4-glycidyloxyphenyl)]propane. Bisphenol A diglycidyl ether. DGEBA. BADGE

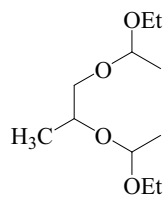


$C_{21}H_{24}O_4$ 340.418
Potential food contaminant arising from its use in epoxy resin coatings for cans, concrete vats and tanks, etc.. d^{21} 1.16. Mp 43°. $Bp_{0.75}$ 225-249° (lit quotes a pressure range). n_D^{20} 1.5703.

Bring, A. *et al., Chem. Listy*, 1956, **50**, 1198-1199; *CA*, **51**, 1110c (*synth*)
Rozentuler, S.M. *et al., Zh. Prikl. Khim. (Leningrad)*, 1973, **46**, 2731-2734; *CA*, **80**, 108924v (*synth*)
Sorokin, V.P. *et al., Polimery (Warsaw)*, 1977, **22**, 315-316; *CA*, **90**, 88110c (*synth*)
Lin, S.C. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1979, **17**, 3095-3119 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **9**, 730-755 (*rev*)
Chem. Technol. Epoxy Resins, 1993, (ed. Ellis, B.), Blackie, 1993, (*rev*)
Losada, P.P. *et al., J. Agric. Food Chem.*, 1997, **45**, 3493-3500 (*anal, bibl*)

1,2-Bis(1-ethoxyethoxy)propane B-129

[67715-79-1]
4,6,9-Trimethyl-3,5,8,10-tetraoxadodecane. FEMA 3534

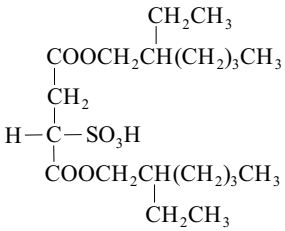


$C_{11}H_{24}O_4$ 220.308
Flavouring agent and adjuvant. Aldehyde generator used for enhancing the flavour of orange drinks. Liq. d_4^{25} 0.92. $Bp_{0.04}$ 47°. n_D^{20} 1.4112. Hydrolyses to acetaldehyde under aq. acidic conditions.

Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-62; **32(2)**, 64-66; 68-70 (*use*)
U.S. Pat., 1981, 4 280 011; *CA*, **95**, 219773z (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 157 (*use*)

1,4-Bis(2-ethylhexyl) sulfosuccinate, 8CI B-130

[10041-19-7]
1,4-Bis(2-ethylhexyl) sulfobutanedioate, 9CI



$C_{20}H_{38}O_7S$ 422.582Log P 6.12 (uncertain value) (calc).

Na salt: [577-11-7] ***Docusate sodium, BAN, INN.*** *Dioctyl sodium sulfosuccinate. Dulcodos. Dyoctol. Klyx. Milkinol. Molcer. Normax. Soliwax. Waxsol. Willoderm. Humifen WT 27G. Lankropol KO 2. Pelex OT. Warcowet 060. Wetaid SR. Vatsol OT. Complemix. Nonit. Solovet. Alcopol O. Karawet DOSS. Gemtex SC. Many other names*
Anionic surfactant used as wetting/dispersing/emulsifying agent in food processing. Hog/poultry scald agent. Used in cheeses, salad dressings, cocoa and dairy products. Waxy solid. Sol. H_2O, org. solvs. Doubtless a mixt. of diastereoisomers.

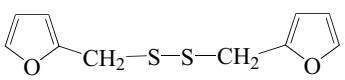
▶ Skin and severe eye irritant. LD_{50} (rat, orl) 1900 mg/kg. WN0525000

[128-49-4, 7491-09-0]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 799A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 897D (*ir*)
Averbakh, K.O. *et al., Zh. Prikl. Khim. (Leningrad)*, 1968, **41**, 2307 (*synth*)
Koenig, H. *et al., Fresenius' Z. Anal. Chem.*, 1970, **251**, 225 (*nmr*)
Ahuja, S. *et al., Anal. Profiles Drug Subst.*, 1973, **2**, 199; 1983, **12**, 713 (*revs*)
Nelan, A.A.M. *et al., Bull. Soc. Chim. Belg.*, 1979, **8**, 31 (*synth, props*)
Moriarty, K.J. *et al., Gut*, 1985, **26**, 1008 (*pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 6012 (*synonyms*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 173-175
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1216
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 883-887 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DJL000

Bis(2-furanylmethyl) disulfide B-131

[4437-20-1]
2,2′-[Dithiobis(methylene)]bisfuran, 9CI. 2,2′-(Dithiodimethylene)difuran. Difurfuryl disulfide. Furfuryl disulfide. FEMA 3146



$C_{10}H_{10}O_2S_2$ 226.32
Flavour component of roasted coffee, roasted sesame seeds and cooked meats. Flavouring ingredient. Liq. with a power-

ful sulfide aroma. d 1.23. Mp 10-11°. $Bp_{0.5}$ 112-115°.

Tressl, R. *et al., J. Agric. Food Chem.*, 1981, **29**, 1078-1082 (*occur*)
Gasser, U. *et al., Z. Lebensm.-Unters. -Forsch.*, 1988, **186**, 489-494; 1990, **190**, 3-8 (*occur*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*occur*)
Firouzabadi, H. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 1131-1134 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 205
Choi, J. *et al., J.O.C.*, 1995, **60**, 3266-3267 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 898-899
Iranpoor, N. *et al., Synthesis*, 1999, 49-50 (*synth*)

Bis(2-furanylmethyl) sulfide B-132

[13678-67-6]
2,2′-(Thiodimethylene)difuran, 9CI. Furfuryl sulfide. Difurfuryl sulfide. FEMA 3238



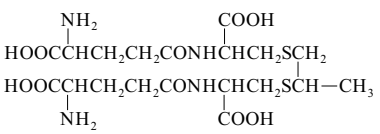
$C_{10}H_{10}O_2S$ 194.254
Present in coffee. Flavouring ingredient. Mp 31-32°. Bp_{14} 135-143°. n_D^{20} 1.5560.

S,S-*Dioxide:* [186685-62-1] *Bis(2-furanylmethyl) sulfone*
$C_{10}H_{10}O_4S$ 226.253
Cryst. Mp 72°.

Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*synth, ir, ms*)
Gol'dfarb, Ya.L. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1967, 2509; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1967, 2387 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 753
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2780
Rozen, S. *et al., J.O.C.*, 1997, **62**, 1457-1462 (*dioxide*)

N,N′-Bis(γ-glutamyl)-3,3′-(1,2-propylenedithio)dialanine B-133

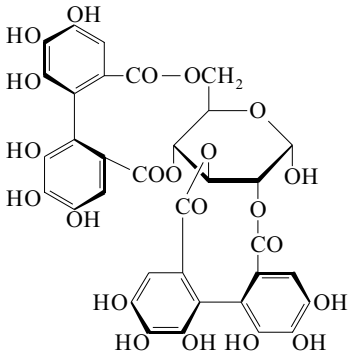
N,N′-*[Propylenebis[thio(1-carboxyethylene)]]diglutamine*



$C_{19}H_{32}N_4O_{10}S_2$ 540.615
Constit. of chives (*Allium schoenoprasum*). Cryst. (Me_2CO aq.).

Matikkala, E.J. *et al., Acta Chem. Scand.*, 1963, **17**, 1799 (*isol*)

2,3:4,6-Bis(hexahydroxydiphenoyl)glucose B-134



(*S,S*)- axial-α-D-Pyranose-*form*

$C_{34}H_{24}O_{22}$ 784.55

(*S,S*)$_{axial}$-α-D-pyranose-*form*
1-O-*(3,4,5-Trihydroxybenzoyl):* [82262-94-0] *1*-O-*Galloyl-2,3;4,6-bis-(S)-hexahydroxydiphenoyl-α-D-glucopyranose.* ***Potentillin***
$C_{41}H_{28}O_{26}$ 936.657
Isol. from *Rubus* spp.. Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{20}$ +108 (c, 0.7 in EtOH). λ_{max} 222 (ε 64600); 258 (ε 35500) (MeOH) (Derep).

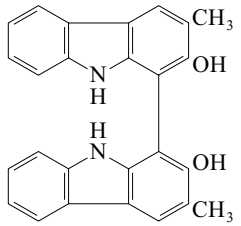
(*S,S*)$_{axial}$-β-D-pyranose-*form*
1-O-*(3,4,5-Trihydroxybenzoyl):* [79786-00-8] *1*-O-*Galloyl-2,3;4,6-bis-(S)-hexahydroxydiphenoyl-β-D-glucopyranose.* ***Casuarictin***
$C_{41}H_{28}O_{26}$ 936.657
Isol. from *Corylus heterophylla* (Siberian filbert). Off-white amorph. powder + $6H_2O$. $[\alpha]_D^{20}$ +35 (c, 0.2 in MeOH).

(2,3-*R*:4,6-*S*)$_{axial}$-β-D-pyranose-*form*
1-O-*(3,4,5-Trihydroxybenzoyl):* [121153-23-9] *1*-O-*Galloyl-2,3(R)-4,6(S)-bis(hexahydroxydiphenoyl)-β-D-glucopyranose.* ***Cuspinin***
$C_{41}H_{28}O_{26}$ 936.657
Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{24}$ -18.2 (c, 0.9 in Me_2CO).

Gupta, R.K. *et al., J.C.S. Perkin 1*, 1982, 2525 (*Potentillin*)
Okuda, T. *et al., J.C.S. Perkin 1*, 1983, 1765 (*Casuarictin*)
Okuda, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2165 (*Potentillin*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1989, **37**, 50 (*Cuspinin*)

1,1′-Bis(2-hydroxy-3-methylcarbazole) B-135

[155519-83-8]
3,3′-Dimethyl-[1,1′-bi-9H-carbazole]-2,2′-diol, 9CI

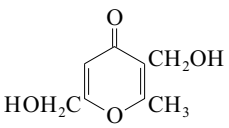


$C_{26}H_{20}N_2O_2$ 392.456
Alkaloid from roots of *Murraya koenigii* (curryleaf tree). Oil.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)
Knölker, H.J. *et al., Synlett*, 1996, 737 (*synth*)

3,6-Bis(hydroxymethyl)-2-methyl-4*H*-pyran-4-one B-136

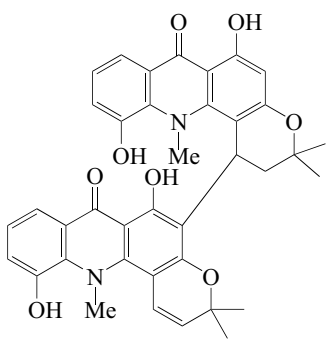
[131123-56-3]
Herierin III



$C_8H_{10}O_4$ 170.165
Constit. of *Hericium erinaceum* (lions mane). Cryst. Mp 122-123°.

Qian, F. *et al., Yaoxue Xuebao*, 1990, **25**, 522-525 (*isol, pmr*)

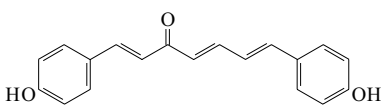
Bis(5-hydroxynoracronycine) B-137



$C_{38}H_{34}N_2O_8$ 646.695
Alkaloid from the roots of *Citrus paradisi* (grapefruit). Yellow cubes (Me_2CO). Mp 207-209°. Racemic λ_{max} 202 ; 231 ; 271 ; 290 (sh) ; 345 (sh) (EtOH).

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 693-696 (*isol, synth, uv, ir, pmr, cmr, ms*)

1,7-Bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one B-138



$C_{19}H_{16}O_3$ 292.334

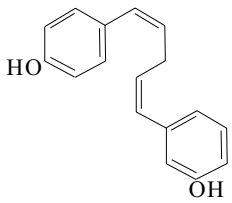
(all-E)-form [149732-52-5]
Constit. of the rhizomes of *Curcuma*

domestica (turmeric). Yellow powder.

Nakayama, R. *et al., Phytochemistry*, 1993, **33**, 501 (*isol, pmr*)

1,5-Bis(4-hydroxyphenyl)-1,4-pentadiene B-139

*Di-(*p*-hydroxystyryl)methane*



$C_{17}H_{16}O_2$ 252.312

(1Z,4Z)-form

Constit. of *Alpinia galanga* (greater galangal) rhizomes.

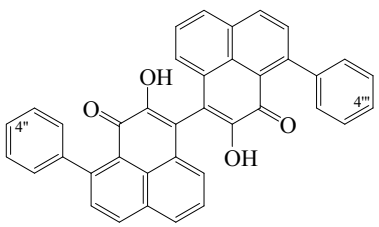
Di-Ac:

Cryst. (C_6H_6/petrol). Mp 140-142°.

Barik, B.R. *et al., Phytochemistry*, 1987, **26**, 2126

3,3′-Bis[2-hydroxy-9-phenyl-1*H*-phenalen-1-one] B-140

*2,2′-Dihydroxy-9,9′-diphenyl-[3,3′-bi-1*H*-phenalene]-1,1′-dione, 9CI. **3,3′-Bisanigorufone***



$C_{38}H_{22}O_4$ 542.589

Constit. of the rhizomes of *Musa acuminata* (dwarf banana). Orange solid.

4″,4‴-Dihydroxy: [190372-82-8] *2,2′-Dihydroxy-9,9′-bis(4-hydroxyphenyl)-[3,3′-bi-1*H*-phenalene]-1,1′-dione. 3,3′-Bis[2-hydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one]. **3,3′-Bis(4″-hydroxyanigorufone)***

$C_{38}H_{22}O_6$ 574.588

Constit. of *Musa acuminata* (dwarf banana). Orange-red cryst. (EtOH). Mp 205-210°. λ_{max} 215 ; 244 ; 274 ; 310 ; 369 ; 429 (MeOH).

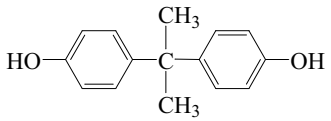
Hoelscher, D. *et al., Phytochemistry*, 1997, **45**, 87-91 (*4″,4‴-dihydroxy*)

Otalvaro, F. *et al., Phytochemistry*, 2002, **60**, 61-66 (*isol, pmr, cmr*)

2,2′-Bis(4-hydroxyphenyl)propane B-141

[80-05-7]

4,4′-(1-Methylethylidene)bisphenol, 9CI. 4,4′-Isopropylidenediphenol, 8CI. Diphenylolpropane. Bisphenol A. Dian. 1,1′-(1-Methylethylidene)bisphenylol, 9CI



$C_{15}H_{16}O_2$ 228.29

Potential food contaminant arising from its use in reusable polycarbonate food containers such as water carboys, baby bottles and kitchen utensils. Insol. H_2O; sol. EtOH; sl. sol. CCl_4. Mp 156-157°. Bp_{13} 250-252°.

▶ Skin and eye irritant. LD_{50} (rat, orl) 3250 mg/kg. Exp. reprod. and teratogenic effects. SL6300000

Di-Ac: [10192-62-8]
$C_{19}H_{20}O_4$ 312.365
Cryst. Mp 79.5-81.5°.

Bis(2-methyl-2-propenoyl): [3253-39-2] *Bisphenol A dimethacrylate*
$C_{23}H_{24}O_4$ 364.44
Mp 72-74°.

Dibenzoyl: [2297-14-5]
$C_{29}H_{24}O_4$ 436.506
Cryst. (EtOH). Mp 153.5°.

Di-Me ether: [1568-83-8] *2,2-Bis(4-methoxyphenyl)propane*
$C_{17}H_{20}O_2$ 256.344
Mp 59-61.5°. Bp_5 190°.

Di-Et ether: [16079-00-8] *2,2-Bis(4-ethoxyphenyl)propane*
$C_{19}H_{24}O_2$ 284.397
Mp 49-50°.

Bis(1,1,2,2-tetrafluoroethyl) ether: [1544-19-0] *1,1′-(1-Methylethylidene)bis[4-(1,1,2,2-tetrafluoroethoxy)benzene]*
$C_{19}H_{16}F_8O_2$ 428.321
$Bp_{0.9}$ 136°. n_D^{25} 1.4640.

Di-2-propenyl ether: [3739-67-1] *1,1′-(1-Methylethylidene)bis[4-(2-propenyloxy)benzene]. 2,2-Bis(*p*-allyloxy)phenylpropane*
$C_{21}H_{24}O_2$ 308.419
Bp_5 120-125°. n_D^{20} 1.5648.

Bis(oxiranylmethyl) ether: 2,2-Bis[4-(2,3-epoxypropoxy)phenyl]propane, B-128

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1119A; **2**, 316B (*ir, dipropenoyl*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 322C; 1296C (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1046A (*ir*)

v. Braun, J. *et al., Annalen*, 1929, **472**, 1 (*synth*)

England, D.C. *et al., J.A.C.S.*, 1960, **82**, 5116 (*bis(tetrafluoroethyl) ether*)

U.K. Pat., 1963, 923 774; *CA*, **58**, 14311f (*Di-2-propenyl ether*)

Takenaka, J. *et al., Kogyo Kagaku Zasshi*, 1967, **70**, 2081; *CA*, **68**, 18759 (*synth*)

Bilik, I.M. *et al., Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 636; *CA*, **67**, 6395 (*synth*)

Encyclopaedia of Polymer Science and Engineering, 2nd edn., Wiley-Interscience, New York, 1986, **6**, 322; 1988, **11**, 648 (*rev, polymers*)

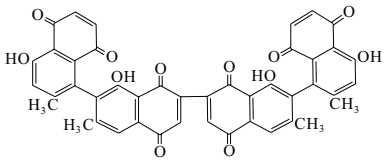
Hileman, B. *et al., Chem. Eng. News*, March 24, 1997, 37 (*rev, tox*)

Biles, J.E. *et al., J. Agric. Food Chem.*, 1997, **45**, 3541-3544 (*anal*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BLD500

Bisisodiospyrin B-142

[30276-87-0]



$C_{44}H_{26}O_{12}$ 746.682

Constit. of roots of *Diospyros lotus* (date plum). Orange prisms. Mp 320°. $[\alpha]_D^{21}$ -678 (c, 0.14 in $CHCl_3$). λ_{max} 257 (log ϵ 4.69) and 444 nm (4.25).

Tetra-Me ether:

Mp 223° dec.

Natori, S. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2308; 2314 (*isol, struct*)

van der Vijver, L.M. *et al., Phytochemistry*, 1974, **13**, 2322 (*isol*)

Lillie, T.J. *et al., J.C.S. Perkin 1*, 1977, 355 (*struct*)

Bis(4-isothiocyanatobutyl) disulfide B-143

[18729-71-0]

Isothiocyanic acid dithiobis(tetramethylene) ester, 9CI

$SCN(CH_2)_4–S–S–(CH_2)_4NCS$

$C_{10}H_{16}N_2S_4$ 292.514

Constit. of salad rocket (*Eruca sativa*). Thick yellow oil.

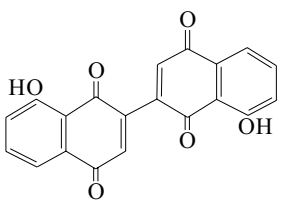
Vinkler, E. *et al., Acta Pharm. Hung.*, 1968, **38**, 6-14; *CA*, **69**, 18773p (*synth*)

Cerny, M.S. *et al., J. Agric. Food Chem.*, 1996, **44**, 3835-3839 (*isol, nmr, ms, synth*)

3,3′-Bisjuglone B-144

[61836-43-9]

8,8′-Dihydroxy[2,2′-binaphthalene]-1,1′,4,4′-tetrone, 9CI. 3,3′-Bijuglone



$C_{20}H_{10}O_6$ 346.295

Constit. of *Juglans regia* (walnut). Orange cryst. (C_6H_6). Mp 270° dec.

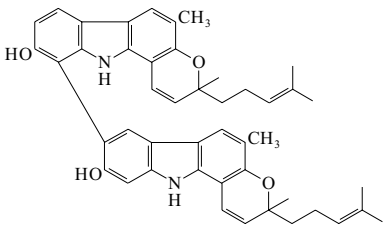
Babu, M.H. *et al., Phytochemistry*, 1978, **17**, 2042-2043 (*isol, uv, ir, ms, struct*)

Laatsch, H. *et al., Annalen*, 1980, 1321-1347 (*synth*)

Tanoue, Y. *et al., Tetrahedron*, 2002, **58**, 99-104 (*synth, pmr, cmr*)

Bismahanine B-145

[155519-87-2]



$C_{46}H_{48}N_2O_4$ 692.896

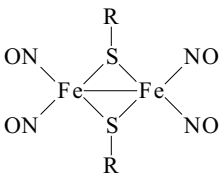
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Oil.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)

Bis(μ-methanethiolato)tetranitrosyldiiron, 10CI B-146

[16071-96-8]

Bis(μ-methylthio)tetranitrosyldiiron. Roussin's red methyl ester. Roussin's red



R = Me

$C_2H_6Fe_2N_4O_4S_2$ 325.92

Exists as an interconverting mixt. of *syn* and *anti* isomers in soln.. Isol. from pickled vegetables consumed in Linxian, China. Fine red-brown or red-black needles (pentane). Mp 92-93° (88-89°). Ir ν_{NO} 1780vs, 1755vs cm^{-1} ($CHCl_3$).

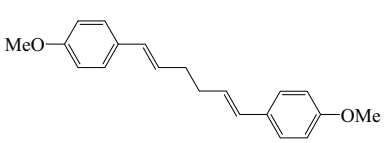
▶ Carcinogenic. NO4740000

[88643-17-8, 88643-72-5]

Li, M.-H. *et al., CA*, 1981, **94**, 25956; 18661; 133390 (*isol, tox*)
Beck, W. *et al., Chem. Ber.*, 1981, **114**, 3184 (*synth, ir, pmr*)
Seyferth, D. *et al., Organometallics*, 1986, **5**, 539 (*synth, pmr, cmr, ir, ms*)
Glidewell, C. *et al., Polyhedron*, 1988, **7**, 1371 (*reactions, epr*)
Liu, J. *et al., Carcinogenesis (London)*, 1989, **10**, 617-620 (*isol, tox*)

1,6-Bis(4-methoxyphenyl)-1,5-hexadiene B-147

1,1′-(1,5-Hexadiene-1,6-diyl)bis[4-methoxybenzene], 9CI. ***Ocimin***



$C_{20}H_{22}O_2$ 294.393

(E,E)-form [72448-90-9]

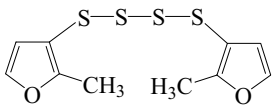
Neolignan from essential oil of *Ocimum americanum* (wild basil). Fluorescent flakes (EtOAc). Mp 170-171°.

Thappa, R.K. *et al., Phytochemistry*, 1979, **18**, 1242
Desai, D.G. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 491 (*synth*)
Khasnis, D.S. *et al., Org. Prep. Proced. Int.*, 1991, **23**, 126 (*synth*)
Ornelas, M.A. *et al., Synth. Commun.*, 1999, **29**, 1401-1403 (*synth*)

Bis(2-methyl-3-furanyl)tetrasulfide B-148

[28588-76-3]

3,3′-Tetrathiobis[2-methylfuran], 9CI, 8CI. FEMA 3260



$C_{10}H_{10}O_2S_4$ 290.452

Flavouring agent for meat products and baked goods.

U.S. Pat., 1977, 4 020 175; *CA*, **81**, 1350204 (*synth, use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1126 (*use*)

Bis(methylthio) selenide B-149

[41884-44-0]

SeS-*Methyl methanesulfeno(selenothioperoxoate), 13CI. [Selenobis(thio)]bismethane, 9CI. 2,4-Dithia-3-selenapentane*

Me–S–Se–S–Me

$C_2H_6S_2Se$ 173.161

Constit. of *Allium* sp..

Cai, X.-J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081 (*occur*)

Bis(methylthio)methane, 9CI B-150

[1618-26-4]

Bismethylmercaptomethane. Formaldehyde dimethylmercaptal. 2,4-Dithiapentane

$MeSCH_2SMe$

$C_3H_8S_2$ 108.228

Odorous constit. of white truffle (*Tuber magnatum*); volatile component of some cheeses and boiled beef aroma. Also found in milk, fish oils, shiitake mushroom, truffles, prawns and lobster. Important off-flavour component of foods. Used in seasonings. Oily liq. with mustard-like odour. d_4^{20} 1.06. Bp 142-143° $Bp_{11.5}$ 41°. n_D^{23} 1.5340.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 264D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 426A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 347D (*ir*)
Böhme, H. *et al., Ber.*, 1941, **74**, 1667 (*synth*)
Schoenberg, A. *et al., Chem. Ber.*, 1967, **100**, 778 (*synth*)
Fiecchi, A. *et al., Tet. Lett.*, 1967, 1681 (*isol, sulfone*)
Sloot, D. *et al., J. Agric. Food Chem.*, 1975, **23**, 356 (*isol*)
Freeman, D.J. *et al., Chem. Ind. (London)*, 1986, 877 (*isol*)
Merck Index, 11th edn., 1989, 1267
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1240

Bis[(methylthio)methyl] disulfide, 9CI B-151

[85544-38-3]

2,4,5,7-Tetrathiaoctane

Me^2SCH_2-^4S-^5S-CH_2^7SMe

$C_4H_{10}S_4$ 186.387

Pale yellow oil. Bp_4 112-120° $Bp_{0.02}$ 83.2-85.8°.

2-Oxide: Methylsulfinylmethyl(methylthiomethyl) disulfide
$C_4H_{10}OS_4$ 202.386

4-Oxide: 2,4,5,7-Tetrathiaoctane 4-oxide. ***Marasmicin***
$C_4H_{10}OS_4$ 202.386
Yellow oil. λ_{max} 206 (log ϵ 4.03); 232 (sh) (log ϵ 3.69) (MeCN).

2,2-Dioxide: [143113-67-1] *Methylsulfonylmethyl(methylthiomethyl) disulfide*
$C_4H_{10}O_2S_4$ 218.386
Needles (Et_2O). Mp 59-60° (55°).

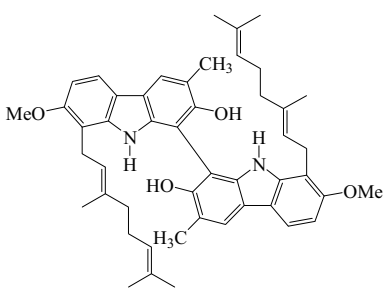
4,4-Dioxide:
$C_4H_{10}O_2S_4$ 218.386
Oil.

2,2,7,7-Tetraoxide: [74963-70-5] *Bis(methylsulfonylmethyl) disulfide*
$C_4H_{10}O_4S_4$ 250.385
Isol. from the edible shiitake mushroom (*Lentinus edodes*).

Altamura, M.R. *et al., J.O.C.*, 1963, **28**, 2438 (*synth*)
Hase, T.A. *et al., Synth. Commun.*, 1982, **12**, 947 (*synth*)
Takazawa, H. *et al., Yakugaku Zasshi*, 1982, **102**, 489 (*tetraoxide*)
Weissflog, E. *et al., Phosphorus Sulfur Relat. Elem.*, 1983, **15**, 27 (*synth*)
Boehme, H. *et al., Sulfur Lett.*, 1984, **2**, 151 (*synth*)
Burton, S.G. *et al., Planta Med.*, 1992, **58**, 295 (*isol, ir, pmr*)
Kubota, K. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 430; 644 (*isol, synth*)
Block, E. *et al., J.O.C.*, 1994, **59**, 2273 (*synth*)
Lim, H. *et al., Phytochemistry*, 1998, **48**, 787-790 (*4,4-dioxide*)
Kubec, R. *et al., Phytochemistry*, 2002, **60**, 21-25 (*Marasmicin*)
Kouokam, J.C. *et al., Phytochemistry*, 2002, **60**, 403-407 (*2-oxide*)

Bismurrayafoline E B-152

[252350-80-4]



$C_{48}H_{56}N_2O_4$ 724.981

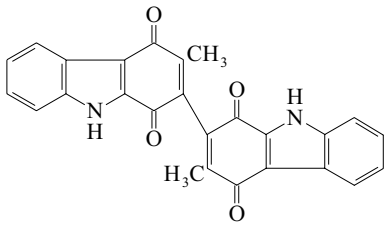
Alkaloid from the leaves of *Murraya*

koenigii (curryleaf tree). Gum.

Nutan, M.T.H. *et al., Fitoterapia*, 1999, **70**, 130-133

Bismurrayaquinone A B-153

[155519-86-1]
*3,3′-Dimethyl-[2,2′-bi-1*H*-carbazole]-1,1′,4,4′(9*H*,9′*H*)-tetrone, 9CI*

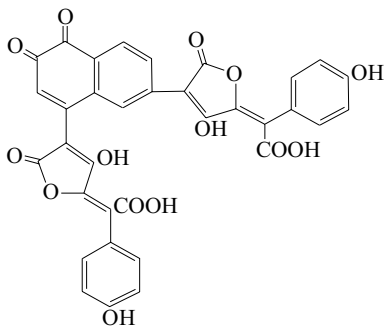


$C_{26}H_{16}N_2O_4$ 420.423
Alkaloid from roots of *Murraya koenigii* (curryleaf tree). Orange powder.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)
Bringmann, G. *et al., Tetrahedron*, 1995, **51**, 9353 (*synth*)
Murphy, W.S. *et al., J.C.S. Perkin 1*, 1998, 4115-4119 (*synth*)

Bisnorbadioquinone A B-154

[90295-70-8]

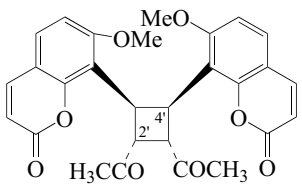


$C_{34}H_{18}O_{14}$ 650.508
Isol. from higher fungus *Xerocomus badius* (kostanjevka).

Steffan, B. *et al., Angew. Chem., Int. Ed.*, 1984, **23**, 445 (*isol, uv, pmr*)

Bisosthenon B-155

[123672-84-4]



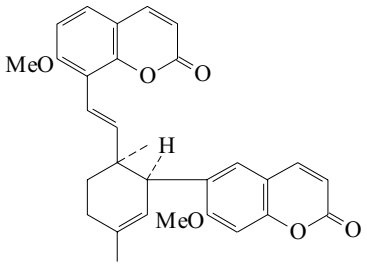
$C_{28}H_{24}O_8$ 488.493
Prisms. Mp 234-237°.

2′,4′-Diepimer: ***Bisosthenon B***
$C_{28}H_{24}O_8$ 488.493
Constit. of *Citrus paradisi* (grapefruit). Oil. $[\alpha]_D$ +24.5 (c, 0.1 in $CHCl_3$). λ_{max} 206 ; 265 (sh) ; 326 (EtOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2102
Takemura, Y. *et al., Heterocycles*, 1997, **45**, 1169 (*Bisosthenon B*)

Bisparasin B-156

[153178-05-3]



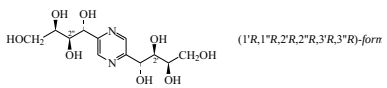
$C_{30}H_{28}O_6$ 484.548
Oil. Racemic.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1657 (*isol, pmr, cmr, struct*)

2,5-Bis(1,2,3,4-tetrahydroxybutyl)pyrazine B-157

[68538-87-4]

[220145-43-7, 220145-44-8, 220145-45-9, 220145-46-0, 220145-47-1]
1,1′-(2,5-Pyrazinediyl)bis-1,2,3,4-butanetetrol, 9CI



$C_{12}H_{20}N_2O_8$ 320.299
(1′R,1″R,2′R,2″R,3′R,3″R)-form [13121-64-7]
D-lyxo-*form*
Beige powder. Mp 109°.
(1′R,1″R,2′S,2″S,3′R,3″R)-form [13185-73-4]
D-arabino-*form*. *D-Fructosazine*
Present in ammonia caramels and soy sauce. Needles (EtOH). Mp 237°. $[\alpha]_D^{20}$ -84.1 (c, 1 in H_2O).
Octa-Ac: [13051-88-2]
Mp 174°. $[\alpha]_D^{11}$ -7.2 (c, 1 in $CHCl_3$).
(1′R,1″R,2′S,2″S,3′S,3″S)-form [41093-14-5] *L*-xylo-*form*. *L-Sorbosazine*
Needles (EtOH). Mp 175-177°. $[\alpha]_D^{20}$ -27 (c, 0.1 in H_2O).
(1′ξ,1″ξ,2′ξ,2″ξ,3′ξ,3″ξ)-form
*2′,2″-Bis-*O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* [165956-47-8] Vibrio alginolyticus *Pyrazine. VAPY*
$C_{28}H_{46}N_4O_{18}$ 726.687
Powder. Sol. MeOH, H_2O. λ_{max} 275 (H_2O).

[68510-02-1]

Fujii, S. *et al., J.O.C.*, 1966, **31**, 2239-2241 (*synth, fructosazine*)
Tsuchida, H. *et al., Agric. Biol. Chem.*, 1973, **37**, 2571-2578 (*Fructosazine, synth, uv, ir*)
Teglia, M.C. *et al., Carbohydr. Res.*, 1973, **26**, 377-384 (*synth, Sorbosazine*)
Tsuchida, H. *et al., Dev. Food Sci.*, 1986, **13**, 85-94 (*occur*)
Tsuchida, H. *et al., CA*, 1990, **113**, 229877r (*occur*)
Sumoto, K. *et al., Bull. Chem. Soc. Jpn.*, 1991, **39**, 792-794 (*Frucosazine, synth, ir, pmr, cmr*)
Yanai, T. *et al., J. Ferment. Bioeng.*, 1995, **80**, 406-407 (*VAPY*)
Japan. Pat., 1995, 95 118 286; *CA*, **124**, 7180w (*VAPY*)
Pat. Coop. Treaty (WIPO), 1999, 9 903 842; *CA*, **130**, 139579s (*synth, lyxo-form*)

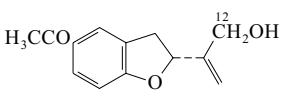
N,N′-Bis(2,2,2-trichloro-1-hydroxyethyl)urea, 9CI, 8CI B-158

[116-52-9]
Dicloralurea, BSI, INN, ISO, USAN. *SKF 1995. DCU, WSSA. Crag Herbicide 2*
$Cl_3CCH(OH)NHCONHCH(OH)CCl_3$
$C_5H_6Cl_6N_2O_3$ 354.83
Vet. food additive, inhibits methane production in herbicide ruminants. Growth stimulant. Herbicide, now superseded. Never marketedLog P 2.86 (calc).
▶ Skin irritant. LD_{50} (rat, orl) 6400 mg/kg. YS2787000

U.S. Pat., 1973, 3 733 417, (*Smith Kline and French*); *CA*, **79**, 52177p (*use*)
Partis, M.D. *et al., J. Chromatogr.*, 1983, **259**, 189 (*hplc*)
Pesticide Manual, 9th edn., 1991, No. 4170
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DGQ200

Bitalin A B-159

[34428-28-9]
1-[2,3-Dihydro-2-[1-(hydroxymethyl)ethenyl]-5-benzofuranyl]ethanone, 9CI. 5-Acetyl-2,3-dihydro-2-(1-hydroxy-2-propen-2-yl)benzofuran. 12-Hydroxytremetone



$C_{13}H_{14}O_3$ 218.252
(R)-form [35844-67-8]
Constit. of *Helichrysum italicum* (curry plant). Liq. $[\alpha]_D$ -61.2 (c, 2 in $CHCl_2$).
O-*Angeloyl:* [65580-28-1]
$C_{18}H_{20}O_4$ 300.354
(S)-form [78548-83-1]
*12-*O-*β-D-Glucopyranoside:*
$C_{19}H_{24}O_8$ 380.394
Constit. of *Helichrysum italicum* (curry plant). Mp 155°. $[\alpha]_D$ -53 (c, 0.1 in MeOH). λ_{max} 233 ; 287 (MeOH).
12-Ac: [134236-63-8] ***12-Acetyloxytremetone***
$C_{15}H_{16}O_4$ 260.289
*12-*O-*(4-Hydroxycinnamoyl)(*E-*):* [158414-61-0] ***12-*p*-Coumaroyloxytremetone***
$C_{22}H_{20}O_5$ 364.397
12-Aldehyde: [70360-18-8] *5-Acetyl-2,3-dihydro-α-methylene-2-benzofuranacetaldehyde, 9CI.* ***12-Oxotremetone***
$C_{13}H_{12}O_3$ 216.236
(±)-form [66614-28-6]
Bp_3 103-105° (bath).

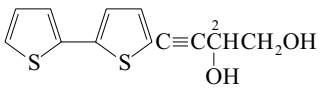
[35844-68-9]

Garcia de Quesda, T. *et al., Phytochemistry*,

1972, **11**, 446 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 179; 668; 683 (*12-Oxotremetone*)
Kawase, Y. *et al., Chem. Lett.*, 1980, 1581 (*synth*)
Le Van, N. *et al., Phytochemistry*, 1981, **20**, 485 (*isol*)
Yamaguchi, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2500 (*synth, pmr*)
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1990, **26**, 409; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 342 (*isol*)
Zdero, C. *et al., Phytochemistry*, 1992, **31**, 155 (*deriv*)
Nieto, M. *et al., An. Asoc. Quim. Argent.*, 1994, **82**, 105-109 (*Parastrephia lepidophylla derivs*)
Sala, A. *et al., J. Nat. Prod.*, 2001, **64**, 1360-1362 (*glucoside*)

4-[2,2′-Bithiophen-5-yl]-3-butyne-1,2-diol, 9CI B-160

[1211-45-6]
5-(3,4-Dihydroxy-1-butynyl)-2,2′-bithiophene



$C_{12}H_{10}O_2S_2$ 250.342
Cryst. (CCl_4/Et_2O). Mp 102°. $[\alpha]_D$ +11 (c, 2.55 in $CHCl_3$) (c, 2.55 in Et_2O).

1-Ac: [95910-62-6] *5-(4-Acetoxy-3-hydroxy-1-butynyl)-2,2′-bithiophene.* ***α-Tertiophene***
$C_{14}H_{12}O_3S_2$ 292.379
Oil.

2-Ac: [1687-88-3] ***5-(3-Acetoxy-4-hydroxy-1-butynyl)-2,2′-bithiophene***
$C_{14}H_{12}O_3S_2$ 292.379
Oil.

Di-Ac: [1233-95-0] ***5-(3,4-Diacetoxy-1-butynyl)-2,2′-bithiophene***
$C_{16}H_{14}O_4S_2$ 334.416
Oil. $[\alpha]_D$ +119 (c, 0.89 in $CHCl_3$). $[\alpha]_{Hg}^{25}$ +183 (c, 0.89 in Et_2O).

1-O-(3-Methylbutanoyl): [58930-56-6] ***5-(3-Hydroxy-4-isovaleryloxy-1-butynyl)-2,2′-bithiophene***
$C_{17}H_{18}O_3S_2$ 334.459
Oil.

2-O-(3-Methylbutanoyl): ***5-(4-Hydroxy-3-isovaleryloxy-1-butynyl)-2,2′-bithiophene***
$C_{17}H_{18}O_3S_2$ 334.459

2-Ketone, Ac: [1222-83-9] ***5-(4-Acetoxy-3-oxo-1-butynyl)-2,2′-bithiophene***
$C_{14}H_{10}O_3S_2$ 290.363
Isol. from *Tagetes erecta* (African marigold). Cryst. (CCl_4). Mp 68°.

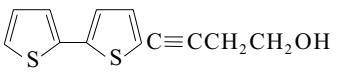
1-Deoxy, 1-chloro: [1020-03-7] ***5-(4-Chloro-3-hydroxy-1-butynyl)-2,2′-bithiophene.*** *1-Chloro-4-[5-(3-thienyl)-2-thienyl]-3-butyn-2-ol, 8CI*
$C_{12}H_9ClOS_2$ 268.787
Isol. from *Tagetes minuta* (Mexican marigold). Solid. Mp 55°.

1-Deoxy, 1-chloro, Ac: [96850-15-6] ***5-(3-Acetoxy-4-chloro-1-butynyl)-2,2′-bithiophene***
$C_{14}H_{11}ClO_2S_2$ 310.824
Yellow oil.

Bohlmann, F. *et al., Chem. Ber.*, 1965, **98**, 155; 876 (*isol, uv, ir, pmr, ord, struct, biosynth*)
Atkinson, R.E. *et al., J.C.S.*, 1965, 7109 (*deriv*)
Bohlmann, F. *et al., Chem. Ber.*, 1976, **109**, 901 (*3-methylbutanoyl*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 192; 1985, **51**, 77 (*isol, derivs*)
Pensl, R. *et al., Z. Naturforsch., C*, 1985, **40**, 3 (*isol, biosynth*)
Chang, C.-T. *et al., Planta Med.*, 1990, **56**, 533
Kagan, J. *et al., Prog. Chem. Org. Nat. Prod.*, 1991, **56**, 87 (*rev*)
Lin, Y.-L. *et al., Chin. Pharm. J. (Taipei)*, 1999, **51**, 201-211; *CA*, **132**, 61618 (*isol, activity*)

4-[2,2′-Bithiophen-5-yl]-3-butyn-1-ol, 9CI B-161

[1137-87-7]
4-[5-(2-Thienyl)-2-thienyl]-3-butyn-1-ol, 8CI. 5-(4-Hydroxy-1-butynyl)-2,2′-bithiophene



$C_{12}H_{10}OS_2$ 234.342
Constit. of the roots of *Tagetes minuta* (Mexican marigold), *Tagetes* spp.. Cryst. (Et_2O/petrol or CCl_4). Mp 68°.

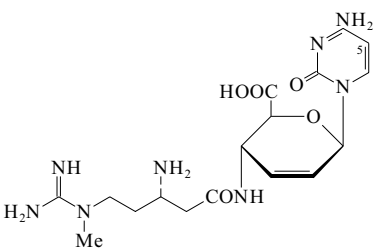
Ac: [1219-28-9]
$C_{14}H_{12}O_2S_2$ 276.38
Isol. from *Tagetes* spp.. Oil. $Bp_{0.001}$ 115°.

3-Methylbutanoyl: [61102-15-6]
$C_{17}H_{18}O_2S_2$ 318.46
Oil.

Bohlmann, F. *et al., Chem. Ber.*, 1962, **95**, 2945; 1964, **97**, 2125
Atkinson, R.E. *et al., J.C.S.*, 1965, 7109 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1976, **15**, 1309 (*isol*)
Rossi, R. *et al., Tetrahedron*, 1984, **40**, 2773 (*synth*)
Kagan, J. *et al., Prog. Chem. Org. Nat. Prod.*, 1991, **56**, 87 (*rev*)

Blasticidin S B-162

[2079-00-7]
Cytovirin. NSC 91770. A 83094C. Antibiotic 21544. Antibiotic A 83094C. Bla-S



$C_{17}H_{26}N_8O_5$ 422.443
Nucleoside-type antibiotic. Contact fungicide used against rice blast disease in Japan. Needles (H_2O). Mp 235° (252-253°) dec. $[\alpha]_D^{11}$ +108.4 (c, 1 in H_2O). pK_{a1} 2.4; pK_{a2} 4.6; pK_{a3} 8; pK_{a4} 0. Hydrol. → Cytosinine λ_{max} 275 (ϵ 14800) (0.1*N* HCl) (Derep). λ_{max} 266 (ϵ 11400) (0.1*N* NaOH) (Derep). λ_{max} 231 (ϵ 8900); 268 (ϵ 7000) (H_2O) (Derep).
▶ LD_{50} (rat, orl) 16 mg/kg. LD_{50} (rat, skn) 3100 mg/kg. EC4900000

Hydrochloride:
Mp 229° dec.

Hydrochloride (1:2):
Mp 195° dec.

Me ester, hydrochloride (1:3):
Mp 206-208.5° dec.

N-*De-Me:* [63257-29-4] ***Demethylblasticidin S***
$C_{16}H_{24}N_8O_5$ 408.416
Sol. H_2O. λ_{max} 274 (H_2O) (Berdy). λ_{max} 274 (ϵ 12900) (HCl) (Berdy). λ_{max} 267 (ϵ 9200) (NAOH) (Berdy).
▶ LD_{50} (mus, orl) 35 mg/kg. MP8930000

3′′-N-Leucyl: [19018-47-4] ***Leucylblasticidin S.*** *Sch 36606. Antibiotic Sch 36606*
$C_{23}H_{37}N_9O_6$ 535.602
Needles (H_2O). Sol. H_2O; fairly sol. MeOH, DMSO; poorly sol. $CHCl_3$, hexane. Mp 252° dec. λ_{max} 269 (ϵ 8000) (H_2O). λ_{max} 276 (ϵ 11000) (HCl) (Berdy).

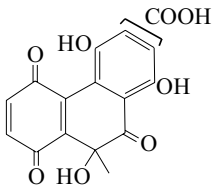
5-Fluoro: [102865-76-9] *Fluoroblasticidin S*
$C_{17}H_{25}FN_8O_5$ 440.433
Powder. Sol. H_2O; poorly sol. butanol, hexane. Mp 225-227°. λ_{max} 280 (ϵ 13500); 282 (ϵ 8020) (HCl) (Berdy). λ_{max} 275 (ϵ 5500) (NaOH) (Berdy). λ_{max} 276 (ϵ 12000) (H_2O) (Berdy).

5-Hydroxymethyl: [123067-52-7] ***5-Hydroxymethylblasticidin S.*** *A 83094B. Antibiotic A 83094B*
$C_{18}H_{28}N_8O_6$ 452.469
Mp 225° dec. λ_{max} 279 (ϵ 11000) (0.01*M* HCl) (Derep). λ_{max} 272 (ϵ 8000) (H_2O) (Derep). λ_{max} 272 (pH 7 buffer) (Berdy).

Yonehara, H. *et al., J. Antibiot., Ser. A*, 1963, **16**, 195
Otake, N. *et al., Tet. Lett.*, 1965, 1411 (*struct*)
Fox, J.J. *et al., Tet. Lett.*, 1966, 897 (*struct*)
Yonehara, H. *et al., Tet. Lett.*, 1966, 3785 (*abs config*)
Seto, H. *et al., Tet. Lett.*, 1966, 3793 (*biosynth*)
Misato, T. *et al., Antibiotics*, (Gottlieb, D. *et al*, Ed.), Springer, N.Y., 1967, **1**, 434 (*rev*)
Seto, H. *et al., Agric. Biol. Chem.*, 1968, **32**, 1299-1305 (*Leucylblasticidin S*)
Seto, H. *et al., J. Antibiot.*, 1977, **30**, 1022 (*isol, deriv*)
Swaminathan, V. *et al., Biochim. Biophys. Acta*, 1981, **655**, 335 (*cryst struct*)
Yonehara, H. *et al., Drugs Pharm. Sci.*, 1984, **22**, 651 (*rev*)
Probhakaran, P.C. *et al., Tet. Lett.*, 1986, **27**, 3815 (*biosynth*)
Kawashima, A. *et al., Agric. Biol. Chem.*, 1987, **51**, 1183 (*Fluoroblasticidin S*)
Dallwag, H. *et al., J. Antibiot.*, 1988, **41**, 1145-1147 (*Leucylblasticidin S*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711 (*rev*)
Larsen, S.H. *et al., J. Antibiot.*, 1989, **42**, 470 (*isol, deriv*)
Zhang, Q. *et al., Tetrahedron*, 2000, **56**, 693-701 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BLX500

Blighinone B-163

[20544-62-1]



$C_{16}H_{10}O_8$ 330.25

Quinone from the fruit pulp of *Blighia sapida* (akee apple). Lemon-yellow cryst. (Py). Mp 360° dec.

Tri-Ac:
Cryst. (Py). Mp 340-344° dec.

Tri-Me ether:
Cryst. (Py). Mp 348-350°.

Garg, H.S. *et al., Tet. Lett.*, 1968, 1549

Blue copper proteins B-164

Type 1 Copper proteins

$[CuN_2S_2]$

A group of metalloproteins which have a single Cu atom at the active site and three characteristic props.: intense blue colour at *ca*. 600 nm, unusually narrow hyperfine coupling in the ESR spectrum of the $Cu^{2\oplus}$ protein, and high reduction potentials (range 184-680 mV).

Amicyanin
Contains 106 amino acids.

Azurin
Contains 128 or 129 amino acids.

Cucumber basic protein
Plantacyanin. CBP
Contains 96 amino acids. Isol. from cucumber.

Plastocyanin
There are a number of Plastocyanins, each containing between 97 and 104 amino acids.

Pseudoazurin
Contains 123 amino acids.

Rusticyanin
Contains 144 amino acids.

Stellacyanin
Contains 107 amino acids.

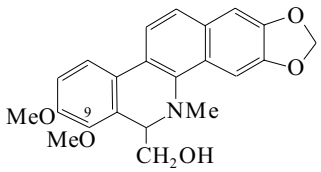
Umecyanin
Contains 125 amino acids. Isol. from roots of horseradish.

Lappin, A.G. *et al., Met. Ions Biol. Syst.*, (Ed. Sigel, H.), Vol. 13, Marcel Dekker, N.Y., 1981, 15 (*rev*)
Copper Proteins Copper Enzymes, (Ed. Lontie, R.), CRC Press, Boca Raton, 1984, (*book*)
Dooley, D.M. *et al., Life Chem. Rep.*, 1987, **5**, 91 (*rev*)
Latour, J.M. *et al., Bull. Soc. Chim. Fr.*, 1988, 508 (*rev*)
Ryden, L. *et al., Prog. Clin. Biol. Res.*, 1988, **274**, 349 (*rev*)
Guss, J.M. *et al., Sciences (N.Y.)*, 1988, 241; 806 (*cryst struct*)
Sykes, A.G. *et al., Adv. Inorg. Chem.*, 1991, **36**, 377 (*rev*)
Gross, E.L. *et al., Adv. Photosynth.*, 1996, **4**, 413-429 (*rev, Plastocyanin*)
Donaire, A. *et al., J.A.C.S.*, 2002, **124**, 13698-13708 (*Pseudoazurin, Rusticyanin, pmr, struct*)

Bocconoline B-165

[32906-88-0]

12,13-Dihydro-1,2-dimethoxy-12-methyl[1,3]benzodioxolo[5,6-c]phenanthridine-13-methanol, 9CI. 8-Hydroxymethyldihydrochelerythrine. Base C†



$C_{22}H_{21}NO_5$ 379.412

Probably an artifact. Pillars (MeOH). Mp 232-233° (215-218°, 221-222°).

O^9-*De-Me:* ***7,8-Dihydro-8-hydroxymethylfagaridine***
$C_{21}H_{19}NO_5$ 365.385
Solid. Poss. artifact.

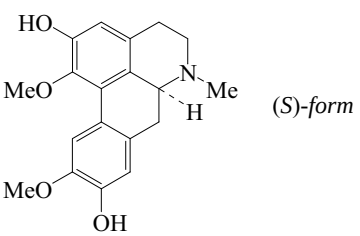
Deoxy: [159465-79-9] ***8-Methyldihydrochelerythrine***
$C_{22}H_{21}NO_4$ 363.412
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Needles (MeOH). Mp 203-205°.

Tani, C. *et al., Yakugaku Zasshi*, 1962, **82**, 755; *CA*, **58**, 5747f (*isol*)
Ishii, H. *et al., Tet. Lett.*, 1971, 2429 (*uv, ir, pmr, ms, struct*)
Novák, V. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 3352 (*isol, uv*)
Ishii, H. *et al., Chem. Pharm. Bull.*, 1978, **26**, 166 (*uv, ir, pmr, ms, struct, synth*)
Itokawa, H. *et al., Phytochemistry*, 1978, **17**, 839 (*isol, uv, ir, pmr, ms*)
Castedo, L. *et al., Heterocycles*, 1981, **16**, 533 (*occur*)
Boulware, R.J. *et al., J. Nat. Prod.*, 1981, **44**, 200 (*7,8-Dihydro-8-hydroxymethylfagaridine*)
Chen, I.S. *et al., J. Nat. Prod.*, 1994, **57**, 1206 (*8-Methyldihydrochelerythrine*)

Boldine B-166

[476-70-0]

5,6,6a,7-Tetrahydro-1,10-dimethoxy-6-methyl-4H-dibenzo[de,g]quinoline-2,9-diol, 9CI. 2,9-Dihydroxy-1,10-dimethoxyaporphine



$C_{19}H_{21}NO_4$ 327.379Log P 2.42 (uncertain value) (calc).

► CE0750000

(S)-form
Alkaloid from *Sassafras* and the leaves of *Peumus boldus* (boldo). Flavouring ingredient. Mp 161-163°. $[\alpha]_D^{13}$ +111 (c, 1.03 in EtOH). Pharmacol. active isomer.

► LD_{50} (mus, orl) 450 mg/kg. CE0750000

N-*De-Me:* [5890-18-6] *2,9-Dihydroxy-1,10-dimethoxynoraporphine.* ***Laurolitsine.*** *Norboldine*
$C_{18}H_{19}NO_4$ 313.352
Alkaloid from *Sassafras* and the leaves of *Peumus boldus* (boldo). Flavouring ingredient. Mp 138-140°. $[\alpha]_D$ +101 (c, 0.69 in EtOH).

► RB5935000

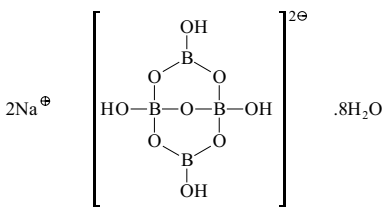
Späth, E. *et al., Ber.*, 1933, **66**, 904 (*isol, struct*)
Nakasato, T. *et al., Chem. Pharm. Bull.*, 1959, **7**, 780 (*Laurolitsine*)
Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 1277 (*isol, pmr, Laurolitsine*)
Tewari, S. *et al., Phytochemistry*, 1972, **11**, 1149 (*isol, pmr, uv, ms, Boldine, Laurolitsine*)
Kupchan, S.M. *et al., Chem. Comm.*, 1976, 91 (*synth*)
Bhakuni, D.S. *et al., J.C.S. Perkin 1*, 1977, 706 (*biosynth*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80 (*cd*)
Asencio, M. *et al., Acta Cryst. C*, 1996, **52**, 1581 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DNZ100

Borax, 11CI, 10CI, 9CI, 8CI B-167

[1303-96-4]

[13840-56-7]

Tincal. Disodium tetraborate decahydrate. Borax decahydrate. Sodium borate, JAN, USAN



$B_4H_{20}Na_2O_{17}$ 381.371

The most important commercial borate. Also formulated as $Na_2O.2B_2O_3.10H_2O$. Listed in the EAFUS Food Additive Database (Jan. 2001) but with no current reported use. Historically used as a food preservative since ca. 1800, common in butter/margarine. Now limited to preservation of caviar. Colourless monoclinic cryst. Sol. H_2O (2 g per 100 cm^3 at 0°, 170 g per 100 cm^3 at 100°) MeOH, polyols; spar. sol. Me_2CO, EtOAc, EtOH. Stable in aq. soln. up to 61° then dehydrates to Disodium tetraborate pentahydrate - complex dehydration reactions depend somewhat on sample's history.

► VZ2275000

Mineral-*form*
Colourless or white to greyish, greenish or bluish cryst.

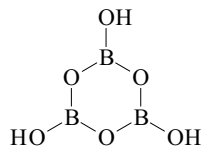
[1344-90-7, 12322-85-9, 12447-40-4, 61028-24-8, 71377-02-1]

Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301 (*Raman*)
Nies, N.P. *et al., J. Chem. Eng. Data*, 1967, **12**, 303 (*synth*)
Thomas, G. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1972, **69**, 1154 (*thermal anal*)
Levy, H.A. *et al., Acta Cryst. B*, 1978, **34**, 3502 (*nd, cryst struct*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **4**, 80 (*manuf, uses, tox*)
Kochergin, V.P. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1641 (*pmr, B-11 nmr*)
Nies, N.P. *et al., Mellor Compr. Treat. Inorg. Theor. Chem.*, 1980, 356 (*rev, bibl*)
Janda, R. *et al., Spectrochim. Acta A*, 1980, **36**, 997 (*ir, Raman*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3155C (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFE500; SFF000

Boric acid (HBO_2), 11CI, 10CI B-168

[13460-50-9]
Boric acid†. *Metaboric acid. E284*



α-*form* (*trimer*)

BHO_2 43.818

Common product of hydrolysis and pyrolysis of many boron compds. Three cryst. forms known. Preservative.

Kracek, F.C. *et al., Am. J. Sci.*, 1938, **35**, 143 (*B_2O_3-H_2O phase diagram, synth*)
Silver, A.H. *et al., J. Chem. Phys.*, 1960, **32**, 959 (*B-11 nmr, α-form, β-form*)
Bray, P.J. *et al., J. Chem. Phys.*, 1961, **35**, 435 (*B-11 nmr, γ-form*)
Zachariasen, W.H. *et al., Acta Cryst.*, 1963, **16**, 380; 385 (*cryst struct, γ-form, β-form*)
Peters, C.R. *et al., Acta Cryst.*, 1964, **17**, 229 (*cryst struct, α-form*)
Bertoluzza, A. *et al., J. Mol. Struct.*, 1980, **64**, 123 (*ir, Raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1980, **5/A**, 224 (*rev, bibl*)

Boric acid (H_3BO_3), 9CI, 8CI, INN, JAN, USAN B-169

[10043-35-3]
Boracic acid. Orthoboric acid

$B(OH)_3$

BH_3O_3 61.833

Common product of hydrol. of many boron compds. containing B−Hal, OR, SR, H, NR_2 etc. bonds. Food contaminant deriving from paper and paperboard in contact with food. V. limited use as an antibacterial agent in caviar. Pearly scales or powder. Mod. sol. hot H_2O, v. spar. sol. cold H_2O. Mp 171°. Component of Aci-Jel, Blinx, Bluboro, Borofax, Collyrium Eye Drops, Wyanoids. ΔH_f° -1094.3 kJ mol^{-1}. Melting point often indefinite owing to gradual dehydration on heating.

▶ Acute exposure affects the gastrointestinal tract, CNS, skin, liver and kidneys. Symptoms of chronic intoxication include anorexia, gastrointestinal disturbances, debility, confusion, dermatitis, menstrual disorders, anaemia, convulsions and alopecia. Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 3000-4000 mg/kg. ED4550000

Mineral-*form*

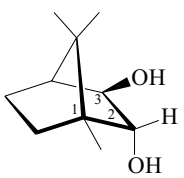
Sassolite

White to grey soft pearly triclinic cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1246A (*ir*)
Zachariasen, W.H. *et al., Acta Cryst.*, 1954, **7**, 305 (*cryst struct*)
Sciarra, E. *et al., J. Am. Pharm. Assoc., Sci. Ed.*, 1960, **49**, 116 (*tox*)
Craven, B.M. *et al., Acta Cryst.*, 1966, **20**, 214 (*nd*)
Nöth, H. *et al., NMR Spectroscopy of Boron Compounds (NMR Basic Principles and Progress)*, Springer Verlag, 1978, (*B-11 nmr*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1980, **5**, 224 (*rev, bibl*)
Butler, L.G. *et al., J. Magn. Reson.*, 1981, **42**, 120 (*nqr*)
Janda, R. *et al., Spectrochim. Acta A*, 1981, **36**, 997 (*ir, Raman*)
Houlsby, R.D. *et al., Antimicrob. Agents Chemother.*, 1986, **29**, 803 (*pharmacol*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *3rd Suppl.*, 1987, **2**, 96 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 365 (*manuf, props, uses*)
Treinen, K.A. *et al., Toxicol. Appl. Pharmacol.*, 1991, **107**, 325 (*tox*)
Heindel, J.J. *et al., Fundam. Appl. Toxicol.*, 1992, **18**, 266 (*tox*)
Von Burg, R. *et al., J. Appl. Toxicol.*, 1992, **12**, 149 (*tox, rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1343
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 644-645 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 291-292
Stokinger, H.E. *et al., Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.)*, Vol. 2, Wiley, 1980, **2B**, 2984 (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMC000

2,3-Bornanediol, 8CI B-170

[13837-85-9, 30128-49-5, 30128-51-9, 30226-61-0, 38226-15-2, 45980-02-7, 56614-57-4, 56614-58-5, 64911-69-9]
1,7,7-Trimethylbicyclo[2.2.1]heptane-2,3-diol, 9CI. 2,3-Camphanediol



(1*R*,2*R*,3*R*)-*form*

$C_{10}H_{18}O_2$ 170.251

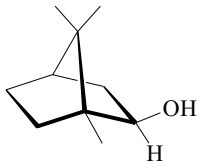
(1*R*,2*R*,3*R*)-*form* [68738-11-4]
(+)-endo,exo-*form*
Cryst. (C_6H_6/petrol). Mp 254-256°. $[\alpha]_D$ +15 (c, 1.5 in EtOH).

2-Ac: [61586-52-5] ***Vulgarole***†
$C_{12}H_{20}O_3$ 212.288
Constit. of oil of *Artemisia vulgaris* (mugwort). Thick oil. Rel. config. only detd., could be the enantiomer.

Nano, G.M. *et al., Planta Med.*, 1976, **30**, 211-215 (*Vulgarole*)

2-Bornanol B-171

[10385-78-1]
1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol. 2-Hydroxybornane. Bingpian



(1*R*,2*R*)-*form*

$C_{10}H_{18}O$ 154.252
Both Borneol and Isoborneol and their acetates and formates are used as flavouring agents.

(1*R*,2*R*)-*form* [10334-13-1]
(-)-Isoborneol. *β-Camphol. Isocamphol. FEMA 2158*
Flavouring agent. Cryst. (petrol). Mp 212° (sealed tube). $[\alpha]_D^{20}$ -32.3 (MeOH).

(1*R*,2*S*)-*form* [464-43-7]
(+)-Borneol. *(+)-Bornyl alcohol. Borneo camphor. FEMA 2157*
Constit. of *Curcuma aromatica* and other plants. Cryst. (petrol). Mp 208°. Bp 212°. $[\alpha]_D^{20}$ +37.7 (c, 5 in EtOH).

▶ ED7060000

Formyl: [7492-41-3] *Bornyl formate. FEMA 2161*
$C_{11}H_{18}O_2$ 182.262
Flavouring agent. Liq. d^{20} 1.01. Bp_{21} 106-108°. n_D^{20} 1.4689.

Butanoyl: [13109-70-1] *Bornyl butyrate. FEMA 3907*
$C_{14}H_{24}O_2$ 224.342
Flavouring agent. d^{18} 0.97. Bp_{22} 141-143°. n_D^{18} 1.4638.

Pentanoyl: [7549-41-9] *Bornyl valerate. FEMA 2164*
$C_{15}H_{26}O_2$ 238.369
Flavouring agent. Bp 249°. n_D^{20} 1.4615.

3-Methylbutanoyl: [76-50-6] *Bornyl isovalerate. FEMA 2165*
$C_{15}H_{26}O_2$ 238.369
Flavouring agent. Oil. d^{18} 0.95. Bp_{26} 151-152°. n_D^{18} 1.4605.

(1*S*,2*R*)-*form* [464-45-9]
(-)-Borneol. *Linderol. Ngai camphor. FEMA 2157*
Constit. of *Blumea balsamifera* (sambong). Cryst. (petrol). Mp 208-209°. Bp 212°. $[\alpha]_D^{20}$ -37.74 (c, 5 in EtOH).

▶ Skin irritant. LD_{50} (rat, orl) 5800 mg/kg. DT5095000

Ac: [5655-61-8] *(-)-Bornyl acetate. FEMA 2159*
$C_{12}H_{20}O_2$ 196.289
Flavouring agent. Sol. MeOH, Et_2O; fairly sol. H_2O. Bp 223-224°. $[\alpha]_D^{20}$ -38.1 (neat).

(1*S*,2*S*)-*form* [16725-71-6]
(+)-Isoborneol. FEMA 2158
Flavouring agent. Cryst. (petrol). Mp 214°. $[\alpha]_D$ +33.89 (EtOH).

(1*RS*,2*RS*)-*form* [6627-72-1]
(±)-Isoborneol
Plates (petrol). Prac. insol. H_2O. Mp 212° (sealed tube).

Formyl: [1200-67-5] *Isobornyl formate. FEMA 2162*

$C_{11}H_{18}O_2$ 182.262
Flavouring agent. d^{18} 1. Bp_{20} 110°. n_D^{20} 1.4717.

Propanoyl: [2756-56-1] *Isobornyl propionate. FEMA 2163*
$C_{13}H_{22}O_2$ 210.316
Flavouring agent. Oil. $d^{15.5}$ 0.98. Bp 245°. n_D^{20} 1.4640.

3-Methylbutanoyl: [7779-73-9] *Isobornyl isovalerate. FEMA 2166*
$C_{15}H_{26}O_2$ 238.369
Flavouring agent. Liq.

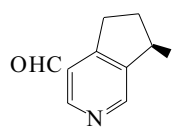
(1*RS*,2*SR*)-*form* [24393-70-2]
(±)-Borneol. FEMA 2157
Flavouring agent. Mp 210-215° subl.
► Fl. p. 66°.

[124-76-5, 507-70-0, 16868-11-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 169B; 169C; 631C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 251A; 251B; 954A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 246A; 246B; 660A (*ir, Ac*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 312; 313 (*occur*)
Oratani, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 1961-1964 (*resoln*)
Gream, G.E. *et al., Aust. J. Chem.*, 1974, **27**, 567-587 (*(+)-Borneol, (-)-Isoborneol, synth*)
Helmchen, G. *et al., Tet. Lett.*, 1974, 1527-1530 (*abs config*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426-432 (*cmr*)
Tadesa, K. *et al., Agric. Biol. Chem.*, 1976, **40**, 1069-1073 (*biosynth*)
Stothers, J.B. *et al., Can. J. Chem.*, 1976, **54**, 1211-1221 (*cmr, biosynth*)
Yamaguchi, S. *et al., Tet. Lett.*, 1977, 89 (*config, pmr*)
Jonsson, S. *et al., J. Chem. Ecol.*, 1988, **14**, 713-721 (*occur*)
Merck Index, 11th edn., 1989, 1339
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1409
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 68; 69; 70; 71; 384; 385; 386 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 292-297; 1435-1440
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMD000; IHY000; NCQ820

Boschniakine B-172

Indicaine



(*R*)-*form*

$C_{10}H_{11}NO$ 161.203

(*R*)-*form* [18070-40-1]
Alkaloid from *Plantago psyllium* (African plantain). Bp_3 80-90°. $[\alpha]_D^{20}$ +21 (c, 0.98 in $CHCl_3$).

Picrate:
Mp 126-128° Mp 156° (dimorph.).

Semicarbazone:
Mp 217-220° (210-224°).

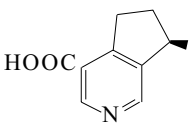
N-*Et:* [32152-74-2] ***Indicainine***
$C_{12}H_{16}NO^{\oplus}$ 190.264The correctness of the struct. has been questioned (D. Gross *et al*).

N-*Et, picrate:*
Mp 125-127°. $[\alpha]_D^{30}$ +14.2 (c, 1.9 in $CHCl_3$).

Sakan, T. *et al., Tetrahedron*, 1967, **23**, 4635 (*uv, ir, synth, struct*)
Torssell, K. *et al., Acta Chem. Scand.*, 1968, **22**, 2715 (*struct*)
Dickinson, E.M. *et al., Tetrahedron*, 1969, **25**, 1523 (*pmr*)
Khakimdzhanov, S. *et al., Khim. Prir. Soedin.*, 1971, **7**, 126; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 121 (*Indicainine*)
Gross, D. *et al., Z. Chem.*, 1973, **13**, 296 (*ms*)

Boschniakinic acid B-173

Plantagonine



(*R*)-*form*

$C_{10}H_{11}NO_2$ 177.202

(*R*)-*form* [21857-97-6]
Alkaloid from *Plantago psyllium* (African plantain). Mp 218-220°. $[\alpha]_D$ +38.6 (+ 30.8).

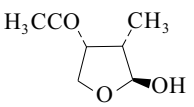
(*S*)-*form* [21913-34-8]
Mp 218-220°. $[\alpha]_D$ -30.1.

(±)-*form*
Mp 226-227°.

Sakan, T. *et al., Tetrahedron*, 1967, **23**, 4635 (*isol, ir, struct, synth*)
Cordell, G.A. *et al., Alkaloids (N.Y.)*, 1977, **16**, 431 (*rev*)

Botryodiplodin B-174

[27098-03-9]
1-(Tetrahydro-5-hydroxy-4-methyl-3-furanyl)ethanone, 9CI. 4-Acetyl-2-hydroxy-3-methyltetrahydrofuran



Absolute configuration

$C_7H_{12}O_3$ 144.17
Mycotoxin prod. by *Botryodiplodia theobromae*, *Penicillium carneoluteus* and *Penicillium roquefortii*. Isol. from *P. roquefortii* infected corn silage. Cryst. (Et_2O). Sol. H_2O, Me_2CO, MeOH, EtOH, Et_2O; fairly sol. C_6H_6, hexane, $CHCl_3$. Mp 50-52°. Anomerises in soln. to a mixt. of 2-epimers λ_{max} 278 (ϵ 25) ($CHCl_3$) (Berdy).
► LD_{50} (mus, ipr) 40-50 mg/kg. OB6005000

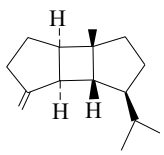
Ac:
Cryst. (Et_2O). Mp 45-47°. $[\alpha]_D$ -104 (c, 0.09 in $CHCl_3$).

[81738-55-8, 95976-07-1, 95976-08-2]

McCurry, P.M. *et al., J.A.C.S.*, 1973, **95**, 5824 (*synth, stereochem*)
Wilson, S.R. *et al., J.O.C.*, 1975, **40**, 3309 (*synth*)
Sakai, K. *et al., CA*, 1979, **90**, 186692p (*synth, abs config*)
Moreau, S. *et al., J.O.C.*, 1982, **47**, 2358 (*isol, cryst struct*)
Renauld, F. *et al., Tetrahedron*, 1984, **40**, 1823; 1985, **41**, 955 (*biosynth, props*)
Kurth, M.J. *et al., J.O.C.*, 1985, **50**, 1840 (*synth*)
Rehnberg, N. *et al., Tet. Lett.*, 1987, **28**, 3589-3592 (*synth*)
Rehnberg, N. *et al., Acta Chem. Scand.*, 1990, **44**, 377 (*synth*)
Nouguier, R. *et al., Tet. Lett.*, 1999, **40**, 3371-3374 (*synth*)
Villar, F. *et al., Tet. Lett.*, 1999, **40**, 3375-3378 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMK290

4(15)-Bourbonene B-175

[5208-59-3]
β-Bourbonene

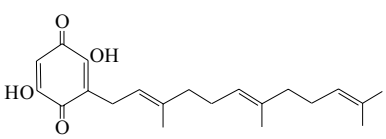


$C_{15}H_{24}$ 204.355
Flavouring agent. Oil. $[\alpha]_D^{20}$ -92.12.

Křepinský, J. *et al., Tetrahedron, Suppl.*, No. 8, 1966, 53 (*struct*)
White, J.D. *et al., J.A.C.S.*, 1968, **90**, 6171 (*synth*)
Tomioka, K. *et al., Tet. Lett.*, 1982, **23**, 3401 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 298-299
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr, cmr*)

Boviquinone 3 B-176

[32916-10-2]
2,5-Dihydroxy-3-(3,7,11-trimethyl-2,6,10-dodecatrienyl)cyclohexadiene-1,4-dione, 9CI. 3-Farnesyl-2,5-dihydroxy-1,4-benzoquinone. Helveticone



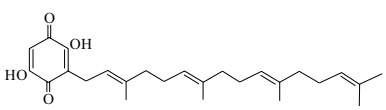
$C_{21}H_{28}O_4$ 344.45

(*E*,*E*)-*form* [34198-83-9]
Pigment from *Chroogomphus rutilus* (pine spike cap). Yellow cryst. (petrol). Mp 98-100°.

Beaumont, P.C. *et al., J.C.S.(C)*, 1971, 2582 (*isol, struct*)
Esser, F. *et al., Z. Naturforsch., B*, 1971, **26**, 336
Mühlbauer, A. *et al., Tet. Lett.*, 1998, **39**, 5167-5170 (*biosynth*)

Boviquinone 4 B-177

[28129-52-4]
3-Geranylgeranyl-2,5-dihydroxy-1,4-benzoquinone. Bovinone



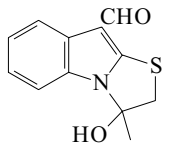
$C_{26}H_{36}O_4$ 412.568

Metabolite of *Boletus (Suillus) bovinus*. Yellow cryst. (AcOH). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 84-85°. λ_{max} 287 (ϵ 20500) (EtOH) (Berdy). λ_{max} 324 (EtOH/NaOH) (Berdy).

Beaumont, P.C. *et al., J.C.S.(C)*, 1969, 2398
Mühlbauer, A. *et al., Tet. Lett.*, 1998, **39**, 5167-5170 (*biosynth*)

Brassicanal B B-178

[126654-63-5]
2,3-Dihydro-3-hydroxy-3-methylthiazolo[3,2-a]indole-9-carboxaldehyde, 9CI



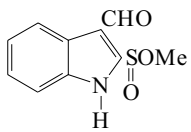
$C_{12}H_{11}NO_2S$ 233.29

Exists in CD_3OD as an equilibrium mixt. of the hemiaminal (illus.) and open-chain keto form. Alkaloid from Chinese cabbage *Brassica campestris* ssp. *pekinensis* inoculated with *Pseudomonas cichorii*. Mp 169-170°. $[\alpha]_D$ 0. λ_{max} 207 (ϵ 25800); 220 (ϵ 25400); 252 (ϵ 24100); 277 (ϵ 14200); 315 (ϵ 11700) (MeOH) (Berdy).

Monde, K. *et al., Chem. Lett.*, 1990, 209 (*isol, uv, ir, pmr, cmr, ms, struct*)

Brassicanal C B-179

[137761-23-0]
Methyl 3-formyl-1H-indole-2-sulfinate, 9CI

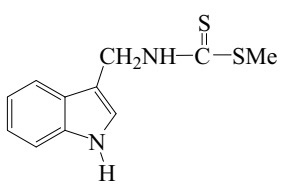


$C_{10}H_9NO_3S$ 223.252
Alkaloid from *Brassica oleracea* (cabbage) inoculated with *Pseudomonas cichorii*. Mp 150-151°. $[\alpha]_D$ -13.3 (c, 1.04 in MeOH). λ_{max} 215 (ϵ 18300); 247 (ϵ 13600); 309 (ϵ 9400) (MeOH) (Berdy).

Monde, K. *et al., Phytochemistry*, 1991, **30**, 2915 (*isol, uv, ir, pmr, cmr, ms, struct*)

Brassinin B-180

[105748-59-2]
Methyl (1H-indol-3-ylmethyl)carbamodithioate, 9CI



$C_{11}H_{12}N_2S_2$ 236.361
Isol. from Chinese cabbage (*Brassica campestris* ssp. *pekinensis*)(Cruciferae) heads inoculated with *Pseudomonas cichorii*. Sol. MeOH, Et_2O, Me_2CO; fairly sol. H_2O. Mp 132-133°. First report of the isol. of sulfur-containing phytoalexins (see also Cyclobrassinin, C-434) λ_{max} 220 (ϵ 30000); 280 (ϵ 6000); 289 (ϵ 5000) (MeOH) (Derep). λ_{max} 218 (ϵ 38300); 236 (ϵ 87400); 268 (ϵ 16100); 287 (ϵ 9070) (MeOH) (Berdy).

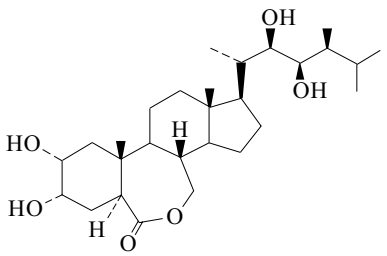
N[1]-Methoxy: [105748-60-5] ***Methoxybrassinin***
$C_{12}H_{14}N_2OS_2$ 266.387
Isol. from *Brassica campestris* ssp. *pekinensis* (Cruciferae) inoculated with *Pseudomonas cichorii*. Viscous oil. λ_{max} 218 (ϵ 37300); 267 (ϵ 15800); 287 (sh) (ϵ 9470); 297 (sh) (ϵ 5740) (MeOH) (Derep). λ_{max} 218 (ϵ 37000); 241 (ϵ 13000); 267 (ϵ 15300) (MeOH) (Berdy). λ_{max} 218 (ϵ 24500); 267 (ϵ 16200) (EtOH) (Berdy).

4-Methoxy: [129602-03-5] ***4-Methoxybrassinin***
$C_{12}H_{14}N_2OS_2$ 266.387
Isol. from white cabbage (*Brassica oleracea* var. *capitata*) (Cruciferae) heads inoculated with *Pseudomonas cichorii*. Amorph. λ_{max} 219 (ϵ 44300); 265 (ϵ 18500) (MeOH) (Berdy).

Takasugi, M. *et al., Chem. Comm.*, 1986, 1077 (*isol, synth, struct, deriv*)
Kawasaki, T. *et al., Heterocycles*, 1990, **31**, 1605 (*synth, Methoxybrassinin*)
Monde, K. *et al., Phytochemistry*, 1990, **29**, 1499 (*4-Methoxybrassinin*)
Somei, M. *et al., Heterocycles*, 1992, **33**, 77 (*synth, Methoxybrassinin*)
Yamada, F. *et al., Heterocycles*, 1993, **36**, 2783 (*synth*)
Kutschy, P. *et al., Tetrahedron*, 1998, **54**, 3549-3566 (*synth*)
Pedras, M.S.C. *et al., Phytochemistry*, 2000, **53**, 161-176 (*rev*)

Brassinolide B-181

[72962-43-7]
2,3,22,23-Tetrahydroxy-24-methyl-B-homo-7-oxacholestan-6-one



$C_{28}H_{48}O_6$ 480.684
Constit. of bee collected rape pollen (*Brassica napus*). Cryst. Mp 274-275°. $[\alpha]_D^{24}$ +41.9 ($CHCl_3$/MeOH, 9:1).

24-Epimer: [78821-43-9] ***24-Epibrassinolide***. *Epibrassinolide R*
$C_{28}H_{48}O_6$ 480.684
Constit. of *Vicia faba* pollen. Cryst. Mp 256-258°.

22,23,24-Triepimer: [78821-42-8] ***Brassinosteroid***. *Epibrassinolide S. Isoepibrassinolide*

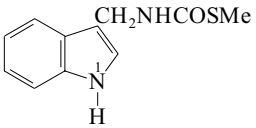
2-Deoxy: [144071-55-6] *3,22,23-Trihydroxy-24-methyl-B-homo-7-oxacholestan-6-one.* ***2-Deoxybrassinolide***
$C_{28}H_{48}O_5$ 464.684
Constit. of seeds of *Apium graveolens* (celery) and *Pisum sativum* (pea).

23-Ketone, 24-epimer: [208346-75-2] ***24-Epi-23-dehydrobrassinolide***
$C_{28}H_{46}O_6$ 478.6683 Stereoisomeric compds. also isol..

Thompson, M.J. *et al., J.O.C.*, 1979, **44**, 5002 (*synth*)
Grove, M.D. *et al., Nature (London)*, 1979, **281**, 216 (*isol, cryst struct*)
Mori, K. *et al., Tetrahedron*, 1982, **38**, 2099 (*synth*)
Sakakibara, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 663 (*synth, bibl*)
Ikekawa, N. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2001 (*synth*)
Donaubaurer, J.R. *et al., J.O.C.*, 1984, **49**, 2833 (*synth*)
Mori, K. *et al., Tetrahedron*, 1984, **40**, 1767 (*synth*)
Singh, H. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 989 (*rev*)
Adam, G. *et al., Phytochemistry*, 1986, **25**, 1787 (*rev*)
Aburatani, M. *et al., Agric. Biol. Chem.*, 1987, **51**, 1909 (*synth*)
Ikekawa, N. *et al., Chem. Pharm. Bull.*, 1988, **36**, 405 (*24-epi-Brassinolide*)
Wei-Shan, Z. *et al., Chem. Comm.*, 1989, 612 (*synth*)
Yokota, T. *et al., Agric. Biol. Chem.*, 1990, **54**, 1107 (*biosynth*)
Zhou, W.-S. *et al., J.C.S. Perkin 1*, 1991, 2827 (*synth*)
Back, T.G. *et al., J.O.C.*, 1991, **56**, 454 (*synth*)
Back, T.G. *et al., Tet. Lett.*, 1991, **32**, 4817 (*synth*)
Zhou, W.-S. *et al., Tet. Lett.*, 1991, **32**, 6745 (*synth*)
Tsubuki, M. *et al., J.C.S. Perkin 1*, 1992, 2643 (*synth*)
Porzel, A. *et al., Magn. Reson. Chem.*, 1992, **30**, 651 (*pmr, cmr*)
Bock, T.G. *et al., Can. J. Chem.*, 1993, **71**, 156 (*synth*)
McMorris, T.C. *et al., J.O.C.*, 1993, **58**, 2338 (*synth*)
Ando, T. *et al., Magn. Reson. Chem.*, 1993, **31**, 94 (*pmr, cmr*)
Schmidt, J. *et al., Phytochemistry*, 1995, **40**, 1041 (*2-Deoxybrassinolide*)
McMorris, T.C. *et al., J.C.S. Perkin 1*, 1996, 295 (*synth*)
Yokota, T. *et al., Phytochemistry*, 1996, **42**, 509 (*2-Deoxybrassinolide*)
Choi, Y.-H. *et al., Phytochemistry*, 1996, **43**, 593; 1997, **44**, 609 (*biosynth*)
Voigt, B. *et al., Tetrahedron*, 1996, **52**, 1997 (*synth*)
Wantanabe, T. *et al., J. Chem. Res., Synop.*, 1997, 360-361 (*synth*)
Stoldt, M. *et al., Magn. Reson. Chem.*, 1997, **35**, 629-636 (*pmr, cmr*)
Schmittberger, T. *et al., Tet. Lett.*, 1997, **38**, 2837 (*synth*)
Yokota, T. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 526-531 (*23-Dehydrobrassinolides*)
Brosa, C. *et al., Tetrahedron*, 1999, **55**, 1793-1798 (*synth*)
Lopez, E.M.F. *et al., Antiviral Chem. Chemother.*, 2000, **11**, 71 (*activity*)
Nomura, T. *et al., Phytochemistry*, 2001, **57**, 171-178 (*biosynth*)

Brassitin B-182

[113866-42-5]
S-*Methyl 1*H-*indole-3-ylmethylcarbamothioate, 9CI*



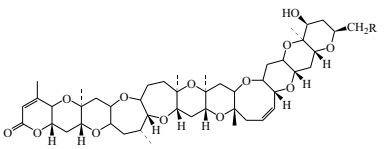
$C_{11}H_{12}N_2OS$ 220.295
Stress metab. from Japanese radish Daikon (*Raphanus sativus* var. *hortensis*, Cruciferae), inoculated with *Pseudomonas cichorii*. Amorph. λ_{max} 218 (ϵ 36800); 271 (ϵ 5910); 277 (ϵ 5910); 287 (ϵ 4830) (MeOH) (Berdy).

1-Methoxy: [113900-63-3] ***Methoxybrassitin***
$C_{12}H_{14}N_2O_2S$ 250.321
Isol. from Chinese cabbage (*Brassica campestris* ssp. *pekinensis*, Cruciferae) inoculated with the bacterium *Pseudomonas cichorii*. Cryst. (Et_2O/EtOH). Mp 94-96°.

Takasugi, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 285 (*Methoxybrassitin*)
Monde, K. *et al., Phytochemistry*, 1995, **39**, 581 (*Brassitin*)
Kutschy, P. *et al., Tetrahedron*, 1998, **54**, 3549-3566 (*synth*)

Brevetoxin B_2 B-183

[173691-95-7]
BTXB2



R = -CH(CH$_2$OH)CH$_2$S(O)CH$_2$CH(NH$_2$)COOH

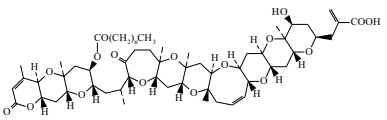
$C_{53}H_{79}NO_{17}S$ 1034.27
Isol. from *Perna canaliculus* (New Zealand green mussel). Amorph. solid. Sol. MeOH. $[\alpha]_D^{25}$ +19 (c, 0.6 in MeCN aq.).
▶ LD_{50} (mus, ipr) 0.306 mg/kg.

N-*Tetradecanoyl:* [260270-43-7] ***Brevetoxin B_{4a}. BTXB4a***
$C_{67}H_{105}NO_{18}S$ 1244.628
Isol. from *Perna canaliculus* (New Zealand green mussel). Isol. as a mixt. with BTXB4b.

N-*Hexadecanoyl:* [260270-44-8] ***Brevetoxin B_{4b}. BTXB4b***
$C_{69}H_{109}NO_{18}S$ 1272.682
Isol. from *Perna canaliculus* (New Zealand green mussel). Isol. as a mixt. with BTXB4a.

Murata, K. *et al., Tetrahedron*, 1998, **54**, 735-742
Morohashi, A. *et al., Nat. Toxins*, 1999, **7**, 45-48 (*Brevetoxin B_4*)

Brevetoxin B_3 B-184



n = 12 and 14

Isol. from the New Zealand green mussel *Perna canaliculus*. Obt. as two homologues λ_{max} 207 (ϵ 19000) (MeOH) (Berdy).

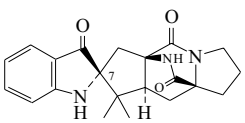
Brevetoxin B_3 C_{64} component [171527-63-2]
$C_{64}H_{96}O_{17}$ 1137.452*n* = 12.

Brevetoxin B_3 C_{66} component [171527-64-3]
$C_{66}H_{100}O_{17}$ 1165.506*n* = 14.

Morohashi, A. *et al., Tet. Lett.*, 1995, **36**, 8995-8998 (*isol, pmr, ms*)

Brevianamide A B-185

[23402-09-7]



Absolute configuration

$C_{21}H_{23}N_3O_3$ 365.431
Diketopiperazine antibiotic. Mycotoxin from *Penicillium brevi-compactum* and some other *Penicillium* spp.. Mp 175-180° ($CHCl_3$ solvate). $[\alpha]_D^{25}$ +413 (EtOH). λ_{max} 234 ; 256 ; 404 (EtOH) (Berdy).

7-Epimer: [38136-92-4] ***Brevianamide B***
$C_{21}H_{23}N_3O_3$ 365.431
From *Penicillium brevi-compactum*. Yellow prisms (DMSO aq.). Mp 324-328° dec. λ_{max} 230 ; 256 ; 400 (MeOH) (Berdy).

Birch, A.J. *et al., Tetrahedron*, 1970, **26**, 2329; 1972, **28**, 2999 (*isol, uv, ir, pmr, ms, struct*)
Coetzer, J. *et al., Acta Cryst. B*, 1974, **30**, 2254 (*cryst struct*)
Baldas, J. *et al., J.C.S. Perkin 1*, 1974, 50 (*biosynth*)
Bird, B.A. *et al., Appl. Environ. Microbiol.*, 1981, **42**, 521; 1982, **43**, 345 (*isol*)
Stocking, E.M. *et al., J.A.C.S.*, 2000, **122**, 9089-9098 (*biosynth*)
Williams, R.M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 711-740 (*rev, synth, biosynth*)

Brevicin 27 B-186

[156409-70-0]
Basic protein, MW 5200 Da. Prod. by *Lactobacillus brevis* SB 27. Bacteriocin.

Benoit, V. *et al., Curr. Microbiol.*, 1997, **34**, 173-179 (*isol*)

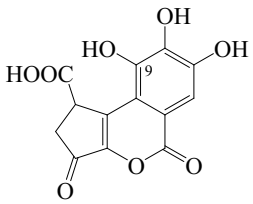
Brevicin 37 B-187

[130588-22-6]
Polypeptide. Prod. by *Lactobacillus brevis* B37. Bacteriocin.

Rammelsberg, M. *et al., J. Appl. Bacteriol.*, 1990, **69**, 177-184 (*isol*)

Brevifolincarboxylic acid B-188

[18490-95-4]
1,2,3,5-Tetrahydro-7,8,9-trihydroxy-3,5-dioxocyclopenta[c][2]benzopyran-1-carboxylic acid, 9CI



$C_{13}H_8O_8$ 292.201
Yellow prisms + H_2O (H_2O). Mp 250° (dec.). $[\alpha]_D^{13}$ -3 (c, 0.4 in Me_2CO aq.). Readily decarboxylates to Brevifolin.

Me ester: [154702-76-8] ***Methyl brevifolincarboxylate***
$C_{14}H_{10}O_8$ 306.228

Et ester: [107646-82-2] *Ethyl brevifolincarboxylate*
$C_{15}H_{12}O_8$ 320.255
Yellow needles (EtOAc/Me_2CO). Mp 250°. λ_{max} 277 (ϵ 21380); 350 (ϵ 14450); 362 (ϵ 14450) (MeOH) (Berdy). λ_{max} 276 (ϵ 21880); 350 (ϵ 9120); 365 (ϵ 8710) (EtOH) (Berdy).

1,3,6-Tri-O-galloyl-β-D-glucopyranosyl ester: ***Euphormisin M_1***
$C_{40}H_{30}O_{25}$ 910.662
Pale brown amorph. powder. $[\alpha]_D$ -20 (c, 1 in MeOH). Esterified at *O*-4 of glucose moiety λ_{max} 215 (log ϵ 4.69); 278 (log ϵ 4.42) (MeOH).

9-Sulfate:
$C_{13}H_8O_{11}S$ 372.266
Constit. of *Punica granatum* (pomegranate). Yellow-brown powder (as K salt). λ_{max} 276 ; 346 (MeOH).

Bernauer, K. *et al., Annalen*, 1954, **588**, 211 (*isol, struct*)
Parveen, N. *et al., Phytochemistry*, 1988, **27**, 3990 (*ester*)
Saijo, R. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2624 (*pmr, cmr, ms*)
Gottlieb, H.E. *et al., Phytochemistry*, 1991, **30**, 2435 (*isol, pmr, cmr*)
Yao, Q.Q. *et al., Yaoxue Xuebao*, 1993, **28**, 829-835 (*isol, Me ester*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1803 (*Euphormisin M_1, isol, pmr, cmr, uv*)
Nawwar, M.A.M. *et al., Phytochemistry*, 1994, **36**, 793 (*isol, pmr, cmr*)
Hussein, S.A.M. *et al., Phytochemistry*, 1997, **45**, 819 (*10-sulfate*)

Brochocin C B-189

[150260-36-9]
Struct. unknown. Bacteriocin prod. by *Brochothrix campestris*.

Siragusa, G.R. *et al., Appl. Environ. Microbiol.*, 1993, **59**, 2326 (*isol*)

Bromelains, BAN, INN, JAN, USAN B-190

[9001-00-7]

[37189-34-7]
Ananase. Bromelase. Extranase. Inflamen. Traumanase. E.C. 3.4.22.32 (stem brome-

lain). E.C. 3.4.22.33 (fruit bromelain)

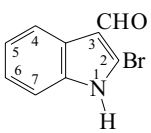
Enzymes with broad specificity for hydrolysis of peptide bonds; stem bromelain is basic, fruit bromelain is acidic. Enzymes occurring in pineapple juice (*Ananas sativus*); used in tenderising meat and chill-proofing beer. Formerly E.C. 3.4.22.4.

▶ LD_{50} (rat, orl) >10000 mg/kg. LD_{50} (rat, ipr) 85.2 mg/kg. Hypersensitivity reactions reported when used therapeutically and from occup. exposure. Adverse gastrointestinal effects. EF8575000

Ger. Pat., 1967, 55 405; *CA*, **67**, 84851x (*isol*)
Murachi, T. *et al., Methods Enzymol.*, 1976, **45**, 475 (*rev*)
Cooreman, W.M. *et al., Pharm. Acta Helv.*, 1976, **51**, 73 (*rev, pharmacol*)
Taussig, S.J. *et al., Med. Hypotheses*, 1980, **6**, 99 (*rev, activity*)
Vellini, M. *et al., Arzneim.-Forsch.*, 1986, **36**, 110 (*pharmacol*)
Boller, T. *et al., Plant Proteolytic Enzymes*, (Dalling, M.J. Ed.), CRC Press, 1986, **1**, 81 (*rev*)
Taussig, S.J. *et al., J. Ethnopharmacol.*, 1988, **22**, 191 (*rev*)
Lotz-Winter, H. *et al., Planta Med.*, 1990, **56**, 249 (*rev, pharmacol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1345
Rowan, A.D. *et al., Methods Enzymol.*, 1994, **244**, 555-568 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 299-300 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMO000

2-Bromo-1*H*-indole-3-carboxaldehyde, 9CI B-191

[119910-45-1]
2-Bromo-3-formylindole



C_9H_6BrNO 224.056
Plant growth enhancer for rice. Prob. of no coml. significance. Solid.

N-*Me:* [156137-02-9]
$C_{10}H_8BrNO$ 238.083
Light tan solid (EtOH). Mp 110-111.5°.

[68770-85-4]

Somei, M. *et al., Heterocycles*, 1988, **27**, 1585 (*synth*)
Japan. Pat., 1990, 02 85 251; *CA*, **113**, 110930n (*synth, activity*)
Showalter, H.D.H. *et al., J. Med. Chem.*, 1997, **40**, 413-426 (*N-Me, pmr*)
De Koning, C.B. *et al., J.C.S. Perkin 1*, 2000, 1705-1713 (*synth, N-Me, ir, pmr, cmr, ms*)

1-Bromo-3-iodo-2-propanone, 9CI B-192

[59227-98-4]
1-Bromo-3-iodoacetone
$BrCH_2COCH_2I$
C_3H_4BrIO 262.873
Minor component of the essential oil of the edible Hawaiian red alga *Asparagopsis taxiformis*.

Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*synth, glc, ms, isol*)

Bromomethane, 9CI B-193

[74-83-9]
Methyl bromide, BSI, ISO, JMAF. R 40B1. Dow Fume MC2. Halon 1001. Terabol. Curafume
H_3CBr
CH_3Br 94.939
Principally used as an insecticidal and nemacidal fumigant, esp. for soil and agricultural produce. Also used as a solvent for extraction of plant oils. Gas with faint chloroform-like odour. Spar. sol. H_2O. Mp -93.7°. Bp 4.5° (3.6°). Forms a hydrate at 0-5°. The signatory countries to the 1995 Montreal Treaty have agreed to phase out the industrial use of methyl bromide by 2010, in the USA its use will be banned after 1st January 2005.

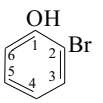
▶ Autoignition temp. 535/537°. Vapour can ignite or explode if strongly heated. Eye irritant and vesicant which can penetrate rubber protection equipment. One of the most toxic organic halides, whose effects are cumulative and may be delayed after exposure. Organs affected after inhalation or percutaneous absorption include nervous system, kidneys and lung. Acute or chronic exposure can be fatal. Exp. carcinogen. OES: long-term 5 ppm; short-term 15 ppm (Sk). PA4900000

[1111-88-2]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 81D (*ir*)
Dougherty, G. *et al., J.A.C.S.*, 1929, **51**, 576 (*synth*)
Egan, C.J. *et al., J.A.C.S.*, 1938, **60**, 2097 (*props*)
Gallant, R.W. *et al., Hydrocarbon Process.*, 1968, **47**, 128 (*rev*)
Kawaguchi, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 53 (*cryst struct*)
Price, C.C. *et al., J.O.C.*, 1973, **38**, 615 (*pmr*)
Ossinger, A.I. *et al., J. Chem. Phys.*, 1976, **65**, 2892 (*ms*)
Jung, M.E. *et al., Tet. Lett.*, 1978, 4483 (*synth*)
Andrews, L. *et al., J.A.C.S.*, 1979, **101**, 7158 (*uv, ir*)
Olah, G.A. *et al., Organometallics*, 1982, **1**, 1485 (*cmr*)
Dangerous Prop. Ind. Mater. Rep., 1985, **5**, 37 (*rev*)
Binbrek, O.S. *et al., J. Phys. Chem.*, 1985, **82**, 1468 (*ir, Raman*)
Bond, J.A. *et al., Toxicol. Appl. Pharmacol.*, 1985, **78**, 259 (*metab*)
IARC Monog., 1986, **41**, 187; *Suppl.* 7, 245; *Suppl.* 6, 386 (*rev, tox*)
Bretherick, L. *et al., Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 567
Pesticide Manual, 9th edn., 1991, No. 8340
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A273
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1129
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 742-744 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3442
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 322
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0410
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 668
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 173
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHR200

2-Bromophenol, 9CI B-194

[95-56-7]



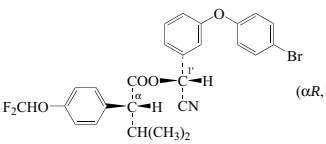
C_6H_5BrO 173.009
Flavour component of marine fish, molluscs and crustaceans. Imparts and intense shrimp-like flavour. Liq. Bp 194°. pK_a 8.45 (25°).

▶ Fl. p. >66°. LD_{50} (mus, orl) 652 mg/kg. SJ7875000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1040A; 1072B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 179B; 247A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 967D; 1004B (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 97 (*synth*)
Pearson, D.E. *et al., J.O.C.*, 1967, **32**, 2358 (*synth*)
Smith, W.B. *et al., Org. Magn. Reson.*, 1976, **8**, 205 (*cmr*)
Brossi, A. *et al., Helv. Chim. Acta*, 1981, **64**, 1672 (*cmr*)
Kim, K. *et al., Chem. Comm.*, 1986, 1159 (*synth*)
Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)
Whitefield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405 (*occur*)

[3-(4-Bromophenoxy)phenyl]-cyanomethyl 4-(difluoromethoxy)-α-(1-methylethyl)benzeneacetate, 9CI B-195

[160791-64-0]
ZXI 8901



(α*R*,1′*R*)-*form*

$C_{26}H_{22}BrF_2NO_4$ 530.365
▶ LD_{50} (rat, orl) >10000 mg/kg.
(α*R*,1′*R*)-*form* [170861-08-2]

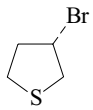
[170861-06-0, 170861-07-1, 171031-56-4]

Sun, G. *et al., Shanghai Huagong*, 1993, **18**, 13-16; *CA*, **122**, 99281q (*synth, activity*)
Pat. Coop. Treaty (WIPO), 1995, 95 18 790, (*Shanghai Zhongxi*); *CA*, **124**, 8415p (*synth, isomers, activity*)
Jin, W-G. *et al., Brighton Crop Prot. Conf. - Pests Dis.*, 1996, 455 (*activity*)

Pesticide Manual, 11th edn., 1997, 759

3-Bromotetrahydrothiophene, 9CI B-196

3-Bromothiolane



(*S*)-*form*

C_4H_7BrS 167.069

(*S*)-*form* [120735-11-7]
Liq. $Bp_{0.4}$ 32°. $[\alpha]_D$ -104.57 (c, 0.53 in $CHCl_3$).

S-*Oxide(*trans-*):* [120735-12-8]
C_4H_7BrOS 183.069
Cryst. (Et_2O/diisopropyl ether). Mp 68-70°. $[\alpha]_D$ -99.94 (c, 5 in $CHCl_3$).

(±)-*form* [39013-66-6]
Liq. $Bp_{0.4}$ 33°.

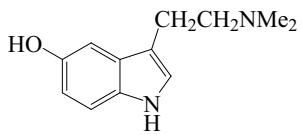
S,S-*Dioxide:* [14008-53-8] *3-Bromosulfolane*
$C_4H_7BrO_2S$ 199.068
Fungicide against black leg of sugar beet seedlings. Solid (Et_2O). Sol. H_2O. Mp 46-47°. Bp_2 132°.

▶ XN0400000

Faith, H.E. *et al., J.O.C.*, 1962, **27**, 2889 (*synth*)
Wilson, G.E. *et al., J.O.C.*, 1973, **38**, 2156 (*synth, pmr, ir, ms*)
Panasenko, A.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1983, 2723; 1984, 1497; 1991, 2035; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1983, 2442; 1984, 1376; 1991, 1799 (*dioxide, pmr, cmr*)
Volkmann, R.A. *et al., J.O.C.*, 1992, **57**, 4352; 1991, 1799 (*S-form, synth, pmr, cmr*)
Ren, X.F. *et al., Tet. Lett.*, 1993, **34**, 1575 (*synth*)
Ren, X.-F. *et al., J.O.C.*, 1995, **60**, 6468 (*dioxide, synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BOG000

Bufotenine B-197

[487-93-4]
*3-(2-Dimethylaminoethyl)-1*H*-indol-5-ol, 9CI. 3-(2-Dimethylaminoethyl)-5-hydroxyindole. Mappine. DM SHT. Cinobufotenine*



$C_{12}H_{16}N_2O$ 204.271
Sol. MeOH, acids, EtOH, bases; fairly sol. Et_2O; poorly sol. H_2O. Mp 146-147°. $Bp_{0.1}$ 320°. λ_{max} 225 ; 274 ; 300 (MeOH) (Berdy). λ_{max} 220 (ϵ 10000); 265 (ϵ 3000) (EtOH) (Berdy).

▶ Adverse systemic effects by intravenous route (psychotropic). LD_{50} (mus, ipr) 290 mg/kg. NM2800000

O-*Sulfate:* [16369-08-7] ***Bufoviridine***. *Dihydrobufothionine*
$C_{12}H_{16}N_2O_4S$ 284.335

O-*β-D-Glucopyranoside:* [64656-15-1] ***Bufotenine* O-*glucoside***
$C_{18}H_{26}N_2O_6$ 366.413
Alkaloid from the leaves of *Citrus unshiu* (satsuma mandarin). $[\alpha]_D$ -58 (c, 0.5 in H_2O). λ_{max} 224 ; 274 (No solvent reported).

N^b-*Oxide:* [1019-44-9] ***Bufotenine* N-*oxide***
$C_{12}H_{16}N_2O_2$ 220.271
Cryst. Mp 214-215°.

N^b-*Me, inner salt:* [487-91-2] ***Bufotenidine***
$C_{13}H_{18}N_2O$ 218.298
Mp 209° (as hydriodide).

Me ether: [1019-45-0] **O-*Methylbufotenine***. N,N-*Dimethyl-5-methoxytryptamine. 5-Methoxy*-N,N-*dimethyltryptamine*
$C_{13}H_{18}N_2O$ 218.298
Prisms (Et_2O/hexane). Mp 69°. Bp_4 208-210°.

▶ Toxic. LD_{50} (mus, ipr) 115 mg/kg. NL7380000

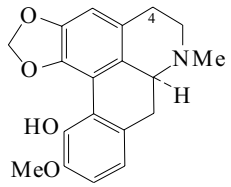
Me ether, picrate:
Orange-yellow cryst. (MeOH/Me_2CO). Mp 176-177°.

Me ether, N^b*-oxide:* **O-*Methylbufotenine* N-*oxide***
$C_{13}H_{18}N_2O_2$ 234.297
Mp 158° (as picrate).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 530D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 663C (*ir*)
Wieland, T. *et al., Annalen*, 1953, **581**, 10 (*isol, uv*)
Stromberg, V.L. *et al., J.A.C.S.*, 1954, **76**, 1707 (*isol, uv*)
Harley-Mason, J. *et al., J.C.S.*, 1954, 1167 (*synth*)
Fish, M.S. *et al., J.A.C.S.*, 1955, **77**, 5892 (*oxide*)
Erspamer, V. *et al., Biochem. Pharmacol.*, 1959, **2**, 270 (*Bufoviridine*)
Pachter, I.J. *et al., J.O.C.*, 1959, **24**, 1285 (*isol, deriv*)
Ghosal, S. *et al., J.O.C.*, 1966, **31**, 2284 (*deriv, uv, ir*)
Paris, R.R. *et al., Ann. Pharm. Fr.*, 1967, **25**, 509 (*oxide*)
Daly, J.W. *et al., J.A.C.S.*, 1967, **89**, 1032 (*pmr*)
Creveling, C.R. *et al., Clin. Chem. (Winston-Salem, N.C.)*, 1968, **14**, 302 (*ms*)
Roseghini, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1976, **54**, 31; 1989, **94**, 455 (*Bufoviridine*)
Sanders-Bush, E. *et al., Life Sci.*, 1976, **19**, 1407 (*metab*)
Schultes, R.E. *et al., Planta Med.*, 1976, **29**, 330
Shaw, G.J. *et al., Biomed. Mass Spectrom.*, 1977, **4**, 348 (*ms*)
Cimino, G. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1978, **61**, 361 (*occur*)
Barlow, R.B. *et al., Br. J. Pharmacol.*, 1980, **69**, 597 (*pharmacol*)
Nishida, R. *et al., Agric. Biol. Chem.*, 1990, **54**, 1853 (*glucoside*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1345
Somei, M. *et al., Heterocycles*, 1997, **46**, 91-94 (*synth*)
Somei, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 87-96 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DPG109

Bulbocapnine B-198

*6,7,7a,8-Tetrahydro-11-methoxy-7-methyl-5*H*-benzo[g]-1,3-benzodioxolo[6,5,4-de]-quinolin-12-ol, 9CI. 11-Hydroxy-10-methoxy-1,2-methylenedioxyaporphine.* N-*Methyllaunobine*



(*S*)-*form*

$C_{19}H_{19}NO_4$ 325.363Log P 2.59 (uncertain value) (calc).

(*S*)-*form* [298-45-3]
Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 201-203°. $[\alpha]_D^{20}$ +232 (c, 0.92 in $CHCl_3$). Pharmacol. active isomer λ_{max} 335 ; 397 (MeOH) (Berdy).

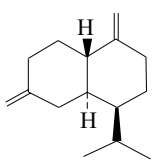
▶ LD_{50} (mus, scu) 195 mg/kg. CE1050000

N-*De-Me:* [20497-21-6] *11-Hydroxy-10-methoxy-1,2-methylenedioxynoraporphine.* ***Launobine***. *Norbulbocapnine*
$C_{18}H_{17}NO_4$ 311.337
Alkaloid from *Laurus nobilis* (bay laurel). Mp 214-215°. $[\alpha]_D^{21}$ +192 (c, 0.95 in $CHCl_3$).

Tomita, M. *et al., Yakugaku Zasshi*, 1963, **83**, 763 (*Launobine*)
Cava, M.P. *et al., J.O.C.*, 1968, **33**, 2443 (*Bulbocapnine, Launobine, isol*)

4(15),10(14)-Bulgaradiene B-199

[15890-31-0]
ϵ-Bulgarene



$C_{15}H_{24}$ 204.355
Constit. of the oil of *Mentha piperita*. $Bp_{4.5}$ 107-115°. $[\alpha]_D^{20}$ -17.1.

Linek, A. *et al., Tet. Lett.*, 1968, 23 (*isol, struct*)
Koster, F.-H. *et al., Annalen*, 1986, 78 (*synth, cmr*)

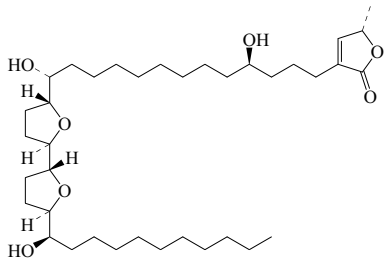
Bulgarican B-200

[86595-74-6]
Prod. by *Lactobacillus bulgaricus*. Shows antimicrobial activity. Sol. H_2O.

Reddy, C.V. *et al., Cult. Diary Prod. J.*, 1983, **18**, 15-19; *CA*, **99**, 68775f (*isol*)

Bullacin B B-201

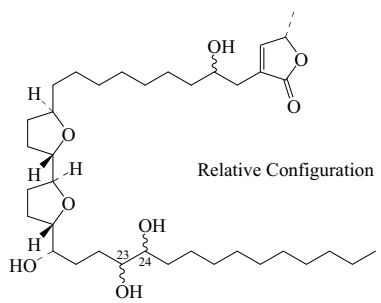
[210230-74-3]



$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona squamosa* (sugar apple). Amorph. powder. $[\alpha]_D^{23}$ +43.8 (c, 0.03 in CH_2Cl_2). λ_{max} 211 (log ϵ 3.79) (MeOH).

Hopp, D.C. *et al., Bioorg. Med. Chem.*, 1998, **6**, 569-573 (*isol*)

Bulladecin B-202

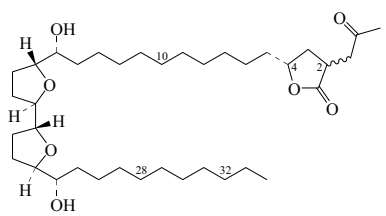


$C_{37}H_{66}O_8$ 638.924
erythro-Config. at C-23, C-24. Constit. of the seeds of *Annona atemoya* (custard apple). Solid. $[\alpha]_D^{20}$ +11 (c, 0.2 in MeOH). λ_{max} 214 (log ϵ 4.85) (MeOH).

Duret, P. *et al., Phytochemistry*, 1998, **48**, 499-506 (*isol, uv, pmr, cmr, ms*)

Bullatacinone B-203

[123012-00-0]
Isorolliniastatin 2. Isoannonareticin



$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona reticulata* (custard apple) and *Annona squamosa* (sugar apple). Cryst. (MeOH). Mp 90.5-90.7°. $[\alpha]_D^{23}$ +12 (c, 0.4 in $CHCl_3$). Log P 8 (uncertain value) (calc). Obt. as a mix of 2,4-*cis*- and *trans*-isomers. Isorolliniastatin 2 is an artifact.

24-Epimer:

[179601-77-5, 179601-78-6] ***Asimicinone***
$C_{37}H_{66}O_7$ 622.924
Constit. of *Asimina triloba* (pawpaw). Obt. as a mixture of 2,4-*cis*- and *trans*-isomers.

24-Epimer, 9-oxo: ***9-Oxoasimicinone***
$C_{37}H_{64}O_8$ 636.908
Constit. of *Annona squamosa* (sugar apple). Amorph. powder. $[\alpha]_D^{23}$ +19.7 (c, 0.1 in CH_2Cl_2). Obt. as a mixture of 2,4-*cis*- and *trans*- isomers λ_{max} 203 (log ϵ 3.55) (MeOH). λ_{max} 203 (ϵ 3550) (MeOH) (Berdy).

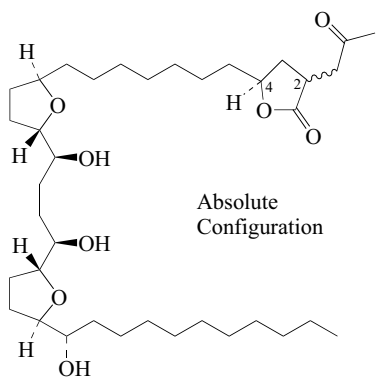
*24-Epimer, 9*R*-hydroxy:* [255900-36-8] ***9-Hydroxyasimicinone***
$C_{37}H_{66}O_8$ 638.924
Constit. of *Annona squamosa* (sugar apple). Wax. $[\alpha]_D$ +19.3 (c, 0.26 in CH_2Cl_2). Obt. as a mixture of 2,4-*cis*- and *trans*- isomers λ_{max} 203 (log ϵ 2.98) (MeOH).

Hui, Y.-H. *et al., J. Nat. Prod.*, 1989, **52**, 463; 1990, **53**, 81 (*isol, pmr, cmr*)
Gu, Z.-M. *et al., Nat. Toxins*, 1994, **2**, 49-55
Laprevote, O. *et al., Tetrahedron*, 1994, **50**, 8479 (*ms, struct*)
Gu, Z.-M. *et al., Phytochemistry*, 1995, **40**, 467-477
Yu, J.G. *et al., Chin. Chem. Lett.*, 1996, **7**, 19-22 (*Isoannonareticin*)
Zhao, G.-X. *et al., Nat. Toxins*, 1996, **4**, 128-134 (*Asimicinone*)
Hopp, D.C. *et al., Bioorg. Med. Chem.*, 1998, **6**, 569-575 (*9-Oxoasimicinone*)
Hopp, D.C. *et al., Phytochem. Anal.*, 1999, **10**, 339-347 (*9-Hydroxyasimicinone*)

Bullatalicinone B-204

[137043-93-7]

[157966-80-8]
Isocherimolin 1



$C_{37}H_{66}O_8$ 638.924
Isocherimolin 1 is an artifact. Mp 125-126°. $[\alpha]_D$ +27 (c, 0.1 in MeOH). Both 2,4-*cis*- and *trans*- isomers isol. λ_{max} 201 (ϵ 6920) (MeOH) (Berdy). λ_{max} 201 (ϵ 714) (EtOH) (Berdy).

23-Epimer: ***20,23*-cis-*Bullatalicinone***
$C_{37}H_{66}O_8$ 638.924
Constit. of unripe fruit of *Rollinia mucosa* (biriba). Amorph. powder. Mp 95-96°. Isol. as a mixt. of 2,4-*cis* and *trans*-isomers to which data refers λ_{max} 202 (log ϵ 3.54) (MeOH).

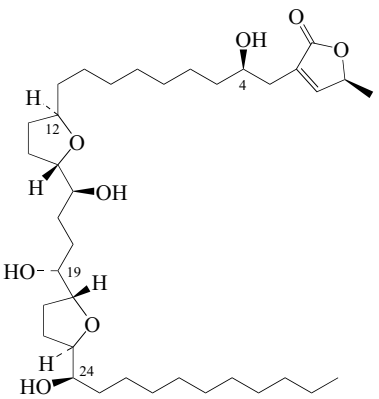
24-Epimer:

[147732-21-6] ***Bullatanocinone***
$C_{37}H_{66}O_8$ 638.924
$[\alpha]_D$ +21.5 (c, 0.2 in $CHCl_3$). 2,4-*cis*- and *trans*- isomers present and have been separated by hplc.

Fang, X.-P. *et al., J. Nat. Prod.*, 1993, **56**, 1095-1100 (*isol*)
Gu, Z.-M. *et al., Tetrahedron*, 1993, **49**, 747
Duret, P. *et al., Heterocycles*, 1994, **39**, 741-749 (*Isocherimolin 1*)
Liaw, C.-C. *et al., J. Nat. Prod.*, 1997, **62**, 1613-1617 (*20,23-cis-Bullatalicinone*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)

Bullatanocin B-205

[150134-21-7, 151637-38-6, 157184-02-6, 159249-82-8]
Annonin IV. Cherimolin 2. Crassiflorin. Purpureacin 1. Squamostatin C



$C_{37}H_{66}O_8$ 638.924
Constit. of *Annona squamosa* (sugar apple), *Annona cherimolia* (cherimoya), *Annona glabra* (pond apple) and *Annona purpurea* (soncoya). Amorph. wax. Mp 107-109° (95-97°). $[\alpha]_D^{25}$ +13.6 (c, 0.28 in CH_2Cl_2). There are still doubts about the stereochemical identity of Purpureacin 1 with Bullatanocin λ_{max} 215 (ϵ 5000) (EtOH) (Derep).

4-Deoxy: [158515-34-5] ***Squamostatin E. 4-Desoxycherimolin 2***
$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona glabra* (pond apple) and *Annona squamosa* (sugar apple). Mp 105-106°. $[\alpha]_D$ +14.7 (c, 0.5 in MeOH).

12-Epimer: [165172-08-7] ***12,15*-cis-*Bullatanocin***
$C_{37}H_{66}O_8$ 638.924

24-Epimer: [152323-84-7] ***Bullatalicin. Annonin VIII. Cherimolin 1. Squamostatin B***†
$C_{37}H_{66}O_8$ 638.924
Constit. of *Annona squamosa* (sugar apple) and *Annona cherimolia* (cherimoya). Amorph. wax. Mp 120-121° (113-116°). $[\alpha]_D$ +64 (c, 0.3 in MeOH). $[\alpha]_D^{25}$ +9.8 (c, 0.29 in CH_2Cl_2). λ_{max} 215 (ϵ 5000) (EtOH) (Derep).

24-Epimer, 4-deoxy: [157184-03-7] ***Squamostatin D***
$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona squamosa* (sugar apple). Mp 112-113.5°. $[\alpha]_D$ +7.9 (c, 0.5 in MeOH).

12,24-Diepimer: [165172-07-6] ***12,15*-cis-*Bullatalicin***
$C_{37}H_{66}O_8$ 638.924
Cryst. (MeCN).

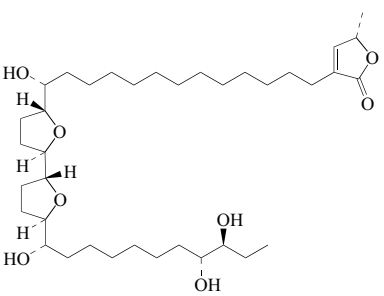
*12,24-Diepimer, 4-deoxy:****12,15*-cis-*Squamostatin D***
$C_{37}H_{66}O_7$ 622.924
Constit. of the seeds of *Annona atemoya* (custard apple). Oil. $[\alpha]_D^{24}$ +19.9 (c, 0.62 in $CHCl_3$).

[125882-64-6]

Nonfon, M. *et al., Phytochemistry*, 1990, **29**, 1951 (*isol, pmr, cmr, ms*)
Rieser, M.J. *et al., J.A.C.S.*, 1992, **114**, 10203 (*abs config*)
Cepleanu, F. *et al., Helv. Chim. Acta*, 1993, **76**, 1379 (*Purpureacin 1*)
Fang, X.-P. *et al., J. Nat. Prod.*, 1993, **56**, 1095 (*pmr, struct*)
Hirayama, K. *et al., Org. Mass Spectrom.*, 1993, **28**, 1516 (*ms*)
Cortes, D. *et al., Phytochemistry*, 1993, **32**, 1467; 1475 (*rev*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1175-1184 (*Squamostatins*)
Pinheiro-Santos, L. *et al., Quim. Nova*, 1994, **17**, 387-390 (*Crassiflorin*)
Shimada, H. *et al., Tet. Lett.*, 1994, **35**, 3961 (*abs config, Squamostatins*)
Gu, Z.-M. *et al., J. Nat. Prod.*, 1995, **41**, 229-236 (*cis-Bullatanocin, cis-Bullatalicin*)
Marshall, J.A. *et al., J.O.C.*, 1998, **63**, 7066-7071 (*synth, Squamostatin D*)
Martin, J.M. *et al., J. Nat. Prod.*, 1999, **62**, 2-4 (*activity, Bullatalicin*)
Chang, F.-R. *et al., Phytochemistry*, 1999, **51**, 883-889 (*cis-Squamostatin D*)

Bullatetrocin B-206

[184288-37-7]



Absolute Configuration

$C_{37}H_{66}O_8$ 638.924
Constit. of *Asimina triloba* (pawpaw).
Wax. $[\alpha]_D^{22}$ +16.3 (c, 0.3 in $CHCl_3$).

He, K. *et al., J. Nat. Prod.*, 1996, **59**, 1029-1034 (*isol, ir, pmr, cmr, ms*)

Butanal, 9CI B-207

[123-72-8]
Butyraldehyde, 8CI. FEMA 2219
$H_3CCH_2CH_2CHO$
C_4H_8O 72.107
Occurs in essential oils, e.g. lavender, hop. Also present in apple, banana, blackberry, hog plum, wheat bread, malt whiskey, red or white wine, tea, toasted oat flakes and other foodstuffs. Flavouring agent. Liq. Produced mainly as intermediate in oxo reaction (hydroformylation of 1-Propene) for manuf. of butanols. d^{25} 0.8. Fp -99. Bp 75°. n_D^{20} 1.3790.

▶ Severe eye, respiratory tract and skin irritant. LD_{50} (rat, orl) 2490 mg/kg. Highly flammable, fl. p. -22/-6°, autoignition temp. 230/218°. ES2275000

[74335-66-3, 74335-67-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 466A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 727C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 552A (*ir*)
Lipp, A. *et al., Annalen*, 1882, **211**, 354 (*synth*)
Dunbar, R.E. *et al., J.O.C.*, 1945, **16**, 501 (*synth*)
Brown, H.C. *et al., J.A.C.S.*, 1961, **83**, 2016 (*synth*)
Hawkes, G.E. *et al., J.O.C.*, 1974, **39**, 1017 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 731 (*rev, tox*)
El-Sherbini, Th.M. *et al., Z. Naturforsch., A*, 1981, **36**, 1334 (*ms*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH, Weinheim, 1985, **A4**, 447 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BSU250
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 736 (*rev*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1508
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 214; 215
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSU250; BSU500

Butane, 9CI B-208

[106-97-8]
E943a
$H_3CCH_2CH_2CH_3$
C_4H_{10} 58.123
Aerosol propellant. Gas. Spar. sol. H_2O, mod. sol. Et_2O, $CHCl_3$. Fp -135. Bp -0.5°. Forms copolymers with 1,3-pentadiene; reactivity ratios; γbut 1.12 + 0.13,γpent 0.32 + 0.08.

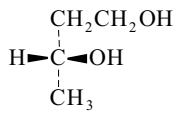
▶ An asphyxiant. Extremely flammable, fl. p. -60°, autoignition temp. 287°. OES: long-term 600 ppm; short-term 750 ppm. EJ4200000

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1D (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1D (*ir*)
Coffin, C.C. *et al., J.A.C.S.*, 1928, **50**, 1427-1437 (*synth*)
Walters, C.J. *et al., Ind. Eng. Chem.*, 1955, **47**, 2544-2547 (*isol*)
Aksnes, D.W. *et al., Acta Chem. Scand.*, 1972, **26**, 3021-3028 (*pmr*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313-321 (*cmr*)
Soboleva, T.V. *et al., Dokl. Akad. Nauk SSSR*, (Chem), 1976, **228**, 619-622; *CA*, **85**, 109042w (*copolym, reactivity ratios*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 910 (*rev*)
Schrumpf, G. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 146 (*conformn*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BOR500
Murphy, W.F. *et al., J. Phys. Chem.*, 1991, **95**, 1124-1139 (*Raman, ir*)
Durig, J.R. *et al., J. Raman Spectrosc.*, 1991, **22**, 683-704 (*Raman, ir*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 43-44
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1187
Boese, R. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 988-992 (*cryst struct*)
Low, L.K. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 267 (*rev, tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 182
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BOR500

1,3-Butanediol, 9CI B-209

[107-88-0]

[25265-75-2]
β-Butylene glycol



(*R*)-*form*

$C_4H_{10}O_2$ 90.122
Solv. for flavouring agents.

▶ Eye irritant. EK0440000

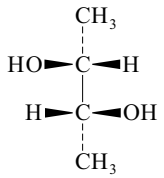
[49662-28-4, 74044-83-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 130D; 131A; 131B; 224A; 600D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 195C; 196A; 196B; 340A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 191B; 191C; 191D; 294B (*ir*)
Lukes, R. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 735 (*synth*)
Pihlaja, K. *et al., Acta Chem. Scand.*, 1969, **23**, 715 (*synth*)
Paquêtte, L.A. *et al., J.O.C.*, 1970, **35**, 2249 (*synth*)
Kirmse, W. *et al., Chem. Ber.*, 1976, **109**, 2296 (*synth*)
Gerlach, H. *et al., Helv. Chim. Acta*, 1976, **59**, 755 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **11**, 956 (*rev*)
Larchevêque, M. *et al., Synth. Commun.*, 1991, **21**, 2295 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 83
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 336-337

2,3-Butanediol, 9CI B-210

[513-85-9]

[25265-75-2]
Dimethylethylene glycol. 2,3-Butylene glycol



(2*R*,3*R*)-*form*

$C_4H_{10}O_2$ 90.122

►LD_{50} (mus, orl) 5462 mg/kg. EK0532000

(2*R*,3*R*)-*form* [24347-58-8]
Isol. from cocoa butter and roots of *Ruta graveolens* (rue). Hygroscopic cryst. Mp 19.7°. Bp_{10} 77.5-77.6°. $[\alpha]_D^{25}$ -13 (neat).

(2*RS*,3*SR*)-*form* [5341-95-7]
meso-*form*
Hygroscopic cryst. (diisopropyl ether). Mp 34.4°. Bp_{742} 181.7° Bp_{16} 89°.

(2ξ,3ξ)-*form*

O-*β*-D-*Glucopyranoside:* [146763-54-4]
$C_{10}H_{20}O_7$ 252.264
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder. $[\alpha]_D^{23}$ -32 (c, 0.2 in MeOH).

O-*[β*-D-*Apiofuranosyl-(1→6)-β*-D-*glucopyranoside]:*
$C_{15}H_{28}O_{11}$ 384.38
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder. $[\alpha]_D^{23}$ -46 (c, 0.2 in MeOH).

[1114-92-7, 4440-89-5, 5341-95-7, 17998-02-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 131C; 131D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 197A; 197B; 197C; 198A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 192A; 192B; 192C (*ir*)
Fulmer, L.M. *et al., Ind. Eng. Chem.*, 1933, **25**, 789; *CA*, **27**, 4021 (*synth*)
Wilson, C.E. *et al., J.A.C.S.*, 1936, **58**, 2396-2402 (*synth*)
Rubin, L.J. *et al., J.A.C.S.*, 1952, **74**, 425-428 (*RR,SS-forms, synth*)
Casanova, J. *et al., Chem. Ind. (London)*, 1961, 1664-1665 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 81; 1992, **16**, 52; 1986, **12**, 80; 1984, **11**, 84; 1979, **7**, 242 (*use*)
Plattner, J.J. *et al., J.A.C.S.*, 1971, **93**, 1758-1761 (*abs config*)
Saucy, G. *et al., J.O.C.*, 1977, **42**, 3206-3208 (*use*)
Enders, D. *et al., Chem. Ber.*, 1991, **124**, 219-226 (*synth*)
Kong, D.Y. *et al., Yaoxue Xuebao*, 1992, **27**, 792; *CA*, **118**, 165184 (*glucoside*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1643-1646 (*isol, glycosides*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BOT000

2,3-Butanedione B-211

[431-03-8]
Biacetyl. Dimethyl diketone. Diacetyl. FEMA 2370

$H_3CCOCOCH_3$

$C_4H_6O_2$ 86.09

Constit. of butter; formed during fermentation. A common constit. of plant oils, prod. of breakdown of carbohydrates. Flavouring additive used in food industry. Also present in apple, orange, plum, okra, walnut, Bourbon vanilla, clary sage, soybean, coffee, honey, rose wine, port wine, cocoa and scallop. Yellowish-green liq. with buttery odour and flavour at low concs. Sol. H_2O, EtOH, Et_2O. d_4^{20} 0.94. Fp 7. Bp 88°. $n_D^{18.5}$ 1.3933. Readily forms dimers and trimers by intermolecular condensation.

►Highly flammable, fl. p. 7°. Skin irritant. LD_{50} (gpg, orl) 990 mg/kg. EK2625000

[17019-25-9, 110828-81-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 423D; **2**, 922B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 657A; 659C; **3**, 489A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 509D (*ir*)
Aldrich Library of NMR Spectra, **2**, 119D (*pmr*)
Rigby, J. *et al., J.C.S.*, 1951, 793-795 (*synth*)
Nerdel, F. *et al., Chem. Ber.*, 1964, **97**, 124-131 (*synth*)
Hagen, K. *et al., J.A.C.S.*, 1973, **93**, 8266-8269 (*struct*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 765-768 (*rev, tox*)
Flatt, S.J. *et al., Synthesis*, 1979, 815-817 (*synth*)
Cerfontain, H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1983, **102**, 9-13 (*uv*)
Grases, F. *et al., Anal. Chim. Acta*, 1984, **166**, 71-78 (*dihydrazone, detn, Tc*)
Bishop, R. *et al., Aust. J. Chem.*, 1987, **40**, 249-255 (*cmr*)
Suszynski, N. *et al., J.O.C.*, 1987, **52**, 2622-2623 (*props*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BOT500
Goodrich, B.S. *et al., J. Chem. Ecol.*, 1990, **16**, 2091-2106 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 800-801 (*use, occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BOT500

1,2-Butanedithiol B-212

[16128-68-0]
FEMA 3528

$H_3CCH_2CH(SH)CH_2SH$

$C_4H_{10}S_2$ 122.255

(±)-*form*
Flavouring agent. Liq. with a sulfur, roast meat odour. d_{20}^{20} 1.31. Bp_{28} 77° Bp_5 49°. n_D^{20} 1.5205.

Simpson, J.D. *et al., Can. J. Res., Sect. B*, 1947, **25**, 25 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 71
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 308

1,3-Butanedithiol, 9CI B-213

[24330-52-7]
1,3-Dimercaptobutane. FEMA 3529

$H_3CCH(SH)CH_2CH_2SH$

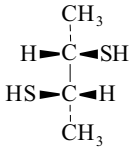
$C_4H_{10}S_2$ 122.255

(±)-*form*
Flavouring agent. Liq. with a meaty odour. d^{26} 1.05. Bp_{10} 64-67°. n_D^{20} 1.5208.

Eliel, E.L. *et al., J.A.C.S.*, 1969, **91**, 2703 (*synth*)
Abatjoglou, A.G. *et al., J.A.C.S.*, 1977, **99**, 8262 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 73
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 308-309

2,3-Butanedithiol B-214

[4532-64-3]
2,3-Dimercaptobutane. FEMA 3477



(2*S*,3*S*)-*form*

$C_4H_{10}S_2$ 122.255

Flavouring agent.

(2*S*,3*S*)-*form*
Bp_{80} 95°. $[\alpha]_D^{25}$ +11.46 (neat).

(2*RS*,3*RS*)-*form*
(±)-form
Bp_{35} 63-65°.
Bis(4-nitrobenzoyl):
Yellow plates ($PhNO_2$/MeOH). Mp 185-186.5°.

(2*RS*,3*SR*)-*form* meso-*form*
Bp_{35} 62-64°.
Bis(4-nitrobenzoyl):
Tan needles (Me_2CO). Mp 154-156°.

[68170-33-2]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 342C (*ir*)
Corey, E.J. *et al., J.A.C.S.*, 1962, **84**, 2939 (*synth, use*)
Drucker, A. *et al., J.O.C.*, 1964, **29**, 360 (*synth*)
Hermann, K. *et al., J.O.C.*, 1979, **44**, 2238 (*use*)
Vriesema, B.K. *et al., J.O.C.*, 1986, **51**, 5169 (*deriv, synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 73
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 309-310

Butanethioic acid, 9CI B-215

[3931-64-4]
Thiobutyric acid

$H_3CCH_2CH_2COSH \Leftrightarrow H_3CCH_2CH_2CSOH$

C_4H_8OS 104.173

Bp 130° (118-119°).

***OH*-form**

O-*Me ester:* [52726-01-9]
$C_5H_{10}OS$ 118.199
Bp 134°. n_D^{20} 1.4640.

Anilide:
$C_{10}H_{13}NS$ 179.285
Needles (AcOH aq.). Mp 32-33°.

***SH*-form**

S-*Me ester:* [2432-51-1] S-*Methyl butanethioate. FEMA 3310*
$C_5H_{10}OS$ 118.199
Flavouring agent. Liq. with a putrid-rancid odour similar to sour cabbage. Bp_{757} 142-142.5°. n_D^{25} 1.4595.

S-*Ph ester:* [18245-73-3]
$C_{10}H_{12}OS$ 180.27
Yellow cryst. Bp_{20} 210-212°. Steam-volatile.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 907B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 730C (*ir*)
Kurihara, T. *et al., CA*, 1959, **53**, 21644b
McFadden, W.H. *et al., Anal. Chem.*, 1965, **37**, 560
Idoux, J.P. *et al., J.O.C.*, 1973, **38**, 4239
Vermeer, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 51
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 591 (*Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1868 (*Me ester*)

1-Butanethiol B-216

[109-79-5]
Butyl mercaptan. Butyl thioalcohol. 1-Mercaptobutane. FEMA 3478

$H_3CCH_2CH_2CH_2SH$

$C_4H_{10}S$ 90.189

Flavouring agent. Present in beef, Cheshire cheese, raw chicken and cooked potatoes. Unpleasant smelling liq. d_4^{25} 0.84. Fp -119. Bp 98-100°. n_D^{25} 1.4403.

▶ Highly flammable, fl. p. 2°. Reacts violently with HNO_3. Eye, skin and respiratory tract irritant. Exp. can cause gastrointestinal disturbances and headache. LD_{50} (rat, orl) 1500 mg/kg. EK6300000

Benzoyl:
$C_{11}H_{14}OS$ 194.297
Liq. Bp_{23} 160°.

S-*Me:* See 1-(Methylthio)butane in *The Combined Chemical Dictionary.*

S-*Ph:* [1126-80-3] *1-(Phenylthio)butane. Butyl phenyl sulfide*
$C_{10}H_{14}S$ 166.287
Liq. d_4^{20} 0.99. Bp_{12} 137-139° Bp_4 94.5-97°. n_D^{20} 1.5463.

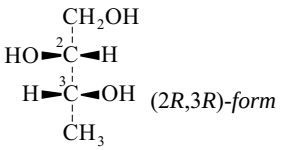
[4779-86-6, 70247-07-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 255C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 411C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 336A (*ir*)
Gray, H.L. *et al., J.A.C.S.*, 1920, **42**, 856 (*synth*)
Bezzi, S. *et al., Gazz. Chim. Ital.*, 1935, **65**, 693 (*synth*)
Ipatieff, V.N. *et al., J.A.C.S.*, 1938, **60**, 2731-2734 (*S-Ph*)
Mathias, S. *et al., J.A.C.S.*, 1950, **72**, 1897 (*props*)
Zinner, H. *et al., Chem. Ber.*, 1953, **86**, 825 (*synth*)
Haines, W.E. *et al., J. Phys. Chem.*, 1956, **60**, 549 (*props, ms, uv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 64
Paukstelis, J.V. *et al., J.O.C.*, 1977, **42**, 3941 (*cmr*)
Siggia, S. *et al., Anal. Chem.*, 1979, **51**, 1259 (*anal, Ag salt*)
Joo, T.H. *et al., J. Mol. Struct.*, 1987, **158**, 265 (*Raman*)
Tomasik, P. *et al., J. Phys. Org. Chem.*, 1991, **4**, 536 (*conformn*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 72
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 310-311
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1607
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 205
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BRR900

1,2,3-Butanetriol, 9CI B-217

[4435-50-1]

[41167-49-1, 61913-75-5, 61913-76-6, 122920-28-9, 138257-33-7]
1-Methylglycerol



(2R,3R)-form

$C_4H_{10}O_3$ 106.121
Liq. with sweet taste. $Bp_{0.4}$ 145°. All reported racemic samples appear to be diastereoisomeric mixts..

(2*R*,3*R*)-*form* [33818-52-9]
1-Deoxy-D-threitol
Hygroscopic syrup. $Bp_{0.15}$ 98-99°. n_D^{26} 1.4604.

Tris(4-nitrobenzoyl): [34290-51-2]
Cryst. ($CHCl_3$/MeOH). Mp 129-131°. $[\alpha]_D^{23}$ -9.05 (c, 2.19 in $CHCl_3$).

(2*R*,3*S*)-*form* *1-Deoxy-L-erythritol*
Constit. of the fruit of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{23}$ -30 (c, 0.3 in H_2O).

(2*S*,3*R*)-*form* [4144-94-9] *1-Deoxy-D-erythritol*
$Bp_{0.05}$ 94°. $[\alpha]_D$ +5.6 (c, 0.033 in MeOH). n_D^{20} 1.4568.

1,3-Dibenzoyl: [195512-74-4]
$C_{18}H_{18}O_5$ 314.337
Oil. $[\alpha]_D$ +51 (c, 0.875 in $CHCl_3$).

Tris(4-nitrobenzoyl): [4233-69-6]
Cryst. + ⅓ $CHCl_3$ ($CHCl_3$/MeOH). Mp 86-88° (loses solv., resolidifies) Mp 159-160° (double Mp).

1,3-Dibenzyl: [114185-05-6]
$C_{18}H_{22}O_3$ 286.37
Oil. $[\alpha]_D$ +28.8 (c, 1.25 in $CHCl_3$).

(2*R*,3*R*)-*form*
Constit. of the fruit of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ +3 (c, 0.1 in MeOH).

Chaby, R. *et al., Tetrahedron*, 1971, **27**, 3197-3205 (*synth*)
Bebault, G.M. *et al., Can. J. Chem.*, 1972, **50**, 3373-3378 (*synth*)
Garson, M.J. *et al., J.C.S. Perkin 1*, 1984, 1021-1026 (*synth, ir*)
Andrews, M.A. *et al., J.O.C.*, 1989, **54**, 5257-5264 (*synth, pmr, cmr, ms*)
Peng, L. *et al., Helv. Chim. Acta*, 1997, **80**, 1494-1512 (*synth, ir, pmr, cmr, ms, 2S,3R-form, dibenzoyl, dibenzyl*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*1-Deoxy-L-erythritol, isol*)

Butanoic acid, 9CI B-218

[107-92-6]
Butyric acid. FEMA 2221

$H_3CCH_2CH_2COOH$

$C_4H_8O_2$ 88.106

Found in fresh and cooked apples, banana, sour cherry, papaya, strawberries, wheat bread, cheeses, butter and coffee. Flavouring agent. Liq. with pungent odour. Misc. H_2O, EtOH, Et_2O. d_4^{20} 0.96. Fp -19 Mp -8°. Bp 163.5°. pK_a 4.82 (25°). n_D^{20} 1.3991. Steam-volatile. Vp 0.84 mmHg (20°).

▶ Corrosive and irritating to skin and eyes. LD_{50} (rat, orl) 2940 mg/kg. ES5425000

Me ester: [623-42-7] *Methyl butyrate. FEMA 2693*
$C_5H_{10}O_2$ 102.133
Found in many fruits, e.g. apple juice, apricot, blackberry, nectarine etc., also present in cheeses, butter, milk, white wine, coffee and black tea. Flavouring ingredient. Liq. with apple-like odour and sweet taste. Sl. sol. H_2O, CCl_4; misc. EtOH, Et_2O. d_4^0 0.92. Mp -95°. Bp 102.3°. n_D^{20} 1.3878. Vp 32 mmHg (25°).

▶ Highly flammable, fl. p. 14°. Skin irritant. LD_{50} (rbt, orl) 3380 mg/kg. ET5500000

Et ester: [105-54-4] *Ethyl butyrate. FEMA 2427*
$C_6H_{12}O_2$ 116.16
Present in many fruits e.g. apple, apricot, banana, plum, tangerine etc. Flavouring ingredient. Liq. with pineapple odour. Sl. sol. H_2O, CCl_4; sol. EtOH, Et_2O. d_4^0 0.9. Fp -93.3. Bp 119.9°. n_D^{20} 1.4000. Vp 15 mmHg (25°).

▶ Flammable. Skin irritant. LD_{50} (rat, orl) 13000 mg/kg. ET1660000

Propyl ester: [105-66-8] *Propyl butyrate. FEMA 2934*
$C_7H_{14}O_2$ 130.186
Present in many fruits, e.g. apple, apricot, banana, melon, papaya etc., also present in Camembert and other cheeses. Flavouring ingredient. Liq. Sl. sol. H_2O; misc. EtOH, Et_2O. d_4^{20} 0.87. Mp -95.2°. Bp_{764} 142-143° Bp_{14} 39°. n_D^{20} 1.4001. Vp 4.5 mmHg (25°).

▶ Flammable, fl. p. 37/40°. ET6200000

Isopropyl ester: [638-11-9] *Isopropyl butyrate. FEMA 2935*
$C_7H_{14}O_2$ 130.186
Present in apricot, kumquat peel oil, American cranberry, papaya, strawberry, spineless monkey orange and sparkling wine. Flavouring ingredient. Liq. Insol. H_2O; sol. EtOH. d_4^{20} 0.86. Bp 129°. n_D^{20} 1.3936. Vp 16 mmHg (25°).

▶ Flammable, fl. p. 24°.

2-Propenyl ester: [2051-78-7] *Allyl butyrate. FEMA 2021*
$C_7H_{12}O_2$ 128.171
Fruit flavouring ingredient. Insol. H_2O; misc. EtOH, Et_2O. d^{20} 0.9. Bp 142° Bp_{15} 44-45°. n_D^{20} 1.4158.

▶ ES5775000

Butyl ester: [109-21-7] *Butyl butyrate. FEMA 2186*
$C_8H_{16}O_2$ 144.213
Present in many fruits, e.g. banana, cherry, melon, plum, also present in

gruyere de comte cheese, cider, soybean etc. Used in fruit flavour compositions. Liq. Insol. H_2O; misc. EtOH, Et_2O. d_4^{20} 0.87. Mp -91.5°. Bp 164.8° Bp_{11} 56-57°. n_D^{20} 1.4075.

▶ Flammable, fl. p. 51/50°. ES8120000

Benzyl ester: [103-37-7] *Phenylmethyl butanoate. Benzyl butyrate. FEMA 2140*
$C_{11}H_{14}O_2$ 178.23
Present in purple and yellow passion fruit, mountain papaya, cherimoya, black tea, Bourbon vanilla and hog plum. Flavouring agent. Oil with apricot-like odour and sweet, pear-like taste. d_4^{20} 1. Bp 238-239° Bp_9 108-110° Bp_3 91-92°. n_D^{20} 1.4930.

[461-55-2, 589-39-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 482A; 604C; 604D; 637B; 711C; 726C; 837C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 752B; 850B; 907A; 907C; 908A; 908B; 908C; 970B; 1166A; 1192A; 1351C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 574A; 613D; 614A; 614B; 614C; 614D; 670C; 761B; 768B; 795C (*ir*)
Grillone, G.B. *et al., Annalen*, 1873, **165**, 127 (*synth*)
Mitchel, J.A. *et al., J.A.C.S.*, 1931, **53**, 321; 1879 (*synth*)
Fr. Pat., 1936, 790 213; *CA*, **30**, 2992 (*synth*)
U.S. Pat., 1936, 2 039 722; *CA*, **30**, 4179 (*synth*)
Ballaus, O. *et al., Monatsh. Chem.*, 1943, **74**, 85 (*esters*)
Zeinalov, B.K. *et al., Azerb. Khim. Zh.*, 1962, 15-21; *CA*, 1963, **59**, 8647g (*benzyl ester*)
Pietsch, R. *et al., Mikrochim. Acta*, 1968, 1287 (*use*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 719 (*rev, tox, Et ester*)
Mondal, M.A.S. *et al., Tetrahedron*, 1974, **30**, 4205 (*synth, ethenyl ester*)
Caswell, L.R. *et al., J.O.C.*, 1976, **41**, 3312 (*uv*)
Terentev, A.B. *et al., Org. Magn. Reson.*, 1977, **9**, 301 (*cmr*)
Williamson, K.L. *et al., J. Magn. Reson.*, 1978, **30**, 367 (*cmr*)
McAdoo, D.J. *et al., J.A.C.S.*, 1978, **100**, 6639 (*ms*)
Delseth, C. *et al., Helv. Chim. Acta*, 1980, **63**, 498 (*O-17 nmr*)
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Sviridov, A.F. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 1650; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1509 (*butyl esters*)
Maccoll, A. *et al., Int. J. Mass Spectrom. Ion Processes*, 1988, **86**, 227 (*ms*)
Yang, H. *et al., Synth. Commun.*, 1994, **24**, 3269 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 80; 264; 331; 359; 956; 1487; 1740; 2341 (*esters, occur, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFY250; BSW000; EHE000; MHY000; BSX250; BQM500; BSV500; SFN600

1-Butanol, 9CI B-219

[71-36-3]

[35296-72-1]
n-*Butyl alcohol, 8CI. FEMA 2178*

$H_3CCH_2CH_2CH_2OH$
$C_4H_{10}O$ 74.122
Flavouring agent. Occurs in essential oils and other plant sources e.g. *Thea sinensis* (tea), *Ribes nigrum* (blackcurrant). Liq. Mod. sol. H_2O. d^{15} 0.81. Fp -90. Bp 117.4°. n_D^{20} 1.3971. Forms constant-boiling mixt. with H_2O, Bp 92°, contg. 37% H_2O.

▶ Flammable, fl. p. 29/35°, autoignition temp. 359°. Eye, skin and respiratory tract irritant. Mild CNS effects by skin absorption and inhalation (headache, dizziness). Can cause dermatitis. LD_{50} (rat, orl) 790 mg/kg. Exp. reprod. effects. OES: short-term 50 ppm. EO1400000

Al salt: See Aluminium butoxide in *The Combined Chemical Dictionary.*

Zr(4+) salt: See Zirconium butoxide in *The Combined Chemical Dictionary.*

Hf(4+) salt: See Tetrabutoxyhafnium in *The Combined Chemical Dictionary.*

Nb(5+) salt: See Pentabutoxyniobium in *The Combined Chemical Dictionary.*

Phenylurethane:
Cryst. Mp 61°.

Ac: [123-86-4] *Butyl acetate. FEMA 2174*
$C_6H_{12}O_2$ 116.16
Flavouring ingredient used in apple flavours. Liq. Sol. EtOH, Et_2CO, Me_2CO; insol. H_2O. d_4^{20} 0.88. Fp -77. Bp 125-126°. n_D^{20} 1.3942.

▶ Eye, skin and respiratory tract irritant. High conc. narcotic. Flammable, fl. p. 22°, autoignition temp. 370/425°. OES: long-term 150 ppm; short-term 200 ppm. AF7350000

4-Methylbenzenesulfonyl: [778-28-9]
$C_{11}H_{16}O_3S$ 228.312
Liq. Bp_2 138-140°.

▶ XT6400000

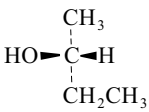
[3999-70-0, 4712-38-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 110A; 601C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 164A; 900A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 156B; 608B (*ir*)
Buchner, E. *et al., Ber.*, 1908, **41**, 1410 (*synth*)
Kagan, M.Ya. *et al., CA*, 1935, **29**, 452 (*synth*)
Vogel, A.I. *et al., J.C.S.*, 1948, 624 (*Ac, synth*)
Chaikin, S.W. *et al., J.A.C.S.*, 1949, **71**, 122 (*synth*)
Bock, R. *et al., Fresenius' Z. Anal. Chem.*, 1953, **138**, 167 (*Ac, use*)
Zomzely, C. *et al., Anal. Chem.*, 1962, **34**, 1414 (*use*)
Biddiscombe, D.P. *et al., J.C.S.*, 1963, 1954 (*purifn, props*)
Andersson, J. *et al., Acta Chem. Scand.*, 1966, **20**, 522 (*isol*)
Dorman, D.E. *et al., J.O.C.*, 1975, **40**, 3729 (*cmr, derivs*)
Choudhary, G. *et al., J. Chromatogr.*, 1976, **128**, 261 (*use*)
Crowder, G.A. *et al., J. Mol. Struct.*, 1977, **42**, 27 (*ir, Raman*)
Ejchart, A. *et al., Org. Magn. Reson.*, 1980, **13**, 368 (*cmr*)
Colosimo, M. *et al., Org. Mass Spectrom.*, 1982, **17**, 286 (*ms*)
Ullmanns Encykl. Tech. Chem., 5. Aufl., 1985, **A4**, 463 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BPW500; BPU750
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 691 (*rev, props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1100
Yamamoto, T. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 555 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 76; 77
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 317-318; 319-320
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 38; 247 (*tox, rev*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 184; 191
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BPW500; BSP750

2-Butanol, 9CI B-220

[78-92-2]

[35296-72-1]
sec-*Butyl alcohol*


(*R*)-*form*

$C_4H_{10}O$ 74.122
Isol. from fruit of blackcurrant (*Ribes nigrum*) and other fruits. Also present in various cheeses, wines, black tea, endive and clary sage. Flavouring agent.

▶ EO1750000

(*S*)-*form* [4221-99-2]
Liq. Bp 99°. $[\alpha]_D^{20}$ +13.87.

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{15}H_{28}O_{10}$ 368.38
Constit. of the roots of cassava (*Manihot esculenta*). Solid + ½H_2O. Mp 114-116°. $[\alpha]_D^{25}$ -65 (c, 0.1 in H_2O).

(±)-*form* [15892-23-6]
Liq. Mod. sol. H_2O. d_4^{22} 0.82. Bp 100°. n_D^{22} 1.3924.

▶ Peroxidisable. Old samples may explode on dist. Highly flammable, fl. p. 14/24°, autoignition temp. 390/405°. Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 6480 mg/kg. Exp. reprod. effects (large doses). OES: long-term 100 ppm; short-term 150 ppm.

Et ether: [2679-87-0] *FEMA 3131*
Flavouring agent. Liq. d^{20} 0.75. Bp 81.2°. n_D^{20} 1.3802.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 118A; 118B; 118C; 601D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 175C; 176A; 176B; 900B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 166B; 166C; 166D; 608C (*ir*)
Aldrich Library of NMR Spectra, **1**, 85D (*pmr*)
Levene, P.A. *et al., J. Biol. Chem.*, 1927, **71**, 465 (*abs config*)
Kenyon, J. *et al., J.C.S.*, 1935, 1072; 1077 (*synth, abs config*)
Leroux, P.J. *et al., J.A.C.S.*, 1951, **73**, 41 (*synth*)
Kantor, S.W. *et al., J.A.C.S.*, 1953, **75**, 1744 (*resoln*)
Brown, H.C. *et al., J.A.C.S.*, 1964, **86**, 397; 1071 (*synth*)

Pollock, G.E. *et al., J. Gas Chromatogr.*, 1965, **3**, 174 (*use*)
Andersson, J. *et al., Acta Chem. Scand.*, 1966, **20**, 522 (*isol*)
Ejchart, A. *et al., Org. Magn. Reson.*, 1981, **15**, 22 (*cmr*)
Colosimo, M. *et al., Org. Mass Spectrom.*, 1982, **17**, 286 (*ms*)
Abe, K. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 3125 (*conformn*)
Brown, H.C. *et al., J.O.C.*, 1988, **53**, 2911 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 691 (*rev, props*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 84 (*Et ether*)
Prawat, H. *et al., Phytochemistry*, 1995, **40**, 1167 (*6-apiosylglucoside*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 337-338 (*Et ether*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 247 (*tox, rev*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 192
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BPV000; BPW750

2-Butanone, 9CI B-221

[78-93-3]
Ethyl methyl ketone. 2-Oxobutane. Methyl ethyl ketone. MEK. FEMA 2170

$H_3CCH_2COCH_3$

C_4H_8O 72.107

Isol. from hop oil (*Humulus lupulus*) white clover (*Trifolium repens*), tea, tomatoes, various fruits and other vegetable sources. Used in the refining and extraction of fats and oils. Flavouring agent. Liq. Part misc. H_2O. d_4^{20} 0.81. Fp -85.9. Bp 79.6°. n_D^{15} 1.3814. Forms constant-boiling mixt. with H_2O, Bp 73.4°, contg. 11.3% H_2O.

► Highly flammable, fl. p. -1°. Peroxidisable. Eye, skin and respiratory tract irritant. Mild CNS effects by inhalation (headache, dizziness). LD_{50} (rat, orl) 2737 mg/kg. Exp. teratogen. OES: long-term 200 ppm; short-term 300 ppm (sk, revised). EL6475000

[10341-59-0, 10341-63-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 405B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 631C; **3**, 488B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 487B (*ir*)
Schramm, J. *et al., Ber.*, 1883, **16**, 1581 (*synth*)
Nef, J.U. *et al., Annalen*, 1900, **310**, 316 (*synth*)
Senderens, J.-B. *et al., Bull. Soc. Chim. Fr.*, 1909, **5**, 480
Meerwein, H. *et al., Annalen*, 1913, **398**, 249 (*synth*)
Takahashi, K. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 1046 (*pmr*)
Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1962, **51**, 938 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 678
Headridge, J.B. *et al., Analyst (London)*, 1969, **94**, 968 (*use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1977, **15**, 627 (*rev, tox*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 903 (*rev*)
Beaupré, P.W. *et al., Mikrochim. Acta*, 1982, **2**, 485 (*use*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A4**, 475 (*rev*)
Rittner, R. *et al., Magn. Reson. Chem.*, 1988, **26**, 51 (*cmr*)
Durig, J.R. *et al., Can. J. Chem.*, 1991, **69**, 1827 (*ir, Raman, conformn*)
Brint, P. *et al., J. Chem. Soc., Faraday Trans.*, 1991, **87**, 3343 (*uv*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1104
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1507
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 186
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EMU500; MKA400; MKA750

2-Butenal B-222

[4170-30-3]
Crotonaldehyde

$H_3CCH{=}CHCHO$

C_4H_6O 70.091Coml. crotonaldehyde is a mixture of (*E*)- and (*Z*)-forms, with the (*E*)-form predominating (>95%); contains hydroquinone as a polym. inhibitor. Undergoes anionic polym. Q/e values for copolym., Q 0.023, e 0.84. Forms phenolic resins by polycondensation with phenols.

► Eye, skin and mucous membrane irritant. Lachrymator and can also cause corneal burns. Exp. carcinogen. LD_{50} (rat, orl) 206 mg/kg. GP9499000

(E)-form [123-73-9]
Isol. from vegetable sources, e.g. tomato juice, strawberry aroma. Lachrymatory liq. Sol. H_2O; v. sol. EtOH, Et_2O, Me_2CO. d_{20}^{20} 0.85. Mp -69°. Bp 102.2° (104°). n_D^{17} 1.4384. Vp 37 mmHg (25°).

► Highly flammable, fl. p. 13°, autoignition temp. 207/230°. Explosive reaction with butadiene. Eye, skin and respiratory tract irritant. Lachrymator. Contact with eyes can also cause corneal burns. LD_{50} (rat, orl) 300 mg/kg. ACGIH TLV: long-term 2 ppm. GP9625000

[1527-96-4]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 362A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 472C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 558C (*ir*)
Fernandez, J.E. *et al., Chem. Rev.*, 1962, **62**, 485 (***rev***)
McGreer, D.E. *et al., Can. J. Chem.*, 1969, **47**, 866 (*isom*)
Fueno, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3290 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 207 (*rev*)
Hommes, H. *et al., Org. Mass Spectrom.*, 1979, **14**, 51 (*ms*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Ullmanns Encykl. Tech. Chem., 5. Aufl., VCH, Weinheim, 1985, **A8**, 83 (*rev*)
Oida, T. *et al., J.C.S. Perkin 1*, 1986, 1715 (*synth, pmr*)
Foote, C.S. *et al., J.A.C.S.*, 1988, **110**, 7167 (*isom, pmr*)
Baldwin, J.E. *et al., J.A.C.S.*, 1988, **110**, 8223 (*synth, pmr*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 165
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1420
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 347
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COB250; COB260

2-Butenoic acid, 9CI B-223

[3724-65-0]
3-Methylacrylic acid. Ethylideneacetic acid

$H_3CCH{=}CHCOOH$

$C_4H_6O_2$ 86.09

► Skin irritant. LD_{50} (rat, orl) 1000 mg/kg. GQ2800000

(E)-form [107-93-7]
Crotonic acid. β-Methacrylic acid. FEMA 3908
Food flavour component. Needles (H_2O or petrol). V. sol. H_2O, EtOH; sol. Et_2O, Me_2CO. Mp 71.4°. Bp 185° (189°). n_D^{20} 1.4457. pK_a 4.61 (25°). Q/e values for copolym., Q 0.017, e 0.89.

► Fl. p. 89°, autoignition temp. 396°. GQ2900000

Et ester: [623-70-1] *Ethyl crotonate. FEMA 3486*
$C_6H_{10}O_2$ 114.144
Component of strawberry aroma, guava fruit and peel (*Psidium guajava*), pineapple, yellow passion fruit and other fruits. Also present in white wine and mussels. Flavouring ingredient. Liq. Insol. H_2O; sol. EtOH, Et_2O. d_4^{20} 0.92. Bp 137° Bp_{15} 38°. n_D^{20} 1.4243.

► Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 3000 mg/kg. Flammable, fl. p. 28°. GQ3500000

2-Methylpropyl ester: [589-66-2] *2-Methylpropyl 2*E*-butenoate. Isobutyl crotonate. FEMA 3432*
$C_8H_{14}O_2$ 142.197
Flavouring ingredient. d^{20} 0.89. Bp 171°. n_D^{20} 1.4291.

Hexyl ester: [19089-92-0] *Hexyl crotonate. FEMA 3354*
$C_{10}H_{18}O_2$ 170.251
Flavouring agent.

2-Propenyl ester: [5453-44-1] *Allyl crotonate*
$C_7H_{10}O_2$ 126.155
Found in roasted filberts (*Corylus avellana*). Bp_{20} 63-65°. n_D 1.4416.

(Z)-form [503-64-0]
Isocrotonic acid. β-Crotonic acid
Used in food preservatives. Needles or prisms (petrol). Sol. H_2O, Et_2O, CS_2, EtOH. d^{20} 1.03. Mp 14.6°. Bp 169° Bp_5 54-55°. n_D^{20} 1.4457. Isom. by sunlight or heat to the (*E*)-isomer.

► Eye, skin and mucous membrane irritant.

[623-68-7, 3246-27-3, 4786-20-3, 7299-91-4, 10487-71-5, 10544-63-5, 18707-60-3, 20474-93-5, 23350-58-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 498C; 641C; 641D; 712D; 732B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 776C; 977B; 977C; 1170B; 1199B (*nmr*)

v. Auwers, K. *et al., Annalen*, 1923, **432**, 46 (*synth*)
v. Auwers, K. *et al., Ber.*, 1923, **56**, 715 (*config*)
Collin, P.J. *et al., Aust. J. Chem.*, 1966, **19**, 317 (*nmr, E-form*)
Hocking, M.B. *et al., Synthesis*, 1971, 482 (*synth*)
Fueno, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3290 (*uv*)
Brouwer, H. *et al., Can. J. Chem.*, 1972, **50**, 601 (*cmr*)
Hocking, M.B. *et al., Can. J. Chem.*, 1972, **50**, 1224 (*isom*)
Org. Synth., 1973, **53**, 123 (*synth*)
Bortolussi, M. *et al., Bull. Soc. Chim. Fr.*, 1975, 2727 (*2-propenyl ester*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 218 (*rev*)
Holmes, J.L. *et al., Org. Mass Spectrom.*, 1979, **14**, 204 (*ms*)
Abou-Zeid, A. *et al., Arab Gulf J. Sci. Res.*, 1984, **2**, 625 (*isol*)
Ger. Pat., 1984, 3 245 111; *CA*, **101**, 191148r (*synth*)
Heathcock, C.H. *et al., J.O.C.*, 1985, **50**, 1190 (*Et ester*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH, Weinheim, 1985, **A8**, 85 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 349; 390 (*esters*)
Merck Index, 12th edn., 1996, No. 5180
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 960-961; 1325; 1446-1447 (*esters, use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COB500; EHO200; COB750; COQ750; COB825

3-Butenoic acid, 9CI B-224

[625-38-7]
Vinylacetic acid. Propene-3-carboxylic acid. Ethenylacetic acid

$H_2C{=}CHCH_2COOH$

$C_4H_6O_2$ 86.09
Liq. Sol. H_2O; misc. EtOH, Et_2O. d_4^{20} 1.01. Mp -39°. Bp 163° Bp_{12} 69-70°. n_D^{15} 1.4257. pK_{a1} 4.37 (23°).

Nitrile: [109-75-1] *3-Butenenitrile, 9CI. Allyl cyanide. Vinylacetonitrile. 3-Cyano-1-propene*
C_4H_5N 67.09
Constit. of mustard oil. Liq. with odour of onions. Sl. sol. H_2O; misc. EtOH, Et_2O. d_4^{20} 0.83. Mp -87°. Bp 119°. n_D^{20} 1.4060. Polym. by radiation or chem. catalysts.

▶ Skin irritant. LD_{50} (rat, orl) 115 mg/kg. EM8050000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 777A; 1358C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 498D; 843A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 46; *Org. Synth., Coll. Vol., 3*, 1955, 851 (*nitrile, synth respectively*)
Griffith, G.H. *et al., J. Mol. Struct.*, 1969, **4**, 255 (*ir, Raman, nitrile*)
Yonemoto, T. *et al., J. Magn. Reson.*, 1973, **12**, 93 (*cmr, nitrile*)
Simchev, G. *et al., Synthesis*, 1975, **9**, 605 (*nitrile*)
Kucukyavuz, Z. *et al., Polymer*, 1990, **31**, 1715 (*polym, nitrile*)

2-Buten-1-ol, 9CI B-225

[6117-91-5]
Crotyl alcohol. 3-Methylallyl alcohol. Crotonyl alcohol

$H_3CCH{=}CHCH_2OH$

C_4H_8O 72.107
Isol. from rapeseed oil.

▶ LD_{50} (rat, orl) 930 mg/kg. Flammable, fl. p. 27/33°, autoignition temp. 349°. EM9275000

(E)-form [504-61-0]
Liq. V. sol. H_2O; misc. EtOH, Et_2O. d^{20} 0.85. Mp -30°. Bp 121.2°. n_D^{20} 1.4288.

(Z)-form [4088-60-2]
Liq. d^{20} 0.87. Bp 122°. n_D^{25} 1.4342.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 138C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 208A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 200D (*ir*)
Young, W.G. *et al., J.A.C.S.*, 1936, **58**, 100 (*synth*)
André, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1950, **231**, 872 (*isol*)
Hatch, L.F. *et al., J.A.C.S.*, 1950, **72**, 727 (*synth*)
Stothers, J.B. *et al., Can. J. Chem.*, 1972, **50**, 1361 (*cmr*)
Rauchschwalbe, G. *et al., Helv. Chim. Acta*, 1975, **58**, 1094 (*synth*)
Kingston, D.G.I. *et al., Org. Mass Spectrom.*, 1975, **10**, 263 (*ms*)
Malhotra, S.L. *et al., J. Macromol. Sci., Part A: Chem.*, 1977, **11**, 1809 (*pmr*)
Denmark, S.E. *et al., J.O.C.*, 1987, **52**, 4031 (*synth*)
Bacon, J.F. *et al., Spectrochim. Acta A*, 1988, **44**, 1243 (*conformn*)
Xu, Y.-C. *et al., Can. J. Chem.*, 1993, **71**, 1152 (*synth, ir, pmr, cmr*)
Glendinning, L. *et al., Bull. Chem. Soc. Jpn.*, 1995, **68**, 2739 (*synth, E-form*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BOY000

3-Buten-1-ol, 9CI B-226

[627-27-0]
Allylcarbinol

$H_2C{=}CHCH_2CH_2OH$

C_4H_8O 72.107
Isol. from rapeseed oil. Liq. Bp_{755} 112.5-113.5° Bp_{12} 28°. n_D^{23} 1.4197.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 139A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 208B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 201B (*ir*)
Grischkevitsch-Trochimovski, E. *et al., J.C.S.*, 1917, **112**, 154 (*synth*)
André, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1950, **231**, 872 (*isol*)
House, H.O. *et al., J.O.C.*, 1974, **39**, 3102 (*synth*)
Wenkert, E. *et al., Org. Magn. Reson.*, 1975, **7**, 51 (*cmr*)
Malhotra, S.L. *et al., J. Macromol. Sci., Part A: Chem.*, 1977, **11**, 1809 (*pmr*)
Rhodes, Y.E. *et al., J.O.C.*, 1978, **43**, 3496 (*synth*)
Marstokk, K.-M. *et al., Acta Chem. Scand., Ser. A*, 1981, **35**, 395 (*conformn*)
Bowen, R.D. *et al., J.C.S. Perkin 2*, 1987, 1019 (*ms*)

3-Butenyl glycosinolate B-227

[19041-09-9]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)-4-pentenimidate], 9CI. ***Gluconapin***

$H_3C{=}CHCH_2CH_2C(SGlc){=}NOSO_3H$

$C_{11}H_{19}NO_9S_2$ 373.404
Isol. from rape seeds and many other *Brassica* spp.. Highly hygroscopic, amorph. solid (as K salt). Mp 125° (K salt). $[\alpha]_D^{25}$ -23.5 (c, 1.8 in H_2O).

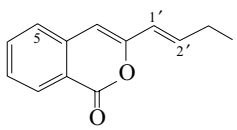
Tetra-Ac:
Cryst. (EtOH) (as K salt). Mp 189° (K salt). $[\alpha]_D^{27}$ -17.1 (c, 1.3 in H_2O).

Salt with Sinapine, S-111: [169272-87-1] ***Boreavan A***. *Sinapinyl gluconapate*
$C_{27}H_{42}N_2O_{14}S_2$ 682.766
Amorph. powder. $[\alpha]_D^{24}$ -8.5 (c, 0.01 in MeOH).

Kjaer, A. *et al., Acta Chem. Scand.*, 1953, **7**, 1271; 1968, **22**, 3324 (*isol, synth*)
Ettlinger, M.G. *et al., J.A.C.S.*, 1955, **77**, 1831 (*occur*)
Hanley, A.B. *et al., J. Sci. Food Agric.*, 1983, **34**, 869 (*isol*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*cmr*)
Sakushima, A. *et al., Phytochemistry*, 1995, **40**, 483-485 (*Boreavan A*)

3-(1-Butenyl)-1*H*-2-benzopyran-1-one, 9CI B-228

3-(1-Butenyl)isocoumarin. Artemidin



$C_{13}H_{12}O_2$ 200.237

(E)-form [29428-84-0]
Constit. of *Artemisia dracunculus* (tarragon). Cryst. (petrol). Mp 48°.

5-Hydroxy: [62268-43-3] *3-(1-Butenyl)-5-hydroxy-1*H*-2-benzopyran-1-one, 9CI.* ***Artemidinol***
$C_{13}H_{12}O_3$ 216.236
Constit. of *Artemisia dracunculus* (tarragon).

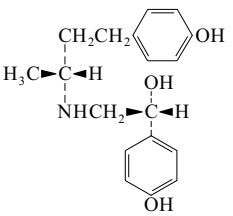
1′,2′-Dihydro, 1′,2′-dihydroxy: [54963-30-3] *3-(1,2-Dihydroxybutyl)-1*H*-2-benzopyran-1-one.* ***Artemidiol***
$C_{13}H_{14}O_4$ 234.251
Constit. of *Artemisia dracunculus* (tarragon). Mp 131.5-133°.

(Z)-form [63898-24-8]
Constit. of *Artemisia dracunculus* (tarragon).

Bohlmann, F. *et al., Chem. Ber.*, 1970, **103**, 2856 (*isol, struct*)
Mallabaev, A. *et al., Khim. Prir. Soedin.*, 1974, **10**, 720; 1976, **12**, 811; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 743; 1976, **12**, 729 (*derivs*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 795 (*isol, struct*)
Chatterjea, J.N. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 359; 992 (*synth*)
Bellina, F. *et al., Tetrahedron*, 2000, **56**, 2533-2545 (*synth*)

Butopamine, INN, USAN B-229

4-Hydroxy-α-[[[3-(4-hydroxyphenyl)-1-methylpropyl]amino]methyl]benzenemethanol, 9CI. 1-(4-Hydroxyphenyl)-2-[1-methyl-3-(4-hydroxyphenyl)propylamino]ethanol



(R,R)-form

$C_{18}H_{23}NO_3$ 301.385Log P 2.03 (calc).

(R,R)-form [66734-12-1]
LY 131126

Hydrochloride: [74432-68-1]
Cryst. (EtOH). Mp 176-176.5°. $[\alpha]_D$ -22.7 (MeOH).

(±)-form [97825-25-7] ***Ractopamine, INN***

Hydrochloride: [90274-24-1] ***Ractopamine hydrochloride, USAN.*** *EL 737. LY 031537. Paylean™. Elanco*
Leanness enhancer for pigs. Approved for use in the USA. Mp 124-129°.

[74433-09-3, 99095-19-9]

Thompson, M.J. *et al., Clin. Pharmacol. Ther. (St. Louis)*, 1980, **28**, 324 (*pharmacol, human*)
Eur. Pat., 1980, 7 205, (*Eli Lilly*); *CA*, **93**, 94972 (*synth, pharmacol*)
Nelson, S. *et al., Curr. Ther. Res.*, 1981, **30**, 405 (*pharmacol*)
Leier, C.V. *et al., J. Lab. Clin. Med.*, 1983, **101**, 955 (*pharmacol*)
U.K. Pat., 1984, 2 133 986, (*Eli Lilly*); *CA*, **102**, 130979m (*synth, props*)
Colbert, W.E. *et al., J. Pharm. Pharmacol.*, 1991, **43**, 844 (*pharmacol*)
Smith, D.J. *et al., Drug Metab. Dispos.*, 1993, **21**, 624 (*metab*)
Turberg, M.P. *et al., J. Assoc. Off. Anal. Chem.*, 1994, **77**, 840 (*hplc*)
Lohr, E. *et al., Food Chem. News*, 2000, **41**, 12; 24 (*use*)

2-Butoxyethanol, 9CI B-230

[111-76-2]
Ethylene glycol butyl ether. Butyl 2-hydroxyethyl ether. Butylcellosolve. Butyloxitol. Chimec NR

$H_3C(CH_2)_3OCH_2CH_2OH$

$C_6H_{14}O_2$ 118.175
Used in food processing as a processing aid, sanitizer, solvent, etc. Liq. Misc. H_2O, most org. solvs. d_{20}^{20} 0.9. Fp -74.8. Bp 171-172°. n_D^{25} 1.4190. Vp 0.76 mmHg (20°).

► Flammable, fl. p. 61/62°, autoignition temp. 238/244°, may form explosive peroxides. Skin and severe eye irritant. Adverse systemic effects by inhalation. LD_{50} (rat, orl) 470 mg/kg. Exp. reprod. and teratogenic effects. MEL: long-term 25 ppm (Sk). KJ8575000

Phosphate (3:1): [78-51-3] *TBEP*
$C_{18}H_{39}O_7P$ 398.476
Liq. Insol. H_2O. d^{25} 1.02. Bp_{10} 255°. n_D^{25} 1.4340.

Ac: [112-07-2]
$C_8H_{16}O_3$ 160.213
Bp 192°.

► KJ8925000

Benzoyl: [5451-76-3]
$C_{13}H_{18}O_3$ 222.283
Liq. $Bp_{14.5}$ 156.5-157°.

4-(Dimethylamino)benzoyl: [67362-76-9]
$C_{15}H_{23}NO_3$ 265.352
$Bp_{1.5}$ 178-181°.

Dodecanoyl: [109-37-5]
$C_{18}H_{36}O_3$ 300.481
d^{20} 0.89. Bp_1 167-169°. n_D^{20} 1.4407.

Octadecanoyl: [109-38-6]
$C_{24}H_{48}O_3$ 384.641
Mp 16°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 223C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 338B; 1048B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 293D; 722C (*ir, Ac*)
Cretcher, L.H. *et al., J.A.C.S.*, 1924, **46**, 1503 (*synth*)
Conn, R.C. *et al., J.A.C.S.*, 1932, **54**, 4370 (*deriv*)
U.S. Pat., 1934, 1 944 530; *CA*, **28**, 2014 (*phosphate*)
Luke, C.L. *et al., Anal. Chem.*, 1954, **26**, 1778; 1956, **28**, 1443
Jankowski, S.J. *et al., Anal. Chem.*, 1961, **33**, 776
Meagher, W.R. *et al., J. Agric. Food Chem.*, 1966, **14**, 374 (*use*)
Illing, H.P.A. *et al., HSE Toxicity Review 10: Glycol Ethers*, HMSO, London, 1985, (*tox, rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 972-973
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 597
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BPJ850; BPM000

1-Butoxy-1-methoxyethane B-231

[75677-94-0]
1-(1-Methoxyethoxy)butane, 9CI. Acetaldehyde butyl methyl acetal

$H_3C(CH_2)_3OCH(OMe)CH_3$

$C_7H_{16}O_2$ 132.202

(±)-form
Aromatic-smelling liq. d_4^{20} 0.84. Bp 130-131.5° Bp_{56} 56.5°. n_D^{20} 1.3890.

(ξ)-form
Detected in strawberry volatiles by gc-ms.

Shoskakovskii, M.F. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1946, **16**, 937 (*synth*)
McFadden, W.H. *et al., J. Chromatogr.*, 1965, **18**, 10 (*isol*)
Gazizova, L.B. *et al., Zh. Org. Khim.*, 1981, **17**, 275; *J. Org. Chem. USSR (Engl. Transl.)*, 1981, **17**, 226 (*synth*)
Borisova, I.A. *et al., Zh. Org. Khim.*, 1982, **18**, 1638; *J. Org. Chem. USSR (Engl. Transl.)*, 1982, **18**, 1432 (*ms*)
Dostovalova, V.I. *et al., Magn. Reson. Chem.*, 1987, **25**, 1 (*cmr*)

Butter acids B-232

[85536-25-0]
FEMA 2171

A mixt. of fatty acids isol. from butter, or an equivalent mixt. of the acids from other sources, comprising oleic/palmitic (50-70%), stearic/myristic acids (ca. 20%), butyric acid (3-4%), linoleic, lauric, caproic, capric and caprylic acids (< 1% each). Flavouring ingredient for baked goods, ice cream, puddings, imitation dairy products, nonalcoholic beverages and candies. Waxy solid.

Et ester: Butter esters. FEMA 2172
Produced by esterification of mixed butter acids with EtOH. Flavouring ingredient for baked goods, fats, oils, ice cream, puddings, imitation dairy products and other foodstuffs. Waxy solid.

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 181-182 (*use, esters*)

Butyl butyryllactate B-233

[7492-70-8]
2-Butoxy-1-methyl-2-oxoethyl butanoate, 9CI. FEMA 2190

$H_3CCH_2CH_2COOCH(CH_3)$-$COO(CH_2)_3CH_3$

$C_{11}H_{20}O_4$ 216.277
Present in fruits of two Korean strawberry cultivars (Bogyojosaeng and suhong). Flavouring ingredient.. Liq. d_4^{20} 0.97. Bp_2 90°. n_D^{20} 1.4215.

Fein, M.L. *et al., Ind. Eng. Chem.*, 1944, **36**, 235-238 (*synth*)
Fein, M.L. *et al., J.A.C.S.*, 1948, **70**, 52-56 (*props*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 247 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 81 (*props, use*)
Park, E.-R. *et al., J. Food Sci. Nutr.*, 2000, **5**, 119-125 (*glc, detn, strawberry*)

Butyl glucosinolate B-234

[35535-42-3]
1-Thio-β-D-glucopyranose 1[N-(sulfooxy)pentanimidate], 9CI

$H_3C(CH_2)_3C(SGlc)=NOSO_3H$

$C_{11}H_{21}NO_9S_2$ 375.42
Present in seeds of *Brassica oleracea* (cabbage).

Kjaer, A. *et al., Phytochemistry*, 1971, **10**, 3155 (*occur*)
Macleod, A.J. *et al., Phytochemistry*, 1989, **28**, 1405 (*occur*)

Butyl isopropyl disulfide B-235

[72437-53-7]
Butyl 1-methylethyl disulfide, 9CI. 2-Methyl-3,4-dithiaoctane

$(H_3C)_2CH–S–S–(CH_2)_3CH_3$

$C_7H_{16}S_2$ 164.335
Constit. of *Allium cepa* (onion).

Gupta, D. *et al., Can. J. Chem.*, 1980, **58**, 1350-1354; 1981, **59**, 543-548 (*synth, ms*)
Misharina, T.A. *et al., CA*, 1994, **120**, 132679j (*isol*)

Butyl 1-(methylthio)propyl disulfide B-236

[183243-87-0]

$H_3CCH_2CH(SMe)–S–S–(CH_2)_3CH_3$

$C_8H_{18}S_3$ 210.428
Constit. of *Allium tuberosum* (Chinese

chives).

Meng, Z. *et al., CA*, 1996, **125**, 326880s (*isol*)

Butyl nitrite, 9CI B-237

[544-16-1]

$H_3C(CH_2)_3ONO$

$C_4H_9NO_2$ 103.121

Preservative for meats. Claimed not to generate nitrosamines as byproducts. Liq. Bp 78° Bp_{43} 24-27°.

▶ LD_{50} (rat, orl) 83 mg/kg. Can cause methaemoglobinaemia-carboxhaemoglobinaemina. Highly flammable, fl. p. 10°. RA0780000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 621A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 479A (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 108 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 97
Netherlands Pat., 1975, 7 416 232, (*Canada Packers*); *CA*, **84**, 57585h (*use*)
Haley, T.J. *et al., Clin. Toxicol.*, 1980, **16**, 317-329 (*pharmacol, tox*)
Moncur, J.H. *et al., Rapid Commun. Mass Spectrom.*, 1988, **2**, 77; *CA*, **112**, 30037r (*use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 935 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1556
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BRV500

Butyl oleate sulfate B-238

[38621-44-2]

Butyl (sulfooxy)-9-octadecenoate, 9CI

$C_{22}H_{42}O_6S$ 434.636

Surfactant. Used in dehydration of grapes to produce raisins and as a coating for citrus fruits.

East Ger. Pat., 1974, 109 042; *CA*, **83**, 116794e (*dyeing, use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 351 (*use*)

Butyl propyl disulfide B-239

[72437-64-0]

4,5-Dithianonane

$H_3CCH_2CH_2–S–S–(CH_2)_3CH_3$

$C_7H_{16}S_2$ 164.335

Constit. of *Allium cepa* (onion) flavour and *Nigella sativa* (black cumin).

Gupta, D. *et al., Can. J. Chem.*, 1980, **58**, 1350-1354; 1981, **59**, 543-548 (*synth, ms*)
Balandrin, M.F. *et al., J. Agric. Food Chem.*, 1988, **36**, 1048-1054 (*isol*)

1-Butylamine B-240

[109-73-9]

1-Butanamine, 9CI. 1-Aminobutane. Norvalamine. FEMA 3130

$H_3CCH_2CH_2CH_2NH_2$

$C_4H_{11}N$ 73.138

Found in mulberry leaves, kale, swede, tomato, wheat bread, cheeses, caviar, raw fatty fish, cooked chicken or beef, beer, cocoa, and other foodstuffs. Flavouring agent. Liq. Sol. H_2O. Bp 78°.

▶ Highly flammable, fl. p. -12°, autoignition temp. 312°. Severe eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 366 mg/kg. LD_{50} (rbt, skn) 850 mg/kg. OES: short-term 5 ppm (Sk). EO2975000

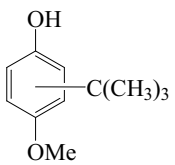
[16999-97-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 281A; 296D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 450C; 475A; 483B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 364D; 380B (*ir*)
Aldrich Library of NMR Spectra, **2**, 2B (*pmr*)
Org. Synth., Coll. Vol., 2, 1943, 319 (*synth*)
Brown, R. *et al., J.C.S.*, 1946, 781 (*synth*)
Betteridge, D. *et al., Anal. Chim. Acta*, 1962, **26**, 101 (*detn, Ag*)
Newman, E.J. *et al., Analyst (London)*, 1963, **88**, 506 (*detn, Mg*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313 (*cmr*)
Faure, R. *et al., Org. Magn. Reson.*, 1980, **14**, 20 (*cmr*)
Colosimo, M. *et al., Org. Mass Spectrom.*, 1982, **17**, 286 (*ms*)
Bowen, R.D. *et al., Org. Mass Spectrom.*, 1985, **20**, 331 (*ms*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 17 (*tox, rev*)

Butylated hydroxyanisole, 8CI B-241

[25013-16-5]

(1,1-Dimethylethyl)-4-methoxyphenol, 9CI. tert-*Butyl-4-methoxyphenol.* tert-*Butylhydroxyanisole. Antioxyne B. BHA. BOA. Embanox. Protex. Sustane 1F. Tenox BHA*



$C_{11}H_{16}O_2$ 180.246

Antioxidant. Used in foods. Mp 104-105°. Used as an undefined mixt. of 2- and 3-*tert*-butyl isomers.

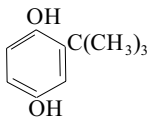
▶ Irritant. Can cause delayed type sensitivity reactions and non-immunogenic skin reactions. Possible human carcinogen (IARC). LD_{50} (rat, orl) 2000 mg/kg. Forestomach-specific nongenotoxic rodent carcinogen. SL1945000

U.S. Pat., 1963, 3 075 832; *CA*, **59**, 12707 (*synth*)
Williams, G.M. *et al., Food Chem. Toxicol.*, 1986, **24**, 1163 (*tox*)
Moch, R.W. *et al., Food Chem. Toxicol.*, 1986, **24**, 1167 (*tox*)
Tobe, M. *et al., Food Chem. Toxicol.*, 1986, **24**, 1223 (*tox*)
IARC Monog., 1986, **40**, 123; *Suppl*. 7, 59 (*rev, tox*)
Grice, H.C. *et al., Food Chem. Toxicol.*, 1988, **26**, 717 (*tox, rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BQI000
Clayson, D.B. *et al., Annu. Rev. Pharmacol. Toxicol.*, 1990, **30**, 441 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 45-46
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1120
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 322-326 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BQI000

2-*tert*-Butyl-1,4-benzenediol, 8CI B-242

[1948-33-0]

2-(1,1-Dimethylethyl)-1,4-benzenediol, 9CI. tert-*Butylhydroquinone. TBHQ. MTBHQ. Tenox 20. Tenox TBHO*



$C_{10}H_{14}O_2$ 166.219

Antioxidant used in food, e.g. oils and fats. Polym. inhibitor. Insol. H_2O; sol. EtOH, Me_2CO, EtOAc. Mp 127-129°.

▶ MX4375000

Di-Ac: [7507-48-4]
$C_{14}H_{18}O_4$ 250.294
Mp 63.5-64.5°.

O^1-*Me:* [88-32-4] *3*-tert-*Butyl-4-methoxyphenol, 8CI. 3-(1,1-Dimethylethyl)-4-methoxyphenol, 9CI*
$C_{11}H_{16}O_2$ 180.246
Mp 65°.

▶ SK1575010

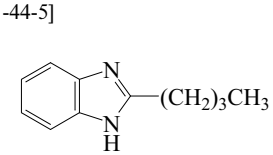
O^4-*Me:* [121-00-6] *2*-tert-*Butyl-4-methoxyphenol. 2-(1,1-Dimethylethyl)-4-methoxyphenol, 9CI*
$C_{11}H_{16}O_2$ 180.246
Mp 62-63°.

▶ LD_{50} (rat, orl) 2910 mg/kg. SK1575000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1108B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 305B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1041D (*ir*)
U.S. Pat., 1949, 2 459 540; *CA*, **43**, 3187 (*synth*)
U.S. Pat., 1957, 2 792 427; *CA*, **51**, 16538 (*O^1-Me*)
Boughton, O.O. *et al., J. Agric. Food Chem.*, 1967, **15**, 751-752 (*glc, nmr*)
Kauffmann, P. *et al., J. Chromatogr.*, 1977, **132**, 356-358 (*purif*)
Dilli, S. *et al., J. Chromatogr.*, 1977, **133**, 363 (*O^1-Me*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 342-343
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BQI010; BRN000; BRM500

2-Butyl-1*H*-benzimidazole B-243

[5851-44-5]



$C_{11}H_{14}N_2$ 174.245

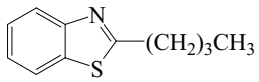
Constit. of chicken eggs. Cryst. (EtOAc/hexane). Mp 153-154°. λ_{max} 243 ; 274 ; 281 (MeOH) (Berdy). λ_{max} 240 ; 268 ; 275

(MeOH/HCl) (Berdy).

Tsuji, K. *et al., Yakugaku Zasshi*, 1976, **96**, 475-478 (*isol*)
Landor, S.R. *et al., J.C.S. Perkin 1*, 1979, 2289-2293 (*synth*)
Kubo, K. *et al., J. Med. Chem.*, 1993, **36**, 1772-1784 (*synth*)

2-Butylbenzothiazole, 9CI B-244

[54798-95-7]

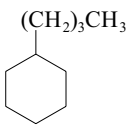


$C_{11}H_{13}NS$ 191.296
Flavour component in roasted coconut and cashew nuts. Liq. d^{25} 1.04. Mp 130° (as picrate). Bp 269°. n_D^{25} 1.5712.

Metzger, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 1692-1696 (*synth*)
Elderfield, R.C. *et al., J.A.C.S.*, 1960, **82**, 1982-1988 (*synth*)
Takei, H. *et al., Chem. Lett.*, 1979, 1447-1450 (*synth*)
Jayalekshmy, A. *et al., J. Sci. Food Agric.*, 1987, **39**, 35-45 (*occur*)
Jayalekshmy, A. *et al., ACS Symp. Ser.*, 1988, **409**, 355-365 (*occur*)
Jayalekshmy, A. *et al., J. Am. Oil Chem. Soc.*, 1991, **68**, 873-880 (*occur*)
Ares, J.J. *et al., Synth. Commun.*, 1991, **21**, 625-633 (*synth, pmr*)

Butylcyclohexane, 9CI, 8CI B-245

[1678-93-9]
1-Cyclohexylbutane

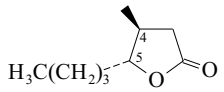


$C_{10}H_{20}$ 140.268
Constit. of the fruit of *Carica papaya* (papaya). d_4^{20} 0.8. Fp -74.7. Bp 180.9° Bp_{12} 640°. n_D^{20} 1.4410.

Adkins, H. *et al., J.A.C.S.*, 1930, **52**, 4349 (*synth*)
Signaigo, F.K. *et al., J.A.C.S.*, 1933, **55**, 3326 (*synth*)
Adv. Chem. Ser., 1955, **15**, 453 (***props***)
Grummitt, O. *et al., J.A.C.S.*, 1956, **78**, 1054 (*synth*)
Adams, J.Q. *et al., Am. Chem. Soc., Div. Pet. Chem., Prepr.*, 1972, **17**, C4 (*cmr*)
Flath, R.A. *et al., J. Agric. Food Chem.*, 1977, **25**, 103 (*isol*)
Corey, E.J. *et al., J.O.C.*, 1978, **43**, 3418 (*synth*)
Lipschutz, B.H. *et al., J.O.C.*, 1984, **49**, 3928 (*synth*)
Baldwin, J.E. *et al., Tetrahedron*, 1986, **42**, 4235 (*synth*)
Wang, T. *et al., Zhiwu Xuebao*, 1986, **28**, 504 (*isol*)

5-Butyldihydro-4-methyl-2(3*H*)-furanone B-246

[39212-23-2]
3-Methyl-4-octanolide. Oaklactone. Quercuslactone. Whisky lactone. FEMA 3803



(4*S*,5*R*)-*form*

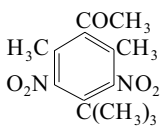
$C_9H_{16}O_2$ 156.224
Stereoisomers are flavour components of whisky and other alcoholic beverages. Used in flavouring candies and soft drinks.
(4*S*,5*R*)-*form* [80041-01-6]
Quercuslactone a
Present in aged spirits. Bp_{16} 123-125° Bp_6 67-68°. $[\alpha]_D^{25}$ +84.5 (c, 2 in MeOH). $[\alpha]_D^{15}$ +79 (c, 1.04 in MeOH).
(4*S*,5*S*)-*form* [80041-00-5]
Quercuslactone b
Present in aged spirits. $[\alpha]_D^{15}$ -87 (c, 0.92 in MeOH).

[39638-67-0, 55013-32-6, 89163-43-9, 99530-35-5]

Masuda, M. *et al., Chem. Lett.*, 1981, 1333 (*struct, uv, cd, ord, bibl*)
Marino, J.P. *et al., Tet. Lett.*, 1985, **26**, 5381 (*synth*)
Günther, C. *et al., Annalen*, 1986, 2112 (*synth, ir, pmr, cmr*)
Bloch, R. *et al., J.O.C.*, 1987, **52**, 4603 (*synth*)
Watanabe, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2914 (*synth*)
Jefford, C.W. *et al., Helv. Chim. Acta*, 1989, **72**, 1362 (*synth*)
Miyata, O. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2579 (*synth*)
Srikrishna, A. *et al., Synth. Commun.*, 1992, **22**, 1127 (*synth*)
Suzuki, Y. *et al., Tet. Lett.*, 1992, **33**, 4931 (*synth*)
Ebata, T. *et al., Heterocycles*, 1993, **36**, 1017 (*synth*)
Takahata, H. *et al., J.O.C.*, 1995, **60**, 5628 (*synth, ir, pmr, cmr*)
Maga, J. *et al., Food Res. Int.*, 1996, **12**, 105-130 (*occur, rev*)
Tsuboi, S. *et al., J.O.C.*, 1998, **63**, 1102-1108 (*synth*)
Masson, E. *et al., J. Agric. Food Chem.*, 2000, **48**, 4306-4309 (*synth*)

4′-*tert*-Butyl-2′,6′-dimethyl-3′,5′-dinitroacetophenone, 8CI B-247

[81-14-1]
*1-[4-(1,1-Dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]ethanone, 9CI. 1-Acetyl-4-*tert*-butyl-2,6-dimethyl-3,5-dinitrobenzene. Musk ketone*

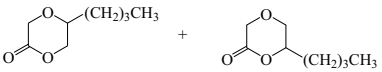


$C_{14}H_{18}N_2O_5$ 294.307
Listed in the EAFUS Food Additive Database (Jan 2001). Cryst. (MeOH). Mp 135.5-136°.

Fuson, R.C. *et al., J.O.C.*, 1947, **12**, 587-595 (*synth, struct*)
Carter, F. *et al., Perfum. Essent. Oil Res.*, 1951, **43**, 296-297; *CA*, **46**, 1718c (*manuf*)
Doepp, D. *et al., Chem. Ber.*, 1975, **108**, 3483-3496 (*photol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1975, **13**, 877 (*tox*)
Padmanabhan, K. *et al., J.C.S. Perkin 2*, 1986, 897-906 (*cryst struct*)
Suzuki, H. *et al., Synthesis*, 1999, 1291-1293 (*synth, ir, pmr, ms*)

5(6)-Butyl-1,4-dioxan-2-one B-248

[65504-95-2]
FEMA 2204

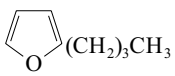


$C_8H_{14}O_3$ 158.197
Mixed isomers used in food flavouring, esp. for fatty foods such as margarine. Liq. with powerful fruity odour and winey-caramellic undertones.

Belg. Pat., 1963, 628 078; *CA*, **60**, 12021f (*synth, use, glc, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 90 (*props, use*)

2-Butylfuran B-249

[4466-24-4]



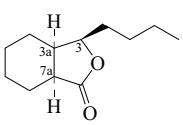
$C_8H_{12}O$ 124.182
Constit. of numerous plant spp. and cooked foods incl. chick pea and carob bean. Liq. Bp 139.5-140.2° Bp_{45} 59°. n_D^{23} 1.4460.

Potts, K.T. *et al., J.C.S.*, 1955, 2675-2686 (*synth*)
Ramanathan, V. *et al., J.O.C.*, 1962, **27**, 1216-1219 (*synth*)
Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223-2235 (*ms*)
Seyfarth, H.E. *et al., Chem. Ber.*, 1968, **101**, 619-622 (*synth*)
Ibragimov, I.I. *et al., Khim. Geterotsikl. Soedin.*, 1973, **9**, 1434-1435; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1973, **9**, 1300 (*synth*)
Akimoto, I. *et al., Synthesis*, 1979, 146-147 (*synth*)
Lissi, E.A. *et al., J. Phys. Chem.*, 1980, **84**, 251-255 (*synth*)
Rembold, H. *et al., J. Agric. Food Chem.*, 1989, **37**, 659-662 (*occur*)
MacLeod, G. *et al., Phytochemistry*, 1992, **31**, 3113-3119 (*occur*)

3-Butylhexahydro-1(3*H*)-isobenzofuranone, 9CI B-250

[3553-34-2]

[153546-49-7, 153546-51-1, 193742-12-0, 193742-13-1]
3-Butylhexahydrophthalide, 8CI



(3*R*,3a*R*,7a*S*)-*form*

$C_{12}H_{20}O_2$ 196.289
(3*R*,3*aR*,7*aS*)-*form* [189504-31-2]
Present in celery, celeriac and fennel.
(3*R*,3*aS*,7*aR*)-*form* [193742-11-9] Not detected in celery or celeriac.
(3*S*,3*aR*,7*aS*)-*form* [114883-66-8]

Present in celery and celeriac. $[\alpha]_D^{20}$ -32.2 (c, 1.66 in $CHCl_3$).

(3*S*,3*aS*,7*aR*)-*form* [124600-37-9]
Cryst. (hexane). Mp 47-48°. $[\alpha]_D^{20}$ -15.6 (c, 2.36 in $CHCl_3$). Not detected in celery or celeriac.

(3*RS*,3*aRS*,7*aSR*)-*form*
Cryst. (hexane). Mp 38-39°. Bp_4 142-148°.

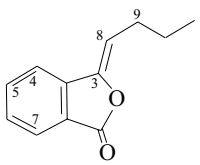
(3*RS*,3*aSR*,7*aRS*)-*form* [6431-21-6]
Oil. $Bp_{0.02}$ 105°. n_D^{18} 1.4761.

(3ξ,3*a*ξ,7*a*ξ)-*form*
Constit. of *Apium graveolens*, and black salsify (*Scorzonera hispanica*).

Mitsuhashi, H. *et al., Tetrahedron*, 1964, **20**, 1971-1982 (*synth*)
Nagai, U. *et al., Tetrahedron*, 1965, **21**, 1433-1440 (*synth*)
Cannone, P. *et al., Tetrahedron*, 1985, **41**, 3695-3704 (*synth, nmr, ms*)
Tanaka, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 2253-2256 (*synth*)
MacLeod, G. *et al., Phytochemistry*, 1991, **30**, 883-888 (*occur*)
Bartschat, D. *et al., J. Agric. Food Chem.*, 1997, **45**, 4554-4557 (*glc, occur, ms*)
Bartschat, D. *et al., J. High Resol. Chromatogr.*, 1997, **20**, 251-256 (*glc, nmr, props*)

3-Butylidene-1(3*H*)-isobenzofuranone, 9CI B-251

[551-08-6]
3-Butylidenephthalide, 8CI. Ligusticum lactone. FEMA 3333



$C_{12}H_{12}O_2$ 188.226
Flavouring ingredient.
► TI3692500

(*E*)-*form* [76681-73-7]
Constit. of *Angelica glauca*. Oil.

(*Z*)-*form* [72917-31-8]
Constit. of *Angelica glauca*. Oil. The samples obt. from *A. glauca* were presumably impure since the isomer of undetermined stereochem. from *Ligusticum* spp. is crystalline.

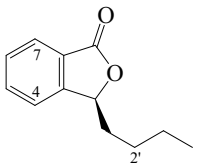
*7-Hydroxy, 7-*O*-β-D-glucopyranoside:* [240823-19-2] *7-β-D-Glucopyranosyloxybutylidenephthalide*
$C_{18}H_{22}O_8$ 366.367
Isol. from elicitor-treated cultures of *Petroselinum crispum* (parsley).

*7-Hydroxy, 7-*O*-(6-*O*-malonyl-β-D-glucopyranoside):* [240823-20-5]
$C_{21}H_{24}O_{11}$ 452.414
Isol. from elicitor-treated cultures of *Petroselinum crispum* (parsley).

Berlingozzi, S. *et al., Gazz. Chim. Ital.*, 1927, **57**, 255 (*synth*)
Mitsuhashi, H. *et al., Chem. Pharm. Bull.*, 1960, **8**, 243 (*isol*)
Banerjee, S.K. *et al., Annalen*, 1982, 699 (*isol*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1983, **21**, 659 (*rev, tox*)
Ogawa, Y. *et al., Synth. Commun.*, 1992, **22**, 315 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 86
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 344-345
Hagemeier, J. *et al., Phytochemistry*, 1999, **51**, 629-635 (*7-glucosyloxy derivs*)
Bellina, F. *et al., Tetrahedron*, 2000, **56**, 2533-2545 (*synth*)

3-Butyl-1(3*H*)-isobenzofuranone, 9CI B-252

[6066-49-5]
3-Butylphthalide, 8CI. FEMA 3334



(*S*)-*form*

$C_{12}H_{14}O_2$ 190.241
Potential nutriceutical.
► Skin irritant. LD_{50} (rat, orl) 2450 mg/kg. TI3692000

(*S*)-*form* [3413-15-8]
Constit. of celery oil (*Apium graveolens*) and lovage (*Levisticum officinale*), also from *Ligusticum acutilobum*. Flavouring agent. d^{20} 1.07. $Bp_{0.1}$ 106-108°. $[\alpha]_D$ -57 (c, 1.96 in $CHCl_3$). n_D^{20} 1.5260.

4-Hydroxy: [74459-24-8]

[74459-23-7] *3-Butyl-4-hydroxy-1(3*H*)-isobenzofuranone, 9CI. 3-Butyl-4-hydroxyphthalide.* ***Chuangxinol***
Cryst. (C_6H_6). Mp 188-190°. $[\alpha]_D$ -88.7 (c, 0.38 in EtOH).

(ξ)-*form*

7-Hydroxy: [135217-23-1] *3-Butyl-7-hydroxy-1(3*H*)-isobenzofuranone. 3-Butyl-7-hydroxyphthalide*
$C_{12}H_{14}O_3$ 206.241
Cryst. Mp 49-50°. $[\alpha]_D$ -45.5 (c, 0.8 in $CHCl_3$).

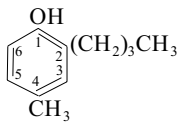
*2′,3′,7-Trihydroxy:3-(2,3-Dihydroxybutyl)-7-hydroxy-1(3*H*)-isobenzofuranone. 3-(2,3-Dihydroxybutyl)-7-hydroxyphthalide*
$C_{12}H_{14}O_5$ 238.24
Cryst. (MeOH). Mp 139-140°. $[\alpha]_D^{22}$ +67 (c, 0.67 in MeOH). λ_{max} 212 (log ϵ 4.39); 237 (log ϵ 3.08); 302 (log ϵ 3.65) (MeOH).

[87421-30-5]

Naves, Y.R. *et al., Helv. Chim. Acta*, 1943, **26**, 1281 (*isol*)
Mitsuhashi, H. *et al., Chem. Pharm. Bull.*, 1963, **11**, 1317; 1966, **14**, 777 (*isol, biosynth*)
Barton, D.H.R. *et al., J.C.S.*, 1963, 1916 (*isol, uv, ir, nmr*)
Nagai, S. *et al., Tetrahedron*, 1965, **21**, 1701 (*abs config*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 251 (*rev, tox*)
Peking Inst. Pharm. Ind., *et al., CA*, 1980, **93**, 114227e (*4-hydroxy*)
Ogawa, Y. *et al., Heterocycles*, 1989, **29**, 865-872 (*S-form, synth, pmr*)
Naito, T. *et al., Phytochemistry*, 1992, **31**, 639 (*4-hydroxy*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 93
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 352-353
Makino, M. *et al., Heterocycles*, 1998, **48**, 1931-1934 (*3-Butyl-7-hydroxyisobenzofuranone*)
Holler, U. *et al., J. Nat. Prod.*, 2002, **65**, 876-882 (*2′,3′,7-trihydroxy*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSH500

2-Butyl-4-methylphenol, 9CI B-253

[6891-45-8]
*2-Butyl-*p*-cresol, 8CI*

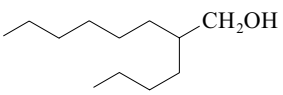


$C_{11}H_{16}O$ 164.247
Antioxidant for lard. d^{20} 0.97. Mp 19°. Bp 228-229° Bp_{15} 124-126°.

Coulthard, C.E. *et al., J.C.S.*, 1930, 291
Grant, M.S. *et al., J.C.S.*, 1959, 2513
Rodamane, I. *et al., CA*, 1964, **61**, 5547f; 1968, **68**, 59203a

2-Butyl-1-octanol B-254

[3913-02-8]
5-Hydroxymethylundecane



$C_{12}H_{26}O$ 186.337
Constit. of *Humulus lupulus* (hops) and *Portulaca oleracea* (purslane). $d_4^{16.5}$ 0.84. Bp_{12} 131-133°. n_D^{16} 1.4435.

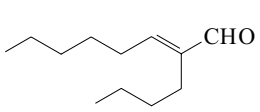
3,5-Dinitrobenzoyl:
Mp 28°.

[35467-05-1]

von Braun, J. *et al., Ber.*, 1929, **62**, 2880 (*synth*)
Bolle, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1951, **233**, 1466 (*synth*)
Pratt, E.F. *et al., J.A.C.S.*, 1954, **76**, 52 (*synth*)
Ohno, M. *et al., CA*, 1965, **62**, 10326e (*synth*)
Kito, T. *et al., CA*, 1978, **89**, 107947d (*synth*)
Paterson, I. *et al., Tet. Lett.*, 1979, 2179 (*synth*)
Krupcik, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 1808 (*glc*)
Rzama, A. *et al., Phytochemistry*, 1995, **38**, 1375 (*isol*)

2-Butyl-2-octenal, 9CI B-255

[13019-16-4]



(*E*)-*form*

$C_{12}H_{22}O$ 182.305
Bp_9 89-91° Bp_{10} 74-76°.

2,4-Dinitrophenylhydrazone: [49563-02-2]
Cryst. (EtOH). Mp 132-133°.

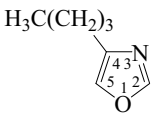
(*E*)-*form* [64935-38-2]
Found in essential oils of *Acorus calamus* (sweet flag) and *Lactuca sativa*.

[99915-14-7]

McElvain, S.M. *et al., J.A.C.S.*, 1954, **76**, 5736 (*synth*)
Lieberman, S.V. *et al., J.A.C.S.*, 1955, **77**, 1114 (*synth*)
Damico, R. *et al., J.O.C.*, 1967, **32**, 2356 (*synth*)
Baker, J.T. *et al., Aust. J. Chem.*, 1972, **25**, 393 (*isol*)
Bradshaw, J.W.S. *et al., Nature (London)*, 1975, **258**, 230 (*isol*)
Grandi, R. *et al., J.O.C.*, 1977, **42**, 1352 (*synth*)
Kuwajima, I. *et al., Chem. Lett.*, 1980, 525 (*synth*)
Pfister, J.R. *et al., Tet. Lett.*, 1980, **21**, 1281 (*synth*)
Casiraghi, G. *et al., J.C.S. Perkin 1*, 1982, 805 (*synth*)
Rossi, R. *et al., Synth. Commun.*, 1992, **22**, 603 (*synth*)

4-Butyloxazole, 9CI B-256

[79886-36-5]



$C_7H_{11}NO$ 125.17
Volatile constit. of ripe tomato. Vegetable-like, green odour. Characterised spectroscopically.

Ho, C.-T. *et al., J. Agric. Food Chem.*, 1981, **29**, 1306-1308 (*synth, ms, odour*)
Ho, C.-T. *et al., Lebensm.-Wiss. Technol.*, 1982, **15**, 340-342 (*occur*)

5-Butyloxazole, 9CI B-257

[77311-06-9]

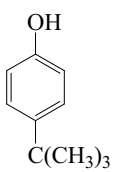
$C_7H_{11}NO$ 125.17
Constit. of roasted peanut volatiles (provisional assignment) and fried bacon. Fatty, animalic, bacon-fatty odour. Characterised spectroscopically.

Lee, M.-H. *et al., J. Agric. Food Chem.*, 1981, **29**, 684-686 (*glc*)
Jin, Q.Z. *et al., Perfum. Flavor.*, 1984, **9**, 25-26 (*synth, aroma, occur*)

4-*tert*-Butylphenol, 8CI B-258

[98-54-4]

[27178-34-3]
4-(1,1-Dimethylethyl)phenol, 9CI. 2-(4-Hydroxyphenyl)-2-methylpropane. FEMA 3918



$C_{10}H_{14}O$ 150.22
Found in oregano. Flavour ingredient. Needles. Mp 99°. Bp 236-238°. pK_{a1} 10.39 (25°). Steam-volatile.
▶ Skin and severe eye irritant. LD_{50} (rat, orl) 2951 mg/kg. SJ8925000

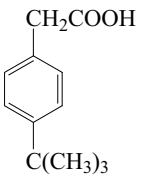
Me ether: [5396-38-3] *1-tert-Butyl-4-methoxybenzene. 4-tert-Butylanisole*
$C_{11}H_{16}O$ 164.247
Bp 215-216° Bp_{730} 222°.

Et ether: [17269-94-2] *1-tert-Butyl-4-ethoxybenzene. 4-tert-Butylphenetole*
$C_{12}H_{18}O$ 178.274
Bp_{730} 233-234°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1077A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 252A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1009B (*ir*)
Cullinane, N.M. *et al., J.C.S.*, 1954, 2942
Adv. Chem. Ser., 1955, **15**, 291 (***props***)
Bowman, R.S. *et al., J.A.C.S.*, 1957, **79**, 87 (*synth, ir*)
Dearden, J.C. *et al., Can. J. Chem.*, 1959, **37**, 1294 (*uv*)
Demerseman, P. *et al., Bull. Soc. Chim. Fr.*, 1971, 201
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 835 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 447
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSE500

4-*tert*-Butylphenylacetic acid, 8CI B-259

[32857-63-9]
4-(1,1-Dimethylethyl)benzeneacetic acid, 9CI



$C_{12}H_{16}O_2$ 192.257
Cryst. (petrol). Mp 79.5-80.5°.

Me ester: [3549-23-3] *FEMA 2690*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient with a roasted, chocolate-like flavour. Used in oral care products. Oil. d_4^{20} 1. $Bp_{2.5}$ 106°.

Et ester: [14062-22-7]
$C_{14}H_{20}O_2$ 220.311
Bp_6 130-131° $Bp_{0.47}$ 95°.

Van der Stelt, C. *et al., J. Med. Pharm. Chem.*, 1961, **4**, 335-339 (*synth*)
U.K. Pat., 1964, 971 700; *CA*, **61**, 14592b (*Me ester, synth*)
Buu-Hoi, N.P. *et al., Chim. Ther.*, 1967, **2**, 39-48 (*Et ester*)
Misharev, A.D. *et al., Org. Mass Spectrom.*, 1981, **16**, 99 (*ms*)
Reichardt, C. *et al., Annalen*, 1983, 721-743 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1737 (*Me ester, use*)
Pat. Coop. Treaty (WIPO), 1999, 9 823 250; *CA*, **129**, 45142w (*Me ester, use*)

2-Butyl-3-phenyl-2-propen-1-al B-260

[7492-44-6]

[128649-17-2, 128649-19-4]

2-(Phenylmethylene)hexanal, 9CI. α-Butylcinnamaldehyde. 2-Benzylidenehexanal. FEMA 2191

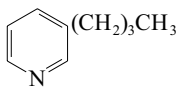
$PhCH{=}C(CHO)(CH_2)_3CH_3$

$C_{13}H_{16}O$
Food flavorant. Liq. with floral odour. $d_4^{15.5}$ 0.83. Bp 265° $Bp_{0.05}$ 78-79° (*E*/*Z* =3:1).

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1980, **18**, 657 (*tox*)
De Kimp, N. *et al., Bull. Soc. Chim. Belg.*, 1990, 41-46 (*synth*)
Dallacker, F. *et al., Chem.-Ztg.*, 1990, **114**, 1-5 (*synth*)

3-Butylpyridine, 9CI B-261

[539-32-2]
Fusarinin†. *Fusarin*†



$C_9H_{13}N$ 135.208
Maillard product. Insol. H_2O. d_4^{20} 0.92. Bp 205-208° Bp_7 82°.
▶ US4056000

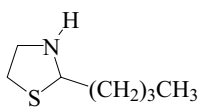
Hydrochloride:
Cryst. (H_2O). Mp 126°.

Picrate:
Cryst. (EtOH). Mp 89-90°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 245A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1517B (*ir*)
Maas, E. *et al., Ber.*, 1914, **47**, 1171
Yabuta, Y. *et al., CA*, 1940, **34**, 3314 (*isol*)
Tamari, K. *et al., Nippon Nogei Kagaku Kaishi*, 1948, **22**, 16
Frank, R.L. *et al., J.A.C.S.*, 1948, **70**, 3482
Plattner, P.A. *et al., Helv. Chim. Acta*, 1954, **37**, 1379
Kyte, C.T. *et al., J.C.S.*, 1960, 4454
Chelucci, G. *et al., J. Het. Chem.*, 1988, **25**, 1761 (*synth, pmr*)

2-Butylthiazolidine, 9CI B-262

[30188-50-2]
2-Butylterahydrothiazole



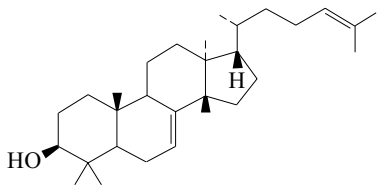
$C_7H_{15}NS$ 145.268

(±)-form
Flavouring ingredient. Bp_4 77-79°.

Asinger, F. *et al., Monatsh. Chem.*, 1970, **101**, 1295-1308 (*synth*)
Ger. Pat., 1974, 2 333 581; *CA*, **80**, 46640p (*use*)
U.S. Pat., 1977, 4 011 233; *CA*, **87**, 23264z (*use*)
Yasuhara, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 2273-2274 (*synth, pmr, ms*)

Butyrospermol B-263

[472-28-6]
Eupha-7,24-dien-3-ol. Basseol



$C_{30}H_{50}O$ 426.724
Isol. from shea nut fat. Cryst. (MeOH). Mp 111-113°. $[\alpha]_D^{19}$ -12 ($CHCl_3$).

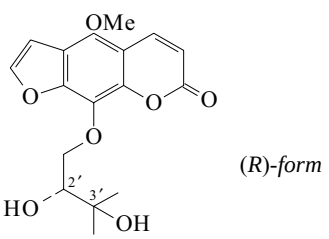
Ac: [1259-21-8]
$C_{32}H_{52}O_2$ 468.762
Cryst. Mp 136-139°. $[\alpha]_D^{19}$ +14 ($CHCl_3$).

Ketone: [81738-57-0] *Eupha-7,24-dien-3-one.* ***Butyrospermone***
$C_{30}H_{48}O$ 424.709
Found in various vegetable oils.

Lawrie, W. *et al., J.C.S.*, 1956, 2029; 3272 (*struct*)
Galbraith, M.N. *et al., Aust. J. Chem.*, 1965, **18**, 226 (*acetate*)
Fedell, E. *et al., J. Am. Oil Chem. Soc.*, 1966, **43**, 254 (*occur*)
Pradhan, B.P. *et al., J. Indian Chem. Soc.*, 1969, **46**, 331 (*isol, struct*)
Murti, V.V.S. *et al., Phytochemistry*, 1972, **11**, 2089 (*acetate*)
Kohle, J.N. *et al., Lipids*, 1982, **17**, 166 (*Butyrospermone*)
Ok, H.O. *et al., Diss. Abstr. Int., B*, 1987, **47**, 3775 (*synth*)
Chaudhuri, K. *et al., J. Nat. Prod.*, 1987, **50**, 1183 (*Butyrospermone*)
De Pascual Teresa, J. *et al., Phytochemistry*, 1987, **26**, 1767 (*pmr, cmr*)
Akihisa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1255 (*pmr, cmr*)

Byakangelicin B-264

[19573-01-4]
*9-(2,3-Dihydroxy-2-methylbutoxy)-4-methoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. Biacangelicin*



(*R*)-*form*

$C_{17}H_{18}O_7$ 334.325Log P 1.34 (calc).
λ_{max} 219 ; 239 ; 246 ; 270 ; 312 (MeOH) (Berdy).

(R)-form [482-25-7]
Constit. of Japanese drug byakusi obt. from *Angelica* spp. Also from lemon oil and other *Citrus* spp.. Pale yellow needles (EtOH). Mp 117-118°. $[\alpha]_D^{25}$ +24.6 (Py). Pharmacol. active isomer.
► Exp. reprod. effects (inhibits action of placental gonadotrophins). LV1049000

2′-O-β-D-Glucopyranoside:
$C_{23}H_{28}O_{12}$ 496.467
Constit. of angelica *Angelica archangelica* root. Cryst. Mp 111-114°. $[\alpha]_D^{25}$ -15 (c, 0.1 in MeOH).

3′-O-β-D-Glucopyranoside:
$C_{23}H_{28}O_{12}$ 496.467
Constit. of angelica root. Cryst. Mp 170-173°. $[\alpha]_D^{25}$ -8 (c, 0.1 in H_2O).

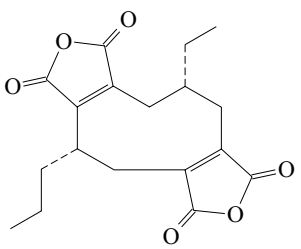
2′-O-(3-Methylbutanoyl):
$C_{22}H_{26}O_8$ 418.443
Constit. of angelica (*Angelica archangelica*) root. Gum. No opt. rotn. or config..

(S)-form
Constit. of common rue (*Ruta graveolens*). Cryst. Mp 124-126°. $[\alpha]_D^{22}$ -19 (MeOH).

Noguchi, T. *et al., Ber.*, 1938, **71**, 344; 1428 (*isol, struct, synth*)
Pakrashi, A. *et al., Indian J. Exp. Biol.*, 1967, **5**, 167 (*pharmacol*)
Neilsen, B.E. *et al., Acta Chem. Scand.*, 1969, **23**, 962 (*abs config*)
Reisch, J. *et al., Planta Med.*, 1969, **17**, 116 (*(-)-Byakangelicin*)
Perel'son, M.E. *et al., Khim. Prir. Soedin.*, 1971, **7**, 576; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 557 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 580 (*occur*)
Fukushima, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1227 (*ms*)
Thastrup, O. *et al., Phytochemistry*, 1983, **22**, 2035 (*glucosides*)
Okuyama, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1084 (*activity*)

Byssochlamic acid B-265

[743-51-1]



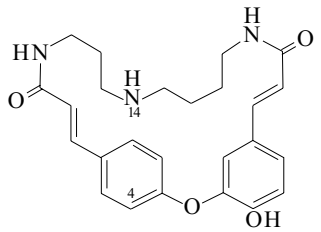
$C_{18}H_{20}O_6$ 332.352
Mycotoxin prod. by *Byssochlamys fulva* and *Byssochlamys nivea*. Prisms (EtOH). Mp 163.5°. $[\alpha]_D$ +108 (c, 0.4 in $CHCl_3$). λ_{max} 244 (ε 9100) (cyclohexane) (Berdy).

Bis-4-bromophenylhydrazide:
Mp 164-166°.

Barton, D.H.R. *et al., J.C.S.*, 1965, 1769; 1787 (*struct, abs config*)
Stork, G. *et al., J.A.C.S.*, 1972, **94**, 4735 (*synth*)
Nieminen, S. *et al., Helv. Chim. Acta*, 1981, **64**, 2791 (*nmr*)
White, J.D. *et al., J.A.C.S.*, 1992, **114**, 9673; 2000, **122**, 8665-8671 (*synth*)

Cadabicine C-1

[99964-83-7]



$C_{25}H_{29}N_3O_4$ 435.522
Alkaloid from the stem bark of the famine food *Cadaba farinosa* (luquata sigmama). Mp 270-272° dec.

N^{14},O-*Di-Ac:* [99964-84-8] ***Cadabicine diacetate***
$C_{29}H_{33}N_3O_6$ 519.596
Rods (MeOH). Mp 265-268°.

4-Methoxy: [126431-38-7] ***Isocodonocarpine***
$C_{26}H_{31}N_3O_5$ 465.548
Off-white cryst. (MeOH). Mp 220-222° dec. CAS gives incorrect name.

4-Methoxy, N^{14}*-Ac:****14*****-N-*****Acetylisocodonocarpine***
$C_{28}H_{33}N_3O_6$ 507.585
Amorph. powder. Mp 234-236°.

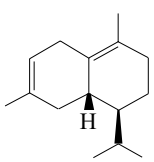
4-Methoxy, N^{14},O-*di-Ac:*
Cryst. (MeOH). Mp 205-207°.

*Me ether:****Cadabicine methyl ether****.* O-*Methylcadabicine*
$C_{26}H_{31}N_3O_4$ 449.549
Alkaloid from the stem bark of the famine food *Cadaba farinosa* (luquata sigmama).

Ahmad, V.U. *et al., Phytochemistry*, 1985, **24**, 2709; 1989, **28**, 2493 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Ahmad, V.U. *et al., J. Nat. Prod.*, 1987, **50**, 1186; 1992, **55**, 1509 (*isol, Cadabicine, Cadabicine diacetate, 14-N-Acetylisocodonocarpine*)
Ahmad, V.U. *et al., Pak. J. Sci. Ind. Res.*, 1992, **35**, 475; *CA*, **119**, 177556n (*Cadabicine methyl ether*)

1(10),3-Cadinadiene C-2

[29350-73-0]
ω-Cadinene

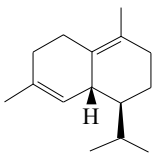


$C_{15}H_{24}$ 204.355
Constit. of *Mentha piperita*. Oil. $Bp_{4.5}$ 115-128°. $[\alpha]_D^{20}$ +92. Originally named δ-Cadinene, which led to confusion with 1(10),4-Cadinadiene, C-3.

Connell, D.W. *et al., Tet. Lett.*, 1968, 519
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr, bibl*)

1(10),4-Cadinadiene C-3

[29350-73-0]
δ-Cadinene



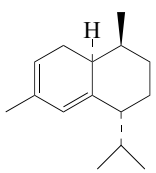
$C_{15}H_{24}$ 204.355
(+)-*form* [483-76-1]
Constit. of the essential oils of ylang-ylang, citronella, cubebs, and sweetflag. Oil. Bp_{10} 133-134°.

Bisepoxide:
Cryst. Mp 86-87°. $[\alpha]_D$ +23 (c, 6.7 in $CHCl_3$).

(±)-*form* *Dysoxylonene*
Bp_{10} 133°.

Herout, V. *et al., Coll. Czech. Chem. Comm.*, 1954, **19**, 118 (*struct*)
Nagasampagi, B.A. *et al., Tet. Lett.*, 1968, 1913 (*struct*)
Nishimura, H. *et al., Agric. Biol. Chem.*, 1981, **45**, 1861 (*synth*)
Davis, G.D. *et al., Phytochemistry*, 1995, **39**, 553 (*biosynth*)
Davis, G.D. *et al., Magn. Reson. Chem.*, 1996, **34**, 156 (*pmr, cmr*)
Alchanati, I. *et al., Phytochemistry*, 1998, **47**, 961-967 (*biosynth*)

3,5-Cadinadiene C-4



(+)-*form*

$C_{15}H_{24}$ 204.355
(+)-*form* [189165-77-3]
Oil.

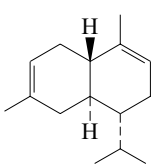
(-)-*form*
Constit. of *Leptospermum scoparium* (red tea). Oil. $[\alpha]_D$ -216.8 (c, 0.14 in $CDCl_3$).

Melching, S. *et al., Phytochemistry*, 1997, **44**, 1291-1296 (*isol, pmr*)

3,9-Cadinadiene C-5

[523-47-7]

[29350-73-0]
β-Cadinene



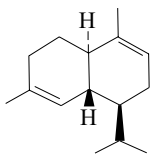
$C_{15}H_{24}$ 204.355
Constit. of *Pinus caribaea*. Mixed cadinene isomers, with β-cadinene usually predominating, occur in several essential oils, esp. ylang-ylang, citronella and cade oil from *Juniper* spp. Cadinene isomers are used as a flavouring agent and/or flavour modifier. Oil.

Fringuelli, F. *et al., J.O.C.*, 1985, **50**, 890 (*synth*)
Barnola, L.F. *et al., Biochem. Syst. Ecol.*, 1994, **22**, 437 (*isol*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 220-221 (*use*)

4,9-Cadinadiene C-6

[24406-05-1]

[29350-73-0]
α-Cadinene



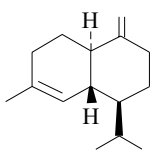
$C_{15}H_{24}$ 204.355
Constit. of *Humulus lupulus* (hops). Oil. $[\alpha]_D^{24}$ -62.4 (c, 0.808 in $CHCl_3$).

Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 1468 (*isol, struct*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 145 (*synth*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr, cmr*)

4,10(15)-Cadinadiene C-7

[483-74-9]

[1460-97-5, 29350-73-0, 30021-74-0, 39029-41-9]
γ-Cadinene



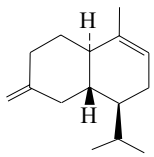
$C_{15}H_{24}$ 204.355
Constit. of citronella oil. Oil. Bp_5 110-115°. $[\alpha]_D^{20}$ +148.

Vig, O.P. *et al., Indian J. Chem.*, 1970, **8**, 29 (*isol, struct*)
Anderson, N.H. *et al., Phytochemistry*, 1970, **9**, 1325-1340 (*pmr*)
Sakurai, H. *et al., Tetrahedron*, 1983, **39**, 883 (*synth*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1997, 2065-2070 (*biosynth*)
Dos Santos, M.H. *et al., Rev. Bras. Cienc. Farm.*, 1999, **35**, 297-300 (*activity*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*cmr*)

4(15),9-Cadinadiene C-8

[66141-11-5]

[29350-73-0]
γ$_1$-Cadinene



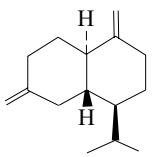
$C_{15}H_{24}$ 204.355
Constit. of citronella oil (*Cymbopogon nardus*). A mixture of cadinene isomers from various essential oils is used as a flavouring agent/flavour modifier. Bp_9 120-121°. $[\alpha]_D$ -19. $n_D^{26.5}$ 1.5155.

Dev, S. *et al., J. Indian Chem. Soc.*, 1949, **26**, 263 (*isol*)
Ghatgey, B.B. *et al., Perfum. Essent. Oil Res.*, 1956, **47**, 157-159 (*isol*)
Irie, T. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 1053-1055 (*isol*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731-1751 (*struct*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 552-554 (*synth*)
Kim, T.C. *et al., Phytochemistry*, 1999, **51**, 793-801 (*occur*)

4(15),10(14)-Cadinadiene C-9

[25548-04-3]

[29350-73-0]
Decahydro-1,6-bis(methylene)-4-(1-methylethyl)naphthalene, 9CI. Decahydro-4-isopropyl-1,6-dimethylenenaphthalene. ***ϵ-Cadinene***



Absolute configuration

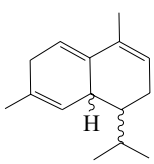
$C_{15}H_{24}$ 204.355
Constit. of *Juniperus communis* (juniper). Oil. Bp_2 99-100°. $[\alpha]_D^{22}$ +50.7 (c, 1.5 in $CHCl_3$).

[1080-67-7, 27542-04-7]

Burk, L.A. *et al., Tetrahedron*, 1976, **32**, 2083 (*bibl*)
Koster, F.-H. *et al., Annalen*, 1986, 78 (*synth, cmr*)
Hagiwara, H. *et al., J.C.S. Perkin 1*, 1993, 2173 (*synth*)

1,4,9-Cadinatriene C-10

[71609-04-6]
1,4,9-Cadalatriene

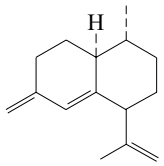


$C_{15}H_{22}$ 202.339
Constit. of *Acorus calamus* (sweet flag). Oil. $Bp_{0.01}$ 80°. $[\alpha]_D^{22}$ -156.4 (c, 1 in $CHCl_3$).

Rohr, M. *et al., Phytochemistry*, 1979, **18**, 328

4(15),5,11-Cadinatriene C-11

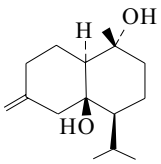
[54274-73-6]
1-Epibicyclosesquiphellandrene. *1-*epi-*Bicyclosesquiphellandrene*



$C_{15}H_{22}$ 202.339
Constit. of *Ocimum basilicum* (sweet basil). Oil.

Terhune, S.J. *et al., Phytochemistry*, 1974, **13**, 1183 (*isol, struct*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1976, **53**, 593 (*synth*)

4(15)-Cadinene-6,10-diol C-12



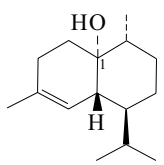
(6β,10α)-*form*

$C_{15}H_{26}O_2$ 238.369
(6β,10α)-*form* [25330-21-6]
Isocalamendiol
Constit. of the rhizomes of *Acorus calamus* (sweet flag). Cryst. (Et_2O/hexane). Mp 72.5-73.5°.
(6β,10β)-*form* [30167-28-3]
Calamendiol. *Calameone*
Constit. of sweet flag essential oil. Cryst. (Et_2O/hexane). Mp 170-171.5°. $[\alpha]_D^{26}$ -4.4 (EtOH).

Yamamura, S. *et al., Tetrahedron*, 1971, **27**, 5419 (*isol, struct*)
Niwa, M. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3148 (*synth*)
Williams, J.R. *et al., J.O.C.*, 1980, **45**, 4479 (*synth*)
Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175 (*isol, pmr, cmr*)

4-Cadinen-1-ol C-13

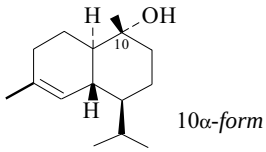
Cubenol



$C_{15}H_{26}O$ 222.37
1α-*form* [21284-22-0]
Constit. of oil of cubeb pepper (*Piper cubeba*). Oil. $Bp_{2.5}$ 170-180° (bath). $[\alpha]_D^{30}$ -30.6.

Ohta, Y. *et al., Tet. Lett.*, 1967, 2073 (*isol, struct*)
Labbé, C. *et al., Phytochemistry*, 1993, **34**, 441 (*isol, pmr, cmr*)
Gijsen, H.J.M. *et al., Tetrahedron*, 1994, **50**, 4745-4754 (*synth*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1997, 2065-2070 (*biosynth*)

4-Cadinen-10-ol C-14



10α-*form*

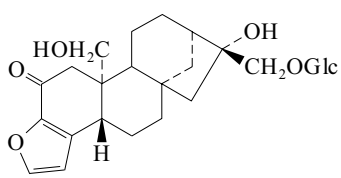
$C_{15}H_{26}O$ 222.37
10α-*form* [481-34-5]
α-Cadinol
Constit. of *Juniperus communis* (juniper). Cryst. Mp 74.5-75°. $[\alpha]_D$ -47 (-38.5).

Me ether: ***α-Cadinol methyl ether***
$C_{16}H_{28}O$ 236.397
Oil. $[\alpha]_D^{24}$ -49 (c, 3.42 in $CHCl_3$).
10β-*form* **T-*Cadinol***
Mp 64-64.5°. $[\alpha]_D$ +3.4 (c, 1.2 in $CHCl_3$). λ_{max} (MeOH) (Berdy).

Nagasampagi, B.A. *et al., Tet. Lett.*, 1968, 1913 (*isol*)
Caine, D. *et al., Tet. Lett.*, 1977, 3107 (*synth*)
Borg-Karlson, A.-K. *et al., Tetrahedron*, 1981, **37**, 425 (*sterochem*)
Bottini, A.T. *et al., J. Nat. Prod.*, 1987, **50**, 732 (*cmr*)
Dupré, S. *et al., Phytochemistry*, 1991, **30**, 1211 (*α-Cadinol methyl ether*)
Claeson, P. *et al., Planta Med.*, 1991, **57**, 352 (*T-Cadinol, pmr, cmr*)
Labbé, C. *et al., Phytochemistry*, 1993, **34**, 441 (*T-Cadinol, pmr, cmr*)
Chang, S.-T. *et al., Phytochemistry*, 2000, **55**, 227-232 (*activity*)

Cafamarine C-15

[42612-19-1]

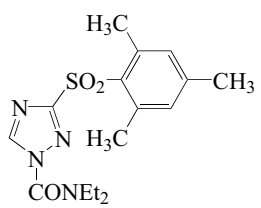


$C_{26}H_{36}O_{10}$ 508.564
Occurs in coffee.

d'Ornano, M. *et al., CA*, 1968, **68**, 36709f (*isol*)
Duc, D.K.M. *et al., Tetrahedron*, 1981, **37**, 2371 (*cmr, struct*)

Cafenstrole C-16

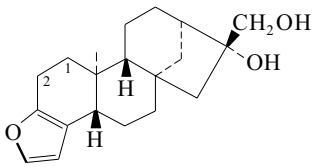
[125306-83-4]
N,N-Diethyl-3-[(2,4,6-trimethylphenyl)-sulfonyl]-1H-1,2,4-triazole-1-carboxamide, 9CI. CH 900



$C_{16}H_{22}N_4O_3S$ 350.441
Cryst. Mp 114-116°.
▶ LD_{50} (rat, orl) >5000 mg/kg.
Eur. Pat., 1989, 332 133, (*Chugai*); *CA*, **112**, 98538k (*synth, activity*)
Kanzaki, M. *et al., Brighton Crop Prot. Conf. - Weeds*, 1991, 923-928 (*activity*)
Pesticide Manual, 11th edn., 1997, 102

Cafestol C-17

[469-83-0]
Cafesterol. Coffeol



$C_{20}H_{28}O_3$ 316.439
Constit. of coffee bean oil. Present in boiled-type coffee beverages. Possesses hypercholesterolaemic activity. Diterpenoid constits. of coffee products are associated with cardiotoxic props.. Cryst. (petrol). Mp 160-162° dec. $[\alpha]_D$ -101 ($CHCl_3$).

1,2-Didehydro: [6894-43-5] ***Kahweol***
$C_{20}H_{26}O_3$ 314.424
Present in boiled type-coffee beverages. May possess hypercholesterolaemic activity. Constit of coffee bean oil. Cryst. Mp 88-90° Mp 143-143.5°. $[\alpha]_D^{20}$ -270. The higher Mp (ref. not accessible) is prob. the correct one referring to a purer sample.

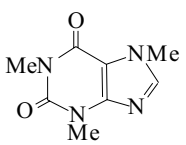
1,2-Didehydro, di-Ac:
Cryst. (MeOH). Mp 115°. $[\alpha]_D^{20}$ -245.

Kaufmann, H.P. *et al., Chem. Ber.*, 1963, **96**, 2489 (*isol, struct, bibl*)
Scott, A.I. *et al., Tetrahedron*, 1964, **20**, 1339 (*Cafestol*)
Duc, D.K.M. *et al., Tetrahedron*, 1981, **37**, 2371 (*cmr*)
Corey, E.J. *et al., Tet. Lett.*, 1987, **28**, 5403 (*synth*)
Ugert, R. *et al., J. Agric. Food Chem.*, 1995, **43**, 2167-2172 (*occur*)

Caffeine, BAN, USAN C-18

[58-08-2]

[5743-12-4]
*3,7-Dihydro-1,3,7-trimethyl-1*H*-purine-2,6-dione, 9CI. 1,3,7-Trimethylxanthine. Theine. Guaranine. Coffeine. Methyltheobromine. Cafipel. FEMA 2224. Many other names*



$C_8H_{10}N_4O_2$ 194.193
Component of coffee beans (*Coffea arabica*), many other *Coffea* spp., chocolate (*Theobroma cacao*), tea (*Camellia thea*), kolanut (*Cola acuminata*) and several other *Cola* spp. and several other plants. Used in many cola-type beverages as a flavour enhancer. Mp 236° (phase transition at 141°). Log P -0.06 (uncertain value) (calc).
▶ Adverse systemic effects (by ingestion and other routes). Human and exp. reprod. effects. LD_{50} (rat, orl) 192 mg/kg.
EV6475000

Perchlorate:
Mp 89°.

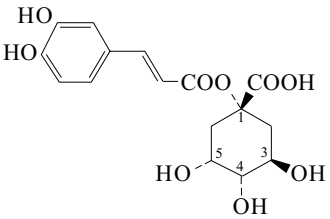
Citrate: [69-22-7] *Caffeine citrate. Cafcit*
Cryst. powder.

[8000-95-1]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 586A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 710B (*ir*)
Fischer, E. *et al., Ber.*, 1895, **28**, 2473; 3135 (*synth*)
Bredereck, H. *et al., Chem. Ber.*, 1950, **83**, 201; 1962, **95**, 1902 (*synth*)
Blout, E.R. *et al., J.A.C.S.*, 1950, **72**, 479 (*ir*)
Sutor, D.J. *et al., Acta Cryst.*, 1958, **11**, 453 (*cryst struct*)
Spiteller, G. *et al., Monatsh. Chem.*, 1962, **93**, 632 (*ms*)
Twanmoh, L.-M. *et al., J. Het. Chem.*, 1973, **10**, 187 (*pmr*)
Nicolau, C. *et al., Z. Naturforsch., C*, 1974, **29**, 475 (*cmr*)
Suzuki, T. *et al., Phytochemistry*, 1976, **15**, 1235 (*biosynth*)
Aranda, J.V. *et al., J. Pediatr.*, 1977, **90**, 467-472 (*Caffeine citrate, use*)
Zubair, M.U. *et al., Anal. Profiles Drug Subst.*, 1986, **15**, 71 (*rev, ir, uv, pmr, cmr, ms, occur, anal*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 921
Arnaud, M.J. *et al., Prog. Drug Res.*, 1987, **31**, 273 (*rev, chem, pharmacol, toxicity*)
Somani, S.M. *et al., Int. J. Clin. Pharmacol., Ther. Toxicol.*, 1988, **26**, 521 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CAK500
Benowitz, N.L. *et al., Annu. Rev. Med.*, 1990, **41**, 277 (*rev, pharmacol*)
IARC Monog., 1991, **51**, 291 (*rev, tox*)
Bott, K. *et al., Chem. Ber.*, 1993, **126**, 1955 (*synth*)
Sitkowski, J. *et al., Spectrochim. Acta A*, 1995, **51**, 839 (*pmr, cmr, N-15 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 363
Caffeine, (ed. Spiller, G.A.), CRC Press, 1998, (*book*)
Carrier, O. *et al., Clin. Pharmacol. Ther. (St. Louis)*, 1998, **44**, 145-151 (*Caffeine citrate, metab*)
Parliment, T.H. *et al., ACS Symp. Ser.*, 2000, **754**,
Bogo, A. *et al., Phytochemistry*, 2000, **54**, 937-939 (*isol, ms*)
Waldvogel, S.R. *et al., Angew. Chem., Int. Ed.*, 2003, **42**, 604-605 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAK500

1-*O*-Caffeoylquinic acid C-19

[1241-87-8]
1-(3,4-Dihydroxycinnamoyl)quinic acid



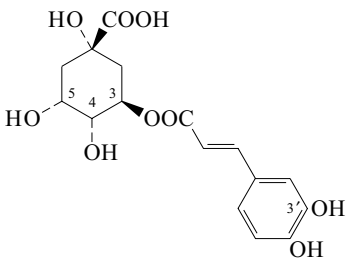
$C_{16}H_{18}O_9$ 354.313
Constit. of coffee. Noncryst. $[\alpha]_D^{15}$ -8.3 (c, 3 in H_2O).

Anhydride:
Cryst. Mp 205-208°. $[\alpha]_D^{25}$ -17 (c, 2 in EtOH).

Scarpati, M.L. *et al., Ann. Chim. (Rome)*, 1958, **48**, 997 (*isol*)
Waiss, A.C. *et al., Chem. Ind. (London)*, 1964, 1984 (*pmr*)
Litinenko, V.I. *et al., Planta Med.*, 1975, **27**, 372 (*rev*)
Sefkow, M. *et al., Eur. J. Org. Chem.*, 2001, 2735-2742 (*synth*)

3-*O*-Caffeoylquinic acid C-20

[327-97-9]
3-(3,4-Dihydroxycinnamoyl)quinic acid. ***Chlorogenic acid****. Caffeylquinic acid. Caffetannic acid. Helianthic acid*



$C_{16}H_{18}O_9$ 354.313
λ_{max} 296 ; 325 (EtOH) (Berdy).
▶ GU8480000
(E)-form
Isol. from Liberian coffee. Nutriceutical with antioxidant props.. Needles + ½ H_2O. Mp 208°. $[\alpha]_D$ -35.2 (H_2O).

Butyl ester: [132741-56-1]
$C_{20}H_{26}O_9$ 410.42
Constit. of *Spondias mombin* (yellow mombin).

1-Me ether: ***3-O-Caffeoyl-1-O-methylquinic acid***
$C_{17}H_{20}O_9$ 368.34
Constit. of *Phyllostachys edulis* (moso bamboo). Powder. Mp 202-203°. $[\alpha]_D^{25}$ -16.9 (c, 0.35 in H_2O). λ_{max} 245 (sh) ; 300 ; 329 (MeOH).

3′-Me ether: [62929-69-5] ***3-O-Feruloylquinic acid***
$C_{17}H_{20}O_9$ 368.34
Constit. of coffee beans. Also from tomato (*Lycopersicon esculentum*) and sunflower (*Helianthus annuus*). Mp 196-197°. $[\alpha]_D^{28}$ -42.8 (EtOH). λ_{max} 325 (ε 19200) (EtOH) (Berdy).

4-Me ether: ***3-O-Caffeoyl-4-O-methylquinic acid***
$C_{17}H_{20}O_9$ 368.34
Constit. of *Phyllostachys edulis* (moso

bamboo). Powder. Mp 200-201°. $[\alpha]_D^{25}$ -47.2 (c, 0.2 in EtOH). Misnamed in ref. λ_{max} 244 (sh) ; 296 ; 328 (MeOH).

3′,4′-Quinone: [24321-18-4] ***Chlorogenoquinone***
$C_{16}H_{16}O_9$ 352.297
Forms coloured adducts with amino acids and peptides, implicated in food discolouration. No phys. props. reported.

3-Epimer: ***3*-O-*Caffeoyl*-muco-*quinic acid***
$C_{16}H_{18}O_9$ 354.313
Constit. of *Asimina triloba* (pawpaw). Powder. λ_{max} 225 ; 325 (MeOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 288C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1235C (*nmr*)
Fischer, H.O.L. *et al., Ber.*, 1932, **65**, 1037-1040 (*struct*)
Corse, J. *et al., Tetrahedron*, 1962, **18**, 1207-1210 (*3-Feruloylquinic acid, isol, derivs*)
Waiss, A.C. *et al., Chem. Ind. (London)*, 1964, 1984-1985 (*pmr*)
Pierpoint, W.S. *et al., Biochem. J.*, 1966, **98**, 567; 1969, **112**, 609 (*Chlorogenoquinone*)
James, N.F. *et al., Biochem. J.*, 1969, **112**, 617 (*Chrorogenoquinone, pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 990 (*occur*)
Schulten, H.R. *et al., Biomed. Mass Spectrom.*, 1974, **1**, 120 (*ms*)
Kelley, C.J. *et al., J.O.C.*, 1976, **41**, 449-455 (*cmr*)
Nagels, L. *et al., Phytochemistry*, 1976, **15**, 703-706 (*biosynth*)
Herrmann, K. *et al., Prog. Chem. Org. Nat. Prod.*, 1978, **35**, 73-132 (*rev*)
Cheminat, A. *et al., Phytochemistry*, 1988, **27**, 2787-2794 (*isol, pmr*)
Corthout, J. *et al., Phytochemistry*, 1992, **31**, 1979-1981 (*isol, butyl ester*)
Ida, Y. *et al., Phytochemistry*, 1994, **35**, 209-215 (*3-Feruloylquinic acid*)
Fuchs, C. *et al., J. Mass Spectrom.*, 1996, **31**, 602-608 (*hplc, ms*)
Haribal, M. *et al., Phytochemistry*, 1998, **49**, 103-108 (*isol, muco isomer*)
Lin, L.-C. *et al., J. Nat. Prod.*, 1999, **62**, 405-408 (*isol, cmr*)
Pauli, G.F. *et al., Magn. Reson. Chem.*, 1999, **37**, 827-836
Sefkow, M. *et al., Eur. J. Org. Chem.*, 2001, 1137-1141 (*synth*)
Kweon, M.-H. *et al., J. Agric. Food Chem.*, 2001, **49**, 4646-4655 (*1-Me ether, 4-Me ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CHK175

4-*O*-Caffeoylquinic acid C-21

[905-99-7]
4-(3,4-Dihydroxycinnamoyl)quinic acid. ***Cryptochlorogenic acid***

$C_{16}H_{18}O_9$ 354.313
Constit. of coffee and sunflowers. Mp 182-184°. $[\alpha]_D$ -75 (-54) (H_2O).

Me ester: [123372-74-7]
$C_{17}H_{20}O_9$ 368.34

[17608-52-5]

Scarpati, M.L. *et al., Tet. Lett.*, 1963, 1147 (*isol*)
Waiss, A.C. *et al., Chem. Ind. (London)*, 1964, 1984 (*pmr*)
Litvinenko, V.I. *et al., Planta Med.*, 1975, **27**, 372 (*rev*)
Machida, K. *et al., Phytochemistry*, 1992, **31**, 3654 (*Me ester*)
Fuchs, C. *et al., J. Mass Spectrom.*, 1996, **31**, 602 (*hplc, ms*)
Nakatani, N. *et al., J. Agric. Food Chem.*, 2000, **48**, 5512-5516 (*isol, pmr, cmr*)
Sefkow, M. *et al., Eur. J. Org. Chem.*, 2001, 2735-2742 (*synth*)

5-*O*-Caffeoylquinic acid C-22

[906-33-2]

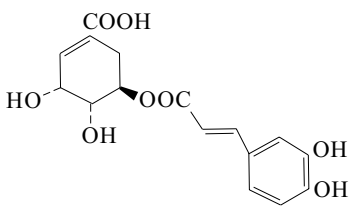
[534-61-2]
5-(3,4-Dihydroxycinnamoyl)quinic acid. ***Neochlorogenic acid***

$C_{16}H_{18}O_9$ 354.313
(*E*)-*form*
Constit. of coffee and many other plants. First isol. from peaches (*Prunus persica*). Mp 177-179° dec. $[\alpha]_D$ -5.4 (EtOH aq.). $[\alpha]_D$ -24.8 (c, 0.49 in MeOH).

Corse, J. *et al., Nature (London)*, 1953, **172**, 771 (*isol*)
Scarpati, M.L. *et al., Tet. Lett.*, 1963, 1147 (*struct*)
Waiss, A.C. *et al., Chem. Ind. (London)*, 1964, 1984 (*pmr*)
Haslam, E. *et al., J.C.S.*, 1964, 2137 (*synth*)
Schaller, D.R. *et al., J. Food Sci.*, 1970, **35**, 762 (*isol*)
Fuchs, C. *et al., J. Mass Spectrom.*, 1996, **31**, 602 (*hplc, ms*)
Pauli, G.F. *et al., Magn. Reson. Chem.*, 1999, **37**, 827-836 (*pmr, cmr*)

3-*O*-Caffeoylshikimic acid C-23

[6082-44-6]
Neodattelic acid. ***Neodactylifric acid***



$C_{16}H_{16}O_8$ 336.298
Constit. of dates (*Phoenix dactylifera*). Cryst. (H_2O). Mp 224-225° dec. $[\alpha]_D^{25}$ -124 (c, 1.16 in EtOH).

Maier, V.P. *et al., Biochem. Biophys. Res. Commun.*, 1964, **14**, 124
Harborne, J.B. *et al., Phytochemistry*, 1974, **13**, 1557
Herrmann, K. *et al., Prog. Chem. Org. Nat. Prod.*, 1978, **35**, 73

4-*O*-Caffeoylshikimic acid C-24

Isodactylifric acid. *Isodattelic acid*

$C_{16}H_{16}O_8$ 336.298
Isol. from unripe dates (*Phoenix dactylifera*). Tentative struct..

3″-Deoxy: ***4*-O-p-*Coumaroylshikimic acid***
$C_{16}H_{16}O_7$ 320.298
Solid.

Maier, V.P. *et al., Biochem. Biophys. Res. Commun.*, 1964, **14**, 124
Saito, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1397-1398 (*p-Coumaroylshikimic acid*)

5-*O*-Caffeoylshikimic acid C-25

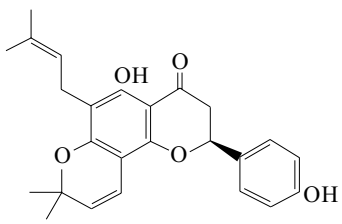
[73263-62-4]
Dattelic acid. *Dactylifric acid*

$C_{16}H_{16}O_8$ 336.298
Isol. from *Pteridium aquilinum* (bracken fern) and from unripe dates (tentative ident.). Mp 300° (dec. at 200°) (224-225°). $[\alpha]_D$ -135 (c, 0.1 in MeOH).

Maier, V.P. *et al., Biochem. Biophys. Res. Commun.*, 1964, **14**, 124
Herrmann, K. *et al., Prog. Chem. Org. Nat. Prod.*, 1978, **35**, 73
Veit, M. *et al., Phytochemistry*, 1992, **31**, 3483 (*occur, pmr*)

Cajaflavanone C-26

Erythrisenegalone

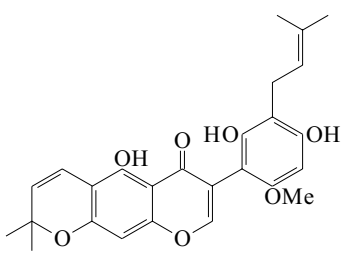


$C_{25}H_{26}O_5$ 406.477
(*S*)-*form* [68236-12-4]
Constit. of *Cajanus cajan* (pigeon pea). Straw-coloured cryst. Mp 129-130° (122-124°). $[\alpha]_D$ -66.6 (c, 1 in $CHCl_3$). $[\alpha]_D$ -5 (c, 1 in $CHCl_3$).
(±)-*form* [68682-03-1]
Light yellow cryst. (C_6H_6/petrol). Mp 138-140°.

Bhanumati, S. *et al., Phytochemistry*, 1978, **17**, 2045 (*isol*)
Jain, A.C. *et al., Tetrahedron*, 1978, **34**, 2607 (*synth*)
Nagar, A. *et al., Tet. Lett.*, 1978, 2031 (*synth*)
Fomum, Z.T. *et al., Phytochemistry*, 1985, **24**, 3075 (*isol*)

Cajaisoflavone C-27

[72578-99-5]
7-[2,4-Dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-5-hydroxy-2,2-dimethyl-2H,6H-benzo[1,2-b:5,4-b′]dipyran-6-one, 9CI



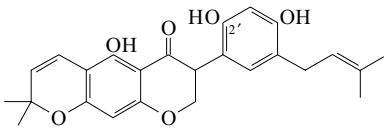
$C_{26}H_{26}O_7$ 450.487
Isol. from root bark of *Cajanus cajan* (pigeon pea). Orange semisolid.

Bhanumati, S. *et al., Phytochemistry*, 1979, **18**, 1254 (*isol, pmr, ms*)

Cajanone C-28

[63006-48-4]
7-[2,4-Dihydroxy-5-(3-methyl-2-butenyl)-

*phenyl]-7,8-dihydro-5-hydroxy-2,2-dimethyl-2*H,*6*H-*benzo[1,2-*b*:5,4-*b′]*dipyran-6-one, 9CI*



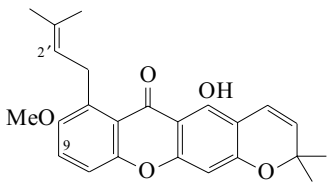
$C_{25}H_{26}O_6$ 422.477
Constit. of *Cajanus cajan* (pigeon pea). Log P 4.93 (uncertain value) (calc). λ_{max} 273 (ϵ 20000); 293 (ϵ 11200) (EtOH) (Berdy).

2′-Me ether: [71765-79-2] ***2′-O-Methylcajanone***
$C_{26}H_{28}O_6$ 436.504
Isol. from root bark of *Cajanus cajan* (pigeon pea). Yellow cryst. solid (EtOAc/petrol). Mp 85°. Opt. inactive.

Preston, N.W. *et al., Phytochemistry*, 1977, **16**, 143 (*isol, uv, pmr, struct*)
Bhanumati, S. *et al., Phytochemistry*, 1979, **18**, 693 (*deriv*)

Calabaxanthone C-29

[39011-96-6]
*5-Hydroxy-8-methoxy-2,2-dimethyl-7-(3-methyl-2-butenyl)-*2H,*6*H-*pyrano[3,2-*b*]*xanthen-6-one, 9CI*



$C_{24}H_{24}O_5$ 392.451
CAS numbering shown. Constit. of *Garcinia mangostana* (mangosteen). Yellow cryst. (EtOH). Mp 172°.

Ac:
Cryst. (MeOH). Mp 147-148°.

Me ether:
Cryst. (Me_2CO). Mp 116-119°.

O-*De-Me:* [106897-03-4] ***Demethylcalabaxanthone***
$C_{23}H_{22}O_5$ 378.424
Constit. of *Garcinia mangostana* (mangosteen). Yellow needles. Mp 85°.

9-Hydroxy: [35349-68-9] ***9-Hydroxycalabaxanthone***
$C_{24}H_{24}O_6$ 408.45
Constit. of *Garcinia mangostana* (mangosteen). Bright yellow cryst. (C_6H_6). Mp 156-156° (152-154°).

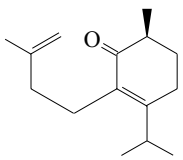
3,4-Dihydro, 9-hydroxy: [19275-46-8] ***3-Isomangostin***
$C_{24}H_{26}O_6$ 410.466
Constit. of *Garcinia mangostana* (mangosteen). Cryst. (C_6H_6). Mp 155-160° (154-155°). λ_{max} 243 (ϵ 39800); 257 (ϵ 34670); 319 (ϵ 30200); 355 (ϵ 13180) (EtOH) (Berdy).

3,4-Dihydro, 3,9-dihydroxy: [184587-72-2] ***Mangostanol***
$C_{24}H_{26}O_7$ 426.465
Constit. of *Garcinia mangostana* (mangosteen). Fine yellow powder (CH_2Cl_2/MeOH). $[\alpha]_D^{28}$ +16.3 (c, 1 in MeOH). λ_{max} 208 (log ϵ 4.39); 242 (log ϵ 4.44); 306 (log ϵ 4.25); 333 (log ϵ 3.94) (MeOH).

2′,3,3′,4-Tetrahydro, 3′,9-dihydroxy: [26063-96-7] ***3-Isomangostin hydrate***
$C_{24}H_{28}O_7$ 428.481
Constit. of *Garcinia mangostana* (mangosteen). Cryst. (CH_2Cl_2). Mp 182-183°.

Somanathan, R. *et al., J.C.S. Perkin 1*, 1972, 1935 (*struct*)
Westerman, P.W. *et al., Org. Magn. Reson.*, 1979, **9**, 631 (*cmr*)
Sen, A.K. *et al., Phytochemistry*, 1980, **19**, 2223; 1981, **20**, 183-185 (*9-Hydroxycalabaxanthone*)
Ampofo, S.A. *et al., Phytochemistry*, 1986, **25**, 2617 (*deriv*)
Mahabusarakam, W. *et al., J. Nat. Prod.*, 1987, **50**, 474 (*Isomangostin, Isomangostin hydrate*)
Chairungsrilerd, N. *et al., Phytochemistry*, 1996, **43**, 1099 (*Mangostanol*)

Calacone C-30



Absolute configuration

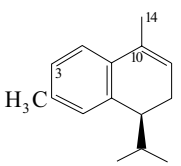
$C_{15}H_{24}O$ 220.354
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D^{20}$ +0.9 (petrol).

Vrkoč, J. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1021; 1343

α-Calacorene C-31

[21391-99-1]

[38599-17-6]
1,2-Dihydro-4,7-dimethyl-1-(1-methylethyl)naphthalene, 9CI. 1,2-Dihydro-1-isopropyl-4,7-dimethylnaphthalene. 7,8-Dihydrocadalene. 3,4-Dihydrocadalene



$C_{15}H_{20}$ 200.323
Constit. of hop, sweet flag, *Juniperus* and other oils. Oil. $[\alpha]_D^{20}$ +52.1.

3-Hydroxy: [60263-12-9] ***3-Hydroxy-α-calacorene***. *5,6-Dihydro-5-isopropyl-3,8-dimethyl-2-naphthol*
$C_{15}H_{20}O$ 216.322
Cryst. (petrol). Mp 103.5°.

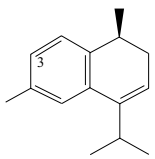
$\Delta^{10,14}$-Isomer, 3-hydroxy: [73484-09-0] ***3-Hydroxy-β-calacorene***
$C_{15}H_{20}O$ 216.322
Oil (as acetate).

Heymes, A. *et al., Recherches*, 1974, **19**, 214 (*synth*)
Bohlmann, F. *et al., Chem. Ber.*, 1976, **109**, 2021 (*3-Hydroxy-α-calacorene*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1675 (*3-Hydroxy-β-calacorene*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr, ms*)

γ-Calacorene C-32

[24048-45-1]

[38599-17-6]
1,2-Dihydro-1,6-dimethyl-4-(1-methylethyl)naphthalene, 9CI. 1,3,5,7-Cadinatetraene, 8CI. 1,2-Dihydro-4-isopropyl-1,6-dimethylnaphthalene. 9,10-Dihydrocadalene. 1,2-Dihydrocadalene



$C_{15}H_{20}$ 200.323
The (*S*)-Config is given in CA but does not appear to be clearly stated in the lit..

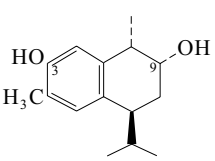
(S)-form
Constit. of *Humulus lupulus* (hops). Oil.

3-Methoxy: ***3-Methoxy-9,10-dihydrocadalene***
$C_{16}H_{22}O$ 230.349
Oil. $[\alpha]_D$ -54.9 (c, 0.69 in $CHCl_3$).

(±)-form
Bp_9 125-126°.

Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2088
Adachi, K. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 651 (*synth*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1986, **39**, 103 (*deriv*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1994, 3277; 1995, 3111 (*biosynth*)

3,9-Calamenenediol C-33



(7α,9α,10α)-*form*

$C_{15}H_{22}O_2$ 234.338

(7α,9α,10α)-form

9-Angeloyl: [72943-95-4]
$C_{20}H_{28}O_3$ 316.439
Oil. $[\alpha]_D^{24}$ +21.7 (c, 4.4 in $CHCl_3$).

9-Angeloyl, 3-Me ether: [72943-96-5]
$C_{21}H_{30}O_3$ 330.466
Oil.

9-Ketone: [155662-80-9] ***3-Hydroxy-9-calamenenone***. *7-Hydroxy-2-calamenenone*
$C_{15}H_{20}O_2$ 232.322
Constit. of *Gossypium hirsutum* (cotton).

(7β,10α)-form

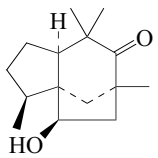
9-Ketone: [155662-81-0]
Constit. of *Gossypium hirsutum* (cotton).

Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1185
Davila-Huerta, G. *et al., Phytochemistry*, 1995, **39**, 531 (*isol, pmr, cmr, ketone*)

Calamensesquiterpinenol C-34

[156158-90-6]

10-Hydroxy-2,6,6,8-tetramethyltricyclo[6.2.1.0^{1,5}]undecan-7-one. Calamenone



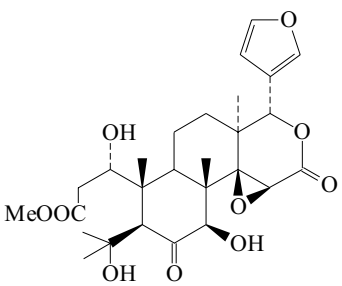
$C_{15}H_{24}O_2$ 236.353

Constit. of the roots of *Acorus calamus* (sweet flag).

Wu, L.J. *et al., CA*, 1994, **121**, 78242s (*isol*)
Wu, L.J. *et al., Yakugaku Zasshi*, 1994, **114**, 182-185 (*isol, struct*)

Calamin C-35

[74751-40-9]



$C_{27}H_{36}O_{10}$ 520.575

Constit. of calamondin seeds (*Citrus reticulata*). Cryst. (MeOH). Mp 162-165°.

Bennett, R.D. *et al., Tetrahedron*, 1981, **37**, 17

Calcium acetate C-36

[62-54-4]

Acetic acid, calcium salt, 8CI. Ethanoic acid, calcium salt. E263

$Ca(OAc)_2$

$C_4H_6CaO_4$ 158.167

Used in foods as a firming agent, acidity regulator, sequestrant, stabiliser and thickener, and nutrient supplement (Ca source). Used as an acidifier/preservative in bread, and in some gelling mixtures. Hygroscopic white powder. V. sol. H_2O (37 g per 100 cm^3 at 0°; 30 g per 100 cm^3 at 100°); spar. sol. EtOH. ΔH_f° -1479 kJ mol^{-1}. Hygroscopic. Dec. on heating to form CaO.

▶ AF7525000

Monohydrate: [5743-26-0]

$C_4H_8CaO_5$ 176.182

Colourless cryst. Dec. on heating → CaO. V. sol. (44 g per 100 cm^3 at 0°; 34 g per 100 cm^3 at 100°); spar. sol. EtOH. ΔH_f° -1772 kJ mol^{-1}.

▶ AF7875000

Dihydrate:

$C_4H_{10}CaO_6$ 194.197

Colourless cryst. Dec. on heating with H_2O loss (-H_2O at 84°) and ultimate formation of CaO. V. sol. H_2O (35 g per 100 cm^3 at 20°; 34 g per 100 cm^3 at 80°); spar. sol. EtOH.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1275D (*ir*)
Rubinshtein, A.M. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1958, **121**, 664 (*thermal dec*)
Walter-Levy, L. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 3320 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 982 (*rev, bibl*)
Stoilova, D. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1976, **9**, 371 (*ir, monohydrate*)
Chill, J. *et al., Thermochim. Acta*, 1980, **40**, 251 (*thermal dec, tga, ms, monohydrate*)
Balimann, G.E. *et al., Philos. Trans. R. Soc. London, A*, 1981, **299**, 643 (*cmr*)
Mu, J. *et al., Thermochim. Acta*, 1981, **49**, 207 (*thermal dec*)
Jagannathan, N.R. *et al., Indian J. Pure Appl. Phys.*, 1984, **22**, 484 (*pmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 665C (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 368-369
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAL750

Calcium bromate C-37

[10102-75-7]

[10235-01-5]

$Ca(BrO_3)_2$

Br_2CaO_6 295.882

Dough conditioner.

Tkachuk, R. *et al., Cereal Chem.*, 1961, **38**, 393-398 (*use*)
Kamman, P.W. *et al., Baker's Dig.*, 1984, **58**, 18-20 (*use*)
Alici, E. *et al., Z. Anorg. Allg. Chem.*, 1992, **608**, 135-144 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 371-372 (*props, use*)

Calcium carbonate, BAN, USAN C-38

[471-34-1]

[3983-19-5, 15187-75-4]

Carbonic acid, calcium salt, 8CI. Chalk. Limestone. E170

$CaCO_3$

$CCaO_3$ 100.087

Used in foods as a neutraliser and leavening agent. Hygroscopic colourless cryst. Prac. insol. H_2O. Mp 1339° (at 1.35 atm). Dec. on heating with loss of CO_2. Dissolves in acids → corresp. calcium salt.

▶ OES: long-term 10 mg/m^3 (total inhalable dust); 4 mg/m^3 (respirable dust). Skin and eye irritant. LD_{50} (rat, orl) 6450 mg/kg. FF9335000

[1317-65-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1271C (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 861 (*rev, bibl*)
Ross, S.D. *et al., Spectrochim. Acta*, 1964, **20**, 781 (*ir*)
Porto, S.P.S. *et al., Phys. Rev.*, 1966, **147**, 608 (*Raman*)
Goldsmith, J.A. *et al., Spectrochim. Acta*, 1966, **22**, 1069 (*ir*)
Langille, D.B. *et al., J. Phys. Chem. Solids*, 1977, **38**, 1149 (*ir, Raman*)
Kummer, P. *et al., Handb. Fillers Reinf. Plast.*, 1978, 81 (*rev, uses*)
Brown, A. *et al., J. Geol. Educ.*, 1980, **28**, 92 (*rev, ir*)
Arai, Y. *et al., Gypsum Lime*, 1981, **170**, 25 (*rev, struct*)
Orwoll, E.S. *et al., Ann. Intern. Med.*, 1982, **97**, 242 (*pharmacol*)
Carr, F.P. *et al., Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley*, 1991, **4**, 796 (*manuf, use*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 52-55
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 373-376; 1580-1581
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1182
Proctor and Hughes' Chemical Hazards of the Workplace, 4th edn., (eds. Hathaway, G.J. et al), Van Nostrand Reinhold, 1996, 102
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, CAO000

Calcium chloride ($CaCl_2$), 8CI C-39

[10043-52-4]

Calcium chloride. Calcium dichloride. E509

$CaCl_2$

$CaCl_2$ 110.983

Orthorhombic. Essentially a distorted rutile-type struct.. Used as a postharvest dip to reduce decay in apples and berries. Added to food as an anticaking agent, curing or pickling agent, firming agent, flavour enhancer, antimrobial, humectant, nutrient supplement, pH control agent, processing aid, stabiliser and thickener, surface active agent, synergist or texturiser. Deliquescent colourless, cubic cryst. V. sol. H_2O (74.5 g per 100 cm^3 at 20°; 159 g per 100 cm^3 at 100°); sol. EtOH, Me_2CO, AcOH. Mp 782°. Bp 1600°. ΔH_f° -796 kJ mol^{-1}. ΔG_f° -748 kJ mol^{-1}. S° 105 J K^{-1} mol^{-1}.

▶ Irritant. EV9800000

Mineral-*form*

Hydrophilite

May be identical to Antarctite or Sinjarite.

Monohydrate: [13477-29-7]

$CaCl_2H_2O$ 128.999

Colourless deliquescent cryst. Dec. on heating with loss of H_2O. V. sol. H_2O (77 g per 100 cm^3 at 0°; 249 g per 100 cm^3 at 100°); sol. EtOH; insol. Me_2CO. ΔH_f° -1109 kJ mol^{-1}; ΔG_f° -1101 kJ mol^{-1}.

▶ Irritant.

Dihydrate: [10035-04-8] ***Sinjarite***

$CaCl_2H_4O_2$ 147.014

Hygroscopic colourless cryst. Dec. on heating with loss of H_2O. V. sol. H_2O (98 g per 100 cm^3 at 0°; 326 g per 100 cm^3 at 60°). V. sol. EtOH (50 g per 100 cm^3 at 80°). ΔH_f° -1403 kJ mol^{-1}.

▶ Irritant. EV9810000

Tetrahydrate: [25094-02-4]

$CaCl_2H_8O_4$ 183.044

Colourless triclinic cryst. Dec. on heating with loss of H_2O. ΔH_f° -2010 kJ mol^{-1}; ΔG_f° -1724 kJ mol^{-1}; S° 213 J K^{-1} mol^{-1}. Struct. comprises $[CaCl_2.4H_2O]_2$ units held together by H-bonds.

▶ Irritant.

Hexahydrate: See Calcium chloride ($CaCl_2$) hexahydrate in *The Combined*

Chemical Dictionary.
Van Bever, A.K. *et al., Z. Kristallogr.*, 1935, **90**, 374 (*cryst struct*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 28, 1957, **B2**, 431; 468; 470 (*rev, bibl*)
Paul, R.C. *et al., J. Indian Chem. Soc.*, 1964, **41**, 541 (*soly*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 104 (*uses*)
Buzagh-Gere, E. *et al., Z. Anorg. Allg. Chem.*, 1973, **400**, 37 (*therm dec, dihydrate*)
Malhotra, K.C. *et al., J. Inorg. Nucl. Chem.*, 1974, **36**, 3767 (*soly*)
Dust, H. *et al., Ullmanns Encykl. Tech. Chem., 4. Aufl.*, 1975, **9**, 81 (*rev, uses*)
Hadenfeldt, C. *et al., Z. Naturforsch., B*, 1975, **30**, 165 (*synth*)
Buzagh-Gere, E. *et al., J. Therm. Anal.*, 1976, **10**, 89 (*therm dec, tetrahydrate*)
Leclaire, A. *et al., Acta Cryst. B*, 1978, **34**, 900; 1980, **36**, 2757 (*polymorphs, tetrahydrate*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **4**, 432 (*rev, uses*)
Vincent, C.A. *et al., Solubility Data Ser.*, 1980, **11**, 74; 140; 240 (*soly*)
Scrosati, B. *et al., Solubility Data Ser.*, 1980, **11**, 296; 337 (*soly*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 693 (*thermochem data*)
Meisingset, K.K. *et al., J. Chem. Thermodyn.*, 1986, **18**, 159 (*thermodyn, phases, tetrahydrate*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 666A; 666B (*haz*)
Garcia, J.M. *et al., J. Agric. Food Chem.*, 1996, **44**, 30-33 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 378-381
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAO750

Calcium diphosphate ($Ca_2P_2O_7$) C-40

[7790-76-3]

[10086-45-0]

Calcium diphosphate. Calcium pyrophosphate ($Ca_2P_2O_7$). Dicalcium pyrophosphate

$Ca_2P_2O_7$

$Ca_2O_7P_2$ 254.099

The dicalcium salt of Diphosphoric acid. Trimorphic, with low temp. (γ, β) and high temp. (α) forms, each metastable at r.t.. Used in foods as a nutrient supplement and pH control agent.

Dihydrate: [17031-92-4]
Cryst. V. insol. H_2O. Triclinic: both Ca atoms are heptacoordinate. Monoclinic and orthorhombic forms also reported.

Tetrahydrate: [17031-93-5]
Colourless tablets. V. insol. H_2O. Monoclinic: both Ca atoms are heptacoordinate with two independent coord. polyhedra. V. nearly eclipsed anion conform..

α-*form*
Monoclinic. Both $Ca^{2\oplus}$ cations are octacoordinate. Anion is in eclipsed form with POP 130°, P–O(t) 151 pm, P–O(bridge) 160 pm.Mp 1352°.

β-*form*
Tetragonal with eclipsed anion conformation for each of two independent POP groups with POP 131°, 138°. Mean P–O(t) 151.8, P–O(bridge) 161.5 pm. Four crystallographically independent $Ca^{2\oplus}$ ions per unit cell having coordination numbers 7 (2 x), 8 (1 x), and 9 (1 x).Yields α-form at 1150-1200°.

γ-*form* At 750-900°, yields β-form.

[17031-92-4, 21349-09-7]

Brown, E.H. *et al., J. Agric. Food Chem.*, 1963, **11**, 214 (*synth*)
Webb, N.C. *et al., Acta Cryst.*, 1966, **21**, 942 (*cryst struct*)
Hezel, A. *et al., Spectrochim. Acta A*, 1967, **23**, 1583 (*ir*)
Steger, E. *et al., Z. Anorg. Allg. Chem.*, 1967, **355**, 131 (*ir*)
Calvo, C. *et al., Inorg. Chem.*, 1968, **7**, 1345 (*cryst struct*)
Mandel, N.S. *et al., Acta Cryst. B*, 1975, **31**, 1730 (*cryst struct*)
Cornilsen, B.C. *et al., J. Inorg. Nucl. Chem.*, 1979, **41**, 602 (*ir, Raman*)
Ann. Rheum. Dis., Suppl. 1, *Proc. Symp. on Crystal-Related Arthropathies* Ed., Dieppe, P., 1983, **42**,
Cornilsen, B.C. *et al., J. Mol. Struct.*, 1984, **117**, 1 (*ir, Raman*)
Davis, N.L. *et al., J. Crystallogr. Spectrosc. Res.*, 1985, **15**, 513 (*cryst struct*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Prabhakar, S. *et al., Chem. Phys. Lett.*, 1987, **139**, 96 (*P-31 nmr*)
Mandel, G.S. *et al., J. Cryst. Growth*, 1988, **87**, 453 (*struct, morphology*)
Schneider, M. *et al., Z. Anorg. Allg. Chem.*, 1989, **576**, 267 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 384-386
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAW450

Calcium hydrogen sulfite C-41

[13780-03-5]

Sulfurous acid calcium salt (2:1). Calcium bisulfite. E227

$Ca(HSO_3)_2$

$CaH_2O_6S_2$ 202.222

Obt. from a soln. of $CaSO_3$ in an aq. soln. of SO_2. Preservative.

Ger. Pat., 1935, 623 181; *CA*, **30**, 2332 (*manuf*)
Simon, A. *et al., Naturwissenschaften*, 1958, **45**, 128 (*Raman*)

Calcium hydroxide ($Ca(OH)_2$), 8CI, INN, USAN C-42

[1305-62-0]

Calcium hydrate. Hydrated lime. Lime water. Slaked lime. E526

$Ca(OH)_2$

CaH_2O_2 74.093

Has CdI_2 struct.. Used in foods as a buffer and firming agent. Colourless hexagonal cryst. Spar. sol. H_2O (0.185 g per 100 cm^3 at 0°; 0.077 g per 100 cm^3 at 100°); insol. EtOH. ΔH_f° -986 kJ mol^{-1}; ΔG_f° -898 kJ mol^{-1}; S° 83.4 J K^{-1} mol^{-1}. Dec. on heating with loss of H_2O. Dissolves in acids to form the corresp. calcium salt. Reacts with atmospheric CO_2 to form $CaCO_3$.

▶ OES: long-term 5 mg/m^3. Corrosive. Severe eye irritant. Respiratory and skin irritant. LD_{50} (rat, orl) 7340 mg/kg. EW2800000

Mineral-*form* [12177-68-3]
Portlandite

Rumpf, E. *et al., Ann. Phys. (Leipzig)*, 1928, **87**, 595 (*cryst struct*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 28, 1961, **B2**, 299 (*rev, bibl*)
Kamisuki, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1345 (*ir*)
Dawson, P. *et al., Solid State Commun.*, 1972, **10**, 41 (*Raman*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, 926 (*synth*)
Holuj, F. *et al., Can. J. Phys.*, 1977, **55**, 654 (*pmr*)
Shpynova, L.G. *et al., Kristallografiya*, 1980, **25**, 967 (*cryst struct, isomorph substitution*)
Ryskin, Ya.I. *et al., CA*, 1981, **94**, 216877 (*ir, Raman*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 704 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 667B (*haz*)
Foreman, P.C. *et al., Int. Endod. J.*, 1990, **23**, 283 (*rev*)
Milosevic, A. *et al., J. Dent. Res.*, 1991, **19**, 3 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1347
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 390-391
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 133
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAT225
Pierce, J.O. *et al., Patty's Ind. Hyg. Toxicol.*, 4th edn., Vol. 2, Wiley, 1993, **2A**, 762 (*tox*)

Calcium hydroxide phosphate ($Ca_5(OH)(PO_4)_3$), 9CI, 8CI C-43

[12167-74-7]

Calcium hydroxide phosphate. Pentacalcium hydroxide triphosphate

$Ca_5(OH)(PO_4)_3$

$Ca_5HO_{13}P_3$ 502.311

V. variable H_2O content with several hydrates (1,2,3,4, and 8 H_2O) claimed. Table salt additive to ensure free-running qualities. Clear, colourless hexagonal cryst. Stable at temps. up to 900°; at higher temps. phosphates e.g. B –Ca_3. Prac. insol. H_2O. (< 0.001 g per 100 cm^3 at 25°). Dissolves in acids.

Mineral-*form* [1306-06-5]
Hydroxyapatite. *Hydroxylapatite. Alveograf. Durapatite. Periograf. Ossopan. Win 40350*
Exists in a variety of cryst. shapes and colours.

[62974-97-4, 72855-61-9, 97329-12-9, 97329-13-0, 97329-14-1, 97329-16-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1267C (*ir*)
Dana's System of Mineralogy, 7th Ed., Wiley N.Y., 1951, 879
Gmelin Handbook Inorg. Chem., *Syst. No.* 28, 1961, **B3**, 1142 (*rev, bibl*)
Lerch, P. *et al., Bull. Soc. Chim. Fr.*, 1968, 1705 (*synth*)
Sudersanan, K. *et al., Acta Chem. Scand.*, 1969, **25**, 1534 (*cryst struct*)
Blakeslee, K.C. *et al., J. Am. Ceram. Soc.*, 1971, **54**, 559 (*ir, Raman*)
Elliott, J.C. *et al., Nature (London)*, 1971, **230**, 72 (*monoclinic-form*)

Fowler, B.O. *et al., Inorg. Chem.*, 1974, **13**, 194; 207 (*synth, ir*)
Young, R.A. *et al., Colloq. Int. C.N.R.S.*, 1975, **230**, 21 (*struct, rev*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 530 (*synth*)
Iqbal, Z. *et al., J. Phys. Chem. Solids*, 1977, **38**, 923 (*ir, Raman*)
Shimabayashi, S. *et al., CA*, 1978, **88**, 163126 (*thermal dec*)
Monma, H. *et al., CA*, 1979, **91**, 48718 (*thermal dec*)
Arends, J. *et al., J. Cryst. Growth*, 1979, **46**, 213; 1987, **84**, 515 (*synth, ir, em*)
Rothwell, W.P. *et al., J.A.C.S.*, 1980, **102**, 2637 (*P-31 nmr*)
Christoffersen, J. *et al., Calcif. Tissue Int.*, 1981, **33**, 557 (*dissoln kinetics*)
Bigi, A. *et al., J. Inorg. Biochem.*, 1981, **15**, 317 (*ir, props*)
Nelson, D.G.A. *et al., Aust. J. Chem.*, 1982, **35**, 715 (*ir, Raman*)
Young, R.A. *et al., Calcif. Tissue Int.*, (Suppl. 2), 1982, **34**, 17 (*synth, ir, bibl*)
Chander, S. *et al., Colloids Surf.*, 1982, **4**, 101 (*dental use*)
Nelson, D.G.A. *et al., J. Ultrastruct. Res.*, 1983, **84**, 1 (*em*)
Pritzkow, W. *et al., Cryst. Res. Technol.*, 1985, **20**, 957 (*synth, cryst struct*)
Dykman, A.S. *et al., Zh. Prikl. Khim. (Leningrad)*, 1986, **59**, 2251; *J. Appl. Chem. USSR (Engl. Transl.)*, 1986, **59**, 2068 (*struct, props*)
Yesinowski, Y.P. *et al., J.A.C.S.*, 1987, **109**, 6274 (*pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAW120

Calcium iodate(*V*) ($Ca(IO_3)_2$) C-44

[7789-80-2]
Iodic acid calcium salt, 8CI. Calcium iodate. Lautarite

$Ca(IO_3)_2$

CaI_2O_6 389.883

Food additive used to enhance poultry and egg production. Oxidiser in bread manuf.. Colourless monoclinic cryst. Spar. sol. H_2O (0.20 g per 100 cm^3 at 15°, 0.67 g per 100 cm^3 at 90°); insol. EtOH. ΔH_f° -1003 kJ mol^{-1}; ΔG_f° -893 kJ mol^{-1}; S° 230 JK^{-1} mol^{-1}. Dec. on heating with loss of I_2 and O_2 forming $Ca_5(IO_6)_2$ at 540-680° and CaO at 700-840°.

►Oxidiser, irritant.

Mineral-*form*
Lautarite
Colourless, yellowish, short prismatic cryst.

Monohydrate: [10031-32-0]
Dec. on heating with H_2O loss. ΔH_f° -1293 kJ mol^{-1}.

Hexahydrate: [10031-33-1] *Hexaaquacalcium diiodate*
Colourless orthorhombic cryst.; dec. on heating with H_2O loss. Spar. sol. H_2O (0.13 g per 100 cm^3 at 0°, 1.2 g per 100 cm^3 at 100°). ΔH_f° -2781 kJ mol^{-1}; ΔG_f° -2268 kJ mol^{-1}; S° 452 J K^{-1} mol^{-1}.

Rocchiccioli, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 1232 (*ir*)
Gmelin Handbook Inorg. Chem., System No. 28, 1961, **B2**, 629; 632; 634 (*rev, bibl, anhydr, hydrates*)
Cinga, M.B. *et al., Acta Cryst.*, 1967, **23**, 1114 (*cryst struct, hexahydrate*)
Bousquet, J. *et al., Bull. Soc. Chim. Fr.*, 1969, 1111 (*soly*)
Sanyal, G.S. *et al., J. Inorg. Nucl. Chem.*, 1977, **39**, 1127 (*thermal dec, anhydr, monohydrate*)
Ghose, S. *et al., Acta Cryst. B*, 1978, **34**, 84 (*cryst struct*)
Shishkin, V.A. *et al., J. Mol. Struct.*, 1982, **83**, 349 (*I-127 nqr, monohydrate*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 392-394 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAT500

Calcium metasilicate ($CaSiO_3$) C-45

[1344-95-2]

[10101-39-0]
Silicic acid calcium salt, 12CI. Calcium metasilicate. Calcium silicate ($CaSiO_3$). C.I. Pigment White 28

$CaSiO_3$

CaO_3Si 116.162

There are 3 normal modifications and a high-pressure modification. The terms α-$CaSiO_3$ and β-$CaSiO_3$ are used ambiguously in the lit. and should be avoided. A hydrous or anhydrous Ca silicate with varying proportions of CaO and SiO_2 is used as an anticaking agent in foodstuffs. Aldrich: 37266-8.

►VV9170000

Mineral-*form* [13983-17-0]
Wollastonite. *Wollastonite-1T. Wollastonite-Tc*
Triclinic low-temp. modification. A chain silicate. Polymorphic.White to greyish cryst. Undergoes a transition to pseudowollastonite above 1125°.

►ZC9750000

Mineral-*form* [14567-51-2]
Parawollastonite. *Wollastonite-2M*
A monoclinic form of wollastonite: related by a simple stacking modification.White or grey cryst.

Mineral-*form* [14567-52-3]
Pseudowollastonite. *Cyclowollastonite*
The high-temp. modification. A ring silicate. Polymorphic.Triclinic transparent colourless cryst. Mp 1544°.

[14404-64-9]

Buerger, M.J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1961, **47**, 1883 (*cryst struct, wollastonite*)
Trojer, F. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1969, **130**, 185 (*cryst struct, high pressure phase*)
Rutstein, M.S. *et al., Am. Mineral.*, 1971, **56**, 877 (*ir*)
Ohashi, Y. *et al., Am. Mineral.*, 1978, **63**, 274 (*cryst struct, wollastonite*)
Deer, W.A. *et al., Rock Forming Minerals*, 2nd edn., Longman, 1978, **2A**, 545 (*rev*)
Yamanaka, T. *et al., Acta Cryst. B*, 1981, **37**, 1010 (*cryst struct, pseudowollastonite*)
Henmi, C. *et al., Am. Mineral.*, 1983, **68**, 156 (*polymorphs, wollastonite*)
Magi, M. *et al., J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)
Hesse, K.-F. *et al., Z. Kristallogr.*, 1984, **168**, 93 (*cryst struct, parawollastonite*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 421-423
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, WCJ000

Calcium oxide (CaO), 8CI C-46

[1305-78-8]
Calcium oxide. Calcium monoxide. Burnt lime. Calcia. Calx. Quicklime. Unslaked lime. E529

CaO

CaO 56.077

NaCl struct. type. Used in food as a pH control agent, nutrient supplement, dough conditioner, and texturising, firming and anticaking agent. Colourless cubic cryst. Mp 2927°. ΔH_f° -635.1 kJ mol^{-1}; ΔG_f° -603.5 kJ mol^{-1}; S° 38.2 J K^{-1} mol^{-1}. Moisture sensitive. Dissolves in $H_2O \rightarrow Ca(OH)_2$; dissolves in acids. Reacts with atmospheric H_2O to form $Ca(OH)_2$ which reacts further with CO_2 to form $CaCO_3$; crude samples of CaO often contain large quantities of $Ca(OH)_2$ and $CaCO_3$.

►Irritant. EW3100000

Mineral-*form*
Lime
Colourless cryst.

[8006-28-8]

Primak, W. *et al., J.A.C.S.*, 1948, **70**, 2043 (*cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1957, **B2**, 278 (*rev, bibl*)
Riboud, P. *et al., Circ. Inf. Tech. -Cent. Doc. Sider.*, 1979, **36**, 559; *CA*, **91**, 94883 (*rev, desulfurisation*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 711 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 669B (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 399-400
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAU500

Calcium oxide silicate ($Ca_3O(SiO_4)$), 10CI C-47

[12168-85-3]

[12141-48-9]
Calcium oxide silicate. Tricalcium silicate. Alite. Basic calcium silicate. C_3S

$Ca_3O(SiO_4)$

Ca_3O_5Si 228.316

Three triclinic, two monoclinic and orthorhombic forms exist. Anticaking agent for table salt. Mp 2150°.

Steinour, H.H. *et al., Chem. Rev.*, 1947, **40**, 391 (*rev*)
Lea, F.M. *et al., The Chemistry of Cement and Concrete*, 3rd Edn., Edward Arnold, London, 1970,
Johansen, V. *et al., Cem. Concr. Res.*, 1972, **2**, 33 (*synth*)
Singh, N.B. *et al., J. Sci. Ind. Res.*, 1976, **35**, 75 (*cryst struct, polymorphs, rev*)
Handke, M. *et al., Ann. Chim. (Paris)*, 1979, **4**, 145 (*ir, Raman*)
Magi, M. *et al., J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2825

Calcium peroxide (CaO_2), 8CI C-48

[1305-79-9]

Calcium peroxide. Perme Ox. Trapzene

$Ca(O_2)$

CaO_2 72.077

CaC_2 struct. Not known in pure state. Coml. product contains up to 75% CaO_2, mixed with CaO, $Ca(OH)_2$, and $CaCO_3$. Flour additive; bleaching agent. White tetragonal cryst. Spar. sol. H_2O. ΔH_f° -653 kJ mol^{-1} (298K). Dissoc. on heating >400° → CaO + O_2; dissolves in H_2O → $Ca(OH)_2$ + H_2O_2 + O_2. Does not melt but dec. 7300°, >400° on heating.

▶ Oxidiser. EW3865000

Octahydrate: [60762-59-6] White cryst. (H_2O). ΔH_f° -3011 kJ mol^{-1} (298K). Thermal dehyd. yields anhyd. CaO_2.

Compd. with hydrogen peroxide (1:2): [12133-34-5]
CaH_4O_6 140.106
White cryst. Reacts. with CO_2 → $CaCO_3$ + H_2O + O_2; thermal dec. yields $Ca(O_2)_2$.

[64544-82-7]

Reisenfeld, E.H. *et al., Z. Anorg. Allg. Chem.*, 1914, **89**, 405 (*synth*)
Kotov, V. *et al., Russ. J. Phys. Chem. (Engl. Transl.)*, 1941, **15**, 1057
Rossini, F.D. *et al., Natl. Bur. Stand. Circ. (U.S.)*, *No.* 500, 1952, 386 (*enthalpy data*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 28, 1957, 318 (*rev, bibl*)
Grigor'eva, N.K. *et al., CA*, 1964, **60**, 14098f; 1967, **66**, 121576p (*synth, props*)
Allamagny, P. *et al., Rev. Chim. Miner.*, 1965, **2**, 645 (*prepn, cryst struct, magnetism, decomp*)
Emons, H.H. *et al., Z. Chem.*, 1965, **5**, 230; 272 (*synth, reactions, H_2O_2 complex*)
Tsentsiper, A.B. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1967, 2563 (*thermal dehyd, octahydrate*)
Blunt, F.J. *et al., Chem. Comm.*, 1969, 278 (*Raman*)
Dubois, D.K. *et al., Baker's Dig.*, 1974, **48**, 40; 59 (*use*)
Eysel, H.H. *et al., Z. Anorg. Allg. Chem.*, 1975, **411**, 97 (*Raman*)
Ballou, E. *et al., Ind. Eng. Chem. Prod. Res. Dev.*, 1977, **16**, 180 (*thermal dec, H_2O_2 complex*)
Ballou, E. *et al., J. Eng. Ind.*, 1978, **100**, 26 (*thermal dec, H_2O_2 complex*)
Brunere, V. *et al., CA*, 1979, **90**, 129714y (*uv-vis*)
Azuma, Y. *et al., Gypsum Lime*, 1979, **162**, 175 (*thermal dec*)
Japan. Pat., 1989, 89 262 713; *CA*, **112**, 174090a (*use*)
Merck Index, 11th edn., 1989, 1696
Ino, K. *et al., Gypsum Lime*, 1990, **224**, 47 (*use*)
Tieckelman, R.E. *et al., Food Technol. (Chicago)*, 1991, **45(1)**, 106 (*dough*)
U.S. Pat., 1991, 5 019 289; *CA*, **115**, 116850z (*use, bleaching agent*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 405-406 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAV500

Calcium phosphate ($Ca(H_2PO_4)_2$) C-49

[7758-23-8]

[10103-46-5]

Calcium phosphate (1:2), 9CI, 8CI. Calcium phosphate†. Calcium bis(dihydrogen phosphate). Monocalcium phosphate

$Ca(H_2PO_4)_2$

$CaH_4O_8P_2$ 234.052

Added to flour as a nutrient source and leavening agent; stabiliser and thickener for fruit jellies, preserves and jams; also used in foods as pH control agent, firming agent, sequestrant and dietary supplement.

▶ TB8527000

Monohydrate: [10031-30-8] Large white shining plates (H_3PO_4). Triclinic. $CaPO_4$ sheets are held together by H_2PO_4 ions and H_2O molecules. Non-equivalent PO_4 groups. Ca ions are 8-coord. When heated, loses $0.5H_2O$ at 170°, and further $0.5H_2O$ at 280°. Structural H_2O lost at 320°, and 430°. Also loses H_2O on grinding.

▶ TB8530000

Tetrahydrate:

[15221-07-5]

Inorg. Synth., 1953, **4**, 18 (*synth*)
Jones, D.W. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1961, **116**, 101 (*ir, cryst struct*)
Berry, E.E. *et al., Spectrochim. Acta A*, 1968, **24**, 1727 (*ir*)
Pechkovskii, V.V. *et al., Zh. Neorg. Khim.*, 1969, **14**, 53; 1979, **24**, 894; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 27; 1979, **24**, 497 (*synth, ir, props*)
Dickens, B. *et al., Acta Cryst. B*, 1971, **27**, 2247; 1973, **29**, 2057 (*cryst struct*)
Schroeder, L.W. *et al., Acta Cryst. B*, 1975, **31**, 9 (*nd, struct*)
Fichter, M. *et al., Spectrochim. Acta B*, 1975, **30**, 417
Pyldme, M. *et al., J. Therm. Anal.*, 1979, **17**, 479 (*props*)
Bertoluzza, A. *et al., J. Raman Spectrosc.*, 1983, **14**, 178 (*props*)
Bertoluzza, A. *et al., J. Mol. Struct.*, 1985, **127**, 35 (*ir, Raman, struct*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Nebelung, A.O. *et al., Sprechsaal*, 1986, **119**, 566 (*props*)
Belton, P.S. *et al., J. Phys. Chem. Solids*, 1988, **49**, 21 (*P-31 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 409-414
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAW110

Calcium phosphate ($Ca(HPO_4)$) C-50

[7757-93-9]

[10103-46-5]

Calcium phosphate (1:1), 9CI, 8CI. Calcium phosphate. Calcium monohydrogen phosphate

$CaHPO_4$

$CaHO_4P$ 136.057

Triclinic lattice. Ca ions coordinated to 7 oxygens (pentagonal pyramid) or to 8 oxygens. Used in foods as a leavening agent, stabiliser and thickener, nutrient, pH control agent, masticatory substance, moisture control agent, emulsifier, and appearance control agent for colours and colour modifiers. White cryst. ΔH_f° -1821 kJ mol^{-1}; ΔG_f° -1680 kJ mol^{-1}; S° 88 J K^{-1} mol^{-1}.

Monohydrate: When shaken with H_2O, → dihydrate → $CaHPO_4$.

1.5-Hydrate: [33849-87-5] At 165° → anhydrous salt.

Dihydrate: [7789-77-7] White cryst. Only slowly sol. H_2O at < 100°. Mp 36°. Monoclinic lattice. Loses H_2O on grinding. ΔH_f° -2410 kJ mol^{-1}; ΔG_f° -2153 kJ mol^{-1}; S° 167 J K^{-1} mol^{-1}.

Mineral-*form* [21063-37-6]
Monetite
Essentially the anhyd. compd. Triclinic lattice.Pale yellowish white translucent cryst., usually flattened with rhombohedral outline.

Mineral-*form* [14567-92-1]
Brushite
Essentially the dihydrate. Monoclinic lattice.Colourless to pale yellow, transparent to translucent cryst., with vitreous lustre.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1268A (*ir*)
Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1951, 660; 704
Inorg. Synth., 1953, **4**, 19 (*synth*)
Petrov, I. *et al., Spectrochim. Acta A*, 1967, **23**, 2637 (*ir*)
Mattingly, G.E.G. *et al., Top. Phosphorus Chem.*, 1967, **4**, 157 (*rev, bibl*)
Francis, M.D. *et al., Calcif. Tissue Res.*, 1971, **6**, 335 (*struct*)
Duff, E.J. *et al., J. Appl. Chem. Biotechnol.*, 1971, **21**, 233 (*synth, props*)
Curry, N.A. *et al., J.C.S.(A)*, 1971, 3725 (*nd, struct*)
Dickens, B. *et al., Acta Cryst. B*, 1972, **28**, 797 (*cryst struct*)
Termine, J.D. *et al., Calcif. Tissue Res.*, 1974, **15**, 55 (*ir, Raman*)
Catti, M. *et al., Acta Cryst. B*, 1977, **33**, 1223; 1980, **36**, 254 (*cryst struct, nd*)
Casciani, F. *et al., J. Solid State Chem.*, 1980, **34**, 385 (*ir, Raman*)
Ohta, M. *et al., J. Cryst. Growth*, 1982, **56**, 562 (*synth, morphology*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Nebelung, A.O. *et al., Sprechsaal*, 1986, **119**, 566 (*use, bioceramics*)
Yesinowski, J.P. *et al., J.A.C.S.*, 1987, **109**, 6274 (*pmr*)
Belton, P.S. *et al., J. Phys. Chem. Solids*, 1988, **49**, 21 (*P-31 nmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 56-60
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1176
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 406-409
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAT210; CAW100

Calcium phosphate ($Ca_3(PO_4)_2$) C-51

[7758-87-4]

[10103-46-5]

Calcium phosphate (3:2), 9CI, 8CI. Calcium phosphate†. Calcium orthophosphate. Bone ash. Bone phosphate of lime. BPL. FEMA 3081

$Ca_3(PO_4)_2$

$Ca_3O_8P_2$ 310.177

There is controversy over the existence of a solid amorphous form. It may be a unique compd. which readily converts to hydroxyapatite or it may be a mixt. of hydroxyapatite and brushite or monetite. Component of flour bleaching mixtures, anticaking agent, dietary supplement, flavouring ingredient. Insol. H_2O (2×10^{-3} g per 100 cm^3 at 25°). ΔH_f° -4121 kJ mol^{-1}; ΔG_f° -3885 kJ mol^{-1}; S° 236 J K^{-1} mol^{-1}.

α-form

High temp.-form

Monoclinic lattice. Struct. consists of columns of cations, and columns of cations + anions with compensating cation vacancies.Mp 1720°. Stable between 1120-1470°.

β-form

Low-temp.-form

Rhombohedral lattice struct. similar to that of α-form except that no cation-cation columns here; a 'tighter' struct. than that of the α-form. Contains 5 distinct $Ca^{2\oplus}$ ions with coord. nos. 6, 7, 8, 8, and 9.Stable below 1120° but in the presence of traces of $M^{2\oplus}$ stabilised to *ca* 1350°. Exists until near r.t. in absence of moisture. Replacement of $Mg^{2\oplus}$ by $Ca^{2\oplus}$ hinders thermal conversion to α-form. Mp 1730°.

[28961-50-4, 64644-52-6]

Eanes, E.D. *et al., Calcif. Tissue Res.*, 1970, **5**, 133 (*props, synth*)
Blumenthal, N.C. *et al., Mater. Res. Bull.*, 1972, **7**, 1181 (*synth, ir*)
Dickens, B. *et al., J. Solid State Chem.*, 1974, **10**, 232 (*struct, synth, β-form*)
Mathew, M. *et al., Acta Cryst. B*, 1977, **33**, 1325 (*cryst struct, α-form*)
Momma, H. *et al., J. Mater. Sci.*, 1980, **15**, 2428 (*synth, props*)
Bigi, A. *et al., J. Inorg. Biochem.*, 1981, **15**, 317 (*props*)
Metsger, D.S. *et al., J. Am. Dent. Assoc.*, 1982, **105**, 1035 (*props, use*)
Akao, M. *et al., J. Mater. Sci.*, 1982, **17**, 343 (*synth, tox*)
Bertoluzza, A. *et al., J. Raman Spectrosc.*, 1983, **14**, 178 (*synth, ir, Raman*)
Tropp, J. *et al., J.A.C.S.*, 1983, **105**, 22 (*P-31 nmr, identity*)
Bonel, G. *et al., J. Phys., Colloq. C*, 1984, **8**, 325 (*rev, structs, ir*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Nebelung, A.O. *et al., Sprechsaal*, 1986, **119**, 566; 1131 (*synth, bioceramics*)
Dykman, A.S. *et al., Zh. Prikl. Khim. (Leningrad)*, 1986, **59**, 2251; *J. Appl. Chem. USSR (Engl. Transl.)*, 1986, **59**, 2068 (*synth*)
Mortier, A. *et al., Thermochim. Acta*, 1987, **113**, 133 (*synth*)
Belton, P.S. *et al., J. Phys. Chem. Solids*, 1988, **49**, 21 (*P-31 nmr*)
Lopatin, S.I. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1989, **25**, 645; *Inorg. Mater. (Engl. Transl.)*, 1989, **25**, 556 (*ms*)
Jakeman, R.J.B. *et al., J. Solid State Chem.*, 1989, **78**, 23 (*P-31 nmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 61-62
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 764
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1176
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 414-417

Calcium phosphinate, 9CI, 8CI C-52

[7789-79-9]

Calcium hypophosphite

$Ca(H_2PO_2)_2$

$CaH_4O_4P_2$ 170.055

Dietary supplement. Monoclinic cryst. (Me_2CO aq.).

Morgunova, E.M. *et al., Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1660; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1602
Myers, K. *et al., J. Phys. Chem.*, 1972, **76**, 3975
Brun, G. *et al., Rev. Chim. Miner.*, 1972, **9**, 581 (*synth, cryst struct*)
Fichter, M. *et al., Spectrochim. Acta B*, 1972, **30**, 417
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 392
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAT250

Calcium silicate (Ca_2SiO_4) C-53

[10034-77-2]

[14981-10-3]

Calcium silicate. Belite. Dicalcium orthosilicate. E552

Ca_2SiO_4

Ca_2O_4Si 172.239

There are 4 principal polymorphs ($\alpha,\alpha',\beta,\gamma$). Anticaking agent.

[1344-95-2, 1344-96-3, 15630-58-7, 17830-10-3, 18536-02-2]

Steinour, H.H. *et al., Chem. Rev.*, 1947, **40**, 391 (*rev*)
Smith, D.K. *et al., Acta Cryst.*, 1965, **18**, 787 (*cryst struct*)
Eysel, W. *et al., Z. Kristallogr.*, 1970, **131**, 322 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 163 (*rev*)
Handke, M. *et al., J. Mol. Struct.*, 1982, **79**, 353 (*ir, Raman*)
Magi, M. *et al., J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)
Barbier, J. *et al., Acta Cryst. B*, 1985, **41**, 383 (*cryst struct*)

Calcium sulfate C-54

[7778-18-9]

[23296-15-3]

Sulfuric acid calcium salt, 8CI. Calcined gypsum. E516

$CaSO_4$

CaO_4S 136.142

Used in foods as an anticaking agent, colouring adjunct, dough strengthener, drying agent, firming agent, formulation aid, leavening agent, nutrient supplement, pH control agent, processing aid, stabiliser, thickener, synergist and texturiser; also used as an additive in the bleaching of flour by benzoyl peroxide. Colourless cryst. Dissolves in acids. Spar. sol. H_2O (0.209 g per 100 cm^3 at 30°; 0.162 g per 100 cm^3 at 100°). Mp 1570°. ΔH_f° -1434 kJ mol^{-1}; ΔG_f° -1322 kJ mol^{-1}; S° 107 J K^{-1} mol^{-1}.

► WS6920000

Hemihydrate: See Calcium sulfate ($CaSO_4$) hemihydrate in *The Combined Chemical Dictionary.*

Dihydrate: See Calcium sulfate dihydrate in *The Combined Chemical Dictionary.*

α-form

Form-I

High temp. form; cubic.

β-form [14798-04-0]

*Form-II. **Anhydrite***

Orthorhombic r.t.-form.White to grey, blue, pink or brownish cryst. Transforms to α-form at 1200°.

γ-form

Form-III

Unstable r.t. modification.

Rossini, F.D. *et al., Natl. Bur. Stand. Circ. (U.S.)*, No. 500, 1952, 390 (*thermochem data*)
Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, No. 539, 1955, **4**, 65 (*cryst struct*)
Krishnan, T.S. *et al., J. Indian Inst. Sci., Sect. A*, 1956, **38**, 207 (*Raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 28, 1961, **B3**, 679 (*rev, bibl*)
Swift, W.M. *et al., ERDA Rept. No.*, ANL-76-122, 1976, ; *CA*, 1977, **87**, 170062 (*rev, thermal dec*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **4**, 437 (*rev, uses*)
Murat, M. *et al., CA*, 1979, **90**, 64553 (*rev, struct*)
Reshetnyak, N.B. *et al., CA*, 1979, **90**, 112525 (*Raman*)
Sunta, C.M. *et al., Radiat. Prot. Dosim.*, 1984, **8**, 25 (*thermoluminescence*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 66-68
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1683
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 427-431
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAX500

Calcium sulfite, 9CI C-55

[10257-55-3]

Sulfurous acid calcium salt. E226

$CaSO_3$

CaO_3S 120.142

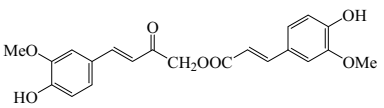
Two modifications known. Preservative. Cryst.

Hemihydrate: [29501-28-8] Cryst. Exists in 3 modifications. Loses H_2O of cryst. at 300-380°.

Schroepfer, L. *et al., Z. Anorg. Allg. Chem.*, 1973, **401**, 1-14 (*cryst struct, ir*)
Lutz, H.D. *et al., Z. Anorg. Allg. Chem.*, 1976, **425**, 134-144 (*synth, ir, Raman*)
Arai, Y. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 738-741 (*synth, cryst struct, phases*)

Harrison, W.D. *et al., Polyhedron*, 1983, **2**, 153-156 (*synth, ir*)

Calebin A C-56



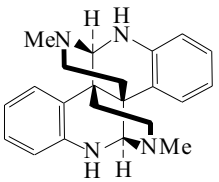
$C_{21}H_{20}O_7$ 384.385

Constit. of the rhizomes of *Cucuma longa* (turmeric). Pale yellow powder. Mp 138-139°. λ_{max} 219 (log ϵ 3.42); 240 (log ϵ 3.44); 339 (log ϵ 3.73) (MeOH).

Kim, D.S.H.L. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 2541-2543 (*synth*)

Park, S.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1227-1231 (*isol, pmr, cmr, ms*)

Calycanthine, 9CI C-57



(+)-*form*

$C_{22}H_{26}N_4$ 346.474

(+)-*form* [595-05-1]

Alkaloid from *Calycanthus floridus* (Carolina allspice) and other *Calycanthus* spp.. Mp 250-251° (anhyd.). $[\alpha]_D$ +684.

Hydrobromide (1:2):

Mp 213-214°.

(-)-*form* [85548-42-1]

Mp 245°. $[\alpha]_D^{25}$ -570 (MeOH).

(±)-*form* [16739-56-3]

Mp 253-258°.

***meso*-form**

Mp 265-268°.

Woodward, R.B. *et al., Proc. Chem. Soc., London*, 1960, 76 (*struct*)

Hamor, T.A. *et al., J.C.S.*, 1962, 194 (*cryst struct*)

Hendrikson, J.B. *et al., Tetrahedron*, 1964, **20**, 565 (*synth, ms, pmr, uv*)

Hall, E.S. *et al., Tetrahedron*, 1967, **23**, 4131 (*synth, ir, uv, ms, pmr*)

Beecham, A.F. *et al., Nature (London), Phys. Sci.*, 1973, **244**, 30 (*config*)

Tokuyama, T. *et al., Tetrahedron*, 1983, **39**, 41 (*isol*)

Adjibade, Y. *et al., Phytochemistry*, 1992, **31**, 317 (*isol, uv, ir, pmr, cmr, ms*)

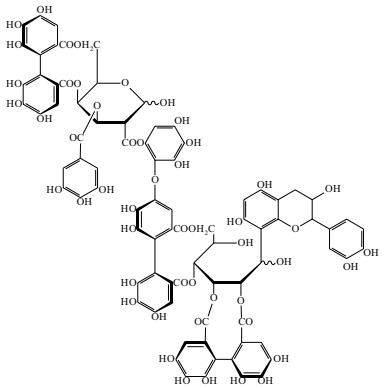
Link, J.T. *et al., J.A.C.S.*, 1996, **118**, 8166 (*synth*)

Arteaga de Garcia, L. *et al., Rev. Colomb. Quim.*, 1997, **26**, 55-57; *CA*, **128**, 110442q (*activity*)

Verotta, L. *et al., J. Nat. Prod.*, 1998, **61**, 392-396 (*isol, pmr, cd*)

Overman, L.E. *et al., J.A.C.S.*, 1999, **121**, 7702-7703 (*synth*)

Camellianin D C-58



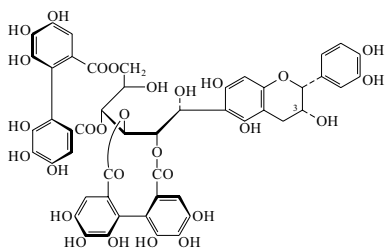
$C_{83}H_{62}O_{50}$ 1859.373

Exists as an equilibrated mixt. of α- and β-anomers. Tannin constit. of *Camellia japonica*.

Okuda, T. *et al., Heterocycles*, 1990, **30**, 1195 (*struct*)

Camelliatannin C C-59

[154524-52-4]



$C_{49}H_{38}O_{28}$ 1074.822

Constit. of the leaves of *Camellia japonica*. Off-white powder + $7H_2O$. $[\alpha]_D$ +119 (c, 1.6 in MeOH). λ_{max} 207 (ϵ 95500); 230 (sh) (ϵ 61660) (MeOH).

3-Epimer: [172723-29-4] ***Stachyuranin B***

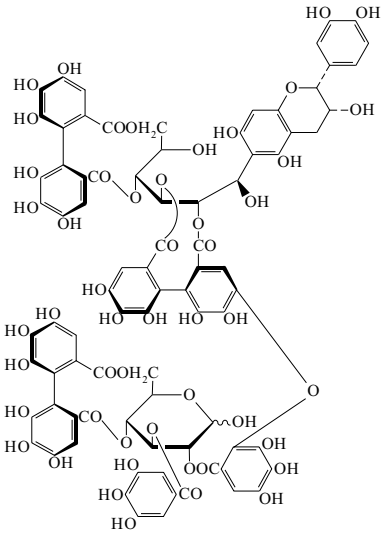
$C_{49}H_{38}O_{28}$ 1074.822

Off-white powder + $8H_2O$. $[\alpha]_D$ +120 (c, 1 in MeOH). λ_{max} 207 (ϵ 93320); 230 (sh) (ϵ 66070); 260 (sh) (ϵ 33880) (MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1629; 2109 (*isol, pmr, cmr*)

Camelliatannin D C-60

[148159-87-9]



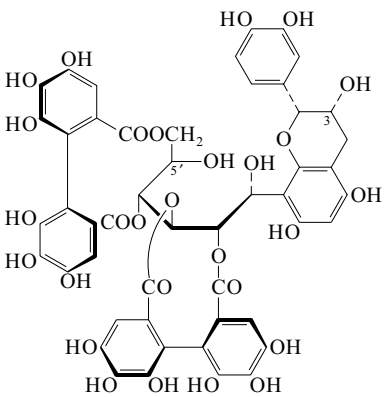
$C_{83}H_{62}O_{50}$ 1859.373

Constit. of the leaves of *Camellia japonica*. Off-white powder + $12H_2O$. $[\alpha]_D$ +46 (c, 0.9 in MeOH). λ_{max} 207 (ϵ 208930); 280 (sh) (ϵ 67610) (MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1995, **43**, 2033 (*isol, struct*)

Camelliatannin E C-61

[148132-92-7]



$C_{49}H_{38}O_{28}$ 1074.822

Constit. of the leaves of *Camellia japonica*. Off-white powder + $6H_2O$. $[\alpha]_D$ +53 (c, 1 in MeOH). λ_{max} 208 (ϵ 97720); 231 (sh) (ϵ 67610); 260 (sh) (ϵ 35480) (MeOH).

*3-Epimer, 5′-*O*-(3,4,5-trihydroxybenzoyl):*

[172617-79-7] ***Stachyuranin A***

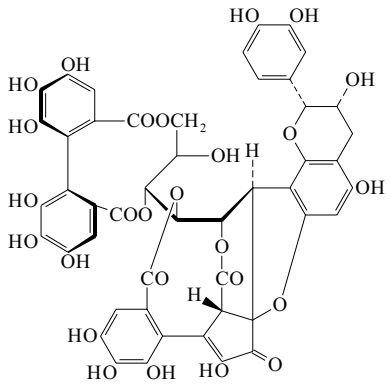
$C_{56}H_{42}O_{32}$ 1226.929

Off-white powder + $7H_2O$. $[\alpha]_D$ -15 (c, 1 in MeOH). λ_{max} 209 (ϵ 109650); 231 (sh) (ϵ 72440); 265 (sh) (ϵ 36310) (MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1629; 2109 (*isol, uv, cd, pmr, cmr*)

Camelliatannin F C-62

[154561-15-6]



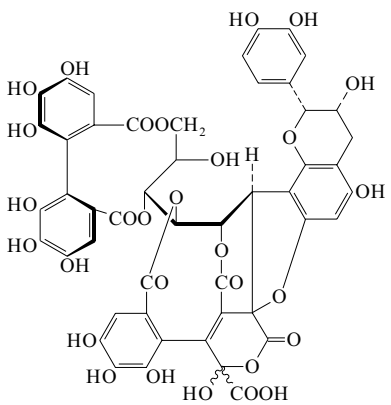
$C_{48}H_{34}O_{26}$ 1026.781

Constit. of the leaves of *Camellia japonica*. Off-white amorph. powder + $4H_2O$. $[\alpha]_D$ -89 (c, 1.6 in MeOH). λ_{max} 209 (ϵ 89125); 230 (sh) (ϵ 58884); 265 (ϵ 31622) (MeOH).

Han, L. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1399 (*isol, uv, cd, pmr, cmr*)

Camelliatannin G C-63

[154524-53-5]



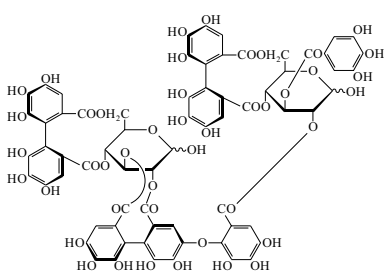
$C_{49}H_{34}O_{29}$ 1086.79

Constit. of the leaves of *Camellia japonica*. Pale yellow amorph. powder + $7H_2O$. $[\alpha]_D$ -245 (c, 1 in MeOH). λ_{max} 213 (ϵ 79430); 234 (sh) (ϵ 57540); 282 (sh) (ϵ 17380) (MeOH).

Han, L. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1398 (*isol, uv, cd, pmr, cmr*)

Camelliatannin H C-64

[148159-86-8]



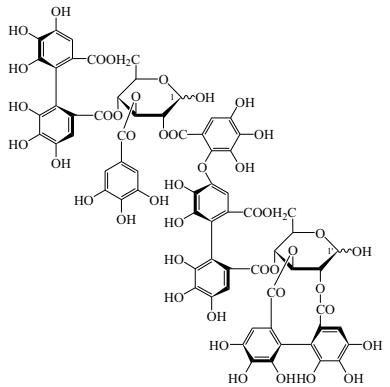
$C_{68}H_{48}O_{44}$ 1569.101

Constit. of the leaves of *Camellia japonica*. Off-white amorph. powder + $8H_2O$. $[\alpha]_D$ +90 (c, 1 in MeOH). λ_{max} 218 (ϵ 100000); 258 (sh) (ϵ 51290); 278 (sh) (ϵ 42660) (MeOH).

Han, L. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1398 (*isol, uv, cd, pmr, cmr*)

Camelliin A C-65

[132731-66-9]



$C_{68}H_{48}O_{44}$ 1569.101

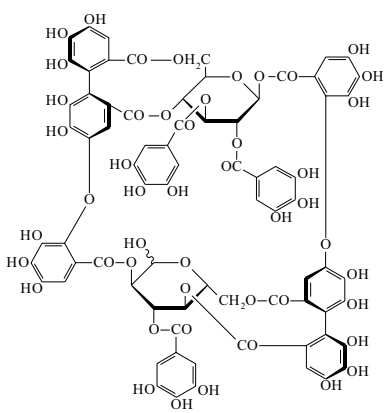
Exists as an equilibrated mixt. of α- and β-anomers. Isol. from the flower buds of *Camellia japonica* and *Camellia sasanqua*. Light brown amorph. powder + $10H_2O$. $[\alpha]_D^{20}$ +53 (c, 0.5 in MeOH).

1-O-(3,4,5-Trihydroxybenzoyl)(1β-):
[159935-08-7] ***Camellioferin A***
$C_{75}H_{52}O_{48}$ 1721.207
Constit. of *Camellia oleifera*. Light brown powder. $[\alpha]_D$ +67 (c, 1 in MeOH).

Yoshida, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2681 (*struct, cd, pmr, cmr*)
Yoshida, T. *et al., Phytochemistry*, 1994, **37**, 241 (*Camellioferin A*)

Camelliin B C-66

[126347-60-2]



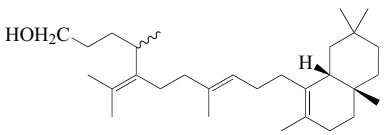
$C_{75}H_{52}O_{48}$ 1721.207

Exists as an equilibrated mixt. of α- and β-anomers (4:1). Isol. from the flower buds of *Camellia japonica* and *Camellia sasanqua*. Off-white amorph. powder + $15H_2O$. $[\alpha]_D^{20}$ -24 (c, 0.8 in MeOH). λ_{max} 224 (ϵ 115000); 276 (ϵ 60000) (MeOH) (Berdy).

Yoshida, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3174; 1990, **38**, 1211; 2681; 1991, **39**, 2247 (*isol, uv, cd, pmr, cmr, pharmacol*)

Camelliol B C-67

[220359-72-8]



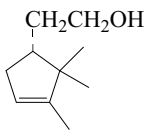
$C_{30}H_{52}O$ 428.74

Constit. of sasanqua oil (*Camellia sasanqua*). Gum. $[\alpha]_D^{25}$ +1.7 (c, 0.4 in $CHCl_3$). Related to Achilleol B, A-102.

Akihisa, T. *et al., J. Nat. Prod.*, 1999, **62**, 265-268 (*isol, pmr, cmr*)

Campholenic alcohol C-68

[1901-38-8]
2,2,3-Trimethyl-3-cyclopentene-1-ethanol, 9CI. FEMA 3741



(R)-form

$C_{10}H_{18}O$ 154.252

(R)-form [52437-39-5]
Bp_{21} 119-121° $Bp_{0.47}$ 65°. $[\alpha]_D^{20}$ +5.4 (c, 2.06 in $CHCl_3$). n_D^{28} 1.4708.

Ac: [52486-39-2]
$Bp_{0.46}$ 65°. $[\alpha]_D^{20}$ -2.1 (neat). n_D^{28} 1.4511.

Aldehyde: [4501-58-0]
Constit. of many essential oils of *Juniperus*, *Eucalyptus* and *Thymus* spp.. $Bp_{12.8}$ 83°. $[\alpha]_D^{20}$ +9.6 (neat).

(S)-form [36789-58-9]
Bp_8 150°. n_D 1.4710.

Ac:
Bp_8 104-106°. n_D^{20} 1.4564.

Aldehyde: [23727-15-3]
$Bp_{12.8}$ 83°. $[\alpha]_D^{22.5}$ -3.7 (neat). n_D 1.4645.

(ξ)-form
Constit. of *Juniperus communis* (juniper). Flavouring ingredient. Oil. $Bp_{0.6}$ 74-76°. $[\alpha]_D$ -1.5 (c, 8 in CCl_4). n_D 1.4736. The opt. rotns. of this isolate and its derivs were too small to allow reliable assignment of abs. config..

Ac: [36789-59-0] *FEMA 3657*
$C_{12}H_{20}O_2$ 196.289
Flavouring ingredient. Constit. of *Juniperus communis* (juniper). Oil with a sweet woody odour. Bp_5 96-97°. $[\alpha]_D$ -1 (c, 8 in CCl_4).

Aldehyde:2,2,3-Trimethyl-3-cyclopenten-1-ylacetaldehyde. ***Campholenic aldehyde.*** *FEMA 3592*
$C_{10}H_{16}O$ 152.236
Flavouring ingredient. Found in *Juniperus communis* (juniper). Oil. d^{20} 0.92.

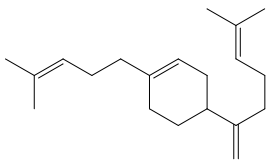
Bp_{10} 77°. $[\alpha]_D^{20}$ -3.1 (CCl_4). Cas no. refers to the (*R*)-enantiomer.

Aldehyde, 3,4-epoxide: [36789-60-3] *1,2,2-Trimethyl-6-oxabicyclo[3.1.0]hexane-3-acetaldehyde, 9CI.* ***Epoxycampholenic aldehyde***
$C_{10}H_{16}O_2$ 168.235
Constit. of *Juniperus communis* (juniper). Oil. Bp_{10} 101-102°. $[\alpha]_D^{20}$ -0.83 ($CHCl_3$). Assigned *trans*-config. of epoxide ring relative to – CH_2CHO group.

Thomas, A.F. *et al., Helv. Chim. Acta*, 1972, **55**, 815-817 (*isol, Ac, aldehyde, aldehyde epoxide*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 102-103; 772
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 433-434; 2842-2843

α-Camphorene C-69

[532-87-6]
4-(5-Methyl-1-methylene-4-hexenyl)-1-(4-methyl-3-pentenyl)cyclohexene, 9CI. Paracamphorene. p-*Camphorene. Dimyrcene*

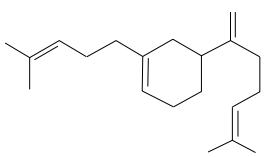


$C_{20}H_{32}$ 272.473
Constit. of *Humulus lupulus* (hops) and *Cymbopogon citratus* (West Indian lemongrass). Oil. $Bp_{0.03}$ 110°.

Lammens, H. *et al., Bull. Soc. Chim. Belg.*, 1968, **77**, 497 (*isol*)
Eisfelder, W. *et al., Annalen*, 1977, 988 (*synth*)
Teresa, J. de P. *et al., An. Quim.*, 1978, **74**, 305 (*synth*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1986, **63**, 507 (*synth*)

γ-Camphorene C-70

[20016-73-3]
m-*Camphorene. Metacamphorene*



$C_{20}H_{32}$ 272.473
Constit. of *Humulus lupulus* (hop). Oil. $Bp_{4.5}$ 176-178°.

Lammens, H. *et al., Bull. Soc. Chim. Belg.*, 1968, **77**, 497

Canavalmine C-71

[70862-15-6]
N,N″-*1,3-Propanediylbis[1,4-butanediamine]. 1,13-Diamino-5,9-diazatridecane*
$H_2N(CH_2)_4NH(CH_2)_3NH(CH_2)_4NH_2$
$C_{11}H_{28}N_4$ 216.369
Isol. from the seeds of *Canavalia gladiata* (sword bean). Viscous oil. $Bp_{0.01}$ 135-140°.

N′-*(3-Aminopropyl):* [129225-31-6] **N′-*(3-Aminopropyl)canavalmine*.** *1,17-Diamino-4,9,13-triazaheptadecane*
$C_{14}H_{35}N_5$ 273.464
Isol. from *Canavalia gladiata* (sword bean).

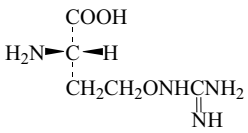
N′-*(4-Aminobutyl):* [129225-32-7] **N′-*(4-Aminobutyl)canavalmine*.** *1,18-Diamino-5,9,14-triazaoctadecane*
$C_{15}H_{37}N_5$ 287.491
Isol. from *Canavalia gladiata* (sword bean).

[107886-53-3, 107886-65-7]

Fujihara, S. *et al., Biochem. Biophys. Res. Commun.*, 1982, **107**, 403 (*isol, synth, ir*)
Aikens, D. *et al., Biophys. Chem.*, 1983, **17**, 67 (*cmr*)
Samejima, K. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3428 (*synth*)
Niitsu, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1032 (*deriv*)
Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1311 (*derivs*)
Schwesinger, R. *et al., Chem. Ber.*, 1994, **127**, 2435 (*synth, pmr*)

Canavanine C-72

O-*[(Aminoiminomethyl)amino]homoserine, 9CI. 2-Amino-4-(guanidinooxy)butanoic acid*



(*S*)-*form*

$C_5H_{12}N_4O_3$ 176.175

(*S*)-*form* [543-38-4]
L-*form*
Stored in large quantities in the seeds of leguminous plants in three subfamilies. Isol. originally from Jackbean (*Canavalia ensiformis*). Cryst. (EtOH). Sol. H_2O. Mp 184°. $[\alpha]_D^{20}$ +7.9 (H_2O). Pharmacol. active enantiomer.
▶ LD_{50} (rat, scu) 5900 mg/kg. ES7002000

Sulfate: [2219-31-0]
Cryst. (EtOH). Mp 172° dec.

Tribenzoyl:
Mp 86° dec.

Picrate:
Mp 163-164°.

(±)-*form* [13269-28-8]
Mp 180-182°. pK_{a1} 2.5; pK_{a2} 6.6; pK_{a3} 9.25 (25°).

Hydrochloride:
Mp 190°.

Hydrochloride (1:2):
Very hygroscopic solid.

Bell, A. *et al., Biochem. J.*, 1960, **75**, 618 (*occur*)
Nakatsu, S. *et al., CA*, 1963, **58**, 752 (*occur*)
Yamada, Y. *et al., Agric. Biol. Chem.*, 1973, **37**, 2201 (*synth*)
Rosenthal, G.A. *et al., Anal. Biochem.*, 1976, **77**, 147 (*isol*)
Rosenthal, G.A. *et al., Q. Rev. Biol.*, 1977, **52**, 155 (*rev*)
Boyar, A. *et al., J.A.C.S.*, 1982, **104**, 1995 (*cryst struct*)
Rosenthal, G.A. *et al., Phytochemistry*, 1991, **30**, 1055 (*biol props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 12026
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKD500

Caneine C-73

$C_{12}H_{24}N_2O_3$ 244.333
Struct. unknown. Constit. of *Canavalia ensiformis* seeds (jack bean). Lustrous needles. Mp 188-189°. Opt. inactive.

Picrate:
Pale yellow needles. Mp 120-121°.

Ackermann, D. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1939, **262**, 103 (*isol*)

Cannagunines C-74

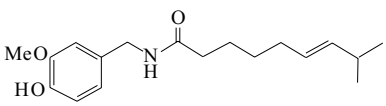
These compounds are erroneous. Claimed alkaloids from fruit of *Vaccinium oxycoccus* (small cranberries).

[35214-92-7, 50906-97-3, 50906-98-4]

Jankowski, K. *et al., Experientia*, 1971, **27**, 1141-1143

Capsaicin C-75

[404-86-4]
N-*[(4-Hydroxy-3-methoxyphenyl)-methyl]-8-methyl-6-nonenamide, 9CI. Natural capsaicin. Axsain. Capsacutin. Capsaiene. Mioton. Zostrix. FEMA 3404*



$C_{18}H_{27}NO_3$ 305.416
Flavouring ingredient. Pungent principle of various *Capsicum* spp. (Solanaceae). Cryst. with a burning pungent taste. Mp 64-65°. $Bp_{0.01}$ 210-220°. Log P 3.5 (uncertain value) (calc). Commercially available Capsaicin is usually the more readily prepd. *n*-nonanoyl analogue (Pseudocapsaicin) λ_{max} (solvent not reported) (Derep). λ_{max} 227 (ε 7000); 281 (ε 2500) (EtOH) (Derep). λ_{max} 227 (ε 7000); 281 (ε 2500) (MeOH) (Berdy).
▶ Skin and mucous membrane irritant. LD_{50} (mus, orl) 47.2 mg/kg. RA8530000

Dihydro: [19408-84-5] ***Dihydrocapsaicin***
$C_{18}H_{29}NO_3$ 307.432
Potential nutriceutical. Cryst. Mp 65.5-65.8°.

(Z)-isomer: [25775-90-0] ***Zucapsaicin, INN, USAN***
Cryst. (Et_2O/hexane). Mp 68.5-69.5°.

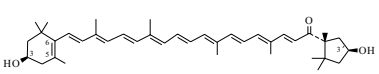
[7553-53-9]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1378C (*nmr*)
Crombie, L. *et al., J.C.S.*, 1955, 1025 (*synth*)
Kosuge, S. *et al., CA*, 1963, **59**, 6724; 1964, **60**, 9827 (*Dihydrocapsaicin*)
Leete, E. *et al., J.A.C.S.*, 1968, **90**, 6837 (*biosynth*)
Bowman, W.R. *et al., Chem. Comm.*, 1969, 1075 (*biosynth*)
Rangoonwala, R. *et al., Pharmazie*, 1969, **24**, 177 (*biosynth*)
Jeso, I. *et al., Chem. Zvesti*, 1975, **29**, 714 (*synth*)
Virus, R.M. *et al., Life Sci.*, 1979, **25**, 1273 (*rev, props*)

Monsereenusorn, Y. *et al., Crit. Rev. Toxicol.*, 1982, **10**, 321 (*rev, props*)
Suzuki, T. *et al., Alkaloids (London)*, 1983, **23**, 227 (*rev*)
Merck Index, 10th edn., 1983, No. 1741
Kaga, H. *et al., J.O.C.*, 1989, **54**, 3477 (*synth, bibl*)
Fuller, R.W. *et al., Arch. Int. Pharmacodyn. Ther.*, 1990, **303**, 147 (*rev, pharmacol*)
Maggi, C.A. *et al., Arch. Int. Pharmacodyn. Ther.*, 1990, **303**, 157 (*pharmacol*)
Kaga, H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 946 (*synth*)
Cordell, G.A. *et al., Ann. Pharmacother.*, 1993, **27**, 330 (*rev*)
Janusz, J.M. *et al., J. Med. Chem.*, 1993, **36**, 2595 (*synth, pharmacol, zucapsaicin*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 756
Kirby, G.W. *et al., Phytochemistry*, 1994, **36**, 185 (*purifn, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 364
Surh, Y.-J. *et al., Life Sci.*, 1995, **56**, 1845 (*rev, tox, metab*)
Fusco, B.M. *et al., Drugs*, 1997, **53**, 909-914 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1374-1375
David, W.I.F. *et al., Chem. Comm.*, 1998, 931-932 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBF750

Capsanthin C-76

[465-42-9]
3,3′-Dihydroxy-β,κ-caroten-6′-one



$C_{40}H_{56}O_3$ 584.881
Constit. of paprika (*Capsicum annuum*) and asparagus (*Asparagus officinalis*). Potential nutriceutical. Red cryst. (petrol). Mp 175-176°. $[\alpha]_{643.8}$ +36 ($CHCl_3$).

3′-Ketone: [28368-01-6] ***Capsanthone***. *3-Hydroxy-β,κ-carotene-3′,6′-dione. Capsanthinone. Ketocapsanthin*
$C_{40}H_{54}O_3$ 582.865
Red rhombs (MeOH aq.). Mp 167°. Identity of Ketocapsanthin not certain.

5α,6α-Epoxide: [29486-21-3] ***Capsanthin 5,6-epoxide***. *5,6-Epoxy-5,6-dihydro-3,3′-dihydroxy-β,κ-caroten-6′-one. Capsanthin monoepoxide*
$C_{40}H_{56}O_4$ 600.88
Constit. of red paprika (*Capsicum annuum*). Red needles. Mp 177-178°. $[\alpha]_D$ +9.4 (C_6H_6).

3-Deoxy: [7044-42-0] ***Cryptocapsin***. *3′-Hydroxy-β,κ-caroten-6′-one. Kryptocapsin*
$C_{40}H_{56}O_2$ 568.881
Constit. of paprika (*Capsicum annuum*). Violet metallic cryst. (EtOAc). Mp 172-174° (160-161°). λ_{max} 486 (ε 112000); 520 (ε 87000) (no solvent reported).

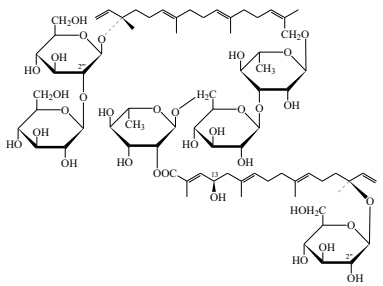
9Z-Isomer, 5α,6α-epoxide: [373386-94-8] ***(9Z)-Capsanthin-5,6-epoxide***
$C_{40}H_{56}O_4$ 600.88
Dark red cryst. (C_6H_6/hexane). Mp 108-110°. λ_{max} 358 (log ε 4.16); 475 (log ε 4.97); 505 (log ε 4.87) (C_6H_6).

[87801-05-6]

Karrer, P. *et al., Carotenoids*, Elsevier, 1950, 240-251 (*rev*)
Barber, M.S. *et al., J.C.S.*, 1961, 4019-4024 (*struct, synth*)
Cholnoky, L. *et al., Tet. Lett.*, 1963, 1257-1259 (*Cryptocapsin, struct*)
Faigle, J.W. *et al., Helv. Chim. Acta*, 1964, **47**, 741-745 (*config*)
De Ville, T.E. *et al., Chem. Comm.*, 1969, 1311-1312 (*abs config*)
De La Mar, R.R. *et al., J. Food Sci.*, 1969, **34**, 287-290 (*Ketocapsanthin*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527-2544 (*abs config*)
Ueda, I. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1974, **140**, 190-217 (*cryst struct*)
Neamtu, G. *et al., CA*, 1979, **93**, 41684q (*occur, Capsanthone*)
Rüttimann, A. *et al., Helv. Chim. Acta*, 1983, **66**, 1939-1958 (*isol, synth, uv, ir, pmr, ms*)
Bowden, R.D. *et al., J.C.S. Perkin 1*, 1983, 1465-1474 (*abs config, synth*)
Parkes, K.E.B. *et al., Tet. Lett.*, 1986, **27**, 2535-2538 (*isol, epoxide*)
Molnár, P. *et al., J. Nat. Prod.*, 2001, **64**, 1254-1255 (*9Z-Capsanthin-5,6-epoxide*)

Capsianoside A C-77

[116107-40-5]
Capsianside A



$C_{76}H_{124}O_{33}$ 1565.796
Struct. revised in 1990. Constit. of fruits of *Capsicum annuum*. Amorph. powder. $[\alpha]_D$ -25.1 (MeOH).

2″-O-β-D-Glucopyranoside: [121940-51-0] ***Capsianoside C***. *Capsianside C*
$C_{82}H_{134}O_{38}$ 1727.938
Constit. of fruits of *Capsicum annuum*. Powder. $[\alpha]_D^{20}$ -21 (c, 0.5 in MeOH).

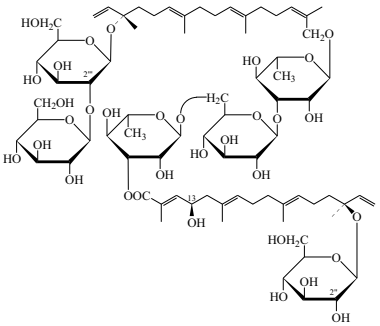
2‴-O-Deglucosyl: ***Capsianoside G***. *Capsianside G*
$C_{70}H_{114}O_{28}$ 1403.654
Constit. of *Capsicum annuum*. Powder. $[\alpha]_D^{20}$ -24.2 (c, 1 in MeOH).

13-Deoxy, 2″-O-β-D-glucopyranoside: [121924-09-2] ***Capsianoside E***. *Capsianside E*
$C_{82}H_{134}O_{37}$ 1711.938
Constit. of fruits of *Capsicum annuum*. Powder. $[\alpha]_D^{19}$ -21.9 (c, 1 in MeOH).

Izumitani, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1299-1307; 1991, **39**, 3258-3260 (*isol, ir, pmr, cmr, ms*)

Capsianoside B C-78

[121924-07-0]
Capsianside B



$C_{76}H_{124}O_{33}$ 1565.796
Constit. of the fruit of *Capsicum annuum*. Powder. $[\alpha]_D^{20}$ -18 (c, 0.7 in MeOH).

2″-O-β-D-Glucopyranosyl: [121924-08-1] ***Capsianoside D***. *Capsianside D*
$C_{82}H_{134}O_{38}$ 1727.938
Constit. of the fruit of *Capsicum annuum*. Powder. $[\alpha]_D^{20}$ -19.9 (c, 0.7 in MeOH).

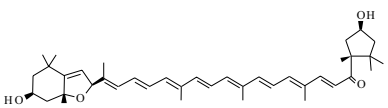
13-Deoxy, 2″-O-β-D-glucopyranosyl: ***Capsianoside F***. *Capsianside F*
$C_{82}H_{134}O_{37}$ 1711.938
Constit. of the fruit of *Capsicum annuum*. Powder. $[\alpha]_D^{19}$ -22.7 (c, 0.6 in MeOH).

2‴-O-Deglucosyl: ***Capsianoside H***. *Capsianside H*
$C_{70}H_{114}O_{28}$ 1403.654
Constit. of *Capsicum annuum*. Powder. $[\alpha]_D^{20}$ -22 (c, 1 in MeOH).

Izumitani, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1299-1307; 1991, **39**, 3258-3260 (*isol, ir, pmr, cmr, ms*)

Capsochrome C-79

[104012-89-7]
5,8-Epoxy-5,8-dihydro-3,3′-dihydroxy-β,κ-caroten-6′-one

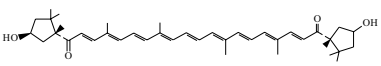


$C_{40}H_{56}O_4$ 600.88
Constit. of red paprika (*Capsicum annuum*). Yellow needles (C_6H_6/petrol). Mp 180-182° (195°).

Karrer, P. *et al., Helv. Chim. Acta*, 1945, **28**, 1143
Parkes, K.F.B. *et al., Tet. Lett.*, 1986, **27**, 2535

Capsorubin C-80

[470-38-2]
3,3′-Dihydroxy-κ,κ-carotene-6,6′-dione. E160



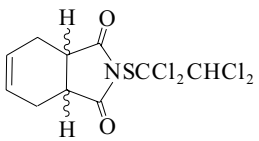
$C_{40}H_{56}O_4$ 600.88
Constit. of paprika (*Capsicum annuum*). Potential nutriceutical. Violet-red plates (petrol). Mp 201°. λ_{max} 468 ; 503 ; 542 (CS_2).

Diketone: [25494-49-9] κ,κ-*Carotene-3,3′,6,6′-tetrone. Capsorubone. Capsorubinidione*
$C_{40}H_{52}O_4$ 596.848
Prod. of oxidn. of pigments from paprika. Black cryst. (C_6H_6/MeOH). Mp 217° (209-210°). λ_{max} 301 ; 378 ; 451 ; 476 ; 510 (hexane).

Barber, M.S. *et al., J.C.S.*, 1961, 4019 (*struct*)
Faigle, J.W. *et al., Helv. Chim. Acta*, 1964, **47**, 741 (*config, pmr*)
Weedon, B.C.L. *et al., Pure Appl. Chem.*, 1973, **35**, 113 (*synth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Rüttimann, A. *et al., Helv. Chim. Acta*, 1983, **66**, 1939 (*synth*)
Lóránd, T. *et al., Helv. Chim. Acta*, 2002, **85**, 1691-1697 (*ir*)

Captafol, ANSI, BSI, ISO C-81

[2425-06-1]
*3a,4,7,7a-Tetrahydro-2-[(1,1,2,2-tetrachloroethyl)thio]-1*H*-isoindole-1,3(2*H*)-dione, 9CI.* N-*(1,1,2,2-Tetrachloroethylthio)-4-cyclohexene-1,2-dicarboximide, 8CI. Tetrachloroethylthiotetrahydrophthalimide. Difolatan, JMAF. Alfloc. Arborseal. Folcid. Foltaf. Haipen 50. Nalco 7046. Proxel EF*



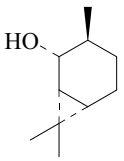
$C_{10}H_9Cl_4NO_2S$ 349.063
Nonsystemic foliar agricultural fungicide, esp. for potatoes. Cryst. Mp 160-161°. Low acute tox.
▶ Skin irritant. Can cause contact dermatitis. OES: long-term 0.1 mg m^{-3} (Sk).
GW4900000

[2939-80-2]

Thomas, W.D. *et al., Phytopathology*, 1962, **52**, 754 (*activity*)
Belg. Pat., 1963, 633 205; *CA*, **60**, 15789c (*synth*)
Etter, G.E. *et al., CA*, 1968, **64**, 66388p (*rev*)
Schuphan, W. *et al., CA*, 1969, **71**, 21121w (*rev*)
Ripley, B.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 1084; 1365
IARC Monog., 1991, **53**, 353 (*rev, tox*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A56
Pesticide Manual, 11th edn., 1997, No. 104
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1415
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBF800

2-Caranol, 8CI C-82

3,7,7-Trimethylbicyclo[4.1.0]heptan-2-ol, 9CI. 2-Caraneol



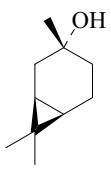
(1*R*,2*R*,3*S*,6*S*)-*form*

$C_{10}H_{18}O$ 154.252
(1*R*,2*R*,3*S*,6*S*)-*form* [16838-54-3]
Bp_1 65°. $[\alpha]_D^{20}$ +18.9 (neat).
(1*R*,2*S*,3*R*,6*S*)-*form* [1636-79-9]
$[\alpha]_D^{20}$ +32.8 (neat).
(1*R*,2*S*,3*S*,6*S*)-*form* [1126-30-3]
$[\alpha]_D^{20}$ +60.4 (neat).
(1*S*,2*R*,3*S*,6*R*)-*form* [5561-13-7]
$[\alpha]_D^{20}$ -34 (neat).
(1*S*,2*S*,3*S*,6*R*)-*form* [15372-82-4]
[18172-72-0]
Bp_1 63-64°. $[\alpha]_D^{20}$ -88.2 (neat).
(1*R*,2*S*,3*S*,6*S*)-*form* [118395-91-8]
Constit. of *Zingiber officinale* (ginger).

Acharya, S.P. *et al., J.A.C.S.*, 1967, **89**, 1925-1932 (*synth, abs config*)
Kuczynski, H. *et al., Tet. Lett.*, 1967, 2371-2376 (*synth*)
Chen, Y. *et al., CA*, 1993, **119**, 34075h (*isol*)

3-Caranol, 8CI C-83

[94268-66-3]
3,7,7-Trimethylbicyclo[4.1.0]heptan-3-ol, 9CI. 3-Caraneol



(1*S*,3*R*,6*R*)-*form*

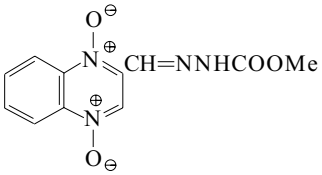
$C_{10}H_{18}O$ 154.252
(1*S*,3*R*,6*R*)-*form* [4017-79-2]
Mp 32-33°. $[\alpha]_D^{30}$ +23.6 (neat).
(1*S*,3*S*,6*R*)-*form* [4017-92-9]
Mp 71.5°. $[\alpha]_D^{23}$ +8.9 (EtOH).
(1*R*,3*R*,6*S*)-*form* [38748-97-9]
Constit. of *Zingiber officinale* (ginger).

[54631-17-3, 69500-37-4]

Gollnick, K. *et al., Tetrahedron*, 1966, **22**, 133-137 (*synth*)
Gollnick, K. *et al., Annalen*, 1969, **721**, 133-153 (*synth, abs config*)
Kokkalou, E. *et al., Planta Med.*, 1988, **54**, 58-59 (*isol*)
Misra, A.N. *et al., Tetrahedron*, 1988, **44**, 6941-6946 (*synth*)

Carbadox, BAN, INN, USAN C-84

[6804-07-5]
Methyl (2-quinoxalinylmethylene)hydrazinecarboxylate N,N′*-dioxide, 9CI. Methyl 3-(2-quinoxalinylmethylene)carbazate* N^1,N^4*-dioxide, 8CI. Fortigro. Getroxel. Mecadox. GS 6244*



$C_{11}H_{10}N_4O_4$ 262.224
Animal growth promoter esp. for pigs. Banned in the EU. Permitted in USA subject to a 45-day withdrawal period (2001). Minute yellow cryst. Insol. H_2O. Mp 239.5-240°.
▶ LD_{50} (rat, orl) 850 mg/kg. Mutagen. Exp. carcinogen. FE2779000

Belg. Pat., 1965, 669 353; *CA*, **65**, 7196 (*synth, props*)
Lojka, J. *et al., &hCesk. Farm.*, 1981, **30**, 278 (*synth*)
Haddadin, M.J. *et al., J.O.C.*, 1985, **50**, 129 (*synth*)
Jager, L.P. *et al., CA*, 1987, **106**, 43265 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 125
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FOI000

Carbamoylphosphonic acid, 8CI C-85

[6874-57-3]
Aminocarbonylphosphonic acid, 9CI. Phosphonoformamide. Dihydroxyphosphinylformamide. Aminooxomethanephosphonic acid
$(HO)_2P(O)CONH_2$
CH_4NO_4P 125.021

Di-Me ester: [33534-83-7] *Dimethyl aminocarbonylphosphonate. (Dimethoxyphosphinyl)formamide. Methafos*
$C_3H_8NO_4P$ 153.074

Mono-Et ester: See Monoethyl (aminocarbonyl)phosphonate in *The Combined Chemical Dictionary.*

Di-Et ester: [31142-29-7] *Diethyl aminocarbonylphosphonate. (Diethoxyphosphinyl)formamide. Etkafos*
$C_5H_{12}NO_4P$ 181.128
Needles (C_6H_6 or EtOAc). Mp 138-139°.

Diisopropyl ester:Diisopropyl aminocarbonylphosphonate. (Diisopropoxyphosphinyl)formamide
$C_7H_{16}NO_4P$ 209.181
Prisms (EtOAc). Mp 95-97°.

Di-Ph ester: [41839-63-8] *Diphenyl aminocarbonylphosphonate. (Diphenoxyphosphinyl)formamide*
$C_{13}H_{12}NO_4P$ 277.216
Prisms (C_6H_6/petrol). Mp 113.5-114.5°.

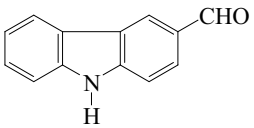
*Bis(diethylamide):*P-*Aminocarbonyl-*N,N,N′,N′*-tetraethylphosphonic diamide*
$C_9H_{22}N_3O_2P$ 235.265
Mp 119-120°.

Nylen, P. *et al., Ber.*, 1924, **57**, 1023 (*diethyl ester*)
Grisely, D.W. *et al., J.O.C.*, 1961, **26**, 2544 (*esters, synth, ir, nmr*)
Bel'skii, V.E. *et al., Zh. Obshch. Khim.*, 1972, **42**, 2427; *J. Gen. Chem. USSR (Engl. Transl.)*, 1972, **42**, 2421 (*diethyl ester, P-31 nmr*)

Gorbatenko, V.I. *et al., Zh. Obshch. Khim.*, 1973, **43**, 1043; *J. Gen. Chem. USSR (Engl. Transl.)*, 1973, **43**, 1035 (*diphenyl ester*)

9*H*-Carbazole-3-carboxaldehyde, 9CI C-86

[51761-07-0]
3-Formylcarbazole. 2-Formylcarbazole (obsol.)



$C_{13}H_9NO$ 195.22
Alkaloid from the roots of *Clausena lansium* (wampee). Pale-yellow needles (C_6H_6), prisms (Me_2CO/hexane). Mp 158-159°.

Hydrazone:
$C_{13}H_{11}N_3$ 209.25
Prisms. Mp 340°.

2,4-Dinitrophenylhydrazone:
Red prisms. Mp 328° dec.

N-*Et:* [7570-45-8]
$C_{15}H_{13}NO$ 223.274
Mp 85-87°.

N-*Et, methylphenylhydrazone:* [75232-44-9]
$C_{22}H_{21}N_3$ 327.428
Cryst. (EtOAc/EtOH). Mp 128-130°.

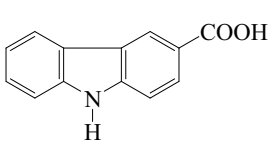
N-*Et, diphenylhydrazone:* [73276-70-7]
$C_{27}H_{23}N_3$ 389.499No phys. props. accessible.

N-*Methoxy:* [117592-01-5] **N-*Methoxy-3-formylcarbazole***
$C_{14}H_{11}NO_2$ 225.246
Yellow oil. First example of an *N*-methoxycarbazole alkaloid.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 681A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 163C (*nmr*)
Carter, P.H. *et al., J.C.S.*, 1957, 2210 (*synth*)
Ger. Pat., 1980, 3019395; *CA*, **94**, 156746z (*N-Et hydrazones*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2377 (*isol, uv, ir, pmr, cmr, ms, struct*)
Kawasaki, T. *et al., Heterocycles*, 1990, **31**, 1605 (*synth, deriv*)
Li, W.-S. *et al., Phytochemistry*, 1991, **30**, 343 (*isol, uv, ir, pmr, cmr, ms*)

9*H*-Carbazole-3-carboxylic acid C-87

[51035-17-7]
2-Carbazolecarboxylic acid (obsol.)



$C_{13}H_9NO_2$ 211.22
Cryst. solid, plates (AcOH). Mp 270-272°.

Me ester: [97931-41-4] ***Methyl 3-carbazolecarboxylate***
$C_{14}H_{11}NO_2$ 225.246
Alkaloid from the roots of *Clausena lansium* (wampee). Plates (MeOH). Mp 175-177°.

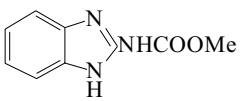
Et ester: [51035-14-4]
$C_{15}H_{13}NO_2$ 239.273
Cryst. solid. Mp 165-168°.

Hydrazide:
$C_{13}H_{11}N_3O$ 225.249
Prisms (Me_2CO). Mp 276-279°.

Carter, P.H. *et al., J.C.S.*, 1957, 2210 (*synth*)
Zelent, B. *et al., Can. J. Chem.*, 1982, **60**, 945 (*synth, ir, pmr, ms*)
Moody, C.J. *et al., J.C.S. Perkin 1*, 1990, 673 (*synth, ir, pmr, ms*)
Li, W.-S. *et al., Phytochemistry*, 1991, **30**, 343 (*isol, ester*)

Carbendazim, BSI, ISO C-88

[10605-21-7]
*Methyl 1*H*-benzimidazol-2-ylcarbamate, 9CI. Derosal. Bavistin. Delsene. Carbendazol, JMAF. MBC. BMC†. Kolfugo. Bengard. Agrizim. Funaben. Battal. Bitosen. Falicarben. Bavistan*

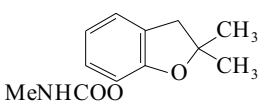


$C_9H_9N_3O_2$ 191.189
Systemic agricultural and horticultural fungicide. Light grey powder. Sol. DMF, spar. sol. most solvs. Mp 302-307° dec.
▶ Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 6400 mg/kg. Mutagenic props.. DD6500000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 186C (*nmr*)
U.S. Pat., 1967, 3 657 443; *CA*, **77**, 57597u
Eckert, J.W. *et al., Pestic. Sci.*, 1979, **10**, 473 (*activity*)
Zaitsev, B.E. *et al., Koord. Khim.*, 1985, **11**, 1490 (*struct*)
Cah. Notes Doc., 1986, **122**, 95 (*rev*)
Grundemann, E. *et al., Magn. Reson. Chem.*, 1986, **24**, 21 (*cmr*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A58
Pesticide Manual, 11th edn., 1997, No. 107
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHC750

Carbofuran, ANSI, BSI, ESA, ISO C-89

[1563-66-2]
2,3-Dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate, 9CI. Furadan. Curaterr. Yaltox. Bay 70143. FMC 10242. Chinufur



$C_{12}H_{15}NO_3$ 221.255
Systemic agricultural insecticide, acaricide and nematocide. Cryst. (cyclohexane). Spar. sol. H_2O. Mp 150-152°.
▶ OES: long-term 0.1 mg m^{-3}. Early symptoms of human exposure incl. headache, lightheadedness, weakness and nausea. Exp. reprod. and teratogenic effects. Exp. decrease in brain acetylcholinesterase activity. FB9450000

3-Hydroxy: [16655-82-6] *2,3-Dihydro-2,2-dimethyl-3,7-benzofurandiol 7-(methylcarbamate)*
$C_{12}H_{15}NO_4$ 237.255
Metab. of Carbofuran in plants, insects and mammals. Cryst. (H_2O). Mp 138-140°.

3-Oxo: [16709-30-1] *2,2-Dimethyl-7-[[(methylamino)carbonyl]oxy]-3(2*H*)-benzofuranone, 9CI*
$C_{12}H_{13}NO_4$ 235.239
Metab. of Carbofuran in plants, insects and mammals. Cryst. (EtOH). Mp 187-188°.

U.K. Pat., 1964, 1 099 691; *CA*, **64**, 3484e
Metcalf, R.L. *et al., J. Agric. Food Chem.*, 1968, **16**, 300-311 (*metabolites*)
Cook, R.F. *et al., J. Agric. Food Chem.*, 1969, **17**, 277 (*glc*)
Cook, R.F. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1973, **7**, 187 (*rev, detn*)
Ferguson, P.W. *et al., Fundam. Appl. Toxicol.*, 1984, **4**, 14 (*metab, tox*)
Hummel, S.V. *et al., Org. Mass Spectrom.*, 1986, **21**, 785 (*ms*)
Barcelo, G. *et al., Synthesis*, 1986, 627 (*synth*)
Dangerous Prop. Ind. Mater. Rep., 1988, **8**, 24 (*rev*)
Patonay, T. *et al., Synth. Commun.*, 1990, **20**, 2865 (*synth, ir*)
Kaloyanova, F.P. *et al., Human Toxicology of Pesticides*, CRC Press, Boca Raton, 1991, 48
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A60
Pesticide Manual, 10th edn., 1994, No. 103
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1153
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBS275

Carbon dioxide C-90

[124-38-9]
Carbon oxide (CO_2). Carbonic anhydride. E290
O=C=O ($D_{\infty h}$)
CO_2 44.01
Final oxidation product of carbon. Forms part of the carbon cycle in nature. Interatomic distance C–O 115.98 pm. Leavening agent, propellant, aerating agent, preservative. Solvent for supercritical extraction e.g. of caffeine in manufacture of caffeine-free instant coffee. Used in carbonation of beverages, in the frozen food industry and as a component of controlled atmosphere packaging (CAD) to inhibit bacterial growth. Esp. effective against Gram-negative spoilage bacteria, e.g. *Pseudomonas*. Colourless, odourless gas. Spar. sol. H_2O, forming H_2CO_3. d 1. Mp -57° under 5 atm. Bp -78.2° Bp -78.5° Subl. -78.46. Log P 0.83 (calc). Liquefies at 20° under 50 atm. pressure. Aq. soln. is acid to litmus. Crit. point 31.3°/72.9atm. Triple pt. -56.6° at 5.11 atm. Reduced to CO by C or H_2. Dissociates above 2000° to CO +O_2.
▶ Above atm. conc. of 6% causes CNS effects. Asphyxiant at higher conc. Contact with solid causes burns and possibly frostbite. OES: long-term 5000

ppm; short-term 15000 ppm. FF6400000

[51-90-1, 1111-72-4, 2537-69-1, 8063-77-2, 10375-59-4, 12181-61-2, 14485-07-5, 18983-82-9]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 759C (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 421; 1972, **3**, 40; 1974, **4**, 41; 1979, **7**, 52; 1981, **9**, 52; 1988, **13**, 65; 1975, **5**, 93; 1977, **6**, 94; 1969, **2**, 141; 1980, **8**, 150; 1972, **3**, 180; 1982, **10**, 274; 1972, **3**, 280; 1984, **11**, 589; 1967, **1**, 1037; 1102 (*use*)
Jaegle, A. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1970, **67**, 687 (*struct*)
Gay, I.D. *et al., J. Phys. Chem.*, 1974, **78**, 38 (*cmr*)
Perizzo, J.J. *et al., CA*, 1975, **82**, 177523s (*ir*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 622 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 1985, **107**, 6123 (*use*)
Behr, A. *et al., Angew. Chem., Int. Ed.*, 1988, **27**, 661 (*rev, use*)
Enzymatic and Model Carboxylation and Reduction Reactions for Carbon dioxide Utilization, (eds., Aresta, M. *et al*), Kluwer Academic Publishers, Dordrecht, 1990, (*book*)
Warnes, M.L. *et al., J. Insect Physiol.*, 1990, **36**, 607
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 35 (*rev*)
Carbon Dioxide Chemistry: Environmental Issues, (Paul, J. *et al*, Eds.), Royal Society of Chemistry, 1994, (*book*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 74-75
Leitner, W. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 2207 (*rev, use*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1187
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0529
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 255
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBU250; CBU500; CBU750

Carbon disulfide, ISO C-91

[75-15-0]
Carbon sulfide (CS_2). Carbon bisulfide. Dithiocarbonic anhydride. Carbon disulphide, BSI

S=C=S ($D_{\infty h}$)

CS_2 76.143

C–S 155.3 pm. Obsolete fumigant against insects in stored grain and potatoes. Highly refracting colourless liq. Misc. EtOH, Et_2O, C_6H_6; spar. sol. H_2O. d_4^0 1.29. Mp -111.6°. Bp 46.5° Bp_{297} 20°. n_D^{15} 1.6315. Forms hemihydrate, dec. at -3°. A black solid form has been prepd. at high press..

► Extremely flammable, fl. p. -30°, autoignition temp. 90°. Toxic by inhalation, skin absorption and ingestion. Acute effects on CNS cause headache, dizziness and can lead to coma, and death by respiratory failure. Prolonged or repeated (chronic) exposure causes peripheral neuropathies, CNS effects and gastrointestinal disturbances. Occup. exposure assoc. with higher incidence of coronary heart disease and male and female reprod. effects. LD_{50} (rat, orl) 3188 mg/kg. Exp. reprod. and teratogenic effects. MEL: long-term 10 ppm (Sk). FF6650000

[12539-80-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 277A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 760B (*ir*)
Bushell, W.J. *et al., Chem. Ind. (London)*, 1961, 1465 (*rev*)
Namasimhachari, N. *et al., Anal. Biochem.*, 1972, **45**, 154 (*use*)
Jungen, C. *et al., Can. J. Phys.*, 1973, **51**, 1471 (*struct*)
Blanquet, G. *et al., Ann. Soc. Sci. Bruxelles*, 1974, **88**, 87 (*struct*)
Namasimhachari, N. *et al., Biomed. Mass Spectrom.*, 1974, **1**, 367 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 94
Verma, B.C. *et al., Mikrochim. Acta*, 1982, **1**, 393 (*use*)
Pesticide Manual, 8th edn., 1987, No. 2030
Dunn, A.D. *et al., Carbon Disulphide in Organic Chemistry*, Ellis Horwood, 1989, (*rev*)
Tominaga, Y. *et al., J. Het. Chem.*, 1989, **26**, 1167 (*rev, use*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 53 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1100
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 986-990 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0532
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 256
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBV500
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 818 (*tox, rev*)

Carbon tetrachloride C-92

[56-23-5]
Tetrachloromethane, 9CI. Carbon chloride†. Perchloromethane. Tetra. F10. R10. Halon 1040

CCl_4

CCl_4 153.822

Grain fumigant. Liq. Sol. EtOH, Et_2O; prac. insol. H_2O. d_4^0 1.63. Mp 21.2° Mp 23.8° Mp 28.6° (trimorph.). Bp 76.74°. n_D^{15} 1.4631.

► Toxic by inhalation and skin contact. Dec. to highly toxic Carbonyl chloride if strongly heated in the presence of air. Production controlled by environmental legislation, illegal in EU from 1996. Eye and skin irritant. Repeated skin exposure can cause dermatitis. Acute and chronic exposure cause gastrointestinal and CNS disturbances. High vapour conc. narcotic. Hepatotoxic and nephrotoxic. Poss. human carcinogen. LD_{50} (rat, orl) 2350 mg/kg. LC_{50} (rat, ihl) 8000 ppm (4h exposure). Exp. carcinogen. Exp. reprod. and teratogenic effects. Non-flammable, autoignition temp. >1000°. OES: long-term 2 ppm (Sk). FG4900000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 84C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 125B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 121B (*ir*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 69
Causley, G.C. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1977, **11**, 383 (*uv*)
IARC Monog., 1979, **20**, 371; *Suppl.* 6, 136; *Suppl.* 7, 143 (*rev, tox*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 2467; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1985, 2282 (*cmr*)
Organo-chlorine Solvents, Royal Society of Chemistry, 1986, 225 (*tox, rev*)
Kalf, G.F. *et al., Annu. Rev. Pharmacol. Toxicol.*, 1987, **27**, 399 (*tox*)
Holmes, J.L. *et al., Int. J. Mass Spectrom. Ion Processes*, 1988, **83**, 285 (*ms*)
Andrews, L. *et al., J. Mol. Struct.*, (*Theochem*), 1989, **200**, 325 (*ms, spectra*)
Chumaevskii, N.A. *et al., Zh. Neorg. Khim.*, 1989, **34**, 1416; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1989, **34**, 798 (*Raman*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 1062 (*rev, synth, props*)
Stevenson, R. *et al., Chem. Br.*, 1992, **28**, 208 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1100
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*rev, occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0316
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 259
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBY000

Carbonic acid C-93

[463-79-6]
$(HO)_2C=O$

CH_2O_3 62.025

Present in aq. solns. of CO_2, the hydration of CO_2 being a slow reaction. Forms a wide range of salts $M[HCO_3]$ and M_2CO_3, some of the most important of which are cross-referenced below.pK_{a1} 6.36; pK_{a2} 10.33 (25°). True diss. const. $[H^{\oplus}][HCO_3^{\ominus}]/H_2CO_3 = 0.00025$.

Mono-NH_4 salt: [1066-33-7] *Ammonium bicarbonate. Ammonium hydrogen carbonate. E503*
CH_5NO_3 79.055
Used in foods as an alkali, dough strengthener, leavening agent, pH control agent and texturizer. White solid. V. sol. H_2O. Mp 107.5° (very rapid heating). Comparatively stable at r.t.; volatile with dec. below Mp (at *ca.* 60°) to $NH_3 + CO_2 + H_2O$. The name E503 is also used for Ammonium carbonate, A-312.

► BO8600000

[71-52-3, 3812-32-6]

Mellor Compr. Treat. Inorg. Theor. Chem., 1925, **6**, 72; 1964, **8/I**, 72 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, ; *Syst. No.* 14, 1973, **C3**, 36 (*bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 1232 (*rev*)
Palmer, D.A. *et al., Chem. Rev.*, 1983, **83**, 651 (*rev*)

Terlouw, J.K. *et al., Angew. Chem., Int. Ed.*, 1990, **29**, 404 (*struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 130-131
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANB250

N-(Carboxyacetyl)alanine, 9CI C-94

N-*Malonylalanine*



$C_6H_9NO_5$ 175.141

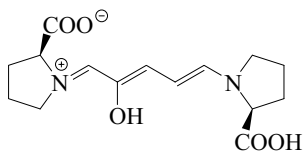
(R)-form [19764-27-3]
D-form
Isol. from seedlings of *Pisum sativum* (pea). Mp 138-140°. $[\alpha]_D^{28}$ +33 (c, 0.38 in H_2O).

Dibenzyl ester: [41087-89-2]
Cryst. (EtOAc/petrol). Mp 43-45°.

Ogawa, T. *et al., Biochim. Biophys. Acta*, 1973, **297**, 60 (*isol, struct, pmr, ir, ms, synth*)
Fukuda, M. *et al., Phytochemistry*, 1973, **12**, 2593 (*isol*)

2-Carboxy-1-[5-(2-carboxy-1-pyrrolidinyl)-2-hydroxy-2,4-pentadienylidene]pyrrolidinium, 9CI C-95

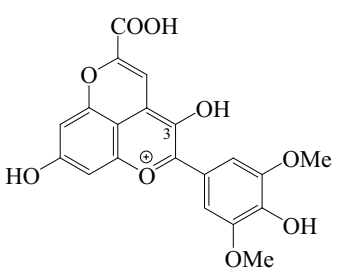
[214150-43-3]
5-(2-Carboxy-1-pyrrolidinyl)-2-hydroxy-2,4-pentadienal (2-carboxypyrrolidine)imine



$C_{15}H_{20}N_2O_5$ 308.333
Likely to be a mesomeric system with (+)-charge delocalised over the two Ns and (-)-charge over the two COOH groups. Maillard product from reaction of L-proline and 2-Furancarboxaldehyde, F-93. Intensely yellow solid.

Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 932-940 (*occur, nmr, ms*)

5-Carboxy-3,8-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)pyrano[4,3,2-*de*]-1-benzopyrylium, 9CI C-96

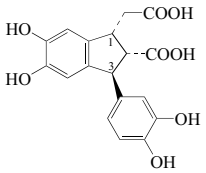


$C_{20}H_{15}O_9^{\oplus}$ 399.333
Adduct of 3,4′,5,7-Tetrahydroxy-3′,5′-dimethoxyflavylium(1+), T-158 and Pyruvic acid, P-632.

3-O-β-D-Glucopyranoside: [209862-95-3]
$C_{26}H_{25}O_{14}^{\oplus}$ 561.475
Constit. of grape pomace. Stable red pigment in wine. CAS no. refers to the chloride λ_{max} 510 (no solvent reported).

Fulcrand, H. *et al., Phytochemistry*, 1998, **47**, 1401-1407 (*isol, uv, pmr, cmr*)

2-Carboxy-3-(3,4-dihydroxyphenyl)-2,3-dihydro-5,6-dihydroxy-1*H*-indene-1-acetic acid C-97



(1*R**,2*R**,3*R**)-*form*

$C_{18}H_{16}O_8$ 360.32

(1R*,2R*,3R*)-form

Di-Me ester: [191280-20-3]
$C_{20}H_{20}O_8$ 388.373
Constit. of the seeds of *Helianthus annuus* (sunflower). Gum. $[\alpha]_D^{24}$ +93.6 (c, 0.25 in MeOH).

(1R*,2S*,3S*)-form

Di-Me ester: [191280-19-0]
Constit. of the seeds of *Helianthus annuus* (sunflower). Gum. $[\alpha]_D^{24}$ +58 (c, 0.25 in MeOH).

Kato, T. *et al., Nat. Prod. Lett.*, 1997, **9**, 161-165 (*isol, pmr, cmr*)

3-(Carboxymethylamino)propanoic acid C-98

[505-72-6]
N-*(Carboxymethyl)-β-alanine, 9CI*. N-*(Carboxyethyl)glycine. Iminopropionicacetic acid*
$HOO^1CCH_2CH_2NHCH_2COOH$
$C_5H_9NO_4$ 147.13
Isol. from *Phaseolus radiatus* var. *typicus*. Cryst. (H_2O or EtOH aq.). Mp 195-198° (191-192°) dec.

Hydrochloride:
Mp 120-122°.

Di-Et ester: [3783-61-7]
$C_9H_{17}NO_4$ 203.238
Oil. Bp 253° sl. dec. Bp_1 98-99°.

Di-Et ester, hydrochloride:
Mp 85-87°.

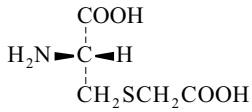
1-Nitrile: [3088-42-4] N-*(2-Cyanoethyl)glycine, 9CI. 3-(Carboxymethylamino)propionitrile*
$C_5H_8N_2O_2$ 128.13
Cryst. Mp 193-195°.

▶ MB9275000

Cocker, W. *et al., J.C.S.*, 1952, 1182 (*deriv*)
McKinney, L.L. *et al., J.A.C.S.*, 1952, **74**, 1942; 5183 (*synth*)
Coburn, M.D. *et al., J. Het. Chem.*, 1965, **2**, 308 (*deriv*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1971, **35**, 1603 (*isol, synth*)
Kawashiro, K. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 1097; 2871 (*synth, ms*)

S-Carboxymethylcysteine, 9CI C-99

[638-23-3]
Carbocisteine, BAN, INN, JAN. *Carbocysteine, USAN. Actithiol. Mucodyne. Thiodril. AHR 3053. LJ 206. Rhinathiol. Many other names*



$C_5H_9NO_4S$ 179.196Log P -2.63 (calc).

▶ LD_{50} (mus, orl) 8400 mg/kg. Exp. reprod. effects. AY4342000

(R)-form [2387-59-9]
L-form
Isol. from radish seedlings. Mp 204-207°. $[\alpha]_D^{24}$ +0.5 (1*M* HCl).

▶ Adverse effects when used therapeutically. LD_{50} (mus, scu) 9000 mg/kg. AY4341000

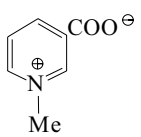
S-*Oxide:*
$C_5H_9NO_5S$ 195.196
Ppt. Mp 190-191° dec. Probably a diastereoisomeric mixture.

S,S-*Dioxide:*
$C_5H_9NO_6S$ 211.195
Mp 193-194° dec.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 502B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 594D (*ir*)
Armstrong, M.D. *et al., J.O.C.*, 1951, **16**, 749 (*synth*)
Schoberl, A. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1956, **304**, 97 (*synth*)
Foye, W.O. *et al., J. Am. Pharm. Assoc.*, 1957, **46**, 273 (*synth*)
Goodman, L. *et al., J.O.C.*, 1958, **23**, 1251 (*synth, oxides*)
Buziassy, C. *et al., Biochim. Biophys. Acta*, 1964, **86**, 185 (*isol*)
Quevanviller, A. *et al., Therapie*, 1967, **22**, 485 (*Carbocysteine*)
Mighell, A.D. *et al., Acta Cryst. B*, 1979, **35**, 1258 (*cryst struct*)
Yokozeki, K. *et al., Agric. Biol. Chem.*, 1988, **52**, 2369 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 745
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBR675; CCH125

3-Carboxy-1-methylpyridinium betaine C-100

[535-83-1]
3-Carboxy-1-methylpyridinium hydroxide inner salt. N-*Methylnicotinic betaine*. ***Trigonelline***. *Gynesis. Coffearin*



$C_7H_7NO_2$ 137.138
Alkaloid from fenugreek (*Trigonella foenum-graecum*) (Leguminosae), and very

many other spp.; also present in coffee beans and many animals. Prisms + $1H_2O$ (EtOH aq.). V. sol. H_2O; sol. MeOH, EtOH; poorly sol. $CHCl_3$, Et_2O. Mp 218° dec. (anhyd.).

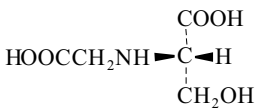
► LD_{50} (rat, orl) 5000 mg/kg. YF6825000

Hydrochloride: [6138-41-6]
Cryst. (EtOH aq.). Mp 257-258° (250°, 245-250° dec.).

Picrate:
Mp 205-206° (198-200°).

Gorter, K. *et al., Annalen*, 1910, **372**, 237 (*isol*)
Späth, E. *et al., Ber.*, 1944, **77**, 362 (*synth*)
Ackermann, D. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1961, **326**, 197 (*occur*)
Wang, S.Y. *et al., Biochemistry*, 1968, **7**, 3740 (*uv*)
Wehrli, F.W. *et al., Helv. Chim. Acta*, 1971, **54**, 229 (*pmr, cmr*)
Ghosal, S. *et al., Planta Med.*, 1973, **23**, 321 (*isol, uv, ir, pmr*)
Merck Index, 9th edn., 1976, No. 9360
Houghton, P.J. *et al., Planta Med.*, 1987, **53**, 262 (*isol*)
Merck Index, 11th edn., 1989, No. 9606
Slattery, M. *et al., Marine Ecol.: Progr. Ser.*, 1997, **161**, 133-144; *CA*, **128**, 119209e (*isol, activity*)
Blunden, G. *et al., Phytochemistry*, 2001, **58**, 451-454 (*occur*)

N-Carboxymethylserine C-101



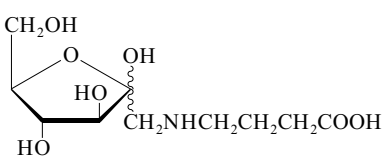
$C_5H_9NO_5$ 163.13

(*S*)-*form* [17136-47-9]
L-form
Isol. from asparagus (*Asparagus officinalis*) shoots. Cryst. (EtOH aq.). Mp 167°. $[\alpha]_D$ +3 (c, 2.2 in H_2O). pK_{a2} 10.4 (80% 2-methoxyethanol aq.). pK_{a1} 1.7; pK_{a2} 2.54; pK_{a3} 8.89 (25°).

Hardegger, E. *et al., Helv. Chim. Acta*, 1968, **51**, 78 (*synth*)
Snyder, R.V. *et al., J. Inorg. Nucl. Chem.*, 1973, **35**, 523
Kasai, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 1483 (*isol*)

1-[(3-Carboxypropyl)amino]-1-deoxyfructose, 9CI C-102

*1-Deoxy-1-(*N*-γ-aminobutyric acid)fructose*



$C_{10}H_{19}NO_7$ 265.263

D-*form* [10003-63-1]
Isol. from stored apricots and peaches. Amorph.

Anet, E.F.L.J. *et al., Aust. J. Chem.*, 1957, **10**, 182 (*isol*)
Tomita, H. *et al., Agric. Biol. Chem.*, 1965, **29**, 959 (*isol, synth*)

N-(3-Carboxypropyl)glutamine, 8CI C-103

γ-Glutamyl-γ-aminobutyric acid
$HOOCCH_2CH_2CH_2NH$-$COCH_2CH_2CH(NH_2)COOH$

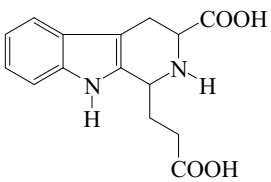
$C_9H_{16}N_2O_5$ 232.236

(*S*)-*form* [3183-72-0]
L-form
Constit. of beet. Cryst. (EtOH aq.). Mp 190-191°. $[\alpha]_D^{17}$ +7.3 (c, 0.9 in H_2O).

Larsen, P.O. *et al., Acta Chem. Scand.*, 1965, **19**, 1071 (*isol, synth*)
Fosker, A.P. *et al., J.C.S.*, 1965, 7305 (*synth*)
Przybylska, J. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Biol.*, 1968, **16**, 615; *CA*, **70**, 75060 (*isol*)
Fowden, L. *et al., Phytochemistry*, 1972, **11**, 2271 (*isol*)
Maguan, S.D.J. *et al., J. Med. Chem.*, 1982, **25**, 1018 (*synth, pharmacol*)

3-Carboxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-1-propanoic acid, 9CI C-104

[192180-84-0, 192180-85-1]
1-(2-Carboxyethyl)-1,2,3,4-tetrahydro-β-carboline-3-carboxylic acid

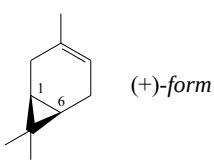


$C_{15}H_{16}N_2O_4$ 288.302
Present in soy and worcester sauces, yeast extract and wine as the (3*S*)-diastereoisomers. Formed by Pictet-Spengler condensation of tryptophan with 4-oxobutanoic acid to give predominantly the *cis*-isomer.. *cis*- and *trans*- isomers have been characterised spectroscopically.

Gutsche, B. *et al., J. Agric. Food Chem.*, 1997, **45**, 2458-2462 (*synth, ms, nmr*)

3-Carene C-105

[13466-78-9]
3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene. ***α-Carene****. Isodiprene*



$C_{10}H_{16}$ 136.236
Flavouring ingredient.

► Skin irritant. LD_{50} (rat, orl) 4800 mg/kg. FH8400000

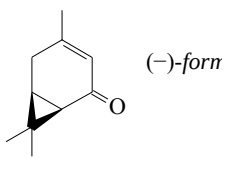
(+)-*form* [498-15-7]
Widespread plant product, found esp. in turpentine oils (from *Pinus* spp.) and oil of galbanum. Oil with pleasant odour. Poorly sol. hexane. Bp_{200} 123-124° $Bp_{7.5}$ 168-169°. Oxidises in air.

(-)-*form* [20296-50-8]
Isol. from root oil of *Kaempferia galanga*. Oil. $[\alpha]_D^{30}$ -5.72.

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 74A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 72B (*nmr*)
Simonsen, J. *et al., J.C.S.*, 1920, **117**, 570 (*struct*)
Sandberg, R. *et al., Ark. Kemi*, 1960, **16**, 255 (*abs config*)
Ryhage, R. *et al., Acta Chem. Scand.*, 1964, **47**, 475 (*ms*)
Wrolstad, R.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 507 (*ir*)
Schweers, W. *et al., Tet. Lett.*, 1968, 4425 (*biosynth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1053 (*rev, tox*)
Banthorpe, D.V. *et al., Phytochemistry*, 1976, **15**, 109 (*biosynth*)
Cocker, W. *et al., J.C.S. Perkin 1*, 1978, 1370 (*synth*)
Akhila, A. *et al., Phytochemistry*, 1980, **19**, 1691 (*biosynth*)
Johnson, C.R. *et al., J.O.C.*, 1987, **52**, 1493 (*synth*)
Misra, A.N. *et al., Tetrahedron*, 1988, **44**, 6941 (*props*)
Denisov, A.Y. *et al., Khim. Prir. Soedin.*, 1992, **28**, 441; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 386 (*pmr, cmr*)
Denisov, A.Y. *et al., Magn. Reson. Chem.*, 1992, **30**, 95; 886 (*pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCK500

3-Caren-5-one C-106

[81800-50-2]
4,7,7-Trimethylbicyclo[4.1.0]hept-3-en-2-one, 9CI



$C_{10}H_{14}O$ 150.22
Constit. of *Kaempferia galanga* (galangal). Oil. No. opt. rotn. reported for natural isolate.

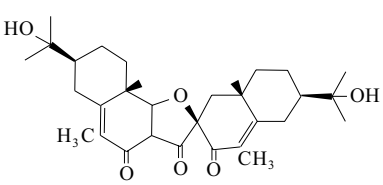
(-)-*form* [22327-32-8]
Oil. $Bp_{0.5}$ 58°. $[\alpha]_D^{20}$ -271 (c, 3.1 in $CHCl_3$).

Semicarbazone:
Prisms (EtOH). Mp 170° (159-161°).

Cocker, W. *et al., J.C.S.(C)*, 1968, 3073; 1971, 1073 (*synth, pmr*)
Kiuchi, F. *et al., Phytochemistry*, 1987, **26**, 3350 (*isol*)

Carindone C-107

[38045-62-4]

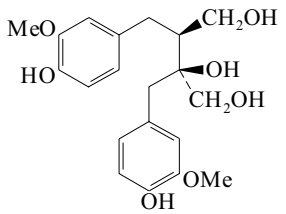


$C_{31}H_{44}O_6$ 512.685
Constit. of *Carissa carandas* (karanda). Cryst. Mp 262°.

Singh, B. *et al., Phytochemistry*, 1972, **11**, 1797

Carinol C-108

[58139-12-1]
2,3-Bis(4-hydroxy-3-methylphenyl)methyl-1,2,4-butanetriol, 9CI. 4,4′,8,9,9′-Pentahydroxy-3,3′-dimethoxylignan

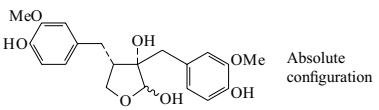


$C_{20}H_{26}O_7$ 378.421
Constit. of roots of *Carissa carandas* (karanda). Amorph. powder. $[\alpha]_D$ -22.4 (c, 1 in EtOH).

Pal, R. *et al., Phytochemistry*, 1975, **14**, 2302 (*isol, struct*)
Khamlach, K. *et al., Heterocycles*, 1990, **31**, 2195 (*synth*)

Carissanol C-109

[87402-76-4]
Tetrahydro-3,4-bis[(4-hydroxy-3-methoxyphenyl)methyl]-2,3-furandiol, 9CI. 4,4′,8,9-Tetrahydroxy-3,3′-dimethoxy-9,9′-epoxylignan

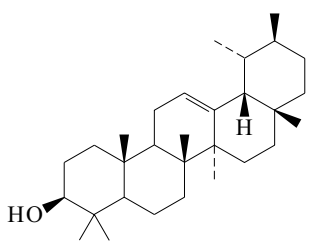


$C_{20}H_{24}O_7$ 376.405
Constit. of *Carissa edulis* (agam). Amorph. powder. $[\alpha]_D^{20}$ -14 (c, 0.7 in EtOH).

Achenbach, H. *et al., Phytochemistry*, 1983, **22**, 749 (*isol, struct*)
Khamlach, K. *et al., Heterocycles*, 1990, **31**, 2195 (*synth*)

Carissol C-110

[101915-51-9]

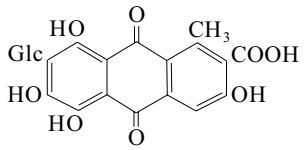


$C_{30}H_{50}O$ 426.724
Constit. of *Carissa carandas* (karanda). Cryst. Mp 118-120°.

Naim, Z. *et al., Pak. J. Sci. Ind. Res.*, 1985, **28**, 378 (*isol, pmr, ms*)

Carmine red C-111

[1260-17-9]
7-Glucopyranosyl-3,4,5,8-tetrahydroxy-1-methylanthraquinone-2-carboxylic acid. Carminic acid. Natural red 4. C. I. 75470. Cochineal. E120. FEMA 2330



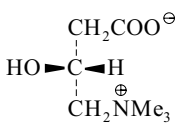
$C_{22}H_{20}O_{13}$ 492.392
Red food colouring. Red cryst. Sol. H_2O, EtOH; sl. sol. Et_2O. λ_{max} 278 (ϵ 31800); 491 (ϵ 7800) (MeOH) (Berdy). λ_{max} 500 (ϵ 6800) (H_2O) (Berdy). λ_{max} 495 (ϵ 5800) (HCl) (Berdy). λ_{max} 540 (ϵ 3450) (NAOH) (Berdy).

Octa-Ac:
Cryst. Mp 189-190° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 246D (*ir*)
Goriushina, V.G. *et al., Zavod. Lab.*, 1957, **23**, 781 (*use*)
Callicoat, D.L. *et al., Anal. Chem.*, 1959, **31**, 1434 (*detn, B*)
Nemodruk, A.A. *et al., Analytical Chemistry of Boron*, Nauka, Moscow, 1964, (*detn, B*)
Bhatia, S.B. *et al., Indian J. Chem.*, 1965, **3**, 92
Mihail, N. *et al., Naturwissenschaften*, 1970, **57**, 500 (*pharmacol*)
Flechon, J. *et al., Bull. Soc. Chim. Fr.*, 1976, 739 (*use*)
Rosenfeld, H.J. *et al., Analyst (London)*, 1979, **104**, 983 (*use*)
Lloyd, A.G. *et al., Food Chem.*, 1980, **5**, 91 (*rev*)
Eisner, T. *et al., Science (Washington, D.C.)*, 1980, **208**, 1039 (*use*)
Fiecchi, A. *et al., J.O.C.*, 1981, **46**, 1511 (*config*)
Ishida, T. *et al., Acta Cryst. C*, 1987, **43**, 1541 (*cryst struct, bibl*)
Allevi, P. *et al., Chem. Comm.*, 1991, 1319 (*synth, bibl*)
Rasimas, J.P. *et al., J. Phys. Chem.*, 1995, **99**, 11333 (*fluoresence*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 647-649
Allevi, P. *et al., J.C.S. Perkin 1*, 1998, 575-582 (*synth, pmr, cmr*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 193

Carnitine, INN C-112

[461-06-3]
3-Carboxy-2-hydroxy-N,N,N-*trimethyl-1-propanaminium hydroxide inner salt, 9CI. β-Hydroxy-γ-butyrotrimethylbetaine. 4-Amino-3-hydroxybutanoic acid trimethylbetaine. Vitamin B_T. Novain*



$C_7H_{15}NO_3$ 161.2

(*R*)-*form* [541-15-1]
L-*form*. ***Levocarnitine, BAN, INN, USAN***
Used in sport and infant nutrition. Present in cotyledons of pea (*Pisum sativum*). Extremely hygroscopic solid (EtOH/Me_2CO). Mp 196-198°. $[\alpha]_D^{25}$ -31.3 (c, 10 in H_2O) (>99% op).
▶ LD_{50} (mus, scu) 9000mg/kg. BP2980000

Hydrochloride: [10017-44-4]
Hygroscopic cryst. Mp 137-139°. $[\alpha]_D^{22}$ -20.4 (H_2O).
▶ LD_{50} (mus, orl) 8000 mg/kg. Exp. reprod. and teratogenic effects (very large doses). BP2979100

Et ester: [40915-13-7] *4-Ethoxy-2-hydroxy*-N,N,N-*trimethyl-4-oxo-1-butanaminium(1+), 9CI*
$C_9H_{20}NO_3^{\oplus}$ 190.262
Needles (Me_2CO) (as chloride). Mp 146°.

O-*Ac:* [3040-38-8]

[14992-62-2]
$C_9H_{17}NO_4$ 203.238
Cryst. (EtOH/Et_2O). Mp 145°. $[\alpha]_D^{20}$ -19.5.
▶ BP2990000

O-*Ac; hydrochloride:* [5080-50-2] *Alcar. Zalcose*
Mp 188-190°.

O-*Propanoyl:* [20064-19-1]

[17298-37-2] *Propionyl-L-carnitine. 3-Carboxy*-N,N,N-*trimethyl-2-(1-oxopropoxy)-1-propanaminium(1+), 9CI*
$C_{10}H_{19}NO_4$ 217.264
Hygroscopic prisms (2-propanol). Mp 146-149° dec. $[\alpha]_D^{22}$ -25.2 (H_2O).

O-*Octanoyl:* [25243-95-2]
$C_{15}H_{29}NO_4$ 287.398
Mp 155-159°.

O-*Hexadecanoyl:* [2364-67-2]

[1935-18-8, 18877-64-0] *3-Carboxy*-N,N,N-*trimethyl-2-[(1-oxohexadecyl)oxy]-1-propanaminium(1+)*
$C_{23}H_{45}NO_4$ 399.613
Mp 177-178° dec. (as hydrochloride). $[\alpha]_D^{20}$ -15 (c, 1 in MeOH).

Me ether:
$C_8H_{17}NO_3$ 175.227
Prisms (Me_2CO) (as hydrochloride). Mp 178°.

(*S*)-*form* [541-14-0] D-*form*
Mp 210-212° dec. $[\alpha]_D$ +30.9.
▶ BP2979850

Hydrochloride: [6645-46-1]
Mp 142° dec.

O-*Propanoyl:* [25518-43-8]
Prisms (2-propanol). $[\alpha]_D$ +25.2 (H_2O).

(±)-*form* [406-76-8]
Mp 195-197° dec.
▶ BP2979900

Hydrochloride: [461-05-2]
Mp 196°.
▶ BP2979140

Amide: [5261-99-4] *Carnitinamide*
$C_7H_{17}N_2O_2^{\oplus}$ 161.223
Mp 207-209° (as chloride).

Nitrile: [18933-33-0] *3-Cyano-2-hydroxy*-N,N,N-*trimethylpropanaminium(1+), 9CI*
$C_7H_{15}N_2O^{\oplus}$ 143.208
Mp 232° dec. (as chloride).

O-*Ac:* [870-77-9]

[14992-62-2]
Mp 187-188°.
▶ BP2985000

O-*Propanoyl:* [25518-45-0]
Mp 169-172° dec.

O-*Dodecanoyl:* [14919-37-0]
$C_{19}H_{37}NO_4^{\oplus}$ 343.506
Mp 170-171° (as chloride).

[56-99-5, 5852-97-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 542C; 777B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1227A; 1276C (*nmr*)
Carter, H.E. *et al., Methods Enzymol.*, 1957, **3**, 660 (*isol*)
Strack, E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1960, **318**, 129; 1970, **351**, 95-98 (*synth, Ac, propanoyl*)
Wolf, G. *et al., Arch. Biochem. Biophys.*, 1961, **92**, 360 (*biosynth*)
Kaneko, T. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 1153 (*abs config*)
Ziegler, H.J. *et al., J.O.C.*, 1967, **32**, 3989-3991 (*O-acyl derivs, palmitoyl hydrochloride*)
Vasil'eva, E.D. *et al., Khim. Prir. Soedin.*, 1969, **5**, 463; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 388 (*synth*)
Strack, E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1970, **351**, 95-98 (*synth, isomers, propanoyl*)
Tomita, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1988 (*cryst struct*)
Bamji, M. *et al., Biochem. Rev.*, 1980, **50**, 99 (*rev*)
Frenkel, R.A. *et al., Carnitine Biosynth., Metab., Funct. [Proc. Virginia Lazenby O'Hara Biochem. Symp.]*, Eds., Academic Press, N.Y., 1980, (*book*)
Boch, K. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 341 (*synth*)
Zhou, B.N. *et al., J.A.C.S.*, 1983, **105**, 5925 (*synth*)
Bremer, J. *et al., Physiol. Rev.*, 1983, **63**, 1420 (*rev*)
Comber, R.N. *et al., Org. Prep. Proced. Int.*, 1985, **17**, 175 (*synth*)
Reboucha, C.J. *et al., Annu. Rev. Nutr.*, 1986, **6**, 41 (*rev*)
Goa, K.L. *et al., Drugs*, 1987, **34**, 1 (*rev*)
Voeffray, R. *et al., Helv. Chim. Acta*, 1987, **70**, 2058 (*synth, ir, pmr, bibl*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 789 (*synonyms*)
Mancini, M. *et al., Arzneim.-Forsch.*, 1992, **42**, 1101-1104 (*propanoyl, pharmacol, bibl*)
L-Carnitine and its Role in Medicine: From Function to Therapy, (Eds. Ferrari, R. *et al*), Academic Press, 1992, (*book*)
Kasai, N. *et al., Tet. Lett.*, 1992, **33**, 1211 (*synth, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1037
Bernabei, I. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 2076 (*synth*)
Weber, H.P. *et al., Acta Cryst. C*, 1995, **51**, 2570 (*cryst struct, Ac*)
Sakuraba, S. *et al., Chem. Pharm. Bull.*, 1995, **43**, 738 (*synth*)
Torielli, L. *et al., J. Cardiovasc. Pharmacol.*, 1995, **26**, 372-380 (*propanoyl, pharmacol, bibl*)
The Carnitine System, (Eds. De Jong, J.W. *et al*), Kluwer, 1995, (*book*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 492
Kabat, M.M. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 2663-2665 (*synth*)
Wiseman, L.R. *et al., Drugs Aging*, 1998, **12**, 243-248 (*propanoyl, rev*)
Rao, K.V. *et al., Neuropharmacology*, 1999, **38**, 383-394 (*Alcar*)
Jain, R.P. *et al., Tet. Lett.*, 2001, **42**, 4437-4440 (*synth*)
Jain, R.P. *et al., Tetrahedron*, 2001, **57**, 6505-6509 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCK650; CCK660

Carnobacteriocins C-113

Peptides. Prod. by *Carnobacterium piscicola*. Bacteriocins with potential food uses.

Carnobacteriocin A [156066-35-2]

[155870-23-8, 155870-24-9]
Prod. by *Carnobacterium piscicola* LV17A. A mixt. of 3 components; the major component A3 is a 53 aminoacid peptide with one disulfide bridge, A2 has a Met oxidised to a sulfoxide, and A1 is a mixt. of peptides derived proteolytically from A3 and A2.

Carnobacteriocin B1 [155982-41-5]
Prod. by *Carnobacterium piscicola* LV17B. An oxidised form of Carnobacteriocin BM1.

Carnobacteriocin B2 [162429-94-9]

[155982-37-9]
Prod. by *Carnobacterium piscicola* LV17B. Contains 48 amino acid residues.

Carnobacteriocin BM1 [156014-92-5]

[165723-95-5]
Pisciocin V1B
Prod. by *Carnobacterium piscicola* LV17B and identical with Pisciocin V1B from the Pisciocin complex prod. by *Carnobacterium piscicola* V1. Contains 43 aminoacid residues.

Quadri, L.E. *et al., J. Biol. Chem.*, 1994, **269**, 12204-12211 (*Carnobacteriocin B*)
Worobo, R.W. *et al., Microbiology (Reading, U.K.)*, 1994, **140**, 517-526 (*Carnobacteriocin A*)
Yang, Y. *et al., Biochemistry*, 1999, **38**, 15437-15447 (*Carnobacteriocin B2, struct*)

Carnocins C-114

Polypeptide bacteriocins.

Carnocin CP 5 [149983-81-3]
Prod. by *Carnobacterium piscicola* CP5.

Carnocin U I49 [142540-01-0]
Prod. by *Carnobacterium piscicola* UI49 isol. from fish.

Stoffels, G. *et al., J. Appl. Bacteriol.*, 1992, **73**, 309-316 (*Carnocin UI 49*)
Mathieu, F. *et al., Biotechnol. Lett.*, 1993, **15**, 587-590 (*Carnocin CP 5*)
Stoffels, G. *et al., Int. J. Food Microbiol.*, 1993, **20**, 199-210 (*Carnocin UI 49*)

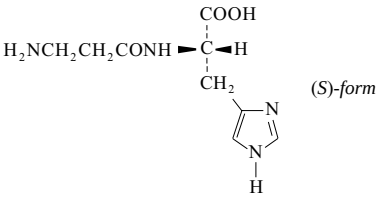
Carnosin C-115

[146103-60-8]
Prod. by *Leuconostoc carnosum* LA44A from vacuum packed Vienna-type sausages. Bacteriocin.

Van Laack, R.L. *et al., Int. J. Food Microbiol.*, 1992, **16**, 183-195 (*isol*)

Carnosine C-116

N-*β-Alanylhistidine, 9CI*



(*S*)-*form*

$C_9H_{14}N_4O_3$ 226.235Log P -4.13 (calc).

(*R*)-*form* [5853-00-9]
D-form
Mp 260°. $[\alpha]_D^{28}$ -20.4 (c, 1.5 in H_2O).

Hydrochloride:
Mp 245°.

N-*Benzyloxycarbonyl:*
$C_{17}H_{20}N_4O_5$ 360.369
Mp 161°. $[\alpha]_D^{24}$ -11 (H_2O).

(*S*)-*form* [305-84-0] *L-form*
Occurs in meats. Needles. Sol. EtOH; fairly sol. MeOH; poorly sol. butanol, hexane. Mp 246-250° dec. $[\alpha]_D^{20}$ +24.1 (c, 1.5 in H_2O). pK_{a1} 2.62; pK_{a2} 6.66; pK_{a3} 9.24 (25°). Log P -4.13 (calc). λ_{max} (H_2O) (Berdy).

▶ LD_{50} (mus, ipr) 9087 mg/kg. Exp. reprod. and teratogenic effects. MS3080000

Hydrochloride: [5852-99-3]
Mp 245°.

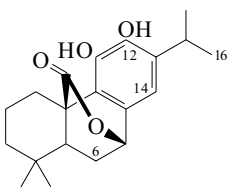
Nitrate: [5852-98-2]
Needles. Mp 219° (222° dec.).

*Sulfate:*Dec. at 238-40°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 86A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 622A (*ir*)
Rinderknecht, H. *et al., J.O.C.*, 1964, **29**, 1968 (*synth*)
Pietta, P.G. *et al., Ann. Chim. (Rome)*, 1968, **58**, 1431 (*synth*)
Barrons, Y. *et al., J. Mol. Struct.*, 1976, **30**, 225 (*cryst struct*)
Itoh, H. *et al., Acta Cryst. B*, 1977, **33**, 2959 (*cryst struct*)
Friedrich, J.O. *et al., Can. J. Chem.*, 1986, **64**, 2132 (*cmr, pmr*)
Boldyrev, A.A. *et al., Adv. Enzyme Regul.*, 1990, **30**, 175 (*rev, biol activity*)
Boldyrev, A.A. *et al., Int. J. Biochem.*, 1990, **22**, 129 (*rev*)
Gaggelli, E. *et al., J.C.S. Perkin 2*, 1990, 401 (*pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCK665

Carnosol C-117

[5957-80-2]
11,12-Dihydroxy-8,11,13-abietatrien-20,7-olide. Picrosalvin



$C_{20}H_{26}O_4$ 330.423

Bitter principle in *Salvia carnosa, Salvia officinalis* (sage), *Salvia triloba* (Greek sage) and *Rosmarinus officinalis* (rosemary). Nutriceutical with anticancer props.. Cryst. (EtOH). Mp 221-226°. $[\alpha]_D$ -66 (EtOH). λ_{max} 210 (ϵ 26300); 283 (ϵ 2510) (EtOH) (Berdy).

Di-Me ether: [25460-12-2] ***11,12-Dimethoxy-8,11,13-abietatrien-20,7-olide***
$C_{22}H_{30}O_4$ 358.477
Constit. of *Salvia columbariae* (California chia). Cryst. ($CHCl_3$). Mp 155-156°. $[\alpha]_D$ -73.5 (c, 0.95 in $CHCl_3$).

6α-Hydroxy: [93780-80-4] *6,11,12-Trihydroxy-8,11,13-abietatrien-20,7-olide.* ***Isorosmanol***
$C_{20}H_{26}O_5$ 346.422
Constit. of *Rosmarinus officinalis* (rosemary). Cryst. Mp 227°.

16-Acetoxy: ***16-Acetoxycarnosol***
$C_{22}H_{28}O_6$ 388.46
Amorph. solid.

12-Deoxy, 14-hydroxy: [92519-82-9] *11,14-Dihydroxy-8,11,13-abietatrien-20,7-olide.* ***Isocarnosol***
$C_{20}H_{26}O_4$ 330.423
Cryst. (MeOH). Mp 216°. $[\alpha]_D^{20}$ -80 (c, 0.2 in $CHCl_3$).

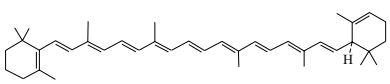
Deoxo:7,20-Epoxy-8,11,13-abietatriene-11,12-diol. ***20-Deoxocarnosol***
$C_{20}H_{28}O_3$ 316.439
Yellow solid (CH_2Cl_2/hexane). Mp 173.5-175.5°. $[\alpha]_D$ -78.8 (c, 1 in $CHCl_3$).

Deoxo, O^{12}*-Me:* ***Deoxycarnosol 12-methyl ether***
$C_{21}H_{30}O_3$ 330.466
Cryst. Mp 188-190°.

Brieskorn, C.H. *et al., J.O.C.*, 1964, **29**, 2293 (*struct, biosynth*)
Narayanan, C.R. *et al., Tet. Lett.*, 1965, 3647 (*stereochem*)
Meyer, W.L. *et al., J.O.C.*, 1976, **41**, 1005 (*synth*)
Nakatani, N. *et al., Agric. Biol. Chem.*, 1984, **48**, 2081 (*Isorosmanol*)
Al-Hazimi, H.M.G. *et al., Phytochemistry*, 1984, **23**, 919 (*Isocarnosol*)
Kelecom, A. *et al., Phytochemistry*, 1984, **23**, 1677 (*Deoxocarnosol*)
Fraga, B.M. *et al., Phytochemistry*, 1986, **25**, 269 (*deriv*)
Luis, J.G. *et al., Phytochemistry*, 1991, **31**, 3272 (*16-Acetoxycarnosol*)
Luis, J.G. *et al., Phytochemistry*, 1994, **35**, 1373 (*di-Me ether*)

α-Carotene C-118

[432-70-2]
β,ϵ-Carotene, 9CI



$C_{40}H_{56}$ 536.882Log P 15.2 (uncertain value) (calc).
λ_{max} 418 ; 442 ; 471 (hexane) (Berdy).

(R)-form [7488-99-5]
Widespread carotenoid, e.g. in carrots and palm oil. Has vitamin A activity but less than that of β-Carotene. Violet prisms (petrol). Mp 187°. $[\alpha]_{643}^{18}$ +385 (C_6H_6). λ_{max} 446 ; 478 ; 511 (CS_2). λ_{max} 418 ; 442 ; 471 (hexane).

5,6-Epoxide: See α-Carotene 5,6-epoxide in *The Combined Chemical Dictionary.*

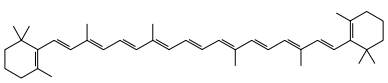
(±)-form
Violet platelets (C_6H_6). Mp 160-162°.

Karrer, P. *et al., Helv. Chim. Acta*, 1933, **16**, 975 (*struct*)
Karrer, P. *et al., Helv. Chim. Acta*, 1950, **33**, 1952 (*synth*)
Tscharner, C. *et al., Helv. Chim. Acta*, 1957, **40**, 1676 (*synth*)
Rüegg, R. *et al., Helv. Chim. Acta*, 1961, **44**, 985 (*synth*)
Strain, H.H. *et al., J.O.C.*, 1961, **26**, 5061 (*ir*)
Goodwin, T.W. *et al., Biochem. J.*, 1965, **97**, 28c (*biosynth*)
Eugster, C.H. *et al., Helv. Chim. Acta*, 1969, **52**, 1729 (*abs config*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1971, **54**, 327 (*uv, cd*)
Kjoesen, H. *et al., Acta Chem. Scand.*, 1972, **26**, 3053 (*pmr, ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1824 (*occur*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 7 (*bibl*)
Broszeit, G. *et al., Liebigs Ann./Recl.*, 1997, 2205-2213 (*synth, pmr, cmr, ir*)

β-Carotene C-119

[7235-40-7]

[116-32-5]
Betacarotene, INN, USAN. *Carotaben. Phenoro. Solatene. β,β-Carotene. Provatene. E160a*



$C_{40}H_{56}$ 536.882
Yellow food colour, dietary supplement, nutrient, Vitamin A precursor. Nutriceutical with antioxidation props.. Deep purple prisms (C_6H_6/MeOH); red rhombs. (petrol). Sol. CS_2, hexane, C_6H_6; fairly sol. MeOH, Et_2O, $CHCl_3$; poorly sol. H_2O. Mp 183° (sealed tube). Log P 15.23 (uncertain value) (calc). Air-sensitive λ_{max} 452 ; 484 ; 520 (CS_2).
► Produces yellow skin discolouration when used therapeutically. FI0329500

5,6-Epoxide: See β-Carotene epoxide in *The Combined Chemical Dictionary.*

5,6:5′,6-Diepoxide: See β-Carotene diepoxide in *The Combined Chemical Dictionary.*

7,7′,8,8′-Tetrahydro: [40772-88-1] *7,7′,8,8′-Tetrahydro-β,β-carotene.* ***η-Carotene***
$C_{40}H_{60}$ 540.914
Isol. from the flavedo of Sinton citrangequat (a *Citrus-Poncirus-Fortunella* hybrid). Poorly characterised λ_{max} 376 ; 397 ; 422 (petrol).

(9Z)-form [19361-58-1]

[13312-52-2]
λ_{max} 276 ; 350 ; 455 (CH_2Cl_2).

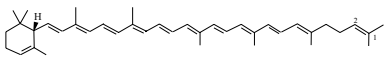
(13Z)-form [6811-73-0]
Neo-β-carotene. Pseudo-α-carotene. β,β-Carotene neo B
Constit. of carrots and other plant spp..

[1465-77-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 54A (*ir*)
Aldrich Library of ^{13}C *and* ^1H *FT NMR Spectra*, 1992, **1**, 71C (*nmr*)
Willstätter, R. *et al., Annalen*, 1907, **355**, 1 (*struct*)
Willstätter, R. *et al., Z. Physiol. Chem.*, 1910, **64**, 47 (*isol*)
Karrer, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1950, **250**, 1920 (*synth*)
Surmatis, J.D. *et al., J.O.C.*, 1961, **26**, 1171 (*synth*)
Sterling, C. *et al., Acta Cryst.*, 1964, **17**, 1224 (*cryst struct*)
Schweiter, U. *et al., Chimia*, 1965, **19**, 294 (*props*)
Yokoyama, H. *et al., Phytochemistry*, 1966, **5**, 1159 (*tetrahydro*)
Yokoyama, H. *et al., J. Agric. Food Chem.*, 1967, **15**, 693 (*tetrahydro*)
Surmatis, J.D. *et al., J.O.C.*, 1969, **34**, 559 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1821 (*occur*)
Johannes, B. *et al., Org. Mass Spectrom.*, 1974, **9**, 1095 (*ms*)
Fischli, A. *et al., Helv. Chim. Acta*, 1975, **58**, 1584 (*synth*)
Ishida, A. *et al., Chem. Lett.*, 1976, 1127 (*synth*)
Bickel, H. *et al., Phytochemistry*, 1976, **15**, 1253 (*biosynth*)
Bramley, P.M. *et al., Phytochemistry*, 1976, **15**, 1913 (*biosynth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*pmr*)
Ninet, L. *et al., Microb. Technol.*, 2nd edn., (eds. Peppler, H.J. *et al*), Academic Press, 1979, **1**, 529 (*manuf, rev*)
Wernly, J. *et al., Chem. Comm.*, 1985, 1221 (*pmr, cmr*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987,
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CCK685
Koyama, Y. *et al., J. Mol. Struct.*, 1989, **193**, 185 (*pmr*)
Bjonland, T. *et al., Phytochemistry*, 1989, **28**, 3347 (*isol, pmr*)
Bernhard, K. *et al., Pure Appl. Chem.*, 1991, **63**, 35 (*synth*)
Senge, M.O. *et al., Z. Naturforsch., C*, 1992, **47**, 474 (*cryst struct*)
Ebenezer, W.J. *et al., J.C.S. Perkin 1*, 1993, 1869 (*9Z-form*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1036
Doering, W. von E. *et al., J.A.C.S.*, 1995, **117**, 2747 (*synth, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 497-500 (*use, props*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1997, 269 (*biosynth*)
Rauchschwalbe, G. *et al., Eur. J. Org. Chem.*, 2001, 3903-3909 (*synth*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 194
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCK685

δ-Carotene C-120

[472-92-4]
ϵ,ψ-Carotene



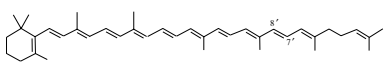
$C_{40}H_{56}$ 536.882
Found in carrots and tomatoes. Red cryst. Mp 172°. $[\alpha]_D^{25}$ +352 (hexane). λ_{max} 280 ; 431 ; 456 ; 488 (no solvent reported).

1′,2′-Epoxide: [58556-44-8] ***δ-Carotene-1,2-epoxide***. *1′,2′-Epoxy-1′,2′-dihydro-ϵ,ψ-carotene*
$C_{40}H_{56}O$ 552.882
Isol. from delta tomatoes. Deep red cryst. (CH_2Cl_2/MeOH). Mp 153-155°. λ_{max} 231 (ϵ 10800) (MeOH) (Derep).

Porter, J.W. *et al., Arch. Biochem. Biophys.*, 1951, **32**, 21 (*isol, struct*)
Kargl, T.E. *et al., Arch. Biochem. Biophys.*, 1960, **88**, 59 (*struct*)
Manchand, P.S. *et al., J.C.S.*, 1965, 2019 (*synth*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1971, **54**, 327 (*abs config*)
Britton, G. *et al., Phytochemistry*, 1975, **14**, 2530 (*occur, epoxide*)
Pfander, H. *et al., Helv. Chim. Acta*, 1980, **63**, 1792 (*synth, uv, pmr, ms*)
Berset, D. *et al., Helv. Chim. Acta*, 1986, **69**, 340 (*occur, uv, pmr, ms, epoxide*)

γ-Carotene C-121

[472-93-5]
β,ψ-Carotene. Sphaerobolin

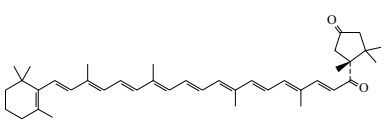


$C_{40}H_{56}$ 536.882
Violet prisms (C_6H_6/petrol). Mp 178° (154°). Log P 15.04 (uncertain value) (calc).

7′,8′-Dihydro: [514-90-9] ***β-Zeacarotene***. *Carotene X. 7′,8′-Dihydro-β,ψ-carotene*
$C_{40}H_{58}$ 538.898
Isol. from sweet corn (*Zea mays*) grains and *Citrus* spp.. Orange-yellow platelets (Me_2CO). Mp 96-97°.

Petzold, E.N. *et al., Arch. Biochem. Biophys.*, 1959, **82**, 117-124 (*β-Zeacarotene, isol*)
Rüegg, R. *et al., Helv. Chim. Acta*, 1961, **44**, 994 (*synth, β-Zeacarotene*)
Williams, R.J.H. *et al., Phytochemistry*, 1965, **4**, 759 (*β-Zeacarotene*)

β,χ-Carotene-3′,6′-dione C-122

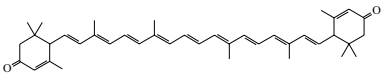


$C_{40}H_{54}O_2$ 566.865
(5′*R*)-*form* [89195-47-1]
Cryptocapsone
Prepd. by Oppenauer oxidn. of red paprika (ex *Capsicum annuum*) capsanthin and cryptocapsin (see Capsanthin, C-76). Fine violet cryst. (C_6H_6/MeOH). Mp 182° (171°). Details of isol. not accessible, not abstracted by CAS λ_{max} 285 ; 295 ; 480 (hexane).

Cholnoky, L. *et al., Tet. Lett.*, 1963, 1257
Neamtu, G. *et al., Stud. Cercet. Biochim.*, 1974, **17**, 41 (*isol*)
Rüttimann, A. *et al., Helv. Chim. Acta*, 1983, **66**, 1939
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 382

ϵ,ϵ-Carotene-3,3′-dione C-123

[28840-14-4]



$C_{40}H_{52}O_2$ 564.85
Constit. of *Sebastes flavidus* and other fish. Also found in chitons. Light red cryst. (CH_2Cl_2/Et_2O). Mp 194°.

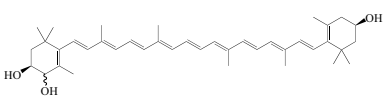
(6*S*,6′*S*)-*form* [97169-05-6]
Isol. from marine fish-eggs and egg yolk. λ_{max} 415 ; 438 ; 468 (petrol).

[57545-55-8, 82880-34-0, 82915-88-6, 97169-05-6]

Surmatis, J.D. *et al., Helv. Chim. Acta*, 1970, **53**, 974 (*synth, uv, pmr*)
Widmer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 958 (*synth*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779 (*isol*)
Ikuno, Y. *et al., J. Chromatogr.*, 1985, **328**, 387 (*resoln*)
Ikuno, Y. *et al., Nippon Suisan Gakkaishi*, 1985, **51**, 2033 (*occur*)
Tsushima, M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **93**, 665 (*occur*)

β,β-Carotene-3,3′,4-triol C-124

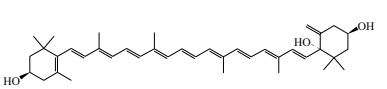
[70800-74-7]



$C_{40}H_{56}O_3$ 584.881
(3*S*,3′*R*,4ξ)-*form* [97134-07-1]
Isol. as a minor constituent from the crustacean *Euchaeta russelli* and from eggs of mackerel, yellow tail, dolphin and flying fish. λ_{max} 423 ; 450 ; 473 (hexane). λ_{max} 425 ; 450 ; 475 (EtOH).

Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **72**, 409 (*isol*)
Matsumo, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779 (*occur, biosynth*)

β,γ-Carotene-3,3′,6′-triol C-125

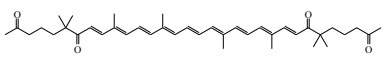


$C_{40}H_{56}O_3$ 584.881
(3*R*,3′*S*,6′*S*)-*form* [334490-57-2]
Prenigroxanthin
Constit. of the ripe pods of red paprika *Capsicum annuum* var. *longum*. λ_{max} 434 ; 457 ; 487 (C_6H_6).

Deli, J. *et al., Tet. Lett.*, 2001, **42**, 1395-1397 (*isol, pmr, cmr*)

β-Carotenone C-126

[20126-74-3]
5,6:5′,6′-Diseco-β,β-carotene-5,5′,6,6′-tetrone

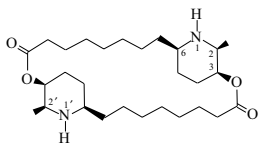


$C_{40}H_{56}O_4$ 600.88
Isol. from *Triphasia trifolia* (limeberry). Purple leaflets (C_6H_6). Mp 174-175°.

Kuhn, R. *et al., Ber.*, 1932, **65**, 894 (*synth*)
Yokoyama, H. *et al., Phytochemistry*, 1968, **7**, 1031 (*isol*)

Carpaine, 9CI C-127

[3463-92-1]



Absolute configuration

$C_{28}H_{50}N_2O_4$ 478.714
Homologue of Azimine. Originally considered to be a monomeric 13-membered cyclic lactone. Alkaloid from leaves of *Carica papaya* (papaya). Cubes (Et_2O). Sol. MeOH, C_6H_6; poorly sol. hexane. Mp 119-120° (117-118.5°). $[\alpha]_D$ +21.65 (c, 1.0 in EtOH). $[\alpha]_{230}^{22}$ -240 (c, 0.12 in MeOH). Log P 4.77 (calc). Prob. formed *in vivo* by dimerisation of Carpamic acid, from which it has been made *in vitro*.

1,2-Didehydro: [72362-02-8] ***Dehydrocarpaine I***. *12,13-Didehydrocarpaine, 9CI*
$C_{28}H_{48}N_2O_4$ 476.698
Alkaloid from the leaves of *Carica papaya* (papaya). Viscous oil.

1,1′,2,2′-Tetradehydro: [72362-03-9] ***Dehydrocarpaine II***. *12,13,25,26-Tetradehydrocarpaine, 9CI*
$C_{28}H_{46}N_2O_4$ 474.682
Alkaloid from the leaves of *Carica papaya* (papaya). Viscous oil.

2-Epimer: [3760-91-6] ***Pseudocarpaine***. *ψ-Carpaine*
$C_{28}H_{50}N_2O_4$ 478.714
Minor alkaloid from leaves of *Carica papaya* (papaya). Cryst. (petrol). Mp 65-68°. $[\alpha]_D^{28}$ +4.95 (c, 1.62 in EtOH). Yields carpamic and pseudocarpamic acids on hydrol..

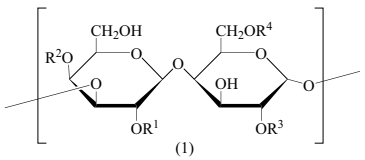
2-Epimer, hydrochloride:
Cryst. (EtOH). Mp 295°.

Greshoff, M. *et al., Ber.*, 1890, **23**, 3537 (*isol*)
Govindachari, T.R. *et al., J.C.S.*, 1954, 1847; 1955, 1563 (*isol, props, Carpaine, Pseudocarpaine*)
Narasimhan, N.S. *et al., Chem. Ind. (London)*, 1956, 1526 (*synth*)
Spiteller-Friedmann, M. *et al., Monatsh. Chem.*, 1964, **95**, 1234 (*ms, struct*)
Coke, J.L. *et al., J.O.C.*, 1965, **30**, 3420 (*abs config*)
Govindachari, T.R. *et al., Tet. Lett.*, 1965, 1907 (*ms, pmr, struct*)
Brown, E. *et al., Chem. Lett.*, 1974, 109 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1975, **97**, 654 (*synth*)

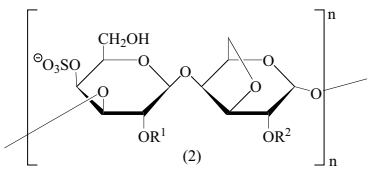
Topuriya, L.I. *et al., Khim. Prir. Soedin.*, 1978, 414; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, 354 (*isol*)
Tang, C.-S. *et al., Phytochemistry*, 1979, **18**, 651 (*Dehydrocarpaines*)
Hanessian, S. *et al., Tet. Lett.*, 1979, 3391 (*synth*)
Natsume, M. *et al., Heterocycles*, 1980, **14**, 169 (*synth*)
Rajnikant, G. *et al., Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. C*, 1998, **9**, 131-137 (*cryst struct*)

Carrageenan C-128

[9000-07-1]
Carrageenin. Carragheen. Genuvisco J. FEMA 2596. E407



(1)



(2)

A complex mixt. of polysaccharides composed of galactans, the proportions of which vary with spp., season and environment. The major structural feature is β(1→3) and α(1→4) linked galactose units with various degrees and sites of sulfation (sulfate ester content 15-40%). The Greek prefixes denote the idealised constitution of different disaccharide units although native carrageenans show variation from these idealised structs. The struct. also varies during life-cycle of the alga. Used for gelling, thickening and emulsion stabilisation of foods (salts may also be used). Sol. H_2O; fairly sol. DMSO; poorly sol. oils, MeOH, hexane. ν component also referred to in the lit. alongside those descr. below.

►FI0700000

μ-*form* [51311-96-7] Structure (1) with R^1 = R^3 = H, R^2 = R^4 = $SO_3^{\ominus}$. Minor fraction of carrageenan samples.

λ-*form* [9064-57-7]
*Picnin A*Structure (1) with R^1 = R^3 = R^4 = $SO_3^{\ominus}$, R^2 = H. Major fraction.

►FI0704000

ϵ-*form* [51311-95-6] Structure (1) with R^1 = R^3 = $SO_3^{\ominus}$, R^2 = R^4 = H.

ι-*form* [9062-07-1] Structure (2) with R^1 = H, R^2 = $SO_3^{\ominus}$. Major fraction.

κ-*form* [11114-20-8] Structure (2) with R^1 = R^2= H. Major fraction.

►FI0703000

ξ-*form* [70431-33-3] Structure (1) with R^1 = R^3= $SO_3^{\ominus}$, R^2 = R^4 = H.

π-*form* [71078-00-7] Structure (1) with R^1 = R^3 = $SO_3^{\ominus}$, R^4 = H, C_4-C_6 pyruvate bridge in left-hand residue.

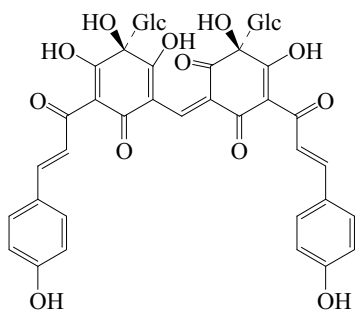
u-*form* Structure (2) with R^1 = R^2 = $SO_3^{\ominus}$.

[8015-95-0, 8036-85-9, 60063-90-3, 64366-24-1]

O'Neill, A.N. *et al., J.A.C.S.*, 1955, **77**, 2837-2839; 6324-6326 (*κ-form, isol, struct*)
Dolan, T.C.S. *et al., J.C.S.*, 1965, 3534-3539 (*λ-form, struct*)
Painter, T.J. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 98-100 (*κ-form, isol*)
Rees, D.A. *et al., Adv. Carbohydr. Chem.*, 1969, **24**, 267-332 (*rev*)
Penman, A. *et al., J.C.S. Perkin 1*, 1973, 2191-2196 (*κ-form, struct*)
Millane, R.P. *et al., Carbohydr. Res.*, 1988, **182**, 1-17 (*κ-form, struct, bibl*)
Falshaw, R. *et al., Carbohydr. Res.*, 1995, **276**, 155-165 (*ξ-form, isol, bibl*)
Chiovitti, A. *et al., Carbohydr. Res.*, 1997, **299**, 229-243 (*isol*)
Arndt, E.R. *et al., Carbohydr. Res.*, 1997, **303**, 73-78 (*cd, struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 500-516 (*props, use*)
Janaswamy, S. *et al., Carbohydr. Res.*, 2001, **335**, 181-194 (*ι-form, struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCL250; CCL350

Carthamin C-129

[36338-96-2]
C.I. Natural Red 26



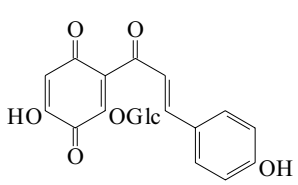
Absolute Configuration

$C_{43}H_{42}O_{22}$ 910.792
Red pigment of flower petals of *Carthamus tinctorius* (safflower). Red needles (Py). Mp 228-230°.

Takahashi, Y. *et al., Tet. Lett.*, 1982, **23**, 5163 (*struct*)
Obara, H. *et al., Chem. Lett.*, 1986, 495 (*synth*)
Nakano, K. *et al., J. Chromatogr.*, 1988, **438**, 61 (*hplc*)
Saito, K. *et al., Biochem. Physiol. Pflanz.*, 1989, **184**, 145 (*isol*)
Sato, S. *et al., Chem. Lett.*, 1996, 833 (*synth, cd, cryst struct, abs config*)
Watanabe, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1179-1183 (*anal*)

Carthamone C-130

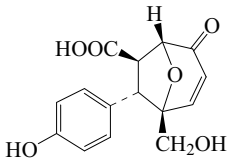
[86579-00-2]



$C_{21}H_{20}O_{11}$ 448.382
Incorr. abstracted in CA as lacking the glucosyl group. Isol. from flowers of *Carthamus tinctorius* (safflower). Red pigment.

Seshadri, T.R. *et al., Curr. Sci.*, 1960, **29**, 54
Harborne, J.B. *et al., Comp. Biochem. of the Flavonoids*, Academic Press, 1967, 80

Cartorimine C-131

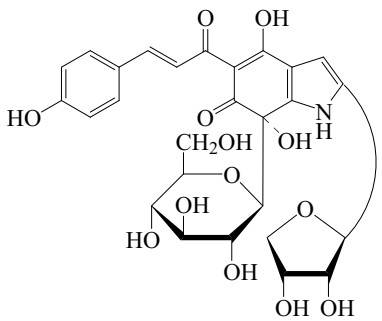


Relative Configuration

$C_{15}H_{14}O_6$ 290.272
Constit. of *Carthamus tinctorius* (safflower). Prims (MeOH). Mp 206-207°. $[\alpha]_D^{25}$ -2.6 (c, 0.005 in MeOH). λ_{max} 225 (log ϵ 4.04) (MeOH).

Yin, H.-B. *et al., J. Nat. Prod.*, 2000, **63**, 1164-1165

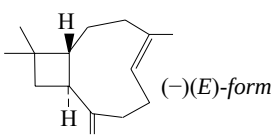
Cartormin C-132



$C_{27}H_{29}NO_{13}$ 575.525
Enolised β-diketone. Constit. of *Carthamus tinctorius* (safflower). Yellow prisms (MeOH). $[\alpha]_D^{27}$ -153.4 (c, 0.01 in Py). Mp >230° dec..

Yin, H.-B. *et al., Tet. Lett.*, 2000, **41**, 1955-1958 (*isol, pmr, cmr, ms, cryst struct*)

3(15),6-Caryophylladiene C-133



(−)(*E*)-*form*

$C_{15}H_{24}$ 204.355

(-)-(*E*)-*form* [87-44-5]
β-Caryophyllene. *β-Humulene (obsol.). Caryophyllene. Tincturoid. FEMA 2252*
Constit. of clove, cinnamon, mint, eucalyptus, thyme, lemon balm and many other oils. The main source is the clove tree *Eugenia caryophyllata*. Flavouring agent. Oil with v. faint odour. $Bp_{9.7}$ 118-119°. $[\alpha]_D^{21}$ -15 (c, 2.6 in $CHCl_3$).

►Skin irritant. Fl. p. 97°. DT8400000

2-Epimer: [68832-35-9] ***2-Epicaryophyllene***. *9βH-Caryophyllene*

$C_{15}H_{24}$ 204.355
Waxy solid. $[\alpha]_D$ +196 ($CHCl_3$).

3β,15-Epoxide: [88395-50-0] ***3,15-Epoxy-6-caryophyllene***
$C_{15}H_{24}O$ 220.354
Constit. of clary sage oil (*Salvia sclarea*). Oil. $[\alpha]_D$ +40 (c, 3.4 in $CHCl_3$).

(-)-(*Z*)-*form* [118-65-0]
γ-Caryophyllene. *Isocaryophyllene*
Widespread in plants (*Jasminum, Origanum* and *Pimpinella* spp.). Oil. $Bp_{14.5}$ 125°. $[\alpha]_D^{24}$ -27.

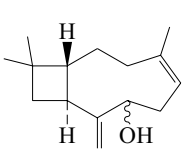
(+)-(*E*)-*form*
(+)-β-Caryophyllene

[33993-33-8, 54061-81-3, 61217-74-1]

Barton, D.H.R. *et al., Q. Rev., Chem. Soc.*, 1957, **11**, 189 (*rev*)
Corey, E.J. *et al., J.A.C.S.*, 1964, **86**, 485 (*synth, bibl*)
Hill, H.C. *et al., J.C.S.(C)*, 1968, 93 (*ms*)
Gollnick, K. *et al., Tet. Lett.*, 1968, 689 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1929 (*occur*)
Croteau, R. *et al., Phytochemistry*, 1972, **11**, 1055 (*biosynth*)
Warnhoff, E.W. *et al., Can. J. Chem.*, 1973, **51**, 3955 (*purifn*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1059 (*rev, tox*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Robertson, J. *et al., Int. Rev. Sci.: Phys. Chem., Ser. Two*, 1975, **11**, 57 (*rev*)
Kumar, A. *et al., Synthesis*, 1976, 461 (*synth*)
Peyron, L. *et al., Riv. Ital. Essenze, Profumi, Piante Off., Aromi, Saponi, Cosmet., Aerosol*, 1977, **59**, 603 (*rev*)
Mauer, B. *et al., Helv. Chim. Acta*, 1983, **66**, 2223 (*epoxide*)
McMurry, J.E. *et al., Tet. Lett.*, 1983, **24**, 1885 (*synth*)
Ohtsuka, Y. *et al., J.O.C.*, 1984, **49**, 2326 (*synth*)
Berry, K.M. *et al., Phytochemistry*, 1985, **24**, 2893 (*2-Epicaryophyllene*)
Hinkley, S.F.R. *et al., Phytochemistry*, 1994, **35**, 1489 (*2-Epicaryophyllene, abs config*)
Suginome, H. *et al., J.C.S. Perkin 1*, 1995, 69 (*synth*)
Fricke, C. *et al., Phytochemistry*, 1995, **39**, 1119 (*(+)-β-Caryophyllene*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 527-528 (*β-Caryophyllene, occur*)
Collado, I.G. *et al., Nat. Prod. Rep.*, 1998, 187-204 (***rev***)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCN000

3(15),6-Caryophylladien-4-ol C-134

[487-87-6]
6,10,10-Trimethyl-2-methylenebicyclo[7.2.0]undec-5-en-3-ol, 9CI. ***β-Betulenol***



Absolute configuration

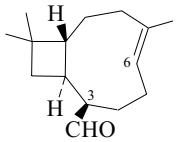
$C_{15}H_{24}O$ 220.354
Constit. of essential oil of peppermint (*Mentha piperita*) and palmarosa (*Cymbopogon martini*). Oil. Bp_{20} 157-158°. $[\alpha]_D^{20}$ -36.

[6040-49-9, 20296-32-6]

Holub, M. *et al., Coll. Czech. Chem. Comm.*, 1959, **24**, 3730 (*struct*)
Treibs, W. *et al., Annalen*, 1960, **634**, 124 (*synth*)
Naves, Y.R. *et al., Parfums, Cosmet. Savons Fr.*, 1970, **13**, 354 (*props*)

6-Caryophyllen-15-al C-135

6,10,10-Trimethylbicyclo[7.2.0]undec-5-ene-2-carboxaldehyde, 9CI



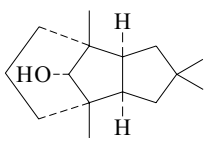
(3*R*,6*E*)-*form*

$C_{15}H_{24}O$ 220.354
(3*R*,6*E*)-*form* [88395-49-7]
Constit. of Clary sage oil (*Salvia sclarea*). Oil. $[\alpha]_D$ +6.7 (c, 1.1 in $CHCl_3$).
(3*S*,6*E*)-*form* [88424-68-4]
From Clary sage oil (*Salvia sclarea*). Oil. $[\alpha]_D$ -21.9 (c, 1.1 in $CHCl_3$).

Maurer, B. *et al., Helv. Chim. Acta*, 1983, **66**, 2223

α-Caryophyllene alcohol C-136

[4586-22-5]
Decahydro-2,2,4,8-tetramethyl-4,8-methanoazulen-9-ol, 9CI. Apollanol



$C_{15}H_{26}O$ 222.37
Constit. of *Cedrus atlantica*. Flavouring ingredient either alone or together with iβ-Caryophyllene alcohol, C-137, with a slightly minty, earthy flavour. Cryst. Mp 118.5-119.5°. Bp_{10} 143-152°. Opt. inactive (*meso-*).

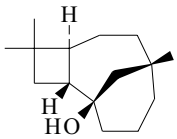
Ac: [17622-35-4]
$C_{17}H_{28}O_2$ 264.407
Flavouring ingredient.

Corey, E.J. *et al., J.A.C.S.*, 1965, **87**, 5733 (*synth*)
Gemmell, K.W. *et al., J.C.S.(B)*, 1970, 947 (*cryst struct*)
Adams, D.R. *et al., J.C.S. Perkin 1*, 1975, 1502 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 111
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 528-530 (*props, use*)

β-Caryophyllene alcohol C-137

[472-97-9]

[58404-89-0, 129445-45-0]
4,4,8-Trimethyltricyclo[6.3.1.0^{2,5}]dodecan-1-ol, 9CI



$C_{15}H_{26}O$ 222.37
Constit. of grapefruit juice, pimento berry, Korean chamchwi and the essential oils of Palmarosa, peppermint, clove, hop, pepper, bergamot and Sicilian sumac fruit (*Rhus coriaria*). Flavouring ingredient either alone or together with α-Caryophyllene alcohol, C-136. Cryst. Mp 94-96°. Bp 287-297°.

Ac: [62532-51-8]

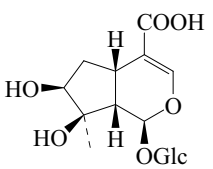
[57082-24-3]
$C_{17}H_{28}O_2$ 264.407
Flavouring ingredient. Not reported in nature. Cryst. with mild fruity and woody odour. d_4^{17} 1.003. Mp 40°. Bp_{10} 149-152°. n_D^{17} 1.4919.

[56747-96-7, 82008-48-8]

Naves, Y. *et al., Parfums, Cosmet. Savons Fr.*, 1970, **13**, 354 (*isol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, 839 (*Ac, use, props*)
Barrow, C.J. *et al., Aust. J. Chem.*, 1988, **41**, 1755 (*pmr, cmr*)
Iwabuchi, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1405-1407 (*synth*)
Vernin, G. *et al., Dev. Food Sci.*, 1994, **34**, 483-500 (*glc, detn, clove oil*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 528; 529; 530 (*props, use, occur, Ac*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 263-264 (*use, props, Ac*)

Caryoptosidic acid C-138

[220271-92-1]



$C_{16}H_{24}O_{11}$ 392.359
Constit. of *Lippia graveolens* (Mexican oregano). $[\alpha]_D^{25}$ -128.6 (c, 1 in MeOH).

Me ester: [139687-24-4] ***Caryoptoside***. *5-Desoxylamiide*
$C_{17}H_{26}O_{11}$ 406.386
Mp 137-139° (as penta-Ac).

6′-(4-Hydroxycinnamoyl)(E-): [220271-93-2] ***Lippioside I***
$C_{25}H_{30}O_{13}$ 538.504
Constit. of *Lippia graveolens* (Mexican oregano). $[\alpha]_D^{25}$ -127.5 (c, 1 in MeOH).

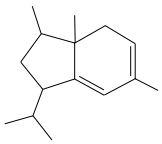
6′-(3,4-Dihydroxycinnamoyl)(E-): [220271-94-3] ***Lippioside II***
$C_{25}H_{30}O_{14}$ 554.504
Constit. of *Lippia graveolens* (Mexican oregano). $[\alpha]_D^{25}$ -126.3 (c, 1 in MeOH).

El-Naggar, L.J. *et al., J. Nat. Prod.*, 1980, **43**, 649 (*Caryoptoside*)
Damtoft, S. *et al., Phytochemistry*, 1992, **31**, 175 (*Caryoptoside*)

Rastrelli, L. *et al., Phytochemistry*, 1998, **49**, 1829-1832 (*Caryoptosidic acid, Lippiosides*)

Cascarilladiene C-139

[59742-39-1]



$C_{15}H_{24}$ 204.355
Constit. of oil of *Croton eleuteria* (cascarilla). Oil.

Claude-Lafontaine, A. *et al., Bull. Soc. Chim. Fr.*, 1976, 88

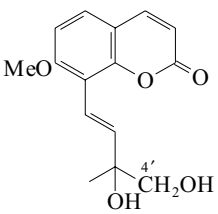
Cascocidin I C-140

Peptide; a 39 amino-acid fragment of bovine α s-2 casein (position 165-203). Isol. from bovine milk. Shows antibacterial activity.

Zucht, H.D. *et al., FEBS Lett.*, 1995, **372**, 185-188

Casegravol C-141

[74474-76-3]



$C_{15}H_{16}O_5$ 276.288
Needles ($CHCl_3$/hexane). Mp 158°. $[\alpha]_D$ 0 ($CHCl_3$).

4′-O-*(3-Methylbutanoyl):* ***Casegravol isovalerate***
$C_{20}H_{24}O_6$ 360.406
Constit. of *Citrus unshiu* (satsuma mandarin). Amorph. solid. $[\alpha]_D$ 0 ($CHCl_3$).

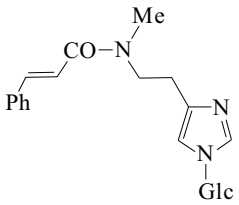
1′,2′-Epoxide, 4′-O-*(3-methylbutanoyl):*
$C_{20}H_{24}O_7$ 376.405
Oil. $[\alpha]_D$ +25 (c, 0.1 in $CHCl_3$).

*(*Z*)-Isomer:* **cis-*Casegravol***
Oil. $[\alpha]_D$ -12.1 (c, 0.102 in $CHCl_3$).

Talapatra, S.K. *et al., Chem. Ind. (London)*, 1980, 154 (*Casegravol*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2217 (*Casegravol isovalerate*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2509 (*cis-Casegravol*)
Quader, M.A. *et al., Phytochemistry*, 1992, **31**, 3083 (*deriv*)

Casimiroedine C-142

N-*[2-(1-β-D-Glucopyranosyl-1*H*-imidazol-4-yl)ethyl]*-N-*methyl-3-phenyl-2-propenamide, 9CI. N*$^{\alpha}$*-Cinnamoyl-N*$^{\alpha}$*-methylhistamine* N-*glucoside*



$C_{21}H_{27}N_3O_6$ 417.461Log P -2.06 (calc).

(E)-form [5853-02-1]
Alkaloid from the seeds of *Casimiroa edulis* (Mexican apple). Cryst. (EtOH). Mp 226.5-228° (223-224°). $[\alpha]_D^{20}$ -21.3 (c, 1.2 in 5% HCl aq.) (-27, -30.7). Pharmacol. active isomer.

Picrate:
Mp 110-112°.

Tetra-O-*Ac:*
Mp 80°.

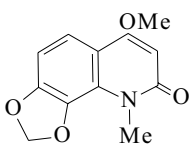
Tetrabenzoyl:
Mp 97-105°. $[\alpha]_D$ +29 (EtOH).

(Z)-form [51013-83-3]
Cryst. (EtOH). Mp 187-189°. $[\alpha]_D^{27}$ +10.65 (c, 1.00 in 1% HCl).

Power, F.B. *et al., J.C.S.*, 1911, 1993 (*isol*)
Aebi, A. *et al., Helv. Chim. Acta*, 1956, **39**, 1495 (*isol, ir, uv*)
Djerassi, C. *et al., Tetrahedron*, 1958, **2**, 168a (*struct*)
Raman, S. *et al., Tet. Lett.*, 1962, 357 (*cryst struct*)
Panzica, R.P. *et al., J.A.C.S.*, 1973, **95**, 8737 (*uv, pmr, ms, synth, struct*)
Reynolds, W.F. *et al., Magn. Reson. Chem.*, 2000, **38**, 366-369 (*pmr, cmr*)

Casimiroin C-143

[477-89-4]
*6-Methoxy-9-methyl-1,3-dioxolo[4,5-*h*]quinolin-8(*9H*)-one, 9CI. 4-Methoxy-1-methyl-7,8-methylenedioxy-2(*1H*)-quinolinone*



$C_{12}H_{11}NO_4$ 233.223
Alkaloid from the seed and bark of *Casimiroa edulis* (Mexican apple). Cryst. (Me_2CO/hexane). Mp 202-203°. λ_{max} 226 ; 236 ; 260 ; 300 (MeOH) (Berdy). λ_{max} 232 ; 262 (ε 8); 465 (EtOH) (Berdy).

Kincl, F.A. *et al., J.C.S.*, 1956, 4163 (*isol, uv, ir*)
Iriarte, J. *et al., J.C.S.*, 1956, 4170 (*isol*)
Meisels, A. *et al., J.A.C.S.*, 1957, **79**, 6328 (*struct*)
Weinstein, B. *et al., Tetrahedron*, 1964, **20**, 1725 (*synth, uv, ir*)

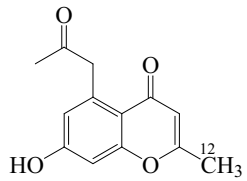
Casoxin D C-144

[134027-58-0]
H-Tyr-Val-Pro-Phe-Pro-Pro-Phe-OH
$C_{47}H_{59}N_7O_9$ 866.025
Isol. from the proteolytic digest of human milk casein.

Yoshikawa, M. *et al., Regul. Pept.*, *Suppl. 1*, 1994, 253
Kato, M. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2056 (*prodn*)

Cassiachromone C-145

[28955-30-8]
*7-Hydroxy-2-methyl-5-(2-oxopropyl)-4*H*-1-benzopyran-4-one, 9CI. 5-Acetonyl-7-hydroxy-2-methylchromone, 8CI*



$C_{13}H_{12}O_4$ 232.235
Isol. from *Rheum* sp. (rhubarb). Yellow-green cryst. (Me_2CO). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 210°. λ_{max} 221 (ε 18000); 243 (ε 16100); 251 (ε 16400); 293 (ε 11400) (MeOH) (Berdy).

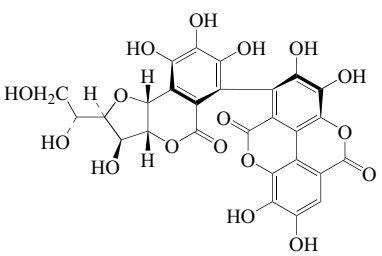
O-*β-D-Glucopyranoside:* [83117-59-3]
$C_{19}H_{22}O_9$ 394.377
Cryst. (EtOAc/petrol). Mp 260° dec.

12-Hydroxy: ***7-Hydroxy-2-hydroxymethyl-5-(2-oxopropyl)-4*H*-1-benzopyran-4-one, 9CI****. 1-(7-Hydroxy-2-hydroxymethyl-4-oxo-4*H*-1-benzopyran-5-yl)-2-propanone*
$C_{13}H_{12}O_5$ 248.235
Solid. λ_{max} 206 (log ε 4.2); 248 (log ε 3.95); 280 (log ε 3.79) (MeOH).

Arora, S. *et al., Tetrahedron*, 1971, **27**, 981 (*isol, pmr, ms, ir, uv*)
Singh, J. *et al., Phytochemistry*, 1982, **21**, 1177 (*glucoside*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3493 (*isol*)
Ingkaninan, K. *et al., J. Nat. Prod.*, 2000, **63**, 315-317 (*12-hydroxy*)

Castacrenin A C-146

[173429-79-3]

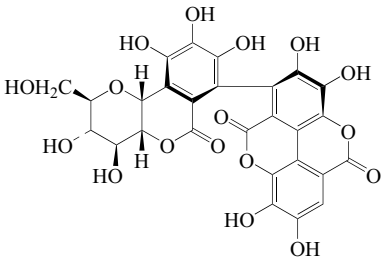


$C_{27}H_{18}O_{17}$ 614.429
Constit. of the heartwood of *Castanea crenata* (Japanese chestnut). Yellow powder + ½H_2O (H_2O). Mp 234-238° (dec.). $[\alpha]_D^{26}$ -47.2 (c, 0.8 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2236-2242 (*isol, pmr, cmr*)

Castacrenin B C-147

[173429-80-6]

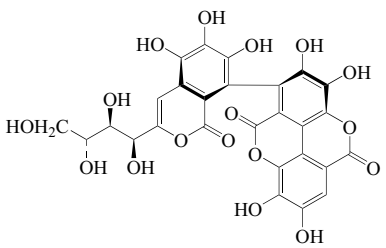


$C_{27}H_{18}O_{17}$ 614.429
Constit. of the heartwood of *Castanea crenata* (Japanese chestnut). Yellow powder + ½H_2O. $[\alpha]_D^{26}$ +46.8 (c, 0.8 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2236-2242 (*isol, pmr, cmr*)

Castacrenin C C-148

[173450-72-1]

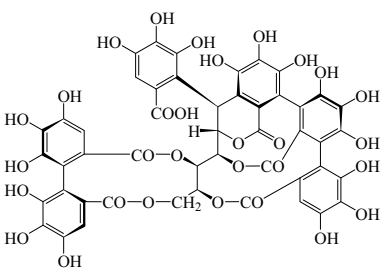


$C_{27}H_{18}O_{17}$ 614.429
Constit. of the heartwood of *Castanea crenata* (Japanese chestnut). Yellow powder + ½H_2O (H_2O). Mp 240-243° (dec.). $[\alpha]_D^{26}$ -7.6 (c, 0.9 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2236-2242 (*isol, pmr, cmr*)

Castacrenin D C-149

[200435-28-5]

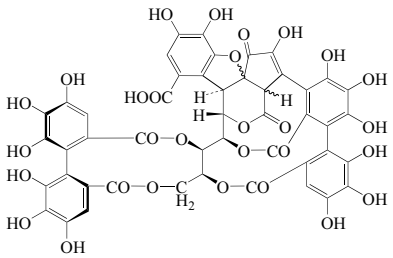


$C_{48}H_{30}O_{30}$ 1086.747
Constit. of the wood of *Castanea crenata* (Japanese chestnut). Amorph. powder + 1H_2O. $[\alpha]_D^{28}$ -29.6 (c, 0.6 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1751-1755 (*isol, pmr, cmr*)

Castacrenin E C-150

[200435-29-6]

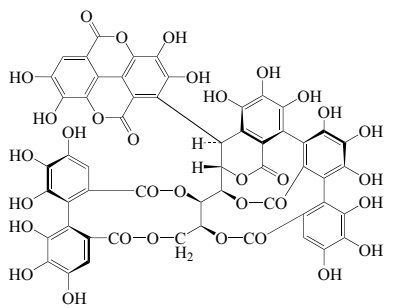


$C_{47}H_{28}O_{29}$ 1056.721
Constit. of the wood of *Castanea crenata* (Japanese chestnut). Amorph. tan powder + 8H_2O. $[\alpha]_D^{28}$ -165.3 (c, 0.7 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1751-1755 (*isol, pmr, cmr*)

Castacrenin F C-151

[200435-36-5]

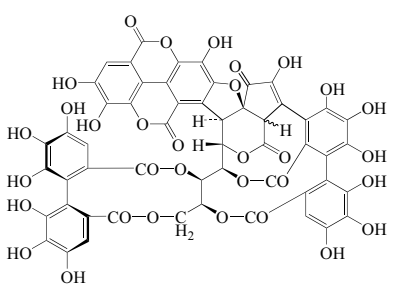


$C_{55}H_{30}O_{33}$ 1218.822
Constit. of the wood of *Castanea crenata* (Japanese chestnut). Amorph. yellow powder + 7H_2O. $[\alpha]_D^{28}$ -105.3 (c, 0.9 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1751-1755 (*isol, pmr, cmr*)

Castacrenin G C-152

[200435-38-7]

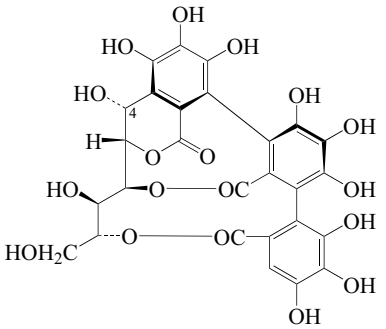


$C_{54}H_{28}O_{32}$ 1188.796
Constit. of the wood of *Castanea crenata* (Japanese chestnut). Amorph. tan powder + 4½ H_2O. $[\alpha]_D^{28}$ -36.3 (c, 0.4 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1751-1755 (*isol, pmr, cmr*)

Castalin C-153

[19086-75-0]

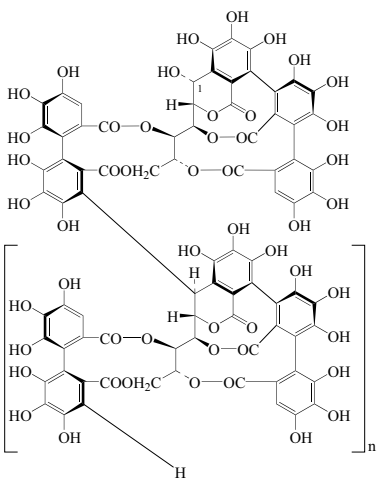


$C_{27}H_{20}O_{18}$ 632.444
Isol. from wood of *Castanea sativa* (sweet chestnut). Off-white amorph. powder. $[\alpha]_D^{17}$ +14.4 (c, 0.46 in H_2O). Gives Vescalin on heating in aq. soln..

4-Epimer: [34112-28-2] ***Vescalin***
$C_{27}H_{20}O_{18}$ 632.444
Isol. from wood of *Castanea sativa* (sweet chestnut). Yellow-brown hygroscopic amorph. solid. $[\alpha]_{Hg}^{25}$ -13 (c, 2 in H_2O).

Mayer, W. *et al., Annalen*, 1967, **707**, 177; 1977, **747**, 51 (*Vescalin*)
Nonaka, G. *et al., J.C.S. Perkin 1*, 1985, 163 (*pmr, cmr*)

Castaneanins C-154



Castaneanin A, n = 2
B, n = 3
D, n = 4

For n = 1 see. Constit. of the heartwood of *Castanea crenata* (Japanese chestnuts).

Castaneanin A [173355-97-0]
$C_{123}H_{74}O_{76}$ 2767.892
n = 2.Tan powder + 3H_2O. $[\alpha]_D$ +9.3 (c, 0.9 in MeOH).

Castaneanin B [173270-91-2]
$C_{164}H_{98}O_{101}$ 3684.518
n = 3.Tan powder + 2H_2O. $[\alpha]_D^{25}$ +24.5 (c, 0.9 in MeOH).

1-Epimer: [173270-92-3] ***Castaneanin C***
$C_{164}H_{98}O_{101}$ 3684.518
Tan powder + 1H_2O. $[\alpha]_D^{25}$ +49.3 (c, 0.8

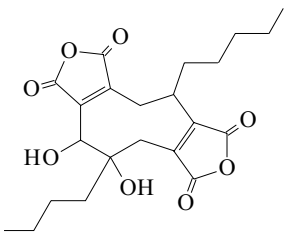
in MeOH).

Castaneanin D [173270-93-4]
$C_{205}H_{122}O_{126}$ 4601.143
n = 4.Tan powder + $2H_2O$. $[\alpha]_D^{25}$ +43.2 (c, 0.8 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2236-2242 (*isol, pmr, cmr*)

Castaneiolide C-155

[125300-50-7]

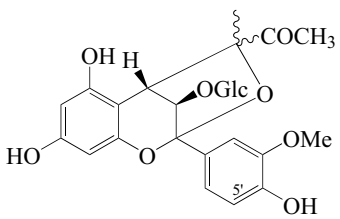


$C_{22}H_{28}O_8$ 420.458
Mycotoxin prod. by the chestnut black root pathogen *Macrophoma castaneicola*. Needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 162-163°. $[\alpha]_D$ -36.5 (c, 0.11 in EtOH). λ_{max} 247 (ϵ 7690) (MeOH) (Derep).

Arai, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2870 (*isol, struct*)

Castavinol C-156

[183607-09-2]



$C_{26}H_{30}O_{13}$ 550.515
Isol. from a Bordeaux red wine.

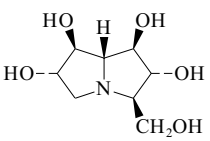
5′-Hydroxy: [183607-17-2] ***5′-Hydroxycastavinol***
$C_{26}H_{30}O_{14}$ 566.515
Isol. from a Bordeaux red wine.

5′-Methoxy: [183607-16-1] ***5′-Methoxycastavinol***
$C_{27}H_{32}O_{14}$ 580.541
Isol. from a Bordeaux red wine. $[\alpha]_D$ +46 (c, 0.2 in H_2O). λ_{max} 269 (no solvent reported).

Castagnino, C. *et al., Tet. Lett.*, 1996, **37**, 7739-7742 (*isol, uv, pmr, cmr*)

Casuarine C-157

[159440-57-0]



Absolute configuration

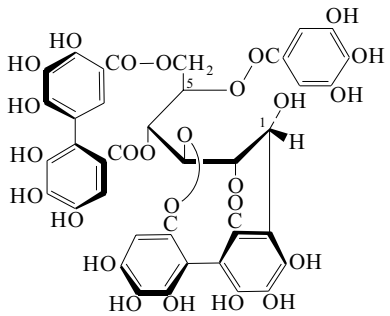
$C_8H_{15}NO_5$ 205.21
Cryst. (EtOH aq.). Mp 181-182°. $[\alpha]_D^{24}$ +16.9 (c, 0.8 in H_2O).

6-O-α-D-Glucopyranoside: [186795-20-0]
Casuarine 6-α-D-glucoside
$C_{14}H_{25}NO_{10}$ 367.352
Alkaloid from *Eugenia jambolana* (jambolan).

Nash, R.J. *et al., Tet. Lett.*, 1994, **35**, 7849 (*isol, pmr, cmr, struct*)
Wormald, M.R. *et al., Carbohydr. Lett.*, 1996, **2**, 169-174 (*6-glucoside*)
Denmark, S.E. *et al., J.O.C.*, 2000, **65**, 2875-2886 (*synth*)

Casuarinin C-158

[79786-01-9]



$C_{41}H_{28}O_{26}$ 936.657
Isol. from *Corylus heterophylla* (Siberian filbert). Pale yellow amorph. powder + $7H_2O$. $[\alpha]_D$ +43.6 (c, 1 in MeOH). λ_{max} 221 (ϵ 74130); 267 (ϵ 32360) (MeOH) (Berdy).

1-Epimer: [81739-27-7] ***Stachyurin***
$C_{41}H_{28}O_{26}$ 936.657
Off-white amorph. powder + $5H_2O$. $[\alpha]_D$ +39 (c, 0.4 in MeOH).

5-Degalloyl: [79786-04-2] *Casuariin. Casauriin (incorr.)*
$C_{34}H_{24}O_{22}$ 784.55
Pale yellow amorph. powder + $4H_2O$. $[\alpha]_D$ +162 (c, 0.5 in MeOH).

1-Epimer, 5-O-degalloyl: [115406-24-1] ***Castanin***. *Tomentosin†. 5-Desgalloylstachyurin*
$C_{34}H_{24}O_{22}$ 784.55
Isol. from *Castanea mollissima* (Chinese chestnut) and *Rhodomyrtus tomentosa* (hill gooseberry). Pale brown amorph. powder. $[\alpha]_D^{20}$ -26.5 (c, 0.8 in MeOH).

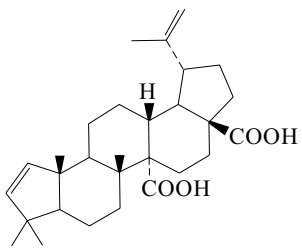
Okuda, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 766 (*struct, uv, pmr*)
Okuda, T. *et al., J.C.S. Perkin 1*, 1983, 1765 (*ir, uv, cd, pmr*)
Feng, H. *et al., Phytochemistry*, 1988, **27**, 1185 (*Castanin*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2151 (*struct, abs config*)
Lee, S.H. *et al., Phytochemistry*, 1990, **29**, 3621 (*5-Desgalloylstachyurin*)
Liu, Y.Z. *et al., Chin. Chem. Lett.*, 1997, **8**, 39-40 (*Tomentosin*)

Catalase, 9CI C-159

[9001-05-2]
Equilase. Caperase. Optidase. E.C. 1.11.1.6
A haemoprotein containing 4 polypeptide subunits of equal size each of which is associated with a ferric protoporphyrin IX prosthetic group. Converts H_2O_2 into O_2 + H_2O; can also act as a peroxidase for which several org. substrates, esp. EtOH, can act as hydrogen donor. Used in the food industry to remove traces of H_2O_2 in the sterilisation of milk for cheese making. A Mn protein containing Mn^{II} in the resting state is called pseudocatalase; enzymes from some microorganisms, e.g. *Penicillium*, that exhibit both catalase and peroxidase activity are sometimes referred to as catalase peroxidase.

Sumner, J.B. *et al., J. Biol. Chem.*, 1937, **121**, 417-424 (*isol*)
Herbert, D. *et al., Biochem. J.*, 1948, **43**, 193-202; 203-205 (*isol*)
Schonbaum, G.R. *et al., The Enzymes*, (Boyer, P. Ed), 3rd Edn., Academic Press, N.Y., 1976, **13C**, 363-408 (*rev*)
Kono, Y. *et al., J. Biol. Chem.*, 1983, **258**, 6015-6019 (*pseudocatalase*)
Merck Index, 12th edn., 1996, 1948
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 541-544 (*use*)

Ceanothenic acid C-160

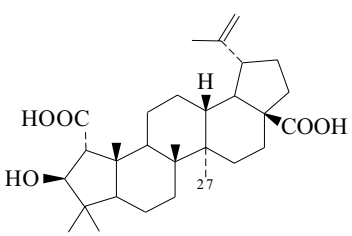


$C_{29}H_{42}O_4$ 454.648
Constit. of *Ceanothus americanus* (New Jersey tea). Cryst. (Et_2O/MeOH). Mp 350-354° dec. $[\alpha]_D$ +39 (c, 1.2 in Py).

de Mayo, P. *et al., Can. J. Chem.*, 1962, **40**, 1632
Eade, R.A. *et al., Aust. J. Chem.*, 1973, **26**, 831 (*isol*)

Ceanothic acid C-161

[21302-79-4]
Emmolic acid. 1(2→3)-Abeo-3-hydroxy-20(29)-lupene-2,28-dioic acid



$C_{30}H_{46}O_5$ 486.69
Constit. of *Ceanothus americanus* (New Jersey tea) and *Zizyphus jujuba* (Chinese date). Cryst. (MeOH). Mp 356-357° dec. (344-346°). $[\alpha]_D$ +38 (c, 2 in EtOH).

3-(3,4-Dihydroxybenzoyl):3-O-Protocatechuoylceanothic acid
$C_{37}H_{50}O_8$ 622.797
Constit. of *Zizyphus jujuba* (Chinese date). Cryst. (as di-Me ether, di-Me

ester). Mp 178-179° (Di-Me ether, di-Me ester). $[\alpha]_D^{23}$ -10 (c, 1.36 in $CHCl_3$) (Di-Me ether, di-Me ester).

27-Carboxylic acid: ***Ceanothetric acid***
$C_{30}H_{44}O_7$ 516.673
Powder (MeOH). $[\alpha]_D^{25}$ +28 (c, 0.4 in MeOH).

27-Carboxylic acid, 28-O-β-D-glucopyranosyl ester: [220623-86-9] ***Hovetrichoside H***
$C_{36}H_{54}O_{12}$ 678.815
Needles. Mp 212-214°. $[\alpha]_D^{25}$ +11.9 (c, 2.2 in MeOH).

27-Hydroxy: ***27-Hydroxyceanothic acid***
$C_{30}H_{46}O_6$ 502.69
Cryst. (MeOH) (as di-Me ester). Mp 253.5-255° (di-Me ester). $[\alpha]_D^{24}$ +24 (c, 1 in $CHCl_3$) (di-Me ester).

1,3-Diepimer: [2739-72-2] ***Isoceanothic acid***
$C_{30}H_{46}O_5$ 486.69
Powder (MeOH/Me_2CO). Mp 320°. $[\alpha]_D$ +38.2 (c, 1.2 in EtOH).

Eade, R.A. *et al., Aust. J. Chem.*, 1971, **24**, 621
Roitman, J.N. *et al., Phytochemistry*, 1978, **17**, 491 (*isol, pmr*)
Kundu, A.B. *et al., Phytochemistry*, 1989, **28**, 3155 (*isol, cmr*)
Lee, S.-S. *et al., J. Nat. Prod.*, 1992, **55**, 602 (*isol, pmr, cmr*)
Lee, S.-S. *et al., Phytochemistry*, 1996, **43**, 847 (*3-(3,4-dihydroxybenzoyl)*)
Li, X.-C. *et al., Phytochemistry*, 1997, **46**, 97-102 (*isol, pmr, cmr, Ceanothetric acid*)
Yoshikawa, K. *et al., Phytochemistry*, 1998, **49**, 2057-2060 (*Hovetrichoside H*)
Jagadeesh, S.G. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 396-398 (*Isoceanothic acid*)

Ceanothine A C-162

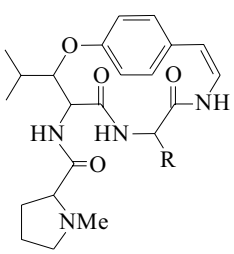
$C_{30}H_{40}N_4O_4$ 520.67

Struct. unknown. Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Needles (CH_2Cl_2/Et_2O). Mp 256-259°. $[\alpha]_D$ -256 (c, 0.5 in $CHCl_3$).

Warnhoff, E.W. *et al., Can. J. Chem.*, 1965, **43**, 2594 (*isol, pmr*)

Ceanothine B C-163

[19471-43-3]
1-Methyl-N-[3-(1-methylethyl)-5,8-dioxo-7-(phenylmethyl)-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-2-pyrrolidinecarboxamide, 9CI



R = CH_2Ph

$C_{29}H_{36}N_4O_4$ 504.628
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Needles ($CHCl_3/Et_2O$). Mp 238.5-240.5°. $[\alpha]_D^{25}$ -293 (c, 0.68 in $CHCl_3$).

Hydroiodide:
Plates (AcOH aq.). Mp 195-200°.

Dihydro:
Mp 263-273° Mp 272-278°. $[\alpha]_D^{25}$ -91 (c, 0.38 in MeOH) (-87).

Warnhoff, E.W. *et al., Can. J. Chem.*, 1965, **43**, 2594 (*isol, ms, pmr*)
Klein, F.K. *et al., J.A.C.S.*, 1968, **90**, 3576 (*ms, struct*)
Servis, R.E. *et al., J.A.C.S.*, 1968, **90**, 4179 (*struct*)
Lagarias, J.C. *et al., J. Nat. Prod.*, 1979, **42**, 663 (*isol, ms*)

Ceanothine C C-164

[18658-42-9]
As Ceanothine B, C-163 with
R = $-CH_2CH(CH_3)_2$ or $-CH(CH_3)CH_2CH_3$

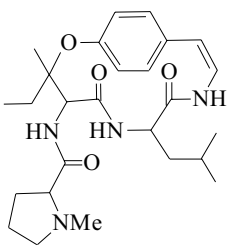
$C_{26}H_{38}N_4O_4$ 470.611

Struct. uncertain. Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Needles ($CHCl_3/Et_2O$). Mp 223-229°. $[\alpha]_D^{25}$ -368 (c, 1.01 in $CHCl_3$).

Warnhoff, E.W. *et al., Can. J. Chem.*, 1965, **43**, 2594 (*isol, uv, ms, pmr*)
Fehlhaber, H.-W. *et al., Z. Anorg. Allg. Chem.*, 1968, **235**, 91 (*ms, struct*)
Servis, R.E. *et al., J.A.C.S.*, 1969, **91**, 5619 (*ms, struct*)

Ceanothine D C-165

[23926-97-8]
N-[3-Ethyl-3-methyl-7-(2-methylpropyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-1-methyl-2-pyrrolidinecarboxamide, 9CI

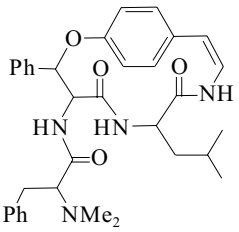


$C_{26}H_{38}N_4O_4$ 470.611
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Cryst. ($CHCl_3/Et_2O$). Mp 227-229°. $[\alpha]_D$ -347 ($CHCl_3$).

Servis, R.E. *et al., J.A.C.S.*, 1969, **91**, 5619 (*isol, pmr, ms, struct*)

Ceanothine E C-166

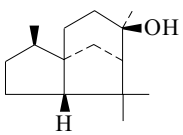
[23926-98-9]
α-(Dimethylamino)-N-[7-(2-methylpropyl)-5,8-dioxo-3-phenyl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]benzenepropanamide, 9CI



$C_{34}H_{40}N_4O_4$ 568.714
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Cryst. (CH_2Cl_2/Et_2O). Mp 238-239°. $[\alpha]_D$ -285 ($CHCl_3$).

Servis, R.E. *et al., J.A.C.S.*, 1969, **91**, 5619 (*isol, ms, struct*)

3-Cedranol C-167



$C_{15}H_{26}O$ 222.37

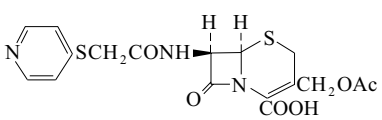
3β-*form* [77-53-2]
Cedrol. *β-Cedrol. Cedar camphor. Cypress camphor*
Needles (MeOH aq.). Mp 86-87°. $[\alpha]_D$ +10.5 (c, 5 in $CHCl_3$).

Ac: [77-54-3]
$C_{17}H_{28}O_2$ 264.407
Flavouring ingredient.
▶ FJ1680000

Hill, H.C. *et al., J.C.S.(C)*, 1968, 93 (*ms*)
Amirthalingam, V. *et al., Acta Cryst.*, Suppl., 1969, 5129 (*cryst struct, abs config*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1975, 745 (*rev*)
Breitholle, E.G. *et al., J.O.C.*, 1978, **43**, 1964 (*synth, bibl*)
Yates, P. *et al., Tetrahedron*, 1981, **37**, 4401 (*synth*)
Joseph-Nathan, P. *et al., J. Nat. Prod.*, 1984, **47**, 924 (*cmr*)
Khan, V.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 41; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 38 (*cryst struct*)
Fang, J.-M. *et al., Phytochemistry*, 1996, **41**, 1361 (*isol, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 548
He, K. *et al., Planta Med.*, 1997, **63**, 158-160 (*activity*)
Engstrom, K. *et al., Potato Res.*, 1999, **42**, 43-50; *CA*, **131**, 348943 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCR250

Cefapirin, BAN, INN C-168

[21593-23-7]
7-[2-(4-Pyridylthio)acetamido]cephalosporanic acid



$C_{17}H_{17}N_3O_6S_2$ 423.47
Active against gram-positive and -negative bacteria (vet. use). FDA approved for use in food producing animals, esp. dairy cattle. Used for the treatment of mastitis in cows. Cryst. (Me_2CO aq.). Mp 155°. Log P -0.32 (calc).

▶ XI0387000

Na salt: [24356-60-3] ***Cephapirin sodium, USAN***. *Sodium cefapirin, JAN. Cefadyl. Cefatrexyl. BL P 1322. Cefaloject*
Cryst. powder.

▶ XI0382000

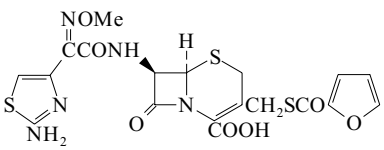
O-*De-Ac:* [38115-21-8]

[104557-24-6]
$C_{15}H_{15}N_3O_5S_2$ 381.433
Potential milk contaminant arising from the metabolism of cefapirin in cattle. Cryst. (DMF).

Ger. Pat., 1970, 2 152 820; *CA*, **77**, 140100x (*deacetyl, purifn*)
U.S. Pat., 1970, 3 503 967; *CA*, **73**, 3921 (*synth*)
Crast, L.B. *et al., J. Med. Chem.*, 1973, **16**, 1413 (*synth, props*)
Goto, S. *et al., Chemotherapy (Basel)*, 1976, **22**, 274 (*props*)
Schanck, A. *et al., Org. Magn. Reson.*, 1979, **12**, 337 (*cmr*)
Miskolczi, I. *et al., Org. Prep. Proced. Int.*, 1982, **14**, 233 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 4333 (*synonyms*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 127
Moats, W.A. *et al., J. Agric. Food Chem.*, 2000, **48**, 498-502 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCX500; HMK000

Ceftiofur, BAN, INN C-169

[80370-57-6]
CM 31916. U 64279



$C_{19}H_{17}N_5O_7S_3$ 523.571
Cephalosporin antibiotic. Veterinary antibacterial agent. FDA approved for treatment of respiratory disorders in beef or dairy cattle and pigs. Log P 0.89 (uncertain value) (calc).

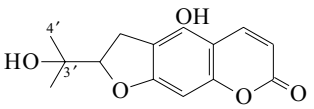
Na salt: [104010-37-9] ***Ceftiofur sodium, USAN***. *Naxcel. U 64279E*

Hydrochloride: [103980-44-5] ***Ceftiofur hydrochloride, USAN***. *Excenel. U 64279A*
Cryst.

Eur. Pat., 1981, 36 812, (*Sanofi*); *CA*, **96**, 68712 (*synth, props*)
Eur. Pat., 1986, 180 372, (*Upjohn*); *CA*, **105**, 133660 (*synth, cryst struct*)
Yancey, R.J. *et al., Am. J. Vet. Res.*, 1987, **48**, 1050 (*props*)
Fed. Regist., 1988, **53**, 5369; 1991, **56**, 12119; 1992, **57**, 41862 (*use*)
Mahrt, C.R. *et al., Am. J. Vet. Res.*, 1992, **53**, 2201 (*tox*)
Tyczkowska, K.L. *et al., J. Chromatogr.*, 1993, **614**, 123 (*hplc*)

Celereoin C-170

[74560-02-4]
5-Hydroxymarmesin



$C_{14}H_{14}O_5$ 262.262
Constit. of *Apium graveolens*. Cryst. Mp 201°. $[\alpha]_D^{21}$ -38 (MeOH).

*3′-*O*-β-D-Glucopyranoside:* [74608-59-6] ***Celereoside***
$C_{20}H_{24}O_{10}$ 424.404
Constit. of *Apium graveolens*. Cryst. Mp 200-201°. $[\alpha]_D^{24}$ -37.27 (MeOH).

5-Me ether: ***5-Methoxymarmesin***
$C_{15}H_{16}O_5$ 276.288
Oil. $[\alpha]_D$ -8 (c, 0.5 in $CHCl_3$).

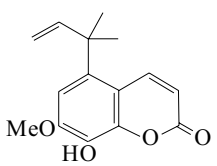
3′-Deoxy, 3′,4′-didehydro: [128836-80-6] ***Elisin***
$C_{14}H_{12}O_4$ 244.246
Needles (EtOAc). Mp 238-240°. $[\alpha]_D^{25}$ +12.8 (c, 0.1 in MeOH).

*5-*O*-(6,7-Epoxy-3,7-dimethyl-3-octenyl):* [74683-02-6] ***Jumutinol***
$C_{24}H_{30}O_6$ 414.497
Cryst. Mp 148-150°.

Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1980, **16**, 250 (*Jumutinol*)
Garg, S.K. *et al., Planta Med.*, 1980, **38**, 186 (*Celereoside*)
Rodighiero, P. *et al., J. Het. Chem.*, 1981, **18**, 447 (*synth*)
Jain, A.K. *et al., Planta Med.*, 1986, 246
Amaro-Luis, J.M. *et al., Planta Med.*, 1990, **56**, 304 (*Elisin*)
Quader, M.A. *et al., Phytochemistry*, 1992, **31**, 3083 (*deriv*)

Celerin C-171

[73815-20-0]
*4-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2*H*-1-benzopyran-2-one*



$C_{15}H_{16}O_4$ 260.289
Constit. of seeds of *Apium graveolens* (celery). Plates (EtOAc/petrol). Mp 158-159.5°. Formerly assigned an incorrect isomeric struct..

Garg, S.K. *et al., Planta Med.*, 1980, **38**, 186 (*isol*)
Murray, R.D.H. *et al., Tetrahedron*, 1984, **40**, 5229 (*struct, synth*)

Cellulase, USAN C-172

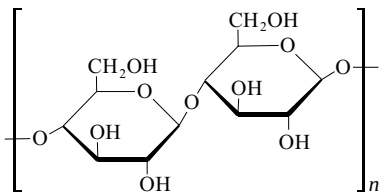
[9012-54-8]
E.C. 3.2.1.4. Endo-1,4-β-glucanase β-glucanase. Endoglucanase

Concentrate of cellulose-splitting enzymes. Enzyme which hydrolyses 1,4-β-D-glucosidic linkages in cellulose, lichenin and cereal β-D-glucans. A carbohydrase and cellulase enzyme prepn. derived from *Aspergillus niger* is used in the prepn. of starch syrups and dextrose, alcoholic drinks, fruit juices, chocolate syrups, bakery products, liq. coffee, dairy products, cereals and spice and flavour extracts. Used in fruit and vegetable processing; breaks down cellulosics for production of fermentable sugars. Component of Kutrase.

Ikeda, R. *et al., Agric. Biol. Chem.*, 1973, **37**, 1153; 1169 (*purifn, props*)
Hurst, P.L. *et al., Biochem. J.*, 1977, **165**, 33; 1978, **169**, 389 (*activity*)
Okada, G. *et al., Agric. Biol. Chem.*, 1985, **49**, 1257 (*purifn, props*)
Teeri, T.T. *et al., Biotechnology*, 1992, **21**, 417-445 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1351
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 464-465
Davies, G.J. *et al., Biochem. Soc. Trans.*, 1998, **26**, 167-173 (*rev, struct*)

Cellulose, 9CI, 8CI C-173

[9004-34-6]
E460



$C_6H_{10}O_5$ 162.142
An unbranched polymer composed of 1,4 β-linked glucopyranose units. Polymeric. Minimum formula given. Native cellulose consists of two different crystal structures, a two-chain monoclinic phase and a single chain triclinic phase. The most abundant organic material found in plants forming the principal constit. of their cell walls giving them structural strength. Anticaking agent, binding agent and other uses in food. Insol. H_2O, most solvs., but forms sol. complexes in conc. aq. $ZnCl_2$, copper-amine solutions and with Fe sodium tartrate solution.

▶ OES: long-term 10 mg m^{-3} for total inhalable dust; 5 mg m^{-3} for respirable dust. OES: short-term 20 mg m^{-3} for total inhalable dust. Reacts vigorously with oxidants. FJ5691460

Poly-O-*sulfate:* [9032-43-3] *Cellulose sulfate*
Used in food thickeners. Sol. H_2O.

Per-Ac: [9004-35-7]

[9012-09-3, 9035-69-2] *Cellulose acetate, 9CI*
Indirect food additive arising by migration from paper and paperboard packaging. Flake or powder. Mp 306° (triacetate form). $[\alpha]_D^{25}$ -20.9 ($CHCl_3$) (as triacetate).

Per-Me ether: [9004-67-5] *Methyl cellulose.*

FEMA 2696. E461
Stabiliser, thickener and emulsifier for foodstuffs.

▶ FJ5959000

Poly-Et ether: [9004-57-3] *Ethyl cellulose. Ethocel*
Stabiliser and thickener for foods. Diluent in food marking inks. Indirect additive arising by migration from paper/paperboard packaging. Powder or granules. Sol. most org. solvs. Only low DS products (1.3) show significant H_2O solubility.

Poly(carboxymethyl) ether: [9000-11-7]

[9045-95-8, 9050-04-8] ***Croscarmellose, BAN, INN***. *Carboxymethyl cellulose. Carmellose, BAN. Carmellose gum. FEMA 2239. E466*
Food additive. Stabiliser, thickener, moisture control agent, emulsifier. Indirect additive arising by migration from cotton fabrics used in food packaging. Amorph. powder. Sol. H_2O. Mp 300°.

▶ Exp. reprod. effects. LD_{50} (rat, orl) 27000 mg/kg. FJ5950000

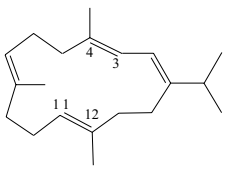
Poly(2-hydroxyethyl, Me) ether: [9032-42-2] *Hydroxyethyl methyl cellulose. HEMC*
HEMC of low hydroxyethyl ratio admitted as food thickening and gelling agent in EU. Better water solubility and electrolyte tolerance than methyl cellulose. Thermally gellable in hot water. Soly. in org. solvs. varies with DS value.

Poly(2-hydroxypropyl, Me) ether: [9004-65-3] *Hydroxypropyl methyl cellulose. HPMC. E463*
Thickening and binding agent approved for food use in USA and EU. Used in deep fried batters. Powder. Sol. H_2O. Thermally gellable in hot water. Sol. in aq. solns. varies with DS value.

[9004-32-4, 9004-57-3, 9004-64-2, 9013-34-7, 55841-00-4, 71138-97-1, 81859-24-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1180B (*ir*)
Malm, C.J. *et al., Ind. Eng. Chem.*, 1951, **43**, 684-688 (*triesters, synth, props*)
Ott, E. *et al., Cellulose and Cellulose Derivatives*, Wiley Interscience, 1954,
Timell, T.E. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 100-103 (*purifn*)
U.S. Pat., 1967, 3342805; *CA*, **67**, 101205j (*2-hydroxypropyl methyl ether*)
Ward, K. *et al., The Carbohydrates*, (eds. Pigman, W. *et al*), Academic Press, 1970, **2A**, 413
Cellulose and other Natural Polymer Systems: Biogenesis, Structure and Degradation, (ed. Brown, R.M.), Plenum Press, 1982,
Delmer, D.P. *et al., Adv. Carbohydr. Chem. Biochem.*, 1983, **41**, 105-153 (*rev, biosynth*)
Cellulose Chemistry and its Applications, (ed. Nevell, T.P.), Ellis Horwood, 1985,
Encyclopaedia of Polymer Science and Engineering, 1985, **1**, 615; **3**, 68; 158; 239 (*rev*)
Xu, Q. *et al., Fenxi Huaxue*, 1985, **13**, 170; *CA*, **103**, 204989j (*carboxymethyl ether*)
Cellulose: Structure, Modification and Hydrolysis, (eds. Young, R.A. *et al*), Wiley, 1986,
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CCU150; CCU250; SFO500; MIF760
Buchanan, C.M. *et al., J.A.C.S.*, 1989, **111**, 7312-7319 (*triesters, cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 476; 545; **6**, 1023; **7**, 292; **8**, 451 (*rev, esters, ethers, phosphate*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 84-87; 88-90; 91-93; 141-142; 306-309
Heiner, A.P. *et al., Carbohydr. Res.*, 1995, **273**, 207-223 (*bibl, struct*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 995; 1536; 1537
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 482; 551; 552; 554; 556; 1385 (*use, derivs*)
Ullmann's Encycl. Ind. Chem., 5th end., **A5**, 375-418; 419-459; 461-488 (*rev, esters, ethers*)

1,3,7,11-Cembratetraene C-174



(*all-E*)-*form*

$C_{20}H_{32}$ 272.473

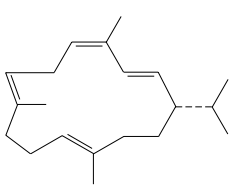
(1*Z*,3*E*,7*E*,11*E*)-*form* [37905-11-6]
γ-Pinacene
Constit. of *Pinus koraiensis* (Korean pine). Oil.

(1*Z*,3*Z*,7*E*,11*E*)-*form* [37905-10-5]
β-Pinacene
Constit. of *Pinus koraiensis* (Korean pine). Oil.

[69743-88-0]

Raldugin, V.A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 604; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 582 (*isol, ir, pmr*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1978, **31**, 2707 (*isol*)
Vanderah, D.J. *et al., J.O.C.*, 1978, **43**, 1614 (*isol*)
Raldugin, V.A. *et al., CA*, 1985, **102**, 149548s (*pmr, cmr, struct*)

2,4,7,11-Cembratetraene C-175

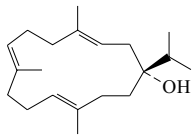


$C_{20}H_{32}$ 272.473

(1*S*,2*E*,4*Z*,7*E*,11*E*)-*form* [1898-13-1]
Cembrene. *Thunbergene. Thumbelene*
Constit. of oil of *Pinus koraiensis* (Korean pine). Cryst. (petrol). Mp 58-59°. $[\alpha]_D^{23}$ +238 (c, 1.1 in $CHCl_3$).

Ibers, J.A. *et al., Acta Cryst.*, 1961, **14**, 1001 (*cryst struct*)
Dauben, W.G. *et al., J.O.C.*, 1965, **30**, 1693 (*uv, ir, pmr, ms, struct*)
Kato, T. *et al., Synth. Commun.*, 1976, **6**, 365 (*synth*)
Forkas, I. *et al., Helv. Chim. Acta*, 1990, **73**, 1980 (*synth*)
Ma, L. *et al., Magn. Reson. Chem.*, 1992, **30**, 1247 (*cmr*)
Li, W. *et al., Chem. Lett.*, 1994, 741 (*synth*)
Pattenden, G. *et al., J.C.S. Perkin 1*, 1996, 57 (*synth*)

3,7,11-Cembratrien-1-ol C-176



(1*R*,3*E*,7*E*,11*E*)-*form*

$C_{20}H_{34}O$ 290.488

(1*R*,3*E*,7*E*,11*E*)-*form* [66648-97-3]
Sarcophytol M
Oil. $[\alpha]_D$ +57 (c, 0.94 in $CHCl_3$).

(1*S*,3*E*,7*E*,11*E*)-*form* [67814-27-1]
Serratol. *Cembrenol*
Constit. of *Boswellia serrata* (Indian olibanum). Oil. Bp_1 150°. $[\alpha]_D^{20}$ -152.2 (c, 0.4 in EtOH).

[67921-02-2]

Pardhy, R.S. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 171 (*isol*)
Klein, E. *et al., Tet. Lett.*, 1978, 349 (*abs config*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 631 (*Sarchophytol M*)
Li, Y. *et al., Tet. Lett.*, 1993, **34**, 2799 (*synth*)
Yue, X. *et al., Bull. Soc. Chim. Belg.*, 1994, **103**, 35 (*synth*)

Centoic acid C-177

$C_{30}H_{48}O_6$ 504.706

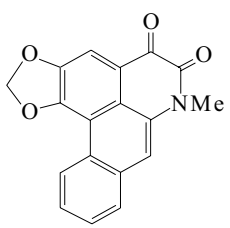
Struct. unknown, prob. terpenoid. Isol. from *Centella asiatica* (Asiatic pennywort). Mp 256-261° dec. (block). $[\alpha]_D^{19}$ +43.5 (c, 0.91 in EtOH). $[\alpha]_D^{19}$ +40.7 (c, 3.31 in Py). Conts. 4 OH groups.

Me ester:
Mp 150-155° (softens at 140°).

Bhattacharyya, S.C. *et al., J. Indian Chem. Soc.*, 1956, **33**, 579-586 (*isol*)

Cepharadione A C-178

[55610-01-0]
*7-Methyl-5*H*-benzo[*g*]-1,3-benzodioxolo[6,5,4-*de*]quinoline-5,6(7*H*)-dione, 9CI*



$C_{18}H_{11}NO_4$ 305.289
Alkaloid from *Piper auritum* (Veracruz pepper). Orange-yellow needles ($CHCl_3$/EtOH). Mp 340-342° dec.

N-*De-Me:* [107882-42-8] ***Norcepharadione A***
$C_{17}H_9NO_4$ 291.262

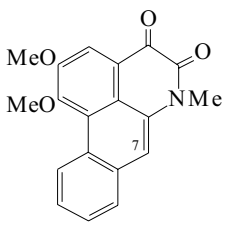
N-*De-Me,* N-*methoxy:* [166833-81-4] ***Artabotrine***. N-*Methoxynorcepharadione A*
$C_{18}H_{11}NO_5$ 321.289
Orange-yellow rods. Mp 287-289°. λ_{max}

220 (ϵ 20900); 235 (ϵ 22390); 280 (ϵ 5750); 300 (ϵ 9800); 310 (ϵ 11000) (MeOH) (Berdy).

Akasu, M. *et al., Tet. Lett.*, 1974, 3609 (*ir, uv, ms, pmr, struct*)
Hänsel, R. *et al., J. Nat. Prod.*, 1975, **38**, 529; *Phytochemistry*, 1976, **15**, 1323 (*isol, uv, ir, ms*)
Kunitomo, J. *et al., Yakugaku Zasshi*, 1981, **101**, 431; *CA*, **95**, 204236c (*isol*)
Achari, B. *et al., Heterocycles*, 1982, **19**, 1203 (*occur*)
Cavé, A. *et al., Plant. Med. Phytother.*, 1986, **20**, 251; *CA*, **106**, 172905x (*Norcepharadione* A)
Wijeratne, E.M.K. *et al., Tetrahedron*, 1995, **51**, 7877 (*Artabotrine*)

Cepharadione B C-179

[55610-02-1]
*1,2-Dimethoxy-6-methyl-4*H*-dibenzo[*de,g*]quinoline-4,5(6*H*)-dione, 9CI*



$C_{19}H_{15}NO_4$ 321.332
Alkaloid from the woody roots of *Piper auritum* (Veracruz pepper). Orange needles (EtOH). Mp 267-268° (255-262°, 263-264°).

N-*De-Me:* [57576-41-7] ***Norcepharadione B***
$C_{18}H_{13}NO_4$ 307.305
Orange cryst. Mp 304-307° dec.

O^2-*De-Me:* [109771-09-7] ***Aristolodione***. *Piperadione*
$C_{18}H_{13}NO_4$ 307.305
Alkaloid *Piper longum* (long pepper). Cryst. ($CHCl_3$/MeOH). Mp 273-276° dec.

O^2-*De-Me, Ac:*
Cryst. (C_6H_6/MeOH). Mp 244-248° dec.

O^2,N-*Di-de-Me:* [82644-81-3] *2-Hydroxy-1-methoxy-4*H*-dibenzo[*de,g*]quinoline-4,5-dione, 9CI*. ***4,5-Dioxodehydroasimilobine***. *Noraristolodione*
$C_{17}H_{11}NO_4$ 293.278
Red needles ($CHCl_3$/MeOH). Mp 310-312°. λ_{max} 246 (ϵ 50100); 292 (sh) (ϵ 13800); 305 (ϵ 18200); 318 (ϵ 19100); 459 (ϵ 17000) (EtOH).

7-Chloro, N-*de-Me:* [149682-95-1] ***7-Chloro-6-demethylcepharadione B***
$C_{18}H_{12}ClNO_4$ 341.75
Alkaloid from *Houttuynia cordata* (Yu Xing Cao).

1-Demethoxy, O^2,N-*di-de-Me:* [138690-43-4] ***Demethoxy-4,5-dioxodehydroasimilobine***
$C_{16}H_9NO_3$ 263.252
Orange needles (MeOH). Mp 283-285°.

Akasu, M. *et al., Tet. Lett.*, 1974, 3609 (*uv, ir, pmr, ms, struct*)
Hänsel, R. *et al., J. Nat. Prod.*, 1975, **38**, 529 (*isol, uv, ir, pmr, ms*)
Akasu, M. *et al., Phytochemistry*, 1975, **14**, 1673 (*uv, ir, pmr, ms, struct, Norcepharadione B*)
Hänsel, R. *et al., Phytochemistry*, 1976, **15**, 1323 (*occur*)
Saá, J.M. *et al., Tet. Lett.*, 1976, 601 (*synth, uv, ir, ms*)
Kunitomo, J. *et al., Yakugaku Zasshi*, 1980, **100**, 337; *CA*, **93**, 95454h (*synth*)
Achari, B. *et al., Heterocycles*, 1982, **19**, 1203 (*Dioxodehydroasimilobine*)
Urzua, A. *et al., J. Nat. Prod.*, 1987, **50**, 305 (*Aristolodione*)
Desai, S.J. *et al., Phytochemistry*, 1988, **27**, 1511 (*Aristolodione*)
Achenbach, H. *et al., J. Nat. Prod.*, 1991, **54**, 1331 (*Demethoxydioxodehydroasimilobine*)
Atanes, N. *et al., J.O.C.*, 1991, **56**, 2984 (*synth, Cepharadione B, Norcepharadione B*)
Jong, T.T. *et al., J. Chin. Chem. Soc. (Taipei)*, 1993, **40**, 301; *CA*, **119**, 135624c (*7-Chloro-6-demethylcepharadione B*)
Suau, R. *et al., Tetrahedron*, 1996, **52**, 11307 (*synth*)
Chia, Y.-C. *et al., J. Nat. Prod.*, 2000, **63**, 1160-1163 (*activity*)

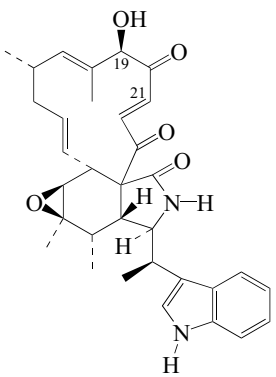
Cerebrosides C-180

RCH(OH)CH(NHCOR′)CH_2O-sugar
Cerebroside is the general name given to monoglycosyl ceramides. On hydrol. they afford a long-chain base such as Sphingenine, a fatty acid (R′COOH) and a sugar (most commonly galactose). These compds. occur as mixtures and are important constits. of lipids of many tissues, esp. brain and nerve. Some members of this class have individual entries, for example see 2-Amino-4-octadecene-1,3-diol, A-283.

Rodd's Chem. Carbon Compd. (2nd edn.), 1976, **1E**, 403
Schmidt, R.R. *et al., Angew. Chem., Int. Ed.*, 1985, **24**, 65 (*synth*)
Kodato, S. *et al., Tetrahedron*, 1989, **45**, 7263 (*synth*)

Chaetoglobosin P C-181

[191403-93-7]



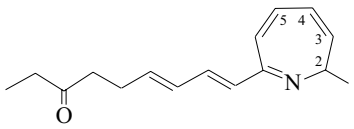
$C_{33}H_{38}N_2O_5$ 542.674
Pale yellow gum.

19-Ketone, 21,22-dihydro: [156980-59-5] ***Chaetoglobosin N***
$C_{33}H_{38}N_2O_5$ 542.674
Isol. from *Phomopsis leptostromiformis* on sweet corn (*Zea mays*). Mp 205°.

Cherton, J.C. *et al., Analusis*, 1994, **22**, 210-216; 217-221 (*deriv, isol, pmr, cmr*)
Donoso, R. *et al., Nat. Prod. Lett.*, 1997, **10**, 49-54 (*isol, pmr, cmr*)

Chalciporone C-182

[112448-74-5]
*2-Methyl-7-(7-oxo-1,3-nonadienyl)-2*H*-azepine*



$C_{16}H_{21}NO$ 243.348
Pungent principle from fruit-bodies of the toxic mushroom *Chalciporus piperatus*. Slightly yellow oil. Sol. MeOH, EtOAc, Et_2O; poorly sol. H_2O. $[\alpha]_D^{22}$ -452 (c, 1.3 in Et_2O). Spontaneously isomerizes to Isochalciporone, e.g. in $CDCl_3$ soln. at r.t. λ_{max} 252 (ϵ 21000); 260 (sh) (ϵ); 270 (sh) (ϵ); 315 (sh) (ϵ) (EtOH) (Derep). λ_{max} 253 (ϵ 21000) (EtOH) (Berdy).

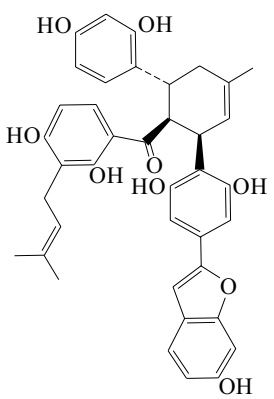
$\Delta^{2,3:4,5}$-Isomer: [112448-72-3] ***Isochalciporone***. *7-Methyl-2-(7-oxo-1,3-nonadienyl)-3*H*-azepine*
$C_{16}H_{21}NO$ 243.348
Constit. of the toxic mushroom *Chalciporus piperatus*. Yellow oil. Sol. MeOH, Et_2O, EtOAc; poorly sol. H_2O. Nonpungent λ_{max} 241 (ϵ 28000); 246 (sh) (ϵ); 292 (ϵ 14700); 328 (sh) (ϵ) (EtOH) (Derep). λ_{max} 241 (ϵ 28000); 292 (ϵ 14700) (EtOH) (Berdy).

*$\Delta^{2,3:4,5}$-Isomer, 12,13-didehydro:7-Methyl-2-(7-oxo-1,3,5-nonatrienyl)-3*H*-azepine.* ***Dehydroisochalciporone***
$C_{16}H_{19}NO$ 241.332
Nonpungent constit. of *Chalciporus piperatus*. Intense-yellow oil. Sol. MeOH, Et_2O, EtOAc; poorly sol. H_2O. λ_{max} 226 (ϵ 21800); 285 (sh) (ϵ); 338 (ϵ 23000) (EtOH) (Derep). λ_{max} 226 (ϵ 21800); 338 (ϵ 23000) (EtOH) (Berdy).

Sterner, O. *et al., Tetrahedron*, 1987, **43**, 1075 (*isol, uv, ir, pmr, cmr, ms, struct*)
Spiteller, P. *et al., J.A.C.S.*, 2001, **123**, 4837-4838 (*biosynth*)

Chalcomoracin C-183

[76472-89-4]



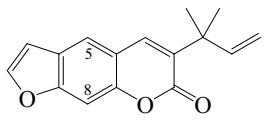
$C_{39}H_{36}O_9$ 648.708
Phytoalexin from diseased white mulberry

(*Morus alba*). Cryst. Mp 183°. $[\alpha]_D$ +194 (Me_2CO). λ_{max} 218 (ϵ 58600); 329 (ϵ 50500); 334 (ϵ 41300) (MeOH) (Berdy).

Takasugi, M. *et al., Chem. Lett.*, 1980, 1573

Chalepensin C-184

[13164-03-9]
*6-(1,1-Dimethyl-2-propenyl)-7*H*-furo[3,2-g][1]benzopyran-7-one, 9CI. 3-(1,1-Dimethylallyl)psoralen. Xylotenin*



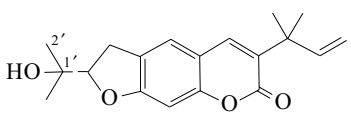
$C_{16}H_{14}O_3$ 254.285
Cryst. (Et_2O/petrol). Mp 89-90° (86°). Log P 3.84 (calc).

5,8-Dimethoxy: [42438-50-6] ***5,8-Dimethoxychalepensin***
$C_{18}H_{18}O_5$ 314.337
Constit. of *Ruta graveolens* (rue). Yellow needles (hexane/EtOAc). Mp 132-134°. λ_{max} 222 (log ϵ 4.44); 241 (log ϵ 4.15); 249 (log ϵ 4.15); 271 (log ϵ 4.32); 313 (log ϵ 4.15) (MeOH).

Reisch, J. *et al., Tet. Lett.*, 1968, 4395 (*isol*)
Joshi, B.S. *et al., Phytochemistry*, 1971, **10**, 480 (*isol, struct*)
González, A.G. *et al., An. Quim.*, 1973, **69**, 1013 (*pmr*)
Arques, J.S. *et al., An. Quim.*, 1974, **70**, 1020 (*isol*)
Delle Monache, F. *et al., Gazz. Chim. Ital.*, 1976, **106**, 681 (*isol*)
Franke, K. *et al., Phytochemistry*, 2001, **56**, 611-621 (*5,8-Dimethoxychalepensin*)

Chalepin C-185

[118389-19-8]
*6-(1,1-Dimethyl-2-propenyl)-2,3-dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-g][1]benzopyran-7-one, 9CI. Rutamarin alcohol*



(*S*)-*form*

$C_{19}H_{22}O_4$ 314.38Log P 3.35 (calc).

(*S*)-*form* [13164-04-0]
Cryst. Mp 118°.
▶LV1051020

Ac: [14882-94-1] ***Rutamarin***. *Chalepin acetate*
$C_{21}H_{24}O_5$ 356.418
Constit. of *Ruta graveolens* (rue). Cryst. Mp 107-108°. $[\alpha]_D^{22}$ +14 (c, 2.3 in $CHCl_3$).
▶LV1045200

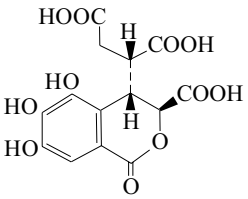
Deoxy, 1′,2′-didehydro: **exo-*Dehydrochalepin***
$C_{19}H_{20}O_3$ 296.365
Constit. of *Ruta graveolens* (rue) roots. Cryst. Mp 100°. $[\alpha]_D^{25}$ +7.4 ($CHCl_3$).

(+)-*form* [33054-89-6]
Heliettin
Mp 165-166°. $[\alpha]_D^{25}$ -29.5 (c, 0.003 in $CHCl_3$). Pharmacol. active isomer.

Reisch, J. *et al., Acta Pharm. Suec.*, 1967, **4**, 179 (*isol*)
Brooker, R.M. *et al., J. Nat. Prod.*, 1967, **30**, 73 (*isol*)
Pozzi, H. *et al., Tetrahedron*, 1967, **23**, 1129 (*isol*)
Burke, B.A. *et al., Heterocycles*, 1981, **16**, 897 (*abs config*)
Sharma, R.B. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 538 (*synth*)
Massanet, G.M. *et al., Heterocycles*, 1987, **26**, 1541 (*synth*)
Reisch, J. *et al., Sci. Pharm.*, 1988, **56**, 171 (*Dehydrochalepin*)
Sharma, R.B. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 247-251 (*biosynth*)

Chebulic acid C-186

[23725-05-5]
*3-Carboxy-3,4-dihydro-5,6,7-trihydroxy-1-oxo-1*H*-2-benzopyran-4-yl-butanedioic acid, 9CI. Split acid*



$C_{14}H_{12}O_{11}$ 356.242

(+)-*form*
Isol. from *Phyllanthus emblica* (emblic). Syrup or amorph. powder. $[\alpha]_D^{20}$ +25.6 (H_2O).

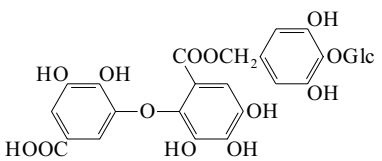
Tri-Me ether, tri-Me ester:
$Bp_{0.001}$ 200-205°. $[\alpha]_D^{20}$ +49.3 (c, 2.3 in MeOH).

(-)-*form*
Yellow-brown. $[\alpha]_D^{25}$ -24.8 (c, 1 in MeOH).

Mayer, W. *et al., Annalen*, 1951, **571**, 1; 15 (*isol, struct, synth*)
Schmidt, O.Th. *et al., Chem. Ber.*, 1952, **85**, 408
Haworth, R.D. *et al., J.C.S.*, 1954, 3611 (*struct*)
King, H.G.C. *et al., Proc. Chem. Soc., London*, 1957, 341 (*isol*)
Haslam, E. *et al., J.C.S.(C)*, 1967, 2381 (*stereochem*)
Schmidt, O.Th. *et al., Annalen*, 1969, **729**, 249 (*isol, struct*)
Schilling, G. *et al., Annalen*, 1981, 603 (*config*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2655 (*abs config*)

Chesnatin C-187

[68735-76-2]

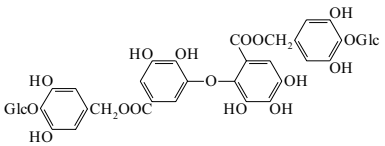


$C_{27}H_{26}O_{18}$ 638.492
A tannin constit. of Japanese chestnut galls (*Castanea crenata*) and from the leaf of *Castanea mollissima* (Chinese chestnut). Needles + ½H_2O (H_2O). $[\alpha]_D^{20}$ -7.3 (c, 1.16 in H_2O). No distinct Mp.

Ozawa, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 1249; 1978, **42**, 1907; 1979, **43**, 1173 (*isol, uv, ir, ms, pmr, cmr*)
Ageta, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 870 (*struct*)
Feng, H. *et al., Phytochemistry*, 1988, **27**, 1185 (*isol*)

Chestanin C-188

[68325-50-8]
MP3. Chestanin A



$C_{40}H_{42}O_{26}$ 938.756
Isol. from Chinese chestnut (*Castanea crenata*) galls caused by the chestnut gall wasp *Dryocosmus kuriphilus*. Sl. yellow powder. $[\alpha]_D^{23}$ -11.8 (c, 1.27 in H_2O). Shows no distinct Mp. Bitter taste.

O-*(3,4,5-Trihydroxybenzoyl)(1):* [115410-38-3] ***Galloylchestanin A***
$C_{47}H_{46}O_{30}$ 1090.86
Off-white amorph. powder + $4H_2O$. $[\alpha]_D^{20}$ -21.5 (c, 1.2 in H_2O). Substd. at the 6-posn. of the left-hand glucose residue.

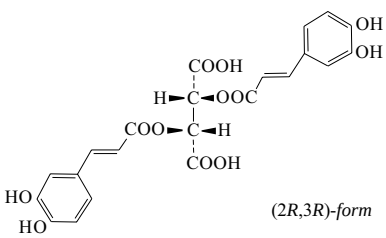
O-*(3,4,5-Trihydroxybenzoyl)(2):* [115410-39-4] ***Galloylchestanin B***
$C_{47}H_{46}O_{30}$ 1090.86
Off-white amorph. powder + $3H_2O$. $[\alpha]_D^{20}$ -18.6 (c, 0.90 in H_2O). Substd. at the 6-posn. of the right-hand glucose residue.

Ozawa, T. *et al., Agric. Biol. Chem.*, 1978, **42**, 1511
Ozawa, T. *et al., Agric. Biol. Chem.*, 1979, **43**, 1173 (*cmr*)
Ageta, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 870 (*Galloylchestanins*)
Feng, H. *et al., Phytochemistry*, 1988, **27**, 1185 (*isol*)

Chicoric acid C-189

[6537-80-0]

[52248-48-3]
2,3-Bis[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]butanedioic acid, 9CI. Dicaffeoyltartaric acid. Cichoric acid



(2*R*,3*R*)-*form*

$C_{22}H_{18}O_{12}$ 474.377

(2*R*,3*R*)-*form* [70831-56-0]
L-Chicoric acid
Constit. of leaves of chicory (*Cichorium intybus*) and endive *Cichorium endivia*. Silky needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 206°. $[\alpha]_D$ -384 (c, 1.07 in MeOH). λ_{max} 318 (MeOH)

(Berdy).

3-Me ether: [99119-75-2] ***Caffeoylferuloyltartaric acid***
$C_{23}H_{20}O_{12}$ 488.404Stereochem. not confirmed.

3,3′-Di-Me ether: [99119-76-3] ***Chicoric acid dimethyl ether***
$C_{24}H_{22}O_{12}$ 502.431Stereochem. not confirmed.

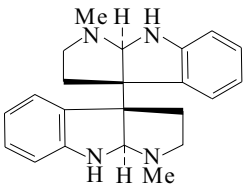
(2*S*,3*S*)-*form*
Isol. from chicory (*Cichorium intybus*) and *Cichorium endivia* (endive). Needles (H_2O). Mp 206°. $[\alpha]_D$ +384 (c, 1.55 in MeOH).

(2*RS*,3*RS*)-*form*
(±)-form
Cryst. (H_2O). Mp 206°.

(2*RS*,3*SR*)-*form* [133520-29-3]
[53797-30-1]
Mesochicoric acid
Cryst. (H_2O). Mp 225°.

Scarpati, M.L. *et al., Tetrahedron*, 1958, **4**, 43-48 (*isol, struct, synth*)
Woeldecke, M. *et al., Z. Naturforsch., C*, 1974, **29**, 360-361 (*isol*)
Cariello, L. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1979, **62**, 159 (*isol*)
Becker, H. *et al., Z. Naturforsch., C*, 1985, **40**, 585-587 (*isol*)
Soicke, H. *et al., Planta Med.*, 1988, **54**, 175-176 (*isol*)
Veit, M. *et al., Phytochemistry*, 1991, **30**, 527-529 (*isol, struct*)
Robinson, W.E. *et al., Antiviral Res.*, 1998, **39**, 101-111 (*activity*)
Zhao, H. *et al., Synth. Commun.*, 1998, **28**, 737-740 (*synth, pmr*)
Lamidey, A.-M. *et al., Helv. Chim. Acta*, 2002, **85**, 2328-2334 (*synth*)

Chimonanthine C-190



(−)-*form*

$C_{22}H_{26}N_4$ 346.474
(-)-form shown.

(+)-*form* [85610-66-8]
Mp 171-172°. $[\alpha]_D^{25}$ +280 (MeOH).

N-*Di-de-Me,* N′,N″-*di-Me:* ***Isochimonanthine***
$C_{22}H_{26}N_4$ 346.474
Needles (EtOAc/petrol). Mp 190-191°. $[\alpha]_D^{27}$ +248 (c, 0.009 in MeOH). λ_{max} 218 (ε 39100); 247 (ε 34000); 305 (ε 15000) (CH_2Cl_2).

(-)-*form* [5545-89-1]
Alkaloid from *Calycanthus floridus* (Carolina allspice). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 188-189°. $[\alpha]_D$ -329. λ_{max} 247 (ε 13600); 303 (ε 5600) (EtOH) (Berdy). λ_{max} 239 ; 294 (EtOH-HCl) (Berdy).

N-*Me:* [5516-85-8] ***Calycanthidine***
$C_{23}H_{28}N_4$ 360.501
Alkaloid from the seeds of *Calycanthus floridus* (Carolina allspice). Mp 142°. $[\alpha]_D^{20}$ -317 (EtOH).

N,N′-*Di-Me:* Folicanthine, F-56

(±)-*form* [4147-36-8]
Mp 183-185°.

meso*-*form [4147-37-9]
Alkaloid from *Calycanthus floridus* (Carolina allspice). Mp 199-202° (176°).

N-*De-Me:* **N-*Demethyl*-meso-*chimonanthine***
$C_{21}H_{24}N_4$ 332.447
Amorph. powder. λ_{max} 245 (log ε 4); 303 (log ε 3.6) (EtOH).

Saxton, J.E. *et al., Proc. Chem. Soc., London*, 1962, 148 (*uv, struct, deriv*)
Hendrikson, J.B. *et al., Tetrahedron*, 1964, **20**, 565 (*synth, ms, pmr*)
Grant, I.J. *et al., J.C.S.*, 1965, 5678 (*cryst struct*)
Hall, E.S. *et al., Tetrahedron*, 1967, **23**, 4131 (*synth, isol, uv, ir, pmr, ms*)
Kirby, G.W. *et al., J.C.S.(C)*, 1969, 1916 (*biosynth*)
Hino, T. *et al., Tet. Lett.*, 1978, 4913 (*synth*)
Tokuyama, T. *et al., Tetrahedron*, 1983, **39**, 41 (*isol*)
Adjibade, Y. *et al., Phytochemistry*, 1992, **31**, 317 (*isol, uv, ir, pmr, cmr, ms*)
Link, J.T. *et al., J.A.C.S.*, 1996, **118**, 8166 (*synth*)
Verotta, L. *et al., J. Nat. Prod.*, 1998, **61**, 392-396 (*isol, pmr, cd*)
Jannic, V. *et al., J. Nat. Prod.*, 1999, **62**, 838-843 (*N-Demethyl-meso-chimonanthine*)
Overman, L.E. *et al., J.A.C.S.*, 1999, **121**, 7702-7703 (*synth*)
Dachriyanus, *et al., Aust. J. Chem.*, 2000, **53**, 159-160 (*Isochimonanthine*)

Chitin-binding protein N C-191

CBP N
Protein, MW approx. 14 kDa. Isol. from grain of barley (*Hordeum vulgare*). Shows antifungal activity *in vitro*.

Hejgaard, J. *et al., Physiol. Plant.*, 1985, **64**, 301-307 (*isol*)
Hejgaard, J. *et al., FEBS Lett.*, 1992, **307**, 389-392 (*isol*)

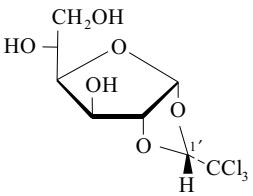
Chitosan C-192

[9012-76-4]
Poly(1,4-β-D-glucopyranosamine), 9CI. Poliglusam, INN, USAN†
Polymer consisting of deacetylated chitin and *N*-acetylated chitan where the deacetylation or *N*-acetylation is partial or unspecified. Obt. from Chitin by methods incl. alkaline hydrol. and thermochemical-chemical treatment. Used in edible coatings for fruit and vegetables and in biodegradable packaging films.. Leaflets. Sol. dil. formic acid, AcOH; insol. H_2O, mineral acids. Typically 80-90% deacylated, though may contain a proportion of insoluble crystallites (Hydrochitin) characterised by higher acetyl content.

Horton, D. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 403 (*synth*)
Muzzarelli, R.A.A. *et al., Anal. Chim. Acta*, 1969, **44**, 234 (*use*)
Chitin Nat. Technol. Proc. Int. Conf. Chitin Chitosan, 3rd, 1985, Plenum Press, 1986, (*book*)
Saito, H. *et al., Macromolecules*, 1987, **20**, 2424 (*cmr*)
Wu, A.C.M. *et al., Methods Enzymol.*, 1988, **161**, 447 (*hplc*)
Chitin Chitosan, (Ed. Skjåk-Braek, G. *et al*), Elsevier, London, 1989, (*book*)
Vårum, K.M. *et al., Carbohydr. Res.*, 1991, **213**, 19 (*cmr*)
Adv. Chitin Chitosan, (Ed. Brine, C.J. *et al*), Elsevier, London, 1992, (*book*)
Nishimura, Y. *et al., Hoshasen Kagaku (Tokyo)*, 1992, **35**, 13 (*rev*)
Raymond, L. *et al., Carbohydr. Res.*, 1993, **246**, 331 (*bibl*)
Rege, P.J. *et al., Carbohydr. Res.*, 1999, **321**, 235-245 (*bibl, props*)
Encycl. Food Sci. Technol., Wiley-Interscience 2nd. Ed., Ed. Francis, F.J., 2000, 579-584 (*use*)

Chloralose, 8CI, BSI, INN, ISO C-193

1,2-O-(2,2,2-Trichloroethylidene)glucofuranose, 9CI. Glucochloralose. Glucochloral. Anhydroglucochloral. Chloralosane. Somio. Aphosal. Dulcidor. Alphakil



(1′*R*)-*form*

$C_8H_{11}Cl_3O_6$ 309.529Log P -0.3 (calc).

(1′*R*)-*form* [15879-93-3]
α-*form. Alphachloralose*
Bird repellant in grain seeds. Needles (EtOH or Et_2O). Mp 187°. $[\alpha]_D^{22}$ +19 (c, 5.00 in EtOH).
▶ Produces a coma (usually non-fatal) in cases of acute human poisoning. LD_{50} (rat, orl) 400 mg/kg. FM9450000

(1′*S*)-*form* [16376-36-6]
β-*form*
Less sol. than α-form. Mp 227-230°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 315C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 201A (*ir*)
Pictet, A. *et al., Helv. Chim. Acta*, 1923, **6**, 621 (*synth, struct*)
Freudenburg, W. *et al., J.A.C.S.*, 1937, **59**, 1955 (*synth, struct*)
Lees, P. *et al., Vet. Rec.*, 1972, **91**, 330 (*pharmacol, tox*)
Belg. Pat., 1979, 875 250; *CA*, **91**, 36002r (*use*)
Sapru, H.N. *et al., Eur. J. Pharmacol.*, 1979, **53**, 151; *CA*, 1979, **90**, 14579f (*use*)
Ger. Pat., 1979, 2 729 739; *CA*, **90**, 153589g (*synth, use*)
Taga, T. *et al., Acta Cryst. B*, 1982, **38**, 1874 (*cryst struct*)
Pesticide Manual, 9th edn., 1991, No. 2130
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A12
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 570
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GFA000
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1306

Chlorine C-194

[7782-50-5]
Dichlorine. E925
Cl_2
Cl 35.453

Atomic No. 17. Ground state electron config. [Ne]$3s^2 3p^5$. Discovered in 1774 by C.W. Scheele. There are 11 Isotopes of which ^{35}Cl and ^{37}Cl are stable and find application in nmr spectroscopy. Abundance: 126 ppm (earth's crust), 19,000 ppm (sea water). Cl–Cl: 199 pm (gas); 198 (solid). Bleaching agent for flour. Greenish-yellow pungent gas combining directly and vigorously with nearly all elements. At 10° 1 vol. H_2O dissolves 3.1 vols. chlorine; sol. organochlorine solvs. Mp -101°. Bp -34.9°. Forms complexes with hydrogen halides and hydrates. Bond energy 243 kJ mol^{-1}.

▶ Respiratory irritant, the liq. burns the skin. Exposure should not exceed 1 ppm. FO2100000

[11094-65-8, 12595-89-0, 14835-24-6, 15721-70-7, 15723-23-6, 16547-50-5, 16904-11-3, 16904-12-4, 16999-02-3, 20337-89-7, 22223-66-1, 22537-15-1, 22537-27-5, 22541-73-7, 24203-47-2, 53664-01-0]

Mellor Compr. Treat. Inorg. Theor. Chem., 1922, **2**, 15; *Suppl.* 1, 262 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 6, 1927, ; *Suppl.*, 1968, **A**, ; *Suppl.*, (1968-1969), **B**, (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1107
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 288 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **1**, 799 (*rev, bibl*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 920 (*rev*)
Merck Index, 11th edn., 1989, No. 2095
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 573-575
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 56; 238
Schmittinger, P. *et al., Chlorine, Principles and Industrial Practice*, Wiley, 2000, (*rev*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 995 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDV750

Chlorine oxide (ClO_2), 11CI C-195

[10049-04-4]
Chlorine oxide†. *Chlorine dioxide. E926*

ClO_2 (C_{2v})

ClO_2 67.452

Paramagnetic, odd electron delocalised over whole molecule. Cl–O 147 pm, angle OClO 118°. In the solid state the dimer is diamagnetic below -84° and involves one bridging Cl–O–Cl interaction. Bleaching agent for flour. Orange-green gas; yellowish-red cryst. Unstable in light, stable in the dark. Insol. H_2O. Mp -59°. Bp 11°. Forms a hydrate.

▶ Explodes in contact with organic materials. Max. safe partial pressure 36 mm. FO3000000

Inorg. Synth., 1953, **4**, 152 (*synth*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 6, 1969, **B2**, 331 (*bibl*)
Clark, A.H. *et al., J.C.S.(A)*, 1970, 46 (*struct*)
Gordon, G. *et al., Prog. Inorg. Chem.*, 1972, **15**, 201 (*rev*)
Compr. Inorg. Chem., Pergamon, 1973, **2**, 1107 (*rev*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 312 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 612
Rehr, A. *et al., Inorg. Chem.*, 1992, **31**, 4740 (*cryst struct, ir, magnetism*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 575-577
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDW450

Chloroacetic acid, 9CI C-196

[79-11-8]
Monochloroacetic acid

$ClCH_2COOH$

$C_2H_3ClO_2$ 94.497

Prohibited from use in food. Cryst. in three forms. V. sol. H_2O; sol. org. solvs. Mp 61.3° (α-form) Mp 56.2° (β-form) Mp 52.5° (γ-form). Bp 189°. pK_a 2.87 (25°).

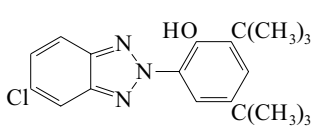
▶ Corrosive skin, eye and mucous membrane irritant. LD_{50} (mus, orl) 165 mg/kg. Toxic in contact with skin. Contamination of 5 to 10% of skin area can be fatal. Fl. p. 150°, autoignition temp. >500°. AF8575000

[3926-62-3, 14526-03-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 508A; 650C; 652A; 713B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 790B; 1007A; 1013A; 1171C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 591B; 700A; 701C (*ir*)
Sadtler Standard C-13 NMR Spectra, 472 (*cmr*)
Kanters, J.A. *et al., Acta Cryst. B*, 1976, **32**, 3328; 3331 (*cryst struct*)
Szyper, M. *et al., Anal. Chim. Acta*, 1976, **85**, 357 (*uv*)
Pesticide Manual, 6th edn., 1979, 105
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Ullmann's Encycl. Ind. Chem., VCH, Weinheim, 1985, **A6**, 537 (*rev*)
Merck Index, 11th edn., 1989, No. 1563
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 165 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1903-1904
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 281
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEE500; CEA000; SFU500; MIF775

5-Chloro-2-(3,5-di-*tert*-butyl-2-hydroxyphenyl)-2*H*-benzotriazole C-197

[3864-99-1]
*2-(5-Chloro-2*H*-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)phenol, 9CI. 2,4-Di*-tert*-butyl-6-(5-chloro-2*H*-benzotriazol-2-yl)phenol, 8CI*



$C_{20}H_{24}ClN_3O$ 357.882

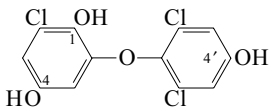
FDA approved for use in food-contact polymers. Pale yellow cryst. (EtOH). Mp 153-154°.

N-*Oxide:* [84755-45-3]
Cryst. (EtOH aq.). Mp 191-193°.

Rosevear, J. *et al., Aust. J. Chem.*, 1982, **35**, 2089; 1984, **37**, 2489 (*synth, uv, pmr*)
Tanimoto, S. *et al., Synthesis*, 1986, 647 (*synth, pmr*)
Food Chem. News, 2002, **43(47)**, 20 (*use*)

2-Chloro-6-(2,6-dichloro-4-hydroxyphenoxy)-1,4-benzenediol C-198

2,3′,6-Trichloro-2′,4,5′-trihydroxydiphenyl ether



$C_{12}H_7Cl_3O_4$ 321.543

1,4-Di-Me ether: [155519-91-8] ***Russuphelin D***
$C_{14}H_{11}Cl_3O_4$ 349.597
Needles. Mp 136-138°. λ_{max} 205 (ε 38900); 286 (ε 6166) (MeOH) (Berdy).

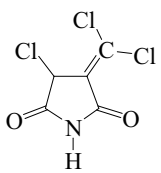
1,4′-Di-Me ether: [155519-92-9] ***Russuphelin E***
$C_{14}H_{11}Cl_3O_4$ 349.597

4,4′-Di-Me ether: [155519-93-0] ***Russuphelin F***
$C_{14}H_{11}Cl_3O_4$ 349.597

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1726

3-Chloro-4-(dichloromethylene)-2,5-pyrrolidinedione, 9CI C-199

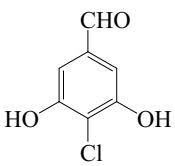
[170660-63-6]



$C_5H_2Cl_3NO_2$ 214.434
Bacterial mutagen produced by chlorination of simulated poultry chiller water. Cryst. (CCl_4). Mp 153-154.5°.

Haddon, W.F. *et al., J. Agric. Food Chem.*, 1996, **44**, 256-263 (*synth, cryst struct*)

4-Chloro-3,5-dihydroxybenzaldehyde C-200



$C_7H_5ClO_3$ 172.567

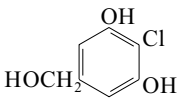
Di-Me ether: [56518-48-0] *4-Chloro-3,5-dimethoxybenzaldehyde*
$C_9H_9ClO_3$ 200.621
Isol. from the mycelium of *Hericium*

erinaceum (lions mane). Cryst. Mp 165-167° (118-120°).

Kompis, I. *et al., Helv. Chim. Acta*, 1977, **60**, 3025 (*synth*)
Okamoto, K. *et al., Phytochemistry*, 1993, **34**, 1445 (*isol*)

4-Chloro-3,5-dihydroxybenzyl alcohol C-201

2-Chloro-5-(hydroxymethyl)-1,3-benzenediol



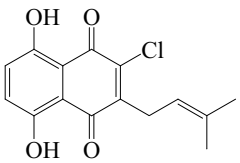
$C_7H_7ClO_3$ 174.583

1,3-Di-Me ether: [152570-76-8] *4-Chloro-3,5-dimethoxybenzyl alcohol*
$C_9H_{11}ClO_3$ 202.637
Isol. from the mycelium of *Hericium erinaceum* (lions mane). Cryst. Mp 83-85°.

Okamoto, K. *et al., Phytochemistry*, 1993, **34**, 1445 (*isol*)

2-Chloro-5,8-dihydroxy-3-prenyl-1,4-naphthoquinone C-202

2-Chloro-5,8-dihydroxy-3-(3-methyl-2-butenyl)-1,4-naphthalenedione, 9CI. ***Chlorosesamone***



$C_{15}H_{13}ClO_4$ 292.718
Constit. of the roots of *Sesamum indicum* (sesame). Red needles (EtOAc/hexane). Mp 129-130°. λ_{max} 217 (log ϵ 4.48); 287 (log ϵ 3.98); 491 (log ϵ 3.82); 514 (log ϵ 3.84); 549 (log ϵ 3.65) (MeOH).

Feroj Hasan, A.F.M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 873-874

Chloroform C-203

[67-66-3]
Trichloromethane, 9CI. R20
$CHCl_3$
$CHCl_3$ 119.377
Indirect food additive arising from adhesives and polymers. Liq. Spar. sol. H_2O. d_4^{25} 1.48. Mp -63.2°. Bp 61.3°. n_D^{20} 1.4467. Log P 1.95 (calc). Nonflammable. Slowly dec. in air and light forming $COCl_2$ (toxic) and other products. Forms hydrate with $18H_2O$, dec. at 1.6°. Forms azeotrope contg. 2.5% H_2O, Bp 56°.

► Vigorous reaction with Me_2CO and base, explosive reaction with some materials. Poss. human carcinogen. Skin, eye and respiratory tract irritant. Adverse systemic effects by inhalation can lead to loss of consciousness, cardiac respiratory failure and death. Hepatotoxic and nephrotoxic. Exp. carcinogen. Exp. reprod. and teratogenic effects. OES: long-term 2 ppm (Sk). Can autoxidise on storage to generate highly toxic phosgene. FS9100000

[865-49-6, 3170-80-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 83A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 122A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 116C (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 130; 1988, **13**, 9; 1990, **15**, 84; 1980, **8**, 92; 1986, **12**, 517 (*use*)
Dykes, M.H.M. *et al., Int. Anesthesiol. Clin.*, 1970, **8**, 357 (*rev, pharmacol*)
Legradi, L. *et al., Mikrochim. Acta*, 1972, 369 (*use*)
IARC Monog., 1979, **20**, 401; *Suppl*. 7, 152; *Suppl*. 6, 155 (*rev, tox*)
Davidson, I.W.F. *et al., Drug Chem. Toxicol.*, 1982, **5**, 87 (*rev, metab, tox*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 2467; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1985, 2282 (*cmr*)
Anderson, A. *et al., J. Chem. Phys.*, 1985, **82**, 99 (*Raman, conformn*)
Hahn, S. *et al., J. Solution Chem.*, 1985, **14**, 129 (*pmr*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A6**, 238 (*rev*)
Organo-chlorine Solvents, Royal Society of Chemistry, 1986, 17 (*tox, rev*)
Tate, R. *et al., Z. Naturforsch., A*, 1986, **41**, 1091 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 1051 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 911
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1134-1138 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 578-579
Turk, E. *et al., Chem. Eng. News*, March 2, 1998, 6 (*haz, autoxidn*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0354
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 303
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CHJ500

10-Chloro-1,16-heptadecadiene-4,6-diyne-3,9-diol C-204

[139035-29-3]
Ginsenoyne B
$H_2C{=}CHCH(OH)C{\equiv}CC{\equiv}CCH_2CH(OH)CHCl(CH_2)_5CH{=}CH_2$
$C_{17}H_{23}ClO_2$ 294.82
Present in ginseng root. Oil. $[\alpha]_D$ -33 (c, 2.0 in $CHCl_3$). λ_{max} 201 ; 230 ; 243 ; 257 ($CHCl_3$).

Di-Ac: [139035-32-8]
Oil. $[\alpha]_D$ +32.8 (c, 2.04 in $CHCl_3$).

Hirakura, K. *et al., Phytochemistry*, 1991, **30**, 3327 (*isol, ir, uv, ms, pmr, cmr*)

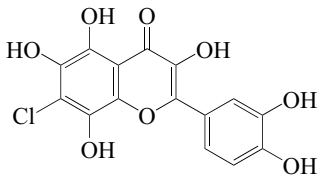
10-Chloro-1-heptadecene-4,6-diyne-3,9-diol C-205

[111103-92-5]
Panaxydol chlorohydrin
$H_2C{=}CHCH(OH)C{\equiv}CC{\equiv}CCH_2CH(OH)CHCl(CH_2)_6CH_3$
$C_{17}H_{25}ClO_2$ 296.836
Isol. from Korean ginseng root. λ_{max} 219 ; 229 ; 242 ; 255 ; 266 (EtOH) (Berdy).

Kitagawa, I. *et al., Yakugaku Zasshi*, 1987, **107**, 495 (*synth*)
Ahn, B.Z. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1989, **322**, 223 (*isol, props, cmr, uv, ir*)
Hirakura, K. *et al., Phytochemistry*, 1991, **30**, 3327 (*isol, pmr*)

7-Chloro-3,3′,4′,5,6,8-hexahydroxyflavone C-206

7-Chloro-3′,4′,5,6,8-pentahydroxyflavonol

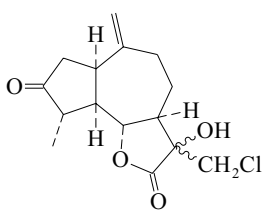


$C_{15}H_9ClO_8$ 352.684

Hexa-Me ether:7-Chloro-3,3′,4′,5,6,8-hexamethoxyflavone
$C_{21}H_{21}ClO_8$ 436.845
Constit. of a *Citrus* sp. (Dancy tangerine). Yellow needles (MeOH). Mp 145-146°.

Chen, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 1235-1238 (*isol, pmr, cmr, ms*)

13-Chloro-11-hydroxy-3-oxo-10(14)-guaien-12,6-olide C-207



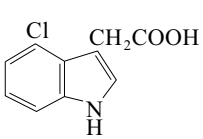
$C_{15}H_{19}ClO_4$ 298.765

(1α,4α,5α,6α,11ξ)-form [83551-02-4]
8-Deoxy-11-hydroxy-13-chlorogrosheimin
Constit. of *Cynara scolymus* (artichoke). Cryst. (EtOAc). Mp 228-230°.

Barbetti, P. *et al., Nat. Prod. Lett.*, 1993, **3**, 21 (*isol, pmr, cmr*)

4-Chloro-1*H*-indole-3-acetic acid C-208

[2519-61-1]



$C_{10}H_8ClNO_2$ 209.631
Auxin from the seeds of *Pisum sativum* (pea) and isol. from *Pinus sylvestris* (Scotch pine). Cryst. (1,2-dichloroethane/EtOH). Mp 179-180°.

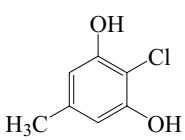
Me ester: [19077-78-2]
$C_{11}H_{10}ClNO_2$ 223.658
Auxin from the seeds of *Pisum sativum* (pea). Cryst (EtOAc/hexane). Mp 120-121°.
Hansch, C. *et al., J.A.C.S.*, 1951, **73**, 3518 (*synth*)
Marumo, S. *et al., Nature (London)*, 1968, **219**, 959 (*isol*)
Magnus, V. *et al., Phytochemistry*, 1997, **46**, 675-681 (*isol*)
Katayama, M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 808-815 (*synth, ir, pmr, ms*)

Chloromethoxymethane, 9CI C-209

[107-30-2]
Chloromethyl methyl ether
$ClCH_2OMe$
C_2H_5ClO 80.514
Used to modify ion-exchange membranes used in the production of grapefruit juice. Liq. d^{25} 1.07. Bp 59.5°.
▶ Human carcinogen (technical grade material). Eye and respiratory tract irritant. LD_{50} (rat, orl) 817 mg/kg. LC_{50} (rat, ihl) 55 ppm (7h exposure). Exp. carcinogen. KN6650000
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 178B (*nmr*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 126E (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 377 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 83; 1977, **7**, 61; 1988, **13**, 76; 1981, **9**, 107; 1976, **6**, 109; 1986, **12**, 116; 1980, **8**, 387; 1982, **10**, 460 (*use*)
IARC Monog., 1974, **4**, 239; *Suppl.* 7, 131; *Suppl.* 6, 159 (*rev, tox*)
Ger. Pat., 1975, 2 431 778; *CA*, **83**, 27558p (*synth*)
Stadlwieser, J. *et al., Synthesis*, 1985, 490 (*use*)
Linderman, R.J. *et al., J.O.C.*, 1994, **59**, 6499 (***synth, bibl***)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1156-1159 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 579-580
Chong, J.M. *et al., Synth. Commun.*, 1998, **28**, 2801-2806 (*synth*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 309
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CIO250

2-Chloro-5-methyl-1,3-benzenediol, 9CI C-210

[56021-31-9]
2-Chloro-5-methylresorcinol, 8CI. 4-Chloro-3,5-dihydroxytoluene

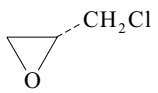


$C_7H_7ClO_2$ 158.584
Prisms (C_6H_6). Mp 138-138.5° (134-136°). λ_{max} 274 (log ϵ 2.99) (MeCN).

1-Me ether: [57074-22-3] *2-Chloro-3-methoxy-5-methylphenol*
$C_8H_9ClO_2$ 172.611
Di-Me ether: [27971-69-3] *2-Chloro-1,3-dimethoxy-5-methylbenzene. 4-Chloro-3,5-dimethoxytoluene*
$C_9H_{11}ClO_2$ 186.637
Isol. from mycelia of *Hericium erinaceum* (lions mane). Cryst. (EtOH). Mp 74-75°.
Büchi, G. *et al., J.O.C.*, 1971, **36**, 1143
Gavin, J. *et al., Helv. Chim. Acta*, 1978, **61**, 352 (*1-Me ether*)
Fitzpatrick, L. *et al., J.C.S. Perkin 1*, 1980, 85-89 (*synth, pmr*)
Henderson, G.B. *et al., J.C.S. Perkin 1*, 1983, 2595-2599 (*synth, pmr*)
Hill, R.A. *et al., J.C.S. Perkin 1*, 1987, 2209-2215 (*synth, di-Me ether*)
Okamoto, K. *et al., Phytochemistry*, 1993, **34**, 1445 (*di-Me ether*)
Monde, K. *et al., J. Nat. Prod.*, 1998, **61**, 913-921 (*isol, uv, ir, pmr, cmr, ms*)

(Chloromethyl)oxirane, 9CI, 8CI C-211

[106-89-8]
α-Epichlorohydrin. 3-Chloropropylene oxide. 1-Chloro-2,3-epoxypropane. Epichlorohydrin



(R)-form

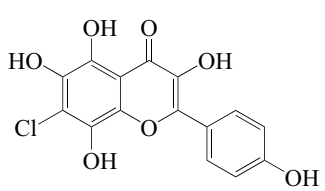
C_3H_5ClO 92.525
Used for cross-linking dextrose units in food starch.
▶ Flammable, fl. p. 41°, autoignition temp. 411°. Toxic by skin contact and inhalation, irritant. Reacts violently with some materials. Possible human carcinogen. Severe eye, skin and respiratory tract irritant. A vesicant and skin sensitiser. Can cause dermatitis. Inhalation may cause respiratory paralysis. Exp. carcinogen and teratogen. Exp. reprod. effects. LD_{50} (mus, orl) 195 mg/kg; LD_{50} (mus, skn) 250 mg/kg. OES: long-term 0.5 ppm; short-term 1.5 ppm. TX4900000
(R)-form [51594-55-9]
Liq. Bp 115-116°. $[\alpha]_D^{22}$ -33 (c, 4.22 in MeOH).
▶ RR0427000
(S)-form [67843-74-7]
Liq. $[\alpha]_D^{20}$ +33 (c, 1.126 in MeOH).
▶ RR0427100
(±)-form [13403-37-7]
Liq. Insol. H_2O; misc. most org. solvs. d_4^{20} 1.18. Fp -57.2. Bp 115-117°. n_D^{20} 1.4382. Vp 16 mmHg (25°).
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 231D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 369B; 369C; 370A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 304C (*ir*)
Fairbourne, A. *et al., J.C.S.*, 1932, 1965 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 233 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 256 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 290
IARC Monog., 1976, **11**, 131; *Suppl.* 6, 286; *Suppl.* 7, 702 (*rev, tox*)
Shapiro, M.J. *et al., J.O.C.*, 1977, **42**, 1435 (*cmr*)
Baldwin, J.J. *et al., J.O.C.*, 1978, **43**, 4876 (*R-form, S-form, synth*)
Abraham, R.J. *et al., Tetrahedron*, 1983, **39**, 4201 (*pmr*)
Nyquist, R.A. *et al., Appl. Spectrosc.*, 1986, **40**, 821 (*ir, Raman*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1986, **6**, 273 (*rev, polymers*)
Pirrung, M.C. *et al., Helv. Chim. Acta*, 1989, **72**, 1301 (*synth*)
Durig, J.R. *et al., J. Mol. Struct.*, 1989, **197**, 143 (*conformn*)
Chen, C.-S. *et al., J.C.S. Perkin 1*, 1990, 2559 (*synth*)
Alkylene Oxides and Their Polymers; Surfactant Science Series, Vol. 35, (Eds. Bailey, F.E. *et al*), Dekker, New York, 1991,
Ellis, M.K. *et al., J.C.S. Perkin 1*, 1991, 747 (*synth, pmr*)
Dargelos, M. *et al., Aust. J. Chem.*, 1992, **45**, 1327 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1102
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2326-2328 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 928-929
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1091
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 298
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAZ500
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 417 (*tox, rev*)

Chloropentafluoroethane C-212

[76-15-3]
[39432-81-0]
Fluorocarbon 115. Freon 115. Arcton 115. CFC 115. Genetron 115
F_3CCClF_2
C_2ClF_5 154.467
Aerating agent for foamed or sprayed food products. Gas. Mp -106°. Bp -37.7°.
▶ Low toxicity. Non-flammable. Substance production controlled by environmental legislation. OES: long-term 1000 ppm. KH7877500
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 126A (*ir*)
Haszeldine, R.N. *et al., J.C.S.*, 1953, 3761
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 580-581
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CJI500

7-Chloro-3,4′,5,6,8-pentahydroxyflavone C-213

7-Chloro-4′,5,6,8-tetrahydroxyflavonol



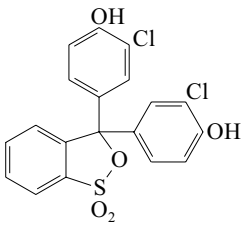
$C_{15}H_9ClO_7$ 336.685
Penta-Me ether:7-Chloro-3,4′,5,6,8-pentamethoxyflavone

$C_{20}H_{19}ClO_7$ 406.819
Constit. of a *Citrus* sp. (Dancy tangerine). Yellow needles (MeOH). Mp 161-162°.

Chen, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 1235-1238

Chlorophenol red C-214

[4430-20-0]
*4,4′-(3*H*-2,1-Benzoxathiol-3-ylidene)-bis[2-chlorophenol], 9CI. 3,3-Bis(3-chloro-4-hydroxyphenyl)3*H*-2,1-benzoxathiole* S,S-*dioxide. 3,3′-Dichlorophenolsulfonephthalein*



$C_{19}H_{12}Cl_2O_5S$ 423.272
Used in the frozen food industry for monitoring storage temperature changes. Greenish-brown cryst. Sol. EtOH; spar. sol. H_2O. Mp 261-262°. Available as sodium salt.

[41350-02-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1023A (*ir*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 200
Harden, W.C. *et al., J.A.C.S.*, 1930, **52**, 4611 (*synth*)
Zombory, L. *et al., Z. Anorg. Allg. Chem.*, 1933, **215**, 255 (*adsorption indicator*)
U.S. Pat., 1958, 2 850 393; *CA*, 1959, **53**, 607a (*use*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, 111 (*use*)

Chlorophyll C-215

[8049-84-1]

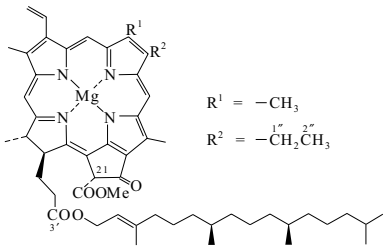
[1406-65-1]
Biophyll. C.I. Natural green 3, 9CI. E140. C.I. 75810

An extract of Chlorophyll a, C-216 and Chlorophyll b, C-217 obt. by solv. extraction of alfalfa meal. The central magnesium atom of the natural chlorophylls may be replaced by copper in the commercial material to obtain blue shaded products, as opposed to yellow shades for the magnesium compd.. Colourant for cosmetics and foodstuffs, esp. meat casings, fats and shortening. Alkaline hydrol. gives C.I. Natural green 5, C-255.

Judah, M.A. *et al., Ind. Eng. Chem.*, 1954, **46**, 2262-2271 (*manuf, rev*)
Colour Index, 3rd edn., 1971, **4**, 4640 (*bibl*)
Wegener, J.W. *et al., Chromatographia*, 1987, **24**, 865-875 (*hplc, detn*)

Chlorophyll a C-216

[479-61-8]
[3,7,11,15-Tetramethyl-2-hexadecenyl 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N^{23},N^{24},N^{25},N^{26}*]magnesium, 9CI*



$C_{55}H_{72}MgN_4O_5$ 893.503
Used in food processing as an appearance control agent for colours. Dark green greasy powder (petrol) or leaflets. Sol. EtOAc, Et_2O; fairly sol. MeOH; poorly sol. hexane. Mp 117-120°. $[\alpha]_D^{20}$ -262 (Me_2CO). Dilute acid removes Mg to form Phaeophytin a. Hydrol. by Chlorophyllase (or warm acid) → Phaeophorbide a. Acid catalysed methanolysis → see Phaeophorbide a. Alkaline hydrol. → Chlorin e_6. Other esters e.g. geranylgeranyl are found in various microorganisms λ_{max} 409 ; 429 ; 498 ; 537 ; 577 ; 613 ; 660 (EtOH) (Berdy).

21-Epimer: [22309-13-3] ***Chlorophyll a′***
$C_{55}H_{72}MgN_4O_5$ 893.503

3′-Free acid: [14897-06-4] ***Chlorophyllide a***
$C_{35}H_{34}MgN_4O_5$ 614.982

21-Hydroxy: [71699-04-2] ***13²-Hydroxychlorophyll a***
$C_{55}H_{72}MgN_4O_6$ 909.502Artifact.

6-Chloro, 21-hydroxy: [91488-37-8] *20-Chloro-13²-hydroxychlorophyll a*. ***Chlorophyll RCI***
$C_{55}H_{71}ClMgN_4O_6$ 943.947Probable artifact.

1″,2″-Didehydro:4-Vinyl-4-desethylchlorophyll a
$C_{55}H_{70}MgN_4O_5$ 891.487

[1406-65-1, 117288-86-5, 118626-30-5]

Woodward, R.B. *et al., J.A.C.S.*, 1960, **82**, 3800 (*synth*)
Fleming, I. *et al., Nature (London)*, 1967, **216**, 151 (*abs config*)
Brockman, H. *et al., Annalen*, 1974, 1007
Chow, H.C. *et al., J.A.C.S.*, 1975, **97**, 7230 (*cryst struct*)
Chem. Biochem. Plant Pigm., (Ed. Goodwin, T.W.), Academic Press, London, 1976, (*book*)
Schoch, S. *et al., Z. Pflanzenphysiol.*, 1977, **83**, 427 (*isol*)
Gleixner, G. *et al., Experientia*, 1982, **38**, 303 (*purifn*)
Bazzaz, M.B. *et al., Tet. Lett.*, 1982, **23**, 1211 (*Divinylchlorophyll a*)
Lotjonen, S. *et al., Org. Magn. Reson.*, 1983, **21**, 757 (*cmr*)
Smith, K.M. *et al., Org. Magn. Reson.*, 1984, **22**, 779 (*pmr*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*rev, biosynth*)
Fujiwara, M. *et al., J. Phys. Chem.*, 1986, **90**, 250; 5646 (*ir, Raman*)
Grotemeyer, J. *et al., J.A.C.S.*, 1986, **108**, 4233 (*ms*)
Tasumi, M. *et al., Adv. Spectrosc. (Chichester, U.K.)*, 1987, **14**, 407 (*rev, ir, Raman*)
Senge, M. *et al., FEBS Lett.*, 1988, **234**, 215 (*Chlorophyll RCI*)
Senge, M. *et al., Z. Naturforsch., C*, 1988, **43**, 515 (*13²-Hydroxychlorophyll a*)
Okazaki, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3303 (*biosynth*)
Grese, R.P. *et al., J. Am. Soc. Mass Spectrom.*, 1990, **1**, 72 (*Chlorophyll RCI*)
Woodward, R.B. *et al., Tetrahedron*, 1990, **46**, 7599 (*synth, rev*)
Giacometti, G. *et al., Gazz. Chim. Ital.*, 1991, **121**, 457 (*pmr*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995, (*bibl, spectra*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 581
Ruediger, W. *et al., Phytochemistry*, 1997, **46**, 1151-1167 (*rev, biosynth*)
Itoh, D. *et al., J. Nat. Prod.*, 2000, **63**, 1090-1093 (*biosynth*)

Chlorophyll b C-217

[519-62-0]
As Chlorophyll a, C-216 with
$R^1 = -CHO$, $R^2 = -CH_2CH_3$

$C_{55}H_{70}MgN_4O_6$ 907.486
Green pigment in leaves of plants together with Chlorophyll a, C-216. Dark green powder (petrol). Reacts as Chlorophyll a with acids and Chlorophyllase to give similar prods., i.e. Phaeophytin b, Phaeophorbide b, P-237 and Me ester. Alkaline hydrol. gives Rhodin g_7. Other esters e.g. geranylgeranyl are found in various microorganisms.

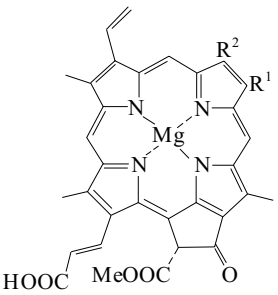
3′-Free acid: [14428-12-7] ***Chlorophyllide b***
$C_{35}H_{32}MgN_4O_6$ 628.966

1′,2′-Didehydro: [89456-97-3] *Divinylchlorophyll b. 4-Desethyl-4-vinylchlorophyll b*
$C_{55}H_{68}MgN_4O_6$ 905.47

Fleming, I. *et al., Nature (London)*, 1967, **216**, 151 (*abs config*)
Shlyk, A.A. *et al., Annu. Rev. Plant Physiol.*, 1971, **22**, 169 (*biosynth*)
Brockmann, H. *et al., Annalen*, 1974, 1007
Serbin, R. *et al., J.A.C.S.*, 1975, **97**, 7237 (*cryst struct*)
Chem. Biochem. Plant Pigm., Goodwin, T.W., Ed., Academic Press, London, 1976, (*book*)
Shioi, Y. *et al., Biochim. Biophys. Acta*, 1983, **756**, 127 (*isol*)
Risch, N. *et al., Tet. Lett.*, 1983, **24**, 173 (*cmr*)
Brereton, R.G. *et al., Tet. Lett.*, 1983, **24**, 5775 (*Divinylchlorophyll b*)
Wu, S.M. *et al., J. Biol. Chem.*, 1985, **260**, 3632 (*struct*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*rev, biosynth*)
Fujiwara, M. *et al., J. Phys. Chem.*, 1986, **90**, 250 (*Raman, ir*)
Lotjonen, S. *et al., Magn. Reson. Chem.*, 1987, **25**, 670 (*pmr*)
Grese, R.P. *et al., J. Am. Soc. Mass Spectrom.*, 1990, **1**, 72 (*ms*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995, (*bibl, spectra*)
Ruediger, W. *et al., Phytochemistry*, 1997, **46**, 1151-1167 (*rev, biosynth*)

Chlorophyll c C-218

Chlorophyllide c



c_1, R^1 = CH=CH_2, R^2 = CH_3

c_2, R^1 = CH_2CH_3, R^2 = CH_3

c_3, R^1 = CH=CH_2, R^2 = COOMe

In spite of their name these are porphyrins, not dihydro derivs. (or chlorins). Widely distributed photosynthetic pigment in marine organisms, e.g. the diatom *Nitzschia closterium*. Cryst. (THF/petrol). λ_{max} 447 ; 578 ; 626 (Et_2O).

Chlorophyll c_1 [18901-56-9]

$C_{35}H_{28}MgN_4O_5$ 608.935

Chlorophyll c_2 [27736-03-4]

$C_{35}H_{30}MgN_4O_5$ 610.951

Chlorophyll c_3 [111308-93-1]

$C_{36}H_{28}MgN_4O_7$ 652.945

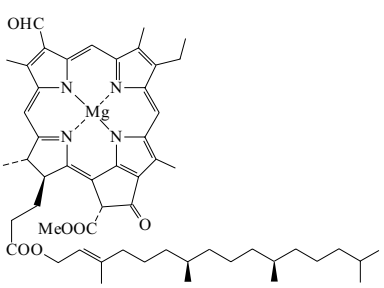
[1406-65-1]

Dougherty, R.C. *et al., J.A.C.S.*, 1970, **92**, 2826
Budzikiewicz, H. *et al., Tetrahedron*, 1971, **27**, 1447 (*isol, ir, pmr, ms, struct*)
Chem. Biochem. Plant Pigm., (Ed. Goodwin, T.W.), Academic Press, London, 1976, (*book*)
Clezy, P.S. *et al., Aust. J. Chem.*, 1978, **31**, 2491 (*synth*)
The Porphyrins, (Ed. Dolphin, D.), Academic Press, N.Y., 1978, (*book*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*rev, biosynth*)
Tasumi, M. *et al., Adv. Spectrosc. (Chichester, U.K.)*, 1987, **14**, 407 (*rev, ir, Raman*)
Fookes, C.J.R. *et al., Chem. Comm.*, 1989, 1827 (*isol, pmr, struct, Chlorophyll c_3*)

Chlorophyll d C-219

[519-63-1]

[3,7,11,15-Tetramethyl-2-hexadecenyl-14-ethyl-9-formyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(2-)-N^{23},N^{24},N^{25},N^{26}]magnesium, 9CI



$C_{54}H_{70}MgN_4O_6$ 895.475

Widely distributed photosynthetic pigment. λ_{max} 445 ; 686 (Et_2O).

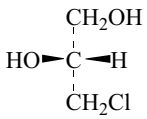
[1406-65-1]

Chem. Biochem. Plant Pigm., Goodwin, T.W., Ed., Academic Press, London, 1976, (*book*)
The Porphyrins, Dolphin, D., Ed., Academic Press, N.Y., 1978, (*book*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*revs, biosynth*)

3-Chloro-1,2-propanediol, 9CI C-220

[96-24-2]

Glycerol α-monochlorohydrin. α-Chlorohydrin. α-Glycerol chlorohydrin. α-Monochlorohydrin. Epibloc. 3-MCPD



(*R*)-*form*

$C_3H_7ClO_2$ 110.54

By-product of vegetable protein hydrolysed by HCl. Identified in some soy sauce products.

▶ Eye irritant. LD_{50} (mus, orl) 160 mg/kg. Exp. reprod. effects (male fertility). TY4025000

(*R*)-*form* [57090-45-6]

$[\alpha]_D^{19}$ -7.4 (c, 1.0 in H_2O).

(*S*)-*form* [60827-45-4]

$Bp_{0.5}$ 80°. $[\alpha]_D^{20}$ +7.3 (c, 1 in H_2O). The pharmacologically active enantiomer showing antifertility activity in mammalian spp..

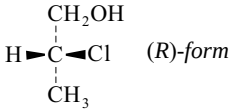
▶ TY4202300

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 169A (*nmr*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 108F (*ir*)
Fairbourne, A. *et al., J.C.S.*, 1931, 445 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 294 (*synth*)
Jones, H.F. *et al., Chem. Ind. (London)*, 1978, 533 (*synth*)
Jones, A.R. *et al., Experientia*, 1981, **37**, 340; 1983, **39**, 784 (*metab*)
Porter, K. *et al., Chem. Biol. Interact.*, 1982, **41**, 95 (*synth, isomers, activity*)
Jones, A.R. *et al., Aust. J. Biol. Sci.*, 1983, **36**, 333 (*rev, pharmacol*)
Brown-Woodman, P.D. *et al., Aust. J. Biol. Sci.*, 1986, **39**, 187 (*activity, tox*)
Narasimhan, S. *et al., Magn. Reson. Chem.*, 1987, **25**, 91 (*cmr*)
Ellis, M.K. *et al., J.C.S. Perkin 1*, 1991, 747 (*synth, pmr*)
Wang, G. *et al., J.O.C.*, 1999, **64**, 1036-1038 (*R-form, synth, pmr, cmr*)
Food Chem. News, 2001, **43(28)**, 9; **43(37)**, 18 (*occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1089; 1173
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDT750; CKU625; CHL875; CIL900

2-Chloro-1-propanol, 9CI C-221

[78-89-7]

Propylene chlorohydrin



(*R*)-*form*

C_3H_7ClO 94.54

▶ Skin and severe eye irritant. LD_{50} (rat, orl) 218 mg/kg; LD_{50} (rbt, skn) 529 mg/kg. Flammable, fl. p. 52°. UA8925000

(*R*)-*form* [37493-14-4]

$[\alpha]_D^{18}$ -2.92.

(*S*)-*form* [19210-21-0]

Bp_{75} 70.3-70.5° Bp_{15} 40-41°.

(±)-*form* [60828-60-6]

Used for etherification of food starch. d^{20} 1.1. Bp 133-134°. n_D^{20} 1.4362.

▶ Highly toxic, flammable.

Me ether: [5390-71-6] *2-Chloro-1-methoxypropane, 9CI*

C_4H_9ClO 108.567

Liq. d^{20} 1. Bp_{756} 98-99°. n_D^{20} 1.4075.

[6145-73-9, 26248-87-3]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 268B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 252B (*ir*)
Smith, L. *et al., CA*, 1921, **15**, 2627 (*synth*)
Dewael, A. *et al., Bull. Soc. Chim. Belg.*, 1925, **34**, 343
Fickett, W. *et al., J.A.C.S.*, 1951, **73**, 5063 (*synth*)
U.K. Pat., 1966, 1 029 607; *CA*, **65**, 7059d (*Me ether*)
East Ger. Pat., 1975, 115 901; *CA*, **87**, 23019y (*synth*)
Schurig, V. *et al., Angew. Chem., Int. Ed.*, 1978, **17**, 937 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 140 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2345-2346
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CKR500

1-Chloro-3,11-tridecadiene-5,7,9-triyn-2-ol C-222

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH(OH)CH_2Cl$

$C_{13}H_{11}ClO$ 218.682

(*E*,*E*)-*form*

Isol. from *Carthamus tinctorius* (safflower). Yellowish cryst (Et_2O/petrol). Mp 83°. $[\alpha]_{Hg}$ -3 (c, 0.33 in Et_2O).

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 3433 (*isol, uv, ir, pmr, ord, struct*)

2-Chloro-3-tridecene-5,7,9,11-tetrayn-1-ol C-223

[65398-34-7]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCHClCH_2OH$

$C_{13}H_9ClO$ 216.666

(*E*)-*form* [71866-99-4]

Chlorohydrin

Isol. from *Carthamus tinctorius* (safflower). Mp 111-112° dec. $[\alpha]_D^{22}$ -88.5 ($CHCl_3$).

Ac:1-Acetoxy-2-chloro-3-tridecene-5,7,9,11-tetrayne

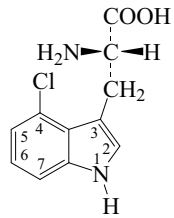
$C_{15}H_{11}ClO_2$ 258.703

Cryst. (Et_2O/petrol). Mp 57.5-58°.

Bohlmann, F. *et al., Chem. Ber.*, 1961, **94**, 3179; 1962, **95**, 2939; 1964, **97**, 809; 1966, **99**, 3433 (*isol, struct, synth, biosynth*)
Andersen, A.B. *et al., Phytochemistry*, 1977, **16**, 1829 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 71 (*isol*)

4-Chlorotryptophan C-224

*2-Amino-3-(4-chloro-1*H*-indol-3-yl)propanoic acid*



(*S*)-*form*

$C_{11}H_{11}ClN_2O_2$ 238.673

(*R*)-*form* [27542-41-2]
D-form
$[\alpha]_D^{15}$ +48 (c, 0.12 in AcOH aq.).

(*S*)-*form* [52448-14-3]
L-form
Isol. from the seed protein of *Pisum sativum* (pea). Also obt. from the seeds of *Vicia faba*. $[\alpha]_D^{15}$ -45 (c, 0.13 in AcOH aq.).

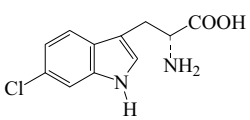
N-*(Carbomethoxyacetyl):*
$C_{15}H_{15}ClN_2O_5$ 338.747
Isol. from *Pisum sativum* (pea).

N-*(Carbethoxyacetyl):*
$C_{16}H_{17}ClN_2O_5$ 352.773
Isol. from *Pisum sativum* (pea).

(±)-*form* [118244-93-2]
Feathery plates (AcOH). Mp 298° dec.

Rydon, H.N. *et al., J.C.S.*, 1955, 3499 (*synth*)
Marumo, S. *et al., Planta*, 1970, **90**, 208 (*isol*)
Japan. Pat., 1973, 73 98 091; *CA*, **80**, 106876g (*isol*)
Thiruvikraman, S.V. *et al., Tet. Lett.*, 1988, **29**, 2339 (*isol, synth*)
Fock, A. *et al., Phytochemistry*, 1992, **31**, 2327 (*isol*)
Lee, M. *et al., J. Het. Chem.*, 1994, **31**, 711 (*cmr, pmr*)

6-Chlorotryptophan, 9CI C-225



(*R*)-*form*

$C_{11}H_{11}ClN_2O_2$ 238.673

(*R*)-*form* [56632-86-1]
D-form
Mp 264° dec. $[\alpha]_D^{23}$ +28 (c, 1 in MeOH).

N^{α}-*Formyl:* [57233-89-3]
$C_{12}H_{11}ClN_2O_3$ 266.683
Cryst. + $1H_2O$. Mp 143-145°. $[\alpha]_D^{23}$ -47 (c, 1 in MeOH).

(±)-*form* [17808-21-8]
Sweetening agent, sweetness 1300x sucrose. Off-white cryst. (AcOH). Mp 278° dec. (285-286°). No indication of coml. use.

N^{α}-*Formyl:* [57233-85-9]
Cryst. (EtOAc). Mp 180-181°.

[33468-35-8]

Fukuda, D.S. *et al., Appl. Microbiol.*, 1971, **21**, 841 (*manuf*)
Yamada, S. *et al., J. Agric. Food Chem.*, 1975, **23**, 653 (*synth, resoln*)
Perry, C.W. *et al., Synthesis*, 1977, 492 (*synth*)
Hengartner, U. *et al., J.O.C.*, 1979, **44**, 3748 (*synth*)
Lee, M. *et al., J. Het. Chem.*, 1994, **31**, 711 (*pmr, cmr*)

Cholecystokinin C-226

[9011-97-6]

[9001-71-2]
Pancreozymin, BAN. *CCK-PZ*

H-Tyr-Ile-Gln-Gln-Ala-Arg-Lys-Ala-Pro-Ser-Gly-Arg-Val-Ser-Met-Ile-Lys-Asn-Leu-Gln-Ser-Leu-Asp-Pro-Ser-His-Arg-Ile-Ser-Asp-Arg-Asp-Tyr(SO_3H)-Met-Gly-Trp-Met-Asp-Phe-NH_2
Struct. shown is Cholecystokinin-39(pig). Cholecystokinin-33(pig) is $\alpha^{7\text{-}39}$ cholecystokinin-39(pig). C-Terminal pentapeptide is identical to that of Gastrin and Caerulin.

[67256-27-3, 79955-77-4, 83381-92-4, 93195-44-9, 96827-04-2, 96827-06-4, 98143-72-7, 103842-53-1, 129202-58-0, 130121-75-4, 139637-56-2, 139873-14-6]

Harper, A.A. *et al., J. Physiol. (London)*, 1943, **102**, 115 (*isol*)
Jorpes, E. *et al., Acta Chem. Scand.*, 1964, **18**, 2408 (*purifn*)
Mutt, V. *et al., Eur. J. Biochem.*, 1968, **6**, 156 (*struct*)
Ondetti, M.A. *et al., J.A.C.S.*, 1970, **92**, 195 (*synth*)
Bodanszky, M. *et al., J.O.C.*, 1972, **37**, 2303 (*synth*)
Takahashi, Y. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1985, **82**, 1931 (*cloning*)
Kurano, Y. *et al., Chem. Comm.*, 1987, 323 (*synth*)
Mutt, V. *et al., Adv. Metab. Disord.*, 1988, **11**, 251 (*rev*)
Cautor, P. *et al., Digestion*, 1989, **42**, 181 (*rev*)
Hughes, J. *et al., The Neuropeptide Cholecystokinin (CCK)*, Ellis Horwood, 1989, (*book*)
Li, C.S. *et al., Neurosci. (Oxford)*, 1992, **48**, 707
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 776
Rehfeld, J.F. *et al., Adv. Cancer Res.*, 1994, **63**, 295 (*rev*)
Reeve, J.R. *et al., Ann. N.Y. Acad. Sci.*, 1994, **713**, 1 (*rev*)
Liddle, R.A. *et al., Gut Pept. 1994*, (Eds. Walsh, J.H. *et al*), Raven Press, 1994, 175 (*rev*)
Crawley, J.N. *et al., Peptides (N.Y.)*, 1994, **15**, 731 (*pharmacol, rev*)

Cholecystokinin 33 C-227

[93443-27-7]
CCK 33

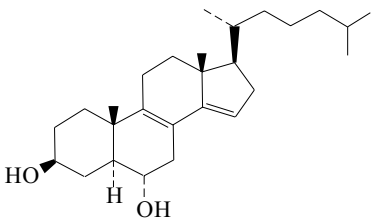
Peptide consisting of 33 amino acid residues with sulfated Tyr at position 27.

Porcine-*form* [67256-27-3]
$[\alpha]_D^{27}$ -70 (c, 0.20 in 1*M* AcOH).

Human-*form* [96827-04-2]

Mutt, V. *et al., Biochem. J.*, 1971, **125**, 57P (*isol*)
Sjodin, L. *et al., Gastroenterology*, 1977, **73**, 1015 (*activity*)
Morgan, K.G. *et al., Am. J. Physiol.*, 1978, **325**, E324 (*activity*)
Rehfeld, J.F. *et al., J. Biol. Chem.*, 1986, **261**, 5832 (*bibl*)
Kurano, Y. *et al., Chem. Comm.*, 1987, 323 (*synth, porcine form*)
Fujii, N. *et al., Chem. Comm.*, 1988, 324 (*bibl, synth, human form*)
Doi, R. *et al., Pancreas*, 1990, **5**, 615 (*pharmacol, human form*)
Penke, B. *et al., Pept. Res.*, 1991, **4**, 289 (*synth*)
Miranda, M.T. *et al., J. Med. Chem.*, 1993, **36**, 1681 (*bibl, activity, analogues*)
Lieverse, R.J. *et al., Gut*, 1995, **36**, 176 (*pharmacol*)

Cholesta-8,14-diene-3,6-diol C-228

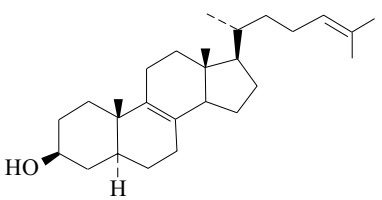


$C_{27}H_{44}O_2$ 400.643

(3β,5α,6α)-*form* [84765-66-2]
Thurberol
Constit. of *Stenocereus thurberi* (organ pipe cactus). Cryst. Mp 190-190.5°. $[\alpha]_D^{24}$ +2 (c, 3 in $CHCl_3$).

Kircher, H.W. *et al., Phytochemistry*, 1982, **21**, 1705

Cholesta-8,24-dien-3-ol, 9CI C-229



$C_{27}H_{44}O$ 384.644

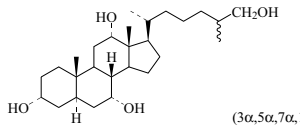
(3β,5α)-*form* [128-33-6]
Zymosterol
Cryst. (MeOH). Mp 110°. $[\alpha]_D^{20}$ +49 (c, 1.0 in $CHCl_3$).

Ac: [2579-07-9]
Cryst. (MeOH). Mp 107-108°. $[\alpha]_D^{20}$ +35 (c, 1.3 in $CHCl_3$).

[6036-87-9, 17137-73-4]

Smedley-MacLean, J. *et al., Biochem. J.*, 1928, **22**, 22 (*isol*)
Heath-Brown, J. *et al., J.C.S.*, 1940, 1482 (*synth*)
Charney, E. *et al., Tetrahedron*, 1965, **21**, 3121 (*ord*)
Terence, J.S. *et al., J. Lipid Res.*, 1968, **9**, 120 (*nmr, ir*)
Ogihara, N. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2724 (*synth, ms*)
Dolle, R.E. *et al., Chem. Comm.*, 1988, 19 (*synth*)

Cholestane-3,7,12,26-tetrol C-230



(3α,5α,7α,12α,25ξ)-*form*

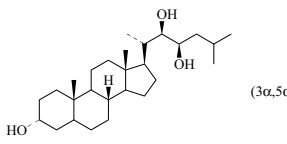
$C_{27}H_{48}O_4$ 436.674

(3α,5α,7α,12α,25ξ)-*form*
27-Deoxy-5α-cyprinol
Isol. from lungfish and carp. Mp 232°. $[\alpha]_D$ +39.

(3α,5β,7α,12α,25ξ)-*form*
27-Deoxy-5β-cyprinol

Anderson, I.G. *et al., Biochem. J.*, 1974, **141**, 485 (*isol*)
Amos, B. *et al., Biochem. J.*, 1977, **161**, 201 (*isol*)

Cholestane-3,22,23-triol C-231



(3α,5α,22*R*,23*R*)-*form*

$C_{27}H_{48}O_3$ 420.674

(3α,5α,22*R*,23*R*)-*form* [378795-16-5]
6-Deoxo-28-nortyphasterol
Constit. of tomato (*Lycopersicon esculentum*). Cryst. (EtOH). Mp 213-214°.

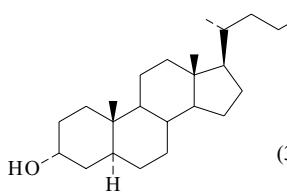
3-Ketone: [378795-15-4] *22,23-Dihydroxycholestan-3-one*
$C_{27}H_{46}O_3$ 418.659
Cryst. (hexane). Mp 146-147°.

(3β,5α,22*R*,23*R*)-*form* [378795-14-3] *6-Deoxo-28-norteasterone*
Cryst. (MeOH). Mp 213-214°.

Yokota, T. *et al., Phytochemistry*, 2001, **58**, 233-238 (*isol, pmr, synth*)

Cholestan-3-ol C-232

[27409-41-2]



(3α,5α)-*form*

$C_{27}H_{48}O$ 388.676

(3α,5α)-*form* [516-95-0]
Epicholestanol. *Epidihydrocholesterin*. *Dihydrin*. *Presteron*
Needles (EtOH). Mp 185-186°. $[\alpha]_D^{20}$ +34 ($CHCl_3$).

► Exp. reprod. and teratogenic effects (large dose). FZ6328000

3-O-*Sulfate:* [56816-66-1]
$C_{27}H_{48}O_4S$ 468.74
Mp 136-137° (as Na salt). $[\alpha]_D^{29}$ +15 (EtOH) (Na salt). CAS No. refers to Na salt.

Ac: [1107-59-1]
$C_{29}H_{50}O_2$ 430.713
Cryst. (MeOH). Mp 96°. $[\alpha]_D$ +30 ($CHCl_3$).

(3β,5α)-*form* [80-97-7]

[17608-41-2] ***Cholestanol***. *Zymostanol*
Occurs in eggs. Leaflets (EtOH). Mp 142-143°. $[\alpha]_D^{22}$ +27.4 ($CHCl_3$).

3-O-*Sulfate:* [1491-96-9]
Mp 174-175.5° (as Na salt). $[\alpha]_D^{29}$ +16.6 (EtOH) (Na salt).

Ac: [1255-88-5]
Prisms (MeOH/EtOAc). Mp 110-111°. $[\alpha]_D^{20}$ +11.5 ($CHCl_3$).

Me ether:3-Methoxycholestane
$C_{28}H_{50}O$ 402.702
Mp 86-87°.

(3α,5β)-*form* [516-92-7] *Epicoprostanol*. *Epicoprosterol*
Mp 107-108°. $[\alpha]_D$ +31 ($CHCl_3$).

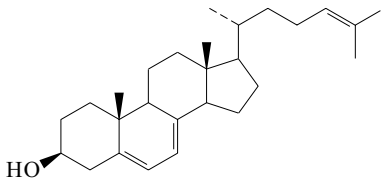
(3β,5β)-*form* [360-68-9]

[17608-41-2] ***Coprostanol***. *Coprosterol*. *Stercorin*
Mp 96-100°. $[\alpha]_D$ +26 ($CHCl_3$).

Ac: [4947-63-1]
Mp 89°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1047D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 566C; 567A (*nmr*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1934, **17**, 1407-1416 (*Epicoprostanol, Coprostanol, synth*)
Barnett, J. *et al., J.C.S.*, 1940, 1390-1393 (*synth*)
Heath-Brown, B. *et al., J.C.S.*, 1940, 1482-1489 (*Zymostanol, synth*)
Org. Synth., Coll. Vol., 2, 1943, 191-193 (*Cholestanol, synth*)
Bergmann, W. *et al., J.O.C.*, 1945, **10**, 580-586 (*Cholestanol, synth*)
Lederer, E. *et al., Helv. Chim. Acta*, 1946, **29**, 1354-1365 (*occur*)
Lieberman, S. *et al., J.A.C.S.*, 1948, **70**, 1427-1432 (*Cholestanol and Epicholestanol sulfates, synth*)
Shoppee, C.W. *et al., J.C.S.*, 1950, 687-689 (*Epicoprostanol, Cholestanol, synth*)
Douglas, G.H. *et al., J.C.S.*, 1959, 1720-1723 (*Epicoprostanol, synth*)
Meittinen, T.A. *et al., Acta Chem. Scand.*, 1967, **21**, 286-290 (*Cholestanol, occur*)
Michnowicz, J. *et al., Org. Mass Spectrom.*, 1972, **6**, 765-783 (*ms*)
Ishige, M. *et al., Can. J. Chem.*, 1973, **51**, 3923-3926 (*Epicoprostanol, synth*)
Eggert, H. *et al., J.O.C.*, 1976, **41**, 71-78 (*cmr*)
Iida, T. *et al., J. Lipid Res.*, 1979, **20**, 279-284 (*pmr*)
Valente, C. *et al., J.O.C.*, 1984, **49**, 44-51 (*Epicholestanol, synth, bibl*)
Zollo, F. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **85**, 559-560 (*Cholestanol, Coprostanol, occur*)
Kanie, K. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 1875-1892 (*Me ether*)
Nakajima, N. *et al., Phytochemistry*, 2002, **60**, 275-279 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EBA100

Cholesta-5,7,24-trien-3-ol, 9CI C-233



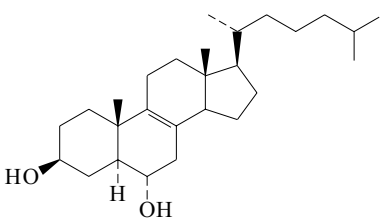
$C_{27}H_{42}O$ 382.628

3β-*form* [1715-86-2]
7,8-Didehydrodesmosterol
Constit. of pig tissues and bakers yeast (*Saccharomyces cerevisiae*). Needles (MeOH). Mp 104-107°. $[\alpha]_D$ -122 (c, 0.77 in $CHCl_3$).

Ac: [17137-77-8]
$C_{29}H_{44}O_2$ 424.665
Cryst. (MeOH). Mp 78-81°.

Scallen, T.J. *et al., Biochem. Biophys. Res. Commun.*, 1965, **21**, 149-151 (*synth*)
Scallen, T.J. *et al., J. Lipid Res.*, 1968, **10**, 121-127 (*isol, synth*)
Barton, D.H. *et al., J.C.S. Perkin 1*, 1974, 1326-1333 (*isol*)
Moreau, J.P. *et al., J.O.C.*, 1974, **39**, 2018 (*synth, ir, pmr, ms*)
Yang, S.S. *et al., Steroids*, 1980, **35**, 329-334 (*synth, uv, ir, pmr, ms*)
Schönauer, K. *et al., Annalen*, 1983, 1031 (*synth, uv, pmr, ms*)
Andreev, A.V. *et al., Khim. Prir. Soedin.*, 1986, **22**, 196; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 182 (*isol*)

Cholest-8-ene-3,6-diol, 9CI C-234



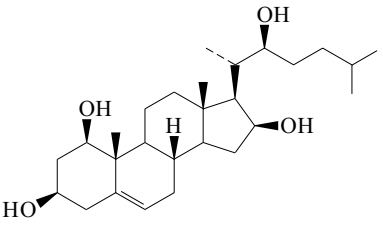
$C_{27}H_{46}O_2$ 402.659

(3β,5α,6α)-*form* [570-92-3]
Peniocerol
Obt. from roots of *Stenocereus thurberi* (organ pipe cactus). Cryst. (MeOH). Mp 181-183°. $[\alpha]_D$ +59 (c, 0.76 in $CHCl_3$).

Di-Ac: [864-15-3]
Needles (Me_2CO). Mp 51.5-52°. $[\alpha]_D$ +45 (c, 0.79 in $CHCl_3$).

Djerassi, C. *et al., J.C.S.*, 1965, 1160 (*isol, ir*)
Knight, J.C. *et al., Phytochemistry*, 1969, **8**, 477 (*isol, ir, pmr*)
Eggert, H. *et al., J.O.C.*, 1981, **46**, 5399 (*cmr*)
Kircher, H.W. *et al., Phytochemistry*, 1982, **21**, 1705 (*isol*)

Cholest-5-ene-1,3,16,22-tetrol C-235



$C_{27}H_{46}O_4$ 434.658

(1β,3β,16β,22*S*)-*form* [142735-57-7] *Alliosterol*
Cryst. (MeOH/EtOAc) or amorph. solid. Mp 200-202°. $[\alpha]_D^{27}$ -60 (c, 0.1 in $CHCl_3$) (-16).

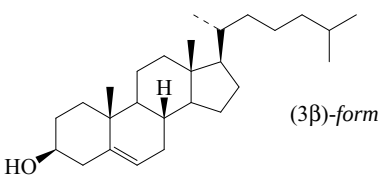
1-O-α-L-*Rhamnopyranoside, 16*-O-β-D-*galactopyranoside:* [289690-78-4]
$C_{39}H_{66}O_{13}$ 742.943
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -25 (c, 0.004 in MeOH).

1-O-*[β-D-Galactopyranosyl-(1→4)-α-L-rhamnopyranoside], 16*-O-β-D-*galactopyranoside:* [289690-79-5]
$C_{45}H_{76}O_{18}$ 905.085
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -2 (c, 0.002 in MeOH).

[142735-58-8]

Fattorusso, E. *et al., J. Agric. Food Chem.*, 2000, **48**, 3455-3462 (*Allium porrum constits*)

Cholest-5-en-3-ol C-236



$C_{27}H_{46}O$ 386.66

► FZ8400000

3α-*form* [474-77-1] *Epicholesterol*
Cryst. (EtOH) or leaflets (Me_2CO). Mp 141.5°. $[\alpha]_D^{30}$ -35 (EtOH).

Ac: [1059-85-4]
$C_{29}H_{48}O_2$ 428.697
Cryst. (MeOH). Mp 85°. $[\alpha]_D$ -12.8 ($CHCl_3$).

3-O-*Sulfate:Epicholesteryl sulfate*
$C_{27}H_{46}O_4S$ 466.724
Mp 163-164° (as pyridine salt).

3β-*form* [57-88-5] ***Cholesterol, BAN, USAN***. *Cholesterin. NSC 8798*
Constit. either free or as esters, of fish liver oils, lard, dairy fats, egg yolk and bran. Pearly leaflets (EtOH aq.). Mp 148.5° (anhyd.). $[\alpha]_D$ -31.12 (Et_2O).

► Exp. reprod. and teratogenic effects (very large doses).

3-O-*Sulfate:Cholesteryl sulfate*
$C_{27}H_{46}O_4S$ 466.724
Mp 170-173° (as Na salt). $[\alpha]_D$ -20.8 (MeOH).

O-β-D-*Glucuronopyranoside:*
$C_{33}H_{54}O_7$ 562.785
Mp 272-274° (242-245°).

Formyl: [4351-55-7] *Cholesteryl formate*
$C_{28}H_{46}O_2$ 414.67
Cryst. (Me_2CO). Mp 96°.

Ac: [604-35-3] *Cholesteryl acetate*
$C_{29}H_{48}O_2$ 428.697
Needles (Me_2CO). Mp 114-115°. $[\alpha]_D^{20}$ -47.4 ($CHCl_3$).

Chloroacetyl: [3464-50-4]
$C_{29}H_{47}ClO_2$ 463.142
Cryst. (EtOH). Mp 160-164°.

Propanoyl: [633-31-8] *Cholesteryl propionate*
$C_{30}H_{50}O_2$ 442.724
Plates (EtOH/Et_2O). Mp 114°. $[\alpha]_D$ -40.9.

Butanoyl: [521-13-1] *Cholesteryl butyrate*
$C_{31}H_{52}O_2$ 456.751
Mp 97-99°. $[\alpha]_D$ -34.8 ($CHCl_3$).

2-Methylpropanoyl: [1180-43-4] *Cholesteryl isobutyrate*
$C_{31}H_{52}O_2$ 456.751
Mp 128-130°. $[\alpha]_D$ -37.4 ($CHCl_3$).

Pentanoyl: [7726-03-6] *Cholesteryl valerate*
$C_{32}H_{54}O_2$ 470.777
Mp 87-89°. $[\alpha]_D$ -34.1 ($CHCl_3$).

Hexanoyl: [1062-96-0] *Cholesteryl caproate*
$C_{33}H_{56}O_2$ 484.804
Cryst. (EtOH or Me_2CO). Mp 92-98° (86-89°).

(S)-14-Methylhexadecanoyl: [19477-24-8] *Carcinolipin*
$C_{44}H_{78}O_2$ 639.099
Cryst. Mp 75°.

► Exp. reprod. effects. FZ7605000

Heptanoyl: [1182-07-6] *Cholesteryl oenanthate*
$C_{34}H_{58}O_2$ 498.831
Mp 106-109°. $[\alpha]_D$ -40 (CCl_4).

Octanoyl: [1182-42-9] *Cholesteryl caprylate*
$C_{35}H_{60}O_2$ 512.858
Mp 104-108°. $[\alpha]_D$ -29 ($CHCl_3$).

Nonanoyl: [1182-66-7] *Cholesteryl pelargonate*
$C_{36}H_{62}O_2$ 526.885
Mp 58° Mp 110-124°. $[\alpha]_D$ -33.2 ($CHCl_3$).

Decanoyl: [1183-04-6] *Cholesteryl caprate*
$C_{37}H_{64}O_2$ 540.911
Mp 80-81°. $[\alpha]_D$ -27 ($CHCl_3$).

Dodecanoyl: [1908-11-8] *Cholesteryl laurate*
$C_{39}H_{68}O_2$ 568.965
Mp 75-77°. $[\alpha]_D$ -23.4 ($CHCl_3$).

Tetradecanoyl: [1989-52-2] *Cholesteryl myristate*
$C_{41}H_{72}O_2$ 597.019
Mp 69-71°. $[\alpha]_D$ -25 ($CHCl_3$).

Hexadecanoyl: [601-34-3] *Cholesteryl palmitate*
$C_{43}H_{76}O_2$ 625.072
Mp 75-77°. $[\alpha]_D$ -25 ($CHCl_3$).

Octadecanoyl: [35602-69-8]

[1184-05-0] *Cholesteryl stearate*
$C_{45}H_{80}O_2$ 653.126
Mp 79-80.5°. $[\alpha]_D$ -24.7 ($CHCl_3$).

9Z-Octadecenoyl: [303-43-5] *Cholesteryl oleate*
$C_{45}H_{78}O_2$ 651.11

9Z,12Z-Octadecadienoyl: [604-33-1] *Cholesteryl lineoleate*
$C_{45}H_{76}O_2$ 649.094
Mp 39-41°. $[\alpha]_D^{20}$ -24 (c, 1 in $CHCl_3$).

9Z,12Z,15Z-Octadecatrienoyl: [2545-22-4] *Cholesterol linolenate*
$C_{45}H_{74}O_2$ 647.078
Mp 32-33°. $[\alpha]_D^{25}$ -24.4.

3-O-*(5Z,8Z,11Z,14Z-Eicosatetraenoyl):* [604-34-2] *Cholesteryl arachidonate*
$C_{47}H_{76}O_2$ 673.116
Cryst. (Et_2O/EtOH). Mp 85-85.5°. $[\alpha]_D$ -23.2.

Tetracosanoyl: [73024-96-1] *Cholesteryl tetracosanoate*
$C_{51}H_{92}O_2$ 737.287

Hexacosanoyl: [87080-57-7] *Cholesteryl hexacosanoate*
$C_{53}H_{96}O_2$ 765.34

Benzoyl: [604-32-0] *Cholesteryl benzoate*
$C_{34}H_{50}O_2$ 490.768
Mp 149-151°. $[\alpha]_D^{20}$ -15 (c, 2 in $CHCl_3$).

Cinnamoyl: [1990-11-0]

[50305-81-2] *Cholesteryl cinnamate*
$C_{36}H_{52}O_2$ 516.806
Mp 159°. $[\alpha]_D$ +0.7 ($CHCl_3$).

4-Methylbenzenesulfonyl: [1182-65-6] *Cholesteryl tosylate*
$C_{34}H_{52}O_3S$ 540.849
Mp 131-132°. $[\alpha]_D$ -42.6 ($CHCl_3$).

Chloroformyl: [7144-08-3] *Cholesteryl chloroformate*
$C_{28}H_{45}ClO_2$ 449.115
Mp 119.5-121°. $[\alpha]_D$ -26.7.

Ethoxyacetyl: ***Chethoxyrol***
$C_{31}H_{52}O_3$ 472.75
Plates (EtOAc/MeOH). Mp 82-83°. $[\alpha]_D^{20}$ -53.8 ($CHCl_3$).

3-Carboxypropanoyl: [1510-21-0] *Cholesteryl hemisuccinate*
$C_{31}H_{50}O_4$ 486.734
Cryst. (AcOH). Mp 177-179°.

Me ether: [1174-92-1] *3β-Methoxycholest-5-ene*
$C_{28}H_{48}O$ 400.687
Cryst. (EtOH). Mp 84.5°. $[\alpha]_D^{20}$ -45.8 ($CHCl_3$).

Et ether:3β-Ethoxycholest-5-ene
$C_{29}H_{50}O$ 414.713
Mp 88.5°. $[\alpha]_D^{21}$ -39 ($CHCl_3$).

3-O-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl):* [164453-91-2]

[2672-47-1] *Cholesteryl ferulate*
$C_{37}H_{54}O_4$ 562.831
Constit. of rice bran oil. Mp 165-166°. $[\alpha]_D^{21}$ +10.3 ($CHCl_3$).

Trimethylsilyl ether: [1856-05-9] *3-(Trimethylsiloxy)cholest-5-ene*
$C_{30}H_{54}OSi$ 458.842
Cryst. Mp 121-123°.

(3β,10α)-*form* [23820-70-4] *10α-Cholesterol*
Needles (MeOH). Mp 118.5-119°. $[\alpha]_D^{25}$ -46 (c, 1.14 in $CHCl_3$).

Ac: [23820-71-5]
Mp 124-124.5°. $[\alpha]_D^{25}$ -47 (c, 1.48 in $CHCl_3$).

(3β,14β)-*form* [57759-45-2] *14β-Cholesterol*
Cryst. (MeOH). Mp 38°. $[\alpha]_D^{21}$ +29

($CHCl_3$).

Ac: [57759-47-4]
Oil.

(3β,14β,17α)-*form* [71869-93-7] *14β,17α-Cholesterol*
Cryst. (hexane). Mp 127-128°. $[\alpha]_D^{23}$ +11 ($CHCl_3$).

(3β,20*S*)-*form* [34026-89-6] *20-Epicholesterol*
Cryst. ($MeOH/Me_2CO$). Mp 152-153°. $[\alpha]_D^{20}$ -54.2 (c, 0.52 in $CHCl_3$).

Ac: [38774-63-9]
$C_{29}H_{48}O_2$ 428.697
Cryst. (MeOH). Mp 90-92°. $[\alpha]_D^{25}$ -53.9 (c, 1 in $CHCl_3$).

(±)-3β-*form* rac-*Cholesterol*
Elongated prisms (MeCN). Mp 149-149.5°.

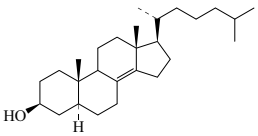
(*ent*-3β)-*form* ent-*Cholesterol*
Mp 146-147°. $[\alpha]_D^{25}$ +40.6 (c, 0.93 in EtOH).

[1256-86-6, 16134-40-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1048B; 1058C; 1059A; 1059B; 1059C; 1059D; 1060A; 1060D; 1064D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 568A; 596C; 597B; 597C; 598A; 598B; 598C; 599A; 599C; 608B (*nmr*)
Page, I.H. *et al., Biochem. Z.*, 1930, **220**, 304 (*fatty acid esters*)
Wagner-Jauregg, T. *et al., Z. Physiol. Chem.*, 1932, **213**, 110 (*deriv*)
Barnett, J. *et al., J.C.S.*, 1940, 1390 (*3α-form, synth*)
King, L.C. *et al., J.A.C.S.*, 1952, **74**, 6238 (*synth*)
Bladon, P. *et al., J.C.S.*, 1952, 2737 (*uv, 3β-form*)
Johnson, D.R. *et al., J.A.C.S.*, 1953, **75**, 52 (*ir, 3β-form*)
Cook, R.P. *et al., Cholesterol (Chem., Biochem. Pathol.)*, Academic Press, N.Y., 1958, (*rev*)
Mahadevan, V. *et al., J. Lipid Res.*, 1962, **3**, 106-110 (*fatty esters*)
Org. Synth., Coll. Vol., 4, 1963, 195 (*purifn*)
Keana, J.F.W. *et al., Steroids*, 1964, **4**, 457 (*synth*)
Johnson, W.S. *et al., Tetrahedron, Suppl.*, No. 8, 1966, 541 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 140; 141 (*purifn, deriv*)
Diekman, J. *et al., J.O.C.*, 1967, **32**, 1005-1012 (*trimethylsilyl ether, synth, uv, ms*)
Edwards, J.T. *et al., J.O.C.*, 1970, **35**, 1426 (*synth, ir, pmr, 3β,10α-form*)
Mulheirn, L.J. *et al., Chem. Soc. Rev.*, 1972, **1**, 259 (*biosynth, 3β-form*)
Hradec, J. *et al., Prog. Biochem. Pharmacol.*, 1975, **10**, 197 (*Carcinolipin*)
Anastasia, M. *et al., J.O.C.*, 1976, **41**, 1064; 1979, **44**, 4983 (*synth, ir, ms, 3β,4β-form*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*pmr*)
Bu'lock, J.D. *et al., Phytochemistry*, 1976, **15**, 1249 (*biosynth*)
Hudec, J. *et al., Tetrahedron*, 1976, **32**, 2475 (*cd*)
Partridge, L.G. *et al., J.O.C.*, 1977, **42**, 2799 (*ms*)
Berman, E. *et al., J.O.C.*, 1977, **42**, 3325 (*cmr*)
Piacenza, L.P.L. *et al., J.O.C.*, 1977, **42**, 3778 (*synth*)
Shieh, H.S. *et al., Nature (London)*, 1977, **267**, 287 (*cryst struct*)
Joseph-Nathan, P. *et al., J.A.C.S.*, 1979, **101**, 1289 (*cmr, 3β-form*)
Anastasia, M. *et al., J.O.C.*, 1979, **44**, 4983 (*synth, ir, pmr, ms, 3β and 14β,17α-form*)
Sawzik, P. *et al., Liq. Cryst., Proc. Int. Conf.*, Pittsburgh, USA, 1979, 171 (*esters*)
Nakahara, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 2499 (*esters*)
Tanabe, M. *et al., J.A.C.S.*, 1980, **102**, 862 (*synth, pmr, 3β,20S-form*)
Meiboom, S. *et al., Phys. Rev. A: Gen. Phys.*, 1981, **24**, 468 (*esters*)
Myant, N.B. *et al., The Biology of Cholesterol and Related Steroids*, Heinemann Medical, London, 1981, (*book*)
Sucrow, W. *et al., Annalen*, 1982, 1897 (*synth, ms*)
Gibbons, G.F. *et al., Biochemistry of Cholesterol*, Elsevier, Amsterdam, 1982, (*book*)
Schneider, H.J. *et al., J.O.C.*, 1982, **47**, 4216 (*cmr*)
Ohmori, M. *et al., Tet. Lett.*, 1982, **23**, 4709 (*synth*)
Goto, R. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3528 (*synth, 3β,20S-form*)
IARC Monog., 1983, **31**, 95; *Suppl.* 7, 161; *Suppl.* 6, 166 (*rev, tox*)
Schmuff, N.R. *et al., J.O.C.*, 1983, **48**, 1404 (*synth, pmr, 3β,20S-form*)
Mikami, K. *et al., Chem. Lett.*, 1985, 115 (*synth, 20S-form*)
Croll, D.H. *et al., J. Chem. Phys.*, 1986, **85**, 7380-7387 (*hexanoyl, cmr*)
Seo, S. *et al., J.C.S. Perkin 1*, 1986, 411 (*pmr, 3β-form*)
Haider, S.I. *et al., J. Nat. Prod.*, 1987, **50**, 261 (*Chethoxyrol*)
Gokel, G.W. *et al., J.O.C.*, 1987, **52**, 2963 (*chloroacetyl*)
Tan, F. *et al., J. Appl. Cardiol.*, 1988, **3**, 67 (*rev, metab*)
Hamilton, J.G.C. *et al., J. Chem. Ecol.*, 1988, **14**, 401 (*oleate*)
Belcher, A. *et al., J. Chem. Ecol.*, 1988, **14**, 1367 (*oleate*)
Ramachandran, R. *et al., J. Magn. Reson.*, 1988, **79**, 357 (*cmr*)
Yeagle, P.L.,.Ed. *et al., The Biology of Cholesterol*, CRC Press, 1988, (*book*)
Hamilton, J.G.C. *et al., J. Insect Physiol.*, 1989, **35**, 873 (*oleate*)
Jarzębski, A. *et al., Steroids*, 1990, **55**, 256 (*20S-form, isol*)
Rychnovsky, S.D. *et al., J.O.C.*, 1992, **57**, 2732 (*ent-form*)
Fernandez, I. *et al., Synlett*, 1993, 489 (*formyl*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 121-122
Cox, P.J. *et al., Acta Cryst. C*, 1996, **52**, 2111 (*cryst struct, tosylate*)
Muhr, P. *et al., Magn. Reson. Chem.*, 1996, **34**, 137 (*pmr*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1409
Nagano, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 944-946 (*biosynth*)
Tian, Y. *et al., Liq. Cryst.*, 1997, **22**, 87-96 (*3-carboxypropanoyl*)
Kumar, A.S. *et al., Tet. Lett.*, 1999, **40**, 823-826 (ent-*Cholesterol, synth*)
Shieh, H.S. *et al., Acta Cryst. E*, 2002, **58**, o79-o80 (*cryst struct*)
Jiang, X. *et al., J.O.C.*, 2002, **67**, 4893-4900 (*Entcholesterol, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCJ500; CMD750

Cholest-8(14)-en-3-ol, 9CI C-237

[18684-35-0]



(3β,5α)-*form*

$C_{27}H_{46}O$ 386.66

(3α,5α)-*form* [35479-87-9]
Cryst. (MeOH). Mp 141-145°.

(3β,5α)-*form* [566-99-4]
Doristerol
Constit. of *Dioscorea batatas* (Chinese yam). Needles (MeOH). Mp 120°. $[\alpha]_D^{23}$ +33 (c, 1 in $CHCl_3$).

Ac: [6562-21-6]
$C_{29}H_{48}O_2$ 428.697
Leaflets (EtOH). Mp 77-78°. $[\alpha]_D^{21}$ +9.5 (c, 1.5 in $CHCl_3$).

Benzoyl: [6673-65-0]
Mp 114°. $[\alpha]_D$ +11 ($CHCl_3$).

(3β,5β)-*form* [16826-38-3]
Needles (Me_2CO/MeCN). Mp 83-85°. $[\alpha]_D^{23}$ +33 (c, 1 in $CHCl_3$).

Ac:
Cryst. (Et_2O/MeOH). Mp 114-115°. $[\alpha]_D^{16}$ +30.5 (c, 0.8 in $CHCl_3$).

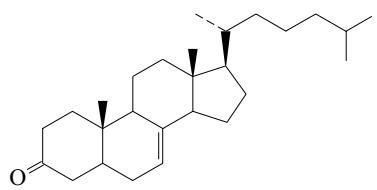
Benzoyl: [16826-39-4]
Cryst. (Me_2CO/MeOH). Mp 96-98°. $[\alpha]_D$ +32 (c, 1 in $CHCl_3$).

[15147-62-3, 26758-20-3]

Johnson, D.R. *et al., J.A.C.S.*, 1953, **75**, 52 (*ir, 3β,5α-form*)
Cohen, C.F. *et al., Steroids*, 1967, **9**, 591 (*synth, 3β,5β-form*)
Breslow, R. *et al., J.A.C.S.*, 1973, **95**, 3251 (*synth, ir, pmr, 3α,5α-form*)
Chu, J.Y.C. *et al., Chem. Comm.*, 1974, 374 (*derivs*)
Iida, T. *et al., Steroids*, 1977, **29**, 453 (*pmr, 3β,5α-form*)
Parish, E.J. *et al., Chem. Phys. Lipids*, 1979, **24**, 167; 1980, **26**, 141 (*synth*)
Tsuda, M. *et al., J.O.C.*, 1979, **44**, 1282; 1290 (*cmr, 3β,5α-form*)
Chorvat, R.J. *et al., J.O.C.*, 1979, **44**, 3974 (*deriv*)
Akihisa, T. *et al., Phytochemistry*, 1991, **30**, 2369 (*isol, pmr, ms*)

Cholest-7-en-3-one, 9CI C-238

[13097-64-8]



$C_{27}H_{44}O$ 384.644

5α-*form* [15459-85-5]
Isol. from butterfat. Plates (MeOH) or needles (Et_2O/MeOH). Mp 148°. $[\alpha]_D^{20}$ +26 (c, 3.94 in $CHCl_3$).

Oxime:
$C_{27}H_{45}NO$ 399.659
Cryst. (EtOAc). Mp 228° dec. $[\alpha]_D$

+24.6 (c, 0.9 in $CHCl_3$).

2,4-Dinitrophenylhydrazone:
Mp 210-212°.

5β-*form* [29374-80-9]
Plates (Me_2CO). Mp 88-90°. $[\alpha]_D^{23}$ +65.4 (c, 0.57 in $CHCl_3$).

Buser, W. *et al., Helv. Chim. Acta*, 1947, **30**, 1379
Evans, D.E. *et al., J.C.S.*, 1956, 4821 (*synth, 5α-form*)
Mazur, Y. *et al., J.A.C.S.*, 1958, **80**, 6296 (*synth, 5α-form*)
Parks, D.W. *et al., Nature (London)*, 1966, **210**, 416
Levchuk, Y.N. *et al., Khim. Prir. Soedin.*, 1969, **5**, 36 (*ord, 5α-form*)
Liston, A.J. *et al., J.C.S.(C)*, 1970, 2117 (*synth, ir, pmr, ord, 5β-form*)
Smith, A.G. *et al., Biomed. Mass Spectrom.*, 1976, **3**, 81 (*ms, 5α-form*)
Emke, A. *et al., J.C.S. Perkin 1*, 1977, 820 (*synth, 5α-form*)
Galbraith, M.N. *et al., Aust. J. Chem.*, 1981, **34**, 2607 (*synth, ir, ms, pmr, 5β-form*)

Choline C-239

[62-49-7]
2-Hydroxy-N,N,N-*trimethylethanaminium(1+), 9CI. (2-Hydroxyethyl)trimethylammonium. Bilineurine. Sincalin. Sinkalin. Amanitin†. Araquine. Arachine*

$Me_3N^{\oplus}CH_2CH_2OH$

$C_5H_{14}NO^{\oplus}$ 104.172
Nutritional supplement. Occurs free and combined in many animal and vegetable foods with highest concentrations found in egg yolk, meat, fish, milk, cereals and legumes.

▶ FZ9625000

Hydroxide: [123-41-1]
$C_5H_{15}NO_2$ 121.179
Syrup, cryst. with difficulty. V. sol. H_2O, EtOH; insol. Et_2O. Strong base, absorbs CO_2 from air. Forms cryst. addn. compds. with H_2PtCl_6 etc..

▶ GA4025500

Chloride: [67-48-1] ***Choline chloride, INN***
$C_5H_{14}ClNO$ 139.624
Deliquescent cryst.

▶ LD_{50} (rat, orl) 3400 mg/kg. KH2975000

O-*(4-Hydroxybenzoyl):* [5094-31-5] ***(4-Hydroxybenzoyl)choline***
$C_{12}H_{18}NO_3^{\oplus}$ 224.279
Alkaloid from white mustard (*Sinapis alba*).

O-*(3,4-Dimethoxybenzoyl):* [15797-38-3]

[95210-18-7] ***Hesperaline***
$C_{14}H_{22}NO_4^{\oplus}$ 268.332
Alkaloid from seeds of damask violet (*Hesperis matronalis* Cruciferae). Mp 182-183° (as iodide).

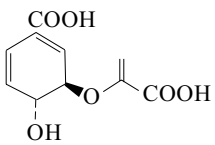
O-*(4-Hydroxy-3-methoxycinnamoyl):*
[85927-25-9]

[22513-68-4, 31545-00-3] ***Feruloylcholine***
$C_{15}H_{22}NO_4^{\oplus}$ 280.343
Constit. of garlic mustard (*Alliaria officinalis*). Mp 203-205° (as chloride). λ_{max} 236 (log ε 4.05); 334 (log ε 4.31) (no solvent reported).

[87-67-2, 23038-04-2, 55357-38-5, 64681-08-9]
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 395D; **2**, 292B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 616C; 859C (*nmr*)
Renshaw, R.R. *et al., J.A.C.S.*, 1910, **32**, 128 (*synth*)
Gmelin, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1967, **300**, 176 (*Hesperaline*)
Byrn, S.R. *et al., J.O.C.*, 1976, **41**, 2283 (*conformn, ir, cryst struct*)
Zeisel, S.H. *et al., Annu. Rev. Nutr.*, 1981, **1**, 195 (*rev*)
Clausen, S. *et al., Phytochemistry*, 1982, **21**, 917 (*4-Hydroxybenzoylcholine*)
Larsen, L.M. *et al., Phytochemistry*, 1983, **22**, 219-222 (*Feruloylcholine*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 199 (*rev*)
Frydenvang, K. *et al., Acta Cryst. C*, 1992, **48**, 1343; 1994, **50**, 617 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1037; 1317
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMF000; CMF500; CMF750

Chorismic acid C-240

[617-12-9]
3-[(1-Carboxyethenyl)oxy]-4-hydroxy-1,5-cyclohexadiene-1-carboxylic acid, 9CI



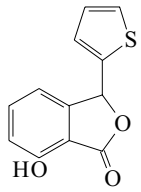
$C_{10}H_{10}O_6$ 226.185
Cryst. + $1H_2O$ (EtOAc/petrol). Mp 148-149°. $[\alpha]_D^{25}$ -295.5 (c, 0.2 in H_2O).

3,4-Didehydro: [81757-66-6] *3-(1-Carboxyvinyl)benzoic acid.* ***Dehydrochorismic acid***
$C_{10}H_8O_6$ 224.17
Isol. from pollen of *Pinus densiflora* (Japanese red pine). Cryst. (H_2O). Mp 178-181° dec. λ_{max} 254 (ε 13000); 286 (ε 3100) (MeOH).

Edwards, J.M. *et al., Aust. J. Chem.*, 1965, **18**, 1227 (*struct, ir, uv, pmr, ms*)
Biochem. Prep., 1968, **12**, 94 (*synth*)
Hill, R.K. *et al., J.A.C.S.*, 1969, **91**, 5893 (*biosynth*)
Pittard, J. *et al., Curr. Top. Cell. Regul.*, 1970, **2**, 29 (*rev*)
Towers, G.H.N. *et al., Filamentous Fungi*, 1976, **2**, 460 (*rev*)
Kobayashi, S. *et al., Agric. Biol. Chem.*, 1982, **46**, 845-847 (*Dehydrochorismic acid*)
McGowan, D.A. *et al., J.A.C.S.*, 1982, **104**, 1153; 7036 (*synth*)
Hoare, J.H. *et al., J.A.C.S.*, 1983, **105**, 6264 (*synth*)
Pawlak, J.L. *et al., J.O.C.*, 1987, **52**, 1765 (*synth*)
Posner, G.H. *et al., J.O.C.*, 1987, **52**, 4836 (*synth*)
Connelly, J.A. *et al., Methods Enzymol.*, 1987, **142**, 422 (*hplc*)
Afshar, C. *et al., Bioorg. Chem.*, 1992, **20**, 323 (*cryst struct*)
Campbell, M.M. *et al., Synthesis*, 1993, 179 (*rev, synth, biosynth*)

Chrycolide C-241

[91362-91-3]
7-Hydroxy-3-(2-thienyl)-1(3H)-isobenzofuranone, 9CI

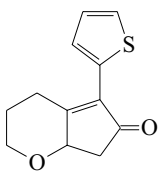


$C_{12}H_8O_3S$ 232.259
Isol. from *Chrysanthemum coronarium* (chop-suey greens) whole plant. Mp 115-116°.

Tada, M. *et al., Agric. Biol. Chem.*, 1984, **48**, 1367 (*isol, ir, uv, cmr, pmr, struct*)

Chrycorin C-242

[91362-90-2]
3,4,7,7a-Tetrahydro-5-(2-thienyl)cyclopenta[b]pyran-6(2H)-one, 9CI



$C_{12}H_{12}O_2S$ 220.292
Isol. from *Chrysanthemum coronarium* (chop-suey greens). Mp 71-72°. $[\alpha]_D^{24}$ +10 (c, 0.6 in MeOH).

Tada, M. *et al., Agric. Biol. Chem.*, 1984, **48**, 1367 (*isol, ir, uv, cmr, pmr, struct*)
Yin, B.-L. *et al., J.C.S. Perkin 1*, 2002, 1746-1747 (*synth, pmr, cmr*)

Chymopapain, BAN, INN, USAN C-243

[9001-09-6]
Chymodiactin. Discase. NSC 107079. BAX 1526

MW = 27000. Isol. from *Carica papaya* (papaya).

▶ LD_{50} (rat, ivn) 92 mg/kg. GC3045600

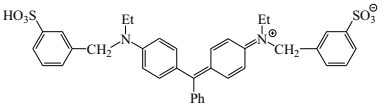
Jansen, E.F. *et al., J. Biol. Chem.*, 1941, **137**, 459 (*isol*)
Ebata, M. *et al., J. Biol. Chem.*, 1962, **237**, 1086 (*isol, cryst*)
Kunimitsu, D.K. *et al., Methods Enzymol.*, 1970, **19**, 244 (*rev*)
Simmons, J.W. *et al., Drug Chem. Toxicol.*, 1984, **7**, 299 (*rev*)
Einarson, T.R. *et al., Drug Intell. Clin. Pharm.*, 1984, **18**, 560 (*rev*)
Brocklehurst, K. *et al., Biochem. J.*, 1985, **228**, 525; 527; 1986, **233**, 119 (*rev*)
Gogan, W.J. *et al., Spine (Philadelphia)*, 1992, **17**, 388 (*clin trial*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1352

C.I. Acid Green 3, 8CI C-244

[6638-02-4]

[4680-78-8]
N-*Ethyl*-N-*[4-[[4-ethyl[(3-sulfophenyl)-methyl]amino]phenyl]phenylmethylene]-2,5-cyclohexadien-1-ylidene-3-sulfobenzenemethanaminium hydroxide inner salt, 9CI. Guinea Green B. C.I. Food Green 1.*

FD and C Green No. 1



$C_{37}H_{36}N_2O_6S_2$ 668.833

Strictly the dye names refer to the di-Na salt. Formerly used for colouring foods. Delisted by FDA in 1970. Dark green powder or bright green cryst (as di-Na salt).

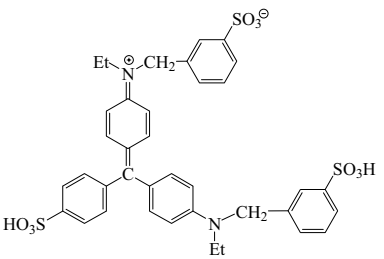
Jones, J.H. *et al., J. Assoc. Off. Agric. Chem.*, 1955, **38**, 977-1010 (*synth, uv, ir, purifn*)
Hansen, W.H. *et al., Food Cosmet. Toxicol.*, 1966, **4**, 389-410 (*tox*)
Fed. Regist., 1970, **35**, 19106; *CA*, **74**, 110481b
Colour Index, 3rd edn., 1971, **4**, 4385 (*props, bibl*)
Oka, H. *et al., J. Chromatogr.*, 1994, **674**, 301-307 (*anal, chromatog, ms*)
Merck Index, 12th edn., 1996, 780-781 (*props, bibl*)

C.I. Acid Green 5 C-245

[25305-94-6]

[5141-20-8]

N-*Ethyl*-N-*[4-[[4-[ethyl[(3-sulfophenyl)-methyl]amino]phenyl](4-sulfophenyl)-methylene]-2,5-cyclohexadien-1-ylidene]-3-sulfobenzenemethanaminium hydroxide inner salt, 9CI. Light Green SF Yellowish. Lissamine Green SF. C.I. Food Green 2. C.I. 42095. Light Green SF. FD and C Green No. 2*



$C_{37}H_{36}N_2O_9S_3$ 748.897

One zwitterionic form shown. Normally encountered as di-Na salt, to which trade names refer. Dye. prohibited from use in food. Reddish-brown powder (as di-Na salt); dissolves in H_2O to a green soln. V. sol. H_2O (di-Na salt). Mp 288° (di-Na salt).

▶ Carcinogen.

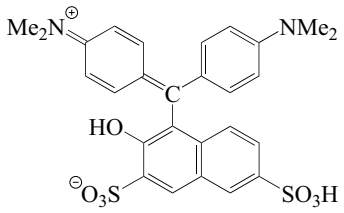
Blangey, L. *et al., Helv. Chim. Acta*, 1942, **25**, 1162-1179 (*synth*)
Hansen, W.H. *et al., Food Cosmet. Toxicol.*, 1966, **4**, 389-410 (*tox*)
Dobozy, O. *et al., Zh. Prikl. Khim. (Leningrad)*, 1966, **39**, 2750-2760; *CA*, **66**, 66566h (*uv*)
Colour Index, 3rd edn., 1971, **4**, 4385 (*synth*)
Liao, W. *et al., Huaxue Shiji*, 1995, **17**, 184-185; *CA*, **123**, 172614c (*synth*)
Wang, Y. *et al., CA*, 1996, **124**, 120098p (*synth*)
Merck Index, 12th edn., 1996, 5508

C.I. Acid Green 50 C-246

[25317-10-6]

[3087-16-9]

N-*[4-[[4-(Dimethylamino)phenyl](2-hydroxy-3,6-disulfo-1-naphthalenyl)methylene]-2,5-cyclohexadien-1-ylidene]-1-methylmethanaminium hydroxide inner salt. Acid brilliant green. Food green S. Green S. Lissamine Green B. C.I. Food green 4. C.I. 44090. E142*



$C_{27}H_{26}N_2O_7S_2$ 554.644

Food colourant . Prohibited in Japan, Canada, USA, Norway, Sweden and Finland. Green cryst. (as Na salt). Strictly the name C.I. Acid green 50 and various synonyms refer to the Na salt.

[84674-88-4]

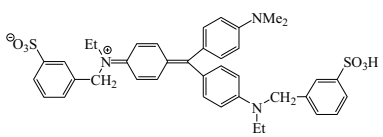
Fierz-David, H.E. *et al., Fundamental Processes of Dye Chemistry*, Interscience, 1949, 307-308
Eur. Pat., 1982, 57 661; 1984, 153 872; *CA*, **98**, 91038f; **104**, 30931m (*synth*)
Gaunt, I.F. *et al., Food Chem. Toxicol.*, 1987, **25**, 969-975; 977-983 (*tox*)
Frazier, R.A. *et al., J. Chromatogr., A*, 2000, **876**, 213-220 (*hplc, anal*)

C.I. Acid Violet 49 C-247

[1694-09-3]

[25329-63-9]

N-*[4-[[4-(Dimethylamino)phenyl][4-[ethyl[(3-sulfophenyl)methyl]amino]phenyl]methylene]-2,5-cyclohexadien-1-ylidene]*-N-*ethyl-3-sulfobenzenemethanaminium inner salt, 9CI. Acid Violet 5B. Acid Violet 6B. Acilon Violet S 4BN. Benzyl Violet 4B. Wool Violet. C.I. Food Violet 2. C.I. 42640. FD and C Violet No. 1*



$C_{39}H_{41}N_3O_6S_2$ 711.901

One zwitterionic form shown. Strictly, the trade names refer to the Na salt. Dye, use now prohibited in food. V. sol. H_2O, sol. EtOH (Na salt).

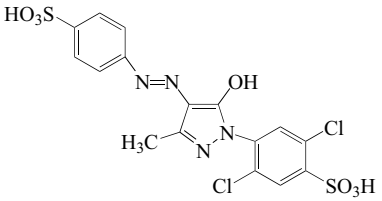
Colour Index, 3rd edn., 1971, **4**, 4397 (*synth*)
Ger. Pat., 1977, 2 651 452; *CA*, **87**, 109417p (*use*)
Minegishi, K. *et al., Toxicol.*, 1977, **7**, 367-383 (*metab*)
Japan. Pat., 1993, 05 216 278; *CA*, **121**, 69460j (*use*)

C.I. Acid Yellow 17 C-248

[25739-65-5]

[6359-98-4]

*2,5-Dichloro-4-[4,5-dihydro-3-methyl-5-oxo-4-[[4-sulfophenyl]azo]-1*H*-pyrazol-1-yl]benzenesulfonic acid, 9CI. Yellow 2G. C.I. Food Yellow 5. C.I. 18965. E 107*



$C_{16}H_{12}Cl_2N_4O_7S_2$ 507.331

Strictly the trade names refer to the di-Na salt. Several tautomers possible incl. oxo-phenylhydrazone; the 9CI name refers to a less probable tautomer. Yellow food colouring; no longer permitted in the EU, USA and Australia. Na salt is polymorphic (7 forms reported).

[95399-60-3]

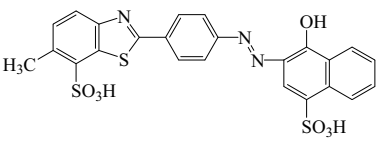
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1001C (*ir*)
Jones, A.V. *et al., J. Food Technol.*, 1968, **3**, 1-14 (*uv*)
Evans, W.H. *et al., J. Sci. Food Agric.*, 1970, **21**, 207-210 (*ir, polymorphism*)
Gaunt, I.F. *et al., Food Cosmet. Toxicol.*, 1971, **9**, 343-353 (*tox*)
Richardson, S.D. *et al., Org. Mass Spectrom.*, 1991, **26**, 826-830 (*ms*)

C.I. Direct Red 45 C-249

[25188-09-4]

[2150-33-6]

2-[4-[(1-Hydroxy-4-sulfo-2-naphthalenyl)azo]phenyl]-6-methyl-7-benzothiazolesulfonic acid, 9CI. C.I. Food Red 13. C.I. 14780



$C_{24}H_{17}N_3O_7S_3$ 555.612

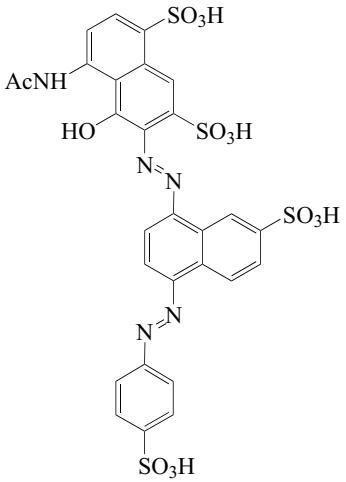
Strictly, the trade names refer to the di-Na salt. Food dye. Di-Na salt v. sol. H_2O; sol. EtOH.

Colour Index, 3rd edn., 1971, **4**, 4070 (*synth*)

C.I. Food Black 1, 8CI C-250

[2519-30-4]

4-(Acetylamino)-5-hydroxy-6-[[7-sulfo-4-[(4-sulfophenyl)azo]-1-naphthalenyl]azo]-1,7-naphthalenedisulfonic acid, 9CI. Brilliant Black BN. C.I. 28440. E151. Black PN



$C_{28}H_{21}N_5O_{14}S_4$ 779.763

Colourant for foodstuffs, hair dyes, cosmetics and printing inks. Food use prohibited in USA, Canada, Japan, Norway and Finland. Normally handled as tetra-Na salt, to which CAS no. and trade names refer.

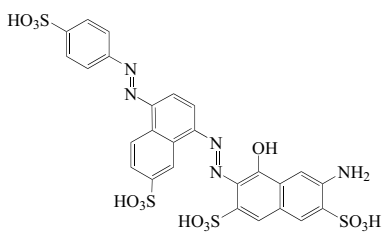
Dickes, G.J. *et al., J. Assoc. Public Anal.*, 1965, **3**, 49-52 (*anal*)
Drake, J.J.P. *et al., Food Cosmet. Toxicol.*, 1977, **15**, 503-508 (*tox*)
Hofer, K. *et al., Z. Lebensm.-Unters. -Forsch.*, 1997, **204**, 32-38 (*anal*)

C.I. Food Black 2, 8CI C-251

[25738-38-9]

[2118-39-0]

6-Amino-4-hydroxy-3-[(7-sulfo-4-[(4-sulfophenyl)azo]-1-naphthalenyl)azo]-2,7-naphthalenedisulfonic acid, 9CI. Black 7984. C.I. 27755. C.I. 27775. E 152



$C_{26}H_{19}N_5O_{13}S_4$ 737.726

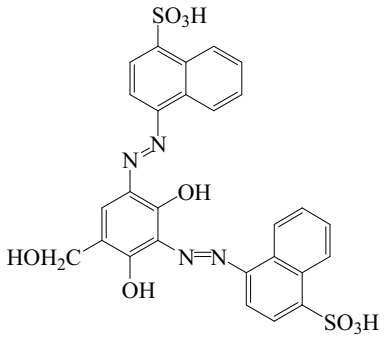
Black food dye; no longer permitted in the EU and not FDA approved. Usually obt. as tetra-Na salt, to which trade names refer.

Pearson, D. *et al., J. Assoc. Public Anal.*, 1967, **5**, 37-38 (*uv*)
Colour Index, 3rd edn., 1971, **4**, 4251
Van Peteghem, C. *et al., J. Chromatogr.*, 1981, **210**, 113-120 (*tlc, detn*)
Joachim, F. *et al., Mutat. Res.*, 1985, **156**, 131-138 (*biochem*)
Gagliardi, L. *et al., J. Chromatogr.*, 1987, **394**, 345-352 (*hplc, detn*)

C.I. Food Brown 3, 8CI C-252

[4553-89-3]

4,4′-[[2,4-Dihydroxy-5-(hydroxymethyl)-1,3-phenylene]bis(azo)]bis-1-naphthalenesulfonic acid, 9CI. Chocolate brown HT. Brown HT. C.I. 20285. E155



$C_{27}H_{20}N_4O_9S_2$ 608.608

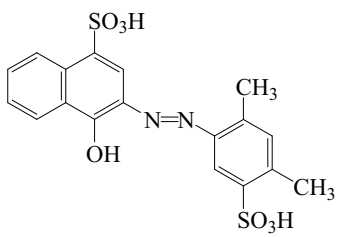
Most names refer to the di-Na salt, to which CAS no. refers. Food colourant. Prohibited in USA, France, Norway and Sweden. Reddish-brown solid (as di-Na salt).

Colour Index, 3rd edn., 1971, **4**, 4146 (*props, synth*)
Chaytor, J.P. *et al., J. Chromatogr.*, 1986, **368**, 450-455 (*hplc, detn in food*)
Gaunt, I.F. *et al., Food Chem. Toxicol.*, 1987, **25**, 999-1007; 1009-1011; 1013-1019 (*tox, metab*)
Spears, K. *et al., J. Assoc. Public Anal.*, 1987, **25**, 47-54 (*detn in food, tlc*)

C.I. Food Red 1 C-253

[4548-53-2]

3-[(2,4-Dimethyl-5-sulfophenyl)azo]-4-hydroxy-1-naphthalenesulfonic acid, 9CI. Ponceau Red SX. Ponceau SX. C.I. 14700. FD and C Red No. 4



$C_{18}H_{16}N_2O_7S_2$ 436.466

Normally obt. as Na salt, to which CAS no. and synonyms refer. Colourant ormerly used in foodstuffs. Red cryst. (EtOH aq.) (as Na salt). Sol. H_2O.

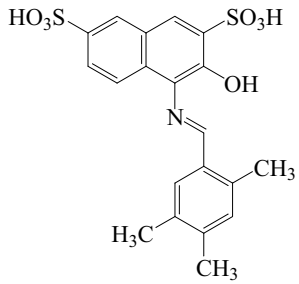
Graichen, C. *et al., J. Assoc. Off. Agric. Chem.*, 1954, **37**, 906-912 (*synth, ir, uv*)
Colour Index, 3rd Edn., 1971, **4**, 4068 (*synth*)
Marmino, D.M. *et al., J. Assoc. Off. Anal. Chem.*, 1974, **57**, 495-507 (*pmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 892-944 (*use*)
Oka, H. *et al., J. Chromatogr., A*, 1994, **674**, 301-307 (*detn, tlc, ms*)

C.I. Food Red 6 C-254

[25738-43-6]

[3564-09-8]

3-Hydroxy-4-[(2,4,5-trimethylphenyl)azo]-2,7-naphthalenedisulfonic acid, 9CI. Ponceau 3R. C.I. 16155. FD and C Red No. 1



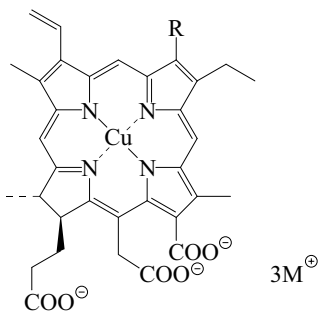
$C_{19}H_{18}N_2O_7S_2$ 450.492

Strictly the trade names refer to the di-Na salt. Former food dye, now delisted by FDA. Dark red powder (EtOH aq.)(as di-Na salt). Di-Na salt sol. H_2O, sl. sol. EtOH.

Steigler, H.W. *et al., Ind. Eng. Chem.*, 1918, **10**, 600 (*synth*)
Whitmore, W.F. *et al., J.A.C.S.*, 1937, **59**, 1501 (*synth*)
Harrow, L.S. *et al., J. Assoc. Off. Agric. Chem.*, 1955, **38**, 172 (*synth*)
Hansen, W.H. *et al., Toxicol. Appl. Pharmacol.*, 1963, **5**, 105 (*tox*)
Pla-Delfina, J.M. *et al., Am. Perfum. Cosmet.*, 1968, **83**, 29 (*synth, tox*)
Parrish, J. *et al., J. Chromatogr.*, 1968, **33**, 542 (*chromatog*)
Rai, J. *et al., Chromatographia*, 1971, **4**, 211 (*tlc*)
Colour Index, 3rd edn., 1971, **4**, 4092 (*synth*)
Segiura, T. *et al., J. Chem. Res., Synop.*, 1980, 164 (*ms*)
Oka, H. *et al., J. Chromatogr.*, 1994, **674**, 301 (*tlc-fab-ms*)

C.I. Natural green 5 C-255

E141. C.I. 75815. Chlorophyllin copper complex. Potassium-sodium-copper chlorophyllin. Sodium-potassium-copper chlorophyllin



R = CH_3, CHO

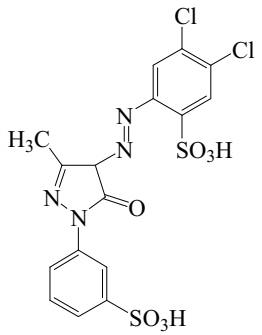
Essentially a mixt. of the copper complexes of Chlorin e_6 and Rhodin g_7 as their tri-K salts. The presence of a small amount of Na ions, acquired during the manuf. process, has given rise to the mixed sodium/potassium nomenclature used for the commercial material. Food and cosmetic colourant. Green-black powder.

Judah, M.A. *et al., Ind. Eng. Chem.*, 1954, **46**, 2262-2271 (*manuf, rev*)

C.I. Pigment Yellow C-256

[65212-84-2]

[65212-76-2]
*4,5-Dichloro-2-[[4,5-dihydro-3-methyl-5-oxo-1-(3-sulfophenyl)-1*H*-pyrazol-4-yl]azo]benzenesulfonic acid, 9CI. 4,5-Dichloro-2-[[5-hydroxy-3-methyl-1-(3-sulfophenyl)-1*H*-pyrazol-4-yl]azo]benzenesulfonic acid*



$C_{16}H_{12}Cl_2N_4O_7S_2$ 507.331

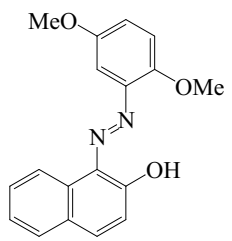
Tautomerism with hydroxypyrazole struct. probable. The name C.I. Pigment Yellow refers to the Ca salt. FDA approved colourant for food contact high density polyethylene and polypropylene resins. Yellow solid (as Ca salt). Ca salt polymorphic.

[65212-77-3]

Ger. Pat., 1976, 2 616 981; *CA*, **88**, 38948v (*synth, use*)
Eur. Pat., 1993, 553 965; *CA*, **119**, 205467e (*polymorphism*)
Anon, *et al., Food Chem. News*, 2000, **41(47)**, 25 (*use*)

C.I. Solvent Red 80 C-257

[6358-53-8]
1-[(2,5-Dimethoxyphenyl)azo]-2-naphthalenol, 9CI. Citrus Red No. 2



$C_{18}H_{16}N_2O_3$ 308.336

Colourant for orange skins. Allowed on fruit which is not to be processed. Use prohibited in orange peel for human consumption. Deep red needles (EtOH). Mp 156°.

Kokkinos, K. *et al., Helv. Chim. Acta*, 1971, **54**, 2744-2747 (*synth, uv*)
Lehmann, G. *et al., Fresenius' Z. Anal. Chem.*, 1987, **328**, 596-597 (*tlc*)
Hope, C. *et al., J. Assoc. Off. Anal. Chem.*, 1989, **72**, 705-707 (*anal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 631-632 (*use*)

Cibulins C-258

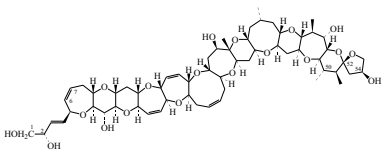
Alkyl propyl sulfoxides
$H_3CCH_2CH_2SOR$

A group of substances with the suggested struct. where R is a long-chain fatty acid residue of varying length. Isol. from onions inoculated with *Botrytis cinerea* and *Fusarium solani*. λ_{max} 210 (MeOH) (Berdy).

Dmitriev, A.P. *et al., CA*, 1989, **110**, 92249d (*isol*)

Ciguatoxin (Pacific) C-259

[11050-21-8]
Pacific Ciguatoxin 1. P-CTX 1B



$C_{60}H_{86}O_{19}$ 1111.328

Earliest known of this group of toxins; sometimes simply known as Ciguatoxin or CTX. Isol. from the moray eel (*Gymnothorax javanicus*) and other fish and shellfish esp. coral reef spp. Present in the dinoflagellate *Gambierdiscus toxicus*. Causes ciguatera food poisoning. *G. toxicus* is the primary cause.

▶ GD0760000

7-Oxo, 6,7-dihydro: [263336-55-6] ***7-Oxociguatoxin***
$C_{60}H_{86}O_{20}$ 1127.327
Isol. from fish.

3ξ-Hydroxy, 7-oxo, 3,4,6,7-tetrahydro: [263336-57-8] ***3,4-Dihydro-3-hydroxy-7-oxociguatoxin***. *3-Hydroxy-7-oxociguatoxin*
$C_{60}H_{88}O_{21}$ 1145.343
Isol. from fish.

4ξ-Hydroxy, 7-oxo, 3,4,6,7-tetrahydro: [287732-85-8] ***3,4-Dihydro-4-hydroxy-7-oxociguatoxin***. *4-Hydroxy-7-oxociguatoxin*
$C_{60}H_{88}O_{21}$ 1145.343
Isol. from fish.

7ξ-Hydroxy, 6,7-dihydro: [263336-56-7] ***6,7-Dihydro-7-hydroxyciguatoxin***. *7-Hydroxyciguatoxin*
$C_{60}H_{88}O_{20}$ 1129.343
Isol. from fish.

54-Deoxy: [139341-09-6] ***54-Deoxyciguatoxin***. *Pacific Ciguatoxin 3. P-CTX 3*
$C_{60}H_{86}O_{18}$ 1095.329
Isol. from *Lycodontis javanicus*, the moray eel (*Gymnothorax javanicus*). λ_{max} 215 (MeOH) (Berdy).

54-Deoxy, 50-hydroxy: [263336-54-5] ***54-Deoxy-50-hydroxyciguatoxin, 9CI***
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

1,2,54-Trideoxy, 1,2-didehydro: [123676-76-6] ***Gambiertoxin 4B***. *GT 4B. Pacific Ciguatoxin 4B. P-CTX 4B. Ciguatoxin 4B*
$C_{60}H_{84}O_{16}$ 1061.314
λ_{max} 223 (ε 22000) (MeCN) (Berdy).

1,2,54-Trideoxy, 52,55-dihydroxy, 52,55-deepoxy, 1,2-didehydro: [287412-00-4] **M-*Secociguatoxin 4A***
$C_{60}H_{86}O_{17}$ 1079.329
Isol. from *Gambierdiscus toxicus*.

52-Epimer: [189013-49-8] ***52-Epiciguatoxin***
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

52-Epimer, 54-deoxy: [142185-85-1] ***Pacific Ciguatoxin 2***. *P-CTX 2*
$C_{60}H_{86}O_{18}$ 1095.329
Isol. from *Lycodontis javanicus* and moray eel. λ_{max} 215 (MeOH) (Berdy).

▶ GD0760100

52-Epimer, 1,2,54-trideoxy, 1,2-didehydro: [66231-73-0] ***Pacific Ciguatoxin 4A***. *P-CTX 4A. Ciguatoxin 4A*
$C_{60}H_{84}O_{16}$ 1061.314
Isol. from *Gambierdiscus toxicus* and *Scarus gibbus*. A toxin isol. from various parrotfish (*Scarus* sp.) and named Scaritoxin or SG 1 probably corresponds to a mixture of CTX 4A and 4B. Amorph. solid. A toxin isol. from various parrotfish (*Scarus* sp.) and named Scaritoxin or SG 1 probably corresponds to a mixture of CTX 4A and 4B λ_{max} 226 (MeOH).

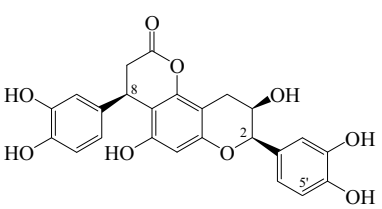
54-Epimer: [287732-40-5] ***54-Epiciguatoxin***
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

52,54-Diepimer: [287732-42-7] ***52,54-Diepiciguatoxin***
$C_{60}H_{86}O_{19}$ 1111.328
Isol. from fish.

Scheuer, P.J. *et al., Bioact. Mol.*, 1989, **10**, 265 (*occur*)
Murata, M. *et al., J.A.C.S.*, 1990, **112**, 4380 (*pmr, struct*)
Lewis, R.J. *et al., Toxicon*, 1991, **29**, 1115 (*isol, derivs*)
Murata, M. *et al., Tet. Lett.*, 1992, **33**, 525 (*cmr, struct*)
Satake, M. *et al., Biosci., Biotechnol., Biochem.*, 1997, **60**, 2103-2105 (*Ciguatoxin 4A*)
Satake, M. *et al., J.A.C.S.*, 1997, **119**, 11325-11326 (*abs config*)
Oguri, H. *et al., Tetrahedron*, 1997, **53**, 3057-3072 (*abs config*)
Yasumoto, T. *et al., J.A.C.S.*, 2000, **122**, 4988-4989 (*ms, occur*)

Cinchonain Ic C-260

[85081-22-7]
*4,8-Bis(3,4-dihydroxyphenyl)-3,4,9,10-tetrahydro-5,9-dihydroxy-2*H*,8*H*-benzo[1,2-b:3,4-b′]dipyran-2-one, 9CI*



$C_{24}H_{20}O_9$ 452.417

Stereochem. revised in 1993.Needles (H_2O). Mp 300°. $[\alpha]_D^{24}$ -25.1 (c, 0.22 in Me_2CO).

3-Epimer:
$C_{24}H_{20}O_9$ 452.417

Needles (H_2O). Mp 240-242°. $[\alpha]_D^{25}$ -12 (c, 0.35 in Me_2CO).

3-Epimer, 5′-hydroxy: [246152-24-9] ***Apocynin D***
$C_{24}H_{20}O_{10}$ 468.416
Brown solid. $[\alpha]_D^{25}$ +45.5 (c, 0.23 in MeOH). λ_{max} 210 (log ϵ 4.52); 230 (sh) ; 270 (log ϵ 3.75) (MeOH).

8-Epimer: [85022-67-9] ***Cinchonain Id***
$C_{24}H_{20}O_9$ 452.417
Needles + $1H_2O$ (H_2O). Mp 182-183°. $[\alpha]_D^{24}$ +29.1 (c, 0.33 in Me_2CO).

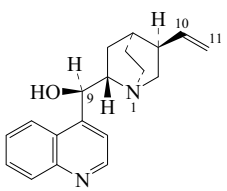
8-Epimer, 9-O-β-D-glucopyranoside: ***Cinchonain Id 7-glucoside***
$C_{30}H_{30}O_{14}$ 614.559
Constit. of *Eriobotrya japonica* (loquat). Pale yellow powder. $[\alpha]_D$ -37.5 (c, 1 in MeOH). Numbering systems vary λ_{max} 284 (log ϵ 3.97); 328 (log ϵ 3.38) (MeOH).

3,8-Diepimer:
$C_{24}H_{20}O_9$ 452.417
Needles (H_2O). Mp 270-272°. $[\alpha]_D^{25}$ +52.4 (c, 0.6 in Me_2CO).

Nonaka, G. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4268 (*isol, pmr, cmr, cd*)
Foo, L.Y. *et al., Phytochemistry*, 1989, **28**, 2477 (*isol*)
Chen, H.F. *et al., Phytochemistry*, 1993, **33**, 183 (*isol, pmr, cmr, config*)
Fan, W. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1049-1050 (*Apocynin D*)
Ito, H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 687-693 (*Cinchonain Id 7-glucoside*)

Cinchonidine C-261

[485-71-2]
*(8α,9*R*)-Cinchonan-9-ol, 9CI. α-Quinidine*



Absolute Configuration

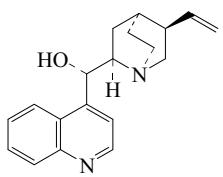
$C_{19}H_{22}N_2O$ 294.396
Stereoisomeric with Cinchonine, C-262. Alkaloid from the leaves of *Olea europaea*. Mp 210.5° (205°). $[\alpha]_D$ -110 (EtOH).
▶ LD_{50} (rat, ipr) 206 mg/kg. GD2975000
Hydrochloride (1:2):
Mp 242°.
Hydroiodide:
Mp 215-220°.
O-*Benzoyl:*
Mp 208-211° (183°).
N[1]-*Benzyl, chloride:* [69257-04-1]
Mp 210° dec. $[\alpha]_D^{20}$ -180 (c, 1.3 H_2O).
Ketone: [14509-68-3] ***Cinchonidinone***. *Cinchonan-9-one. Cinchoninone*
$C_{19}H_{20}N_2O$ 292.38
10,11-Dihydro: [485-64-3] ***Hydrocinchonidine***. *(8α,9*R*)-10,11-Dihydrocinchonan-9-ol, 9CI. 10,11-Dihydrocinchonidine. Cinchamidine*
$C_{19}H_{24}N_2O$ 296.411
Leaflets (EtOH). Mp 232° (229°). $[\alpha]_D$ -98.4 (EtOH).
10,11-Dihydro; hydrochloride:
Prisms + $2H_2O$. V. sol. H_2O. Mp 202.3° (anhyd.). $[\alpha]_D$ -98.4.

[524-61-8, 5948-98-1]

Goutarel, R. *et al., Helv. Chim. Acta*, 1950, **33**, 150 (*ir*)
Lyle, G.G. *et al., Tetrahedron*, 1967, **23**, 3253 (*config*)
Kamath, B.R. *et al., Indian J. Chem.*, 1968, **6**, 510 (*uv*)
Battersby, A.R. *et al., Chem. Comm.*, 1971, 30; 31 (*biosynth*)
Schneider, G. *et al., Planta Med.*, 1972, **22**, 109 (*isol*)
Moreland, C.G. *et al., J.O.C.*, 1974, **39**, 2413 (*cmr*)
Oleksyn, B. *et al., Acta Cryst. B*, 1982, **38**, 1832 (*cryst struct*)
Ihara, M. *et al., Chem. Comm.*, 1986, 573 (*synth, deriv*)
Bürgi, T. *et al., J.A.C.S.*, 1998, **120**, 12920-12926 (*pmr, conformn*)

Cinchonine C-262

[118-10-5]
*(9*S*)-Cinchonan-9-ol, 9CI*



Absolute Configuration

$C_{19}H_{22}N_2O$ 294.396
Stereoisomeric with Cinchonidine, C-261. Alkaloid from the leaves of *Olea europaea*. Cryst. Mp 264° Mp 255°. $[\alpha]_D$ +229 (EtOH). Log P 2.64 (calc).
▶ LD_{50} (rat, ipr) 152 mg/kg. GD3500000
Hydrochloride: [5949-11-1]

[24302-67-8]
Mp 217-218°.

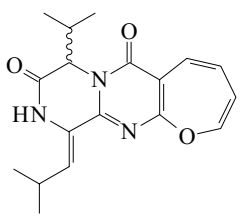
Sulfate: [5949-16-6]
Mp 206°.
▶ GD3800000
N-*Me:*
Mp 269-270° (iodide).
O-*Benzoyl:*
Mp 106-107°.
N-*Benzyl, chloride:* [69221-14-3]
Mp 256° dec.
10,11-Dihydro: [485-65-4] ***Hydrocinchonine***. *(9*S*)-10,11-Dihydrocinchonan-9-ol, 9CI. 10,11-Dihydrocinchonine. Cinchotine. ψ-Cinchonine. Pseudocinchonine. Cinchonifine*
$C_{19}H_{24}N_2O$ 296.411
Alkaloid from *Olea europaea*. Prisms. Mp 268-269°. $[\alpha]_D^{14}$ +204.5 (EtOH). Log P 3.12 (calc).
10,11-Dihydro; hydrochloride:
Mp 220-221°.
N-*[4-(Trifluoromethyl)benzyl], bromide:* [95088-20-3]

[205441-34-5] N-*[4-(Trifluoromethyl)benzyl]cinchoninium bromide*
$C_{27}H_{28}BrF_3N_2O$ 533.43
Mp 245°. Comly. available.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 864C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 439A (*nmr*)
Hesse, O. *et al., Ber.*, 1871, **4**, 818; 1883, **16**, 58 (*isol*)
Rabe, P. *et al., Ber.*, 1908, **41**, 62 (*struct*)
Potratz, A.H. *et al., Anal. Chem.*, 1949, **21**, 1276 (*detn, Bi*)
Goutarel, R. *et al., Helv. Chim. Acta*, 1950, **33**, 150 (*ir*)
Lyle, G.G. *et al., Tetrahedron*, 1967, **23**, 51; 3253 (*uv, ord, config, pmr*)
Kamath, B.R. *et al., Indian J. Chem.*, 1968, **6**, 510 (*uv*)
Battersby, A.R. *et al., Chem. Comm.*, 1971, 30; 31 (*biosynth*)
Schneider, G. *et al., Planta Med.*, 1972, **22**, 109 (*isol, uv, deriv*)
Norwitz, G. *et al., Anal. Chim. Acta*, 1974, **69**, 59 (*use*)
Moreland, C.G. *et al., J.O.C.*, 1974, **39**, 2413 (*cmr*)
Oleksyn, B. *et al., Acta Cryst. B*, 1979, **35**, 440 (*cryst struct*)
Ihara, M. *et al., Chem. Comm.*, 1986, 573 (*synth, deriv*)
Hughes, O.L. *et al., J.O.C.*, 1987, **52**, 4745 (*trifluoromethylbenzyl bromide, synth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 5156-5158 (*trifluoromethylbenzyl, bromide, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1998, **13**, 323; 1989, **14**, 326; 1990, **15**, 340 (*trifluoromethylbenzyl bromide, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMP925

Cinereain C-263

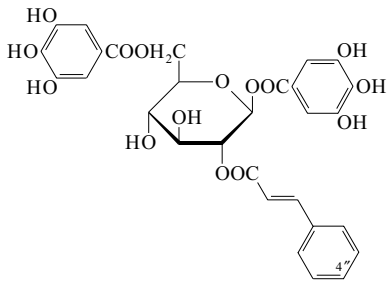
[117013-51-1]
*10,11-Dihydro-8-(1-methylethyl)-11-(2-methylpropylidene)-6*H*-oxepino[2,3-*d*]pyrazino[1,2-*a*]pyrimidine-6,9(8*H*)-dione, 9CI*



$C_{18}H_{21}N_3O_3$ 327.382
Isol. from *Botrytis cinerea* on sunflower seed. Ruby-red cryst. (Me_2CO). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 201-203°. λ_{max} 238 (ϵ 10471); 276 (ϵ 8710); 371 (ϵ 1230) (EtOH) (Berdy).

Cutler, H.G. *et al., Agric. Biol. Chem.*, 1988, **52**, 1725 (*isol, struct, props*)

2-Cinnamoyl-1,6-digalloylglucose C-264

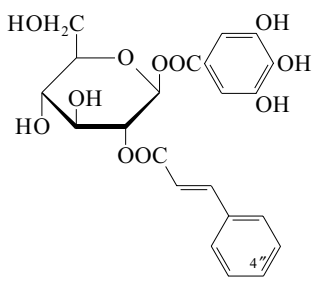


$C_{29}H_{26}O_{15}$ 614.515

β-D-Pyranose-*form* [94356-17-9]
Isol. from commercial rhubarbs (*Rheum* sp.). Off-white amorph. powder + $^3/_2H_2O$. $[\alpha]_D^{24}$ -95.2 (c, 1.29 in Me_2CO).

4″-Hydroxy: [115713-49-0] *2*-O-*(4-Hydroxycinnamoyl)-1,6-di*-O-*galloyl-β-D-glucopyranose*
$C_{29}H_{26}O_{16}$ 630.515
Isol. from commercial rhubarbs (*Rheum* sp.). Needles + $3^1/_2H_2O$ (H_2O). Mp 179-181°. $[\alpha]_D^{28}$ -112.8 (c, 0.53 in Me_2CO).
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461 (*struct, pmr, cmr*)
Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1473 (*deriv*)

2-Cinnamoyl-1-galloylglucose C-265



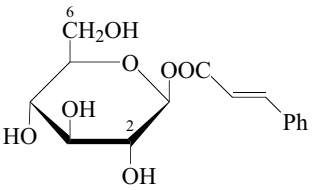
$C_{22}H_{22}O_{11}$ 462.409

β-D-Pyranose-*form* [56994-83-3]
Isol. from commercial rhubarbs (*Rheum* spp.). Needles (MeOH). Mp 190-193°. $[\alpha]_D^{19}$ -125.2 (c, 1 in MeOH).

4″-Hydroxy: [94356-18-0] *2*-O-*(4-Hydroxycinnamoyl)-1*-O-*galloyl-β-D-glucopyranoside*
$C_{22}H_{22}O_{12}$ 478.409
Isol. from *Rheum* spp.. Needles + $1H_2O$ (H_2O). Mp 181-183°. $[\alpha]_D^{24}$ -124.5 (c, 1.33 in Me_2CO).
Kahiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461 (*struct, pmr, cmr*)

1-*O*-Cinnamoylglucose C-266

[41682-52-4]



$C_{15}H_{18}O_7$ 310.303

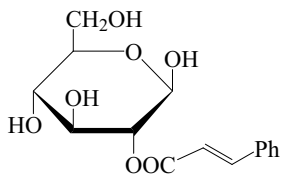
β-D-(*E*)-*form* [40004-96-4]
Constit. of *Vaccinium vitis-idaea* (cowberry). Amorph. powder.

6-O-*α-L-Arabinofuranosyl:* [181373-66-0]
$C_{20}H_{26}O_{11}$ 442.419
Constit. of *Psidium guajava* (guava). Amorph. powder.

6-O-*β-D-Glucopyranosyl:* [181373-65-9] *1*-O-*Cinnamoyl-β-D-gentiobiose*
$C_{21}H_{28}O_{12}$ 472.445
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. powder.

Yoshimoto, K. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2065 (*cmr*)
Plusquellec, D. *et al., Tetrahedron*, 1986, **42**, 2457 (*synth*)
Achenbach, H. *et al., Phytochemistry*, 1988, **27**, 1835 (*isol*)
Latza, S. *et al., J. Agric. Food Chem.*, 1996, **44**, 1367 (*isol*)
Latza, S. *et al., Phytochemistry*, 1996, **43**, 481 (*isol, synth, ir, pmr, cmr*)

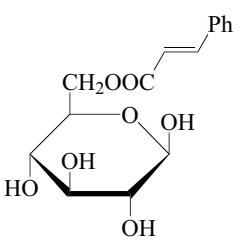
2-*O*-Cinnamoylglucose C-267



$C_{15}H_{18}O_7$ 310.303

β-D-Pyranose-(*E*)-*form* [94356-16-8]
Constit. of commercial rhubarb, *Rheum* sp.. Needles (H_2O). Mp 156.5-158°. $[\alpha]_D^{20}$ +49.7 (c, 0.87 in MeOH).
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461-3470

6-*O*-Cinnamoylglucose C-268



$C_{15}H_{18}O_7$ 310.303

β-D-*form* [64461-84-3] Possible artifact.

1-O-*(3,4,5-Trihydroxybenzoyl):* [115746-69-5] ***6-Cinnamoyl-1-galloylglucose***
$C_{22}H_{22}O_{11}$ 462.409
Isol. from commercial rhubarb (*Rheum* spp.). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ +3.3 (c, 0.64 in Me_2CO).

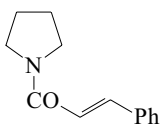
1,2-Bis(3,4,5-trihydroxybenzoyl): [115746-70-8] ***6-Cinnamoyl-1,2-digalloylglucose***
$C_{29}H_{26}O_{15}$ 614.515
Isol. from commercial rhubarbs (*Rheum* spp.). Off-white amorph. powder + $^1/_2H_2O$. $[\alpha]_D^{20}$ -76.9 (c, 0.75 in Me_2CO).

[64461-97-8]

Weinges, K. *et al., Annalen*, 1977, 1053 (*isol*)
Yoshimoto, K. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2065 (*cmr*)
Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1473 (*1,2-digalloyl*)

1-Cinnamoylpyrrolidine, 8CI C-269

[19202-21-2]
1-(1-Oxo-3-phenyl-2-propenyl)pyrrolidine, 9CI. Cinnamic acid pyrrolidide

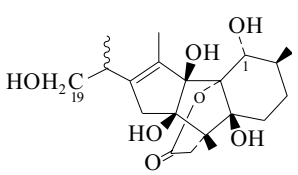


$C_{13}H_{15}NO$ 201.268

(*E*)-*form* [52438-21-8]
Alkaloid from the roots of kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liber damage (2002). Needles (petrol). Mp 101-103° (94-95°).
Achenbach, H. *et al., Chem. Ber.*, 1970, **103**, 2535 (*isol, uv, ir, ms, synth, struct*)
Engel, P. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1974, **139**, 207 (*cryst struct*)
Huang, Y.Z. *et al., Tet. Lett.*, 1987, **28**, 2159 (*synth*)
Rajeswari, S. *et al., Tet. Lett.*, 1987, **28**, 5099 (*synth*)
Son, T. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 1251 (*synth*)
Lindsay, C.M. *et al., J.C.S. Perkin 1*, 1988, 569 (*synth*)
Ohta, A. *et al., Heterocycles*, 1991, **32**, 965 (*synth*)

Cinncassiol A C-270

[73599-11-8]
Sincassiol†



$C_{20}H_{30}O_7$ 382.453

Cinncassiol A (from *Cinnamomum* spp.) and Sincassiol (from *Cassia* sp.) appear to be identical but this is not completely clear. Constit. of *Cinnamomum cassia* (Chinese cinnamon). Cryst. (MeOH aq.). Mp 172-174°. $[\alpha]_D^{32}$ +30.2 (c, 1.1 in MeOH).

19-O-*β-D-Glucopyranoside:* [73599-12-9]
$C_{26}H_{40}O_{12}$ 544.595
Constit. of *Cinnamomum* spp.. Powder.

Mp 95-99°. $[\alpha]_D^{25}$ +5.6 (c, 2.8 in MeOH).

19-Deoxy: [65230-04-8] ***Anhydrocinnzeylanol***
$C_{20}H_{30}O_6$ 366.453
Isol. from *Cinnamomum cassia* (Chinese cinnamon). Cryst. (C_6H_6/EtOAc). Mp 205-207°. $[\alpha]_D^{28}$ +56.4 (c, 0.5 in MeOH).

19-Deoxy, 1-Ac: [68799-62-2] ***Anhydrocinnzeylanine***
$C_{22}H_{32}O_7$ 408.491
Isol. from *Cinnamomum cassia* (Chinese cinnamon). Cryst. (C_6H_6/EtOAc). Mp 195-199°. $[\alpha]_D^{16}$ +88.7 (c, 1 in MeOH).

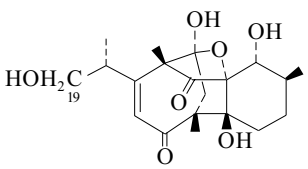
19-Deoxy, 1-ketone: [346414-64-0] ***Anhydrocinnzeylanone***
$C_{20}H_{28}O_6$ 364.438

[75765-19-4]

Yagi, A. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1432 (*isol, struct*)
Japan. Pat., 1980, 80 49 370; *CA*, **93**, 239708 (*Sincassiol*)
Nakao, K. *et al., Yakugaku Zasshi*, 1981, **101**, 1052 (*ms*)
Fraga, B.M. *et al., Phytochemistry*, 2001, **56**, 315-320 (*Anhydrocinnzeylanone*)

Cinncassiol C_1 C-271

[73613-35-1]
Cinncassiol C



$C_{20}H_{28}O_7$ 380.437
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Cryst. (MeOH). Mp 204-207°. $[\alpha]_D$ -3.6 (MeOH).

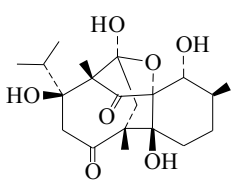
19-O-β-D-Glucopyranoside:
$C_{26}H_{38}O_{12}$ 542.579
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Amorph. powder. $[\alpha]_D$ +14.5 (c, 0.97 in MeOH).

19-Deoxy: [73599-14-1] *Cinncassiol C_2*
$C_{20}H_{28}O_6$ 364.438
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Needles (MeOH aq.). Mp 219-221°. $[\alpha]_D$ +30.5 (c, 0.82 in MeOH).

Nohara, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1969
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2686

Cinncassiol C_3 C-272

[64979-94-8]

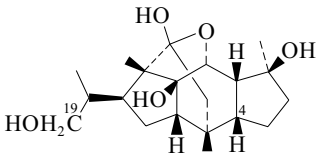


$C_{20}H_{30}O_7$ 382.453
Constit. of cinnamoni cortex, the dried bark of *Cinnamomum cassia* (Chinese cinnamon). Needles (MeOH). Mp 221-222°. $[\alpha]_D^{21}$ +6.1 (c, 0.33 in MeOH).

Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2686

Cinncassiol D_1 C-273

[77353-84-5]



$C_{20}H_{32}O_5$ 352.47
Constit. of cinnamomi cortex, the dried bark of *Cinnamomum cassia* (Chiense cinnamon). Powder. $[\alpha]_D^{26}$ -11.6 (c, 0.81 in MeOH).

19-O-β-D-Glucopyranosyl: ***Cinncassiol D_1 glucoside***
$C_{26}H_{42}O_{10}$ 514.612
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Powder. $[\alpha]_D$ -4.1 (c, 0.29 in MeOH).

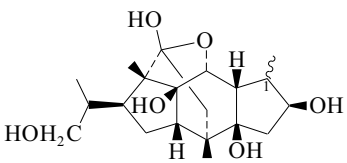
4β-Hydroxy: [77751-33-8] ***Cinncassiol D_2***
$C_{20}H_{32}O_6$ 368.469
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Powder. $[\alpha]_D^{16}$ -15.4 (c, 0.94 in MeOH).

4β-Hydroxy, 19-O-β-D-glucopyranoside:- ***Cinncassiol D_2 glucoside***
$C_{26}H_{42}O_{11}$ 530.611
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Powder. $[\alpha]_D^{17}$ -3.2 (c, 0.44 in MeOH).

Nohara, T. *et al., Tet. Lett.*, 1980, 2647 (*cryst struct*)
Nohara, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2451 (*cryst struct*)

Cinncassiol D_3 C-274

[80178-41-2]

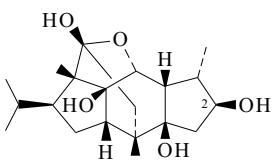


$C_{20}H_{32}O_6$ 368.469
Constit. of cinnamomi cortex, the dried bark of *Cinnamomum cassia* (Chinese cinnamon). Powder. $[\alpha]_D^{27}$ -10.1 (c, 0.79 in MeOH).

Nohara, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2451

Cinncassiol D_4 C-275

[84807-46-5]



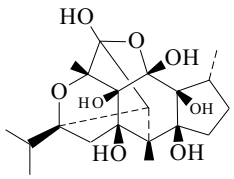
$C_{20}H_{32}O_5$ 352.47
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Amorph. powder. $[\alpha]_D^{26}$ -16.3 (c, 0.49 in MeOH).

2-O-β-D-Glucopyranoside:
$C_{26}H_{42}O_{10}$ 514.612
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Amorph. powder. $[\alpha]_D^{26}$ -12.5 (c, 0.88 in MeOH).

Nohara, T. *et al., Phytochemistry*, 1982, **21**, 2130

Cinncassiol E C-276

[98751-76-9]

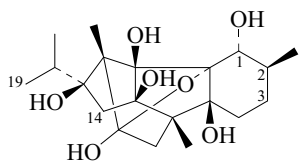


$C_{20}H_{30}O_8$ 398.452
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Cryst. (MeOH). Mp 195-198°. $[\alpha]_D$ -20.4 (c, 2 in MeOH).

Nohara, T. *et al., Phytochemistry*, 1985, **24**, 1849

Cinnzeylanol C-277

[62394-04-1]
3-Deoxyryanodol



$C_{20}H_{32}O_7$ 384.469
Constit. of the dried bark of *Cinnamomum zeylanicum* (cinnamon) and of *Cinnamomum cassia* (Chinese cinnamon). Cryst. (EtOAc/C_6H_6). Mp 278-279°. $[\alpha]_D^{26}$ +60.8 (c, 1.3 in MeOH).

1-Ac: [62203-47-8] ***Cinnzeylanine***
$C_{22}H_{34}O_8$ 426.506
Constit. of *Cinnamomum zeylanicum* (cinnamon) and *Cinnamomum cassia* (Chinese cinnamon). Cryst. (EtOAc/C_6H_6). Mp 265-267°. $[\alpha]_D^{27}$ +45 (c, 2 in MeOH).

2,3-Didehydro, 1-ketone: [346414-65-1] ***2,3-Didehydrocinnzeylanone***
$C_{20}H_{28}O_7$ 380.437

19-Hydroxy: [73599-13-0] ***Cincassiol B***
$C_{20}H_{32}O_8$ 400.468
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Powder. $[\alpha]_D^{17}$ +22.7 (c, 0.44 in MeOH).

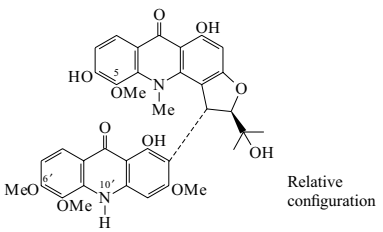
19-Hydroxy, 19-β-D-glucopyranoside:
$C_{26}H_{42}O_{13}$ 562.61
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Powder. $[\alpha]_D^{16}$ -20 (c, 0.15 in MeOH).

14α-Acetoxy, 1-deoxy, 3-oxo: ***Garajonone***
$C_{22}H_{32}O_9$ 440.489

Isogai, A. *et al., Acta Cryst. B*, 1977, **33**, 623 (*cryst struct*)
Isogai, A. *et al., Agric. Biol. Chem.*, 1977, **41**, 1779 (*isol*)
Yagi, A. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1432
Nohara, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2682 (*Cincassiol B*)
Fraga, B.M. *et al., Phytochemistry*, 2001, **56**, 315-320 (*Garajonone, 2,3-Didehydrocinnzeylanone*)

Citbismine B C-278

[169055-77-0]



Relative configuration

$C_{36}H_{34}N_2O_{11}$ 670.671
Alkaloid from roots of Marsh grapefruit (*Citrus paradisi*) and Hirado-buntan (*Citrus grandis*). Yellow cubes (Me_2CO). Mp 336-344°. $[\alpha]_D$ 0 ($CHCl_3$).

$N^{10'}$*-Me:* [169055-79-2] ***Citbismine C***
$C_{37}H_{36}N_2O_{11}$ 684.698
From roots of *Citrus paradisi* (grapefruit) and *Citrus grandis* (pummelo). Yellow cubes (Me_2CO). Mp 314-326°. Opt. inactive.

$O^{6'}$*-De-Me,* $N^{10'}$*-Me:* [173429-82-8] ***Citbismine E***
$C_{36}H_{34}N_2O_{11}$ 670.671
From roots of *Citrus paradisi* (grapefruit) and *Citrus grandis* (pummelo). Pale yellow oil. Opt. inactive.

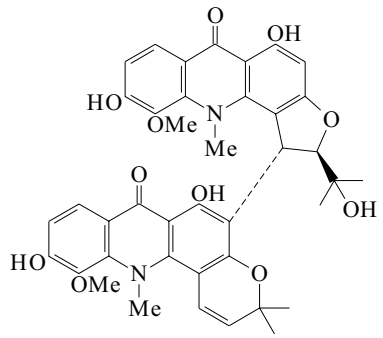
6-Deoxy, O^5*-de-Me:* [161068-61-7] ***Citbismine A***
$C_{35}H_{32}N_2O_{10}$ 640.645
Alkaloid from roots of *Citrus paradisi* (Marsh grapefruit) and *Citrus grandis* (pummelo). Yellow cubes (DMSO). Mp 335-336°. $[\alpha]_D$ 0 (DMSO).

6-Deoxy, O^5*-de-Me,* $N^{10'}$*-Me:* ***Citbismine F***
$C_{36}H_{34}N_2O_{10}$ 654.672
Alkaloid from *Citrus paradisi* (Marsh grapefruit). Yellow cubes. Mp 330-341° (dec.). $[\alpha]_D$ 0 ($CHCl_3$). λ_{max} 222 (log ϵ 3.87); 266 (log ϵ 4.28); 275 (log ϵ 4.27); 334 (log ϵ 3.77); 390 (log ϵ 3.41) (EtOH).

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1548; 1995, **43**, 1340 (*Citbismine A, Citbismine B, isol, uv, ir, pmr, cmr, ms, cryst struct*)
Ju-ichi, M. *et al., Heterocycles*, 1996, **42**, 237 (*Citbismine E*)
Takemura, Y. *et al., Heterocycles*, 1999, **51**, 851-855 (*Citbismine F*)

Citbismine D C-279

[173429-81-7]

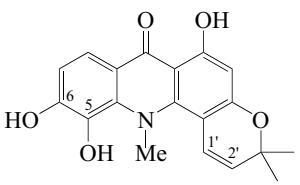


$C_{40}H_{38}N_2O_{11}$ 722.747
Alkaloid from roots of Marsh grapefruit (*Citrus paradisi*). Pale yellow oil. Opt. inactive.

Ju-ichi, M. *et al., Heterocycles*, 1996, **42**, 237 (*isol, uv, ir, pmr, ms, struct*)

Citracridone III C-280

[139219-98-0]
*3,12-Dihydro-6,10,11-trihydroxy-3,3,12-trimethyl-7*H*-pyrano[2,3-*c*]acridin-7-one, 9CI*



$C_{19}H_{17}NO_5$ 339.347
Acridone numbering shown.Yellow cubes (CH_2Cl_2). Mp 135-140°.

5-Me ether: [81525-61-3] ***Citracridone I***
$C_{20}H_{19}NO_5$ 353.374
Alkaloid from the root bark of *Citrus sinensis* var. *brasiliensis* (navel orange). Orange plates (Me_2CO). Mp 275-278°.

5-Me ether, N*-de-Me:* [172335-13-6] ***Acrifoline***†. N*-Demethylcitracridone I*
$C_{19}H_{17}NO_5$ 339.347
Yellow amorph. powder.

6-Me ether: [90846-44-9] ***3,12-Dihydro-6,11-dihydroxy-10-methoxy-3,3,12-trimethyl-7*H*-pyrano[2,3-*c*]acridin-7-one, 9CI***. *2′,2′-Dimethyl(pyrano-5′,6′:3:4)-1,5-dihydroxy-6-methoxy-10-methylacridone*
$C_{20}H_{19}NO_5$ 353.374
Alkaloid from the roots of *Citrus decumana* (pummelo). Cryst. (MeOH). Mp 260°.

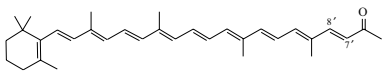
5,6-Di-Me ether: [81525-62-4] ***Citracridone II***
$C_{21}H_{21}NO_5$ 367.401
Yellow needles (Et_2O). Mp 161-163°.

1′,2′-Dihydro, 1′,2′-dihydroxy (trans-)*, 5-Me ether:* [161043-20-5] ***Dihydroxycitracridone I***
$C_{20}H_{21}NO_7$ 387.388
Isol. from roots of grapefruit plants. Yellow cubes. Mp 235-238°. $[\alpha]_D$ +107 (c, 0.056 in EtOH).

Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1983, **31**, 895; 901 (*isol, uv, ir, pmr, ms, struct*)
Wu, T.-S. *et al., Phytochemistry*, 1983, **22**, 1493 (*isol*)
Basa, S.C. *et al., J. Nat. Prod.*, 1984, **47**, 325 (*6-Me ether*)
Ju-ichi, M. *et al., Heterocycles*, 1991, **32**, 1781 (*isol, pmr, cmr, struct*)
Takemura, Y. *et al., Heterocycles*, 1995, **41**, 187-190 (*Dihydroxycitracridone I*)
Ono, T. *et al., J. Nat. Prod.*, 1995, **58**, 1629-1631 (*Acrifoline*)

Citranaxanthin C-281

[3604-90-8]
6′-Methyl-6′-apo-β-caroten-6′-one



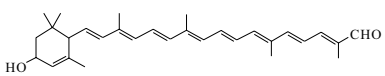
$C_{33}H_{44}O$ 456.71
Constit. of Sinton citrangequat (a *Citrus-Poncirus-Fortunella* hybrid). Cryst. (petrol). Mp 156°.

7′,8′-Dihydro, 8′-hydroxy: [15446-86-3] *7′,8′-Dihydro-8′-hydroxy-6′-methyl-6′-apo-β-caroten-6′-one.* ***7′,8′-Dihydro-8′-hydroxycitraniaxanthin****. 8′,9′-Dihydro-8′-hydroxycitraniaxanthin (incorr.)*
Isol. from Sinton citrangequat. Cryst. (petrol). Mp 146-147°.

Yokoyama, H. *et al., J.O.C.*, 1965, **30**, 2481; 1966, **31**, 3452 (*isol, biosynth*)
Stewart, I. *et al., Phytochemistry*, 1973, **12**, 2947
Bremser, W. *et al., Org. Magn. Reson.*, 1974, **6**, 433 (*cmr*)

α-Citraurin C-282

3-Hydroxy-8′-apo-ϵ-caroten-8′-al

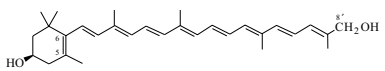


$C_{30}H_{40}O_2$ 432.645
Constit. of avocado (*Persea americana*). Cryst. (MeOH). Mp 153°. $[\alpha]_D^{18}$ +372 (C_6H_6).

Karrer, P. *et al., Helv. Chim. Acta*, 1938, **21**, 445 (*synth*)
Gross, J. *et al., Phytochemistry*, 1973, **12**, 2259 (*occur*)

β-Citraurol C-283

[57593-78-9]
8′-Apo-β-carotene-3,8′-diol. β-Citraurinol



$C_{30}H_{42}O_2$ 434.661
Constit. of citrus hybrid peel.

Di-Ac:
Cryst. (petrol/MeOH). Mp 92°.

8′-Aldehyde: [650-69-1] *3-Hydroxy-8′-apo-β-caroten-8′-al.* ***β-Citraurin***
$C_{30}H_{40}O_2$ 432.645
Constit. of orange peel. Cryst. (EtOH or Et_2O/petrol). Mp 146-147°.

*8′-Aldehyde, 5*R*,6*S*-epoxide:* [71869-83-5]
5,6-Epoxy-3-hydroxy-8′-apo-β-caroten-8′-al. ***β-Citraurin epoxide.*** *Apo-8′-violaxanthal*
$C_{30}H_{40}O_3$ 448.644
Isol. from orange peel. Cryst. (C_6H_6/petrol). Unnatural (5*S*,6*R*)-diastereoisomer also prepd. (Mp 158°) λ_{max} 424 ; 448 ; 477 (hexane).

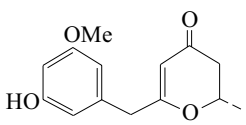
8′-Deoxy: [58947-97-0] *8′-Apo-β-caroten-3-ol.* ***β-Citraurinene***
$C_{30}H_{42}O$ 418.661
Constit. of citrus peel. Orange cryst. (CH_2Cl_2/petrol). Mp 141°.

[75715-17-2, 75715-18-3]

Leuenberger, U. *et al., J.O.C.*, 1976, **41**, 891-892 (*β-Citraurol*)
Leuenberger, U. *et al., Phytochemistry*, 1976, **15**, 227-229 (*β-Citraurinene*)
Pfander, H. *et al., Pure Appl. Chem.*, 1979, **51**, 565-580 (*synth*)
Pfander, H. *et al., Helv. Chim. Acta*, 1980, **63**, 716-727; 1377-1382 (*abs config, synth, biosynth*)
Molnár, P. *et al., Phytochemistry*, 1980, **19**, 633-637 (*β-Citraurin epoxide*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 483; 484 (*bibl*)
Deli, J. *et al., Helv. Chim. Acta*, 1998, **81**, 1815-1820 (*β-Citraurin, pmr, cmr*)
Lóránd, T. *et al., Helv. Chim. Acta*, 2002, **85**, 1691-1697 (*ir*)

Citreovirenone C-284

[103955-68-6]

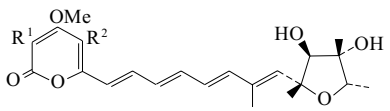


$C_{14}H_{16}O_4$ 248.278
Mycotoxin prod. by the rice storage mould *Penicillium citreo-viride* B. Oil. $[\alpha]_D^{30}$ -109.5 (c, 0.66 in $CHCl_3$). λ_{max} 209 (ε 20000); 222 (sh) (ε 7000); 267 (ε 12000) (MeOH) (Derep).

Shizuri, Y. *et al., Chem. Lett.*, 1986, 1129 (*isol, struct, nmr*)

Citreoviridin C-285

[25425-12-1]
Citreoviridin A



$R^1 = H, R^2 = CH_3$

$C_{23}H_{30}O_6$ 402.486
Metab. of *Penicillium citreo-viride, Penicillium toxicarium, Penicillium ochrosalmoneum* and *Aspergillus terreus*. Isol. from mouldy rice. Toxin formerly responsible for epidemic-like occurrences of cardiac beriberi in East Asia. Deep yellow cryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 107-111°. λ_{max} 204 (ε 17000); 235 (ε 10200); 286 (ε 24600); 294 (ε 27100); 388 (ε 48000); 398 (sh) (ε 46000) (EtOH) (Derep). λ_{max} 205 (ε 14100); 238 (ε 10000); 294 (ε 24500); 390 (ε 45000) (MeOH) (Berdy). λ_{max} 234 (ε 10200); 294 (ε 27100); 388 (ε 48000) (EtOH) (Berdy).

▶ LD_{50} (mus, orl) 29 mg/kg. LD_{50} (mus, ipr) 7.2 mg/kg , LD_{50} (mus, scu) 11 mg/kg. Exp. reprod. and teratogenic effects.. UQ1235000

Ac:
Cryst. Mp 99-101°.

Saito, M. *et al., Microb. Toxins*, 1971, **6**, 299 (*rev*)
Nagel, D.W. *et al., Phytochemistry*, 1972, **11**, 3215 (*biosynth*)
Sakabe, N. *et al., Tetrahedron*, 1977, **33**, 3077 (*struct*)
Linnett, P.E. *et al., Biochem. J.*, 1978, **170**, 503 (*props*)
Franck, B. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 461 (*isol*)
Steyn, P.S. *et al., J.C.S. Perkin 1*, 1982, 2175 (*biosynth*)
Steyn, P.S. *et al., Chem. Comm.*, 1985, 1531 (*biosynth*)
Nishiyama, S. *et al., Tet. Lett.*, 1985, **26**, 231 (*synth, abs config*)
Williams, D.R. *et al., J.O.C.*, 1987, **52**, 5067 (*synth*)
Suh, H. *et al., J.A.C.S.*, 1988, **110**, 470 (*synth*)
Hatakeyama, S. *et al., J.A.C.S.*, 1988, **110**, 5201 (*synth*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, (*rev*)
Bowden, M.C. *et al., J.C.S. Perkin 1*, 1991, 1947 (*synth*)
Whang, K. *et al., J.O.C.*, 1991, **56**, 7174 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 876
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMS500

Citreoviridin C C-286

[74145-78-1]
As Citreoviridin, C-285 with
$R^1 = CH_3$, $R^2 = H$
$C_{23}H_{30}O_6$ 402.486
Mycotoxin prod. by the common soil organism *Aspergillus terreus*. λ_{max} 204 (ε 17000); 235 (ε 10200); 286 (ε 24600); 294 (ε 27100); 388 (ε 48000); 398 (sh) (ε 46000) (EtOH) (Derep).

Saito, M. *et al., Microb. Toxins*, 1971, **6**, 299 (*rev*)
Sakabe, N. *et al., Tetrahedron*, 1977, **33**, 3077 (*struct*)
Linnett, P.E. *et al., Biochem. J.*, 1978, **170**, 503 (*props*)
Franck, B. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 461 (*isol*)
Steyn, P.S. *et al., Chem. Comm.*, 1985, 1531 (*biosynth*)
Nishiyama, S. *et al., Tet. Lett.*, 1985, **26**, 231 (*config, synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 876

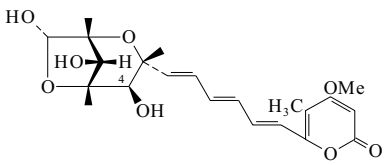
Citreoviridin D C-287

[74145-79-2]
As Citreoviridin, C-285 with
$R^1 = R^2 = CH_3$
$C_{24}H_{32}O_6$ 416.513
Mycotoxin prod. by the common soil organism *Aspergillus terreus*. λ_{max} 204 (ε 17000); 235 (ε 10200); 286 (ε 24600); 294 (ε 27100); 388 (ε 48000); 398 (sh) (ε 46000) (EtOH) (Derep).

Saito, M. *et al., Microb. Toxins*, 1971, **6**, 299 (*rev*)
Sakabe, N. *et al., Tetrahedron*, 1977, **33**, 3077 (*struct*)
Linnett, P.E. *et al., Biochem. J.*, 1978, **170**, 503 (*props*)
Franck, B. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 461 (*isol*)
Steyn, P.S. *et al., Chem. Comm.*, 1985, 1531 (*biosynth*)
Nishiyama, S. *et al., Tet. Lett.*, 1985, **26**, 231 (*config, synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 876

Citreoviridinol A_1 C-288

[94161-12-3]



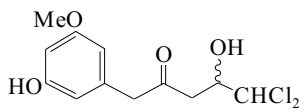
$C_{22}H_{28}O_8$ 420.458
Mycotoxin prod. by *Penicillium pedemontanum*.

4-Epimer: [94122-10-8] ***Citreoviridinol A_2***
$C_{22}H_{28}O_8$ 420.458
Mycotoxin of *Penicillium pedemontanum*.

Rebuffat, S. *et al., Org. Mass Spectrom.*, 1984, **19**, 349 (*ms*)

Citreovirone C-289

[103955-67-5]
5,5-Dichloro-4-hydroxy-1-(3-hydroxy-5-methoxyphenyl)-2-pentanone, 9CI

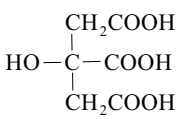


$C_{12}H_{14}Cl_2O_4$ 293.146
Mycotoxin prod. by the rice storage mould *Penicillium citreo-viride*. Oil. $[\alpha]_D^{30}$ +21.8 (c, 4.0 in $CHCl_3$). λ_{max} 209 (ε 14000); 222 (sh) (ε 7000); 280 (ε 1000) (MeOH) (Derep).

Shizuri, Y. *et al., Chem. Lett.*, 1986, 1129 (*isol, struct, nmr*)

Citric acid C-290

[77-92-9]
2-Hydroxy-1,2,3-propanetricarboxylic acid, 9CI. 2-Hydroxytricarballylic acid. E330. FEMA 2306



$C_6H_8O_7$ 192.125
Occurs in the free state in lemons, currants, beetroot etc. and the seeds and juices of many flowers and plants. Commercially produced by large-scale fermentation of sugars using the mould *Aspergillus nigus*. Constit. of fruit drinks, pharmaceutical syrups. Flavouring ingredient. Primary function as an acid, acidity regulator, antioxidant, preservative and sequestrant. One of the most widely used food additives. Its clean taste makes it applicable in soft drinks, sugar confectionery, preserves, soups and sauces. Cryst. + $1H_2O$ (H_2O), losing H_2O at 70-75°. V. sol. H_2O, EtOH; mod. sol. Et_2O. Mp 135° (monohydrate) Mp 153° (anhyd.). pK_{a1} 3.13; pK_{a2} 4.78; pK_{a3} 6.43 (25°).

▶ Eye and skin irritant. LD_{50} (rat, orl) 6730 mg/kg. GE7350000

Mono-Na salt: [18996-35-5]

[994-36-5] *Sodium dihydrogen citrate. Bicitra*
Preservative. Hygroscopic solid. Mp 212°.

▶ LD_{50} (rat, ipr) 1348 mg/kg. GE7950000

Di-Na salt: [144-33-2]

[994-36-5, 6132-05-4] *Disodium hydrogen citrate. Alkacitron*
Preservative. Solid + $1\frac{1}{2}H_2O$. Mp 149° dec.

Tri-Na salt: [68-04-2]

[994-36-5] *Sodium citrate. Trisodium citrate. Citrosodine. E331. FEMA 3026*
Used in food processing as an emulsifying agent, pH control agent, colour control agent, flavouring agent and modifier. Used in conjunction with ascorbate or erythorbate derivs. as a cure accelerator in processed meat products. Cryst. + $2H_2O$. Mp 300°. Pentahydrate also known.

▶ GE8300000

Mono-K salt: [866-83-1] *Potassium dihydrogen citrate*
Preservative. Cryst. powder. Sol. H_2O.

Tri-K salt: [866-84-2]

[7778-49-6] *Potassium citrate. Tripotassium citrate. Urocit K. E332*
Alkalising and buffering agent. Used in foods, beverages and oral pharmaceutical formulations. More sol. than Na salts; also used in low-Na foods and as a potassium source in nutritional supplements. Cryst. + H_2O. Mp 275° dec. CAS no. refers to anhydr. form.

Ca salt (2:3): [813-94-5]

[5785-44-4] *Calcium citrate. Citracal. E333*
$C_{12}H_{10}Ca_3O_{14}$ 498.437
Emulsifier in foods, dietary supplement. Cryst. + $4H_2O$. Loses H_2O of crystallisation at 100-120°.

Mn salt: [10024-66-5] *Manganese citrate*
Dietary supplement. Pale orange or pinkish white powder.

Tri-NH_4 salt: [3458-72-8] *Ammonium citrate. Triammonium citrate. E380*
Emulsifier and acidity regulator used in the food industry.

Tri-Et ester: [77-93-0] *Triethyl citrate. FEMA 3083. E1505*
$C_{12}H_{20}O_7$ 276.286
Used in foods as a flavouring agent, solvent and surface-active agent. Oil with a bitter taste. Sl. sol. H_2O. d^{25} 1.14. Bp 294° Bp_1 127°.

▶ LD_{50} (rat, orl) 5900 mg/kg. GE8050000

1-Isopropyl ester: [101396-15-0]

[1321-57-9, 39413-05-3, 135630-69-2]
$C_9H_{14}O_7$ 234.205
Sequestrant, antioxidant, solvent and vehicle in margarine manuf.. Isopropyl citrate for food use is a mixt. of the 1- and 2- isomers together with smaller amts. of di- and triisopropyl citrates.

2-Isopropyl ester: [83966-24-9]

[1321-57-9, 39413-05-3]
$C_9H_{14}O_7$ 234.205
Sequestrant and antioxidant for margarine and other foodstuffs. Plasticiser for food contact packaging. Cryst. (Me_2CO/hexane). Mp 126-128°. Food grade material is a mixt. of the 1- and 2- isopropyl esters.

2-Octadecyl ester:2-Stearyl citrate
$C_{24}H_{44}O_7$ 444.607
Antioxidant, sequestrant and emulsifier for use in margarine. Plasticiser for food contact packaging. Cryst. (toluene). Mp 80.4-80.9°. Food grade material is a mixt. of mono-, di- and triesters prepared by esterification of citric acid with stearyl alcohol.

Ac, tributyl ester: [77-90-7] *Acetyl tributyl citrate. ATBC. FEMA 3080*
$C_{20}H_{34}O_8$ 402.484
Flavouring ingredient. Plasticiser used in packaging films for food. Liq. with a faint, sweet herbaceous odour and mild fruity flavour. Bp_1 165-170°. Mp >330°.

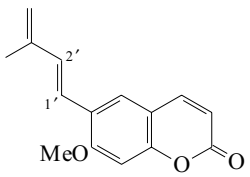
Me ether, tri-Me ester:
$C_{10}H_{16}O_7$ 248.232
Bp_{12} 159-160°.

[126-44-3, 3012-65-5, 3458-72-8, 4450-94-6, 5949-29-1, 6100-05-6, 6132-04-3, 7693-13-2, 10402-15-0, 80238-46-6, 80300-24-9, 101996-63-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 524B; 555B; 555D; 665A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 814A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 719D (*ir*)
v. Pechmann, H. *et al., Annalen*, 1891, **261**, 162 (*synth*)
Bülow, C. *et al., Ber.*, 1918, **51**, 1246 (*synth*)
Challenger, F. *et al., Ind. Chem.*, 1929, **5**, 181 (*bibl*)
U.S. Pat., 1936, 2 047 669; *CA*, **30**, 6128 (*synth*)
U.S. Pat., 1937, 2 066 892; *CA*, **31**, 1045 (*isol*)
U.S. Pat., 1945, 2 389 766; *CA*, **40**, 5757 (*Ca salt, manuf*)
Rudy, H. *et al., Pharmazie*, 1949, **4**, 393-399 (*Ca salt, rev*)
Cheng, K.L. *et al., Anal. Chem.*, 1961, **33**, 783 (*use*)
Hulanicki, A. *et al., Talanta*, 1962, **9**, 549 (*use*)
Gilbert, D.J. *et al., Chemistry*, 1968, **41**, 29 (*ester*)
Food Chemicals Codex, 2nd Ed., Vol. II, 1972, 204 (*anal*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 877 (*occur*)
Schulz, G. *et al., Ullmanns Encykl. Tech. Chem., 4. Aufl.*, 1975, **9**, 624 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ADD750; CMS750; TJP750
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 354 (*rev*)
Venkateshwarlu, M. *et al., Powder Diffr.*, 1993, **8**, 173-174 (*cryst struct*)
Grewal, H.S. *et al., Biotechnol. Adv.*, 1995, **13**, 209 (*rev, manuf*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADD750; MRL000; TNL000; DXC400; CMS750; PLB750; TJP750

Citrubuntin C-291

[74794-83-5]
7-Methoxy-6-(3-methyl-1,3-butadienyl)-2H-1-benzopyran-2-one, 9CI. Dehydrosuberosin. Suberodiene



$C_{15}H_{14}O_3$ 242.274
Constit. of *Citrus grandis* (pummelo). Powder (Et_2O) or pale yellow prisms (CH_2Cl_2/EtOAc). Mp 118-120° (115-117°).

1′S,2′S-Epoxide: [23631-16-5] *7-Methoxy-6-[3-(1-methylethenyl)oxiranyl]-2H-1-benzopyran-22-one, 9CI. 6-(1,2-Epoxy-3-methyl-3-butenyl)-7-methoxycoumarin.* ***Thamnosmin***
$C_{15}H_{14}O_4$ 258.273
Plates (EtOAc/hexane). Mp 101-104°. $[\alpha]_D^{23}$ -17.3 ($CHCl_3$).

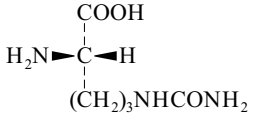
1′,2′-Dihydro, 1′,2′-dihydroxy: [60094-90-8] *6-(1,2-Dihydroxy-3-methyl-3-butenyl)-7-methoxy-2H-1-benzopyran-2-one, 9CI.* ***Thamnosmonin***
$C_{15}H_{16}O_5$ 276.288
Cryst. (EtOH). Mp 162-164°. $[\alpha]_D^{26}$ +187 (c, 0.6 in MeOH). Config. not establ..

[114032-21-2]

Kutney, J.P. *et al., Tetrahedron*, 1972, **28**, 5091 (*isol, struct, Thamnosmin*)
González, A.G. *et al., An. Quim.*, 1973, **69**, 1013; *CA*, **80**, 145231 (*pmr, Thamnosmin*)
Chang, P.T.O. *et al., J. Nat. Prod.*, 1976, **39**, 134 (*Thamnosmonin*)
Reisch, J. *et al., Annalen*, 1988, 543; 1990, 931 (*synth, pmr, cmr, ir, ms*)
Wu, T.S. *et al., Phytochemistry*, 1988, **27**, 3717 (*Citrubuntin*)

Citrulline C-292

N^5-(Aminocarbonyl)ornithine, 9CI. N^5-Carbamoylornithine, 8CI. 2-Amino-5-ureidovaleric acid. 5-Ureidoornithine. Stimol



$C_6H_{13}N_3O_3$ 175.187Log P -4.59 (calc).

(*S*)-*form* [372-75-8]

L-form
Occurs in the juice of watermelon (*Citrullus vulgaris*). Prisms (MeOH aq.). Mp 222°. $[\alpha]_D^{25}$ +22 (c, 2 in 1*M* HCl). pK_{a1} 2.43; pK_{a2} 9.41 (25°, 0.1*M* NaCl). Pharmacol. active enantiomer.

Hydrochloride:
$[\alpha]_D^{22}$ +17.9 (c, 2 in H_2O). Dec. at 185°.

Cu salt:
Blue prisms. Mp 257-258°.

2-N-*Benzoyl, Me ester:*
$C_{14}H_{19}N_3O_4$ 293.322Dec. at 120°.

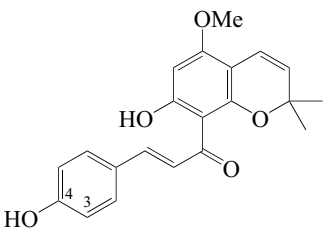
2-N-*Benzoyl, amide:*
$C_{13}H_{18}N_4O_3$ 278.31Dec. at 140°.

[627-77-0]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1279C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 784B (*ir*)
Biochem. Prep., 1953, **3**, 100; 104 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1964, **18**, 2412 (*ord*)
Dunnill, P.M. *et al., Phytochemistry*, 1965, **4**, 933 (*occur*)
Ashida, T. *et al., Acta Cryst. B*, 1972, **28**, 1367 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2391 (*occur*)
Msall, M. *et al., N. Engl. J. Med.*, 1984, **310**, 1500 (*pharmacol*)
Wakamiya, T. *et al., Tetrahedron*, 1984, **40**, 235 (*isol, bibl*)
Toffoli, P. *et al., Acta Cryst. C*, 1987, **43**, 945 (*cryst struct*)
Drauz, K. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 712 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1038

Citrunobin C-293

[126026-23-1]



$C_{21}H_{20}O_5$ 352.386

Chalcone-type numbering shown. Constit. of *Citrus sinensis* (orange) and *Citrus nobilis* (King orange). Red plates (Et_2O). Mp 182-184°.

4-Me ether:
$C_{22}H_{22}O_5$ 366.413
Yellow powder. λ_{max} 290 ; 362 ($CHCl_3$).

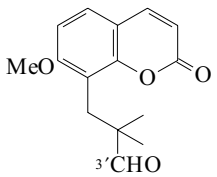
3-Methoxy, 4-Me ether:
$C_{23}H_{24}O_6$ 396.439
Yellow powder. λ_{max} 294 ; 372 ($CHCl_3$).

3,5-Dimethoxy, 4-Me ether: [194607-72-2]
$C_{24}H_{26}O_7$ 426.465
Yellow powder. λ_{max} 286 ; 352 (MeOH).

Wu, T.-S. *et al., Phytochemistry*, 1989, **28**, 3558 (*isol, pmr, cmr*)
Passador, E.A.P. *et al., Phytochemistry*, 1997, **45**, 1533-1537 (*deriv*)
Tomazela, D.M. *et al., Phytochemistry*, 2000, **55**, 643-651 (*derivs, pmr, cmr*)

Citrusal C-294

[5980-07-4]
*8-(2,2-Dimethyl-3-oxopropyl)-7-methoxy-2*H*-1-benzopyran-2-one, 9CI. 7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin*



$C_{15}H_{16}O_4$ 260.289

Constit. of grapefruit peel oil (*Citrus paradisi*). Fine needles (EtOAc/hexane). Mp 137-138°.

3′-Carboxylic acid: [112397-12-3]
Paniculin†
$C_{15}H_{16}O_5$ 276.288
Needles (MeOH). Mp 236-238°.

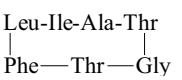
5-Methoxy: [74158-07-9] ***Seselinal***
$C_{16}H_{18}O_5$ 290.315
Needles (Me_2CO/hexane). Mp 174-175°.

5-Methoxy, 3′-carboxylic acid: [117007-26-8] *5,7-Dimethoxy-α,α-dimethyl-2-oxo-2*H*-1-benzopyran-8-propanoic acid.*
Murraculatin
$C_{16}H_{18}O_6$ 306.315
Needles (Me_2CO). Mp 217-218°.

Fisher, J.F. *et al., Tetrahedron*, 1966, **22**, 1489 (*isol, ir, uv, pmr, ms*)
Chatterjea, A. *et al., Chem. Ind. (London)*, 1976, 410 (*synth, uv, ir, pmr, ms*)
Banerjee, S.K. *et al., Phytochemistry*, 1980, **19**, 281 (*Seselinal*)
Wu, T.S. *et al., Phytochemistry*, 1988, **27**, 2357 (*Murraculatin*)
Imai, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 358 (*Paniculin*)
Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, 1991, **58**, 83 (*Citrusal*)
Rajnikant, G.K.N. *et al., Mol. Cryst. Liq. Cryst.*, 1993, **3**, 61 (*Seselinal, cryst struct*)

Citrusin I C-295

[139626-28-1]



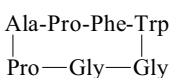
$C_{34}H_{53}N_7O_9$ 703.834

Isol. from unripe *Citrus unshiu* (satsuma mandarin). Cryst. Mp 300°. $[\alpha]_D^{22}$ -25.92 (c, 0.03 in MeOH).

Matsubara, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 2923 (*isol, pmr, cmr, ms*)

Citrusin II C-296

[139626-29-2]



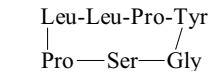
$C_{37}H_{44}N_8O_7$ 712.804

Isol. from *Citrus sinensis* (orange). Cryst. Mp 213-215°. $[\alpha]_D^{22}$ -75.16 (c, 0.15 in MeOH).

Matsubara, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 2923 (*isol, pmr, cmr, ms*)

Citrusin III C-297

[139626-30-5]



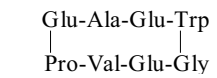
$C_{36}H_{53}N_7O_9$ 727.856

Isol. from *Citrus sinensis* (orange). Cryst. Mp 160-163°. $[\alpha]_D^{22}$ -103.09 (c, 0.14 in MeOH).

Matsubara, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 2923 (*isol, pmr, cmr, ms*)

Citrusin IV C-298

[139626-31-6]



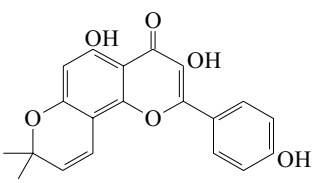
$C_{41}H_{55}N_9O_{14}$ 897.937

Isol. from *Citrus sinensis* (orange). Yellow cryst. Mp 220-221°. $[\alpha]_D^{22}$ +5.58 (c, 0.05 in MeOH).

Matsubara, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 2923 (*isol, pmr, cmr, ms*)

Citrusinol C-299

[112516-43-5]
*3,5-Dihydroxy-2-(4-hydroxyphenyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-b′]dipyran-4-one, 9CI*



$C_{20}H_{16}O_6$ 352.343

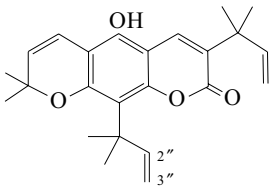
Isol. from root bark of king orange (*Citrus nobilis*). Yellow needles + $1H_2O$ (Me_2CO). Mp 252-254°.

3,6-Di-Me ether: [157072-30-5] *2-(4-Hydroxyphenyl)-3,6-dimethoxy-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-b′]dipyran-4-one*
$C_{22}H_{20}O_6$ 380.396
Constit. of the fruits of tangerine (*Citrus reticulata* cv. *blanco*). Mp 225-226°.

Wu, T.S. *et al., Phytochemistry*, 1987, **26**, 3094 (*isol*)
Saxena, V.K. *et al., Phytochemistry*, 1994, **36**, 1039 (*di-Me ether*)

Clausarin C-300

[62770-67-6]
*3,10-Bis(1,1-dimethyl-2-propenyl)-5-hydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-b:5′,4′-b′]dipyran-2-one, 9CI*



$C_{24}H_{28}O_4$ 380.483
Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 208° dec. λ_{max} 232 ; 282 ; 338 (MeOH) (Berdy).

Ac:
$C_{26}H_{30}O_5$ 422.52
Mp 120°.

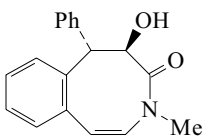
2″,3″-Epoxide: ***Oxaclausarin***
$C_{24}H_{28}O_5$ 396.482
Oil. $[\alpha]_D$ -32.3 (c, 0.192 in EtOH).

*6,7-Dihydro, 6,7-dihydroxy (*trans-*):* ***Clausarinol***
$C_{24}H_{30}O_6$ 414.497
Constit. of a cross hybrid of *Citrus paradisi* (grapefruit) and *Citrus tangerina* (tangerine). Oil. $[\alpha]_D$ -27.8 (c, 0.07 in $CHCl_3$).

Anwer, F. *et al., Experientia*, 1977, **33**, 412 (*isol, struct*)
Bhatia, S.K. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 1090 (*synth*)
Murray, R.D.H. *et al., Tetrahedron*, 1984, **40**, 3133 (*synth*)
Ju-ichi, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2252 (*Oxaclausarin*)
Takemura, Y. *et al., Chem. Pharm. Bull.*, 1996, **44**, 804 (*Clausarinol*)
Yenjai, C. *et al., Planta Med.*, 2000, **66**, 277-281 (*activity*)

ζ-Clausenamide C-301

[136173-85-8]
*5,6-Dihydro-5-hydroxy-3-methyl-6-phenyl-3-benzazocin-4(3*H*)-one, 9CI*

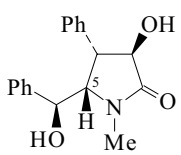


$C_{18}H_{17}NO_2$ 279.338
Alkaloid from *Clausena lansium* (wampee).

Yang, M. *et al., Chin. Chem. Lett.*, 1991, **2**, 291; *CA*, **115**, 155059 (*isol, struct*)

Clausenamide C-302

[119616-14-7]
3-Hydroxy-5-(hydroxyphenylmethyl)-1-methyl-4-phenyl-2-pyrrolidinone, 9CI. Lansimide 4



$C_{18}H_{19}NO_3$ 297.353
λ_{max} 257 (ϵ 500) (MeOH) (Berdy).

(±)-*form* [103541-15-7]
Isol. from the leaves of *Clausena lansium* (wampee). Needles. Mp 239-240°.

Di-Ac:
Cubes. Mp 165-167°.

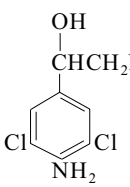
1′-Me ether: [119518-25-1] ***Lansimide 3***
$C_{19}H_{21}NO_3$ 311.38
Constit. of *Clausena lansium* (wampee).

1′,5-Diepimer: [114528-82-4] ***Neoclausenamide***
Isol. from *Clausena lansium* (wampee). Cubes. Mp 205-216°.

Lakshmi, V. *et al., Indian Drugs*, 1988, **26**, 105 (*Lansimides*)
Yang, M. *et al., Phytochemistry*, 1988, **27**, 445 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Rao, E.C. *et al., Chin. Chem. Lett.*, 1994, **5**, 267-268 (*synth*)
Huang, D.F. *et al., Chin. Chem. Lett.*, 1994, **5**, 371-372 (*synth*)
Wang, J.-Q. *et al., J.C.S. Perkin 1*, 1996, 209-212 (*synth, cryst struct, Neoclausenamide*)
Cappi, M.W. *et al., Chem. Comm.*, 1998, 1159-1160 (*synth*)

Clenbuterol, BAN, INN C-303

[37148-27-9]
*4-Amino-3,5-dichloro-α-[[(1,1-dimethylethyl)amino]methyl]benzenemethanol, 9CI. 1-(4-Amino-3,5-dichlorophenyl)-2-*tert*-butylaminoethanol. Spiropent. Ventipulmin. NAB 365. Many other names*



$C_{12}H_{18}Cl_2N_2O$ 277.192
Potential food contaminant arising from its illicit use to improve carcass quality and productivity in cattle. Approved tocolytic agent for cows in several European countries. Log P 2.38 (calc).
▶ LD_{50} (rat,orl) 159 mg/kg. Exp. reprod. and teratogenic effects. DA4726600

(+)-*form* [50499-60-0]
Cryst. (H_2O). Mp 127-128.5°. $[\alpha]_{364}^{20}$ +244 (c, 2.28 in $CHCl_3$). Abs. configs. not detd. (1994).

Hydrochloride: [50310-83-3]
Cryst. (Et_2O). Mp 197.5-198°. $[\alpha]_{364}^{20}$ +126 (c, 2.15 in H_2O).

(-)-*form* [50306-03-1]
Cryst. (H_2O). $[\alpha]_{364}^{20}$ -243 (c, 2.65 in $CHCl_3$). Active isomer.

Hydrochloride: [50310-85-5]
Cryst. (Et_2O). Mp 187-188° dec. $[\alpha]_{364}^{20}$ -126 (c, 2.72 in H_2O).

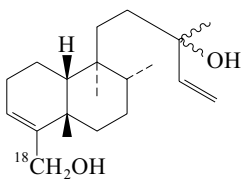
(±)-*form* [50306-01-9]

Hydrochloride: [69930-61-6]
Powder (2-propanol). Mp 174-175.5°.

[21898-19-1]

Keck, J. *et al., Arzneim.-Forsch.*, 1972, **22**, 861; 869 (*synth, pharmacol*)
Ger. Pat., 1972, 2 212 600; *CA*, **79**, 146177 (*resoln*)
Engelhardt, G. *et al., Arzneim.-Forsch.*, 1976, **26**, 1403 (*props*)
Baehring-Kuhlmey, S.R. *et al., Drugs of Today (Barcelona)*, 1978, **14**, 59; 1981, **17**, 335 (*revs*)
Tschan, M. *et al., Eur. J. Clin. Pharmacol.*, 1979, **15**, 159 (*props*)
Carpy, A. *et al., Acta Cryst. B*, 1980, **36**, 2837 (*cryst struct*)
Martin, P. *et al., Eur. J. Pharmacol.*, 1985, **117**, 127 (*pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2492 (*synonyms*)
Lafontan, M. *et al., Reprod., Nutr., Dev.*, 1988, **28**, 61 (*rev, anabolic props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1241
Panoyan, A. *et al., J. Agric. Food Chem.*, 1995, **43**, 2716-2718 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VHA350

3,14-Clerodadiene-13,18-diol C-304



$C_{20}H_{34}O_2$ 306.487

(*ent*-5α,13ξ)-*form* [56497-92-8]
Sagittariol
Constit. of *Sagittaria sagittifolia* (arrowhead). Cryst. (C_6H_6/hexane). Mp 109°. $[\alpha]_D$ +41 ($CHCl_3$).

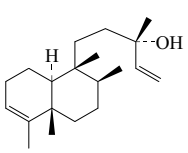
18-(2-Pyrrolecarbonyl): [174756-41-3]
Nakamurol D
$C_{25}H_{37}NO_3$ 399.572
Pale yellow oil. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{25}$ -8.5 (c, 1.2 in $CHCl_3$).

13-Epimer: [329689-18-1] ***Deacetylrigidusol***
$C_{20}H_{34}O_2$ 306.487
Gum. $[\alpha]_D^{24}$ -21.1 (c, 1.21 in $CHCl_3$).

13-Epimer, 18-Ac: [329688-58-6] ***Rigidusol***
$C_{22}H_{36}O_3$ 348.525
Gum. $[\alpha]_D^{24}$ -31.8 (c, 0.11 in $CHCl_3$).

Sharma, S.C. *et al., Phytochemistry*, 1975, **14**, 1055; 1984, **23**, 1194 (*Sagittariol*)
Shoji, N. *et al., J. Nat. Prod.*, 1996, **59**, 448 (*Nakamurol D*)
Morales, G. *et al., Phytochemistry*, 2000, **55**, 863-866 (*Rigidusol, Deacetylrigidusol*)

3,14-Clerodadien-13-ol C-305



(5β,8α*H*,13*S*)-*form*

$C_{20}H_{34}O$ 290.488

(5β,8α*H*,13*S*)-*form* [272777-78-3]
(+)-Kolavelool
Oil. $[\alpha]_D^{18}$ +59.1 (c, 0.68 in $CHCl_3$).

(*ent*-5β,8α*H*,13*S*)-*form* [19941-81-2]
Kolavelool
Oil. $[\alpha]_D^{24}$ -40.4 ($CHCl_3$).

(*ent*-5α,8α*H*,13ξ)(1)-*form* [374925-73-2]
Oil. $[\alpha]_D^{19}$ -24.2 (c, 1 in $CHCl_3$).

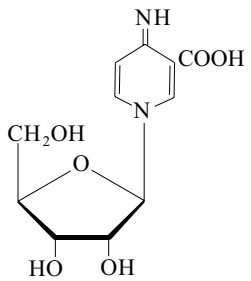
(*ent*-5α,8α*H*,13ξ)(2)-*form*
18-Deoxysagittarol
Constit. of *Sagittaria sagittifolia* (arrowhead). Viscous liq.

(*ent*-5α,8β*H*,13ξ)-*form* [16910-19-3]
Plathyterpol
Oil. $Bp_{0.2}$ 142-144°. $[\alpha]_D$ -28 (c, 0.2 in $CHCl_3$). The stereochemical assignment may be incorrect.

King, T.J. *et al., Chem. Comm.*, 1967, 575; 1969, 683 (*Plathyterpol*)
Misra, R. *et al., Tet. Lett.*, 1968, 2685 (*synth*)
Anthonsen, T. *et al., Acta Chem. Scand.*, 1969, **23**, 1068 (*Kolavelool*)
Juneja, R.K. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 748 (*18-Deoxysagittarol*)
Nagashima, F. *et al., J. Nat. Prod.*, 2001, **64**, 1309-1317 (*Jungermannia infusca constits*)

Clitidine C-306

[63592-84-7]
1,4-Dihydro-4-imino-1-β-D-ribofuranosyl-3-pyridinecarboxylic acid. Chrytidine



$C_{11}H_{14}N_2O_6$ 270.241
Mp 189-191° (monohydrate). $[\alpha]_D^{24}$ -50.6 (c, 1.0 in H_2O). λ_{max} 267 (ε 14500) (H_2O at pH 2) (Derep). λ_{max} 271 (ε 15100) (H_2O at pH 12) (Derep). λ_{max} 271 (ε 12590) (H_2O) (Derep).

▶ Toxic.

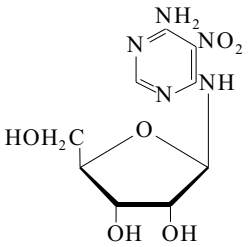
5′-Phosphate: [65411-71-4] ***Clitidine 5′-monophosphate***. *Clitidine 5′-mononucleotide*
$C_{11}H_{15}N_2O_9P$ 350.221
$[\alpha]_D^{18}$ -43.5 (c, 0.4 in H_2O). λ_{max} 268 (log ε 4.31) (H_2O).

3′,5′-Dibenzoyl:
Mp 160-161°.

Konno, K. *et al., Tet. Lett.*, 1977, 481 (*synth, struct, pmr, ms*)
Tono-oka, S. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 212-216 (*synth*)
Konno, K. *et al., Tetrahedron*, 1982, **38**, 3281 (*abs config*)
Yamano, K. *et al., Phytochemistry*, 1994, **35**, 897-899 (*5′-phosphate*)
Shirahama, H. *et al., Heterocycles*, 1998, **47**, 661-664 (*tautom, cryst struct*)

Clitocine C-307

[105798-74-1]
N-(6-Amino-5-nitro-4-pyrimidinyl)-β-D-ribofuranosylamine, 9CI. 6-Amino-5-nitro-4-imino-β-D-ribofuranosylpyrimidine

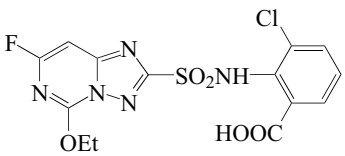


$C_9H_{13}N_5O_6$ 287.232
Nucleoside isol. from the mushroom *Clitocybe inversa* (edibility unknown). Sol. MeOH, EtOAc; poorly sol. cyclohexane. Mp 228-230°. λ_{max} 255 (ε 7950); 330 (ε 2190) (EtOH) (Derep). λ_{max} 255 (ε 7450); 330 (ε 2190) (EtOH) (Berdy).

Kubo, I. *et al., Tet. Lett.*, 1986, **27**, 4277 (*isol, uv, ir, pmr, cmr, ms*)
Larson, S.B. *et al., Acta Cryst. C*, 1988, **44**, 1076 (*cryst struct*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711 (*rev*)
Kamikawa, T. *et al., Chem. Comm.*, 1988, 195 (*synth*)
Palmer, C.F. *et al., Tet. Lett.*, 1990, **31**, 279 (*synth*)

Cloransulam C-308

[159518-97-5]
3-Chloro-2-[[(5-ethoxy-7-fluoro[1,2,4]-triazolo[1,5-c]pyrimidin-2-yl)sulfonyl]amino]benzoic acid, 9CI



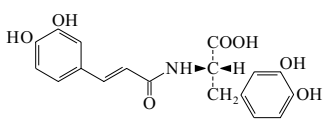
$C_{14}H_{11}ClFN_5O_5S$ 415.789

Me ester: [147150-35-4] ***Cloransulam-methyl, BSI***. *XDE 565*
$C_{15}H_{13}ClFN_5O_5S$ 429.815
Pre- and post-emergence broad-leaved herbicide for use in soya beans.

U.S. Pat., 1992, 5 163 995, (*Dow Elanco*); *CA*, **118**, 213106f (*synth, activity*)
Wolt, J.D. *et al., J. Agric. Food Chem.*, 1996, **44**, 324-332 (*metab*)
Pesticide Manual, 11th edn., 1997, 155

Clovamide C-309

N-*[3-(3,4-Dihydroxyphenyl)-1-oxo-2-propenyl]-3-hydroxytyrosine, 9CI*. N-*(3,4-Dihydroxycinnamoyl)DOPA*. N-*Caffeoyl DOPA*



(S,E)-form

$C_{18}H_{17}NO_7$ 359.335

(*S,E*)-*form* [53755-02-5]
Isol. from cocoa liquor (*Theobroma cacao*) and red clover (*Trifolium pratense*). Natural antioxidant. Amorph. powder or oil. Mp 125-130°. $[\alpha]_D^{18}$ -30.9 (c, 0.5 in H_2O).

Tetra-Me ether, Me ester: [64803-83-4] Mp 152-153°. $[\alpha]_D^{22}$ +137 (c, 1 in $CHCl_3$).

(*S,Z*)-*form* [53755-03-6]
Isol. from *Trifolium pratense* (red clover). Oil. $[\alpha]_D^{19}$ +28.7 (c, 0.57 in H_2O).

Tetra-Me ether, Me ester: [64803-85-6] Syrup. $[\alpha]_D^{16}$ +83 (c, 1 in $CHCl_3$).

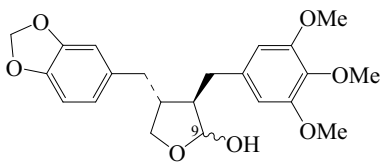
[120094-83-9]

Yoshihara, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 1107; 1977, **41**, 1679 (*isol*)
Van Heerden, F.R. *et al., Phytochemistry*, 1980, **19**, 2125 (*isol, cmr, synth*)
Robiot, G. *et al., J. Nat. Prod.*, 1988, **51**, 596 (*synth*)
Sanbongi, C. *et al., J. Agric. Food Chem.*, 1998, **46**, 454-457 (*S,E-form, isol cacao, hplc, pmr, cmr*)

Clusin C-310

[86992-94-1]

[72627-54-4]
4-(1,3-Benzodioxol-5-ylmethyl)tetrahydro-3-[(3,4,5-trimethoxyphenyl)methyl]-2-furanol, 9CI. 9-Hydroxy-3,4,5-trimethoxy-3′,4′-methylenedioxy-9,9′-epoxylignan



$C_{22}H_{26}O_7$ 402.443
Constit. of *Piper cubeba* (cubeb pepper). Gum. $[\alpha]_D$ -34.4 (c, 1.0 in $CHCl_3$).

Me ether: **O-*Methyl-α-clusin***
$C_{23}H_{28}O_7$ 416.47
Oil. $[\alpha]_D^{23}$ -19.3 (c, 0.1 in $CHCl_3$).

Et ether: [93395-17-6] *9-Ethoxy-3,4,5-trimethoxy-3′,4′-methylenedioxy-9,9′-epoxylignan*
$C_{24}H_{30}O_7$ 430.497
Gummy solid. $[\alpha]_D^{36}$ -31.6 (MeOH).

9-Epimer, Me ether: **O-*Methyl-β-clusin***
$C_{23}H_{28}O_7$ 416.47
Oil. $[\alpha]_D^{23}$ -3.5 (c, 0.2 in $CHCl_3$).

Koul, S.K. *et al., Phytochemistry*, 1983, **22**, 999-1000; 1984, **23**, 2099-2101

Cobalt(*II*) chloride ($CoCl_2$), 8CI C-311

[7646-79-9]
Cobalt chloride†. *Cobalt dichloride. Cobaltous chloride. Cobatope-57. Cobatope-60*

$CoCl_2$

Cl_2Co 129.839

Has $CdCl_2$ struct.. Formerly approved as a food additive but now prohibited. Pale blue hygroscopic cryst. Sol. H_2O, polar org. solvs. Mp 735°. Bp 1049°. Turns pink on exp. to moist air. Paramagnetic (also hydrates).

▶ Human systemic effects by ingestion include anorexia, gastrointestinal disturbances, cardiomyopathy, thyroid enlargement and weight loss. LD_{50} (rat, orl) 80 mg/kg. Exp. cardiotoxic. Exp. reprod. and teratogenic effects. MEL:

long-term 0.1 mg m^{-3} (as Co). GF9800000

Dihydrate: [16544-92-6]
Violet-pink solid. Octahedral polymeric struct. with bridging Cl.

Hexahydrate: [7791-13-1] *Hexaaquacobalt(2+) chloride. Cobalt(*II*) chloride hexahydrate*
$Cl_2CoH_{12}O_6$ 237.93
Red monoclinic cryst. Sol. H_2O, Me_2CO. Mp 86°. Best considered as chloride salt of Hexaaquacobalt(*II*)(2+).

▶ LD_{50} (rat, orl) 766 mg/kg. Exp. reprod. and teratogenic effects. GG0200000

Compd. with graphite: [12672-50-3]
Intercalation compd.; contains an excess of Cl in the stoichiometry.

[1332-82-7, 14543-09-0, 29377-09-1, 66828-02-2, 115526-21-1]

Sidgwick, N.V. *et al., The Chemical Elements and their Compds.*, Oxford, 1950, 1379
Osthoff, W. *et al., J.A.C.S.*, 1954, **76**, 4732 (*synth*)
Remy, H. *et al., Treatise Inorg. Chem.*, Elsevier, 1956, **2**, 297
Young, R.S. *et al., Cobalt - Its Chemistry, Metallurgy and Uses*, (Ed.), ACS Monograph Ser. No. 149, Reinhold N.Y., 1960, 76
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **3**, 1660 (*synth*)
Underwood, E.J. *et al., Nutr. Rev.*, 1975, **33**, 65
Wells, A.F. *et al., Structural Inorg. Chem.*, 5th Ed., Oxford, 1984, 413; 675; 682 (*struct*)
Elinder, C.-G. *et al., Handb. Toxicol. Met.*, (Eds. Friberg, L. *et al*), 2nd edn., Elsevier, 1986, **2**, 211 (*tox, rev*)
Speck, J.S. *et al., Synth. Met.*, 1989, **34**, 211-216 (*rev, compd with graphite, struct*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1291-1293 (*use*)
Touzain, P. *et al., Synth. Met.*, 1996, **79**, 241-251 (*compd with graphite, synth*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1565
Beliles, R.P. *et al., Patty's Ind. Hyg. Toxicol.*, 4th edn., Vol. 2, Wiley, 1993, **2C**, 1973 (*tox, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, CNB599; CNB800

Cobalt(*II*) sulfate ($CoSO_4$), 8CI C-312

[10124-43-3]

[10393-49-4]
Cobalt sulfate†. *Cobaltous sulfate*

$CoSO_4$
CoO_4S 154.997
Once used in fermented malt beverages as a foam stabiliser; now prohibited from use in food. Dark bluish solid. Sol. H_2O. Anhydrous compd. dec. at 735°.

▶ GG3100000

Monohydrate:
Red cryst. Sol. H_2O.

Hexahydrate: [16591-12-1] *Hexaaquacobalt(2+) sulfate. Cobalt(*II*) sulfate hexahydrate*
$CoH_{12}O_{10}S$ 263.088
Orange-pink cryst. Sol. H_2O. Hygroscopic; contains $[Co(OH_2)_6]^{2\oplus}$ cations. Dec. at 95° (-$2H_2O$).

Heptahydrate: [10026-24-1] *Cobalt vitriol.* ***Bieberite***
Red cryst. Sol. H_2O, MeOH, EtOH. Mp 96.8°. Formulated as $[Co(OH_2)]_6SO_4$.-H_2O.

▶ GG3200000

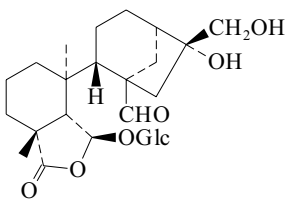
Double salt with ammonium sulfate, hexahydrate: [13586-38-4]
Red cryst. Sol. H_2O.

[15136-97-7, 60459-08-7]

Remy, H. *et al., Treatise Inorg. Chem.*, Elsevier, 1956, **2**, 300 (*synth, props*)
Nobukazu, O. *et al., Nippon Kagaku Zasshi*, 1966, **87**, 363 (*pe*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **6**, 503
Merck Index, 11th edn., 1989, No. 2443
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 646
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNE125

Coccinin C-313

[132242-50-3]



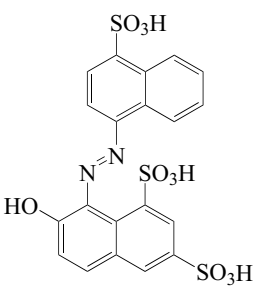
$C_{26}H_{40}O_{11}$ 528.595
Constit. of *Phaseolus coccineus* (scarlet runner bean). Plates (butanol aq.). Mp 190-193°. $[\alpha]_D$ +19.9 (MeOH).

Yamashita, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2905 (*isol, pmr, cmr, cryst struct*)

Cochineal Red A C-314

[7244-14-6]

[2611-82-7]
7-Hydroxy-8-[(4-sulfo-1-naphthalenyl)azo]-1,3-naphthalenedisulfonic acid, 9CI. Acid Scarlet 3R. Brilliant Ponceau 3R. Brilliant Scarlet 3R. Coccine. New coccine. Food Red No. 102. Naphthalene Scarlet 4R. Neucoccin. Ponceau 4R. Strawberry Red. C.I. Acid Red 18. C.I. Food Red 7. C.I. 16255. E124

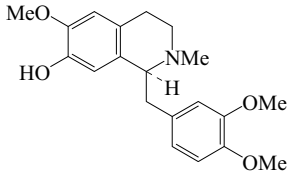


$C_{20}H_{14}N_2O_{10}S_3$ 538.536
Strictly the trade names apply to the tri-Na salt. Synthetic food colouring. Bright red powder (as tri-Na salt).

Colour Index, 3rd edn., 1971, **4**, 4074 (*synth*)

Pearson, D. *et al., J. Assoc. Public Anal.*, 1973, **11**, 135-138 (*chromatog*)
Meyer, O. *et al., Toxicology*, 1975, **5**, 201-207 (*tox*)
Gelbcke, M. *et al., Anal. Lett.*, 1980, **13**, 975-984 (*cmr*)
Fogg, A.G. *et al., Analyst (London)*, 1981, **106**, 883-889; 1986, **111**, 831-835 (*anal*)
Yamada, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 494-499 (*hplc, pmr, cmr*)

Codamine C-315



(*S*)-*form*

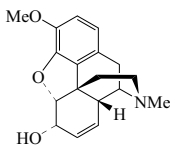
$C_{20}H_{25}NO_4$ 343.422

(*S*)-*form* [21040-59-5]
Minor constit. of opium. Cryst. (petrol). Mp 126-127°. $[\alpha]_D^{15}$ +66.1 (c, 1 in EtOH).

Brockmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1965, **54**, 1531 (*isol*)
Cassels, B.K. *et al., Tetrahedron*, Suppl. 8, 1966, 485-490 (*synth, resoln*)
Benn, M.H. *et al., Phytochemistry*, 1972, **11**, 461-464 (*isol*)
Hoshino, O. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1302-1306 (*pmr*)

Codeine, BAN, USAN C-316

[76-57-3]
7,8-Didehydro-4,5-epoxy-3-methoxy-17-methylmorphinan-6-ol, 9CI. Methylmorphine. Codicept. Kodein. Tussipan



Absolute Configuration

$C_{18}H_{21}NO_3$ 299.369
Opium alkaloid (*Papaver somniferum*) (content ca. 1%). Prisms (Et_2O or C_6H_6), octahedra or rhombic prisms + H_2O (H_2O). Sol. EtOH, $CHCl_3$, Me_2CO; spar. sol. CCl_4, H_2O. Mp 155°. $[\alpha]_D$ -137.8 (EtOH). Log P 0.82 (uncertain value) (calc). Also used as complex with sulfonated styrene-divinylbenzene copolymer (Codeine polistirex, USAN).

▶ Human and exp. reprod. effects. Exp. teratogen. LD_{50} (rat, orl) 427 mg/kg. QD0893000

Hydrochloride: [1422-07-7]
Prisms + $2H_2O$ (H_2O). Mp 287° (as dihydrate). $[\alpha]_D^{22.5}$ -108.2 (H_2O).

▶ LD_{50} (rat, orl) 750 mg/kg. QD1050000

Sulfate salt: [6854-40-6]

[1420-53-7] ***Codeine sulfate, USAN***
Needles + $3H_2O$. Component of Copavin.

Phosphate salt: [41444-62-6]

[52-28-8] ***Codeine phosphate, BAN, JAN, USAN.*** *Brochodine. Codeinfos. Codeisan. Codeophen. Codlin. Duraspan. Paveral. Sedantole. Solcodein. Vixaton*

$C_{18}H_{21}NO_6P$ 378.341
Needles + $\frac{1}{2}H_2O$. Component of Proval and Migraleve.

Compd. with calcium bis(2-acetylsalicylate): [81648-77-3] *Paxidine*

N-*Oxide:* [3688-65-1] ***Codeine* N-*oxide***. *Codeigene. Codeine aminoxyde. Genocodein*
$C_{18}H_{21}NO_4$ 315.368
Alkaloid from *Papaver somniferum* (opium poppy). Platelets (H_2O). Mp 231-232°.

▶ QD1260000

N-*Oxide; hydrochloride:*
Cryst. Mp 219-220°. $[\alpha]_D^{20}$ -105.8 (c, 2 in H_2O).

6-O-*β*-*D*-*Glucuronopyranoside:* [20736-11-2]
$C_{24}H_{29}NO_9$ 475.494
Mp 274-275° dec. (hemihydrate). $[\alpha]_D^{20}$ -224 (c, 1 in H_2O).

Ac: [6703-27-1]
Prisms (Et_2O). Mp 133.5°.

▶ LD_{50} (mus, scu) 99 mg/kg. QD0960000

3-Pyridinecarboxylate: See Nicocodine in *The Combined Chemical Dictionary.*

6-Ketone: [467-13-0] *7,8-Didehydro-4,5-epoxy-3-methoxy-17-methylmorphinan-6-one.* ***Codeinone***
$C_{18}H_{19}NO_3$ 297.353
Prisms (EtOAc). Mp 181.5-182.5°. $[\alpha]_D^{20}$ -205 (EtOH). Subl. under reduced pressure.

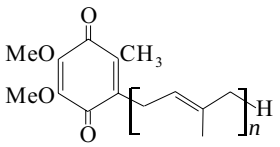
▶ LD_{50} (mus, scu) 11 mg/kg. QD2169000

[5913-76-8, 6059-47-8]

Findlay, S.P. *et al., J.A.C.S.*, 1950, **72**, 3247 (*Codinone, synth*)
Bentley, K.W. *et al., Chemistry of the Morphine Alkaloids*, Oxford Univ. Press, 1954, 57-97 (*isol, props, uv, synth*)
Kartha, G. *et al., Acta Cryst.*, 1962, **15**, 326-333 (*cryst struct, abs config*)
Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1964, **53**, 1549-1550 (*glc, chromatog*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1965, **18**, 1799-1806 (*pmr*)
Wheeler, D.M.S. *et al., J.A.C.S.*, 1967, **89**, 4494-4501 (*ms*)
DeAngelis, G.G. *et al., Tetrahedron*, 1969, **25**, 5099-5112 (*ord*)
Parker, H.I. *et al., J.A.C.S.*, 1972, **94**, 1276-1282 (*biosynth*)
Weller, D.D. *et al., J. Med. Chem.*, 1976, **19**, 1171-1175 (*synth*)
Carroll, F.I. *et al., J.O.C.*, 1976, **41**, 996-1001 (*cmr*)
Phillipson, J.D. *et al., Phytochemistry*, 1976, **15**, 1297-1301 (*oxide*)
Muhtadi, F.J. *et al., Anal. Profiles Drug Subst.*, 1981, **10**, 93 (*rev, phosphate*)
Whittle, B.J.R. *et al., Gut*, 1981, **22**, 798 (*Paxidine*)
Moos, W.H. *et al., J.O.C.*, 1983, **48**, 227-238 (*synth*)
White, J.D. *et al., Tetrahedron*, 1983, **39**, 2393-2397 (*synth, ir, pmr*)
Quiding, H. *et al., Eur. J. Clin. Pharmacol.*, 1986, **30**, 673 (*metab*)
Canfield, D.V. *et al., Acta Cryst. C*, 1987, **43**, 977-979 (*cryst struct*)
Ishida, T. *et al., Drug Metab. Dispos.*, 1991, **19**, 895 (*Codeinone, metab*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1069
Nair, M.M. *et al., Spectrosc. Lett.*, 1997, **30**, 497-505 (*pmr, cmr*)
White, J.D. *et al., J.O.C.*, 1999, **64**, 7871-7884 (*synth*)
Rukhman, I. *et al., Tetrahedron*, 2001, **57**, 1083-1092 (*6-glucuronoside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNF500; CNG500; CNG675; CNF750; CNG750

Coenzyme Q C-317

Mitoquinone. Ubiquinone



A group of related substances having n = 1-12; the main naturally occurring homologues have n = 6-10. Subscript number (≡Ubiquinone no.) indicates n. For lowest homologue, see 2,3-Dihydroxy-5-methyl-1,4-benzoquinone. In redox bioequilibrium with the reduced forms (hydroquinones), the CAS nos. for some of which are given in this entry.

Coenzyme Q_4 [4370-62-1]
Ubiquinone 4
$C_{29}H_{42}O_4$ 454.648
Isol. from various yeasts. Red oil.

Coenzyme Q_6 [1065-31-2]
Ubiquinone 6. Ubiquinone 30
$C_{39}H_{58}O_4$ 590.885
Isol. from bakers' yeast (*Saccharomyces cerevisiae*). Orange-yellow cryst. (EtOH) or red oil. Mp 19-20° (16°).

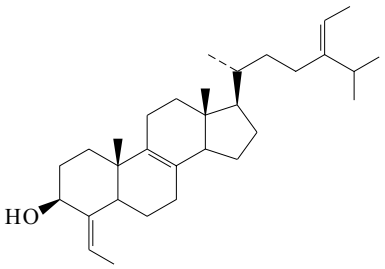
Coenzyme Q_{10} [303-98-0]
Ubiquinone 10. Ubiquinone 50. Ubidecarenone, BAN, INN. NSC 140865. Many other names
$C_{59}H_{90}O_4$ 863.358
Isol. from beef heart. Orange cryst. (MeOH or EtOH) at low temp. Mp 49.9°. Log P 20.24 (uncertain value) (calc).

▶ Exp. reprod. and teratogenic effects. DK3900000

[606-06-4, 727-81-1, 1173-76-8, 4370-62-1, 24663-35-2, 24663-36-3, 75763-46-1]

Gale, P.H. *et al., Biochem. Biophys. Res. Commun.*, 1963, **12**, 414 (*Coenzyme Q_{10} (H-10)*)
Gale, P.H. *et al., Biochemistry*, 1963, **2**, 196 (*Coenzyme Q_{10} (H-10)*)
Mahler, H.R. *et al., Biochemistry*, 1964, **3**, 893-895 (*Coenzyme Q_6, isol*)
Lavate, W.V. *et al., J. Biol. Chem.*, 1965, **240**, 524 (*Coenzyme Q_{10} (H-10)*)
Greenberg, S.M. *et al., Med. Clin. North Am.*, 1988, **72**, 243 (*rev, pharmacol*)
Tran, M.T. *et al., Pharmacotherapy (Carlisle, Mass.)*, 2001, **21**, 797-806 (*Coenzyme Q_{10}, rev*)
Ferrante, R.J. *et al., J. Neurosci.*, 2002, **22**, 1592-1599 (*Coenzyme Q_{10}, pharmacol*)
Lipshutz, B.H. *et al., J.A.C.S.*, 2002, **124**, 14282-14283 (*Coenzyme Q_{10}, synth*)

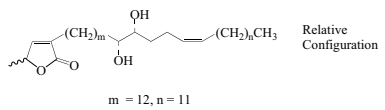
Coffeasterene C-318



$C_{31}H_{50}O$ 438.735
Dubious struct., no more recent work reported. Isol. from coffee bean oil. Mp 164°. $[\alpha]_D$ +4.
Kaufmann, H.P. *et al., Fette, Seifen, Anstrichm.*, 1964, **66**, 461; *CA*, **61**, 14722h

Cohibin A C-319

[189508-31-4]



$C_{35}H_{64}O_4$ 548.888
Constit. of the roots of *Annona muricata* (soursop). Powder. Mp 60-62°. $[\alpha]_D$ +12 (c, 0.1 in MeOH). Obt. as a mixture with Cohibin B to which the data refers λ_{max} 212 (log ϵ 2.82) (MeOH).
Gleye, C. *et al., Phytochemistry*, 1997, **44**, 1541 (*isol, uv, pmr, cmr, ms*)

Cohibin B C-320

[189508-32-5]
As Cohibin A, C-319 with
m = 10, n = 13
$C_{35}H_{64}O_4$ 548.888
Constit. of *Annona muricata* (soursop). Obt. as a mixture with Cohibin A.
Gleye, C. *et al., Phytochemistry*, 1987, **44**, 1541 (*isol, uv, pmr, cmr, ms*)

Cohibin C C-321

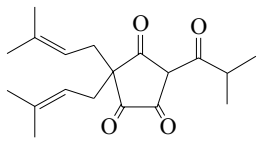
As Cohibin A, C-319 with
m = 14, n = 11
$C_{37}H_{68}O_4$ 576.942
Obt. as a mixt. with Cohibin D, C-322 to which data refers. Constit. of *Annona muricata* (soursop). Waxy solid. λ_{max} 214 (log ϵ 3.62) (MeOH).
Gleye, C. *et al., J. Nat. Prod.*, 2000, **63**, 1192-1196

Cohibin D C-322

As Cohibin A, C-319 with
m = 11, n = 14
$C_{37}H_{68}O_4$ 576.942
Obt. as a mixt. with Cohibin C, C-321. Constit. of *Annona muricata* (soursop).
Gleye, C. *et al., J. Nat. Prod.*, 2000, **63**, 1192-1196

Cohulupone C-323

[1891-34-5]
3,3-Bis(3-methyl-2-butenyl)-5-(2-methyl-1-oxopropyl)-1,2,4-cyclopentanetrione, 9CI



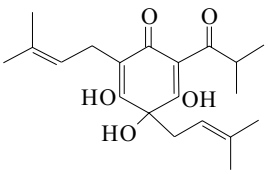
$C_{19}H_{26}O_4$ 318.412
Constit. of hops. Oil. $Bp_{0.0001}$ 100°.

2,3-Diaminonaphthalene deriv.:
Orange cryst. (MeOH). Mp 135°.

Wright, D. *et al., J.C.S.*, 1963, 1769 (*synth*)
Forsén, S. *et al., Acta Chem. Scand.*, 1964, **18**, 513 (*ir, pmr, tautom*)
Borremans, F. *et al., Org. Magn. Reson.*, 1975, **7**, 415 (*cmr*)

Cohumulone C-324

[511-25-1]
3,4,5-Trihydroxy-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-2,5-cyclohexadien-1-one, 9CI



$C_{20}H_{28}O_5$ 348.438
Constit. of hops. Yellow wax. Sol. MeOH, Et_2O; fairly sol. H_2O. $[\alpha]_D^{27}$ -208.5. λ_{max} 230 ; 283 ; 312 ; 335 (MeOH) (Berdy).

Howard, G.A. *et al., Chem. Ind. (London)*, 1954, 514 (*synth*)
Howard, G.A. *et al., J.C.S.*, 1954, 2400 (*struct*)
Borremans, F. *et al., Org. Magn. Reson.*, 1975, **7**, 415 (*cmr*)
Drawert, F. *et al., Phytochemistry*, 1976, **15**, 1695 (*biosynth*)
Zuurbier, K.W.M. *et al., Phytochemistry*, 1995, **38**, 77 (*biosynth*)

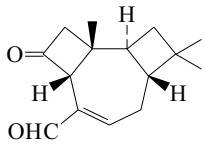
Colicin E3 C-325

[11032-90-9]
Composed of 2 proteins, A and B. Protein A is a special kind of RNase and is made up of 551 amino acid residues; it is protected by an immunity protein (protein B) which contains 84 amino acid residues. Prod. by *Escherichia coli*. Bacteriocin; kills sensitive *E. coli* cells.

Jakes, K.J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1974, **71**, 3380-3384 (*isol*)
Hirose, A. *et al., J. Biochem. (Tokyo)*, 1976, **79**, 305-311 (*isol*)
Mochitate, K. *et al., J. Biochem. (Tokyo)*, 1981, **89**, 1609-1618 (*Protein B, struct*)
Masaki, H. *et al., J. Mol. Biol.*, 1985, **182**, 217-227 (*struct*)
Frolow, F. *et al., J. Biol. Chem.*, 1990, **265**, 10196-10197 (*cryst struct*)

Collybial C-326

[164300-75-8]
2,10,10-Trimethyl-4-oxotricyclo[7.2.0.0^{2,5}]undec-6-ene-6-carboxaldehyde, 9CI



$C_{15}H_{20}O_2$ 232.322
Constit. of *Collybia confluens* (clustered tough shank). Needles. Sol. MeOH, Me_2CO, Et_2O; poorly sol. H_2O. Mp 121°. λ_{max} 236 (ε 8571) (MeOH) (Berdy).

Simon, B. *et al., Z. Naturforsch., C*, 1995, **50**, 173 (*isol, pmr, cmr*)

Colneleic acid C-327

9-(1,3-Nonadienyloxy)-8-nonenoic acid, 9CI
$H_3C(CH_2)_4CH{=}CHCH{=}CH\text{-}O\text{-}CH{=}CH(CH_2)_6COOH$
$C_{18}H_{30}O_3$ 294.433
(2′E,4′Z,8E)-form [52761-34-9]
Product of the enzymic oxidation of potato lipids. Isol. as the Me ester by glc.

[52077-21-1]

Galliard, T. *et al., Biochem. J.*, 1972, **129**, 743 (*isol*)
Curtis, R.R. *et al., Chem. Phys. Lipids*, 1973, **11**, 11 (*synth*)
Galliard, T. *et al., Chem. Phys. Lipids*, 1973, **11**, 173 (*isol*)
Crombie, L. *et al., Chem. Comm.*, 1987, 502; 503 (*biochem*)
Corey, E.J. *et al., J.O.C.*, 1990, **55**, 1670 (*synth*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1991, 567 (*synth, pmr, cmr, ms*)

Colnelenic acid C-328

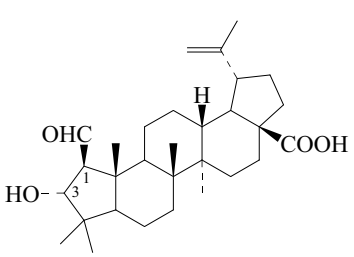
9-(1,3,6-Nonatrienyloxy)-8-nonenoic acid, 9CI
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH{=}CH\text{-}O\text{-}CH{=}CH(CH_2)_6COOH$
$C_{18}H_{28}O_3$ 292.417
(2′E,4′Z,7′Z,8E)-form [52591-16-9]
Product of enzymic oxidation of potato lipids. Isol. as the Me ester by glc.

[52077-22-2]

Galliard, T. *et al., Chem. Phys. Lipids*, 1973, **11**, 173 (*isol, pmr, uv, ir, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1991, 567 (*synth, pmr, cmr, ms*)

Colubrinic acid C-329

[67594-73-4]
Zizyberanalic acid



$C_{30}H_{46}O_4$ 470.691
Constit. of *Zizyphus jujuba* (Chinese date). Cryst. (EtOAc). Mp 282-284° (263-265°). $[\alpha]_D^{20}$ +3 (c, 1.15 in Py).

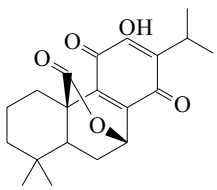
Me ester: [67594-78-9]
$C_{31}H_{48}O_4$ 484.718
Cubic cryst. (petrol/Et_2O). Mp 173-180° (dec.). $[\alpha]_D^{25}$ -39 (c, 0.2 in $CHCl_3$).

3-Deoxy, 1,3-didehydro: [125456-52-2] ***Zizyberenalic acid***
$C_{30}H_{44}O_3$ 452.676
Cryst. Mp 214-216°. $[\alpha]_D^{18}$ +24 (c, 0.5 in MeOH). λ_{max} 239 (log ε 3.48); 266 (sh) (log ε 3.22) (no solvent reported).

Roitman, J.N. *et al., Phytochemistry*, 1978, **17**, 491 (*isol, ir, ms, pmr*)
Baxter, R. *et al., Phytochemistry*, 1988, **27**, 2350 (*isol, cryst struct*)
Kundu, A.B. *et al., Phytochemistry*, 1989, **28**, 3155 (*isol, pmr, cmr, ms*)
Lee, S.-S. *et al., Phytochemistry*, 1997, **46**, 549-554 (*Zizyberenalic acid*)

Columbaridione C-330

[156162-09-3]

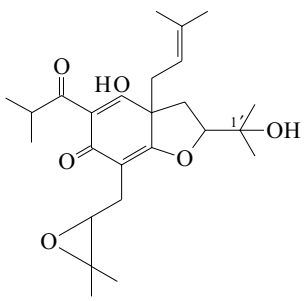


$C_{20}H_{24}O_5$ 344.407
Constit. of *Salvia columbariae* (California chia). Orange oil.

Luis, J.G. *et al., Phytochemistry*, 1994, **36**, 251 (*isol, pmr, cmr*)

Colupdox a C-331

[35923-67-2]



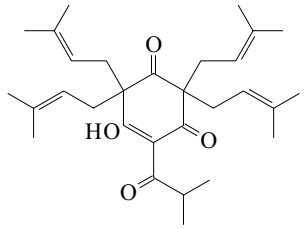
$C_{25}H_{36}O_6$ 432.556
Enolised β-diketone. Isol. from hops.

1′-Deoxy: [36136-11-5] ***Colupox b***
$C_{25}H_{36}O_5$ 416.556
Isol. from hops.

Kokubo, E. *et al., Proc. Am. Soc. Brew. Chem.*, 1971, 265 (*isol*)
Kokubo, E. *et al., CA*, 1973, **78**, 159926 (*struct*)

Colupone C-332

[16658-23-4]
5-Hydroxy-2,2,6,6-tetrakis(3-methyl-2-butenyl)-4-(2-methyl-1-oxopropyl)-4-cyclohexene-1,3-dione, 9CI



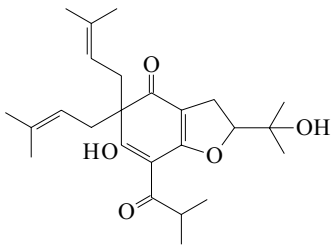
$C_{30}H_{44}O_4$ 468.675

Congener of Lupulone, L-123. Found in hops.

Elvidge, J.A. *et al., J.C.S.(C)*, 1969, 1839 (*pmr, uv, ir*)

Colupox a C-333

[18944-21-3]



$C_{25}H_{36}O_5$ 416.556

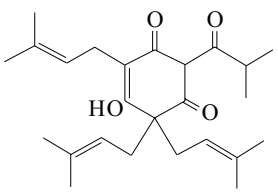
Isol. from hops. V. pale yellow oil. Racemic.

[22592-22-9]

Cahill, D.M. *et al., J.C.S.(C)*, 1969, 938 (*synth*)
Kokubo, E. *et al., Proc. Am. Soc. Brew. Chem.*, 1971, 265 (*isol*)
Kokubo, E. *et al., CA*, 1973, **78**, 159926 (*struct*)

Colupulone C-334

[468-27-9]



$C_{25}H_{36}O_4$ 400.557

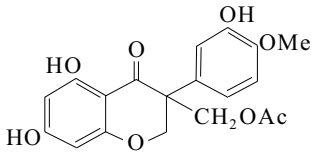
Constit. of the resin of English hops. Cryst. (MeOH). Sol. MeOH, Et_2O; fairly sol. H_2O. Mp 92-93°. λ_{max} 228 ; 280 ; 338 (MeOH) (Berdy).

Collins, M. *et al., J.C.S.(C)*, 1971, 3814 (*struct*)
Borremans, F. *et al., Org. Magn. Reson.*, 1975, **7**, 415 (*cmr*)

Comosin C-335

[99877-69-7]

3-[(Acetyloxy)methyl]-2,3-dihydro-5,7-dihydroxy-3-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI



$C_{19}H_{18}O_8$ 374.346

Constit. of *Muscari comosum* (tassel hyacinth). Vitreous solid.

Adinolfi, M. *et al., Phytochemistry*, 1985, **24**, 2423
Adinolfi, M. *et al., Magn. Reson. Chem.*, 1986, **24**, 663 (*pmr, cmr*)

Concanavalin A C-336

[11028-71-0]

Con A

[CaMn]

A phytagglutinin or lectin. Isol. from jackbeans, *Canavalia ensiformis*. Each subunit of Con A contains one $Ca^{2\oplus}$ and one $Mn^{2\oplus}$ ion. MW = 27000. Contains 283 amino acid residues.

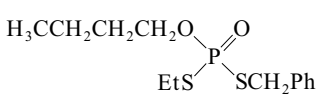
► LD_{50} (mus, ivn) 50 mg/kg. Exp. reprod. and teratogenic effects. GK6890000

Goldstein, I.J. *et al., Methods Carbohydr. Chem.*, 1972, **6**, 106 (*isol, use*)
Bittiger, H. *et al., Concanavalin A Tool. 1976*, Wiley, Chichester, U.K., 1976, (*book*)
Hardman, K.D. *et al., Immunochem. Proteins*, 1977, **2**, 373 (*rev*)
Shoham, M. *et al., FEBS Lett.*, 1978, **95**, 54 (*struct*)
Liener, I.E. *et al., The Lectins: Properties, Functions, and Applications in Biology and Medicine*, Academic Press, 1986, (*book*)
Parker, C.W. *et al., Methods Enzymol.*, 1987, **150**, 29 (*rev, props*)
Arrondo, J.L.R. *et al., Biochim. Biophys. Acta*, 1988, **952**, 261 (*ir*)
Hansen, J.E.S. *et al., AIDS*, 1989, **3**, 635 (*anti-HIV activity*)
Adv. Lectin Res., (Ed. Franz, H.), Springer-Verlag, Berlin, Vol 2, 1989, (*book*)
Sharon, N. *et al., Lectins*, Routledge, Chapman and Hall, N.Y., 1989, (*book*)
Lin, S.L. *et al., Biochemistry*, 1990, **29**, 3599 (*cryst struct*)
Kalnin, N.N. *et al., Biopolymers*, 1990, **30**, 1273 (*struct, ir*)
Kalghatgi, K. *et al., J. Chromatogr.*, 1990, **499**, 267 (*hplc*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNH625

Conen C-337

[27949-52-6]

O-*Butyl* S-*ethyl*-S-*(phenylmethyl) phosphorodithioate, 9CI*. S-*Benzyl* O-*butyl* S-*ethyl phosphorodithioate, 8CI*. S-*Benzyl* O-*butyl* S-*ethyl dithiophosphate*



$C_{13}H_{21}O_2PS_2$ 304.413

► LD_{50} (rat, orl) 870 mg/kg. TD5100000

(±)-*form*

Fungicide, used against rice blast. Oil. n_D^{20} 1.5392. Prob. of no coml. significance.

Fr. Pat., 1969, 1 560 374; *CA*, **72**, 90043 (*synth*)
Kawamura, Y. *et al., CA*, 1971, **91**, 191459 (*glc*)
Reddy, P.P. *et al., Sci. Cult.*, 1972, **38**, 144 (*activity*)
Mikami, A. *et al., CA*, 1975, **82**, 81279 (*anal*)

Conglutinin C-338

[170834-56-7]

Protein containing 351 amino acid residues. Isol. from bovine serum. $Ca^{2\oplus}$-dependent lectin.

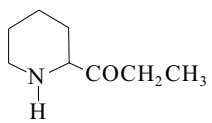
[137366-53-1, 148847-26-1, 154103-32-9]

Kawasaki, N. *et al., J. Biochem. (Tokyo)*, 1985, **98**, 1309-1320 (*isol*)
Strang, C.J. *et al., Biochem. J.*, 1986, **234**, 381-389 (*struct*)
Lee, Y.M. *et al., J. Biol. Chem.*, 1991, **266**, 2715-2723 (*struct*)

Conhydrinone C-339

[97073-23-9]

1-(2-Piperidinyl)-1-propanone, 9CI. 2-Propanoylpiperidine. 1′-Oxoconiine



$C_8H_{15}NO$ 141.213

Maillard product from L-proline and monosaccharides.

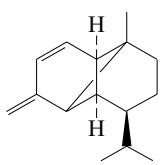
(±)-*form* [38726-76-0]

Hydrochloride: [38726-77-1] Mp 249-250°.

Hydrobromide: [38726-78-2] Mp 228-229°.

Leete, E. *et al., J.A.C.S.*, 1972, **94**, 5472 (*isol, struct, synth*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*occur*)

2,4(15)-Copadiene C-340



$C_{15}H_{22}$ 202.339

(1α,6α,7α*H*)-*form* [27597-38-2]

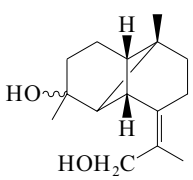
Copadiene

Constit. of the essential oil of *Cyperus rotundus* (nutgrass). Oil. Bp_1 130-140° (bath). $[\alpha]_D$ +17.3 ($CHCl_3$).

Kapadia, V.H. *et al., Tet. Lett.*, 1967, 4661

7(11)-Copaene-4,12-diol C-341

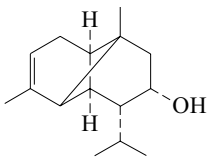
10-Copene-3,12-diol



$C_{15}H_{24}O_2$ 236.353

(3ξ,7(11)*Z*)-*form*
Constit. of *Ocimum americanum* (wild basil). Viscous mass.
Upadhyay, R.K. *et al., Phytochemistry*, 1991, **30**, 691 (*isol, pmr*)

3-Copaen-8-ol C-342
α-Copaen-8-ol

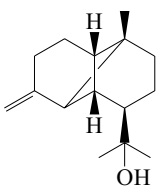


$C_{15}H_{24}O$ 220.354

8α-*form* [58569-25-8]
Isol. from root of *Angelica archangelica* (angelica).
8-Ketone:3-Copaen-8-one. ***α-Copaen-8-one***
$C_{15}H_{22}O$ 218.338
Oil. $[\alpha]_D^{24}$ +14 (c, 0.53 in $CHCl_3$).

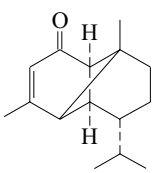
8β-*form*
Oil.
Taskinen, J. *et al., Acta Chem. Scand., Ser. B*, 1975, **29**, 999
Tamayo-Castillo, G. *et al., Phytochemistry*, 1989, **28**, 938
Weyerstahl, P. *et al., Annalen*, 1993, 1117 (*isol, pmr, cmr*)

4(15)-Copaen-11-ol C-343
[133587-94-7]
3(15)-Copen-11-ol



$C_{15}H_{24}O$ 220.354
Constit. of *Ocimum americanum* (wild basil). Viscous mass.
Upadhyay, R.K. *et al., Phytochemistry*, 1991, **30**, 691 (*isol, pmr*)

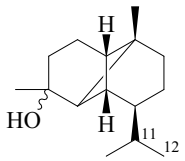
3-Copaen-2-one C-344



$C_{15}H_{22}O$ 218.338

(1α*H*,6α*H*,7β*H*)-*form* [1209-91-2]
Mustakone
Constit. of *Cyperus rotundus* (nutgrass). Oil. Bp_1 128-129°. $[\alpha]_D^{25}$ -42.5 (c, 1.85 in $CHCl_3$).
2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 141-142°.
Kapadia, V.H. *et al., Tetrahedron*, 1965, **21**, 607 (*isol*)
Nyasse, B. *et al., Phytochemistry*, 1988, **27**, 3319 (*isol, pmr*)

4-Copanol C-345
3-Copanol



$C_{15}H_{26}O$ 222.37
Cadinane numbering used.

3ξ-*form*
Constit. of *Ocimum americanum* (wild basil). Cryst. Mp 102°. $[\alpha]_D^{21}$ +0.62 (c, 0.2 in $CHCl_3$).
11,12-Didehydro: ***11-Copaen-4-ol****. 11-Copen-3-ol*
$C_{15}H_{24}O$ 220.354
Constit. of *Ocimum americanum* (wild basil). Viscous mass.
Upadhyay, R.K. *et al., Phytochemistry*, 1991, **30**, 691 (*isol, pmr, cmr*)

Copper(*I*) iodide (CuI) C-346
[7681-65-4]
Copper iodide†*. Cuprous iodide*
CuI
CuI 190.451
Polymorphic. γ-CuI (zinc blende struct.) exists below 420°, β-CuI (wurtzite struct.) between 402 and 440°, and α-CuI (cubic) above 440°. Dietary iodine supplement for use in table salt and animal feed. Air- and light-stable white cryst. V. insol. H_2O. Mp 606°. Bp 1290°.

[24401-69-2]

Krug, J. *et al., Z. Naturforsch., A*, 1952, **7**, 369 (*cryst struct, polymorphs*)
Inorg. Synth., 1960, **6**, 3 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 169 (*use*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 975 (*synth*)
Matsumoto, K. *et al., Talanta*, 1975, **22**, 695 (*ms*)
Burns, G. *et al., Solid State Commun.*, 1977, **24**, 753 (*Raman*)
Becker, K.D. *et al., J. Chem. Phys.*, 1978, **68**, 3785 (*nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 105 (*rev*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1346 (*use*)
Merck Index, 12th edn., 1996, No. 2732
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, COF680

Copper(*II*) sulfate C-347
[7758-98-7]

[10124-44-4, 18939-61-2]
Copper sulfate, BSI†*. Cupric sulfate, USAN*

$CuSO_4$
CuO_4S 159.61
Hygroscopic white rhomb. cryst. or amorph. powder. V. sol. H_2O; sol. MeOH, glycerol; sl. sol. EtOH. Mp 200°. Dec. above 560°; forms CuO at 650°.
▶ Ingestion of large amounts of copper salts (15-75 mg Cu) causes gastrointestinal disturbances. Haemolysis, hepatotoxic and nephrotoxic effects, and death also result from acute exposure. Chronic copper toxicity usually only encountered with inherited metabolic copper disorders (e.g. Wilson's disease). LD_{50} (rat, orl) 300 mg/kg. Exp. reprod. and teratogenic effects. GL8800000

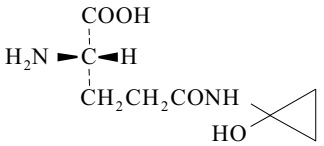
Mineral-*form* [24270-43-7]
Chalcocyanite, 9CI*. Chalcokyonite. Blue Copperas. Chalcanthite*
V. hygroscopic pale green, sky-blue or yellowish-brown orthorhombic cryst. V. sol. H_2O. Pure artificial cryst. are colourless.
Pentahydrate: [7758-99-8] *Hydrocyanite. Pentaaquasulfatocopper(*II*). Bluestone. Blue vitriol. Roman vitriol. Salzburg vitriol*
Used in foods as a nutrient supplement and processing aid. Blue cryst. (H_2O). V. sol. H_2O; sol. MeOH, glycerol; sl. sol. EtOH. Loses $2H_2O$ at 30°, two more at 110°, becomes anhyd. by 250°. Acidic: 0.2*M* aq. soln. has pH 4.0.
▶ GL8900000

[33772-44-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1259D; 1262C (*ir*)
Palache, C. *et al., Dana's System of Mineralogy*, Wiley, 7th edn., 1951, **2**, 429 (*rev*)
Kakohana, H. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1952, **1**, 85 (*anal*)
Geballe, T.H. *et al., J.A.C.S.*, 1952, **74**, 3513 (*magnetism*)
Berg, D. *et al., J.A.C.S.*, 1952, **74**, 4704 (*solns, conductivity*)
Meloche, V.W. *et al., J. Inorg. Nucl. Chem.*, 1958, **6**, 104 (*ir*)
Rama Rao, B. *et al., Acta Cryst.*, 1961, **14**, 321 (*cryst struct*)
Almodovar, I. *et al., Phys. Rev.*, 1965, **138**, 153 (*magnetism*)
Stringer, H.C.W. *et al., Drugs*, 1973, **6**, 413 (*pharmacol*)
Industrial Chemicals, (Eds. Lowenheim, F.A. *et al*), 4th Ed., Wiley Interscience, N.Y., 1975, 280 (*manuf*)
Copper in the Environment, (ed. Nriagu, J.O.), J. Wiley, 1979, (*book*)
Varghese, J.N. *et al., Acta Cryst. B*, 1985, **41**, 184 (*cryst struct*)
Aaseth, J. *et al., Handb. Toxicol. Met.*, (Eds., Friberg, L. *et al*), 2nd edn., Elsevier, 1986, **2**, 233 (*tox, rev*)
Wildner, M. *et al., Mineral. Petrol.*, 1988, **39**, 201 (*cryst struct, synthetic*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1038
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1365 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 668-669
Pesticide Manual, 12th edn., 2000, 171
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNP250; CNP500

Coprine C-348

N^5-*(1-Hydroxycyclopropyl)glutamine, 9CI*



$C_8H_{14}N_2O_4$ 202.21

(*S*)-*form* [58919-61-2]

L-form

Present in the mod. toxic ink cap mushroom *Coprinus atramentarius* (common ink cap). Produces an oversensitivity to ethanol in some people. Mp 197-199°. $[\alpha]_D^{25}$ +7.6 (c, 4.1 in H_2O).

Et ether:

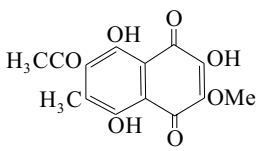
Cryst. (H_2O/MeOH/EtOH). Mp 183-184°. $[\alpha]_D$ +5.2 (c, 7.8 in H_2O).

Hatfield, C.M. *et al., J. Nat. Prod.*, 1975, **35**, 489 (*struct*)
Lindberg, P. *et al., J.C.S. Perkin 1*, 1977, 684 (*isol, synth*)
Kienzler, T. *et al., Helv. Chim. Acta*, 1992, **34**, 1078 (*synth*)

Cordeauxione C-349

[1228-77-9]

2-Acetyl-4,7,8-trihydroxy-6-methoxy-3-methyl-1,5-naphthalenedione, 9CI. 7-Acetyl-2,5,8-trihydroxy-3-methoxy-6-methyl-1,4-naphthoquinone. Cordeauxiaquinone



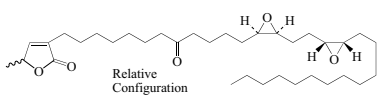
$C_{14}H_{12}O_7$ 292.245

Tautomeric. Isol. from leaf hairs of *Cordeauxia edulis* (yehib). Garnet-red prisms. Mp 194°.

Lister, J.H. *et al., Helv. Chim. Acta*, 1955, **38**, 215 (*isol, uv, ir*)
Fehlmann, M. *et al., Helv. Chim. Acta*, 1965, **48**, 305 (*cryst struct*)
Hanumaiah, T. *et al., Phytochemistry*, 1985, **24**, 1811 (*isol*)

Corepoxylone C-350

[154272-51-2]



$C_{35}H_{60}O_5$ 560.856

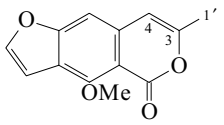
Constit. of *Annona muricata* (soursop). Powder. $[\alpha]_D$ +36.8 (c, 0.08 in $CHCl_3$).

Gromek, D. *et al., Tetrahedron*, 1993, **49**, 5247-5252 (*isol, uv, ir, pmr, cmr, ms*)

Coriandrin C-351

[116408-80-1]

*4-Methoxy-7-methyl-5*H*-furo[2,3-g][2]benzopyran-5-one, 9CI*



$C_{13}H_{10}O_4$ 230.22

Constit. of *Coriandrum sativum* (coriander). Needles (MeOH). Mp 142-143°. λ_{max} 286 ; 298 ; 340 (MeOH) (Berdy).

3,4-Dihydro: [116383-99-4] ***Dihydrocoriandrin***

$C_{13}H_{12}O_4$ 232.235

Constit. of *Coriandrum sativum* (coriander).

1′-Hydroxy: [177795-32-3] *7-Hydroxymethyl-4-methoxy-5*H*-furo[2,3-g][2]benzopyran-5-one.* ***Coriandrone C***

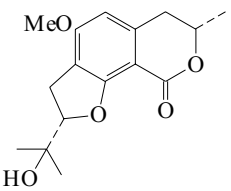
$C_{13}H_{10}O_5$ 246.219

Constit. of *Coriandrum sativum* (coriander). Needles. Mp 142-143°.

Ceska, O. *et al., Phytochemistry*, 1988, **27**, 2083
Kraus, G.A. *et al., J.O.C.*, 1994, **59**, 4735 (*synth, pmr*)
Taniguchi, M. *et al., Phytochemistry*, 1996, **42**, 843 (*Coriandrone C*)
Mal, D. *et al., Tet. Lett.*, 2000, **41**, 3677-3680 (*synth*)

Coriandrone A C-352

[139906-03-9]



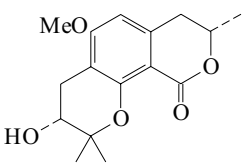
$C_{16}H_{20}O_5$ 292.331

Constit. of *Coriandrum sativum* (coriander). Cryst. Mp 102-103°.

Baba, K. *et al., Phytochemistry*, 1991, **30**, 4143 (*isol, pmr, cmr, cryst struct*)

Coriandrone B C-353

[139906-04-0]



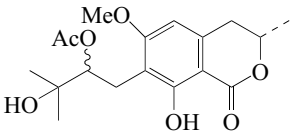
$C_{16}H_{20}O_5$ 292.331

Constit. of *Coriandrum sativum* (coriander). Cryst. Mp 213-214°.

Baba, K. *et al., Phytochemistry*, 1991, **30**, 4143 (*isol, pmr, cmr, cryst struct*)

Coriandrone D C-354

[177795-33-4]



$C_{18}H_{24}O_7$ 352.383

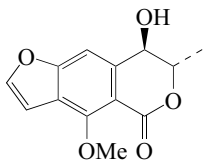
Constit. of *Coriandrum sativum* (coriander) (Umbelliferae). Prisms. Mp 172-173°. λ_{max} 223 (log ϵ 4.34); 273 (log ϵ 4.06); 300 (sh) (log ϵ 3.57) (MeOH).

Taniguchi, M. *et al., Phytochemistry*, 1996, **42**, 843-846 (*isol, uv, ir, cd, pmr, cmr*)

Coriandrone E C-355

[177795-34-5]

*7,8-Dihydro-8-hydroxy-4-methoxy-7-methyl-5*H*-furo[2,3-g][2]benzopyran-5-one*



$C_{13}H_{12}O_5$ 248.235

Constit. of *Coriandrum sativum* (coriander) (Umbelliferae). Needles. Mp 148-150°. λ_{max} 232 (log ϵ 4.59); 259 (sh) (log ϵ 3.84); 306 (log ϵ 3.33) (MeOH).

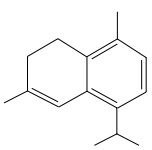
Taniguchi, M. *et al., Phytochemistry*, 1996, **42**, 843-846 (*isol, uv, ir, cd, pmr, cmr*)

α-Corocalene C-356

[20129-39-9]

[38599-17-6]

1,2-Dihydro-3,8-dimethyl-5-(1-methylethyl)naphthalene. 1,2-Dihydro-5-isopropyl-3,8-dimethylnaphthalene

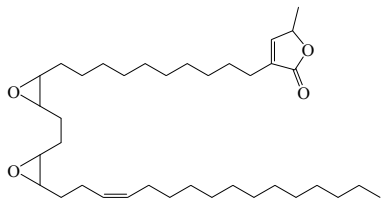


$C_{15}H_{20}$ 200.323

Constit. of the oil of hops (*Humulus lupulus*). Oil.

Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2088
Ngo, K.-S. *et al., J. Chem. Res., Synop.*, 1998, 80-81 (*synth, pmr, cmr*)

Coronin C-357

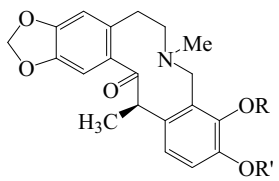


$C_{37}H_{64}O_4$ 572.91
Constit. of the roots of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +12 (c, 0.15 in $CHCl_3$). λ_{max} 210 (log ϵ 3.65) (MeOH).

Gleye, C. *et al., Planta Med.*, 2001, **67**, 570-572

Corycavamine C-358

4,6,7,14-Tetrahydro-5,14-dimethylbis[1,3]benzodioxolo[4,5-c:5′,6′-g]azecin-13(5H)-one, 9CI. Corycavine



(*R*)-form

RR' = —CH_2—

$C_{21}H_{21}NO_5$ 367.401
The name Corycavine was applied to the racemate.

(*R*)-*form* [521-85-7]
Mp 148-149°. $[\alpha]_D^{20}$ +167 ($CHCl_3$).

(*S*)-*form* [144606-40-6]
Needles. Mp 145-146°. $[\alpha]_D^{25}$ -170 (c, 1.3 in $CHCl_3$).

(±)-*form* [521-87-9]
Plates (EtOH). Mp 221-222°.

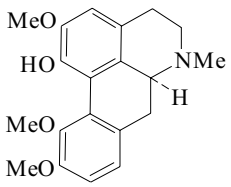
Hydrochloride:
Mp 219°.

Methiodide:
Mp 220°.

Gardmer, J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1902, **240**, 81 (*isol*)
Späth, E. *et al., Ber.*, 1927, **60**, 1892 (*struct*)
Kametani, T. *et al., Phytochemistry*, 1971, **10**, 1881 (*isol*)
Nonaka, G. *et al., Yakugaku Zasshi*, 1973, **93**, 87 (*isol*)
Takao, N. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2859 (*biosynth*)
Iwasa, K. *et al., J.O.C.*, 1981, **46**, 4744 (*abs config*)
Kamigauchi, M. *et al., Helv. Chim. Acta*, 1987, **70**, 1482 (*cryst struct, pmr*)
Kamigauchi, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1992, **325**, 585 (*cd, abs config, resoln*)

Corydine C-359

1-Hydroxy-2,10,11-trimethoxyaporphine. Glaucentrine



(*S*)-form

$C_{20}H_{23}NO_4$ 341.406Log P 2.69 (uncertain value) (calc).

(*S*)-*form* [476-69-7]
Mp 149°. $[\alpha]_D^{25}$ +204 (c, 0.6 in EtOH). Pharmacol. active isomer.

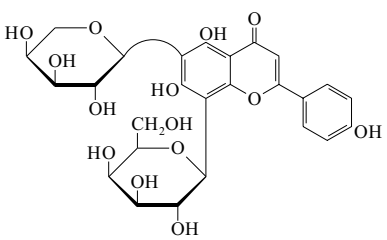
▶CE1057000

N-*De-Me:* [26931-78-2] *1-Hydroxy-2,10,11-trimethoxynoraporphine.* ***Norcorydine***
$C_{19}H_{21}NO_4$ 327.379
Alkaloid from *Annona squamosa* (sugar apple). Noncryst. Mp 249-251° (as hydrochloride). $[\alpha]_D$ +156 (MeOH). $[\alpha]_D^{23}$ +190 (c, 0.2 in $CHCl_3$).

Johns, S.R. *et al., Aust. J. Chem.*, 1970, **23**, 363 (*Norcorydine*)
Tackie, A.N. *et al., J. Nat. Prod.*, 1974, **37**, 6 (*Norcorydine*)
Hoquemiller, R. *et al., J. Nat. Prod.*, 1981, **44**, 551 (*Norcorydine, occur*)
Urzúa, A. *et al., Phytochemistry*, 1982, **21**, 773 (*Norcorydine, isol, ir, pmr, ms*)

Corymboside C-360

[73543-87-0]
6-α-L-Arabinopyranosyl-8-β-D-galactopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 6-Arabinopyranosyl-8-galactopyranosyl-4′,5,7-trihydroxyflavone. 6-Arabinopyranosyl-8-galactopyranosylapigenin. 6-Arabinosyl-8-galactosylapigenin

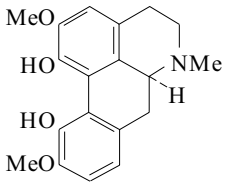


$C_{26}H_{28}O_{14}$ 564.499
Isol. from *Triticum aestivum* (wheat) (as acyl derivs.). Yellow powder. $[\alpha]_D$ +79 (c, 0.67 in H_2O).

Besson, E. *et al., Phytochemistry*, 1979, **18**, 1899
Wagner, H. *et al., J. Nat. Prod.*, 1980, **43**, 583 (*isol, derivs*)
Gaffield, W. *et al., Phytochemistry*, 1984, **22**, 1317 (*cd*)

Corytuberine C-361

1,11-Dihydroxy-2,10-dimethoxyaporphine



(*S*)-form

$C_{19}H_{21}NO_4$ 327.379
Log P 2.42 (uncertain value) (calc).
λ_{max} 208 (ϵ 31600); 226 (ϵ 25100); 276 (ϵ 5010); 318 (ϵ 5010) (EtOH/KOH) (Derep).
λ_{max} 222 (ϵ 25100); 268 (ϵ 10000); 306 (ϵ 3160) (EtOH) (Derep).

(*S*)-*form* [517-56-6]
Mp 240°. $[\alpha]_D^{20}$ +286 (c, 0.1 in EtOH). Pharmacol. active isomer.

Di-Ac:
Mp 72°.

N-*Me:* [2141-09-5] ***Magnoflorine****. Thalictrine. Esholine. Escholine. Corytuberine methosalt*
$C_{20}H_{24}NO_4^{\oplus}$ 342.414
Mp 248-249° (as iodide). $[\alpha]_D^{20}$ +193 (c, 0.20 in MeOH) (iodide). Iodide shows grinding-induced polymorphism. Many lit. references where Magnoflorine has supposedly been identified may be in error because of the similarity in props. to λ_{max} 227 (log ϵ 4.68); 275 (log ϵ 3.99); 315 (log ϵ 3.96) (H_2O) (iodide).

N-*De-Me:1,11-Dihydroxy-2,10-dimethoxynoraporphine.* ***Muricinine***
$C_{18}H_{19}NO_4$ 313.352
Alkaloid from *Annona muricata* (soursop). Tentative struct., not well characterised.

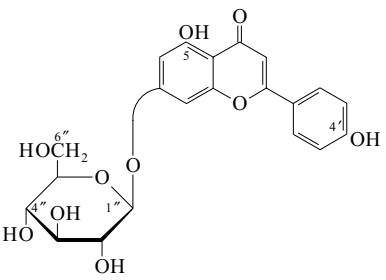
(±)-*form* [71630-07-4]
Mp 242°.

Hydrochloride:
Mp 250° dec.

Dobbie, J.J. *et al., J.C.S.*, 1893, **63**, 485-488 (*isol*)
Gulland, J.M. *et al., J.C.S.*, 1928, 1834-1838 (*synth*)
Späth, E. *et al., Ber.*, 1931, **64**, 2038-2048 (*synth*)
Manske, R.H.F. *et al., Alkaloids (N.Y.)*, 1954, **4**, 142-143 (*Muricinine*)
Nakano, T. *et al., Chem. Pharm. Bull.*, 1954, **2**, 329-334 (*Magnoflorine*)
Tomita, M. *et al., Yakugaku Zasshi*, 1957, **77**, 157 (*Magnoflorine*)
Albonico, S.M. *et al., J.C.S.(C)*, 1966, 1340-1342 (*ord, abs config*)
Jackson, A.H. *et al., J.C.S.(C)*, 1966, 2222-2229 (*pmr*)
Slavic, J. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 3514-3520 (*Esholine*)
Dominguez, X.A. *et al., Phytochemistry*, 1974, **13**, 680 (*Magnoflorine*)
Kametani, T. *et al., J.A.C.S.*, 1977, **99**, 3805-3808 (*synth*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80-85 (*cd*)
Hoard, M.S. *et al., Phytochemistry*, 1996, **43**, 1129-1133 (*Magnoflorine, polymorphism*)
Barbosa-Filho, J.M. *et al., Phytochemistry*, 1997, **44**, 959-961 (*Magnoflorine, isol, pmr, cmr*)

Cosmosiin C-362

[578-74-5]
7-O-β-D-Glucopyranosyloxy-4′,5-dihydroxyflavone. Apigenin 7-O-glucoside. Cosmetin. Apigetrin



$C_{21}H_{20}O_{10}$ 432.383
Yellow needles (EtOH or Me_2CO). Mp 178° Mp 203° Mp 229-232°. $[\alpha]_D$ -64 (Py). Forms a dihydrate, Mp 218-220°.

2″-Ac: [75357-75-4] *Apigenin 7-O-(2″-O-acetylglucoside)*
$C_{23}H_{22}O_{11}$ 474.42
Isol. from *Matricaria chamomilla* (German chamomile). No phys. props. reported.

6″-Ac: [72741-92-5] *Apigenin 7-O-(6″-O-acetylglucoside)*
$C_{23}H_{22}O_{11}$ 474.42
Isol. from *Matricaria chamomilla* (German chamomile). No phys. props. reported.

2″,3″-Di-Ac: [84323-20-6]
$C_{25}H_{24}O_{12}$ 516.457
Isol. from *Matricaria chamomilla* (German chamomile). No phys. props. reported.

3″,4″-Di-Ac: [84323-21-7]
$C_{25}H_{24}O_{12}$ 516.457
Isol. from *Matricaria chamomilla* (German chamomile). No phys. props. reported.

6″-O-Malonyl:6″-Malonylcosmosiin
$C_{24}H_{22}O_{13}$ 518.43
Isol. from *Petroselinum crispum* (parsley). No phys. props. reported.

6″-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl): [173356-77-9] *6″-O-(3-Hydroxy-3-methylglutaroyl)cosmosiin*. ***Chamaemeloside***
$C_{27}H_{28}O_{14}$ 576.51
Constit. of the flowers of *Chamaemelum nobile* (Roman chamomile). Amorph. yellow powder. $[\alpha]_D^{20}$ -74.5 (c, 0.2 in Py). λ_{max} 268 (ϵ 20780); 333 (ϵ 24200) (MeOH).

6″-O-(4-Hydroxycinnamoyl): [61237-19-2] ***Terniflorin***. *Echinacin*
$C_{30}H_{26}O_{12}$ 578.528
Isol. from *Pogostemon cablin* (patchouli). Cryst. Mp 261-263°. Identity of samples not certain. Mp. refers to Echinacin.

O-(2,3-Dihydroxycinnamoyl): [35397-62-7] ***Anthemoside***
$C_{30}H_{26}O_{13}$ 594.528
Constit. of *Anthemis nobilis* (Roman chamomile). Posn. of esterification not determined.

4′-O-(3,4-Dihydroxycinnamoyl): [20196-92-3] ***Piperitoside***
$C_{30}H_{26}O_{13}$ 594.528
Isol. from *Mentha piperita* (peppermint) leaves. Mp 251-253°. $[\alpha]_D^{18}$ -63.

3″-O-(3,4-Dihydroxycinnamoyl): [79366-62-4] *3″-O-Caffeoylcosmosiin*
$C_{30}H_{26}O_{13}$ 594.528
Isol. from leaves of *Perilla frutescens* (perilla). No phys. props. reported.

6″-O-α-L-Rhamnopyranosyl: [552-57-8] *Apigenin 7-O-rutinoside*. ***Isorhoifolin***
$C_{27}H_{30}O_{14}$ 578.526
Isol. from leaves of *Citrus paradisi* (grapefruit) and other plant spp.. Small needles (MeOH). Mp 269-270°. $[\alpha]_D^{23}$ -98.2 (c, 1.19 in Py).

6″-O-α-L-Rhamnopyranosyl, 4′-O-(3,4-dihydroxycinnamoyl): [14637-28-6] ***Menthoside***. *Apigenin 7-O-rutinoside 4′-O-caffeate*
$C_{36}H_{36}O_{17}$ 740.67
Isol. from *Mentha piperita* (peppermint) leaves. Cryst. (EtOH). Mp 271-273°. $[\alpha]_D^{18}$ -89 (c, 0.1 in DMF).

2″-β-D-Apiofuranosyl: [26544-34-3] ***Apiin***. *7-(2-Apiosylglucosyl)apigenin*
$C_{26}H_{28}O_{14}$ 564.499
Constit. of parsley (*Petroselinum crispum*) and of the flowers of *Anthemis nobilis* (Roman chamomile). First isol. in 1843. Cryst. (EtOH). Mp 236-237°. $[\alpha]_D$ -130 (c, 0.12 in MeOH). λ_{max} 267 (ϵ 15136); 342 (ϵ 19950) (MeOH) (Berdy).

2″-β-D-Apiofuranosyl, 6″-Ac: ***6″-Acetylapiin***
$C_{28}H_{30}O_{15}$ 606.536
Constit. of parsley. Powder. $[\alpha]_D^{25}$ -151.6 (c, 0.4 in MeOH). λ_{max} 269 (log ϵ 4); 334 (log ϵ 4.1) (MeOH).

2″-β-D-Apiofuranosyl, 6″-O-malonyl: [60478-75-3] ***6″-Malonylapiin***
$C_{29}H_{30}O_{17}$ 650.546
Isol. from parsley.

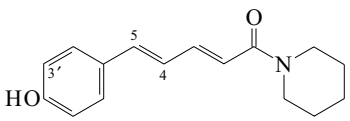
O″-Galacturonosyl: [126254-76-0]
$C_{27}H_{28}O_{16}$ 608.509
Isol. from *Cuminum cyminum* (cumin).

[36790-49-5, 86546-87-4, 105815-90-5]

Teoule, R. *et al., Bull. Soc. Chim. Fr.*, 1960, 2116-2123 (*glycosides, synth*)
Aritomi, M. *et al., Chem. Pharm. Bull.*, 1963, **11**, 1225-1228 (*Terniflorin*)
Hulyalkar, R.H. *et al., Can. J. Chem.*, 1965, **43**, 2085 (*Apiin*)
Gella, E.V. *et al., Farm. Zh. (Kiev)*, 1966, **21**, 58-66; 1967, **22**, 80-85; *CA*, **65**, 13810; **68**, 49985 (*Menthoside, Piperitoside*)
Nordby, H.E. *et al., Phytochemistry*, 1968, **7**, 1653-1657 (*Isorhoifolin*)
Wagner, H. *et al., Chem. Ber.*, 1969, **102**, 2083-2088 (*Isorhoifolin*)
Ezekiel, A.D. *et al., J.C.S.(C)*, 1971, 2907 (*Apiin, synth*)
Herisset, A. *et al., Plant. Med. Phytother.*, 1971, **5**, 234-239 (*Anthemoside*)
Schmid, R.D. *et al., Tetrahedron*, 1972, **28**, 3259 (*Apiin, ms*)
Kreuzaler, F. *et al., Phytochemistry*, 1973, **12**, 1149-1152 (*malonate*)
Kunde, R. *et al., Planta Med.*, 1979, **37**, 124-130 (*6″-acetate*)
Redaelli, C. *et al., Phytochemistry*, 1980, **19**, 985-986; 1982, **21**, 1828-1830 (*acetates*)
Ishikura, N. *et al., Agric. Biol. Chem.*, 1981, **45**, 1855-1860 (*deriv*)
Stein, W. *et al., Z. Naturforsch., C*, 1985, **40**, 469-473 (*6″-Malonylcosmosiin*)
Singh, K.N. *et al., Chem. Ind. (London)*, 1986, 713-714 (*Echinaticin, Echinacin*)
Eckey-Kaltenbach, H. *et al., Phytochemistry*, 1993, **34**, 687 (*6″-Malonylapiin*)
Tschan, G.M. *et al., Phytochemistry*, 1996, **41**, 643-646 (*Chamaemeloside*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1039-1044 (*6″-Acetylapiin*)

Coumaperine C-363

[76733-91-0]
1-[5-(4-Hydroxyphenyl)-1-oxo-2,4-pentadienyl]piperidine, 9CI. N-*[5-(4-Hydroxyphenyl)-2,4-pentadienoyl]piperidine. 5-(4-Hydroxyphenyl)-2,4-pentadienoic acid piperidide*



$C_{16}H_{19}NO_2$ 257.332
Isol. from the fruits of pepper (*Piper nigrum*) (Piperaceae). Cryst. (Me_2CO). Mp 199.5-200.5°.

Ac: [76733-93-2]
Needles (Et_2O). Mp 127-128°.

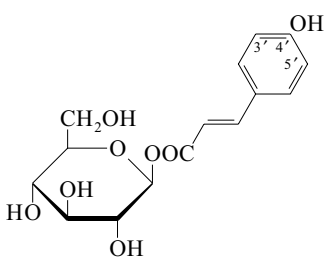
3′-Methoxy: [77795-15-4] ***Feruperine***
$C_{17}H_{21}NO_3$ 287.358
Alkaloid from pepper (*Piper nigrum*) (Piperaceae). Pale yellow needles (C_6H_6). Mp 159°.

3′-Methoxy, 4′,5′-dihydro: [77795-17-6] ***Dihydroferuperine***
$C_{17}H_{23}NO_3$ 289.374
Alkaloid from pepper (*Piper nigrum*) (Piperaceae). Cryst. (petrol). Mp 78°.

Nakatani, N. *et al., Agric. Biol. Chem.*, 1980, **44**, 2831 (*isol, ms, uv, ir, pmr, struct, synth*)
Inatani, R. *et al., Agric. Biol. Chem.*, 1981, **45**, 667 (*Feruperine, Dihydroferuperine*)

1-*O*-*p*-Coumaroylglucose C-364

*Glucose 1-[3-(4-hydroxyphenyl)-2-propenoate], 9CI. 1-*O-p-*Hydroxycinnamoylglucose*



$C_{15}H_{18}O_8$ 326.302

β-D-*form* [7139-64-2]
Isol. from many plants, e.g. *Solanum* and *Fragaria* spp.. Platelets (H_2O). Mp 212°. $[\alpha]_D^{20}$ -7.95 (50% MeOH aq.).

2-O-Sulfate:
$C_{15}H_{18}O_{11}S$ 406.367Isol. as mixt. with the 6-sulfate.

3-O-Sulfate:
$C_{15}H_{18}O_{11}S$ 406.367

6-O-*Sulfate:*
$C_{15}H_{18}O_{11}S$ 406.367
Isol. from *Pteridium aquilinum* (bracken fern).

2′-Hydroxy, 4′-Me ether: [145227-80-1]
$C_{16}H_{20}O_9$ 356.329
Constit. of *Matricaria chamomilla* (German chamomile).

3′-Hydroxy: [14364-08-0] ***1*-O-*Caffeoylglucose***
$C_{15}H_{18}O_9$ 342.302
Present in many plants, e.g. *Solanum*, *Raphanus* etc. spp.. Amorph. Mp 96-98°. $[\alpha]_D$ -47 (EtOH).

3′-Hydroxy, 6-O-*sulfate:*
$C_{15}H_{18}O_{12}S$ 422.366
Isol. from *Pteridium aquilinum* (bracken fern).

3′-Hydroxy, 6-O-*β-D-glucopyranosyl:****1*-O-*Caffeoyl-β-gentiobiose***
$C_{21}H_{28}O_{14}$ 504.444
Amorph. yellow powder. $[\alpha]_D^{15}$ -26 (c, 0.3 in MeOH).

3′-Hydroxy, 3-O-*(3,4,5-trihydroxybenzoyl):****1*-O-*Caffeoyl-3*-O-*galloyl-β-D-glucopyranose***
$C_{22}H_{22}O_{13}$ 494.408
Amorph. yellow powder. $[\alpha]_D^{15}$ -48.9 (c, 0.8 in MeOH).

*3′-Hydroxy, 3,4-bis(3,4,5-trihydroxybenzoyl):****1*-O-*Caffeoyl-3,4-di*-O-*galloyl-β-D-glucopyranose***
$C_{29}H_{26}O_{17}$ 646.514
Amorph. yellow powder + 2½ H_2O. $[\alpha]_D^{15}$ -74.9 (c, 0.4 in MeOH).

3′-Hydroxy, 4,6-bis(3,4,5-trihydroxybenzoyl):1-O-*Caffeoyl-4,6-di*-O-*galloyl-β-D-glucopyranose*
$C_{29}H_{26}O_{17}$ 646.514
Amorph. yellow powder + $3H_2O$. $[\alpha]_D^{15}$ -177.8 (c, 0.2 in MeOH).

3′-(β-D-Glucopyranosyloxy): [62018-87-5]
$C_{21}H_{28}O_{14}$ 504.444
Amorph. yellow powder. $[\alpha]_D^{15}$ -438.4 (c, 0.5 in MeOH).

3′-Methoxy: [7196-71-6] ***1*-O-*Feruloylglucose***
$C_{16}H_{20}O_9$ 356.329
Present in *Solanum*, *Raphanus*, etc. spp.. Short prisms (EtOH). Mp 123-126°. $[\alpha]_D^{20}$ -13.9 (H_2O).

*3′,5′-Dimethoxy:****1*-O-*Sinapoylglucose***
$C_{17}H_{22}O_{10}$ 386.355
Present in rhubarb (*Rheum rhaponticum*) and cabbage (*Brassica oleracea*).

[13080-40-5, 18030-39-2, 29744-33-0, 38621-53-3, 51463-98-0]

Birkofer, L. *et al., Naturwissenschaften*, 1960, **47**, 469 (*isol, synth, Feruloylglucose*)
Harborne, J.B. *et al., Biochem. J.*, 1961, **81**, 242 (*occur*)
Birkofer, L. *et al., Z. Naturforsch., B*, 1961, **16**, 249 (*occur, synth*)
Asen, S. *et al., Phytochemistry*, 1962, **1**, 169 (*occur*)
Harborne, J.B. *et al., Phytochemistry*, 1964, **3**, 421 (*occur*)
Cooper-Driver, G. *et al., Phytochemistry*, 1975, **14**, 2506 (*6-sulfate*)
Litvinenko, V.I. *et al., Planta Med.*, 1975, **27**, 372 (*rev, Feruloylglucose*)
Imperato, F. *et al., Phytochemistry*, 1976, **15**, 1786 (*3′-glucosyloxy*)
Herrmann, K. *et al., Prog. Chem. Org. Nat. Prod.*, 1978, **35**, 73 (*rev*)
Jiang, Z.-H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 887-892 (*3′-glucosyloxy, 1-caffeoylgentiobiose, caffeoylgalloylglucoses*)

2-*O*-*p*-Coumaroylglucose C-365

2-O-*(4-Hydroxycinnamoyl)glucose*
$C_{15}H_{18}O_8$ 326.302

D-*form* [110351-44-5]
Isol. from various commercial rhubarbs (*Rheum* sp.). Needles (H_2O). Mp 204-206°. $[\alpha]_D^{27}$ +32.8 (c, 0.3 in MeOH). $[\alpha]_D^{20}$ +27.3 → +51.8 (c, 1 in MeOH).

6-O-*Sulfate:*
$C_{15}H_{18}O_{11}S$ 406.367

β-D-*form*

1,6-Bis(3,4,5-trihydroxybenzoyl):2-O-p-*Coumaroyl-1,6-digalloyl-β-D-glucopyranoside*
$C_{29}H_{26}O_{16}$ 630.515
Isol. from various commercial rhubarbs (*Rheum* sp.). Needles (H_2O). Mp 179-181°. $[\alpha]_D^{28}$ -112.8 (c, 0.53 in Me_2CO).

Imperato, F. *et al., Chem. Ind. (London)*, 1981, 691 (*sulfate*)
Shimomura, H. *et al., Phytochemistry*, 1987, **26**, 1981 (*isol, pmr*)
Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1473 (*isol, pmr, cmr*)

6-*O*-*p*-Coumaroylglucose C-366

6-O-*(4-Hydroxycinnamoyl)glucose*
$C_{15}H_{18}O_8$ 326.302

D-*form* [114297-65-3]
Isol. from various commercial rhubarbs (*Rheum* sp.). Needles (H_2O). Mp 184-186°. $[\alpha]_D^{24}$ +30.1 (c, 0.72 in MeOH). $[\alpha]_D$ +32 → +39 (80% dioxan aq.). λ_{max} 313 (EtOH).

*3′,5′-Dimethoxy:****6*-O-*Sinapoylglucose***
$C_{17}H_{22}O_{10}$ 386.355
Powder (MeOH). Mp 129-131°.

β-D-Pyranose-*form*

1,2-Bis(3,4,5-trihydroxybenzoyl):6-O-p-*Coumaroyl-1,2-digalloylglucose*
$C_{29}H_{26}O_{16}$ 630.515
Isol. from various commercial rhubarbs. Amorph. powder + $3H_2O$. $[\alpha]_D^{21}$ -68.7 (c, 0.95 in Me_2CO).

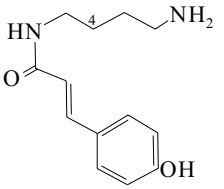
*3′-Hydroxy, 1,3,4-tris(3,4,5-trihydroxybenzoyl):****6*-O-*Caffeoyl-1,3,4-tri*-O-*galloyl-β-D-glucopyranose***
$C_{36}H_{30}O_{21}$ 798.62
Amorph. yellow powder + 2½H_2O. $[\alpha]_D^{15}$ +14.9 (c, 0.6 in MeOH).

[149998-27-6, 149998-28-7]

Watanabe, S. *et al., Agric. Biol. Chem.*, 1966, **30**, 420 (*synth*)
Shimomura, H. *et al., Phytochemistry*, 1988, **27**, 641 (*isol*)
Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1473 (*isol, cmr, pmr*)
Lou, H. *et al., Phytochemistry*, 1993, **32**, 1283 (*6-Sinapoylglucose*)
Jiang, Z.-H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 887-892 (*6-Caffeoyl-1,3,4-trigalloylglucose*)

4-Coumaroylputrescine C-367

[34136-53-3]
4-Hydroxycinnamoylputrescine



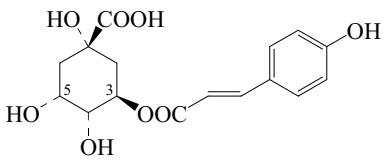
$C_{13}H_{18}N_2O_2$ 234.297
Alkaloid from *Pennisetum americanum* (pearl millet), *Zea mays* (sweet corn), *Persea gratissima* (avocado) and *Lycopersicon esculentum* (tomato). Faint yellow needles + $1H_2O$ (H_2O). Mp 182-183.5°.

*4*S-*Hydroxy:* [24177-22-8] ***4-Coumaroyl-2-hydroxyputrescine***
$C_{13}H_{18}N_2O_3$ 250.297
Alkaloid from *Triticum aestivum* (wheat). Geom. of double bond not defined λ_{max} 293 ; 316 (H_2O) (Berdy). λ_{max} 309 ; 363 (NAOH) (Berdy).

Stoessl, A. *et al., Tet. Lett.*, 1969, 2807 (*deriv*)
Mizusaki, S. *et al., Phytochemistry*, 1971, **10**, 1347 (*isol, synth*)
Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*occur*)

3-*O*-*p*-Coumaroylquinic acid C-368

1,4,5-Trihydroxy-3-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]cyclohexanecarboxylic acid, 9CI



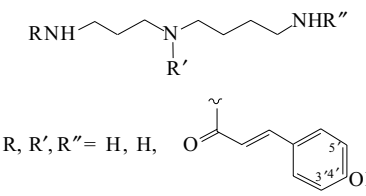
$C_{16}H_{18}O_8$ 338.313
Found in cider apples, tea, cacao etc.. Needles (H_2O). Mp 247-248°. $[\alpha]_D^{20}$ -53.6 (c, 1.04 in MeOH).

1-Me ether:
Needles (H_2O). Mp 248°. $[\alpha]_D^{22}$ -47.5 (c, 0.5 in EtOH).

Williams, A.H. *et al., Chem. Ind. (London)*, 1958, 1200 (*isol*)
Haslam, E. *et al., J.C.S.*, 1961, 5153-5156 (*synth*)

4-Coumaroylspermidine C-369

[70185-59-0]
(4-Hydroxycinnamoyl)spermidine



$C_{16}H_{25}N_3O_2$ 291.392
These alkaloids have not been fully characterised and the regioisomeric compositions may not correspond.

3′-Hydroxy: [58994-15-3] ***Caffeoylspermidine***
$C_{16}H_{25}N_3O_3$ 307.392

Alkaloid from *Pennisetum americanum* (pearl millet).

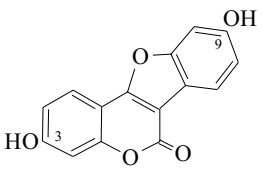
3′-Methoxy: [70185-60-3] ***Feruloylspermidine***
$C_{17}H_{27}N_3O_3$ 321.419
Alkaloid from *Ananas comosus* (pineapple) and *Lycopersicon esculentum* (tomato).

3′,5′-Dimethoxy: [70185-62-5] ***Sinapoylspermidine***
$C_{18}H_{29}N_3O_4$ 351.445

Delétang, J. *et al., Ann. Tab., Sect. 2*, 1974, **11**, 123; *CA*, **84**, 147656m (*struct*)
Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*occur*)

Coumestrol C-370

[479-13-0]
*3,9-Dihydroxy-6*H*-benzofuro[3,2-c][1]benzopyran-6-one, 9CI. 3,9-Dihydroxycoumestan. 7,12-Dihydroxycoumestan (obsol.). 3,9-Dihydroxy-6-oxopterocarpen (obsol.). 6′,7-Dihydroxybenzofuro[3′,2′,3,4]coumarin (obsol.). Cumostrol*



$C_{15}H_8O_5$ 268.225
Isol. from *Medicago* spp., *Glycine max* (soybean), *Pisum sativum* (pea), *Spinacia oleracea* (spinach), *Brassica oleracea* (cabbage), *Dolichos biflorus* (papadi), *Melilotus alba* (white melilot), *Phaseolus* spp. (inc. lima beans, pinto beans) and *Vigna unguiculata* (all Leguminosae). Potential nutriceutical. Sol. bases; fairly sol. MeOH, $CHCl_3$, Et_2O; poorly sol. H_2O, C_6H_6, CCl_4, acids. Mp 385°. Log P 3.12 (calc). Subl. at 325°. Shows blue fluorescence λ_{max} 208 ; 243 ; 343 (MeOH) (Berdy). λ_{max} 243 ; 307 ; 343 (EtOH) (Berdy). λ_{max} 250 ; 280 ; 310 ; 385 (NaOH) (Berdy).

▶ Exp. reprod. and teratogenic effects. DF8077000

3-O-β-D-Glucopyranoside: [92631-72-6] ***Coumestrin***
$C_{21}H_{18}O_{10}$ 430.367
Constit. of *Glycine max* (soybean). Oil.

3-Me ether: ***3-O-Methylcoumestrol***
$C_{16}H_{10}O_5$ 282.252
Isol. from alfalfa (*Medicago sativa*). Cryst. (Me_2CO/MeOH). Mp 331-332°.

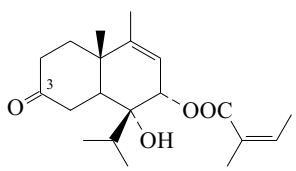
9-Me ether: [1690-62-6] ***9-O-Methylcoumestrol***. *3-Hydroxy-9-methoxycoumestan*
$C_{16}H_{10}O_5$ 282.252
Isol. from *Cicer arietinum* (chickpea), *Myroxylon balsamum* (Tolu balsam), *Pisum sativum* (pea) *and Trifolium pratense* (red clover). Needles (Me_2CO/MeOH). Mp 338-339°.

9-Me ether, 3-O-β-D-glucopyranoside: ***Licoagroside C***
$C_{22}H_{20}O_{10}$ 444.394
Needles (MeOH). Mp 245-247°. $[\alpha]_D^{24}$ -23.1 (c, 0.4 in MeOH). λ_{max} 211 (log ϵ 4.21); 242 (log ϵ 4.2); 337 (log ϵ 4.26) (MeOH).

Di-Me ether: [3172-99-4] ***Di-O-methylcoumestrol***. *3,9-Dimethoxy-6-oxopterocarpen. 3,9-Dimethoxycoumestan*
$C_{17}H_{12}O_5$ 296.279
Microcryst. (MeOH). Mp 200-201° (195-198°).

Bikoff, E.M. *et al., J.A.C.S.*, 1958, **80**, 3969 (*struct*)
Micheli, R.A. *et al., J. Med. Chem.*, 1962, **5**, 321 (*pharmacol*)
Schauer, H. *et al., Dtsch. Apoth. -Ztg.*, 1964, **104**, 987 (*rev, props*)
Jurd, L. *et al., J.O.C.*, 1964, **29**, 3036 (*synth*)
Bickoff, E.M. *et al., J. Agric. Food Chem.*, 1965, **13**, 596 (*deriv*)
Harper, S.H. *et al., J.C.S.(C)*, 1969, 1109 (*Coumestrin*)
Dewick, P.M. *et al., Phytochemistry*, 1970, **9**, 775 (*biosynth*)
De Alencar, R. *et al., Phytochemistry*, 1972, **11**, 1517
Donnelly, D.M.X. *et al., J.C.S. Perkin 1*, 1973, 1737 (*9-O-Methylcoumestrol*)
Kappe, T. *et al., Z. Naturforsch., B*, 1974, **29**, 292 (*synth*)
Kurosawa, K. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1955 (*synth*)
Murray, R.D.H. *et al., The Natural Coumarins*, J.Wiley, 1982, 320 (*biol, prop*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Jurd, L. *et al., Aust. J. Chem.*, 1984, **37**, 1127 (*9-O-Methylcoumestrol*)
Le-Van, N. *et al., Phytochemistry*, 1984, **23**, 1204 (*Coumestrin*)
Setchell, K.D.R. *et al., J. Chromatogr.*, 1987, **386**, 315 (*hplc*)
Pandit, S.B. *et al., Synth. Commun.*, 1988, **18**, 157 (*synth*)
Hiroya, K. *et al., J.C.S. Perkin 1*, 2000, 4339-4346 (*synth*)
Li, W. *et al., Phytochemistry*, 2001, **58**, 595-598 (*Licoagroside C*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COF350

Crispanone C-371



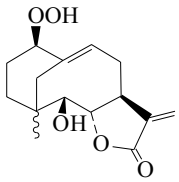
$C_{20}H_{30}O_4$ 334.455
Constit. of *Petroselinum crispum* (parsley).

Deoxo: ***Crispane***
$C_{20}H_{32}O_3$ 320.471
Constit. of *Petroselinum crispum* (parsley).

Spraul, M.H. *et al., Phytochemistry*, 1992, **31**, 3109 (*isol, pmr, cmr*)

Crispolide C-372

[83217-86-1]
1β-Hydroperoxy-5β-hydroxy-4,14-cyclo-9,11-germacradien-12,6α-olide

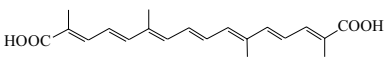


$C_{15}H_{20}O_5$ 280.32
Constit. of *Tanacetum vulgare* var. *crispum*. Amorph. powder. $[\alpha]_D^{24}$ -20 (c, 0.90 in Py).

Appendino, G. *et al., Phytochemistry*, 1982, **21**, 1099

Crocetin C-373

2,6,11,15-Tetramethyl-2,4,6,8,10,12,14-hexadecaheptaenedioic acid. 8,8′-Diapo-8,8′-carotenedioic acid. Nyctanthin. α-Crocetin. Gardenidin†



$C_{20}H_{24}O_4$ 328.407

(all-*E*)-*form* [27876-94-4]
Red cryst. (Ac_2O). Mp 285-287°. λ_{max} 411 ; 436 ; 464 (Py).

Mono-Me ester: [25368-09-6] *β-Crocetin*
$C_{21}H_{26}O_4$ 342.434
Cryst. ($CHCl_3$). Mp 218°.

Di-Me ester: [5892-54-6] ***γ-Crocetin***
$C_{22}H_{28}O_4$ 356.461
Isol. from saffron. Orange-red cryst. ($CHCl_3$/MeOH). Mp 222-225°.

Mono-β-D-glucopyranosyl ester: [58050-17-2]
$C_{26}H_{34}O_9$ 490.549
Isol. from saffron. λ_{max} 419 ; 440 ; 468 (Py).

[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [55750-85-1] ***Crocin 3***
$C_{32}H_{44}O_{14}$ 652.691
Isol. from saffron. Red prismatic needles (MeOH). Mp 204-208°. λ_{max} 418 ; 439 ; 467 (Py). λ_{max} 430 ; 455 (MeOH).

β-D-Glucopyranosyl Me diester: [55750-86-2] ***Crocin 4***
$C_{27}H_{36}O_9$ 504.576
Isol. from saffron (*Crocus sativus*). Light red microprisms (Me_2CO). Mp 230-236°. λ_{max} 435 ; 460 (MeOH).

Di-β-D-glucopyranosyl ester: [57710-64-2]
$C_{32}H_{44}O_{14}$ 652.691
Isol. from saffron (*Crocus sativus*). Wine red cryst. λ_{max} 425 ; 447 ; 475 (Py).

[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] diester: [42553-65-1] ***α-Crocin***. *Crocin. Gardenin*
$C_{44}H_{64}O_{24}$ 976.975
The colouring principle of saffron. Red cryst. (MeOH) or brown-red needles. Mp 215° (186° dec.). $[\alpha]_D^{21}$ +1760 (H_2O). Log P -5.64 (uncertain value) (calc).

▶ HL7380000

[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] β-D-glucopyranosyl diester: [55750-84-0] ***Crocin 2***
$C_{38}H_{54}O_{19}$ 814.833
Isol. from saffron (*Crocus sativus*).

Dark red rectangular prisms (MeOH). Mp 208-210°. λ_{max} 410 ; 440 (ε 84000); 460 (EtOH) (Berdy). λ_{max} 421 ; 443 ; 471 (Py).

[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl] [β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] diester: [90332-59-5] *Crocetin β-gentiobiosyl β-neapolitanosyl ester*
$C_{50}H_{74}O_{29}$ 1139.117

Bis[β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl] diester: [90332-60-8] *Crocetin dineapolitanosyl ester*
$C_{56}H_{84}O_{34}$ 1301.259

(8*Z*)-*form*
cis-*Crocetin*
Occurs as glycoside in saffron.

Di-Me ester:
Cryst. (MeOH). Mp 141°.

Sigma-Aldrich Library of Stains, Dyes and Indicators, 644
Karrer, P. *et al., Helv. Chim. Acta*, 1932, **15**, 1218; 1399 (*struct*)
Inhoffen, H.H. *et al., Annalen*, 1953, **580**, 7 (*synth, isom*)
Duquenois, P. *et al., Bull. Soc. Pharm. Strasbourg*, 1972, **15**, 149 (*rev*)
Pfander, H. *et al., Helv. Chim. Acta*, 1975, **58**, 1608; 2233 (*isol, struct, glycosides*)
Dhingra, V.K. *et al., Indian J. Chem.*, 1975, **13**, 339 (*glycosides*)
Dhingra, V.K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 231 (*glycosides*)
Quinkert, G. *et al., Chem. Ber.*, 1977, **110**, 3582 (*synth*)
Pfander, H. *et al., Helv. Chim. Acta*, 1979, **62**, 1944 (*synth*)
Pfander, H. *et al., J. Chromatogr.*, 1982, **234**, 443 (*hplc*)
Matheson, I.B.C. *et al., Photochem. Photobiol.*, 1982, **36**, 1 (*photochem*)
Pfander, H. *et al., Phytochemistry*, 1982, **21**, 1039 (*biosynth*)
Rychener, M. *et al., Helv. Chim. Acta*, 1984, **67**, 386 (*neapolitanosyl esters*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 538 (*bibl*)

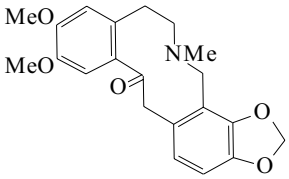
Crofelemer, USAN C-374

[148465-45-6]
Provir™. Virend. SP 303
Oligomeric proanthocyanidin.

Wyde, P.R. *et al., Antiviral Res.*, 1993, **20**, 145-154; **21**, 37-45 (*pharmacol*)
Holodniy, M. *et al., Am. J. Gastroenterol.*, 1999, **94**, 3267-3273 (*phase II study*)
Gabriel, S.E. *et al., Am. J. Physiol.*, 1999, **276**, G58-G63 (*pharmacol*)

Cryptopine C-375

[482-74-6]
4,6,7,13-Tetrahydro-9,10-dimethoxy-5-methylbenzo[e]1,3-dioxolo[4,5-l][2]benzazecin-12(5H)-one, 9CI. Cryptocavine. Thalisopyrine



$C_{21}H_{23}NO_5$ 369.416
Prisms (Py/EtOH). Mp 221-223°.
▶ Highly toxic. DF4935300

Perchlorate:
Mp 226-228°.

Picrate:
Mp 163°.

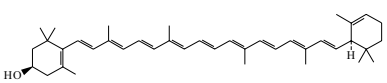
O^3*-De-Me:* [89117-94-2] ***Izmirine***
$C_{20}H_{21}NO_5$ 355.39

13-Oxo: [15215-66-4] ***13-Oxocryptopine***. *14-Oxocryptopine*
$C_{21}H_{21}NO_6$ 383.4
Alkaloid from *Papaver somniferum* (opium poppy). Cryst. (Me_2CO). Mp 185-186°. The 13-(or14-) position is the methylene carbon adjoining the carbonyl group.

Haworth, R.D. *et al., J.C.S.*, 1926, 1769 (*synth*)
Dolejš, L. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 2479 (*ms*)
Ma, J.C.N. *et al., Can. J. Chem.*, 1965, **43**, 1849 (*pmr*)
Hanuš, V. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 1759 (*13-Oxocryptopine*)
Hruban, L. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 3414 (*uv*)
Hall, S.R. *et al., Acta Cryst. B*, 1968, **24**, 346 (*cryst struct*)
Brochmann-Hanssen, E. *et al., Planta Med.*, 1970, **18**, 366 (*isol, deriv*)
Nakashima, T.T. *et al., Org. Magn. Reson.*, 1973, **5**, 9 (*cmr*)
Guinaudeau, H. *et al., J. Nat. Prod.*, 1983, **46**, 934 (*Izmirine*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 522

α-Cryptoxanthin C-376

[24480-38-4]
β,ε-Caroten-3-ol, 9CI. Physoxanthin. Zeinoxanthin. α-Kryptoxanthin

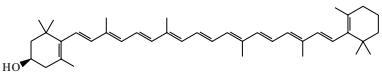


$C_{40}H_{56}O$ 552.882
Constit. of *Capsicum annuum* and maize (*Zea mays*), peach, plum and citrus juices. Natural food colorant. Dark red needles (C_6H_6/MeOH). Mp 175-176° (157.5-158.5°). $[\alpha]_D^{25}$ -508.3 (c, 0.36 in Me_2CO).

Bodea, C. *et al., Annalen*, 1959, **622**, 188 (*isol*)
Petzold, E.N. *et al., Arch. Biochem. Biophys.*, 1960, **86**, 163 (*isol*)
Goodfellow, D. *et al., Chem. Comm.*, 1970, 1578 (*synth*)
Loeber, D.E. *et al., J.C.S.(C)*, 1971, 404 (*synth*)
Stewart, I. *et al., J. Agric. Food Chem.*, 1977, **25**, 1132-1137 (*occur*)
Bodea, C. *et al., Phytochemistry*, 1978, **17**, 2037 (*struct*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 60 (*bibl*)

β-Cryptoxanthin C-377

[472-70-8]
β,β-Caroten-3-ol. Cryptoxanthin. 3-Hydroxy-β-carotene. Caricaxanthin. Neocryptoxanthin. β-Krypoxanthin. Cryptoxanthol



$C_{40}H_{56}O$ 552.882
Isol. from papaya (*Carica papaya*) and many other higher plants, also from fish eggs. Cryst. (C_6H_6/EtOH), metallic prisms or needles (C_6H_6). Mp 172-173° (169°). λ_{max} 452 ; 480 (no solvent reported).

Hexadecanoyl: [25671-24-3] *β-Cryptoxanthin palmitate*
$C_{56}H_{86}O_2$ 791.294
Cryst. (C_6H_6/MeOH). Mp 114°.

5R,6S-Epoxide: [188116-19-0]

[29291-23-4] *5,6-Epoxy-5,6-dihydro-β,β-caroten-3-ol*. ***Cryptoxanthin epoxide***
$C_{40}H_{56}O_2$ 568.881
Isol. from yellow paprika (*Capsicum annuum* var. *Lycopersiforme*), peel of ripe persimmon (*Diospyros kaki*), mature fruit of peach (*Prunus persica*) and ripe peel of a mandarin hybrid (*Citrus reticulata*). Cryst. (C_6H_6/petrol). Mp 154°. Absolute stereochem. of isolate from *C. annuum* determined by Molnar *et al*. (1997). Stereochem of isolates and synthetic epoxide prior to this date unknown.

5′ξ,6′ξ-Epoxide: [29291-23-4] *5′,6′-Epoxy-5′,6′-dihydro-β,β-caroten-3-ol*
$C_{40}H_{56}O_2$ 568.881
Isol. from *Citrus reticulata* (mandarin). Cryst. (C_6H_6/hexane). Mp 158-160°.

5,5′,6,6′-Diepoxide: Violaxanthin, V-40

7,8-Didehydro: [76207-91-5]

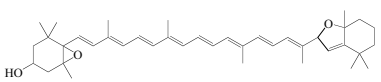
[162302-60-5] *7,8-Didehydro-β,β-caroten-3-ol, 9CI. 7,8-Didehydrocryptoxanthin.* ***Allobetaxanthin***
Cryst. ($MeOH/Et_2O$). Mp 173°. λ_{max} 452 (ε 155000) (Me_2CO).

Karrer, P. *et al., Helv. Chim. Acta*, 1946, **29**, 229-233 (*epoxide, synth*)
Isler, O. *et al., Helv. Chim. Acta*, 1957, **40**, 456-467 (*synth*)
Entschel, R. *et al., Helv. Chim. Acta*, 1958, **41**, 983-987 (*palmitate*)
Bodea, C. *et al., Annalen*, 1963, **666**, 189-191 (*ir*)
Subbarayan, C. *et al., Anal. Biochem.*, 1965, **12**, 275-281 (*epoxide*)
De Ville, T.E. *et al., Chem. Comm.*, 1969, 1311-1312 (*abs config*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527-2544 (*struct*)
Loeber, D.E. *et al., J.C.S.(C)*, 1971, 404-408 (*synth*)
Pfander, H. *et al., Chimia*, 1972, **27**, 103-104 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1837 (*occur*)
Cooper, R.D.G. *et al., J.C.S. Perkin 1*, 1975, 2195-2204 (*synth*)
Lassertois, D. *et al., Phytochemistry*, 1978, **17**, 411-415 (*epoxide, isol*)

Litchfield, C. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **66**, 359-365 (*Allobetaxanthin*)
Farin, D. *et al., Phytochemistry*, 1983, **22**, 403-408 (*5,6-epoxide, 5′,6′-epoxide, isol*)
Ebert, G. *et al., Phytochemistry*, 1985, **24**, 29-32 (*epoxide, isol*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 335 (*isol*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 55 (*bibl*)
Godoy, H.T. *et al., Food Chem.*, 1990, **36**, 281-286 (*5,6-epoxide*)
Haugan, J.A. *et al., Acta Chem. Scand.*, 1994, **48**, 899-904 (*Allobetaxanthin, synth*)
Molnar, P. *et al., Helv. Chim. Acta*, 1997, **80**, 221-229 (*epoxide*)

Cryptoxanthin 5,6:5′,8′-diepoxide C-378

[55965-22-5]
5,6:5′,8′-Diepoxy-5,5′,6,8′-tetrahydro-β,β-caroten-3-ol

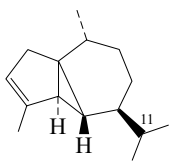


$C_{40}H_{56}O_3$ 584.881
Structure assignment is tentative. Isol. from juice of Shamouti orange (*Citrus sinensis*) and mature fruit of peach (*Prunus persica*).

Gross, J. *et al., J. Food Sci.*, 1971, **36**, 466 (*isol*)
Lessertois, D. *et al., Phytochemistry*, 1978, **17**, 411-415 (*isol*)

3-Cubebene C-379

Cubebene



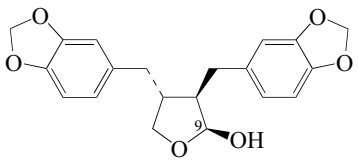
$C_{15}H_{24}$ 204.355
(5α,6β,7β,10α)-*form* [17699-14-8]
α-Cubebene
Constit. of oil of cubeb pepper (*Piper cubeba*). Oil. $[\alpha]_D^{30}$ -20 ($CHCl_3$).

11-Hydroxy:3-Cubeben-11-ol. ***11-Hydroxy-α-cubebene***
$C_{15}H_{24}O$ 220.354
Oil.

Piers, E. *et al., Can. J. Chem.*, 1971, **49**, 12 (*synth*)
Tanaka, A. *et al., J.C.S. Perkin 1*, 1972, 1721 (*synth*)
Martin, S.S. *et al., Phytochemistry*, 1976, **15**, 113 (*biosynth*)
Thiessen, W.E. *et al., Acta Cryst. B*, 1977, **33**, 3838 (*cryst struct*)
Connolly, J.D. *et al., Phytochemistry*, 1982, **21**, 233 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1153 (*11-hydroxy*)

Cubebin C-380

[18423-69-3]
3,4-Bis(1,3-benzodioxol-5-ylmethyl)tetrahydro-2-furanol, 9CI. 9-Hydroxy-3,4:3′,4′-bis(methylenedioxy)-9,9′-epoxylignan. β-Cubebin



$C_{20}H_{20}O_6$ 356.374
Isol. from unripe fruit of *Piper cubeba* (cubeb pepper). Cryst. (EtOH or C_6H_6). Mp 131-132°. $[\alpha]_D^{14}$ -17.1 (Me_2CO). $[\alpha]_D^{14}$ -45.7 ($CHCl_3$). Readily epimerises at C-9.

Et ether: [146830-09-3] **O-*Ethylcubebin***
$C_{22}H_{24}O_6$ 384.428
Constit. of *Piper cubeba* (cubeb pepper). Visc. solid.

9-Epimer: [112458-74-9] *α-Cubebin*
$C_{20}H_{20}O_6$ 356.374

Me ether:9-Methoxy-3,4:3′,4′-bis(methylenedioxy)-9,9′-epoxylignan. **O-*Methyl-β-cubebin***
$C_{21}H_{22}O_6$ 370.401
Amorph. solid. $[\alpha]_D$ -2.2 (c, 0.2 in $CHCl_3$).

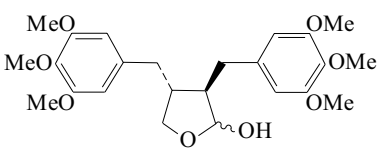
*9-Epimer, Me ether:***O-*Methyl-α-cubebin***
Oil. $[\alpha]_D$ -17.9 (c, 0.2 in $CHCl_3$).

[112448-61-0, 112448-62-1]

Freudenburg, K. *et al., Tetrahedron*, 1961, **15**, 115 (*stereochem*)
Chatterjee, A. *et al., J. Indian Chem. Soc.*, 1968, **45**, 723
Burden, R.S. *et al., J.C.S.(C)*, 1969, 693 (*ord*)
Batterbee, J.E. *et al., J.C.S.(C)*, 1969, 2470 (*synth*)
Chen, W.M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1987, **320**, 374-376 (*struct, isom*)
Badheka, L. *et al., Phytochemistry*, 1987, **26**, 2033 (*O-Ethylcubebin*)
Rehnberg, N. *et al., J.O.C.*, 1990, **55**, 4340 (*synth*)
Conserva, L.M. *et al., Phytochemistry*, 1990, **29**, 257-260 (*isol*)
De Almeida Blumenthal, E.E. *et al., Phytochemistry*, 1997, **46**, 745-749 (*O-Methylcubebins*)
Bastos, J.K. *et al., Planta Med.*, 1999, **65**, 541 (*activity*)
Borsato, M.L.C. *et al., Phytochemistry*, 2000, **55**, 809-813 (*activity*)

Cubebinin C-381

[96238-92-5]
Tetrahydro-3,4-bis[(3,4,5-trimethoxyphenyl)methyl]-2-furanol, 9CI. 9-Hydroxy-3,3′,4,4′,5,5′-hexamethoxy-9,9′-epoxylignan



$C_{24}H_{32}O_8$ 448.512
Constit. of *Piper cubeba* (cubeb pepper). Gum. $[\alpha]_D^{25}$ -23.3 (c, 0.3 in $CHCl_3$).

Prabhu, B.R. *et al., Phytochemistry*, 1985, **24**, 329
Lalami, K. *et al., Heterocycles*, 1988, **27**, 1131 (*synth*)

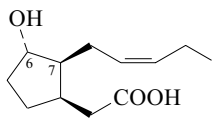
Cucumisin C-382

[82062-89-3]
E.C. 3.4.21.25
Protein. Constit. of the fruit of *Cucumis melo* var. Prince.

Kaneda, M. *et al., J. Biochem. (Tokyo)*, 1975, **78**, 1287 (*isol*)
Yamagata, H. *et al., J. Biol. Chem.*, 1994, **269**, 32725-32731 (*struct*)
Kaneda, M. *et al., Biotechnol. Appl. Biochem.*, 1995, **22**, 215-222 (*isol*)

Cucurbic acid C-383

[58240-50-9]
3-Hydroxy-2-(2-pentenyl)cyclopentaneacetic acid



$C_{12}H_{20}O_3$ 212.288
Constit. of *Cucurbita pepo*. Gum.

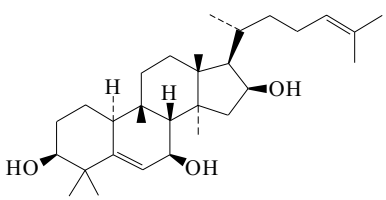
7-Epimer: [146143-02-4] **7-*Isocucurbic acid***
$C_{12}H_{20}O_3$ 212.288

6,7-Diepimer: [120330-52-1] ***6-Epi-7-isocucurbic acid***
$C_{12}H_{20}O_3$ 212.288
Constit. of *Vicia faba* and *Juglans regia* (walnut). Oil. $[\alpha]_D^{22}$ +6.1 (c, 0.1 in EtOH).

6,7-Diepimer, O-*β*-D-*glucopyranoside:* [176486-13-8]
$C_{18}H_{30}O_8$ 374.43
Constit. of *Perilla frutescens* (perilla). Paste. $[\alpha]_D$ -31.3 (c, 0.2 in MeOH).

Fukui, H. *et al., Agric. Biol. Chem.*, 1977, **41**, 175 (*isol*)
Kitahara, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 1129 (*synth*)
Miersch, O. *et al., Phytochemistry*, 1989, **28**, 339; 1999, **50**, 517-523 (*isol*)
Fujita, T. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 732-735 (*glucoside, pmr, cmr*)

Cucurbita-5,24-diene-3,7,16-triol C-384



$C_{30}H_{50}O_3$ 458.723
(3β,7β,16β)-*form*
Hydroxyhebevinogenin

3-O-*β*-D-*Xylopyranoside:* [101365-11-1]
Hebevinoside IX
$C_{35}H_{58}O_7$ 590.839
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder.

16-O-*β*-D-*Glucopyranoside, 3*-O-*β*-D-

xylopyranoside: [101365-08-6] ***Hebevinoside VI***
$C_{41}H_{68}O_{12}$ 752.981
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D^{23}$ +56 (c, 0.54 In Py).
▶ LD_{50} (mus, ipr) 66 mg/kg.

16-O-(4-O-Acetyl-β-D-glucopyranoside), 3-O-β-D-xylopyranoside: [138995-51-4] ***Hebevinoside XII***
$C_{43}H_{70}O_{13}$ 795.018
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D^{22}$ +60 (c, 0.36 in Py). λ_{max} 200 (MeCN) (Berdy).

16-O-(6-O-Acetyl-β-D-glucopyranoside), 3-O-β-D-xylopyranoside: [89203-39-4] ***Hebevinoside III***
$C_{43}H_{70}O_{13}$ 795.018
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. Sol. MeOH, butanol, Me_2CO. Mp 204-205° (as hepta-Ac). $[\alpha]_D^{20}$ +89 (c, 0.058 in MeOH).

16-O-(6-O-Acetyl-β-D-glucopyranoside), 3-O-(4-O-acetyl-β-D-xylopyranoside): [89456-98-4] ***Hebevinoside II***
$C_{45}H_{72}O_{14}$ 837.055
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. Sol. MeOH, butanol, Me_2CO. $[\alpha]_D$ +30 (c, 0.20 in Me_2CO).
▶ Toxic.

16-O-(6-O-Acetyl-β-D-glucopyranoside), 3-O-(3,4-di-O-acetyl-β-D-xylopyranoside): [138995-53-6] ***Hebevinoside XIV***
$C_{47}H_{74}O_{15}$ 879.093
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D^{24}$ +15 (c, 0.4 in $CHCl_3$). λ_{max} 200 (MeCN) (Berdy).

16-O-(4,6-Di-O-acetyl-β-D-glucopyranoside), 3-O-β-D-xylopyranoside: [101770-14-3] ***Hebevinoside VII***
$C_{45}H_{72}O_{14}$ 837.055
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D^{20}$ +82 (c, 0.22 in Me_2CO).

16-O-(4,6-Di-O-acetyl-β-D-glucopyranoside), 3-O-(4-O-acetyl-β-D-xylopyranoside): [101365-10-0] ***Hebevinoside VIII***
$C_{47}H_{74}O_{15}$ 879.093
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D$ +36.5 (c, 0.52 in $CHCl_3$).

16-O-(4,6-Di-O-acetyl-β-D-glucopyranoside), 3-O-(3,4-di-O-acetyl-β-D-xylopyranoside): [138995-52-5] ***Hebevinoside XIII***
$C_{49}H_{76}O_{16}$ 921.13
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D^{21}$ +35 (c, 0.42 in $CHCl_3$). λ_{max} 200 (MeCN) (Berdy).

O^7-Me:3-Methoxycucurbita-5,24-diene-3,16-diol. Methoxyhebevinogenin
$C_{31}H_{52}O_3$ 472.75

O^7-Me, 3-O-β-D-xylopyranoside: [101365-06-4] ***Hebevinoside IV***
$C_{36}H_{60}O_7$ 604.866
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Needles (MeOH). Mp 172-173°.
▶ Toxic.

O^7-Me, 16-O-β-D-glucopyranoside, 3-O-β-D-xylopyranoside: [101365-12-2] ***Hebevinoside X***
$C_{42}H_{70}O_{12}$ 767.008
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D$ +63 (c, 0.49 in MeOH).

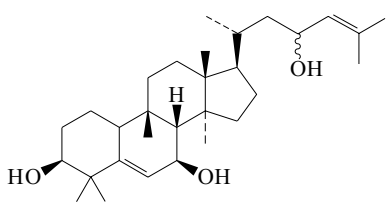
O^7-Me, 16-O-(6-O-acetyl-β-D-glucopyranoside), 3-O-β-D-xylopyranoside: [87396-30-3] ***Hebevinoside I***
$C_{44}H_{72}O_{13}$ 809.045
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. Sol. MeOH, butanol, Me_2CO.

O^7-Me, 16-O-(6-O-acetyl-β-D-glucopyranoside), 3-O-(4-O-acetyl-β-D-xylopyranoside): [101365-07-5] ***Hebevinoside V***
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Needles (MeOH). Mp 165-166°. $[\alpha]_D^{20}$ +83 (c, 0.053 in $CHCl_3$).
▶ Toxic.

O^7-Me, 16-O-(4,6-di-O-acetyl-β-D-glucopyranoside), 3-O-β-D-xylopyranoside: [101365-13-3] ***Hebevinoside XI***
$C_{46}H_{74}O_{14}$ 851.082
Toxic constit. of the toxic mushroom *Hebeloma vinosophyllum*. Amorph. powder. $[\alpha]_D^{20}$ +65 (c, 0.17 in MeOH).

Fujimoto, H. *et al., Chem. Pharm. Bull.*, 1986, **34**, 88-99; 1987, **35**, 2254-2260; 1991, **39**, 1958-1961 (*isol, struct, cryst struct*)

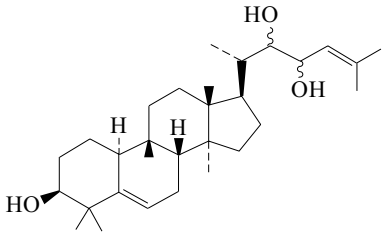
Cucurbita-5,24-diene-3,7,23-triol C-385



$C_{30}H_{50}O_3$ 458.723
(3β,7β,22ξ)-*form*
7-O-β-D-Glucopyranoside:
$C_{36}H_{60}O_8$ 620.865
Constit. of *Momordica charantia* (bitter melon). Amorph. powder. $[\alpha]_D$ +89 (c, 0.43 in MeOH).

Fatope, M.O. *et al., J. Nat. Prod.*, 1990, **53**, 1491 (*isol, pmr, cmr*)

Cucurbita-5,24-diene-3,22,23-triol C-386

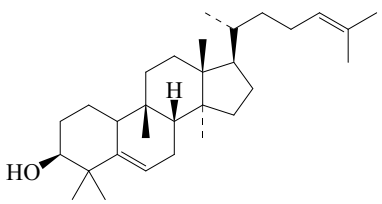


$C_{30}H_{50}O_3$ 458.723
(3β,22ξ,23ξ)-*form*
Prisms (MeOH). Mp 189-192.5°. $[\alpha]_D^{20}$ +37.4 (c, 1.01 in $CHCl_3$/MeOH).

3-O-β-Gentiobioside: [78887-73-7] ***Momordicoside D***
$C_{42}H_{70}O_{13}$ 783.007
Constit. of *Momordica charantia* (bitter melon). Needles (MeCN aq.). Mp 199-200°. $[\alpha]_D^{20}$ -1.26 (c, 1.59 in MeOH/$CHCl_3$).

Miyahara, Y. *et al., Chem. Pharm. Bull.*, 1981, **29**, 1561

Cucurbita-5,24-dien-3-ol C-387



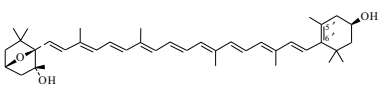
$C_{30}H_{50}O$ 426.724
3β-*form* [128779-09-9]
Constit. of pumpkin seeds.

[35012-08-9]

Shimizu, N. *et al., J.O.C.*, 1984, **49**, 709 (*synth*)
Nes, W.D. *et al., Chem. Comm.*, 1991, 1272 (*pmr, cmr, cryst struct*)

Cucurbitaxanthin A C-388

[103955-77-7]
3,6-Epoxy-5,6-dihydro-β,β-carotene-3′,5-diol. Zeaxanthin 3,6-epoxide (incorr.)

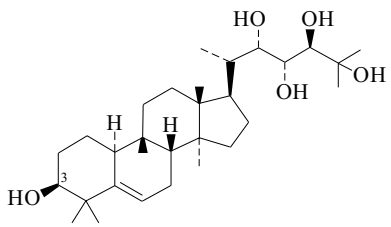


$C_{40}H_{56}O_3$ 584.881
Constit. of pumpkin (*Cucurbita maxima*) and of paprika (*Capsicum annuum* var. *longum*) fruits. Orange needles. Mp 175-176° (164-165°). λ_{max} 434 ; 457 ; 487 (C_6H_6).

5′α,6′α-Epoxide: [107390-61-4] *3,6:5′,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3′,5-diol.* ***Cucurbitaxanthin B***
$C_{40}H_{56}O_4$ 600.88
Isol. from pumpkin (*Cucurbita maxima*) and from paprika fruits. Orange needles. Mp 181-182° (164-166°). λ_{max} 415 ; 438 ; 468 (Et_2O).

Matsuno, T. *et al., Phytochemistry*, 1980, **25**, 2837 (*isol, deriv*)
Parkes, K.E.B. *et al., Tet. Lett.*, 1986, **27**, 2535 (*isol*)
Deli, J. *et al., Helv. Chim. Acta*, 1993, **76**, 952 (*synth, deriv*)
Deli, J. *et al., Helv. Chim. Acta*, 1996, **79**, 1435 (*isol, pmr, cmr, cd*)

Cucurbit-5-ene-3,22,23,24,25-pentol C-389



$C_{30}H_{52}O_5$ 492.738

(3β,22*S*,23*R*,24*R*)-*form*
Cryst. (MeOH). Mp 193-195°. $[\alpha]_D^{20}$ +48.1 (c, 0.94 in $CHCl_3$/MeOH).

3-O-*β*-D-*Glucopyranoside:* [134886-64-9] ***Momorcharaside B***
$C_{36}H_{62}O_{10}$ 654.88
Constit. of *Momordica charantia* (bitter melon). Mp 186-189°.

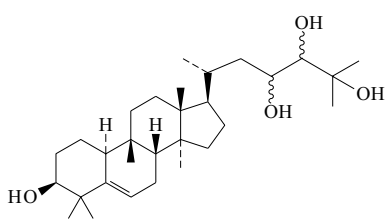
3-O-*[β*-D-*Glucopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [75801-95-5] ***Momordicoside A***
$C_{42}H_{72}O_{15}$ 817.022
Constit. of *Momordica charantia* (bitter melon). Cryst. (MeOH). Mp 181-187° dec. $[\alpha]_D^{20}$ +1.05 (c, 0.96 in $CHCl_3$/MeOH).

3-O-*[β*-D-*Galactopyranosyl-(1→6)-β*-D-*galactopyranoside]:* [135126-59-9] ***Momorcharaside A***
$C_{42}H_{72}O_{15}$ 817.022
Constit. of *Momordica charantia* (bitter melon). Mp 170-172°. $[\alpha]_D^{19}$ +0.8 (c, 1.8 in MeOH).

3-O-*[6*-O-*β*-D-*Glucopyranosyl-4*-O-*β*-D-*xylopyranosyl-β*-D-*glucopyranoside]:* [75799-04-1] ***Momordicoside B***
$C_{47}H_{80}O_{19}$ 949.138
Constit. of *Momordica charantia* (bitter melon). Cryst. (MeOH/$CHCl_3$). Mp 238-242° dec. $[\alpha]_D^{20}$ +6.15 (c, 0.98 in $CHCl_3$/MeOH).

Okabe, H. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2753
Zhu, Z.J. *et al., Yaoxue Xuebao*, 1990, **25**, 898-903; *CA*, **115**, 64133w (*Momorcharasides*)

Cucurbit-5-ene-3,23,24,25-tetrol C-390



$C_{30}H_{52}O_4$ 476.738

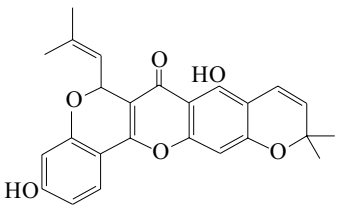
(3β,23ξ,24ξ)-*form*
Plates (MeOH). Mp 223-225°. $[\alpha]_D^{20}$ +55.8 (c, 1.96 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [78887-72-6] ***Momordicoside C***
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Momordica charantia* (bitter melon). Needles (MeOH aq.). Mp 224-227°. $[\alpha]_D^{20}$ +13.9 (c, 1.15 in MeOH).

Miyahara, Y. *et al., Chem. Pharm. Bull.*, 1981, **29**, 1561

Cudraflavone A C-391

[96843-73-1]
Isocyclomorusin



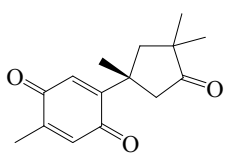
$C_{25}H_{22}O_6$ 418.445
Isol. from *Artocarpus altilis* (breadfruit). Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 265-272° (244-245°). $[\alpha]_D^{19}$ +27.3 (c, 0.147 in $CHCl_3$). $[\alpha]_D^{25}$ +30 (c, 0.29 in Me_2CO).

5′-Hydroxy: [114339-95-6] ***5′-Hydroxycudraflavone A***
$C_{25}H_{22}O_7$ 434.445
Cryst. ($CHCl_3$/hexane). Mp 235-237°. $[\alpha]_D^{20}$ +13.8 (c, 1.1 in Me_2CO). λ_{max} 232 (ϵ 16600); 293 (ϵ 15850); 392 (ϵ 10960) (MeOH) (Berdy).

Fujimoto, T. *et al., Planta Med.*, 1984, **50**, 218 (*isol, struct*)
Messana, I. *et al., Planta Med.*, 1987, **53**, 541 (*deriv*)
Chen, C.-C. *et al., J. Nat. Prod.*, 1993, **56**, 1594 (*isol, pmr, cmr*)

2,5-Cuparadiene-1,4,10-trione C-392

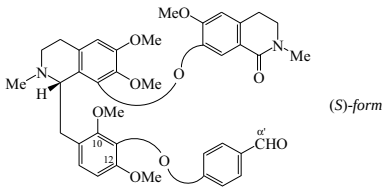
[306951-08-6]
Enokipodin B



$C_{15}H_{18}O_3$ 246.305
Metab. of *Flammulina velutipes* (velvet shank). $[\alpha]_D^{24}$ -63 (c, 0.05 in MeOH).

Ishikawa, N.K. *et al., Phytochemistry*, 2000, **54**, 777-782 (*isol, pmr, cmr*)

Curacautine C-393



(*S*)-*form*

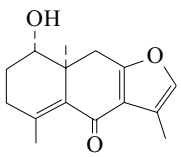
$C_{39}H_{42}N_2O_9$ 682.769

(ξ)-*form*
10-Demethoxy: [172924-26-4] ***Secoisotetrandrine***
$C_{38}H_{40}N_2O_8$ 652.743
Alkaloid from leaves of *Laurelia sempervirens* (Peruvian nutmeg). $[\alpha]_D^{20}$ +2.73 (c, 1.1 in $CHCl_3$). Abs. config. shown as *S*- in the lit., but apparently without evidence.

Schmeda-Hirschmann, G. *et al., Phytochemistry*, 1996, **41**, 339-341 (*Secoisotetrandrine*)

Curcolone C-394

[17015-43-9]
1α-Hydroxyfuranoeudesm-4-en-6-one. Nehipetol

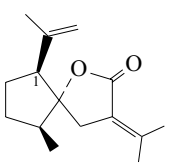


$C_{15}H_{18}O_3$ 246.305
Constit. of *Curcuma zedoaria* (zedoary). Cryst. (MeOH). Mp 139-139.5° (152-154°). $[\alpha]_D$ +13.7 (c, 3.8 in $CHCl_3$). λ_{max} 261 (log ϵ 3.92); 290 (log ϵ 3.85) (EtOH).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1065-1066; 1968, **16**, 827-831 (*isol, struct, abs config*)
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1976, **50**, 1931

Curcumanolide A C-395

[97550-04-4]



$C_{15}H_{22}O_2$ 234.338
Constit. of the crude drug zedoary (*Curcuma zedoaria*). Oil. $[\alpha]_D$ -33 (c, 1.2 in $CHCl_3$).

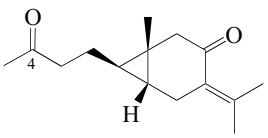
1-Epimer: [97452-55-6] ***Curcumanolide B***
$C_{15}H_{22}O_2$ 234.338
From *Curcuma zedoaria* (zedoary). Oil. $[\alpha]_D$ +24.2 (c, 1.4 in $CHCl_3$).

Shiobara, Y. *et al., Phytochemistry*, 1985, **24**, 2629
Shiobara, Y. *et al., Tet. Lett.*, 1985, **26**, 913 (*ir, pmr, cmr, ms, struct*)

Firman, K. *et al., Phytochemistry*, 1988, **27**, 3887-3891 (*isol*)
Hirukawa, T. *et al., Chem. Lett.*, 1992, 2343-2344 (*synth*)
Kato, T. *et al., Chem. Lett.*, 1992, 2343-2344 (*synth*)
Honda, T. *et al., J.C.S. Perkin 1*, 1994, 3567 (*synth*)
Fujita, T. *et al., J.O.C.*, 1997, **62**, 3824-3830 (*synth*)

Curcumenone C-396

[100347-96-4]



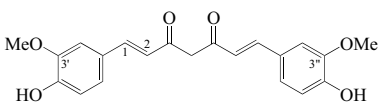
$C_{15}H_{22}O_2$ 234.338
Constit. of the crude drug zedoary (*Curcuma zedoaria*). Oil. $[\alpha]_D$ -12.7 (c, 1.1 in MeOH).

4S-Alcohol: ***4S-Dihydrocurcumenone***
$C_{15}H_{24}O_2$ 236.353
Constit. of zedoary (*Curcuma zedoaria*). Oil. $[\alpha]_D^{27}$ -5.1 ($CHCl_3$).

Shiobara, Y. *et al., Phytochemistry*, 1985, **24**, 2629 (*Curcumenone*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1186-1188 (*Dihydrocurcumenone*)
Matsuda, H. *et al., Tetrahedron*, 2001, **57**, 8443-8453 (*abs config*)

Curcumin C-397

[458-37-7]
1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, 9CI. Diferuloylmethane. Curcuma yellow. E100. C.I. Natural Yellow 3



$C_{21}H_{20}O_6$ 368.385
Isol. from *Curcuma zedoaria* (zedoary) and other *Curcuma* spp. flavouring ingredient. Natural colouring matter used extensively in Indian curries etc. Nutriceutical with anticancer and antiinflammatory props.. Orange prisms. Mp 183°. Log P 2.05 (calc).

▶ MI5230000

Di-Ac:
Cryst. Mp 170-171°.

Dibenzoyl:
Cryst. Mp 210°.

O-*De-Me:* [149732-51-4] ***1-(3,4-Dihydroxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione***
$C_{20}H_{18}O_6$ 354.359
Constit. of the rhizomes of *Curcuma domestica* (turmeric). Orange powder.

1,2-Dihydro: [76474-56-1] *5-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-4,6-heptadien-3-one, 9CI.* ***Dihydrocurcumin.*** *Letestuianin B*
$C_{21}H_{22}O_6$ 370.401
Constit. of *Curcuma longa* (turmeric). Yellow cryst. + ½ H_2O. Mp 179-180°. Enolised β-diketone λ_{max} 250 (log ε 4.1); 260 (sh) ; 280 (log ε 3.84); 305 (log ε 3.73); 375 (log ε 4.39) (EtOH).

5′-Methoxy: ***5′-Methoxycurcumin***
$C_{22}H_{22}O_7$ 398.412
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Yellow powder. Mp 145-146°.

Demethoxy: [22608-11-3] *1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, 9CI.* p-*Hydroxycinnamoylferuloylmethane.* ***Demethoxycurcumin***
$C_{20}H_{18}O_5$ 338.359
Isol. from *Curcuma zedoaria* (zedoary), *Curcuma longa (turmeric)*, *Curcuma xanthorrhiza* (Java turmeric). Orange-yellow powder. Mp 168°.

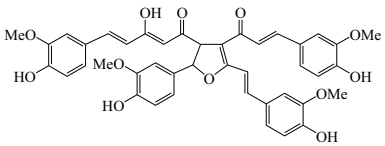
Bis(demethoxy): [22608-12-4] *1,7-Bis(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, 9CI.* p,p′-*Dihydroxydicinnamoylmethane.* ***Bisdemethoxycurcumin***
$C_{19}H_{16}O_4$ 308.333
Isol. from *Curcuma zedoaria* (zedoary) and *Curcuma longa* (turmeric). Yellow plates + H_2O (EtOH). Mp 224°.

Bis(demethoxy), 1,2-dihydro:1,7-Bis(4-hydroxyphenyl)-5-hydroxy-4,6-hepadien-3-one. 1,7-Bis(4-hydroxyphenyl)-1-heptene-3,5-dione
$C_{19}H_{18}O_4$ 310.349
Yellow needles (Et_2O/C_6H_6). Mp 148-149°. λ_{max} 215 (sh) ; 225 (sh) ; 362 (log ε 4.4) (MeOH).

[24939-16-0, 33171-05-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 52C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 800B (*nmr*)
Lampe, V. *et al., Ber.*, 1918, **51**, 1347 (*synth*)
Srinivasan, K.R. *et al., J. Pharm. Pharmacol.*, 1953, **5**, 448 (*derivs*)
Spicer, G.S. *et al., Anal. Chim. Acta*, 1958, **18**, 231 (*detn, B*)
Umland, F. *et al., Fresenius' Z. Anal. Chem.*, 1963, **197**, 151 (*detn, Ni*)
Jentzsch, K. *et al., Sci. Pharm.*, 1968, **36**, 251; *CA*, **70**, 90793h (*isol*)
Sastry, B.S. *et al., Res. Ind.*, 1970, **15**, 258; *CA*, **75**, 75063e (*isol*)
Kuroyagi, M. *et al., Yakugaku Zasshi*, 1970, **90**, 1467; *CA*, **74**, 61612a (*isol*)
Dyrssen, D.W. *et al., Anal. Chim. Acta*, 1972, **60**, 139 (*detn, B*)
Roughley, P.J. *et al., J.C.S. Perkin 1*, 1973, 2379-2388 (*biosynth*)
Karig, F. *et al., Dtsch. Apoth. -Ztg.*, 1975, **115**, 325; *CA*, **83**, 65372f (*derivs*)
Quint, P. *et al., Fresenius' Z. Anal. Chem.*, 1977, **285**, 356; 1979, **295**, 269 (*detn, B*)
Kashina, C. *et al., Heterocycles*, 1977, **7**, 241 (*synth*)
Wahlstrom, B. *et al., Acta Pharmacol. Toxicol.*, 1978, **43**, 86 (*metab*)
Holder, G.M. *et al., Xenobiotica*, 1978, **8**, 761 (*metab*)
Ravindranath, V. *et al., Phytochemistry*, 1980, **19**, 2031-2032 (*Dihydrocurcumin*)
Tønnesen, H.H. *et al., Acta Chem. Scand., Ser. B*, 1982, **36**, 475 (*cryst struct, bibl*)
Cheng, K.L. *et al., Handbook of Organic Analytical Reagents*, CRC Press, Boca Raton, 1982, 511 (*use*)
Ammon, H.P.T. *et al., Planta Med.*, 1991, **57**, 1-7 (*rev, pharmacol*)
Jitoe, A. *et al., J. Agric. Food Chem.*, 1992, **40**, 1337-1340 (*occur*)
Masuda, T. *et al., Phytochemistry*, 1992, **31**, 3645 (*5′-Methoxycurcumin*)
Nakayama, R. *et al., Phytochemistry*, 1993, **33**, 501 (*O-de-Me*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2856-2858
Dong, H. *et al., J. Nat. Prod.*, 1998, **61**, 142-144 (*isol, uv, ir, pmr, cmr, ms*)
Syu, W.-J. *et al., J. Nat. Prod.*, 1998, **61**, 1531-1534 (*isol, synth*)
Khar, A. *et al., FEBS Lett.*, 1999, **445**, 165-168 (*antitumour props*)

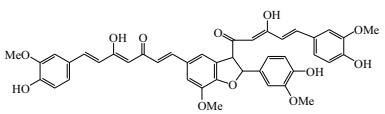
Curcumin dimer 1 C-398



$C_{42}H_{38}O_{12}$ 734.755
Constit. of the rhizomes of *Curcuma longa* (turmeric). Yellow powder.

Masuda, T. *et al., J. Agric. Food Chem.*, 2002, **50**, 2524-2530 (*isol, pmr*)

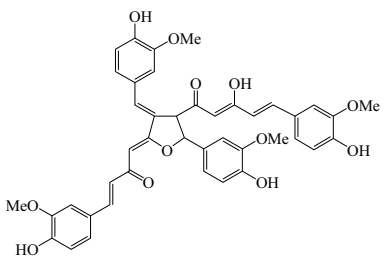
Curcumin dimer 2 C-399



$C_{42}H_{38}O_{12}$ 734.755
Constit. of the rhizomes of *Curcuma longa* (turmeric). Yellow solid.

Masuda, T. *et al., J. Agric. Food Chem.*, 2002, **50**, 2524-2530 (*isol, pmr, cmr*)

Curcumin dimer 3 C-400

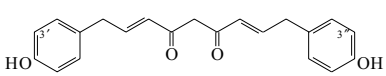


$C_{42}H_{38}O_{12}$ 734.755
Constit. of the rhizomes of *Curcuma longa* (turmeric). Yellow powder.

Masuda, T. *et al., J. Agric. Food Chem.*, 2002, **50**, 2524-2530 (*isol, pmr, cmr*)

Curcumin III C-401

[91884-88-7]
1,9-Bis(4-hydroxyphenyl)-2,7-nonadiene-4,6-dione, 9CI



$C_{21}H_{20}O_4$ 336.387
Isol. from the rhizomes of *Curcuma longa* (turmeric). Yellow pigment. Log P 2.39

(calc).

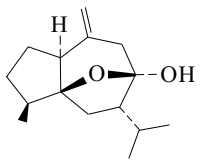
3′-Methoxy: [91884-87-6] ***Curcumin II***
$C_{22}H_{22}O_5$ 366.413
Isol. from the rhizomes of *Curcuma longa* (turmeric). Yellow pigment. Log P 2.24 (calc).

3′,3″-Dimethoxy: [91884-86-5] ***Curcumin I***
$C_{23}H_{24}O_6$ 396.439
Isol. from the rhizomes of *Curcuma longa* (turmeric). Yellow pigment. Log P 2.09 (calc).

Gorchakova, N.K. *et al., Farmatsiya (Moscow)*, 1984, **33**, 12; *CA*, **101**, 126880 (*isol, props*)
Nagabhusan, M. *et al., Mutat. Res.*, 1988, **202**, 163 (*props*)
Babu, K.V.D. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 674 (*synth*)
Ruby, A.J. *et al., Cancer Lett. (Shannon, Irel.)*, 1995, **94**, 79-83 (*antitumour props*)

Curcumol C-402

[4871-97-0]
5,8-Epoxy-10(14)-guaien-8-ol

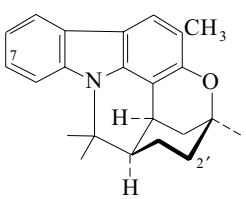


$C_{15}H_{24}O_2$ 236.353
Constit. of *Curcuma zedoaria* (zedoary). Cryst. Poorly sol. hexane. Mp 141-142°. $[\alpha]_D$ -32.26 (c, 2.127 in $CHCl_3$). Log P 3.4 (uncertain value) (calc).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1966, **14**, 1241-1249 (*isol, struct*)
Inayama, S. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3783-3786 (*cryst struct, abs config*)
Harimaya, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 843 (*isol, pmr, cryst struct*)
Phan, M.G. *et al., Tap Chi Hoa Hoc*, 2000, **38**, 91-94 (*activity*)

Currayangine C-403

9a,10,11,12,13,13a-Hexahydro-2,9,9,12-tetramethyl-1,12-epoxy-9H-indolo[3,2,1-de]phenanthridine, 9CI. Curryangine. Mahanimbidine. Murrayazoline



$C_{23}H_{25}NO$ 331.457

(+)-form
Needles (Me_2CO). Mp 276-278°. $[\alpha]_D^{25}$ +2.25 (c, 0.4 in $CHCl_3$).

2′-Hydroxy: [125287-09-4] ***Murrayazolinol***
$C_{23}H_{25}NO_2$ 347.456
Minor alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Mp 290°. The OH-config. does not appear to have been detd..

2′-Hydroxy, picrate: [125409-38-3]
Cryst. (C_6H_6). Mp 335°.

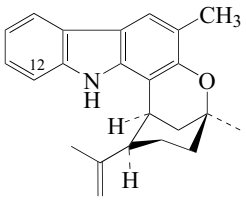
7-Hydroxy: [172617-68-4] ***Murrayamine E***
$C_{23}H_{25}NO_2$ 347.456
Prisms (MeOH). Mp 275-276° dec. $[\alpha]_D$ +39.68 (c, 0.133 in $CHCl_3$).

(±)-form [25488-37-3]
Alkaloid from the leaves and stem bark of *Murraya koenigii* (curryleaf tree). Cubes (C_6H_6). Mp 266° (260-262°).

Dutta, N.L. *et al., Indian J. Chem.*, 1969, **7**, 1061; 1168 (*uv, pmr, struct, synth*)
Kureel, S.P. *et al., Tet. Lett.*, 1969, 3857 (*uv, ir, pmr, ms, struct*)
Bordner, J. *et al., Experientia*, 1972, **28**, 1406 (*uv, cryst struct*)
Narasimhan, N.S. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 430 (*uv, ir, pmr, struct, synth*)
Bhattacharyya, P. *et al., J. Indian Chem. Soc.*, 1978, **55**, 308 (*uv, ir*)
Furukawa, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4132 (*isol, uv, ir, pmr, ms, struct*)
Bhattacharyya, L. *et al., J. Indian Chem. Soc.*, 1989, **66**, 140 (*Murrayazolinol*)
Wu, T.-S. *et al., Phytochemistry*, 1995, **40**, 1817 (*Murrayamine E*)

Currayanine C-404

[25488-33-9]
1,2,3,4,5,13-Hexahydro-5,7-dimethyl-2-(1-methylethenyl)-1,5-methanooxocino[3,2-a]carbazole, 9CI. Cyclomahanimbine. Murrayazolidine. Curryanine



$C_{23}H_{25}NO$ 331.457
Alkaloid from the leaves and stem bark of *Murraya koenigii* (curryleaf tree). Needles (hexane). Mp 137° Mp 146°. Probably an artifact. Obt. by brief acid or prolonged heat treatment of Mahanimbine, M-32.

N-Me:
Mp 169-170°.

Dihydro:
Mp 136-137° Mp 146°.

11-Hydroxy: [172548-90-2] ***Murrayamine D***
$C_{23}H_{25}NO_2$ 347.456
Oil.

12-Methoxy: [183130-90-7] ***Murrayamine H***
$C_{24}H_{27}NO_2$ 361.483
Syrup. λ_{max} 218 ; 243 ; 255 ; 301 ; 329 (MeOH).

Kureel, S.P. *et al., Tet. Lett.*, 1969, 3857 (*uv, ir, pmr, ms, struct*)
Chakraborty, D.P. *et al., Chem. Ind. (London)*, 1970, 593; 1974, 260 (*uv, ir, pmr, struct, synth*)
Bandaranayake, W.M. *et al., J.C.S. Perkin 1*, 1974, 998 (*struct, pmr, synth*)
Narasimhan, N. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 430 (*uv, ir, pmr, struct, synth*)
Reisch, J. *et al., Phytochemistry*, 1992, **31**, 2877 (*cryst struct*)
Wu, T.-S. *et al., Phytochemistry*, 1995, **40**, 1817; 1996, **43**, 785 (*Murrayamine D, Murrayamine H*)

Curvacin A C-405

[146239-44-3]
Polypeptide containing 41 amino acid residues. Prod. by *Lactobacillus curvatus* LTH 1174. Bacteriocin.

Tichaczek, P.S. *et al., Syst. Appl. Microbiol.*, 1992, **15**, 460-468 (*isol*)
Tichaczek, P.S. *et al., Arch. Microbiol.*, 1993, **166**, 279-283 (*struct*)

Curvacitins C-406

Proteins. Prod. by *Lactobacillus curvatus*. Bacteriocins with poss. food uses.

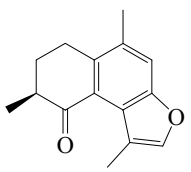
Curvaticin FS47 [157243-19-1]
Prod. by *Lactobacillus curvatus* FS47.

Curvaticin 13 [152742-61-5]
Prod. by *Lactobacillus curvatus* SB13.

Sudirman, I. *et al., Curr. Microbiol.*, 1993, **27**, 35-40 (*Curvaticin 13*)
Garver, K.L. *et al., Appl. Environ. Microbiol.*, 1994, **60**, 2191-2195 (*Curvaticin FS47*)

Curzeone C-407

[104068-56-6]
7,8-Dihydro-1,5,8-trimethylnaphtho[2,1-b]furan-9(6H)-one, 9CI



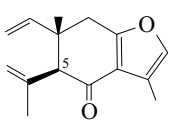
$C_{15}H_{16}O_2$ 228.29

(S)-form
Constit. of *Curcuma zedoaria* (zedoary). Cryst. Mp 72-74° (66-67°). $[\alpha]_D^{26}$ +61.5 (+24).

Shiobara, Y. *et al., Phytochemistry*, 1986, **25**, 1351-1353
Yang, C. *et al., Chin. Trad. Herbal Drugs*, 1998, **29**, 154-156 (*abs config*)

Curzerenone C-408

[20493-56-5]
Zedoarone



$C_{15}H_{18}O_2$ 230.306
Constit. of *Curcuma zedoaria* (zedoary). Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ 0. Log P 3.85 (calc). λ_{max} 272 (log ϵ 3.44) (EtOH). λ_{max} 276 (ϵ 5623) (EtOH) (Berdy). λ_{max} 264 (ϵ 3550) (hexane) (Berdy).

5-Epimer: [20085-85-2] ***5-Epicurzerenone.*** *5-epi-Curzerenone*
$C_{15}H_{18}O_2$ 230.306
From *Curcuma zedoaria* (zedoary). Oil. $[\alpha]_D$ 0. λ_{max} 220 (log ϵ 3.92); 270 (log ϵ 3.44) (EtOH).

[19956-58-2]

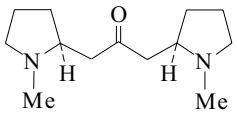
Fukushima, S. *et al., Yakugaku Zasshi*, 1968, **88**, 792-794; 1970, **90**, 863-869 (*isol, pharmacol*)

Hikino, H. *et al., J.C.S. Perkin 1*, 1975, 478-484 (*isol, struct*)
Miyashita, M. *et al., J.O.C.*, 1984, **49**, 3728 (*synth, bibl*)
Phan, M.G. *et al., Tap Chi Hoa Hoc*, 2000, **38**, 91-94 (*activity*)

Cuscohygrine C-409

[454-14-8]

[46727-05-3]
1,3-Bis(1-methyl-2-pyrrolidinyl)-2-propanone, 9CI. Cuskhygrine. Bellaradine. Hellaradine



$C_{13}H_{24}N_2O$ 224.345

Stereochem. not fully established. Natural Cuscohygrine is either the *meso*-form (illus.) or a mixt. of *meso*- and (±)-forms. Like other related alkaloids it appears to racemise and epimerise readily. It is unknown in opt. active form but opt. active dihydrocuscohygrine is known which suggests that the opt. active form may be present in the plant. The correct struct. was assigned by Liebermann in 1896 but for some years an incorrect alternative was put forward by Hess. Hellaradine appears to be a misprint in *CA* for Bellaradine. Alkaloid from the root of *Cyphomandra betacea* (tree tomato). Oil; cryst. + $3\frac{1}{2}H_2O$. d_4^{16} 0.98. Mp 40-41° (hydrate). $n_D^{18.4}$ 1.4845.

Methiodide:
Mp 244°.

Oxime:
Mp 53-54°.

[72407-34-2]

Liebermann, C. *et al., Ber.*, 1889, **22**, 675; 1896, **29**, 2050 (*isol, struct*)
Späth, E. *et al., Monatsh. Chem.*, 1948, **79**, 119 (*synth*)
Rapoport, H. *et al., J.O.C.*, 1949, **14**, 664 (*synth, struct*)
Anet, E. *et al., Nature (London)*, 1949, **163**, 289 (*synth*)
Galinovsky, F. *et al., Monatsh. Chem.*, 1951, **82**, 551; 1953, **84**, 798 (*synth, stereochem, bibl*)
El-Olemy, M.M. *et al., J. Nat. Prod.*, 1966, **29**, 58 (*synth*)
McGraw, B.A. *et al., Phytochemistry*, 1978, **17**, 257; 1979, **18**, 189 (*biosynth*)
Narasimhan, N.J. *et al., CA*, 1980, **92**, 42185u (*synth*)
Evans, W.C. *et al., Phytochemistry*, 1980, **19**, 2351 (*occur*)
Turner, C.E. *et al., Phytochemistry*, 1981, **20**, 1403 (*isol, stereochem, bibl*)
Leete, E. *et al., J.A.C.S.*, 1982, **104**, 1403 (*biosynth*)
Leete, E. *et al., Phytochemistry*, 1983, **22**, 699 (*biosynth*)
Ghani, A. *et al., Indian J. Pharm. Sci.*, 1985, **47**, 127; *CA*, **104**, 3308q (*occur*)
Stapper, C. *et al., J.O.C.*, 2002, **67**, 6456-6460 (*synth*)

Cyanocarbamodithioic acid, 9CI C-410

[108-04-3]
Cyanocarbonimidodithioic acid. Cyanodithioimidocarbonic acid. Cyanimidodithiocarbonic acid

$(HS)_2C{=}NCN \Leftrightarrow HSC(S)NHCN$

$C_2H_2N_2S_2$ 118.183

Esistence of free acid doubtful.

Di-Na salt: [138-93-2]
Antimicrobial agent used to control microorganisms in sugar cane and sugar beet mills.

Di-K salt: [13145-41-0]
Mp 217-225°.

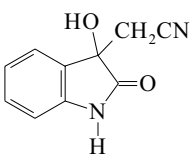
Di-Me ester: [10191-60-3] *Dimethyl cyanodithioiminocarbonate. DMT*
$C_4H_6N_2S_2$ 146.237
Cryst. (MeOH aq.). Mp 51-52.5°.

[34318-05-3, 35092-86-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 867A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1394C (*nmr*)
Hantzch, A. *et al., Annalen*, 1904, **331**, 265 (*synth*)
Timmons, R.J. *et al., J.O.C.*, 1967, **32**, 1566 (*synth, use*)
Jensen, K.A. *et al., Acta Chem. Scand.*, 1968, **22**, 1107 (*synth, use*)
Thalev, W.A. *et al., J.O.C.*, 1971, **36**, 14 (*synth, K salt*)
Wobig, D. *et al., Annalen*, 1972, **764**, 125 (*synth, use*)
Wittenbrook, L.S. *et al., J.O.C.*, 1973, **38**, 465 (*synth, use*)
Gattow, G. *et al., Z. Anorg. Allg. Chem.*, 1977, **433**, 211; **434**, 115 (*synth, ir*)
Klasinc, L. *et al., Gazz. Chim. Ital.*, 1980, **110**, 287 (*di-Me ester, pmr, uv*)
Yokoyama, M. *et al., J.C.S. Perkin 1*, 1988, 2309 (*di-Me ester, ir, pmr*)
Tominaga, Y. *et al., J. Het. Chem.*, 1991, **28**, 1039 (*di-Me ester, use, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 890-891 (*use*)
Marble, L.K. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 473-476 (*di-Me ester, synth, pmr, cmr*)

3-Cyanomethyl-3-hydroxy-1*H*-indol-2(3*H*)-one C-411

*2,3-Dihydro-3-hydroxy-2-oxo-1*H*-indole-3-acetonitrile, 9CI. 3-Cyanomethyl-3-hydroxy-2-oxo-1*H*-indole*



$C_{10}H_8N_2O_2$ 188.185

(-)-*form* [137761-24-1]
Alkaloid from brassicas inoculated with *Pseudomonas cichorii*. $[\alpha]_D$ -37.1 (c, 0.21 in MeOH).

(±)-*form* [137761-25-2]
Mp 162-163°.

Hallmann, G. *et al., Chem. Ber.*, 1962, **95**, 1138 (*synth*)
Monde, K. *et al., Phytochemistry*, 1991, **30**, 2915 (*isol, uv, ir, pmr, ms*)

3-[(Cyanophenylmethyl)amino]-3-oxopropanoic acid, 9CI C-412

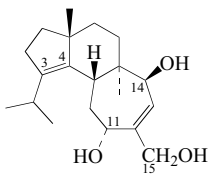


$C_{11}H_{10}N_2O_3$ 218.212

(*S*)-*form* [161470-12-8]
Metab. of Phoxim formed by soybean plants and cell cultures. Cryst. (EtOH/CH_2Cl_2).

Höhl, H.-U. *et al., J. Agric. Food Chem.*, 1995, **43**, 1052-1056 (*occur, synth*)

3,12-Cyathadiene-11,14,15-triol C-413



(11α,14β)-*form*

$C_{20}H_{32}O_3$ 320.471

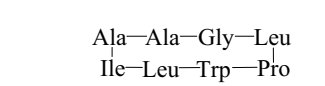
(11α,14β)-*form* [70116-99-3]
Cyathatriol
Powder (Me_2CO). Mp 172-173°.

*15-Aldehyde, 11-Ac, 14-*O*-β-D-xylopyranoside:* [291532-17-7] ***Erinacine P. Herical***
$C_{27}H_{40}O_8$ 492.608
Metab. of *Hericium erinaceum* (lion's mane) and *Hericium ramosum*.
Amorph. solid or oil. $[\alpha]_D^{25}$ -52.4 (c, 0.23 in MeOH). $[\alpha]_D^{25}$ -35.9 ($CHCl_3$). Erinacine P and Herical appear to be identical but this is not confirmed λ_{max} 206 (ϵ 7500); 228 (ϵ 6900) (MeOH).

(11β,14β)-*form*
*15-Aldehyde, 11-Et ether, 14-*O*-β-D-xylopyranoside:* [157397-40-5] ***Erinacine D***
$C_{27}H_{42}O_7$ 478.625
Metab. of *Hericium erinaceum* (lion's mane). Cryst. Mp 121-123°.

Steglich, W. *et al., DECHEMA-Monogr.*, 1993, **129**, 3-4 (*Herical*)
Kawagishi, H. *et al., Heterocycl. Commun.*, 1996, **2**, 51-54 (*Erinacine D*)
Kenmoku, H. *et al., Tet. Lett.*, 2000, **41**, 4389-4393 (*Erinacine P*)
Anke, T. *et al., Z. Naturforsch., C*, 2002, **57**, 263-271 (*Erinacine P, biosynth, pmr, cmr, ms*)

Cyclo(alanylalanylglycylleucylprolyltryptophylleucylisoleucyl) C-414



$C_{42}H_{63}N_9O_8$ 822.015

Constit. of the fruit peel of *Citrus medica* var. *sarcodactylis*. Powder. $[\alpha]_D^{24}$ -81.1 (c,

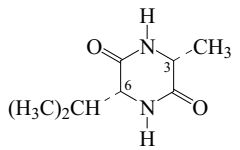
0.15 in MeOH). λ_{max} 224 (ϵ 13300); 282 (ϵ 4400) (MeOH).

Matsumoto, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 857-860 (*isol, pmr, cmr*)

Cyclo(alanylvalyl) C-415

[22160-42-5]

[125410-17-5]
3-Methyl-6-(1-methylethyl)-2,5-piperazinedione, 9CI. 3-Isopropyl-6-methyl-2,5-dioxopiperazine. Cyclo(valylalanyl). Alanine valine anhydride



(3*R*,6*R*)-*form*

$C_8H_{14}N_2O_2$ 170.211

(3*R*,6*R*)-*form*

[55904-06-8]
(+)-cis-*form*. *D-form*
Cryst. (H_2O). Mp 268-270°. $[\alpha]_D$ +48.9 (H_2O).

(3*R*,6*S*)-*form* [15136-27-3]
(+)-trans-*form*
Cryst. (H_2O). Mp 272-275°. $[\alpha]_D$ +38.6 (H_2O).

(3*S*,6*R*)-*form*

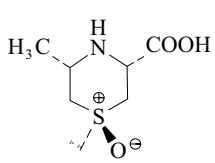
[55904-05-7]
(-)-trans-*form*
Cryst. (H_2O). Mp 273-276°. $[\alpha]_D$ -26.7 (H_2O).

(3*S*,6*S*)-*form* [15136-26-2]
(-)-cis-*form*. *L-form*
Cryst. (H_2O). Mp 268-270°. $[\alpha]_D$ -43.2 (c, 0.5 in H_2O).

(3ξ,6ξ)-*form*
Isol. from roasted cocoa.
Nitecki, D.E. *et al., J.O.C.*, 1968, **33**, 864-866 (*synth*)
Slater, G. *et al., J. Chem. Res.*, 1972, **64**, 166-169 (*glc*)
Pickenhagen, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1078-1086 (*occur, synth*)
Kricheldorf, H.R. *et al., Org. Magn. Reson.*, 1980, **13**, 52-58 (*cmr, N-15 nmr*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 233-237 (*synth*)
Qin, W.-J. *et al., Chung Ts'ao Yao*, 1981, **12**, 5-9; *CA*, **95**, 156423n (*occur*)
Thomas, A.R. *et al., Tetrahedron*, 1991, **47**, 497-506 (*synth, ir, pmr, cmr*)
Wabnitz, P.A. *et al., Int. J. Mass Spectrom. Ion Processes*, 1996, **154**, 193-201 (*ms*)

Cycloalliin C-416

[455-41-4]
5-Methyl-3-thiomorpholinecarboxylic acid 1-oxide, 9CI



Absolute configuration

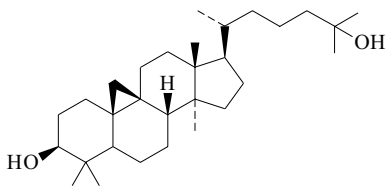
$C_6H_{11}NO_3S$ 177.224

Constit. of onion (*Allium cepa*). $[\alpha]_D^{20}$ -17.4 (H_2O).

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1959, **19**, 2257 (*synth, biosynth*)
Palmer, K.J. *et al., Acta Cryst. B*, 1972, **28**, 2615 (*cryst struct, abs config*)

Cycloartane-3,25-diol C-417

9,19-Cyclolanostane-3,25-diol

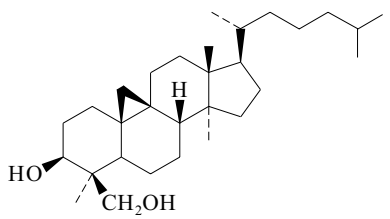


$C_{30}H_{52}O_2$ 444.74

3β-*form* [26525-84-8]
Constit. of mature wheat straw (*Triticum aestivum*).
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523

Cycloartane-3,29-diol C-418

9,19-Cyclolanostane-3,29-diol

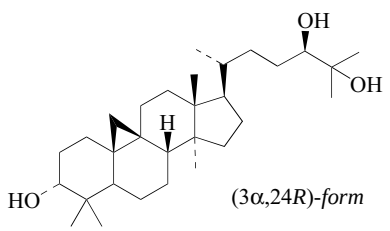


$C_{30}H_{52}O_2$ 444.74

3β-*form* [157772-00-4]
Constit. of *Mangifera indica* (mango). Cryst. Mp 196-198°. $[\alpha]_D$ +34.9 (c, 0.18 in $CHCl_3$).
Khan, M.A. *et al., J. Nat. Prod.*, 1994, **57**, 988 (*isol, pmr, cmr*)

Cycloartane-3,24,25-triol C-419

9,19-Cyclolanostane-3,24,25-triol



(3α,24*R*)-*form*

$C_{30}H_{52}O_3$ 460.739

(3α,24*R*)-*form*
Cryst. (MeOH). Mp 201-202°. $[\alpha]_D^{20}$ +35.9 (c, 0.33 in MeOH).

(3β,24*R*)-*form*

24-Ac: [339155-11-2]
$C_{32}H_{54}O_4$ 502.776
Cryst. ($CHCl_3$/hexane). Mp 160°.

3-Tetradecanoyl: [357419-30-8]
$C_{44}H_{78}O_4$ 671.098
Amorph. solid.

3-Hexadecanoyl: [357419-31-9]
$C_{46}H_{82}O_4$ 699.151
Cryst. Mp 81-82° .

24,25-Isopropylidene: [57576-30-4]
$C_{33}H_{56}O_3$ 500.804
Cryst. Mp 189°.

3-Ketone:24,25-Dihydroxycycloartan-3-one
$C_{30}H_{50}O_3$ 458.723
Cryst. (EtOH/hexane). Mp 150-152°. $[\alpha]_D^{20}$ +13.1 (c, 1.1 in $CHCl_3$).

(3β,24*S*)-*form*

25-Me ether: [357419-12-6] *25-Methoxycycloartane-3,24-diol*
$C_{31}H_{54}O_3$ 474.766
Cryst. Mp 140-145°. $[\alpha]_D$ +29 (c, 0.4 in $CHCl_3$).

25-Me ether, 3-hexadecanoyl: [357419-26-2]
$C_{47}H_{84}O_4$ 713.178
Amorph. solid.

(3β,24ξ)-*form* [110044-47-8]
Constit. of *Mangifera indica* (mango). Cryst. (C_6H_6). Mp 154-156°. $[\alpha]_D^{30}$ 0 (c, 0.8 in $CHCl_3$). Isol. as a mixt. of C-24 epimers.

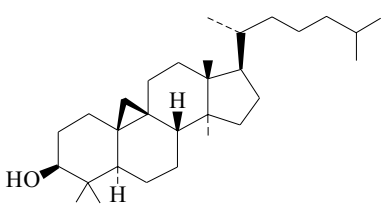
3-Ketone:
$C_{30}H_{50}O_3$ 458.723
Constit. of *Artocarpus heterophyllus* (jackfruit). Cryst. Mp 142-144°. $[\alpha]_D$ +17 (c, 0.36 in $CHCl_3$). Isol. as a mixt. of C-24 epimers.

[155060-47-2, 155060-48-3]

Anjaneyulu, V. *et al., Phytochemistry*, 1985, **24**, 2359
Arriaga-Giner, F.J. *et al., Z. Naturforsch., C*, 1991, **46**, 507 (*acetonide*)
Barik, B.R. *et al., Phytochemistry*, 1994, **35**, 1001 (*isol, pmr, cmr*)
Della Greca, M. *et al., Phytochemistry*, 1994, **35**, 1017 (*isol, pmr, cmr*)
Inada, A. *et al., J. Nat. Prod.*, 1995, **58**, 1143 (*isol, pmr, cmr*)
Inada, A. *et al., Phytochemistry*, 1997, **46**, 379-381 (*3α,24R-form*)
Bhattacharyya, K. *et al., Acta Cryst. C*, 2000, **56**, 979-980 (*3-ketone, cryst struct*)
Ukiya, M. *et al., J. Agric. Food Chem.*, 2001, **49**, 3187-3197 (*Chrysanthemum morifolium constits*)
Hisham, A. *et al., Phytochemistry*, 2001, **56**, 331-334 (*24-Ac*)

Cycloartanol C-420

[4657-58-3]
9β,19-Cyclolanostan-3β-ol. Cycloartan-3β-ol



$C_{30}H_{52}O$ 428.74
Minor constit. of rice bran oil. Cryst. (MeOH aq.). Mp 101-102°. $[\alpha]_D$ +45 (c, 3.59 in $CHCl_3$). Log P 10.8 (uncertain value) (calc).

Ac: [4575-74-0]
$C_{32}H_{54}O_2$ 470.777

Cryst. ($CHCl_3$/MeOH). Mp 132-133°. $[\alpha]_D$ +57 (c, 5.31 in $CHCl_3$).

*3-(2-Methylbutanoyl)(*R-*):* [207606-42-6]
$C_{35}H_{60}O_2$ 512.858
Cryst. Mp 123-124°. $[\alpha]_D^{20}$ +67 ($CHCl_3$).

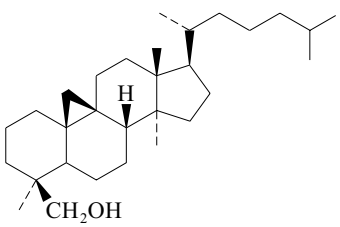
3-(4-Hydroxy-3-methoxycinnamoyl): [20972-10-5] *Cycloartanyl ferulate*
$C_{40}H_{60}O_4$ 604.912
Constit. of rice bran oil.

3-Ketone: [4936-10-1] *Cycloartan-3-one.* ***Cycloartanone***
$C_{30}H_{50}O$ 426.724

Shimizu, M. *et al., Chem. Pharm. Bull.*, 1960, **8**, 108 (*isol*)
Altenburger, E. *et al., Helv. Chim. Acta*, 1965, **48**, 704 (*synth*)
Audier, H.E. *et al., Tet. Lett.*, 1966, 4341 (*ms*)
Berti, G. *et al., Tet. Lett.*, 1967, 125 (*isol*)
Endo, T. *et al., CA*, 1968, **69**, 37319n (*isol, ferulate*)
Imhof, R. *et al., Chem. Comm.*, 1969, 852 (*synth*)
Khuong-Huu, F. *et al., Tet. Lett.*, 1975, 1787 (*cmr*)
Ageta, H. *et al., Phytochemistry*, 1984, **23**, 2875 (*isol, acetate*)
Böhme, F. *et al., Phytochemistry*, 1997, **45**, 1041-1044 (*Cycloartanone, ms*)
Tellez, N. *et al., Molecules*, URL:http://www.mdpi.org/molbank/m0049.htm, 1998, **3**, M49; *CA*, **129**, 14430j (*2-methylbutanoate*)

Cycloartan-29-ol C-421

[157772-01-5]
9,19-Cyclolanostan-29-ol

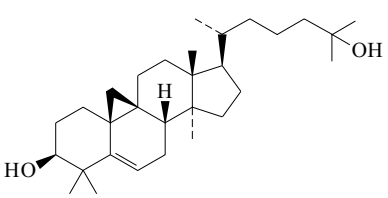


$C_{30}H_{52}O$ 428.74
Constit. of *Mangifera indica* (mango). Cryst. Mp 180-182°. $[\alpha]_D$ +27.38 (c, 0.21 in $CHCl_3$).

Khan, M.A. *et al., J. Nat. Prod.*, 1994, **57**, 988 (*isol, pmr, cmr*)

Cycloart-5-ene-3,25-diol C-422

9,19-Cyclolanost-5-ene-3,25-diol



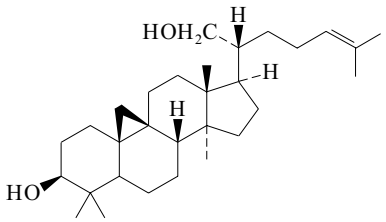
$C_{30}H_{50}O_2$ 442.724

3β-*form* [151676-48-1]
Constit. of mature wheat straw (*Triticum aestivum*).

Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523 (*isol*)

Cycloart-24-ene-3,21-diol C-423

9,19-Cyclolanost-24-ene-3,21-diol



$C_{30}H_{50}O_2$ 442.724

3β-*form* [125292-57-1]
Cryst. ($CHCl_3$). Mp 130°. $[\alpha]_D^{21}$ +41 (c, 0.96 in $CHCl_3$).

21-Aldehyde: [125292-62-8] ***3-Hydroxycycloart-24-en-21-al***
$C_{30}H_{48}O_2$ 440.708
Cryst. (Me_2CO). Mp 79-81°. $[\alpha]_D^{21}$ +47 (c, 0.28 in $CHCl_3$).

21-Carboxylic acid: [125302-31-0] ***3-Hydroxycycloart-24-en-21-oic acid***
$C_{30}H_{48}O_3$ 456.707
Constit. of *Lansium domesticum* (langsat). Cryst. ($CHCl_3$). Mp 185-186° (181°). $[\alpha]_D^{21}$ +23 (c, 0.48 in $CHCl_3$) (+18.7).

21-Aldehyde, 3-ketone: [125292-61-7] ***3-Oxocycloart-24-en-21-al***
$C_{30}H_{46}O_2$ 438.692
Cryst. (Me_2CO). Mp 80-82°. $[\alpha]_D^{21}$ +20 (c, 0.72 in $CHCl_3$).

Nishizawa, M. *et al., Tet. Lett.*, 1989, **30**, 5615 (*cryst struct*)
Achenbach, H. *et al., Phytochemistry*, 1992, **31**, 4263 (*isol, pmr, cmr*)

Cycloart-24-ene-3,26-diol C-424

9,19-Cyclolanost-24-ene-3,26-diol

$C_{30}H_{50}O_2$ 442.724

(3β,24*E*)-*form* [64396-81-2] ***Mangiferadiol***
Constit. of *Mangifera indica* (mango). Needles (C_6H_6). Mp 154-155°. $[\alpha]_D^{30}$ +51 (c, 1 in $CHCl_3$).

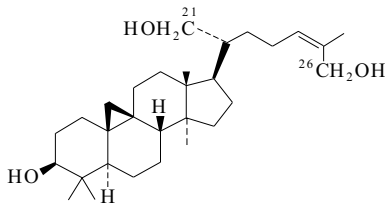
Di-Ac:
Needles (MeOH). Mp 74-77°. $[\alpha]_D^{30}$ +107.7 (c, 0.7 in $CHCl_3$).

3-Ketone, 26-aldehyde: [105986-49-0] ***3-Oxocycloart-24-en-26-al***
$C_{30}H_{46}O_2$ 438.692
Amorph. solid. $[\alpha]_D^{25}$ +25 (c, 0.06 in $CHCl_3$).

Corsano, S. *et al., Tet. Lett.*, 1965, 2377 (*synth*)
Anjaneyulu, V. *et al., Phytochemistry*, 1985, **24**, 2359 (*isol, pmr, cmr*)
Cabrera, G.M. *et al., J. Nat. Prod.*, 1996, **59**, 343 (*isol, pmr, cmr*)

Cycloart-24-ene-3,21,26-triol C-425

9β,19-Cyclolanost-24-ene-3,21,26-triol



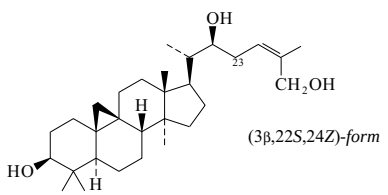
$C_{30}H_{50}O_3$ 458.723

(3β,24*Z*)-*form*
Cryst. (EtOAc/hexane). Mp 170°. $[\alpha]_D^{25}$ +43 (c, 1.02 in MeOH).

3,26-Di-O-*gentibioside:* [100182-36-3] ***Quadrangulosside***
$C_{54}H_{90}O_{23}$ 1107.291
Constit. of *Passiflora quadrangularis* (giant grandilla). Amorph. powder. Mp 164-165° dec. $[\alpha]_D^{25}$ -11 (c, 0.89 in MeOH).

Orsini, F. *et al., Phytochemistry*, 1986, **25**, 191

Cycloart-24-ene-3,22,26-triol C-426



(3β,22*S*,24*Z*)-*form*

$C_{30}H_{50}O_3$ 458.723

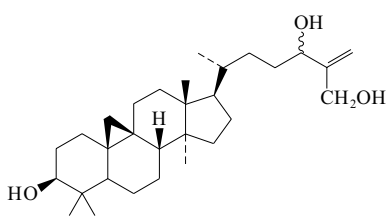
(3α,22ξ,24*E*)-*form*
26-Carboxylic acid: ***3,22-Dihydroxycycloart-24-en-26-oic acid***
$C_{30}H_{48}O_4$ 472.707
Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 218-220°. $[\alpha]_D^{30}$ +27.5 (c, 0.8 in $CHCl_3$).

(3β,22*S*,24*E*)-*form*
26-Carboxylic acid:
Constit. of *Mangifera indica* (mango).

Anjaneyulu, V. *et al., Phytochemistry*, 1989, **28**, 1471
Yoshimitsu, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2465

Cycloart-25-ene-3,24,27-triol C-427

9,19-Cyclolanost-25-ene-3,24,27-triol



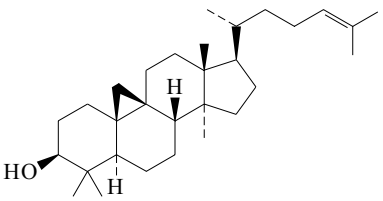
$C_{30}H_{50}O_3$ 458.723

(3β,24ξ)-*form*
Constit. of *Mangifera indica* (mango). Cryst. (C_6H_6/hexane). Mp 190-192°. $[\alpha]_D^{20}$ +18.8 (c, 1.2 in $CHCl_3$). Isolated as a mixture of C-24 epimers.

Anjaneyulu, V. *et al., Phytochemistry*, 1985, **24**, 2359

Cycloart-24-en-3-ol C-428

9,19-Cyclo-9β-lanost-24-en-3-ol



$C_{30}H_{50}O$ 426.724

3β-*form* [469-38-5]
Cycloartenol. *Artosenol*. *Handianol*
Constit. of *Artocarpus integrifolia* fruits and *Solanum tuberosum* (potato). Cryst. (EtOH). Mp 115° (dry) Mp 99° (solvated). $[\alpha]_D$ +54 ($CHCl_3$).

Ac:Cycloartenyl acetate
$C_{32}H_{52}O_2$ 468.762
Mp 122°. $[\alpha]_D$ +57 (c, 1.97 in $CHCl_3$).

*3-*O*-(4-Hydroxycinnamoyl)(*E*-):****Arundinol***
$C_{39}H_{56}O_3$ 572.87
Cryst. (EtOAc/petrol). Mp 245°. $[\alpha]_D$ +3.52 (MeOH).

*3-(4-Hydroxy-3-methoxycinnamoyl):****Oryzanol A***
$C_{40}H_{58}O_4$ 602.896
From rice bran oil (*Oryza sativa*). Cryst. Mp 148-150°. $[\alpha]_D$ +40 (c, 1 in $CHCl_3$). Oryzanol B was a mixt. of Oryzanol A and Oryzanol C (see under 24-Methylenecycloartan-3-ol, M-404).

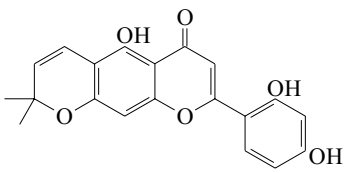
3-Ketone: [511-63-7] *9,19-Cyclolanost-24-en-3-one*. ***Cycloartenone***. *Artostenone*. *Cycloart-24-en-3-one*
$C_{30}H_{48}O$ 424.709
Mp 109°. $[\alpha]_D$ +24 (c, 3.39 in $CHCl_3$).

*3-*O*-(3,4-Dihydroxycinnamoyl)(*E*-):*
[75884-34-3] ***Caffeoylcycloartenol***
$C_{39}H_{56}O_4$ 588.869
Constit. of *Phalaris canariensis* (canary grass).

Chapon, S. *et al., Bull. Soc. Chim. Fr.*, 1952, 456 (*isol*)
Bentley, H.R. *et al., J.C.S.*, 1953, 3673 (*isol, struct*)
Barton, D.H.R. *et al., J.C.S.*, 1954, 2715 (*struct*)
Irvine, D.S. *et al., J.C.S.*, 1955, 1316 (*struct*)
Shimizü, M. *et al., Chem. Pharm. Bull.*, 1960, **8**, 108 (*isol*)
Capella, P. *et al., Nature (London)*, 1961, **190**, 167 (*isol*)
Ardenne, M. *et al., Experientia*, 1963, **19**, 178 (*ms*)
Galbraith, M.N. *et al., Aust. J. Chem.*, 1965, **18**, 226 (*acetate*)
Fedeli, E. *et al., J. Am. Oil Chem. Soc.*, 1966, **43**, 254 (*occur*)
Aplin, R.T. *et al., J.C.S.(B)*, 1966, 1078 (*ms*)
Barton, D.H.R. *et al., Chem. Comm.*, 1968, 643 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2035 (*occur*)
Radics, L. *et al., Tet. Lett.*, 1975, **48**, 4287 (*cmr*)
Boar, R.B. *et al., J.C.S. Perkin 1*, 1979, 563 (*synth*)
De Pascual Teresa, J. *et al., Phytochemistry*, 1987, **26**, 1767 (*pmr, cmr*)
Seo, S. *et al., J.C.S. Perkin 1*, 1988, 2407 (*biosynth*)
Milon, A. *et al., Helv. Chim. Acta*, 1989, **72**, 1 (*pmr, cmr*)
Majumder, P.L. *et al., J. Indian Chem. Soc.*, 1991, **68**, 88 (*Arundinol*)
Dominguez, X.A. *et al., Planta Med.*, 1992, **58**, 382 (*Caffeoylcycloartenol*)
Akihisha, T. *et al., J. Agric. Food Chem.*, 2000, **48**, 2313-2319 (*activity*)

Cycloartocarpesin C-429

[23806-61-3]
*8-(2,4-Dihydroxyphenyl)-5-hydroxy-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b′*]dipyran-6-one, 9CI*

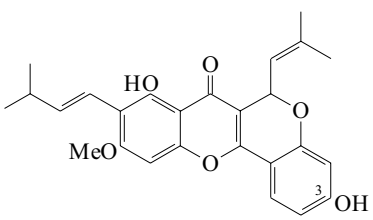


$C_{20}H_{16}O_6$ 352.343
Isol. from *Artocarpus heterophyllus* (jackfruit).

Parthasarathy, P.C. *et al., Indian J. Chem.*, 1969, **7**, 101 (*isol, uv, pmr, ms*)
Rao, A.V.R. *et al., Indian J. Chem.*, 1972, **10**, 905; 989 (*isol, ms*)
Fujimoto, T. *et al., Planta Med.*, 1985, 190 (*isol*)

Cycloartocarpin C-430

[5912-09-4]
*3,8-Dihydroxy-10-methoxy-9-(3-methyl-1-butenyl)-6-(2-methyl-1-propenyl)-6*H*,7*H*-[1]benzopyrano[4,3-*b*][1]benzopyran-7-one. Isoartocarpin*†



$C_{26}H_{26}O_6$ 434.488
The name Cycloartocarpin has been assigned to two isomeric compds..

Di-Me ether:
$[\alpha]_D^{25}$ +1.19 (c, 2.25 in $CHCl_3$).

O-*De-Me:* [145682-71-9] ***Cyclocommunin***. *Isocyclomulberrin*
$C_{25}H_{24}O_6$ 420.461
Isol. from the rootbark of *Artocarpus communis* and stems of *Artocarpus altilis* (breadfruit). Yellow powder (C_6H_6). Mp 277-279° (270-271°). $[\alpha]_D^{25}$ +53 (c, 0.31 in Me_2CO).

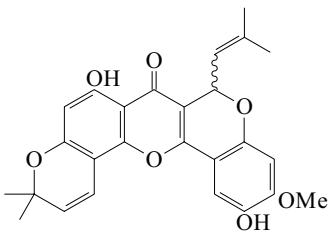
O-*De-Me, tri-Ac:* [145643-99-8]
Pale yellow needles. Mp 173-175°.

O-*De-Me, 3-Me ether:* [156127-37-6] ***Cycloartocarpin***†
$C_{26}H_{26}O_6$ 434.488
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow microneedles (Me_2CO/cyclohexane). Mp 262-264°.

Dave, K.G. *et al., Tet. Lett.*, 1962, 9 (*isol*)
Nair, P.M. *et al., Tet. Lett.*, 1964, 125 (*isol*)
Rao, A.V.R. *et al., Indian J. Chem.*, 1972, **10**, 989 (*ms*)
Lin, C.N. *et al., Phytochemistry*, 1992, **31**, 2922 (*Cyclocommunin*)
Chen, C.C. *et al., J. Nat. Prod.*, 1993, **56**, 1594 (*Isocyclomulberrin*)
Lu, C.-M. *et al., Phytochemistry*, 1994, **35**, 781 (*isol, pmr, cmr*)

Cycloartomunin C-431

[135023-19-7]
*6,12-Dihydroxy-11-methoxy-3,3-dimethyl-8-(2-methyl-1-propenyl)-3*H*,7*H*,8*H*-bis[1]benzopyrano[4,3-*b*:6′,5′-*e*]pyran-7-one, 9CI*



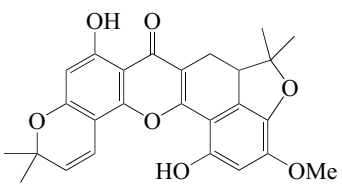
$C_{26}H_{24}O_7$ 448.471
Isol. from the root bark of *Artocarpus communis* (breadfruit). Yellow needles (MeOH). Mp 278-280°.

Di-Ac:
Needles ($CHCl_3$). Mp 274-276°.

Lin, C.-N. *et al., Phytochemistry*, 1991, **30**, 1669; 1996, **41**, 1215 (*isol, uv, pmr, cmr*)

Cycloartomunoxanthone C-432

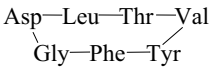
[135023-20-0]



$C_{26}H_{24}O_7$ 448.471
Constit. of the roots of *Artocarpus communis* (breadfruit). Dark yellow powder. Mp 264-266°. λ_{max} 224 (log ε 4.13); 253 (log ε 4); 280 (log ε 4.1); 311 (sh) (log ε 3.76); 384 (log ε 3.85) (MeOH).

Lin, C.N. *et al., Phytochemistry*, 1991, **30**, 1669-1671 (*isol, uv, cmr*)

Cyclo(aspartylleucylthreonylvalyltyrosylphenylalanylglycyl) C-433

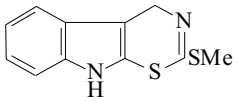


$C_{39}H_{53}N_7O_{11}$ 795.888
Constit. of the fruit peel of *Citrus medica* var. *sarcodactylis*. Powder. $[\alpha]_D^{24}$ -22.3 (c, 0.25 in MeOH). λ_{max} 212 (ε 14200); 278 (ε 1800) (MeOH).

Matsumoto, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 857-860 (*isol, pmr, cmr, ms*)

Cyclobrassinin C-434

[105748-58-1]
4,9-Dihydro-2-(methylthio)-1,3-thiazino[6,5-b]indole, 9CI



$C_{11}H_{10}N_2S_2$ 234.345
Isol. from Chinese cabbage (*Brassica campestris* ssp. *pekinensis*)(Cruciferae) heads inoculated with *Pseudomonas cichorii*. Mp 136-137°. First report of the isol. of sulfur-containing phytoalexins (see also Brassinin, B-180) λ_{max} 204 (ϵ 24700); 227 (ϵ 34000); 284 (ϵ 7830); 294 (ϵ 8170) (MeOH) (Berdy). λ_{max} 220 (ϵ 19200); 270 (ϵ 13200) (EtOH) (Berdy).

S-*Oxide:* [128722-96-3] *4,9-Dihydro-2-(methylsulfinyl)-1,3-thiazino[6,5-b]indole, 9CI.* ***Cyclobrassinin sulfoxide***
$C_{11}H_{10}N_2OS_2$ 250.345
Isol. from leaves of brown mustard *Brassica juncea* (Cruciferae). Pale yellow grains. Mp 188-190°.

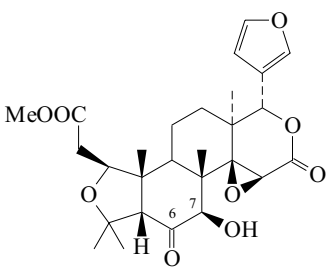
9-N-*Methoxy:* ***Sinalbin B***
$C_{12}H_{12}N_2OS_2$ 264.372
Isol. from *Sinapis alba* (white mustard). λ_{max} 231 (log ϵ 4.13); 275 (log ϵ 3.8) (CH_2Cl_2).

9-N-*Methoxy,* S-*oxide:* ***Sinalbin A***
Isol. from *Sinapis alba* (white mustard). λ_{max} 231 (log ϵ 4.33); 280 (log ϵ 3.96) (CH_2Cl_2).

Takasugi, M. *et al., Chem. Comm.*, 1986, 1077 (*isol, synth, struct*)
Devys, M. *et al., Phytochemistry*, 1990, **29**, 1087 (*isol, ir, pmr, ms, struct, oxide*)
Kutschy, P. *et al., Tetrahedron*, 1998, **54**, 3549-3566 (*synth*)
Pedras, M.S.C. *et al., Phytochemistry*, 2000, **53**, 161-176 (*rev*)
Pedras, M.S.C. *et al., Phytochemistry*, 2000, **55**, 213-216 (*Sinalbins*)

Cyclocalamin C-435

[74751-39-6]

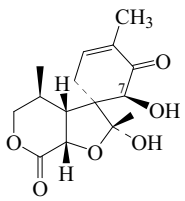


$C_{27}H_{34}O_9$ 502.56
Constit. of calamondin seeds (*Citrus reticulata* var. *austera* x *Fortunella* sp.). Gum.

7-Ketone, 6β-alcohol: [111004-32-1] ***Isocyclocalamin***
$C_{27}H_{34}O_9$ 502.56
Constit. of a *Citrus reticulata*/*Fortunella* hybrid.

Bennett, R.D. *et al., Tetrahedron*, 1981, **37**, 17 (*Cyclocalamin*)
Herman, Z. *et al., Phytochemistry*, 1987, **26**, 2247 (*Isocyclocalamin*)
Hasegawa, S. *et al., Phytochemistry*, 1988, **27**, 1349 (*biosynth*)

Cyclocalopin A C-436



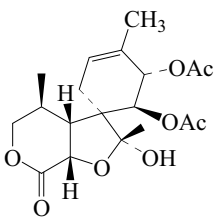
Relative Configuration

$C_{15}H_{20}O_6$ 296.319
Bitter principle isol. from *Boletus calopus* and other *Boletus* spp.. Cryst. Mp 165°. $[\alpha]_D^{25}$ -34.5 (c, 0.2 in $CHCl_3$). λ_{max} 211 (log ϵ 2.57); 243 (log ϵ 2.8) (EtOH). λ_{max} 200 (log ϵ 2.51); 241 (log ϵ 2.65) (MeCN).

7-Ac: O-*Acetylcyclocalopin A*
$C_{17}H_{22}O_7$ 338.357
Major bitter principle from *Boletus calopus* and other *Boletus* spp.. Cryst. Mp 190°. $[\alpha]_D^{25}$ -29.1 (c, 0.35 in $CHCl_3$). λ_{max} 218 (log ϵ 2.37); 273 (log ϵ 2.64) (EtOH). λ_{max} 238 (log ϵ 2.51); 332 (log ϵ 1.12) (MeCN).

Hellwig, V. *et al., Eur. J. Org. Chem.*, 2002, 2895-2904 (*isol, uv, cd, ir, pmr, cmr, cryst struct*)

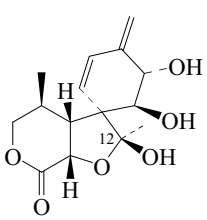
Cyclocalopin B C-437



$C_{19}H_{26}O_8$ 382.41
Isol. from *Boletus calopus* and other *Boletus* spp.. Oil. $[\alpha]_D^{33}$ +18.7 (c, 0.1 in $CHCl_3$). λ_{max} 201 (log ϵ 3.09) (MeCN).

Hellwig, V. *et al., Eur. J. Org. Chem.*, 2002, 2895-2904 (*isol, cd, pmr, cmr, ms*)

Cyclocalopin C_1 C-438

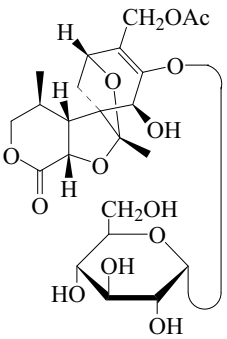


$C_{15}H_{20}O_6$ 296.319
Isol. from *Boletus radicans*. Oil. $[\alpha]_D^{33}$ +168.6 (c, 0.12 in $CHCl_3$). Obt. as a 2:1 mixt. with Cyclocalopin C_2 to which the data refers λ_{max} 228 (log ϵ 3.18); 240 (sh) (log ϵ 2.94) (MeCN).

12-Epimer: ***Cyclocalopin C₂***
$C_{15}H_{20}O_6$ 296.319
Isol. from *Boletus radicans*.

Hellwig, V. *et al., Eur. J. Org. Chem.*, 2002, 2895-2904 (*isol, pmr, cmr, ms*)

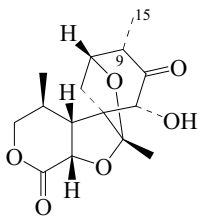
Cyclocalopin D C-439



$C_{23}H_{32}O_{13}$ 516.498
Isol. from *Boletus calopus* and other *Boletus* spp.. Cryst. Mp 110°. $[\alpha]_D^{25}$ +109.7 (c, 0.26 in MeOH). λ_{max} 212 (log ϵ 3.01); 244 (log ϵ 1.91) (MeOH).

Hellwig, V. *et al., Eur. J. Org. Chem.*, 2002, 2895-2904 (*isol, cd, ir, pmr, cmr, ms*)

Cyclocalopin E C-440



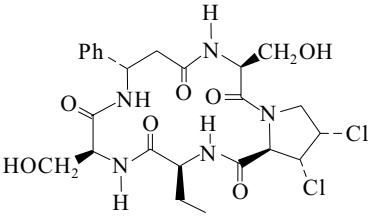
$C_{15}H_{20}O_6$ 296.319
Isol. from *Boletus calopus* and other *Boletus* spp.. Cryst. Mp 183°. $[\alpha]_D^{33}$ +38 (c, 1.1 in MeCN). λ_{max} 226 (sh) (log ϵ 2.19); 283 (log ϵ 1.9) (MeCN).

9,15-Didehydro: ***Cyclocalopin F***
$C_{15}H_{18}O_6$ 294.304
Isol. from *Boletus calopus* and other *Boletus* spp.. Obt. as a mixt. with Cyclocalopin E.

Hellwig, V. *et al., Eur. J. Org. Chem.*, 2002, 2895-2904 (*isol, cd, ir, pmr, cmr, ms*)

Cyclochlorotine C-441

[12663-46-6]
Cyclic[3-phenyl-β-alanylseryl-3,4-dichloroprolylaminobutyrylseryl], 9CI



$C_{24}H_{31}Cl_2N_5O_7$ 572.444

Mycotoxin prod. by the common food storage mould *Penicillium islandicum*. Needles (MeOH). Mp 255° dec. $[\alpha]_D^{16}$ -92.9 (MeOH). Similar chemical and biological characteristics to Islanditoxin, I-66 λ_{max} 250 (ϵ 4550); 257 (ϵ 5000); 265 (ϵ 4670) (EtOH) (Derep).

▶ GU2100000

Yoshioka, H. *et al., Chem. Lett.*, 1973, 1319 (*cryst struct*)

Enomoto, M. *et al., Mycotoxins*, (I.F.H. Purchase Ed.), Elsevier, Amsterdam, 1974, 303 (*rev*)

Ghosh, A.C. *et al., Appl. Environ. Microbiol.*, 1978, **35**, 1074 (*manuf*)

Anderegg, R.J. *et al., Biomed. Mass Spectrom.*, 1979, **6**, 129 (*ms*)

Ghosh, A.C. *et al., J. Het. Chem.*, 1980, **17**, 1809 (*rev*)

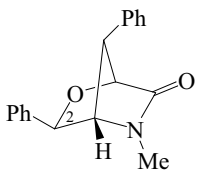
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 708

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COW750

Cycloclausenamide C-442

[103541-16-8]

5-Methyl-3,7-diphenyl-2-oxo-5-azabicyclo[2.2.1]heptan-6-one, 9CI



$C_{18}H_{17}NO_2$ 279.338

Obt. as a pair of C-2 epimers. Isol. from the leaves of *Clausena lansium* (wampee). Prisms. Mp 164-166°. $[\alpha]_D^{24.5}$ -40 (c, 0.255 in MeOH).

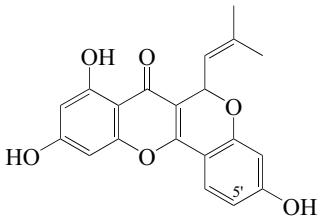
Yang, M. *et al., Phytochemistry*, 1988, **27**, 445-450 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Zhao, B. *et al., Yaoxue Xuebao*, 2001, **36**, 373-376 (*cryst struct, conformn*)

Cyclocommunol C-443

[145643-96-5]

3,8,10-Trihydroxy-6-(2-methyl-1-propenyl)-6H,7H-[1]benzopyrano[4,3-b]benzopyran-7-one, 9CI



$C_{20}H_{16}O_6$ 352.343

Isol. from the root bark of *Artocarpus communi* (breadfruit). Yellow powder (C_6H_6). Mp 160-162°.

5′-Hydroxy: [180845-64-1] ***Cyclochampedol***

$C_{20}H_{16}O_7$ 368.342

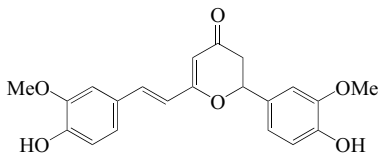
Yellow cryst. ($CHCl_3$/MeOH). Mp 205-206°. $[\alpha]_D^{25}$ +141.6 (c, 0.1 in MeOH). λ_{max} 212 (log ϵ 4.64); 269 (log ϵ 4.42); 315 (sh) (log ϵ 3.98); 399 (log ϵ 4.29) (MeOH). λ_{max} 269 (ϵ 26300); 315 (ϵ 9600); 399 (ϵ 19500) (MeOH) (Berdy). λ_{max} 214 (ϵ 97770); 276 (ϵ 30900); 438 (ϵ 34670) (MeOH-NaOH) (Berdy).

Lin, C.-N. *et al., Phytochemistry*, 1992, **31**, 2922 (*isol, pmr, cmr*)

Achmad, S.A. *et al., J. Nat. Prod.*, 1996, **59**, 878 (*Cyclochampedol*)

Cyclocurcumin C-444

[153127-42-5]



$C_{21}H_{20}O_6$ 368.385

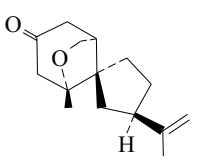
Constit. of the rhizome of *Curcuma longa* (turmeric). Yellow gum. λ_{max} 233 (log ϵ 4.4); 262 (log ϵ 4.28); 373 (log ϵ 4.89) (EtOH).

Kiuchi, F. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1640-1643 (*isol, uv, ir, pmr, cmr, ms*)

Cyclodehydroisolubimin C-445

[72055-93-7]

4,10-Epoxy-11-spirovetiven-2-one



$C_{15}H_{22}O_2$ 234.338

Constit. of potatoes infected with *Phytophthora infestans*. Oil. $[\alpha]_D^{26}$ -6.5 (c, 0.46 in $CHCl_3$).

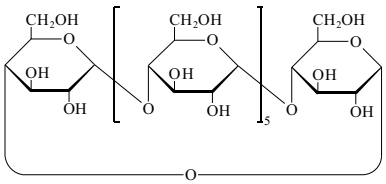
Coxon, D.T. *et al., Chem. Comm.*, 1979, 348

β-Cyclodextrin, 9CI C-446

[7585-39-9]

[68168-23-0]

*Cycloheptakis-(1→4)-(α-D-glucopyranose). Cycloheptaamylose. Cyclomaltoheptaose. **Betadex, INN, USAN**. Beta cyclodextrin, USAN. Cycloheptaglucan. Cycloheptamaltose. β-Schardinger dextran. E459*



$C_{42}H_{70}O_{35}$ 1134.994

GRAS status for use as a flavour carrier or protectant in food. Monoclinic cryst. + H_2O (H_2O). Mp 260° dec. $[\alpha]_D$ +162.5 (c, 1.0 in H_2O). Forms cryst. complexes with propanol and iodine.

▶ GU2293000

French, D. *et al., J.A.C.S.*, 1942, **64**, 1651-1653 (*cryst struct*)

French, D. *et al., J.A.C.S.*, 1949, **71**, 353 (*isol*)

Barker, S.A. *et al., J.C.S.*, 1954, 171-176 (*ir*)

French, D. *et al., Adv. Carbohydr. Chem.*, 1957, **12**, 189 (*rev*)

Casu, B. *et al., Tetrahedron*, 1968, **24**, 803; *Carbohydr. Res.*, 1979, **76**, 59

Colson, P. *et al., J.A.C.S.*, 1974, **96**, 8081 (*conformn, cmr*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 151

Bender, M.L. *et al., Cyclodextrin Chemistry*, Springer-Verlag, 1978,

Lindner, K. *et al., Carbohydr. Res.*, 1982, **99**, 103 (*cryst struct*)

Szejtli, J. *et al., Cyclodextrins and Their Inclusion Complexes*, Budapest, 1982,

Ueno, A. *et al., Tet. Lett.*, 1982, **23**, 3451

Clarke, R.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1988, **46**, 205 (*rev, complexes*)

Gidley, M.J. *et al., J.A.C.S.*, 1988, **110**, 3820-3829 (*cmr*)

Sophianopoulos, A.J. *et al., Anal. Chem.*, 1992, **64**, 2652 (*purifn*)

Shieh, W.J. *et al., J. Macromol. Sci., Part A: Pure Appl. Chem.*, 1996, **33**, 673-683 (*rev*)

Irie, T. *et al., J. Pharm. Sci.*, 1997, **86**, 147-162 (*rev, tox*)

D'Souza, V.T. *et al., Chem. Rev.*, 1998, **98**, 1743-1753 (*rev*)

Schneider, H.J. *et al., Chem. Rev.*, 1998, **98**, 1755-1785 (*pmr, cmr*)

Osvath, R. *et al., Food Chem. News*, 2001, **43(16)**, 6 (*use*)

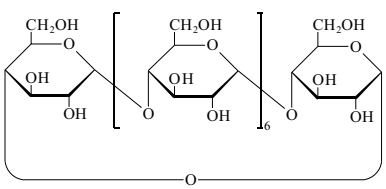
Food Chem. News, 2001, **43(40)**, 8-9 (*use*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COW925

γ-Cyclodextrin, 9CI, 8CI C-447

[17465-86-0]

Cyclooctakis-(1→4)-(α-D-glucopyranose). Cyclooctaamylose. Cyclomaltooctaose



$C_{48}H_{80}O_{40}$ 1297.136

Stabiliser, emulsifier, carrier and formula-

tion aid. Generally recognised as safe (GRAS) in the USA. $[\alpha]_D$ +177.4 (c, 1.0 in H_2O). Forms cryst. complexes with propanol and iodine.

Hexadeca-Ac:
$C_{80}H_{112}O_{56}$ 1969.731
$[\alpha]_D$ +138.5 (c, 1.0 in $CHCl_3$).

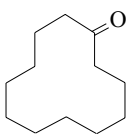
Tetracosa-O-Me:
$C_{72}H_{128}O_{40}$ 1633.779
Rod-shaped cryst. +2 or 4.5 H_2O. Sol. cold H_2O, spar. sol. hot H_2O. Cryst. with difficulty.

2,2′,2″,2‴,2⁗,2⁗′,2⁗″,2⁗‴-Octaepimer: [130322-69-9] *γ-Cyclomannin. Cyclooctakis-(1→4)-(α-D-mannopyranose)*
$C_{48}H_{80}O_{40}$ 1297.136
$[\alpha]_D^{23}$ +27.2 (c, 0.3 in H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 198B (*ir*)
French, D. *et al., J.A.C.S.*, 1949, **71**, 353 (*isol*)
French, D. *et al., Adv. Carbohydr. Chem.*, 1957, **12**, 189 (*rev*)
Takeo, K. *et al., Chem. Lett.*, 1973, 1233 (*conformn, cmr*)
Bender, M.L. *et al., Cyclodextrin Chemistry*, Springer-Verlag, 1978,
Bender, H. *et al., Carbohydr. Res.*, 1983, **124**, 225 (*synth*)
Takahashi, Y. *et al., Carbohydr. Res.*, 1987, **169**, 127 (*synth*)
Clarke, R.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1988, **46**, 205 (*rev, complexes*)
Mori, M. *et al., Tet. Lett.*, 1990, **31**, 3191 (*γ-Cyclomannin*)
Shieh, W.J. *et al., J. Macromol. Sci., Part A: Pure Appl. Chem.*, 1996, **33**, 673-683 (*rev*)
Irie, T. *et al., J. Pharm. Sci.*, 1997, **86**, 147-162 (*rev, toxicol, safety*)
D'Souza, V.T. *et al., Chem. Rev.*, 1998, **98**, 1743-1753 (*rev*)
Schneider, H.J. *et al., Chem. Rev.*, 1998, **98**, 1755-1785 (*pmr, cmr*)
Aree, T. *et al., Carbohydr. Res.*, 2000, **328**, 399-407 (*tetracosa-Me, cryst struct*)
Osvath, R. *et al., Food Chem. News*, 2000, **42**, 7-8 (*use*)

Cyclododecanone, 9CI C-448

[830-13-7]



$C_{12}H_{22}O$ 182.305
Constit. of *Panax notoginseng* (sanchi).
Mp 59°. Bp_{12} 125°.

Oxime: [946-89-4]
$C_{12}H_{23}NO$ 197.32
Mp 132°.

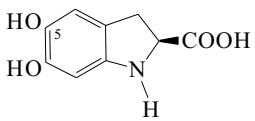
2,4-Dinitrophenylhydrazone:
Orange prisms. Mp 145-146°.

Semicarbazone:
Mp 226-227°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 400D; *CA*, **108**, 218998b (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 438C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 524A (*ir*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1926, **9**, 256; 1949, **32**, 544 (*synth*)
Kosswig, K. *et al., Ullmanns Encykl. Tech. Chem., 4. Aufl.*, 1975, **9**, 675 (*rev*)
Ohtsuha, Y. *et al., Chem. Pharm. Bull.*, 1983, **31**, 454 (*synth*)
Lu, Q. *et al., Zhongcaoyao*, 1988, **19**, 5-7; *CA*, **108**, 218998b (*isol*)
Rawdah, T.N. *et al., Tetrahedron*, 1990, **46**, 4101 (*conformn*)

Cyclodopa C-449

[18791-20-3]
2,3-Dihydro-5,6-dihydroxy-1H-indole-2-carboxylic acid, 9CI. Leucodopachrome



$C_9H_9NO_4$ 195.174

(S)-form [18766-67-1]
$[\alpha]_D^{25}$ -92 (c, 1.65 in 20% HCl).

5-O-β-D-Glucopyranoside: [71242-23-4] ***Cyclodopa glucoside***
$C_{15}H_{19}NO_9$ 357.316
Occurs in red beet cabbage juice. Mp 159.5-162.5°. $[\alpha]_D^{20.5}$ -110.7 (H_2O, pH 3). pK_{a3} 9.42.

Tri-Ac, Me ester:
Mp 94-96° (after drying). $[\alpha]_D^{20}$ -61 (c, 1.03 in $CHCl_3$).

(±)-form

Tri-Ac, Me ester:
Mp 157.5-158.5°.

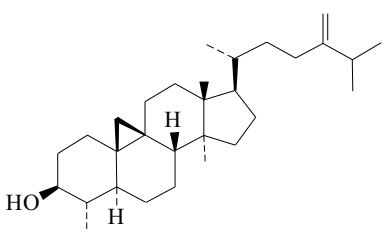
(ξ)-form

O⁵,N,N-Tri-Me: [165329-95-3]
$C_{12}H_{15}NO_4$ 237.255
$[\alpha]_D^{25}$ -12 (c, 0.001 in MeOH).
Zwitterion.

Wyler, H. *et al., Helv. Chim. Acta*, 1962, **45**, 638; 1968, **51**, 1476; 1984, **67**, 1348
Ciminiello, P. *et al., J. Nat. Prod.*, 1995, **58**, 689 (*tri-Me*)

Cycloeucalenol C-450

[469-39-6]
4,14-Dimethyl-9,19-cycloergost-24(28)-en-3-ol, 9CI. 4,14,24-Trimethyl-9,19-cyclocholest-24(28)-en-3-ol. 24-Methylene-29-norcycloartan-3-ol



$C_{30}H_{50}O$ 426.724
Cryst. (petrol). Mp 138-139°. $[\alpha]_D$ +45 ($CHCl_3$).

3-O-β-D-Glucopyranoside:
$C_{36}H_{60}O_6$ 588.866
Amorph. solid. Mp 231-234°. $[\alpha]_D$ +24.7 (c, 0.14 in MeOH).

Ac: [10376-42-8] *Cycloeucalenyl acetate*
$C_{32}H_{52}O_2$ 468.762
Mp 108-109°. $[\alpha]_D$ +55.

3-(2R-Methylbutanoyl): [306971-70-0]
$C_{35}H_{58}O_2$ 510.842
Cryst. Mp 132-134°. $[\alpha]_D^{20}$ +47 (c, 0.68 in $CHCl_3$).

3-O-(4-Hydroxy-3-methoxy-E-cinnamoyl): [156555-51-0] ***Jatrocurin***
$C_{40}H_{58}O_4$ 602.896

3-Ketone: [1255-12-5] *24-Methylene-29-norcycloartan-3-one.* ***Cycloeucalenone***
$C_{30}H_{48}O$ 424.709
Constit. of *Musa sapientum* (banana).

24R,28-Dihydro:24-Methyl-29-norcycloartan-3-ol. ***Cycloeucalanol***
$C_{30}H_{52}O$ 428.74
Needles (MeOH). Mp 141-142°.

24R,28-Dihydro, Ac:
Cryst. (MeOH). Mp 107.5-108°. $[\alpha]_D^{25}$ +70.9 (c, 0.9 in $CHCl_3$).

24S,28-Dihydro:
$C_{30}H_{52}O$ 428.74
Needles (MeOH). Mp 152-153°.

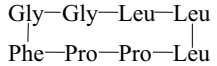
24R,28-Dihydro, 3-ketone:24-Methyl-29-norcycloartan-3-one. ***Cycloeucalanone***
$C_{30}H_{50}O$ 426.724
Constit. of *Musa sapientum* (banana).

3-Epimer: ***3-Epicycloeucalenol***
$C_{30}H_{50}O$ 426.724
Constit. of *Musa sapientum* (banana) fruit peel. Cryst. Mp 121-122°.

4-Epimer, 3-ketone: [190206-62-3] *24-Methylene-28-norcycloartan-3-one.* ***4-Epicycloeucalenone****. Cycloabyssinone*
$C_{30}H_{48}O$ 424.709
Isol. from *Musa sapientum* (banana).
Cryst. Mp 130-131°.

Cox, J.S.G. *et al., J.C.S.*, 1959, 514 (*struct*)
Amorós-Marín, L. *et al., J.O.C.*, 1959, **24**, 411 (*isol*)
Atallah, A.M. *et al., Phytochemistry*, 1975, **14**, 1529 (*biosynth*)
Itoh, T. *et al., Phytochemistry*, 1977, **16**, 1448 (*isol*)
Conner, A.H. *et al., Phytochemistry*, 1981, **20**, 2543 (*isol*)
Ageta, H. *et al., Phytochemistry*, 1984, **23**, 2875 (*isol, acetate*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1914; 1986, **34**, 2479 (*isol, pmr, cmr, struct*)
Akihisa, T. *et al., Lipids*, 1986, **21**, 494-497 (*Cycloeucalenone*)
Talapatra, S.K. *et al., J. Indian Chem. Soc.*, 1993, **70**, 543 (*Jatrocurin*)
Tavares, O.S. *et al., Fitoterapia*, 1995, **66**, 551 (*isol, ir, pmr, cmr*)
Akihisa, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 744-746 (*4-Epicycloeucalenone*)
De Paula, J.R. *et al., Phytochemistry*, 1997, **44**, 1449 (*glucoside*)
Böhme, F. *et al., Phytochemistry*, 1997, **45**, 1041-1044 (*Cycloeucalanone, ms*)
Akihisa, T. *et al., Phytochemistry*, 1998, **47**, 1107-1110 (*3-Epicycloeucalenol*)
Nohemi, T.A. *et al., Molecules*, 2000, **5**, M163; *CA*, **133**, 362845h (*Espeletia barclayana constit*)
Baldé, A.M. *et al., Fitoterapia*, 2001, **72**, 438-440 (*Cycloabyssinone*)

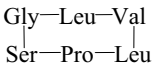
Cyclo(glycylglycylleucylleucylleucylprolylprolylphenylalanyl) C-451



$C_{41}H_{62}N_8O_8$ 794.99
Constit. of the fruit peel of *Citrus aurantium*. Powder. $[\alpha]_D^{23}$ -109.6 (c, 0.3 in MeOH). λ_{max} 228 (ϵ 7500); 280 (ϵ 1700) (MeOH).

Matsumoto, T. *et al., Heterocycles*, 2002, **56**, 477-482 (*isol, pmr, cmr*)

Cyclo(glycylleucylvalylleucylprolylseryl) C-452

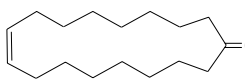


$C_{27}H_{46}N_6O_7$ 566.696
Constit. of the fruit peel of *Citrus aurantium*. Powder. $[\alpha]_D^{23}$ -123.6 (c, 0.23 in MeOH). λ_{max} 226 (ϵ 6100) (MeOH).

Matsumoto, T. *et al., Heterocycles*, 2002, **56**, 477-482 (*isol, pmr, cmr*)

9-Cycloheptadecen-1-one C-453

[74244-64-7]
Civetone



(*Z*)-*form*

$C_{17}H_{30}O$ 250.423

(*E*)-*form* [1502-37-0]
Mp 37.5-38.5°.

Semicarbazone:
Mp 190-191°.

(*Z*)-*form* [542-46-1] *FEMA 3425*
Flavouring ingredient. Cryst. with an obnoxious animal gland odour which can be pleasant at extreme dilutions. Mp 32.5°. Bp_{742} 342° Bp_2 158-160°.

▶ Skin irritant. GU2990000

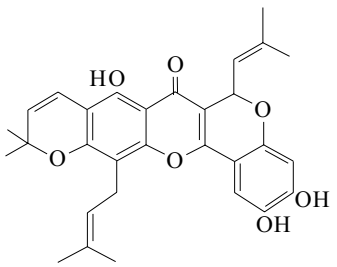
Oxime:
$C_{17}H_{31}NO$ 265.438
Mp 92°.

Semicarbazone:
Mp 187°.

Ruzicka, L. *et al., Helv. Chim. Acta*, 1926, **9**, 230 (*synth*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1927, **10**, 695 (*synth*)
Mathur, H.H. *et al., J.C.S.*, 1963, 114 (*synth*)
Opdyke, D.L.S. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 727 (*rev, tox*)
Tsuji, J. *et al., Tet. Lett.*, 1977, 3285 (*synth, nmr, ir*)
Seoane, E. *et al., Chem. Ind. (London)*, 1978, 165 (*synth*)
Abad, A. *et al., An. Quim.*, 1982, **78**, 304 (*synth*)
Bernardinelli, G. *et al., Helv. Chim. Acta*, 1982, **65**, 730 (*cryst struct*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 133
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 745-746
Tanabe, Y. *et al., Adv. Synth. Catal.*, 2002, **344**, 507-510 (*Z-form, synth, ir, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMU850

Cycloheterophyllin C-454

[36545-53-6]
*2,3,8-Trihydroxy-11,11-dimethyl-13-(3-methyl-2-butenyl)-6-(2-methyl-1-propenyl)-6*H,*7*H,*11*H-*bis[1]benzopyrano[4,3-b:6′,7′-e]pyran-7-one, 9CI*



$C_{30}H_{30}O_7$ 502.563
Isol. from bark of *Artocarpus heterophyllus* (jackfruit). Yellow cryst. (MeOH). Mp 205-206°. λ_{max} 206 ; 239 ; 295 ; 384 (MeOH) (Berdy).

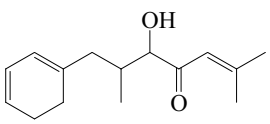
Tri-Me ether: [34144-08-6]
Cryst. (MeOH). Mp 168-169°. $[\alpha]_D$ +20 (c, 1.0 in $CHCl_3$).

2-Deoxy: [182052-09-1] ***Artelastochromene***
$C_{30}H_{30}O_6$ 486.563
Yellow solid. Mp 238-240°. λ_{max} 202 (log ϵ 5.2); 296 (log ϵ 4.3); 375 (log ϵ 402) (MeOH).

[34144-07-5]

Rao, A.V.R. *et al., Indian J. Chem.*, 1971, **9**, 7 (*isol*)
Parthasarathy, M.R. *et al., Phytochemistry*, 1979, **18**, 506 (*cmr*)
Kijjoa, A. *et al., Phytochemistry*, 1996, **43**, 691-694 (*Artelastochromene*)

7-(1,3-Cyclohexadienyl)-5-hydroxy-2,6-dimethyl-2-hepten-4-one C-455



$C_{15}H_{22}O_2$ 234.338
Constit. of the oil of turmeric, *Curcuma longa*.

Jayaprakasha, G.K. *et al., Z. Naturforsch., C*, 2001, **56**, 40-44

Cyclohexane C-456

[110-82-7]
Hexamethylene. Hexahydrobenzene



C_6H_{12} 84.161
Diluent in colour additive mixtures for food use. Liq. Prac. insol. H_2O; sol. MeOH; misc. most org. solvs. d_4^{20} 0.78. Mp 6.5°. Bp 81°. n_D^{20} 1.4262.

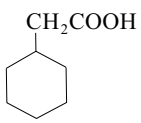
▶ Highly flammable, fl. p. -20°, autoignition temp. 245°. Eye, skin and respiratory tract irritant. High vapour conc. narcotic. OES: long-term 100 ppm; short-term 300 ppm.. GU6300000

[1735-17-7, 3170-58-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 33D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 46C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 48D (*ir*)
Zelinsky, N. *et al., Ber.*, 1911, **44**, 3123 (*synth*)
Schoorel, G.F. *et al., J. Inst. Pet. Technol.*, 1932, **18**, 179 (*rev*)
Seyer, W.F. *et al., Ind. Eng. Chem.*, 1939, **31**, 759 (*purifn*)
Barton, D.H.R. *et al., Nature (London)*, 1954, **172**, 1096 (*conformn*)
Adv. Chem. Ser., 1955, **15**, 441 (***props***)
Kahn, R. *et al., Acta Cryst. B*, 1973, **29**, 131 (*cryst struct*)
Bacon, M.R. *et al., J.A.C.S.*, 1973, **95**, 2413 (*pmr, cmr*)
Eilers, J.E. *et al., J.A.C.S.*, 1975, **97**, 1319 (*struct*)
Cross, B.P. *et al., Org. Magn. Reson.*, 1977, **10**, 82 (*cmr*)
Herman, J.A. *et al., Org. Mass Spectrom.*, 1982, **17**, 143 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CPB000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1101
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 746-747
Longacre, S.L. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 225 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2307
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 355
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CPB000

Cyclohexaneacetic acid C-457

[5292-21-7]
Hexahydrophenylacetic acid. FEMA 2347



$C_8H_{14}O_2$ 142.197
Flavouring ingredient. Needles (HCOOH) with waxy, fatty odour. Spar. sol. H_2O. Mp 33° (27°). Bp 244-246° Bp_{13} 135°.

▶ GU6490000

Me ester: [14352-61-5]
$C_9H_{16}O_2$ 156.224
Bp 200-202° Bp_{15} 90-95°.

Et ester: [5452-75-5]
$C_{10}H_{18}O_2$ 170.251

▶ GU6555000

2-Propenyl ester: [4728-82-9] *Allyl cyclohexylacetate. FEMA 2023*
$C_{11}H_{18}O_2$ 182.262
Flavouring ingredient. Liq. with an intense fruity aroma. Bp_1 66°. n_D^{20} 1.4574.

Chloride: [23860-35-7]
$C_8H_{13}ClO$ 160.643

Bp_{23} 98-100°.

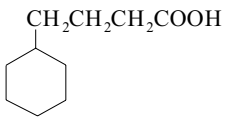
Amide: [1503-87-3]
$C_8H_{15}NO$ 141.213
Cryst. (MeOH aq.). Mp 171-172°.
▶ GU6350000

Nitrile: [4435-14-7] *(Cyanomethyl)cyclohexane*
$C_8H_{13}N$ 123.197
Bp 215°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 537A; 628C; 629C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 830A; 957C; 958A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 602B; 653C; 653D (*ir*)
Wallach, O. *et al., Annalen*, 1908, **359**, 311 (*synth*)
Darzens, G. *et al., C. R. Hebd. Seances Acad. Sci.*, 1911, **153**, 774
Sabatier, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1913, **156**, 425
Kindler, K. *et al., Annalen*, 1943, **554**, 9 (*synth*)
Hara, S. *et al., Tet. Lett.*, 1978, 2891 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 19 (*2-propenyl ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 134
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 82-83 (*2-propenyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 747-748

Cyclohexanebutanoic acid, 9CI C-458

[4441-63-8]
4-Cyclohexylbutyric acid



$C_{10}H_{18}O_2$ 170.251
Insol. H_2O. Mp 31°. Bp_{20} 169° Bp_4 136-139° $Bp_{0.6}$ 109-111°. n_D^{38} 1.4592. pK_a 4.92. Metal salts sol. many org. solvs..

Me ester: [15972-01-7]
$C_{11}H_{20}O_2$ 184.278
Bp_{24} 124°.

Et ester: [17851-38-6]
$C_{12}H_{22}O_2$ 198.305
$Bp_{0.8}$ 83-87°. n_D^{20} 1.4582.

2-Propenyl ester: [7493-65-4] *2-Propenyl cyclohexanebutanoate. Allyl cyclohexanebutyrate. FEMA 2024*
$C_{13}H_{22}O_2$ 210.316
Flavouring ingredient. Liq. with pineapple aroma. Bp_1 104°. n_D^{20} 1.4608.

Chloride:
$C_{10}H_{17}ClO$ 188.696
Bp_2 115-120°.

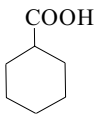
Anhydride:
$C_{20}H_{34}O_3$ 322.487
$Bp_{0.5}$ 169-172°.

[61886-29-1, 62638-03-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 537D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 831A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 602D (*ir*)
Hiers, G.S. *et al., J.A.C.S.*, 1926, **48**, 2391; 2392 (*synth*)
Cairns, T.L. *et al., J.A.C.S.*, 1948, **70**, 1689 (*synth*)
Seldner, A. *et al., Am. Perfumer Essent. Oil Rev.*, 1949, **54**, 295-296 (*allyl ester, props*)
Isbell, H.S. *et al., NBS Monogr. (U.S.)*, No. 54, 1962, ; *CA*, **58**, 2305 (*use*)
Niyazov, A.N. *et al., CA*, 1974, **81**, 11328 (*glc, pmr, ir*)
Ger. Pat., 1975, 2 437 382; *CA*, **83**, 19056 (*use*)
U.S. Pat., 1976, 3 957 514; *CA*, **85**, 184868 (*use*)
Braeunlich, G. *et al., Z. Chem.*, 1989, **29**, 417-418 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 20 (*allyl ester, use*)
Zikan, V. *et al., Coll. Czech. Chem. Comm.*, **27**, 2704-2705 (*synth*)

Cyclohexanecarboxylic acid, 9CI C-459

[98-89-5]
Hexahydrobenzoic acid. Naphthenoic acid. Naphthenic acid. FEMA 3531



$C_7H_{12}O_2$ 128.171
Flavouring ingredient. Prisms with a cheese-like odour. V. sol. EtOH, Et_2O, $CHCl_3$, C_6H_6; spar. sol. H_2O. Mp 20-21° Mp 31-32°. Bp 232-333° Bp_{13} 120-121°.
▶ LD_{50} (rat, orl) 3265 mg/kg. GU8370000

Me ester: [4630-82-4] *FEMA 3568*
$C_8H_{14}O_2$ 142.197
Flavouring ingredient. Liq. with a cheese-like odour. d^{20} 0.99. Bp 183° Bp_{15} 73°. n_D^{20} 1.4433.
▶ GU8599000

Et ester: [3289-28-9] *FEMA 3544*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient. Oil with a cheese-like odour. d_4^{20} 0.96. Bp 194° Bp_2 50.5-51°. n_D^{20} 1.4419.

4-Bromophenacyl ester:
Mp 91-92°.

Chloride: [2719-27-9]
$C_7H_{11}ClO$ 146.616
Bp 179-180° Bp 184° Bp_{17} 76°. n_D^{15} 1.4766.

Amide: [1122-56-1]
$C_7H_{13}NO$ 127.186
Prisms (H_2O). V. sol. EtOH, Et_2O. Mp 185-186°.
▶ Skin irritant. GU7875500

Nitrile: [766-05-2] *Cyclohexanecarbonitrile. Cyanocyclohexane. Cyclohexyl cyanide*
$C_7H_{11}N$ 109.171
Bp 184-185° Bp_{16} 75-77°.

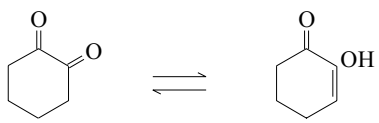
Anhydride: [22651-87-2]
$C_{14}H_{22}O_3$ 238.326
Mp 25°. Bp 280-283°.

[3198-23-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 536B; 629B; 745A; 748D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 957A; 1220C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 600D; 655A; 774D (*ir*)
Lumsden, J.S. *et al., J.C.S.*, 1905, **87**, 90
Hiers, G.S. *et al., J.A.C.S.*, 1926, **48**, 2392 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 364 (*synth*)
Szego, L. *et al., Anal. Chim. Acta*, 1968, **42**, 1 (*detn, Ca*)
Schoellkopf, U. *et al., Annalen*, 1972, **766**, 130 (*synth*)
Gurski, R.N. *et al., CA*, 1972, **76**, 59039s (*synth*)
White, D.R. *et al., Chem. Comm.*, 1974, 988 (*synth*)
Souma, Y. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3335 (*synth*)
Morita, T. *et al., Chem. Comm.*, 1978, **20**, 874 (*synth*)
Williamson, K.L. *et al., J. Magn. Reson.*, 1978, **30**, 367 (*cmr*)
Olah, G.A. *et al., Synthesis*, 1978, 929-930 (*Et ester*)
Corey, E.J. *et al., Tet. Lett.*, 1979, 399 (*synth*)
Rao, C.G. *et al., Org. Prep. Proced. Int.*, 1980, **12**, 225-228 (*Et ester*)
Bakke, J.M. *et al., J. Chem. Ecol.*, 1983, **9**, 513
Davis, C.R. *et al., J.O.C.*, 1993, **58**, 6843 (*Me ester, synth, pmr, cmr, ms, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 134; 224; 492
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 748; 961; 1748
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CPB050

1,2-Cyclohexanedione, 9CI C-460

[765-87-7]
2-Hydroxy-2-cyclohexen-1-one



$C_6H_8O_2$ 112.128
Flavour material for food. Cryst. (petrol). Mod. sol. H_2O. Mp 38-40°. Bp 193-195° Bp_{17} 85°. pK_a 10.3 (20°, 40% enol form).
▶ Explosion has resulted when prepd. by HNO_3 oxidn. of cyclohexanol. Irritant. GV0340000

Dioxime: [492-99-9] *Nioxime. Nyoxime*
$C_6H_{10}N_2O_2$ 142.157
Needles (H_2O), cryst. (dioxan). Sol. EtOH, dioxan; sl. sol. H_2O. Mp 187-188° dec. pK_{a2} 12.16 (25°).

Bis-2,4-dinitrophenylhydrazone: [1468-24-2]
Mp 233-234°.

Bisthiosemicarbazone: See 1,2-Cyclohexanedione bis(thiosemicarbazone) in *The Combined Chemical Dictionary.*

Bis(2-pyridylhydrazone): See 1,2-Cyclohexanedione bis(2-pyridylhydrazone) in *The Combined Chemical Dictionary.*

Bisbenzoylhydrazone: See 1,2-Cyclohexanedione bisbenzoylhydrazone in *The Combined Chemical Dictionary.*

Mono(di-Me acetal): [38461-13-1] *2,2-Dimethoxycyclohexanone, 9CI*

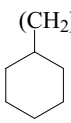
$C_8H_{14}O_3$ 158.197
Liq. $Bp_{2.1}$ 66-69°.

Bis(di-Me acetal): [163125-34-6] *1,1,2,2-Tetramethoxycyclohexane, 9CI*
$C_{10}H_{20}O_4$ 204.266
Liq. $Bp_{0.8}$ 76°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 450B; **2**, 923C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 490C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 542B (*ir*)
Rauh, E.G. *et al., J.O.C.*, 1945, **10**, 199-203 (*synth*)
Monnier, D. *et al., Anal. Chim. Acta*, 1959, **20**, 444-455 (*dioxime, detn, Ni*)
Org. Synth., Coll. Vol., 4, 1963, 229-232 (*dioxime, synth*)
Lenard, J. *et al., Anal. Biochem.*, 1969, **29**, 203-209 (*use, peptide sequence anal*)
Kowalski, C. *et al., J.O.C.*, 1978, **43**, 2601-2608 (*di-Me ketal, synth, ir, pmr*)
Rao, D.V. *et al., J.O.C.*, 1979, **44**, 456-458 (*synth*)
Nazarenko, A.Yu. *et al., Zh. Anal. Khim.*, 1982, **37**, 1469-1472 (*dioxime, detn, Fe*)
Caubere, P. *et al., J.O.C.*, 1986, **51**, 1419-1427 (*synth*)
Koul, S. *et al., J.C.S. Perkin 1*, 1995, 2969-2988 (*Di-Me ketal synth, ir, pmr, cmr, ms*)
Grice, P. *et al., J.C.S. Perkin 1*, 1997, 351-363 (*bis(di-Me ketal), synth, ir, pmr, ms, use*)
Org. Synth., 1998, **75**, 170-176 (*bis(di-Me ketal), synth, ir, pmr, cmr*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2240
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 356

Cyclohexanehexanoic acid, 9CI, 8CI C-461

[4354-56-7]
6-Cyclohexylhexanoic acid



$C_{12}H_{22}O_2$ 198.305
Cryst. (Me_2CO). Mp 33°. Bp_4 127.5-128°.

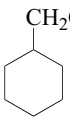
S-*Benzylthiuronium salt:*
Cryst. (EtOH). Mp 155.5°.

2-Propenyl ester: [7493-66-5] *2-Propenyl cyclohexanehexanoate. Allyl cyclohexanehexanoate. FEMA 2025*
$C_{15}H_{26}O_2$ 238.369
Flavouring ingredient.

Tanaka, A. *et al., Chem. Pharm. Bull.*, 1960, **8**, 1063-1066 (*synth*)
Ryozo, G. *et al., Nippon Kagaku Zasshi*, 1967, **88**, 678-683; *CA*, **68**, 86865z (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 20 (*allyl ester, use*)
Semino, G. *et al., Riv. Ital. Essenze, Profumi, Piante Off., Aromi, Saponi, Cosmet., Aerosol*, 1997, 86-95; *CA*, **128**, 22005n (*allyl ester, use*)

Cyclohexanepentanoic acid, 9CI C-462

[5962-88-9]
Cyclohexylvaleric acid, 8CI



$C_{11}H_{20}O_2$ 184.278
d 0.96. Mp 16-17°. Bp_{50} 203° $Bp_{0.5}$ 126-127°. n_D^{20} 1.4661.

Et ester: [17851-39-7]
$C_{13}H_{24}O_2$ 212.331
d_4^{20} 0.95. Bp_{19} 148-153°. n_D^{21} 1.4673.

2-Propenyl ester: [7493-68-7] *2-Propenyl cyclohexanepentanoate. Allyl cyclohexanevalerate. FEMA 2027*
$C_{14}H_{24}O_2$ 224.342
Flavouring ingredient. Liq. with characteristic fruity aroma. Bp_1 119°. n_D^{22} 1.4605.

4-Bromophenacyl ester:
Mp 81°.

Chloride:
$C_{11}H_{19}ClO$ 202.723
Bp_{15} 139°.

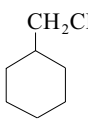
Amide:
$C_{11}H_{21}NO$ 183.293
Leaves (C_6H_6). Mp 122-123°.

[16076-64-5]

Hiers, G.S. *et al., J.A.C.S.*, 1926, **48**, 2385 (*synth*)
Smith, H.A. *et al., J.A.C.S.*, 1945, **67**, 272 (*synth*)
Baker, R.H. *et al., J.A.C.S.*, 1946, **68**, 1283 (*synth*)
Heilbron, I. *et al., J.C.S.*, 1949, 742 (*chloride, amide, synth*)
English, J. *et al., J.A.C.S.*, 1950, **72**, 4187 (*synth*)
Cousseau, J. *et al., Bull. Soc. Chim. Fr.*, 1967, 4702 (*Et ester, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 21 (*2-propenyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 85-86 (*2-propenyl ester*)

Cyclohexanepropanoic acid, 9CI C-463

[701-97-3]
3-Cyclohexylpropionic acid. Hexahydrohydrocinnamic acid. Octahydrocinnamic acid



$C_9H_{16}O_2$ 156.224
d_4^{20} 1. Mp 16°. Bp 275-280° $Bp_{0.3}$ 89°. n_D^{20} 1.4634.

Me ester: [20681-51-0]
$C_{10}H_{18}O_2$ 170.251
d_0^{16} 0.96. Bp 222-224°.

Et ester: [10094-36-7] *FEMA 2431*
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient. Liq. with sweet, pineapple-like taste at high dilution. d_0^{17} 0.94. Bp 231°. n_D^{17} 1.4520.

Propyl ester: [16595-06-5]
$C_{12}H_{22}O_2$ 198.305
d_0^{15} 0.93. Bp 251-252°. n_D^{15} 1.4550.

2-Propenyl ester: [2705-87-5] *Allyl 3-cyclohexylpropionate. Ananolide. FEMA 2026*
$C_{12}H_{20}O_2$ 196.289
Pineapple flavourant. Liq. with pineapple-like odour. d_{25}^{25} 0.95. Bp_1 91°. n_D^{20} 1.4600.

▶ LD_{50} (mus, orl) 970-1083 mg/kg.
GV6735000

Ph ester:
$C_{15}H_{20}O_2$ 232.322
Bp_{31} 195°. n_D^{14} 1.5030.

Chloride: [39098-75-4]
$C_9H_{15}ClO$ 174.67
Bp_{35} 124-126° Bp_{17} 108°.

Amide: [4361-29-9]
$C_9H_{17}NO$ 155.239
Needles (MeOH). Mp 120°.

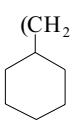
Hydrazide:
$C_9H_{18}N_2O$ 170.254
Cryst. (MeOH). Mp 92°.

Phenylhydrazide:
$C_{15}H_{22}N_2O$ 246.352
Mp 155-156°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 537B; 629D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 830C; 958B; 958C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 602C; 656A; 656B (*ir*)
Adams, R. *et al., J.A.C.S.*, 1928, **50**, 1972 (*synth*)
de Bennerville, P.L. *et al., J.A.C.S.*, 1940, **62**, 283 (*synth, Et ester*)
Finkbeiner, H.L. *et al., J.O.C.*, 1962, **27**, 3395 (*synth*)
Bestmann, H.J. *et al., Chem. Ber.*, 1966, **99**, 1906 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Matsumoto, N. *et al., Tet. Lett.*, 1975, 3643 (*synth, cmr*)
Liu, S.-H. *et al., J.O.C.*, 1977, **42**, 3209 (*Et ester*)
Fischli, A. *et al., Helv. Chim. Acta*, 1979, **62**, 48 (*synth, ir, pmr, ms*)
Japan. Pat., 1980, 80 76 843; *CA*, **93**, 238930y (*synth, allyl ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGC500

Cyclohexaneundecanoic acid C-464

11-Cyclohexylundecanoic acid



$C_{17}H_{32}O_2$ 268.439
Minor constit. of butterfat and sheep perinephric fat. Mp 55.4-56.6°.

Me ester: [19096-10-7]
$C_{18}H_{34}O_2$ 282.465
$Bp_{0.3}$ 120-124.5°.

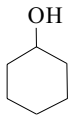
Anilide:
$C_{23}H_{37}NO$ 343.551
Mp 84.9-86.6°.

Hiers, G.S. *et al., J.A.C.S.*, 1926, **48**, 2385 (*synth*)
Schogt, J.C.M. *et al., J. Lipid Res.*, 1965, **6**, 466
Hanson, R.P. *et al., Chem. Ind. (London)*, 1967, 1640

Hanson, R.P. *et al., J. Sci. Food Agric.*, 1967, **18**, 225 (*isol*)

Cyclohexanol, 9CI C-465

[108-93-0]
Hexahydrophenol



$C_6H_{12}O$ 100.16
Needles or liq. Sol. EtOH, Et_2O, mod. sol. H_2O, misc. nonpolar solvs. d_4^{20} 0.96. Mp 24°. Bp 161°. n_D^{22} 1.4650. Hygroscopic.

▶ Fl. p. 68°, autoignition temp. 300°. Severe eye irritant. Inhalation can cause conjunctival irritation, and olfactory and respiratory system changes. Exp. hepatotoxic and nephrotoxic effects. LD_{50} (rat, orl) 2060 mg/kg. OES: long-term 50 ppm. GV7875000

Formyl: [4351-54-6] *FEMA 2353*
$C_7H_{12}O_2$ 128.171
Flavouring ingredient. d_4^0 1.01. Bp 162-163°. n_D^{24} 1.4417.

▶ Flammable, fl. p. 42°.

Ac: [622-45-7] *FEMA 2349*
$C_8H_{14}O_2$ 142.197
Flavouring agent. Present in sauerkraut, soybean and onion. Liq. with fruity aroma. d_4^{15} 0.98. Bp 175°.

▶ Fl. p. 58°, autoignition temp. 330°. AG5075000

Propanoyl: [6222-35-1] *Cyclohexyl propionate. FEMA 2354*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient. Liq. d_4^{20} 0.95. Bp_{750} 193°. n_D^{20} 1.4430.

Butanoyl: [1551-44-6] *Cyclohexyl butanoate. FEMA 2351*
$C_{10}H_{18}O_2$ 170.251
Used in food flavouring. Oily liq. with floral odour. d 0.95. Bp 212°. n_D^{25} 1.4423.

3-Methylbutanoyl: [7774-44-9] *Cyclohexyl 3-methylbutanoate. Cyclohexyl isovalerate. FEMA 2355*
$C_{11}H_{20}O_2$ 184.278
Used in fruit food flavouring. d 0.93. Bp 223°. n_D^{25} 1.4418.

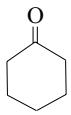
Pentanoyl: [1551-43-5] *Cyclohexyl pentanoate. Cyclohexyl valerate*
$C_{11}H_{20}O_2$ 184.278
Used in blackcurrant fruit flavouring. d_4^{25} 0.93. Bp_6 93°. n_D^{25} 1.4439.

[66522-78-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 157C; 628B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 232A; 952B (*nmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CPF000
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 136-139 (*propanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 749; 753; 756 (*esters, occur, props*)

Cyclohexanone, 9CI C-466

[108-94-1]
Ketocyclohexane. Oxocyclohexane. Nadone. Sextone. FEMA 3909



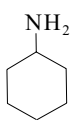
$C_6H_{10}O$ 98.144
Food flavourant. Present in various plant spp. e.g. *Cistus ladaniferus* (labdanum). Oily liq. with peppermint/acetone odour. Mod. sol. H_2O. d_4^{20} 0.95. Mp -45° (-32°). Bp 155° Bp_{15} 47°. n_D^{20} 1.4500. pK_a 16.7.

▶ Flammable, fl. p. 43°, autoignition temp. 420°. Forms explosive peroxide with H_2O_2. Eye, skin and respiratory tract irritant. Inhalation causes conjunctival irritation, and olfactory and respiratory system changes. LD_{50} (rat, orl) 1535 mg/kg. Exp. reprod. effects. CNS depressant at high vapour conc. OES: long-term 25 ppm; short-term 100 ppm. GW1050000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 432C; 1372A; **2**, 923B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 669A; **3**, 490B; 545A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 517C; 1578A (*ir*)
Baeyer, A. *et al., Ber.*, 1893, **26**, 231 (*synth*)
Nakata, H. *et al., Org. Mass Spectrom.*, 1970, **4**, 211 (*ms*)
Frechet, J.M.J. *et al., J.O.C.*, 1978, **43**, 2618 (*synth*)
Fry, A.J. *et al., J.O.C.*, 1979, **44**, 349 (*synth*)
Macháček, V. *et al., J.C.S. Perkin 2*, 1982, 355 (*cmr*)
IARC Monog., 1989, **47**, 157 (*rev, tox*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4780 (*tox, rev*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2282
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 358
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CPC000; HLI500

Cyclohexylamine C-467

[108-91-8]
Cyclohexanamine, 9CI. Aminocyclohexane. Hexahydroaniline



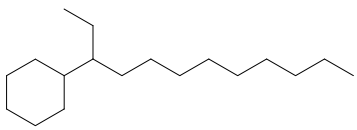
$C_6H_{13}N$ 99.175
Food contaminant arising from its use as a boiler water additive. Liq. with strong amine odour. Misc. H_2O, org. solvs. d_{25}^{25} 0.87. Fp -18. Bp 134° Bp_{71} 65° Bp_{20} 36.4°. n_D^{25} 1.4565. Strong base. Forms azeotrope with H_2O contg. 55.8% H_2O, Bp 96.4°.

▶ Flammable, fl. p. 21/31°, autoignition temp. 260°. Vapour irritates eyes and respiratory tract. Liquid is corrosive to skin and eyes. Toxic by skin absorption causing gastrointestinal effects. LD_{50} (rat, orl) 156 mg/kg. LD_{50} (rbt, skn) 277 mg/kg. Exp. reprod. and teratogenic effects. OES: long-term 10 ppm (Sk). GX0700000

Carswell, T.S. *et al., Ind. Eng. Chem.*, 1937, **29**, 1247-1251 (*bibl*)
Org. Synth., Coll. Vol., 2, 1943, 318-320 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CPF500
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 750

3-Cyclohexyldodecane C-468

[13151-83-2]
(1-Ethyldecyl)cyclohexane, 9CI

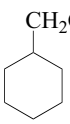


$C_{18}H_{36}$ 252.482
Isol. from *Panax quinquefolium* (American ginseng).

Traditional Chinese Medicines, (ed. Milne, G.A.), Ashgate, 1999, 1414

2-Cyclohexylethanol C-469

[4442-79-9]
Cyclohexaneethanol, 9CI



$C_8H_{16}O$ 128.214
Liq. d_4^{20} 0.92. Bp 206-209° Bp_{12} 97-100°. n_D^{20} 1.4647.

Ac: [21722-83-8] *Cyclohexylethyl acetate. FEMA 2348*
$C_{10}H_{18}O_2$ 170.251
Flavouring ingredient. Liq. Bp_{15} 104°.

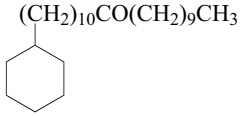
3,5-Dinitrobenzoyl:
Cryst. Mp 70.5°.

Phenylurethane:
Cryst. Mp 119.5-120.5°.

Hiers, G.S. *et al., J.A.C.S.*, 1926, **48**, 1089-1093; 2385-2393 (*synth*)
Adkins, H. *et al., J.A.C.S.*, 1930, **52**, 4349-4358 (*synth, phenylurethane*)
Huston, R.C. *et al., J.O.C.*, 1941, **6**, 123-133 (*synth, dinitrobenzoyl*)
Olah, G.A. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 92-93 (*synth*)
Eliel, E.L. *et al., J.O.C.*, 1981, **46**, 1959-1962 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 135 (*Ac*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 748-749 (*Ac*)

1-Cyclohexyl-11-heneicosanone C-470

[182141-50-0]
(11-Oxoheneicosanyl)cyclohexane

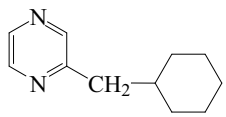


$C_{27}H_{52}O$ 392.707
Constit. of *Centella asiatica* (Asiatic pennywort).

Srivastava, R. *et al., Indian Drugs*, 1996, **33**, 233-234 (*isol*)

(Cyclohexylmethyl)pyrazine C-471

[28217-92-7]
FEMA 3631

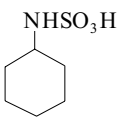


$C_{11}H_{16}N_2$ 176.261
Flavouring ingredient. Possesses fungicidal and acaricidal activity. No commercial useage in agriculture. d_4^{25} 1.52. Bp_4 98-100°.

Ger. Pat., 1969, 1 913 726; *CA*, **72**, 20872a (*fungicide use*)
U.S. Pat., 1975, 3 914 227; *CA*, **84**, 31129n (*food use, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 139 (*use, props*)

Cyclohexylsulfamic acid, 9CI C-472

[100-88-9]
*Cyclohexanesulfamic acid. Cyclohexylamine-*N*-sulfonic acid.* ***Cyclamic acid, BAN, USAN****. Cyclamate. Hexamic acid. Asugryn. E952*



$C_6H_{13}NO_3S$ 179.24
Artificial sweetening agent, usually employed as Na or Ca salt (cyclamate). Use suspended in some countries, including USA, because of possible weak carcinogenic activity (disputed). Permitted in EU at levels of 250-1600 ppm in food products. Cryst. Mp 169-170°. pK_a 1.71 (25°). Log P 1.16 (uncertain value) (calc). Sweetness approx. 30 × sucrose. Not permitted (1997) in USA.

▶ GV6950000

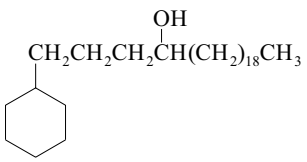
Na salt: [139-05-9] ***Sodium cyclamate, BAN****. Sucaryl sodium. Sucrosa*
Non-nutritive sweetener. Cryst. So. H_2O.

[139-06-0, 5897-16-5, 7757-85-9, 7758-04-5]

U.S. Pat., 1942, 2 275 125; *CA*, **36**, 4292 (*synth*)
Audrieth, L.F. *et al., J.O.C.*, 1944, **9**, 89-101 (*synth*)
U.S. Pat., 1945, 2 383 617, (*du Pont de Nemours*); *CA*, **40**, 357[9] (*synth, sodium cyclamate*)
Richards, R.K. *et al., J. Am. Pharm. Assoc.*, 1951, **40**, 1-6 (*use, sodium cyclamate*)
Wicker, R.J. *et al., Chem. Ind. (London)*, 1966, 1708-1716 (*rev*)
IARC Monog., 1980, **22**, 55; 171; *Suppl.* 7, 178 (*rev, tox*)
Suenaga, A. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2079-2084 (*metab, sodium cyclamate*)
Nicholson, L.J. *et al., Int. J. Cancer*, 1988, **42**, 295-298 (*tox, sodium cyclamate*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CPQ625; SGC000
Bopp, B.A. *et al., Food Sci. Technol.*, 1991, **48**, 71-95 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 446-447
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1358
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 383; 1621; 2295 (*salts*)
Encycl. Food Sci. Technol., Wiley-Interscience, 2000, 2245-2264 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CPQ625; SGC000

1-Cyclohexyl-4-tricosanol C-473

α-Nonadecylcyclohexanebutanol, 9CI

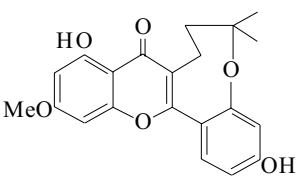


$C_{29}H_{58}O$ 422.777
(-)-*form* [151454-21-6]
Constit. of *Papaver somniferum* (opium poppy). Mp 110°. $[\alpha]_D$ -3 (c, 1 in Py).

Bhakuni, R.S. *et al., J. Indian Chem. Soc.*, 1992, **69**, 889 (*isol*)

Cyclointegrin C-474

[60791-48-2]

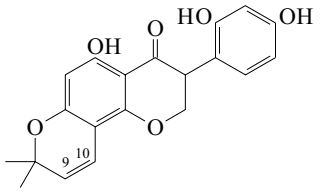


$C_{21}H_{20}O_6$ 368.385
Isol. from heartwood of *Artocarpus integer* (champedak). Yellow cryst. (Me_2CO/C_6H_6). Mp 260°.

Pendse, A.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 69 (*isol*)

Cyclokievitone C-475

[74175-82-9]
*3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5-hydroxy-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-b′]dipyran-4-one, 9CI. 1′′,2′′-Dehydrocyclokievitone*



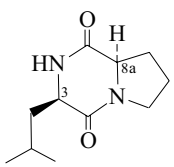
$C_{20}H_{18}O_6$ 354.359
Isol. from pods of *Phaseolus vulgaris* (kidney bean) and from other *Phaseolus* spp.. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 270 ; 355 (MeOH) (Berdy).

9,10-Dihydro, 9-hydroxy: [104363-15-7]
Cyclokievitone hydrate
$C_{20}H_{20}O_7$ 372.374
Isol. from *Phaseolus mungo* (black gram). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 294 (MeOH) (Berdy).

Woodward, M.D. *et al., Phytochemistry*, 1979, **18**, 2007 (*isol, uv, pmr, ms*)
O'Neill, M.J. *et al., Z. Naturforsch., C*, 1983, **38**, 693; 1984, **39**, 888 (*isol*)

Cyclo(leucylprolyl) C-476

[5654-86-4]
Hexahydro-3-(2-methylpropyl)pyrrolo[1,2a]pyrazine-1,4-dione. Prolylleucyldiketopiperazine. Gancidin W. Maculosin 6



(3*R*,8a*R*)-*form*

$C_{11}H_{18}N_2O_2$ 210.275
Diketopiperazine antibiotic.
(3*R*,8*aR*)-*form*
D,D-form
Amorph. solid.
(3*R*,8*aS*)-*form* [36238-67-2]
Cryst. Sol. MeOH, EtOAc. Mp 148-149° (119-122°). $[\alpha]_D^{31}$ -105.5 (c, 0.5 in EtOH).
(3*S*,8*aS*)-*form* [2873-36-1]
L,L-form
Prod. by microorganisms. Bitter component of sake and contributes to the flavour of beer. Cryst. Mp 168-172° (158-159°). $[\alpha]_D^{25}$ -133 (c, 1 in EtOH) (lit. gives a temp. range). $[\alpha]_D^{21}$ -144 (c, 0.5 in H_2O).

▶ LD_{50} (mus, ivn) 80 mg/kg. UY8708800

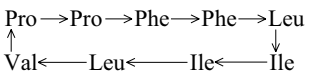
[19943-30-7, 43041-29-8]

Kodaira, Y. *et al., Agric. Biol. Chem.*, 1961, **25**, 261
Nitecki, D.E. *et al., J.O.C.*, 1968, **33**, 864 (*synth*)
Siemion, I.Z. *et al., Org. Magn. Reson.*, 1971, **3**, 545 (*synth, nmr*)
Vicar, J. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 4060; 1973, **38**, 1940 (*synth, ir, pmr*)
Karle, I.L. *et al., J.A.C.S.*, 1972, **94**, 81 (*cryst struct*)
Takahashi, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 927
Bycroft, B.W. *et al., Chem. Comm.*, 1975, 988 (*synth*)
Davies, D.B. *et al., J.C.S. Perkin 2*, 1976, 187 (*conformn*)

Pancoska, P. *et al., Coll. Czech. Chem. Comm.*, 1977, **44**, 1296 (*cd*)
Jain, T.C. *et al., Heterocycles*, 1977, **7**, 341 (*isol, struct, uv, ms*)
Bjoerkman, S. *et al., J. Med. Chem.*, 1979, **22**, 931 (*synth*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 233 (*synth*)
Schmidtz, F.J. *et al., J.O.C.*, 1983, **48**, 3941 (*isol, ms, pmr, synth, bibl*)
Ayer, W.A. *et al., Can. J. Chem.*, 1986, **64**, 904 (*isol*)
Kricheldorf, H.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 21 (*cmr*)
Adamczeski, M. *et al., J. Nat. Prod.*, 1995, **58**, 201 (*isol, pmr, cmr, bibl*)

Cyclolinopeptide A C-477

[33302-55-5]

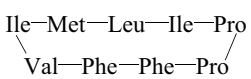


$C_{57}H_{85}N_9O_9$ 1040.353
Isol. from flax oil (*Linum usitatissimum*). Cryst. Mp 243°. $[\alpha]_D$ -111.1 (c, 0.23 in MeOH).

Kaufmann, H.P. *et al., Chem. Ber.*, 1959, **92**, 2805 (*isol*)
Kessler, H. *et al., Angew. Chem., Int. Ed.*, 1986, **25**, 997 (*props*)
Di Blasio, B. *et al., J.A.C.S.*, 1989, **111**, 9089 (*conformn, cryst struct, bibl*)
Tancredi, T. *et al., Biopolymers*, 1991, **31**, 761 (*cd, pmr, conformn*)
Morita, H. *et al., Tetrahedron*, 1999, **55**, 967-976 (*isol*)
Matsumoto, T. *et al., Tetrahedron*, 2002, **58**, 5135-5140 (*cryst struct, conformn*)

Cyclolinopeptide B C-478

[193139-41-2]



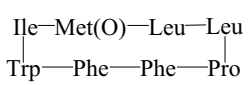
$C_{56}H_{83}N_9O_9S$ 1058.393
Cyclic peptide. Constit. of flax (*Linum usitatissimum*). Powder. $[\alpha]_D$ -104.1 (c, 0.2 in MeOH). λ_{max} 218 (ϵ 10050); 267 (ϵ 250) (MeOH).

S-*Oxide:* ***Cyclolinopeptide C***
$C_{56}H_{83}N_9O_{10}S$ 1074.392
Constit. of flax (*Linum usitatissimum*). Powder. $[\alpha]_D$ -109.7 (c, 0.21 in MeOH). λ_{max} 218 (ϵ 11000); 268 (ϵ 245) (MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 967-976 (*isol, uv, ir, pmr, cmr, activity*)
Matsumoto, T. *et al., Tetrahedron*, 2002, **58**, 5135-5140 (*cryst struct, conformn*)

Cyclolinopeptide D C-479

[222527-66-4]

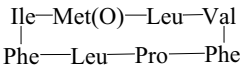


$C_{57}H_{77}N_9O_9S$ 1064.356
Cyclic peptide. Constit. of *Linum usitatissimum* (flax). Powder. $[\alpha]_D$ -75 (c, 0.2 in MeOH). λ_{max} 229 (ϵ 10070); 280 (ϵ 4630) (MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 967-976 (*isol, uv, pmr, cmr*)

Cyclolinopeptide E C-480

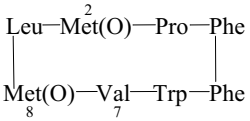
[222527-67-5]



$C_{51}H_{76}N_8O_9S$ 977.276
Cyclic peptide. Incorrect MF in the ref.. Constit. of *Linum usitatissimum* (flax). Powder. $[\alpha]_D$ -75.5 (c, 0.2 in MeOH). λ_{max} 218 (ϵ 8690); 267 (ϵ 300) (MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 967-976 (*isol, uv, pmr, cmr*)

Cyclolinopeptide F C-481



$C_{55}H_{73}N_9O_{10}S_2$ 1084.368
Constit. of the seeds of *Linum usitatissimum* (flax). Powder. $[\alpha]_D$ -71.4 (c, 0.21 in MeOH). λ_{max} 228 (log ϵ 4.02); 280 (log ϵ 3.65) (MeOH).

7-L-Isoleucine analogue: ***Cyclolinopeptide G***
$C_{56}H_{75}N_9O_{10}S_2$ 1098.395
Constit. of the seeds of *Linum usitatissimum* (flax). Powder. $[\alpha]_D$ -66.6 (c, 0.2 in MeOH). λ_{max} 219 (log ϵ 3.96); 281 (log ϵ 3.65) (MeOH).

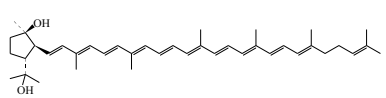
8-L-Methionine analogue: ***Cyclolinopeptide I***
$C_{55}H_{73}N_9O_9S_2$ 1068.369
Constit. of the seeds of *Linum usitatissimum* (flax). Powder. $[\alpha]_D$ -60.6 (c, 0.2 in MeOH). λ_{max} 228 (log ϵ 4); 281 (log ϵ 3.65) (MeOH).

2-L-Methionine, 7-L-isoleucine analogue:- ***Cyclolinopeptide H***
$C_{56}H_{75}N_9O_9S_2$ 1082.395
Constit. of the seeds of *Linum usitatissimum* (flax). Powder. $[\alpha]_D$ -87.7 (c, 0.15 in MeOH). λ_{max} 229 (log ϵ 3.94); 281 (log ϵ 3.62) (MeOH).

Matsumoto, T. *et al., Phytochemistry*, 2001, **57**, 251-260

2,6-Cyclolycopene-1,5-diol C-482

2-(3,7,12,16,20,24-Hexamethyl-1,3,5,7,9,11,13,15,17,19,23-pentacosaundecaenyl)-3-hydroxy-α,α,3-trimethylcyclopentanemethanol, 9CI. 1,5-Dihydroxyiridanyllycopene



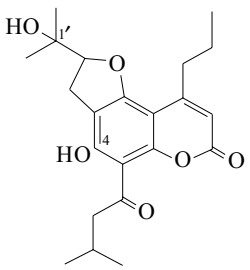
$C_{40}H_{58}O_2$ 570.897
(1R,2S,3R)-form [189131-36-0]

[189131-37-1]
Cryst. (hexane). Mp 78° dec.

Khachik, F. *et al., Anal. Chem.*, 1992, **64**, 2111-2122; 1997, **69**, 1873-1881 (*detn, hplc, uv*)
Khachik, F. *et al., ACS Symp. Ser.*, 1998, **701**, 71-85 (*formn, detn*)
Traber, B. *et al., Tetrahedron*, 1998, **54**, 9011-9022 (*synth, bibl, uv, pmr, cmr, ir, ms*)

Cyclomammein C-483

[30390-03-5]
*2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-5-(3-methyl-1-oxobutyl)-9-propyl-7*H*-furo[2,3-f][1]benzopyran-7-one, 9CI. Mammea B/BA cyclo F*



$C_{22}H_{28}O_6$ 388.46
Found in seeds of *Mammea americana* (mamey). Cryst. ($CHCl_3$/hexane). Mp 128.5-129.5°.

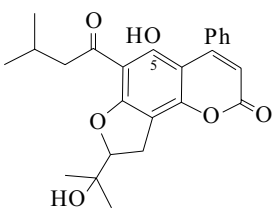
4-Ac: [38789-18-3]
Cryst. ($CHCl_3$/hexane). Mp 126-129°.

1′-Hydroperoxide:
$C_{22}H_{28}O_7$ 404.459
Isol. from *Mammea americana* (mamey). Mp 133°. Contains -OOH in place of the aliphatic OH gp. Shows sl. opt. activity.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2241; 1987, 317 (*isol, ir, pmr, synth*)
Finnegan, R.E. *et al., J. Pharm. Sci.*, 1972, **61**, 1599 (*isol, ir, uv, pmr*)

Cyclomammeisin C-484

[30563-62-3]
*8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9CI. 8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-isovaleryl-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 8CI. Mammea A/AA cyclo F*



$C_{25}H_{26}O_6$ 422.477
Constit. of *Mammea americana* (mamey). Yellow cryst. (Et_2O/hexane). Mp 115-117° Mp 148-150°.

5-Ac:
Cryst. ($CHCl_3$/hexane). Mp 145-146°.

*1′-Deoxy, 1′,2′-didehydro:8,9-Dihydro-5-hydroxy-8-(1-methylethenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one.* ***Mam-***

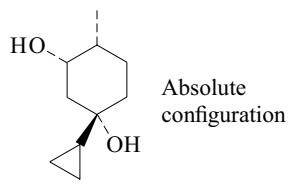
mea AIAA deshydrocyclo F
$C_{25}H_{24}O_5$ 404.462
Amorph. yellow solid. λ_{max} 230 (log ϵ 3.79); 283 (log ϵ 4.04); 346 (log ϵ 3.61) (EtOH).

*9-Methoxy:8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-9-methoxy-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one.* ***Mammea AIAA methoxycyclo F***
$C_{26}H_{28}O_7$ 452.503
Amorph. yellow solid. Possesses *trans*-config. λ_{max} 245 (log ϵ 4.01); 282 (log ϵ 4.04); 349 (log ϵ 3.65) (EtOH).

Finnegan, R.A. *et al., J. Pharm. Sci.*, 1972, **61**, 1603 (*isol, synth, ir, uv, pmr*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248 (*isol, pmr, uv, ms, ir*)
Bandaranayake, W.M. *et al., Phytochemistry*, 1975, **14**, 265 (*isol, ir, uv, pmr, ms*)
Guilet, D. *et al., J. Nat. Prod.*, 2001, **64**, 563-568 (*isol, pmr, cmr*)

9,10-Cyclo-*p*-menthane-2,4-diol C-485

[83133-21-5]
1-Cyclopropyl-4-methyl-1,3-cyclohexanediol, 9CI

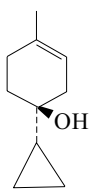


$C_{10}H_{18}O_2$ 170.251
Constit. of pistachio (*Pistacia vera*). Oil. $[\alpha]_D$ +21 (c, 1.2 in $CHCl_3$).

Mangoni, L. *et al., Phytochemistry*, 1982, **21**, 811

9,10-Cyclo-*p*-menth-1-en-4-ol C-486

1-Cyclopropyl-4-methyl-3-cyclohexen-1-ol, 9CI

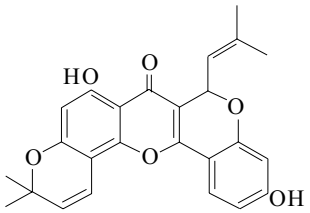


$C_{10}H_{16}O$ 152.236
(*S*)-*form* [83133-20-4]
Constit. of pistachio (*Pistacia vera*).

Monaco, P. *et al., Phytochemistry*, 1982, **21**, 2408 (*isol*)
Mangoni, L. *et al., Phytochemistry*, 1982, **21**, 811 (*synth*)

Cyclomorusin C-487

[62596-34-3]
*6,11-Dihydroxy-3,3-dimethyl-8-(2-methyl-1-propenyl)-3*H*,7*H*,8*H*-bis[1]benzopyrano[4,3-b:6′,5′-e]pyran-7-one, 9CI. Cyclomulberrochromene*

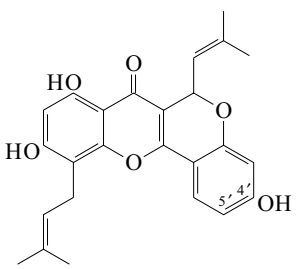


$C_{25}H_{22}O_6$ 418.445
Isol. from the root bark of *Morus alba* (white mulberry). Also from *Artocarpus altilis* (breadfruit). Pale yellow prisms (MeOH). Mp 256-257° (233-234°). $[\alpha]_D^{20}$ +20 (c, 0.15 in MeOH). λ_{max} 223 (ϵ 28300); 283 (ϵ 27000); 353 (ϵ 15400) (MeOH) (Berdy).

Deshpande, V.H. *et al., Indian J. Chem.*, 1974, **12**, 431 (*isol*)
Nomura, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1394-1402 (*isol, pmr*)
Nomura, T. *et al., Heterocycles*, 1979, **12**, 1289 (*struct*)
Nomura, T. *et al., Planta Med.*, 1983, **49**, 90 (*isol*)
Chen, C.-C. *et al., J. Nat. Prod.*, 1993, **56**, 1594 (*isol, pmr*)
Lin, C.-N. *et al., Phytochemistry*, 1996, **41**, 1215-1217 (*cmr*)

Cyclomulberrin C-488

[19275-51-5]
*3,8,10-Trihydroxy-11-(3-methyl-2-butenyl)-6-(2-methyl-1-propenyl)-6*H*,7*H*-[1]benzopyrano[4,3-b][1]benzopyran-7-one, 9CI*



$C_{25}H_{24}O_6$ 420.461
Isol. from the bark of *Morus* spp. Also isol. from *Artocarpus altilis* (breadfruit). Mp 231-232° Mp 245-246°. λ_{max} 214 (ϵ 39600); 274 (ϵ 21000); 370 (ϵ 16000) (EtOH) (Berdy).

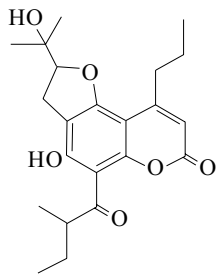
5′-Methoxy: [145643-97-6] ***Dihydroisocycloartomunin***
$C_{26}H_{26}O_7$ 450.487
Isol. from the root bark of *Artocarpus communis* (breadfruit). Yellow needles (C_6H_6). Mp 250-252°.

5′-Hydroxy, 4′-Me ether: [152130-62-6] ***Cycloaltilisin***
$C_{26}H_{26}O_7$ 450.487
Constit. of *Artocarpus altilis* (breadfruit). Mp 186-188°. $[\alpha]_D^{25}$ +99 (c, 0.36 in Me_2CO).

Deshpande, V.H. *et al., Tet. Lett.*, 1968, 1715 (*isol*)
Deshpande, V.H. *et al., Indian J. Chem.*, 1972, **10**, 681; 1974, **12**, 431 (*isol*)
Nomura, T. *et al., Heterocycles*, 1979, **12**, 1289 (*struct*)
Lin, C.-N. *et al., Phytochemistry*, 1992, **31**, 2922 (*Dihydroisocycloartomunin*)
Chen, C.-C. *et al., J. Nat. Prod.*, 1993, **56**, 1594 (*Cycloaltilisin*)
Lin, C.-N. *et al., Phytochemistry*, 1996, **41**, 1215 (*cmr, Dihydroisocycloartomunin*)

Cycloneomammein C-489

[30390-04-6]
*2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-5-(2-methyl-1-oxobutyl)-9-propyl-7*H*-furo[2,3-f][1]benzopyran-7-one, 9CI. Mammea B/BB cyclo F*

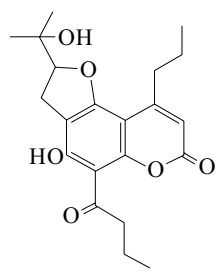


$C_{22}H_{28}O_6$ 388.46
Constit. of seeds of *Mammea americana* (mamey). Cryst. ($CHCl_3$/hexane). Mp 130-131°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2241; 1987, 317 (*isol, ir, pmr, ms, synth*)
Finnegan, R.E. *et al., J. Pharm. Sci.*, 1972, **61**, 1599 (*isol, ir, uv, pmr*)

Cyclonormammein C-490

[30563-61-2]
Mammea B/BC cyclo F

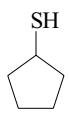


$C_{21}H_{26}O_6$ 374.433
Constit. of *Mammea americana* (mamey). Cryst. ($CHCl_3$/hexane). Mp 129.5-131.5°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2241; 1987, 317 (*isol, struct, synth*)

Cyclopentanethiol, 9CI C-491

[1679-07-8]
Mercaptocyclopentane. Cyclopentyl sulfide. Cyclopentyl mercaptan. FEMA 3262



$C_5H_{10}S$ 102.2
Flavouring ingredient. d_4^{20} 0.95. Bp 131.5-132° Bp_{745} 129-131°. n_D^{20} 1.4882 (1.4902). Strong odour (stench).

▶ GY4701000

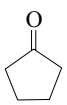
S-*Me:* See (Methylthio)cyclopentane in *The Combined Chemical Dictionary.*

S-*Et:* [7133-13-3] *(Ethylthio)cyclopentane, 9CI. Cyclopentyl ethyl sulfide, 8CI*
$C_7H_{14}S$ 130.254
Oil. Bp 176-177° Bp_{12} 60°. n_D^{20} 1.4852.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 417C (*pmr*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 417C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 341B (*ir*)
Aldrich Library of FT-NMR Spectra, **3**, 341B (*ir*)
Loevenich, J. *et al., Ber.*, 1929, **62**, 3084 (*synth, derivs*)
Lanum, W.J. *et al., J. Chem. Eng. Data*, 1969, **14**, 93 (*props, derivs*)
Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1970, **89**, 593 (*synth*)
Tanner, D.D. *et al., Can. J. Chem.*, 1973, **51**, 3366 (*synth*)
Wladislaw, B. *et al., J.C.S. Perkin 2*, 1980, 453 (*ir*)
Cerny, M. *et al., Coll. Czech. Chem. Comm.*, 1983, **48**, 1749 (*ms*)
Sandorfy, C. *et al., Phosphorus Sulfur Relat. Elem.*, 1983, **16**, 287 (*pe*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 140
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 756

Cyclopentanone, 9CI C-492

[120-92-3]
Adipic ketone. Dumasine. FEMA 3910



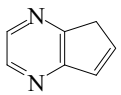
C_5H_8O 84.118
Found in various foods, incl. potato and tomato, and cooked foods, e.g. butter, meats, coffee, roasted peanut. Flavouring ingredient. Liq. with pleasant ethereal/peppermint odour. Spar. sol. H_2O (0.1%); sol. EtOH, Et_2O. Fp -58. Bp 130°. n_D^{20} 1.4366. pK_a 16.7 (25°).

▶ Flammable, fl. p. 26/31°. Mixtures with HNO_3 or H_2O_2 may explode. Skin and severe eye irritant. GY4725000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 430D; **2**, 923A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 396C; 666C; **3**, 490A (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 192-194 (*synth*)
Vanden Heuvel, W.J.A. *et al., Anal. Chem.*, 1964, **36**, 1550-1560 (*use*)
Gallardo-Herrero, R. *et al., Bull. Soc. Chim. Fr.*, 1973, 2231-2236 (*uv*)
Hawkes, G.E. *et al., J.O.C.*, 1974, **39**, 1017-1028 (*cmr*)
Girard, C. *et al., Tet. Lett.*, 1974, 3329-3332 (*synth*)
Hass, J.R. *et al., Org. Mass Spectrom.*, 1976, **11**, 697-711 (*ms*)
Cortese, N.A. *et al., J.O.C.*, 1978, **43**, 3985-3987 (*synth*)
Keeffe, J.R. *et al., J.A.C.S.*, 1990, **112**, 4862-4868 (*tautom*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 371-372 (*use, occur*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 365; 366 (*JR*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CPW500; CPW750

5*H*-Cyclopentapyrazine, 9CI, 8CI C-493

[25042-83-5]

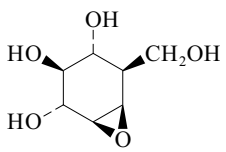


$C_7H_6N_2$ 118.138
Constit. of shoyu (soy sauce). Mauvish liq. with burnt, maple syrup taste. Bp_{10} 78-80°.

Flament, I. *et al., Helv. Chim. Acta*, 1976, **59**, 2314-2326 (*synth, ms, ir, pmr*)
Nunomura, N. *et al., Agric. Biol. Chem.*, 1978, **42**, 2123-2128 (*occur*)

Cyclophellitol C-494

[126661-83-4]
3,4,5-Trihydroxy-7-oxabicyclo[4.1.0]heptane-2-methanol. 2,3-Epoxy-4,5,6-trihydroxy-1-cyclohexanemethanol. 1,2-Anhydro-3-deoxy-3-(hydroxymethyl)inositol



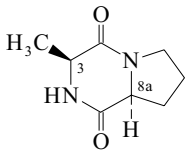
Absolute configuration

$C_7H_{12}O_5$ 176.169
Plates (H_2O). Mp 149-151°. $[\alpha]_D^{27}$ +103 (c, 0.5 in H_2O).

Atsumi, S. *et al., J. Antibiot.*, 1990, **43**, 49; 1579 (*isol, pmr, cmr, cryst struct, props*)
Tatsuta, K. *et al., J. Antibiot.*, 1991, **44**, 456 (*synth, props*)
Moritz, V. *et al., Tet. Lett.*, 1992, **33**, 5243 (*synth*)
Akiyama, T. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 3760 (*synth*)
Sato, K. *et al., Chem. Lett.*, 1994, 37 (*synth*)
Shing, T.K.M. *et al., J.C.S. Perkin 1*, 1994, 2017 (*synth, pmr*)
McDevitt, R.E. *et al., J.O.C.*, 1994, **59**, 3250 (*synth*)
Schlessinger, R.H. *et al., J.O.C.*, 1995, **60**, 16 (*synth*)
Jung, M. *et al., J.O.C.*, 1995, **60**, 3280 (*synth*)
Acena, J.L. *et al., J.O.C.*, 1997, **62**, 3360 (*synth*)
Ziegler, F.E. *et al., J.O.C.*, 1998, **63**, 426-427; 7920-7930 (*synth*)
Trost, B.M. *et al., Chem. Eur. J.*, 2001, **7**, 3768-3777 (*synth*)
Marco-Contelles, J. *et al., Eur. J. Org. Chem.*, 2001, 1607-1618 (*rev,synth,chem*)

Cyclo(prolylalanyl) C-495

Hexahydro-3-methylpyrrolo[1,2-a]pyrazine-1,4-dione, 9CI



(3*S*,8a*S*)-*form*

$C_8H_{12}N_2O_2$ 168.195

(3*S*,8a*S*)-*form* [36357-32-1]
*L,L-form. (3*S-trans*)-form*
Isol. from cocoa. Mp 153-156°. $[\alpha]_{Hg}^{20}$ -160 (c, 1 in EtOH).

(3*S*,8a*R*)-*form* [19943-29-4]
*D,L-form. (3*S-cis*)-form*
Mp 162-166°. $[\alpha]_D^{22}$ -85.

(3*R*,8a*S*)-*form* [36238-64-9]
*L,D-form. (3*R-cis*)-form*
Mp 139-142°.

[19943-28-3, 65556-33-4]

Westley, J.W. *et al., Anal. Chem.*, 1968, **40**, 1888 (*glc, chromatog, pmr*)
Siemion, I.Z. *et al., Org. Magn. Reson.*, 1971, **3**, 545 (*synth, pmr*)
Young, P.E. *et al., J.A.C.S.*, 1976, **98**, 5365 (*synth, pmr, cmr*)
Izumiya, N. *et al., Pept. Chem.*, 1977, **15**, 49 (*pharmacol*)
Cotrait, M. *et al., Cryst. Struct. Commun.*, 1979, **8**, 819 (*cryst struct*)
Grove, J.F. *et al., Phytochemistry*, 1981, **20**, 815 (*isol*)
Schmitz, F.J. *et al., J.O.C.*, 1983, **48**, 3941 (*isol, pmr, ms*)
Langhammer, M. *et al., Fresenius' Z. Anal. Chem.*, 1986, **324**, 5 (*ms*)

Cyclopropane, 9CI, INN, USAN C-496

[75-19-4]
Trimethylene



C_3H_6 42.08
Gas with ethereal odour. Mod. sol. H_2O, v. sol. EtOH, Et_2O. Mp -126°. Bp -34°. Log P 1.68 (calc).

▶ Extremely flammable. Autoignition temp. 498°. GZ0690000

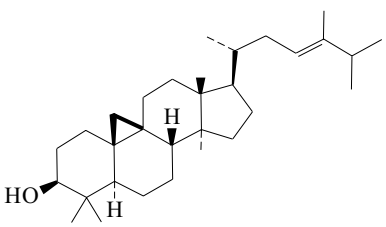
[2417-82-5]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 48B (*ir*)
Hass, H.B. *et al., Ind. Eng. Chem.*, 1936, **28**, 1178 (*synth*)
Simmons, H.E. *et al., J.A.C.S.*, 1958, **80**, 5323 (*synth*)
Weitkamp, H. *et al., Tetrahedron*, 1964, **20**, 2125 (*pmr*)
Crecely, K.M. *et al., J. Chem. Phys.*, 1970, **74**, 2680 (*cmr*)
Marsmann, M. *et al., Tetrahedron*, 1971, **27**, 4377 (*struct*)
Etsten, B.E. *et al., Textb. Vet. Anesth.*, 1971, 81 (*pharmacol*)
Org. Synth., 1972, **52**, 22 (*synth*)
Neff, W.B. *et al., Anesthesiology*, 1974, **41**, 313 (*bibl, use*)
Teratake, S. *et al., Chem. Lett.*, 1975, **12**, 1333 (*synth*)

van de Sande, C.C. *et al., J.A.C.S.*, 1975, **97**, 4617 (*ms*)
Price, H.L. *et al., Pharmacol. Basis Ther., 5th edn.*, 1975, 81 (*rev, pharmacol*)
Teratake, S. *et al., CA*, 1978, **88**, 50332x
Yamamoto, S. *et al., J. Phys. Chem.*, 1985, **89**, 3298 (*struct*)
Wong, H.N.C. *et al., Chem. Rev.*, 1989, **89**, 165 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 108 (*use*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 912
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQD750
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1124
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 367

Cyclosadol C-497

[25850-61-7]
24-Methylcycloart-23-en-3β-ol



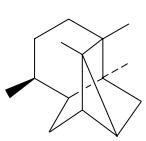
$C_{31}H_{52}O$ 440.751
Constit. of *Zea mays* (sweet corn). Cryst. (MeOH). Mp 132-134°. $[\alpha]_D$ +41 ($CHCl_3$).

Ac: [24278-47-5] *24-Methylcycloart-23-en-3β-yl acetate*
$C_{33}H_{54}O_2$ 482.788
Constit. of *Zea mays* (sweet corn). Cryst. (MeOH). Mp 121-122°. $[\alpha]_D$ +50 ($CHCl_3$).

Pinhas, H. *et al., Bull. Soc. Chim. Fr.*, 1969, 2037 (*isol*)
Itoh, T. *et al., Phytochemistry*, 1981, **20**, 1353 (*isol, pmr, cmr, ms*)
Shimizu, N. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 1425 (*synth*)
Guo, D. *et al., Tet. Lett.*, 1996, **37**, 6823 (*biosynth*)

Cycloseychellene C-498

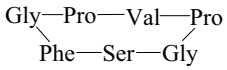
[52617-34-2]



$C_{15}H_{24}$ 204.355
Constit. of *Pogostemon cablin* (patchouli). Oil.

Terhune, S.J. *et al., Tet. Lett.*, 1973, 4705 (*isol*)
Welsh, S.C. *et al., J.O.C.*, 1981, **46**, 4819; 1985, **50**, 2676 (*struct, synth*)
Niwa, H. *et al., Tet. Lett.*, 1983, **24**, 937 (*synth*)
Akhila, A. *et al., Phytochemistry*, 1988, **27**, 2105 (*biosynth*)

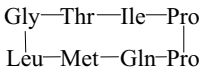
Cyclosquamosin A C-499



$C_{31}H_{43}N_7O_8$ 641.723
Constit. of the seeds of *Annona squamosa* (sugar apple). Powder. $[\alpha]_D^{20}$ -74.7 (c, 0.83 in MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 7509-7518

Cyclosquamosin B C-500

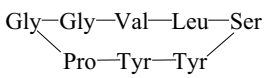


$C_{38}H_{63}N_9O_{10}S$ 838.036
Constit. of the seeds of *Annona squamosa* (sugar apple). Powder. $[\alpha]_D^{20}$ -53.8 (c, 0.58 in MeOH).

S-*Oxide:* ***Cyclosquamosin C***
$C_{38}H_{63}N_9O_{11}S$ 854.035
Constit. of the seeds of *Annona squamosa* (sugar apple). Powder. $[\alpha]_D^{20}$ -94 (c, 0.1 in MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 7509-7518

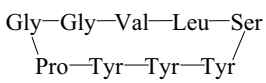
Cyclosquamosin D C-501



$C_{41}H_{56}N_8O_{11}$ 836.94
Constit. of the seeds of *Annona squamosa* (sugar apple). Powder. $[\alpha]_D^{20}$ -36.4 (c, 0.11 in MeOH). λ_{max} 278 (ε 2560) (MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 7509-7518

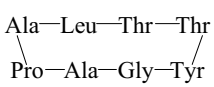
Cyclosquamosin E C-502



$C_{50}H_{65}N_9O_{13}$ 1000.116
Constit. of the seeds of *Annona squamosa* (sugar apple). Powder. $[\alpha]_D^{20}$ -10.9 (c, 1.4 in MeOH). λ_{max} 278 (ε 7440) (MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 7509-7518

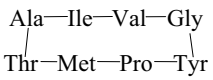
Cyclosquamosin F C-503



$C_{36}H_{54}N_8O_{11}$ 774.87
Constit. of the seeds of *Annona squamosa* (sugar apple). Powder. $[\alpha]_D^{20}$ -38.2 (c, 1.11 in MeOH). λ_{max} 278 (ε 1750) (MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 7509-7518

Cyclosquamosin G C-504

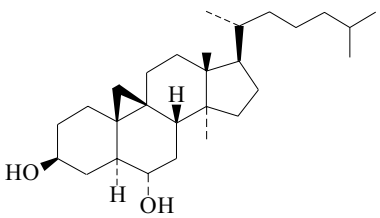


$C_{39}H_{60}N_8O_{10}S$ 833.017
Constit. of the seeds of *Annona squamosa* (sugar apple). Powder. $[\alpha]_D^{20}$ -37.1 (c, 0.14 in MeOH). λ_{max} 278 (ε 1840) (MeOH).

Morita, H. *et al., Tetrahedron*, 1999, **55**, 7509-7518

Cyclostenol C-505

[84765-67-3]
14α-Methyl-9,19-cyclo-5α,9β-cholestane-3β,6α-diol

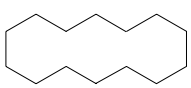


$C_{28}H_{48}O_2$ 416.686
Constit. of *Stenocereus thurberi* (organ pipe cactus). Cryst. Mp 222-223°. $[\alpha]_D^{24}$ +42 (c, 3 in $CHCl_3$).

Kircher, H.W. *et al., Phytochemistry*, 1982, **21**, 1705

Cyclotetradecane C-506

[295-17-0]

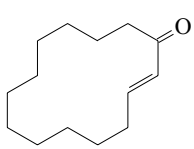


$C_{14}H_{28}$ 196.375
Constit. of *Glycyrrhiza glabra* (licorice) and *Rosa* spp.. Cryst. (EtOH aq. or by subl.). Mp 56.2°.

Ruzicka, L. *et al., Helv. Chim. Acta*, 1930, **13**, 1152 (*synth*)
Borgen, T. *et al., J.C.S. Dalton*, 1970, 1340 (*conformn*)
Herzschuh, R. *et al., J. Phys. Chem.*, 1980, **322**, 21 (*ms*)
Chen, Y. *et al., Chromatographia*, 1987, **23**, 502 (*isol*)
Drotloff, H. *et al., J.A.C.S.*, 1987, **109**, 7797 (*synth, cmr, cryst struct*)
Shannon, V.L. *et al., J.A.C.S.*, 1989, **111**, 1947 (*ir, Raman, conformn*)
Sakagami, H. *et al., CA*, **118**, 232572w (*isol*)

2-Cyclotetradecen-1-one, 9CI C-507

[55395-12-5]



(*E*)-*form*

$C_{14}H_{24}O$ 208.343
Geom. isom. not well defined. Bitterness

depressant for flavourings. Bp 107-109°.

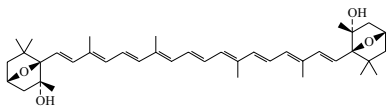
Semicarbazone:
Cryst. (MeOH). Mp 165-166°.

[73639-28-8]

Ingraham, R.B. *et al., Can. J. Res., Sect. B*, 1950, **28**, 453; *CA*, **45**, 6181e (*synth*)
Leonard, N.J. *et al., J.A.C.S.*, 1958, **80**, 6039 (*synth*)
U.S. Pat., 1980, 4 183 965; *CA*, **92**, 203426r (*synth, use*)

Cycloviolaxanthin C-508

[136624-30-1]
3,6:3′,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-carotene-5,5′-diol

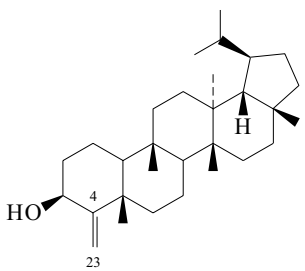


$C_{40}H_{56}O_4$ 600.88
Isol. from red paprika *Capsicum annuum* var. *longum nigrum*. Pale red cryst. (C_6H_6/hexane). Mp 193-194°. λ_{max} 427 ; 453 ; 483 (C_6H_6).

Deli, J. *et al., Helv. Chim. Acta*, 1991, **74**, 819; 1996, **79**, 1435 (*isol, pmr, uv, cd*)

Cymbopogonol C-509

[60816-94-6]
D:A-Friedo-4(23)-lupen-3β-ol



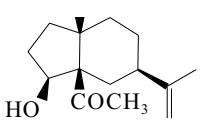
$C_{30}H_{50}O$ 426.724
Constit. of *Cymbopogon citratus* (West Indian lemongrass). Cryst. (EtOH). Mp 191-193°. $[\alpha]_D$ +15.9 ($CHCl_3$).

4α,23-Dihydro, 3-ketone: [57789-30-7]
Cymbopogone
$C_{30}H_{50}O$ 426.724
Isol. from *Cymbopogon citratus* (West Indian lemongrass). Cryst. (EtOH). Mp 262-265°.

Yokoyama, Y. *et al., Chem. Lett.*, 1979, 1463 (*synth, cryst struct*)
Yokoyama, Y. *et al., Tet. Lett.*, 1980, 3701 (*struct*)

Cyperolone C-510

[13741-46-3]

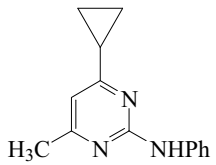


$C_{15}H_{24}O_2$ 236.353
Constit. of *Cyperus rotundus* (nutgrass). Cryst. + H_2O. Mp 41-42°. $Bp_{0.1}$ 120° (bath). $[\alpha]_D$ +31.4 ($CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1966, **14**, 1439; 1441; 1967, **15**, 1349 (*isol, ir, pmr, ord, struct, synth*)
Kapadia, V.H. *et al., Tet. Lett.*, 1967, 4661

Cyprodinil C-511

[121552-61-2]
4-Cyclopropyl-6-methyl-N-phenyl-2-pyrimidinamine, 9CI. 2-Anilino-4-cyclopropyl-6-methylpyrimidine. Chorus. Unix. CGA 219417

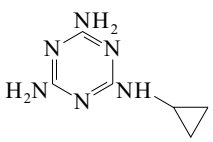


$C_{14}H_{15}N_3$ 225.293
Fungicide. Beige powder. Mp 76°. pK_a 4.4.
▶ LD_{50} (rat, orl) >2000 mg/kg.

Eur. Pat., 1989, 310 550, (*Ciba-Geigy*); *CA*, **111**, 52481n (*synth, activity*)
Heye, U.J. *et al., Brighton Crop Prot. Conf. - Pests Dis.*, 1994, **2**, 501-508 (*activity*)
Heye, U.J. *et al., Crop Prot.*, 1994, **13**, 541-549 (*activity*)
Masner, P. *et al., Pestic. Sci.*, 1994, **42**, 163-166 (*activity*)
Bocquet, G. *et al., Phytoma*, 1994, **458**, 53-55 (*activity*)
Eur. Pat., 1995, 655 441; *CA*, **123**, 55916s (*synth, activity*)
Cobras, P. *et al., J. Agric. Food Chem.*, 1997, **45**, 2708-2710 (*detn*)
Pesticide Manual, 12th edn., 2000, No. 203

Cyromazine, ANSI, BAN, BSI, INN, ISO C-512

[66215-27-8]
N-*Cyclopropyl-1,3,5-triazine-2,4,6-triamine, 9CI. CGA 72662. Larvadex. Vetrazine*



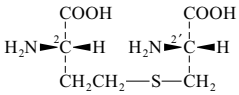
$C_6H_{10}N_6$ 166.185
Ectoparasiticide. Insect growth regulator. Specific activity against dipterous larvae. FDA approved for use in livestock. Cryst. Mp 219-222°. Log P -0.04 (calc).
▶ LD_{50} (rat, orl) 3387 mg/kg. XZ1056500

[72393-96-5, 76311-36-9]

Hall, R.D. *et al., J. Econ. Entomol.*, 1980, **73**, 564 (*activity*)
U.S. Pat., 1980, 4 225 598; *CA*, **94**, 59795g (*synth, activity*)
Hart, R.J. *et al., Aust. Vet. J.*, 1982, **59**, 104 (*activity*)
Binnington, K.C. *et al., Pestic. Biochem. Physiol.*, 1987, **27**, 201 (*activity*)
Pesticide Manual, 9th edn., 1991, 217

Cystathionine C-513

[6899-07-6]
S-*(2-Amino-2-carboxyethyl)homocysteine, 9CI. 2-Amino-4-[(2-amino-2-carboxyethyl)thio]butanoic acid. Homocysteine-cysteine sulfide*


(2*S*,2′*S*)-*form*

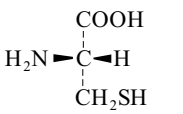
$C_7H_{14}N_2O_4S$ 222.265
Note that the assignment of stereoisomers to the D or L series depends on whether the config. is referred to the cysteine or to the homocysteine residue.

(2*S*,2′*R*)-*form* [56-88-2]
L-Cystathionine
Isol. from *Phallus impudicus* (common stinkhorn). Mp 282-283° dec. $[\alpha]_D^{20}$ +24.5 (c, 1 in 1*N* HCl).

Schoberl, A. *et al., Annalen*, 1956, **599**, 23 (*synth*)
McHale, D. *et al., J.C.S.*, 1960, 2847 (*synth*)
Warren, R.J. *et al., J. Assoc. Off. Anal. Chem.*, 1966, **49**, 1083 (*ir*)
Snow, M.L. *et al., J.O.C.*, 1967, **32**, 246 (*synth*)
Perry, T.L. *et al., Nature (London)*, 1968, **219**, 178 (*N-Acetylcystathionine*)
Jung, G. *et al., Eur. J. Biochem.*, 1973, **35**, 436 (*cd, abs config*)
Chen, C.-S. *et al., Biochim. Biophys. Acta*, 1978, **538**, 534 (*cryst struct*)
Shiraiwa, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1081-1085 (*synth, pmr, cmr*)

Cysteine, INN C-514

2-Amino-3-mercaptopropanoic acid, 9CI. 3-Mercaptoalanine. Thioserine (obsol.). NSC 8746. Cys. E920. FEMA 3263


(*R*)-*form*

$C_3H_7NO_2S$ 121.16
Uniquely among the common amino acids, in Cysteine (and Cystine) the biologically important L-form has the *R*-config. according to the Cahn-Ingold-Prelog convention (CH_2SH has higher priority than COOH).

(*R*)-*form* [52-90-4]
L-form
Detoxicant, dietary supplement, dough strengthener, yeast nutrient for leavened bakery products. Flavouring agent. Enzymic browning inhibitor. Dimorphic monoclinic or orthorhombic cryst. V. sol. H_2O, AcOH, NH_3. Mp 178° dec. $[\alpha]_D^{25}$ -16.5 (c, 2 in H_2O). $[\alpha]_D$ +26.5 (5*M* HCl). pK_{a1} 1.92; pK_{a2} 8.35; pK_{a3} 10.46 (SH). Isoelectric point 5.02. Sulfurous taste. Oxid. rapidly to Cystine, C-516.
▶ LD_{50} (rat, orl) 1890 mg/kg. Exp. reprod. effects (large dose). HA1600000

Hydrochloride: [52-89-1]

[7048-04-6] ***Cysteine hydrochloride, USAN***
Dietary supplement, nutrient. Dough conditioner. Mp 175-178° dec.
▶ LD_{50} (mus, ipr) 1250 mg/kg. HA2275000

S-*Me:* [7728-98-5]

[1187-84-4] *3-(Methylthio)alanine.* S-*Methylcysteine*
$C_4H_9NO_2S$ 135.187
Occurs in all members of the genus *Allium*, at least two genera of *Brassicaceae* family (*Brassica* and *Raphanus*) and sporadically in the families *Compositae, Leguminosae* and *Umbelliferae*. Found in kidney bean seeds (*Phaseolus vulgaris*). Mp 234-236° dec. (207-211°). $[\alpha]_D^{26}$ -32 (H_2O).

► AY7175000

S-*Et,* S-*oxide:* [17795-08-3] *3-(Ethylsulfinyl)alanine, 9CI.* S-*Ethylcysteine sulfoxide.* ***Ethiin***
$C_5H_{11}NO_3S$ 165.213
Constit. of numerous *Allium* spp.. Cryst. (EtOH aq.). Mp 157-159° dec. Config. at S not determined.

S-*Propyl:* [1115-93-1]
$C_6H_{13}NO_2S$ 163.24
Occurs as γ-glutamyl peptide in garlic. $[\alpha]_D$ -24.9 (H_2O).

S-*2-Propenyl:* [21593-77-1] S-*Allylcysteine*
$C_6H_{11}NO_2S$ 161.224
Occurs in garlic. Potential nutriceutical. Sol. H_2O. Mp 218°. $[\alpha]_D$ -16.4 (H_2O).

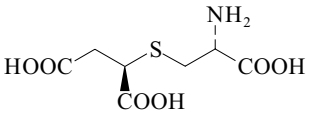
[2139-94-8, 10318-18-0, 16597-46-9, 17929-81-6, 17929-82-7, 32443-99-5, 32443-99-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 591D; 675D; **2**, 251C; 251D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 891C; 1074C (*nmr*)
Du Vigneaud, V. *et al., J.A.C.S.*, 1930, **52**, 4500-4504 (*S-benzyl, synth*)
Turner, R.B. *et al., J.A.C.S.*, 1950, **72**, 628-629 (*synth*)
Thompson, J.F. *et al., Nature (London)*, 1956, **178**, 593 (*S-Me, isol*)
Suzuki, T. *et al., Chem. Pharm. Bull.*, 1961, **9**, 251-252 (*S-Allylcysteine*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1879 (*rev*)
Tominga, T. *et al., J. Biochem. (Tokyo)*, 1963, **54**, 220-221 (*S-Me, isol*)
Fowden, L. *et al., Annu. Rev. Biochem.*, 1964, **33**, 173 (*occur, derivs*)
Martin, R.B. *et al., J.A.C.S.*, 1965, **87**, 1065-1070 (*pmr*)
Saggers, B.A. *et al., J. Clin. Pathol.*, 1966, **19**, 313; *CA*, **65**, 9533b
Martens, J. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 668 (*synth*)
Dangerous Prop. Ind. Mater. Rep., 1983, **3**, 14 (*tox, rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 319 (*deriv, synonyms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CQK250
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 16183; 577; 579; 607
Axelsson, B.S. *et al., J.C.S. Perkin 1*, 1994, 807-815 (*synth, derivs*)
Görbitz, C.H. *et al., Acta Cryst. C*, 1996, **52**, 1756-1759 (*D-form, cryst struct*)

S-Cysteinosuccinic acid C-515

[34317-60-7]
[(2-Amino-2-carboxyethyl)thio]butanedioic acid, 9CI. [(2-Amino-2-carboxyethyl)thio]succinic acid, 8CI. 2-Amino-3-(1,2-dicarboxyethylthio)propanoic acid.

ADC. KI-II



$C_7H_{11}NO_6S$ 237.233
Isol. from seeds of *Vigna radiata* (mung bean). Mp 125-126° dec Mp 132-134° dec. (AcOH solvate). All four diastereoisomers have been synth..

Bis(dicyclohexylamine) salt:
Cryst. + $5H_2O$. Mp 118-119°.

(1′*R*,2*R*)-*form* [148406-44-4]
Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. Mp 103-105° Mp 125-126°. $[\alpha]_D^{20}$ +55 (c, 0.5 in H_2O) (synthetic). Obt. as a mixt. with (1′*S*,2*R*)-form.

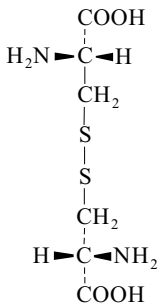
(1′*S*,2*R*)-*form* [148406-45-5]
Mp 98-101° Mp 125-127°. $[\alpha]_D^{20}$ -110 (c, 0.5 in H_2O) (synthetic). Obt. as a mixt. with (1′*R*,2*R*).

[153144-85-5, 153144-86-6]

Calam, D.H. *et al., Biochem. J.*, 1963, **86**, 226-231 (*synth, isol*)
Kasai, T. *et al., Phytochemistry*, 1986, **25**, 679-682 (*isol*)
Fushiya, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 484-486 (*isol, pmr, synth, abs config*)
Shiraiwa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1364-1369 (*synth, ir, pmr*)

Cystine, 9CI, USAN C-516

[24645-67-8]
3,3′-Dithiobis[2-aminopropanoic acid]. 3,3′-Dithiodialanine. 3,3′-Dithiobisalanine



(*R,R*)-*form*

$C_6H_{12}N_2O_4S_2$ 240.304
Disulfide corresponding to Citrulline, C-292.

► HA2600000

(*R,R*)-*form* [56-89-3]
L-form
Flavouring ingredient; dietary supplement. Plates or prisms. Sol. hot H_2O, mineral acids and aq. alkali. Mp 258-261° dec. (sealed tube). $[\alpha]_D^{25}$ -232 (c, 1 in 5*M* HCl). pK_{a3} 7.85; pK_{a4} 9.85 (25°). *N*-Protected derivs. useful in peptide synth. are listed elsewhere.

► Exp. reprod. effects (large dose). HA2690000

Hydrochloride (1:2): [30925-07-6]

[34760-60-6] Dec. by H_2O.

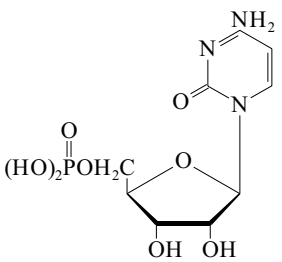
(*RS*)-(*RS*)-*form* [923-32-0]
(±)-form
Flavouring ingredient. Mp 260°.

[13059-63-7, 22671-21-2, 90350-38-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 596B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 894B (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 188 (*synth*)
Levintow, L. *et al., J. Biol. Chem.*, 1950, **184**, 55
Atkinson, R.O. *et al., J.C.S.*, 1953, 580 (*synth*)
Arnstein, H.R.V. *et al., Biochem. J.*, 1954, **57**, 360
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., Vol. 3, 1961, 1879 (*rev*)
Fujiwara, S. *et al., Bull. Chem. Soc. Jpn.*, 1963, **36**, 578; 1964, **37**, 344 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Bartle, K.D. *et al., Biochim. Biophys. Acta*, 1968, **160**, 106 (*pmr*)
Schoberl, A. *et al., Chem. Ber.*, 1969, **102**, 1767 (*synth*)
Rambarke, P. *et al., CA*, 1972, **77**, 62313c (*synth*)
Jones, D.D. *et al., Acta Cryst. B*, 1974, **30**, 1220 (*cryst struct*)
Kleemann, A. *et al., Annalen*, 1982, 1995 (*resoln*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CQK325
Axelsson, B.S. *et al., J.C.S. Perkin 1*, 1994, 807 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 760-762
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQK325

Cytidine 5′-(dihydrogen phosphate), 9CI, 8CI C-517

[63-37-6]
5′-Cytidylic acid, 9CI, 8CI. Cytidine 5′-phosphoric acid



$C_9H_{14}N_3O_8P$ 323.199
Isol. from biol. sources, e.g. *Phaseolus aureus* (mung bean) seedlings. Mp 233° dec. (monohydrate).

► HA3980000

Ba salt: [13435-44-4]
$[\alpha]_D^{16}$ +11.4 (c, 0.33 in H_2O).

Dibrucine salt:
Mp 215° dec.

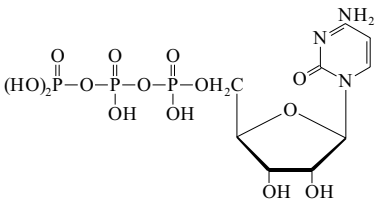
[6757-06-8, 25249-24-5, 30811-80-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 838A (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 717C (*nmr*)
Michelson, A.M. *et al., J.C.S.*, 1949, 2476 (*synth*)
Beaucamp, K. *et al., Biochem. Z.*, 1966, **344**, 121 (*cryst struct*)
Dorman, D.E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1970, **65**, 19; *CA*, **72**, 107074r (*cmr*)

Ohtsuka, E. *et al., Nucleic Acids Res.*, 1974, **1**, 323
Takaku, O. *et al., Agric. Biol. Chem.*, 1975, **39**, 2373 (*pmr*)

Cytidine 5′-triphosphate C-518

[65-47-4]
Cytidine 5′-(tetrahydrogen triphosphate), 9CI. Cytidine 5′-triphosphoric acid



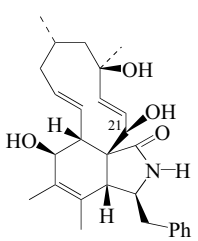
$C_9H_{16}N_3O_{14}P_3$ 483.158
Found in cheese and liver. Cryst. powder (as Na salt).
▶ HA3914000

[1637-76-9, 7358-19-2, 18609-48-8, 20764-52-7, 24951-83-5, 27908-30-1, 34973-27-8, 34973-28-9, 36051-68-0, 36792-26-4, 40147-56-6, 50694-74-1, 54619-78-2, 61994-39-6, 69113-64-0, 75898-70-3, 75898-71-4, 75898-74-7, 81012-87-5, 84495-58-9, 86527-73-3, 87015-26-7, 90290-70-3, 90290-71-4, 90290-72-5, 90290-73-6, 90290-80-5, 91999-08-5, 123334-07-6]

Bergkvist, R. *et al., Acta Cryst.*, 1956, **10**, 1303; 1957, **11**, 1457 (*isol*)
Tanaka, K. *et al., Chem. Pharm. Bull.*, 1962, **10**, 220 (*synth*)
Moffat, J.G. *et al., Can. J. Chem.*, 1964, **42**, 599-604 (*synth*)
Lee, G.C.Y. *et al., J.A.C.S.*, 1972, **94**, 951 (*tautom, pmr*)
Labotka, R.J. *et al., J.A.C.S.*, 1976, **98**, 3699 (*P-31 nmr*)
Iio, M. *et al., Agric. Biol. Chem.*, 1977, **41**, 155-160 (*synth*)
Takaku, H. *et al., Chem. Lett.*, 1977, 655 (*synth*)
Jost, W. *et al., Anal. Biochem.*, 1983, **135**, 120 (*chromatog*)
Scheller, K.H. *et al., J.A.C.S.*, 1983, **105**, 5891 (*pmr*)
Kehr, J. *et al., Fresenius' Z. Anal. Chem.*, 1986, **325**, 466 (*hplc*)
Veda, T. *et al., J. Chromatogr.*, 1987, **386**, 273 (*hplc*)
Hammer, D.F. *et al., Anal. Biochem.*, 1988, **169**, 300 (*hplc*)
Simon, E.S. *et al., Tet. Lett.*, 1988, **29**, 1123 (*synth*)
Lim, C.K. *et al., J. Chromatogr.*, 1989, **461**, 259 (*hplc*)
Simon, E.S. *et al., J.A.C.S.*, 1989, **111**, 8920-8921 (*synth*)

Cytochalasin O C-519

[108050-26-6]
Cytochalasin O_{pho}

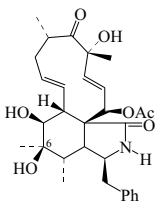


$C_{28}H_{37}NO_4$ 451.605
Mycotoxin prod. by *Phomopsis* sp.. Needles (Me_2CO/hexane). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 187-188°. $[\alpha]_D$ +59.6 (MeOH). λ_{max} 206 (ϵ 20800) (MeOH) (Berdy).

O^{21}-Ac: [108050-28-8] ***Cytochalasin N***†. *Cytochalasin N_{pho}*
$C_{30}H_{39}NO_5$ 493.642
Mycotoxin from *Phomopsis* sp.. Powder (Me_2CO). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 253-254°. $[\alpha]_D$ +85.4 (MeOH). λ_{max} 208 (ϵ 19800) (MeOH) (Berdy).

Tomioka, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 902 (*isol, struct*)

Cytochalasin O C-520



Absolute Configuration

$C_{30}H_{39}NO_7$ 525.641
Needles (toluene/methanol). Mp 258-265°. $[\alpha]_D^{23}$ -39.3 (c, 1.0 in MeOH).

6-Epimer: ***Cytochalasin P***†
$C_{30}H_{39}NO_7$ 525.641
Needles (Me_2CO/petrol). Mp 169-173°. $[\alpha]_D^{23}$ -35.8 (c, 1.0 in MeOH).

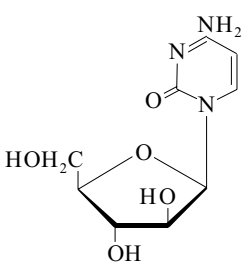
6,18-Diepimer, 17-deoxo: [108050-27-7] ***Cytochalasin P***†. *Cytochalasin P_{pho}*
$C_{30}H_{41}NO_6$ 511.657
Prod. by *Phomopsis* sp.. Cryst. ($CHCl_3$). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 117-118°. $[\alpha]_D$ -116 (MeOH). λ_{max} 208 (ϵ 15200) (MeOH) (Berdy).

[119179-33-8]

Tomioka, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 902 (*Cytochalasin Ppho*)
Edwards, R.L. *et al., J.C.S. Perkin 1*, 1989, 57 (*isol, ir, pmr, cmr, struct*)
Merifield, E. *et al., J.C.S. Perkin 1*, 1999, 3269-3283 (*synth, config*)

Cytosine arabinoside C-521

4-Amino-1-arabinofuranosyl-2(1H)-pyrimidinone, 9CI. Arabinosylcytosine. 4-Amino-1-arabinofuranosyl-2-oxo-1,2-dihydropyrimidine. Arabinofuranosylcytosine. Cyclocide



$C_9H_{13}N_3O_5$ 243.219
β-D-Furanose-*form* [147-94-4]
Cytarabine, BAN, INN, JAN, USAN. *Alexan. Aracytidine. Ara-C. Aracytin. Cytosar-U. Tarabine. NSC 63878. U 19920*
Isol. from the mushroom *Xerocomus nigromaculatus* of unknown palatability. Prisms (EtOH aq.). Sol. H_2O, MeOH. Mp 212-213° Mp 223-224°. $[\alpha]_D^{25}$ +155.2 (c, 0.7 in H_2O). Log P -3.08 (calc). λ_{max} 197 (ϵ 24550); 272 (ϵ 12020) (H_2O) (Berdy).
▶ Skin and eye irritant. Adverse systemic effects when used therapeutically. Exp. reprod. and teratogenic effects. LD_{50} (mus, orl) 3150 mg/kg ; LD_{50} (mus, orl) 3150 mg/kg. HA5425000

Hydrochloride: [69-74-9] ***Cytarabine hydrochloride, USAN***
Cryst. (EtOH aq.). Mp 188-193°. $[\alpha]_D^{25}$ +131 (c, 0.7 in H_2O).
▶ Eye irritant. LD_{50} (mus, orl) 826 mg/kg. HA5500000

[116459-64-4]

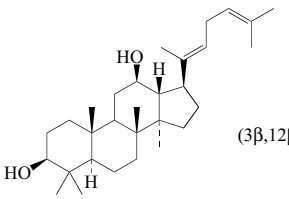
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 830D (*ir*)
Walwick, E.R. *et al., Proc. Chem. Soc., London*, 1959, 84 (*synth*)
Shen, T.Y. *et al., J.O.C.*, 1965, **30**, 835 (*synth*)
Roberts, W.K. *et al., J.O.C.*, 1967, **32**, 816 (*synth*)
Tolman, R.L. *et al., J. Med. Chem.*, 1971, **14**, 1112 (*synth*)
Tougard, P. *et al., Acta Cryst. B*, 1974, **30**, 86 (*cryst struct*)
Beranek, J. *et al., Nucleic Acid Chem.*, 1978, **1**, 239; 249; 255 (*synth*)
Krenitsky, T.A. *et al., Carbohydr. Res.*, 1981, **97**, 139 (*synth*)
Hruska, F.E. *et al., Can. J. Chem.*, 1982, **60**, 3026 (*pmr, cmr*)
Creasey, W.A. *et al., Antibiotics (N.Y.)*, 1983, **6**, 12 (*rev*)
Pallavicini, M.G. *et al., Pharmacol. Ther.*, 1984, **25**, 207 (*rev, pharmacol*)
Takahashi, A. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1313 (*isol, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQQ750; AQR000; EAU075

Pleurotus ostreatus Cytotoxic constituent C-522

POCT
Glycoprotein. MW 22000. Isol. from *Pleurotus ostreatus*. Cytotoxic.

Hua, L. *et al., CA*, 1994, **120**, 94960j (*isol*)

Dammara-20(22),24-diene-3,12-diol D-1



(3β,12β,20*E*)-*form*

$C_{30}H_{50}O_2$ 442.724

(3β,12β,20*E*)-*form* [166241-39-0] ***Quasipanaxadiol***
$[\alpha]_D$ +15 ($CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [74964-14-0] ***Ginsenoside Rg$_5$***
$C_{42}H_{70}O_{12}$ 767.008
Isol. from ginseng. Powder (C_6H_6/MeOH).

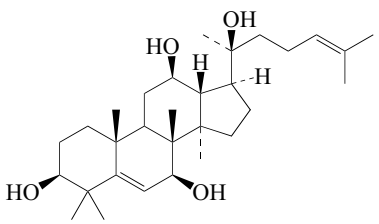
(3β,12β,20*Z*)-*form*

3-O-*β-D-Glucopyranoside:* [105558-26-7] ***Ginsenoside Rh$_3$***
$C_{36}H_{60}O_7$ 604.866
Isol. from ginseng. Powder. Mp 255-257°. $[\alpha]_D^{27}$ +7 (c,0.78 in MeOH).

[89951-13-3, 108266-93-9]

Atopkina, L.N. *et al., Carbohydr. Res.*, 1988, **177**, 101-109 (*glucoside, synth, pmr, cmr*)
Zhang, S. *et al., Planta Med.*, 1990, **56**, 298-300 (*Ginsenoside Rh3*)
Kim, S.I. *et al., Arch. Pharmacal Res.*, 1996, **19**, 551 (*Ginsenoside Rg5*)
Japan. Pat., 1996, 96 291 194 (*Quasipanaxadiol*)

Dammara-5,24-diene-3,7,12,20-tetrol D-2



$C_{30}H_{50}O_4$ 474.723

(3β,7β,12β,20*S*)-*form*

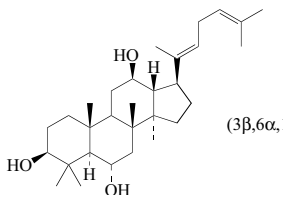
20-O-*β-D-Glucopyranoside:* [343780-68-7] ***Ginsenoside Rh$_7$***
$C_{36}H_{60}O_9$ 636.865
Constit. of leaves of *Panax ginseng* (ginseng). Powder. $[\alpha]_D^{21}$ +30.1 (c, 0.1 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [193976-63-5] ***Notoginsenoside G.*** *Vinaginsenoside R23*
$C_{48}H_{80}O_{19}$ 961.149
Constit. of *Panax notoginseng* (sanchi) and *Panax vietnamensis* (Vietnamese ginseng). Cryst. (MeOH aq.). Mp 204-206°. $[\alpha]_D^{21}$ +39.2 (c, 0.1 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [208764-54-9] ***Quinquenoside IV***
$C_{54}H_{90}O_{24}$ 1123.291
Constit. of *Panax quinquefolium* (American ginseng). Cryst. (MeOH aq.). Mp 190-192°. $[\alpha]_D^{28}$ +39.1 (c, 0.25 in MeOH).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1056-1062; 1998, **46**, 647-654 (*isol, pmr, cmr*)
Minh Duc, N. *et al., Stud. Plant Sci.*, 1999, **6**, 77-82 (*Vinaginsenoside R23*)
Dou, D.-Q. *et al., Chem. Pharm. Bull.*, 2001, **49**, 442-446 (*Ginsenoside Rh$_7$*)

Dammara-20(22),24-diene-3,6,12-triol D-3



(3β,6α,12β,20*E*)-*form*

$C_{30}H_{50}O_3$ 458.723

(3β,6α,12β,20*E*)-*form*
Isol. from ginseng. Powder (MeOH aq.). Mp 131-132°. $[\alpha]_D$ +40 (c, 0.2 in MeOH).

6-O-*β-D-Glucopyranoside:* [174721-08-5] ***Ginsenoside Rh$_4$***
$C_{36}H_{60}O_8$ 620.865
Isol. from ginseng. Cryst. (MeOH aq.). Mp 160-161°. $[\alpha]_D$ +28.2 (c, 1.0 in MeOH).

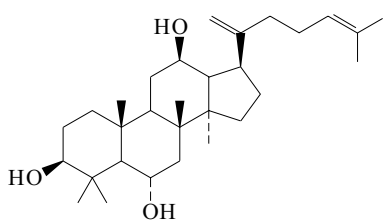
6-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* ***(20E)-Ginsenoside F$_4$***
$C_{42}H_{70}O_{12}$ 767.008
Isol. from ginseng. Amorph. powder. Mp 177-181°. $[\alpha]_D^{22}$ -7.93 (c, 0.28 in MeOH).

(3β,6α,12β,20*Z*)-*form*

6-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [126223-28-7] ***Ginsenoside F$_4$***. *Ginsenoside Rg$_4$*
$C_{42}H_{70}O_{12}$ 767.008
Isol. from ginseng. Powder. Mp 177-180°. $[\alpha]_D^{20}$ -10.8 (c, 0.5 in MeOH).

Zhang, S. *et al., Planta Med.*, 1990, **56**, 298
Ryu, J.H. *et al., Arch. Pharmacal Res.*, 1996, **19**, 335; *CA*, **125**, 270438j (*20E-Ginsenoside F4*)
Baek, N.-I. *et al., Planta Med.*, 1996, **62**, 86 (*Giasenoxide Rh4*)

Dammara-20,24-diene-3,6,12-triol D-4



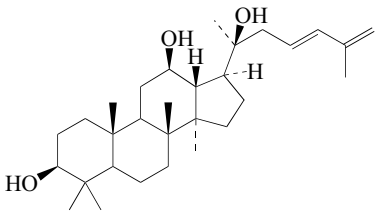
$C_{30}H_{50}O_3$ 458.723

(3β,6α,12β)-*form*

6-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [147419-93-0] ***Ginsenoside Rg$_6$***
$C_{42}H_{70}O_{12}$ 767.008
Isol. from ginseng. Amorph. Mp 173-176°. $[\alpha]_D^{23}$ -9.48 (c, 0.28 in MeOH).

Zhao, Y.Q. *et al., Chin. Chem. Lett.*, 1992, **3**, 887
Rya, J.-H. *et al., Phytochemistry*, 1997, **44**, 931 (*Ginsenoside Rg$_6$*)

Dammara-23,25-diene-3,12,20-triol D-5



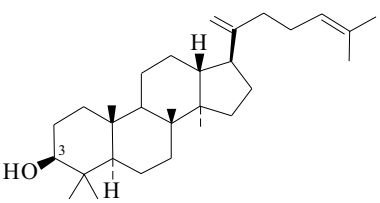
$C_{30}H_{50}O_3$ 458.723

(3β,12β,20*S*,23*E*)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [196302-61-1] ***Quinquenoside L1***
$C_{48}H_{80}O_{18}$ 945.149
Constit. of *Panax quinquefolium* (American ginseng). Cryst. Mp 208-210°.

Wang, J. *et al., CA*, 1997, **127**, 275353d (*isol, pmr, cmr*)
Wang, J.-H. *et al., J. Asian Nat. Prod. Res.*, 2001, **3**, 123-130; *CA*, **135**, 208196g (*isol, pmr, cmr*)

Dammara-20,24-dien-3-ol D-6



$C_{30}H_{50}O$ 426.724

3β-*form* [20460-34-8] ***Dammaradienol***. *Dammadienol*
Constit. of *Inula helenium* (elecampane). Cryst. (MeOH). Mp 136-138°. $[\alpha]_D$ +47 (c, 0.6 in $CHCl_3$).

Ac:
$C_{32}H_{52}O_2$ 468.762
Cryst. (EtOH). Mp 153°. $[\alpha]_D^{20}$ +72.5 (c, 0.5 in $CHCl_3$).

3-Ketone: [16883-32-2] ***Dammadienone***
$C_{30}H_{48}O$ 424.709
Cryst. (MeOH). Mp 79-80°. $[\alpha]_D$ +90 (c, 0.6 in $CHCl_3$).

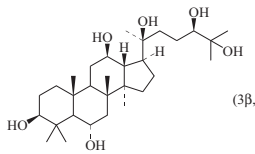
24,25-Epoxy: [1838-52-4] ***Aglaiol***. *24S,25-Epoxydammar-20-en-3β-ol*
$C_{30}H_{50}O_2$ 442.724
Cryst. (petrol). Mp 113-114°. $[\alpha]_D^{30}$ +53 (c, 0.2 in $CHCl_3$).

[52914-32-6]

Mills, J.S. *et al., J.C.S.*, 1956, 2196 (*isol*)

Corbett, R.E. *et al., Aust. J. Chem.*, 1964, **17**, 712 (*acetate*)
Shiengthong, D. *et al., Tetrahedron*, 1965, **21**, 925 (*isol, Aglaiol*)
Boar, R.B. *et al., J.C.S. Perkin 1*, 1977, 510 (*struct*)
Leong, Y.-W. *et al., Phytochemistry*, 1999, **50**, 849-857 (*pmr, cmr*)

Dammarane-3,6,12,20,24,25-hexol D-7



(3β,6α,12β,20*S*,24*R*)-*form*

$C_{30}H_{54}O_6$ 510.753

(3β,6α,12β,20*S*,24R)-*form*

6,20-Di-O-*β*-D-*glucopyranoside:* [226713-28-6] ***Vinaginsenoside R22***
$C_{42}H_{74}O_{16}$ 835.037
Constit. of *Panax vietnamensis* (Vietnamese ginseng).

(3β,6α,12β,20*S*,24S)-*form*

6,20-Di-O-*β*-D-*glucopyranoside:* [226713-20-8] ***Vinaginsenoside R21***
$C_{42}H_{74}O_{16}$ 835.037
Constit. of *Panax vietnamensis* (Vietnamese ginseng).

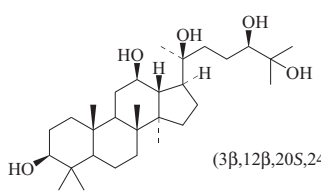
(3β,6α,12β,20*S*,24ξ)-*form* [156006-35-8]
Needles (MeOH aq.). Mp 169-171°. $[\alpha]_D^{28}$ +28.1 (c, 0.53 in MeOH).

6-O-*β*-D-*Glucopyranoside:* [156398-71-9] ***Vinaginsenoside R12***
$C_{36}H_{64}O_{11}$ 672.895
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{18}$ +29.3 (c, 1.6 in MeOH).

6,20-Di-O-*β*-D-*glucopyranoside:* ***Notoginsenoside J***
$C_{42}H_{74}O_{16}$ 835.037
Constit. of *Panax notoginseng* (sanchi). Cryst. (MeOH aq.). Mp 205-207°. $[\alpha]_D^{28}$ +9.3 (c, 0.3 in MeOH).

Duc, N.M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 634 (*Vinaginsenoside R12*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1056-1062 (*Notoginsenoside J*)
Minh Duc, N. *et al., Stud. Plant Sci.*, 1999, **6**, 77-82 (*Vinaginsenosides R21 and R22*)

Dammarane-3,12,20,24,25-pentol D-8



(3β,12β,20*S*,24*R*)-*form*

$C_{30}H_{54}O_5$ 494.754

(3β,12β,20*S*,24ξ)-*form*

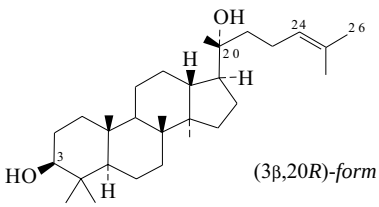
3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [336161-28-5] ***Quinquenoside F1***
$C_{42}H_{74}O_{15}$ 819.038
Constit. of fruit of *Panax quinquefolius* (American ginseng).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β*-D-*glucopyranoside:* [156398-72-0] ***Vinaginsenoside R13***
$C_{48}H_{84}O_{20}$ 981.18
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{27}$ +2.2 (c, 0.47 in MeOH).

Duc, N.M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 634 (*isol, pmr, cmr*)
Fujita, S. *et al., Phytochemistry*, 1995, **39**, 591 (*isol, pmr, cmr*)
Arriaga, F.J. *et al., Z. Naturforsch., C*, 1996, **51**, 423; 750; 1997, **52**, 292-294 (*acetonides, isol, pmr, cmr*)
Hao, X. *et al., Zhongcaoyao*, 2000, **31**, 801-803; *CA*, **134**, 323447f (*Quinquenoside F1*)

Dammar-24-ene-3,20-diol D-9

[19132-83-3]



(3β,20*R*)-*form*

$C_{30}H_{52}O_2$ 444.74

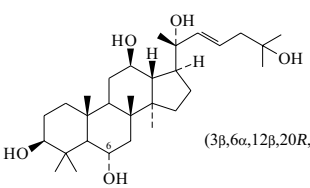
(3β,20*S*)-*form* [14351-29-2]
Dammarenediol II
Cryst. (MeOH aq. or $MeNO_2$). Mp 131-133°. $[\alpha]_D$ +33 (c, 1.2 in $CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β*-D-*glucopyranoside:* [156012-92-9] ***Vinaginsenoside R3***
$C_{48}H_{82}O_{17}$ 931.166
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Needles (MeOH aq.). Mp 254-256° dec. $[\alpha]_D^{18}$ -15 (c, 0.6 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [193977-08-1] ***Notoginsenoside I***
$C_{54}H_{92}O_{22}$ 1093.308
Constit. of *Panax notoginseng* (sanchi). Cryst. (MeOH aq.). Mp 209-211°. $[\alpha]_D^{24}$ +0.8 (c, 0.1 in MeOH).

Minh Duc, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 115 (*Vinaginsenoside R3*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1056-1062 (*Notoginsenoside I*)

Dammar-22-ene-3,6,12,20,25-pentol D-10



(3β,6α,12β,20*R*,22*E*)-*form*

$C_{30}H_{52}O_5$ 492.738

(3β,6α,12β,20*R*,22*E*)-*form*

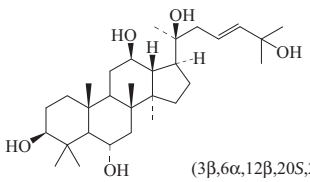
6-O-*β*-D-*Glucopyranoside:* [175889-50-6] ***Notoginsenoside R9***
$C_{36}H_{62}O_{10}$ 654.88
Constit. of *Panax notoginseng* (sanchi). Powder. $[\alpha]_D^{18}$ +27 (c, 0.32 in MeOH).

(3β,6α,12β,20*S*,22*E*)-*form*

6-O-*β*-D-*Glucopyranoside:* [175484-14-7] ***Notoginsenoside R8***
$C_{36}H_{62}O_{10}$ 654.88
Constit. of *Panax notoginseng* (sanchi). Powder. $[\alpha]_D^{18}$ +29 (c, 0.45 in MeOH).

Zhao, P. *et al., Phytochemistry*, 1996, **41**, 1411 (*isol, pmr, cmr*)

Dammar-23-ene-3,6,12,20,25-pentol D-11



(3β,6α,12β,20*S*,23*E*)-*form*

$C_{30}H_{52}O_5$ 492.738

(3β,6α,12β,20*S*,23*E*)-*form*

6-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β*-D-*glucopyranoside:* [125310-00-1] ***Majoroside F6***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax japonicus* var. *major*. Powder. Mp 182.5-184°.

6,20-Di-O-*β*-D-*glucopyranoside:* [259795-18-1]
$C_{42}H_{72}O_{15}$ 817.022
Constit. of *Panax notoginseng* (sanchi). Amorph. powder. Mp 208-212°. $[\alpha]_D^{21}$ +31.2 (c, 0.25 in MeOH).

25-Hydroperoxide:25-Hydroperoxydammar-23-ene-3,6,12,20-tetrol
$C_{30}H_{52}O_6$ 508.737

25-Hydroperoxide, 20-O-*β*-D-*glucopyranoside:* [343780-67-6] ***Ginsenoside Rh6***
$C_{36}H_{62}O_{11}$ 670.879
Constit. of leaves of *Panax ginseng* (ginseng). Powder. $[\alpha]_D^{21}$ +21.8 (c, 0.1 in MeOH).

(3β,6β,12β,20*S*,23*E*)-*form*

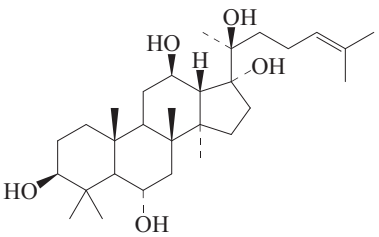
6,20-Di-O-*β*-D-*glucopyranoside:* [226712-34-1] ***Vinaginsenoside R15***
$C_{42}H_{72}O_{15}$ 817.022
Constit. of *Panax vietnamensis* (Vietnamese ginseng).

6-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β*-D-*glucopyranoside:* [193976-69-1] ***Notoginsenoside H***
$C_{47}H_{80}O_{19}$ 949.138
Constit. of *Panax notoginseng* (sanchi). Cryst. (MeOH aq.). Mp 201-203°. $[\alpha]_D^{25}$ +14.9 (c, 0.1 in MeOH).

Wang, D.Q. *et al., Yaoxue Xuebao*, 1989, **24**, 633-636; *CA*, **112**, 95498m (*Majoroside F6*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1056-1062 (*Notoginsenoside H*)
Ma, W.G. *et al., Phytochemistry*, 1999, **52**, 1133-1139 (*6,10-diglucoside*)

Minh Duc, N. *et al., Stud. Plant Sci.*, 1999, **6**, 77-82 (*Vinaginsenoside R15*)
Dou, D.-Q. *et al., Chem. Pharm. Bull.*, 2001, **49**, 442-446 (*Ginsenoside Rh_6*)

Dammar-24-ene-3,6,12,17,20-pentol D-12



$C_{30}H_{52}O_5$ 492.738

(3β,6α,12β,17α,20*S*)-*form*

20-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]*, *6*-O-*β-D-xylopyranoside:* [251101-57-2]
$C_{47}H_{80}O_{19}$ 949.138
Constit. of *Cyclanthera pedata* (achoccha).

20-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]*, *6*-O-*β-D-xylopyranoside:* [251101-56-1]
$C_{53}H_{90}O_{23}$ 1095.28
Constit. of *Cyclanthera pedata* (achoccha).

20-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]*, *6*-O-*β-D-glucopyranoside:* [251101-58-3]
$C_{54}H_{92}O_{24}$ 1125.306
Constit. of *Cyclanthera pedata* (achoccha).

20-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]*, *3*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]*, *6*-O-*β-D-xylopyranoside:* [251101-59-4]
$C_{65}H_{110}O_{33}$ 1419.564
Constit. of *Cyclanthera pedata* (achoccha).

De Tommasi, N. *et al., J. Agric. Food Chem.*, 1999, **47**, 4512-4519 (*isol, pmr, cmr*)

Dammar-25-ene-3,6,12,20,24-pentol D-13

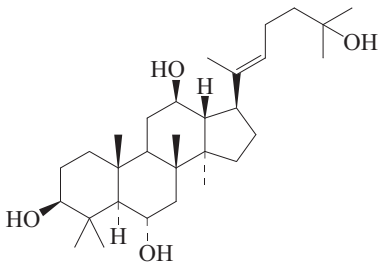
$C_{30}H_{52}O_5$ 492.738

(3β,6α,12β,20*S*,24ξ)-*form*

20-O-*β-D-Glucopyranoside:* [69987-14-0] ***Ginsenoside M_{7cd}***
$C_{36}H_{62}O_{10}$ 654.88
Isol. from ginseng. Powder + $1\frac{1}{2}H_2O$. $[\alpha]_D^{21}$ +29 (c, 0.33 in MeOH).

Yahara, S. *et al., Chem. Pharm. Bull.*, 1979, **27**, 88

Dammar-20(22)-ene-3,6,12,25-tetrol D-14



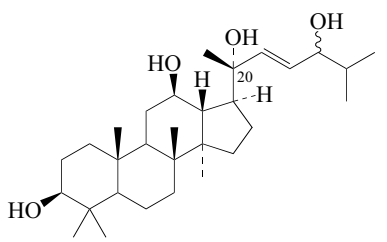
$C_{30}H_{52}O_4$ 476.738

(3β,6α,12β,20*E*)-*form*

6-O-*β-D-Glucopyranoside:* [97744-96-2] ***Sanchinoside B_1***
$C_{36}H_{62}O_9$ 638.88
Constit. of *Panax notoginseng* (sanchi). Powder. Mp 144-146°.

Wei, J. *et al., Yaoxue Xuebao*, 1985, **20**, 288-293

Dammar-22-ene-3,12,20,24-tetrol D-15



(3β,12β,20*S*,22*E*,24ξ)-*form*

$C_{30}H_{52}O_4$ 476.738

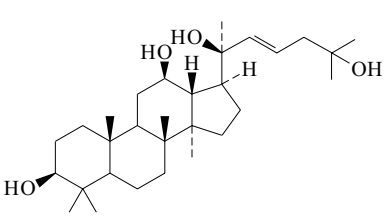
(3β,12β,20*S*,22*E*,24ξ)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]*, *20*-O-*β-D-glucopyranoside:* [125310-01-2] ***Bipinnatifidusoside F_2***
$C_{48}H_{82}O_{19}$ 963.164

3,20-Di-O-*β-D*-glucopyranoside: [114019-98-6] ***Majoroside F_3***
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax japonicus* (Japanese ginseng).

Feng, B. *et al., CA*, 1988, **108**, 183641a (*Majoroside F_3*)
Wang, D.Q. *et al., Yaoxue Xuebao*, 1989, **24**, 593-599; *CA*, **113**, 187990q (*Bipinnatifidusoside F_2*)

Dammar-22-ene-3,12,20,25-tetrol D-16



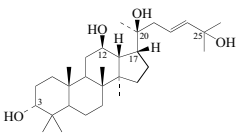
$C_{30}H_{52}O_4$ 476.738

(3β,12β,20*S*,22*E*)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]*, *20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [171746-13-7] ***Koryoginsenoside Rg_2***
$C_{54}H_{92}O_{24}$ 1125.306
Isol. from ginseng. Amorph. powder. $[\alpha]_D^{22}$ +12 (c, 0.04 in MeOH).

Kim, D.S. *et al., Phytochemistry*, 1995, **40**, 1493

Dammar-23-ene-3,12,20,25-tetrol D-17



(3α,12β,20*S*,23*E*)-*form*

$C_{30}H_{52}O_4$ 476.738

(3α,12β,20*S*,23*E*)-*form* [38736-83-3] ***Betulafolienetetrol B***
Cryst. ($CHCl_3$). Mp 130-133°. $[\alpha]_D$ -4.9 ($CHCl_3$).

3-Malonyl, 12-Ac: [147199-49-3]
$C_{35}H_{56}O_8$ 604.823
Amorph. powder. $[\alpha]_D^{24}$ -18 (c, 0.0074 in $CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]*, *20*-O-*β-D-glucopyranoside:* [156042-22-7] ***Vinaginsenoside R8***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{25}$ +14 (c, 1 in MeOH).

(3β,12β,20*S*,23*E*)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]*, *20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [193895-21-5] ***Notoginsenoside A***
$C_{54}H_{92}O_{24}$ 1125.306
Constit. of *Panax notoginseng* (Sanchi). Cryst. (MeOH aq.). Mp 197-200°. $[\alpha]_D^{24}$ +18.9 (c, 0.1 in MeOH).

25-Hydroperoxide, 3-O-*[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]*, *20*-O-*β-D-glucopyranoside:* [193976-50-0]

[207351-71-1] ***Notoginsenoside E***. *Vinaginsenoside R19*
$C_{48}H_{82}O_{20}$ 979.164
Constit. of *Panax notoginseng* (Sanchi) and *Panax vietnamensis* (Vietnamese ginseng). Cryst. (MeOH aq.). Mp 202-204°. $[\alpha]_D^{24}$ +19.2 (c, 0.1 in MeOH).

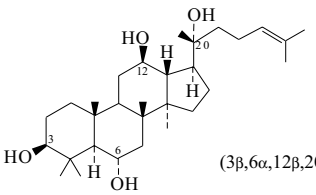
(3β,12β,20*S*,23ξ)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]*, *20*-O-*β-D-glucopyranoside:* [93376-72-8] ***Ginsenoside M_{6a}***
$C_{48}H_{82}O_{19}$ 963.164
Isol. from *Panax ginseng* (ginseng).

3,20-Di-O-*β-D*-glucopyranoside: [114019-99-7] ***Majoroside F_4***
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax japonicus* (Japanese ginseng).

Ikekawa, N. *et al., Phytochemistry*, 1972, **11**, 3037-3079
Feng, B. *et al., CA*, 1988, **108**, 183641a (*Majoroside F_4*)
Rickling, B. *et al., Planta Med.*, 1993, **59**, 76-79 (*isol, pmr, cmr, malonate*)
Minh Duc, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 115 (*Vinaginsenoside R8*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1039-1045; 1056-1062 (*Notoginsenosides*)
Minh Duc, N. *et al., Stud. Plant Sci.*, 1999, **6**, 77-82 (*Vinaginsenoside R19*)

Dammar-24-ene-3,6,12,20-tetrol D-18



(3β,6α,12β,20*R*)-*form*

$C_{30}H_{52}O_4$ 476.738

(3β,6α,12β,20*R*)-*form* [1453-93-6]
*(20*R*)-Protopanaxatriol*
Cryst. ($CHCl_3$). Sol. MeOH, butanol. Mp 233-235°. $[\alpha]_D^{16}$ -8.2 ($CHCl_3$).

Glycoside (1): ***Panaxoside B***
Glycoside from *Panax ginseng* (ginseng). Struct. unknown. Data inaccessible.

Glycoside (2): ***Panaxoside C***
$C_{48}H_{82}O_{17}$ 931.166
Glycoside from *Panax ginseng* (ginseng). Cryst. (1-butanol/butanone). Mp 185-187°. $[\alpha]_D$ -4.3 (c, 2.76 in MeOH). Struct. unknown. On hydrol. gives glucose and rhamnose ratio 3:1. The MF given here is required by a glycoside with 3 Glc and 1 Rha, but that does not correspond with the anal. figures given.

(3β,6α,12β,20*S*)-*form* [34080-08-5]
*(20*S*)-Protopanaxatriol*
Noncryst. Sol. MeOH, butanol. $[\alpha]_D^{21}$ +42.9 ($CHCl_3$).

6-O-β-D-Xylopyranoside, 20-O-β-D-glucopyranoside: [98474-75-0] ***Pseudoginsenoside RT_3***
$C_{41}H_{70}O_{13}$ 770.996
Constit. of *Panax pseudo-ginseng*. Amorph. powder (EtOH/EtOAc). $[\alpha]_D^{24}$ +30.9 (c, 1.15 in MeOH).

6-O-β-D-Glucopyranoside: [63223-86-9] ***Ginsenoside Rh_1***. *Sanchinoside B_2*
$C_{36}H_{62}O_9$ 638.88
Isol. from *Panax* spp.. Powder + $1^1/_2H_2O$. $[\alpha]_D^{22}$ +20 (c, 0.88 in MeOH).

6-O-β-D-Glucopyranoside, 20-O-[α-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [87741-78-4] ***Notoginsenoside R6***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax notoginseng* (ginseng). Amorph. powder. $[\alpha]_D^{17}$ +44.3 (c, 0.5 in MeOH).

6-O-β-D-Glucopyranoside, 20-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [87741-76-2] ***Notoginsenoside R3***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax notoginseng* (ginseng). Amorph. powder. $[\alpha]_D^{16}$ +23.7 (c, 0.97 in MeOH).

6-O-[2-Butenoyl-(→6)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [171674-97-8] ***Koryoginsenoside R_1***
$C_{46}H_{76}O_{15}$ 869.097
Constit. of *Panax ginseng* (ginseng). Amorph. powder. $[\alpha]_D^{24}$ +39.5 (c, 0.05 in MeOH).

20-O-β-D-Glucopyranoside: [53963-43-2] ***Ginsenoside F_1***
$C_{36}H_{62}O_9$ 638.88
Isol. from *Panax* spp.. Powder + $1H_2O$. $[\alpha]_D^{25}$ +36.6 (c, 1.12 in MeOH).

3,20-Di-O-β-D-glucopyranoside: [177745-52-7] ***Ginsenoside I_a***
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax ginseng* (ginseng). Powder. Mp 190-191°.

6,20-Di-O-β-D-glucopyranoside: [22427-39-0] ***Ginsenoside A_2***. *Panaxoside A*. *Sanchinoside C_1*. *Ginsenoside Rg_1*
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax ginseng* (ginseng). Powder. Mp 194-196.5°. $[\alpha]_D^{19.5}$ +32 (Py).

▶ LD_{50} (mus, ipr) 405 mg/kg. LY9537200

20-O-[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]: ***Ginsenoside F_5***
$C_{41}H_{70}O_{13}$ 770.996
Constit. of *Panax ginseng* (ginseng). Powder. Mp 189-190°.

20-O-[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]: [62025-50-7] ***Ginsenoside F_3***
$C_{41}H_{70}O_{13}$ 770.996
Isol. from *Panax* spp.. Powder + $3H_2O$. $[\alpha]_D^{25}$ +26.5 (c, 0.98 in MeOH).

6-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside]: [80418-25-3] ***Notoginsenoside R_2***
$C_{41}H_{70}O_{13}$ 770.996
Constit. of *Panax notoginseng* (ginseng). Powder. $[\alpha]_D^{15}$ +10.3 (c, 1.0 in MeOH).

6-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [80418-24-2] ***Notoginsenoside R_1***
$C_{47}H_{80}O_{18}$ 933.138
Constit. of roots of *Panax notoginseng* (ginseng). Needles (H_2O). Mp 215-217°. $[\alpha]_D^{25}$ +15 (c, 1.0 in MeOH).

6-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [52286-74-5] ***Ginsenoside C***. *Chikusetsusaponin I*. *Ginsenoside R_{g2}*
$C_{42}H_{72}O_{13}$ 785.023
Constit. of *Panax ginseng* (ginseng). Cryst. (EtOH). Mp 187-189°. $[\alpha]_D^{30}$ +5.5 (c, 1 in MeOH).

6-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [52286-59-6] ***Ginsenoside B_2***. *Chikusetsusaponin IVc*. *Ginsenoside R_e*
$C_{48}H_{82}O_{18}$ 947.165
Constit. of *Panax ginseng* (ginseng) and *Panax japonicum* (Japanese ginseng). Needles (EtOH aq.). Mp 201-203°. $[\alpha]_D^{30}$ 0 (c, 1 in MeOH).

▶ LY9536700

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [68406-26-8] ***Ginsenoside R_{b3}***
$C_{53}H_{90}O_{23}$ 1095.28
Constit. of *Panax ginseng* (ginseng). Powder (2-propanol). Mp 193-195°. $[\alpha]_D^{28}$ +19.4 (c, 1 in MeOH).

▶ LZ5857000

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: Vinaginsenoside R4
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{18}$ +28.4 (c, 0.7 in MeOH).

6-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [52286-58-5] ***Ginsenoside R_f***
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax ginseng* (ginseng). The first pure ginseng constit. to show nearly all the activities of the plant extract. Powder (Me_2CO). Mp 197-198°. $[\alpha]_D^{30}$ +7 (c, 1 in MeOH).

▶ LY9536900

6-O-[α-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [350586-56-0] ***Notoginsenoside N***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of roots of *Panax notoginseng* (ginseng). Cryst. (MeOH aq.). Mp 186-188°. $[\alpha]_D^{22}$ +50 (c, 0.3 in MeOH).

6-O-[α-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [394246-74-3] ***Notoginsenoside M***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of the roots of *Panax notoginseng* (ginseng). Cryst. (MeOH aq.). Mp 187-189°. $[\alpha]_D^{24}$ +24.7 (c, 0.3 in MeOH).

20-Me ether, 6-O-β-D-glucopyranoside: [340270-88-4] ***Ginsenoside Rh_5***
$C_{37}H_{64}O_9$ 652.907
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. solid. $[\alpha]_D^{25}$ +32.4 (c, 2.39 in MeOH).

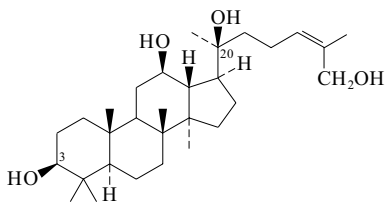
12-Ketone:3,6,20-Trihydroxydammar-24-en-12-one
$C_{30}H_{50}O_4$ 474.723

12-Ketone, 20-O-β-D-glucopyranoside: [343780-69-8] ***Ginsenoside Rh_8***
$C_{36}H_{60}O_9$ 636.865
Constit. of leaves of *Panax ginseng* (ginseng). Powder.

Uvarova, N.I. *et al., Khim. Prir. Soedin.*, 1965, **1**, 82; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 63 (*Panaxosides*)
Nagai, Y. *et al., Tetrahedron*, 1971, **27**, 881 (*isol, struct*)
Sanada, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2407; 1978, **26**, 1694 (*isol, Ginsenoside R_e*)
Lin, T.D. *et al., Chem. Pharm. Bull.*, 1976, **24**, 253 (*isol*)
Yahara, S. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2204; 1979, **27**, 88 (*Ginsenosides*)
Lin, T.-D. *et al., J. Chin. Chem. Soc. (Taipei)*, 1979, **26**, 29 (*Chikusetsusaponin IV_c*)
Zhou, J. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2844 (*isol*)

Matsuura, H. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2281 (*Notoginsenosides R3 and R6*)
Tanaka, O. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2323 (*Pseudoginsenoside RT$_3$*)
Minh Duc, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 115 (*Vinaginsenoside R4*)
Kim, D.-S. *et al., Phytochemistry*, 1995, **40**, 1493-1497 (*Koryoginsenoside R, Ginsenoside Rg$_1$*)
Dou, D.Q. *et al., J. Chin. Pharm. Sci.*, 1996, **5**, 48-52; *CA*, **126**, 328059a (*Ginsenoside F5*)
Dou, D. *et al., Planta Med.*, 1996, **62**, 179-181 (*Ginsenoside I$_a$*)
Yoon, S.-R. *et al., Chem. Pharm. Bull.*, 1998, **48**, 1144-1147 (*Ginsenosides R$_f$ and R$_{g2}$, assay*)
Battellina, L. *et al., Pharm. Pharmacol. Commun.*, 1998, **4**, 411-413 (*activity*)
Elyakov, G.B. *et al., Planta Med.*, 1999, **65**, 30-34 (*activity*)
Dou, D.-Q. *et al., Chem. Pharm. Bull.*, 2001, **49**, 442-446 (*Ginsenoside Rh$_8$*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1452-1456 (*Notoginsenosides M,N*)
Tran, Q.L. *et al., J. Nat. Prod.*, 2001, **64**, 456-461 (*Ginsenoside Rh$_5$*)
Teng, R. *et al., Magn. Reson. Chem.*, 2002, **40**, 483-488 (*pmr, cmr*)

Dammar-24-ene-3,12,20,26-tetrol D-19



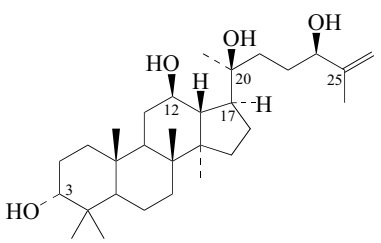
$C_{30}H_{52}O_4$ 476.738

(3β,12β,20*S*)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [218917-14-7] ***Vinaginsenoside R24***. *Quinquenoside L$_2$*
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax vietnamensis* (Vietnamese ginseng) and *Panax quinquefolium* (American ginseng).

Minh Duc, N. *et al., Stud. Plant Sci.*, 1999, **6**, 77-82 (*Vinaginsenoside R24*)

Dammar-25-ene-3,12,20,24-tetrol D-20



(3α,12β,20*S*,24*R*)-*form*

$C_{30}H_{52}O_4$ 476.738

(3β,12β,20*S*,24*R*)-*form*

3,20-Di-O-β-D-glucopyranoside: [215720-23-3] ***Ginsenoside Ib***. *Ginsenoside Rg$_7$*
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax ginseng* (ginseng). Cryst. Mp 187-188°.

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [114128-16-4] ***Majoroside F$_1$***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax japonicus* (Japanese ginseng) and *Panax vietnamensis* (Vietnamese ginseng). Powder. $[\alpha]_D^{25}$ +9.3 (c, 0.9 in MeOH).

24-Hydroperoxide, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [227758-58-9] ***Ginsenoside I***
$C_{48}H_{82}O_{20}$ 979.164
Constit. of *Panax ginseng* (ginseng).

(3β,12β,20*S*,24*S*)-*form*

3,20-Di-O-β-D-glucopyranoside: [114019-97-5] ***Majoroside F$_2$***
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax japonicus* (Japanese ginseng). Mp 186-189°.

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [156042-23-8] ***Vinaginsenoside R9***
$C_{48}H_{82}O_{19}$ 963.164
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{25}$ +10.5 (c, 0.6 in MeOH).

24-Hydroperoxide, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [227758-59-0] ***Ginsenoside II***
$C_{48}H_{82}O_{20}$ 979.164
Constit. of *Panax ginseng* (ginseng).

(3β,12β,20*S*,24ξ)-*form*

24-Ketone, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-β-D-glucopyranoside: [223710-06-3] ***Ginsenoside III***. *Vinaginsenoside R20*
$C_{48}H_{80}O_{19}$ 961.149
Constit. of *Panax ginseng* (ginseng) and *Panax vietnamensis* (Vietnamese ginseng). Cryst. Mp 203-205°.

24-Ketone, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [193895-26-0] ***Notoginsenoside B***
$C_{54}H_{90}O_{24}$ 1123.291
Constit. of *Panax notoginseng* (ginseng). Cryst. (MeOH aq.). Mp 201-204°. $[\alpha]_D^{23}$ +17.8 (c, 0.1 in MeOH).

24-Hydroperoxide, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [193895-49-7] ***Notoginsenoside C***
$C_{54}H_{92}O_{25}$ 1141.306
Constit. of *Panax notoginseng* (ginseng). Cryst. (MeOH aq.). Mp 199-202°. $[\alpha]_D^{22}$ +14.4 (c, 0.1 in MeOH).

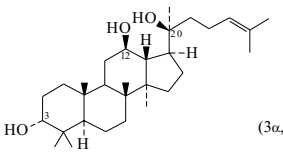
(3β,12β,20ξ,24ξ)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-β-D-glucopyranoside: [93376-73-9] ***Ginsenoside M$_{6\text{-}bc}$***
$C_{48}H_{82}O_{19}$ 963.164
Isol. from *Panax ginseng* (ginseng).

Feng, B. *et al., CA*, 1988, **108**, 183641a (*Majorosides*)
Minh Duc, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 115 (*Vinaginsenoside R9*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1039-1045 (*Notoginsenosides*)
Dou, D. *et al., Zhongguo Yaowu Huaxue Zazhi*, 1997, **7**, 202-204; *CA*, **130**, 335321r (*Ginsenoside Ib*)
Qiu, F. *et al., Chin. Chem. Lett.*, 1998, **9**, 643-645 (*Ginsenoside III*)
Dou, D.Q. *et al., Chem. Pharm. Bull.*, 2001, **49**, 442-446 (*Ginsenoside Ib*)
Qiu, F. *et al., J. Asian Nat. Prod. Res.*, 2001, **3**, 235-240; *CA*, **135**, 329254h (*Ginsenosides I and II*)

Dammar-24-ene-3,12,20-triol D-21

[465-07-6, 53368-76-6]



(3α,12β,20*S*)-*form*

$C_{30}H_{52}O_3$ 460.739
C(20)-configs. in this series are variable and difficult to determine.

(3α,12β,20*S*)-*form*

[6892-79-1]
Betulafolienetriol
Isol. from *Panax ginseng* (ginseng). Cryst. Mp 236-238° (197-198°). $[\alpha]_D$ +20.5 (c, 1 in $CHCl_3$). Not. isol. On hydrolysis, glycosides undergo cyclisation to 20,25-Epoxydammarane-3,12-diol, E-72.

3-Malonyl, 12-Ac: [147199-47-1]
$C_{35}H_{56}O_7$ 588.823
Amorph. powder. $[\alpha]_D^{24}$ -18.2 (c, 0.005 in $CHCl_3$).

3-Ketone: [51116-90-6] ***12,20-Dihydroxydammar-24-en-3-one***
$C_{30}H_{50}O_3$ 458.723
Cryst. Mp 202-202°. $[\alpha]_D^{19}$ +56 (c, 0.93 in $CHCl_3$).

3-Ketone, 12-Ac: [127750-93-0]
$C_{32}H_{52}O_4$ 500.76
Oil. $[\alpha]_D^{25}$ +48 (c, 0.15 in CH_2Cl_2).

(3β,12β,20*R*)-*form* [7755-01-3]

[30636-90-9] *(20*R*)-Protopanaxadiol*
Sol. MeOH, butanol. Mp 236-238°. $[\alpha]_D$ +20.5 ($CHCl_3$). Artifact.

3-O-β-D-Glucopyranoside: [112246-15-8] ***(20R)-Ginsenoside Rh$_2$***
$C_{36}H_{62}O_8$ 622.881
Isol. from *Panax ginseng* (ginseng). Cryst. Mp 278-280°.

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [38243-03-7] ***(20R)-Ginsenoside Rg$_3$***
$C_{42}H_{72}O_{13}$ 785.023
Isol. from *Panax ginseng* (ginseng). Cryst. (MeOH aq.). Mp 192-194°. $[\alpha]_D^{20}$ +8.5 (c, 1.0 in MeOH).

(3β,12β,20*S*)-*form*

[30636-90-9] ***Protopanaxadiol***
Sapogenin of Ginsenosides R_{b1}, R_{b2} and

R_e from *Panax ginseng* (ginseng). Cryst. Sol. MeOH, butanol. Mp 199-200°.

3-O-*β*-D-*Glucopyranoside:* [78214-33-2] ***Ginsenoside Rh$_2$***
$C_{36}H_{62}O_8$ 622.881
Isol. from *Panax ginseng* (ginseng).

3-O-*β*-D-*Glucopyranoside, 20*-O-*[α-arabinofuranosyl-(1→6)-β-glucopyranoside]:* [88105-29-7] ***Notoginsenoside F$_e$***
$C_{47}H_{80}O_{17}$ 917.139
Constit. of leaves of *Panax notoginseng* (ginseng). Needles (MeOH). Mp 179-184°. $[\alpha]_D^{27}$ -0.3 (c, 0.8 in MeOH).

3-O-*β*-D-*Glucopyranoside, 20*-O-*[α*-L-*arabinopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [259795-17-0]
$C_{47}H_{80}O_{17}$ 917.139
Constit. of *Panax notoginseng* (ginseng). Amorph. powder. Mp 189-192°. $[\alpha]_D^{21}$ +34.5 (c, 0.08 in MeOH).

3-O-*β*-D-*Glucopyranoside, 20*-O-*[β*-D-*xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80321-63-7] ***Gynosaponin I***. *Gypenoside IX*. *Notoginsenoside F$_d$*
$C_{47}H_{80}O_{17}$ 917.139
Constit. of *Panax notoginseng* (ginseng). Cryst. + $3H_2O$. Mp 183-185°. $[\alpha]_D^{27}$ +1 (c, 3 in MeOH). $[\alpha]_D^{22}$ +14.2 (c, 1.5 in H_2O).

3-O-*β*-D-*Glucopyranoside, 20*-O-*[α*-L-*rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80330-76-3] ***Gynosaponin J***. *Gypenoside X*
$C_{48}H_{82}O_{17}$ 931.166
Cryst. + $4H_2O$. Mp 189-191°. $[\alpha]_D^{22}$ +13.3 (c, 1.5 in MeOH).

3-O-*β*-D-*Glucopyranoside, 20*-O-*[β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80321-69-3] ***Gynosaponin S***. *Gypenoside XVII*
$C_{48}H_{82}O_{18}$ 947.165
Constit. of *Panax* spp.. Powder. Mp 179-181°. $[\alpha]_D^{22}$ +20.6 (c, 1.4 in MeOH).

3,20-Di-O-*β*-D-*glucopyranoside:* [62025-49-4] ***Ginsenoside F$_2$***
$C_{42}H_{72}O_{13}$ 785.023
Isol. from *Panax* spp.. Powder + $2^1/_2H_2O$. $[\alpha]_D^{25}$ +21.1 (c, 1.14 in MeOH).

3-O-*[β*-D-*Xylopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*β*-D-*glucopyranoside:* [226712-37-4] ***Vinaginsenoside R16***
$C_{47}H_{80}O_{17}$ 917.139
Constit. of *Panax vietnamensis* (Vietnamese ginseng).

3-O-*[β*-D-*Xylopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[β*-D-*xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80321-67-1] ***Gynosaponin Q***
$C_{52}H_{88}O_{21}$ 1049.255

3-O-*[β*-D-*Xylopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[α*-L-*rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80321-68-2] ***Gynosaponin R***. *Protopanaxadiol 20-rutinoside 3-sambubioside*
$C_{53}H_{90}O_{21}$ 1063.281

3-O-*[β*-D-*Xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [59252-86-7] ***Chikusetsusaponin Ia***
$C_{41}H_{70}O_{12}$ 754.997
Constit. of *Panax japonicum* (Japanese ginseng). Cryst. ($CHCl_3$/MeOH/EtOAc). Mp 194°. $[\alpha]_D^{16}$ -3.5 (c, 1.4 in $CHCl_3$).

20-O-*[β*-D-*Xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80325-22-0] ***Gynosaponin M***. *Gypenoside XIII*
$C_{41}H_{70}O_{12}$ 754.997
Cryst. + $1.5H_2O$. Mp 158-160°. $[\alpha]_D^{22}$ +25.7 (c, 1.0 in MeOH).

3-O-*[α*-L-*Rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside], 20*-O-*β*-D-*glucopyranoside:* [80321-64-8] ***Gynosaponin K***. *Gypenoside XI*
$C_{48}H_{82}O_{17}$ 931.166
Cryst. + $3H_2O$. Mp 187-189°. $[\alpha]_D^{22}$ +13.4 (c, 1.8 in MeOH).

3-O-*[α*-L-*Rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside], 20*-O-*[β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80321-72-8] ***Gypenoside I-EH***. *Progynosaponin A$_2$*
$C_{54}H_{92}O_{22}$ 1093.308

3,20-Bis-O-*[α*-L-*rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80321-62-6] ***Gynosaponin G***. *Gypenoside VII*
$C_{54}H_{92}O_{21}$ 1077.308
Cryst. + $3H_2O$. Mp 192-194°. $[\alpha]_D^{22}$ +1.63 (c, 2.0 in MeOH).

20-O-*[α*-L-*Rhamnopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [80330-77-4] ***Gynosaponin N***. *Gypenoside XIV*. *Protopanaxadiol rutinoside*
$C_{42}H_{72}O_{12}$ 769.024
Cryst. + $2H_2O$. Mp 165-170°. $[\alpha]_D^{22}$ +25 (c, 1.3 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-α*-L-*arabinopyranoside], 20*-O-*[β*-D-*xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [105214-49-1] ***Gypenoside LVIII***
$C_{52}H_{88}O_{21}$ 1049.255
Cryst. + $5H_2O$. Mp 181-183°. $[\alpha]_D^{22}$ +8.9 (c, 2.4 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*xylopyranoside], 20*-O-*[β*-D-*xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [88480-44-8] ***Gypenoside XV***
$C_{52}H_{88}O_{21}$ 1049.255
Powder. Mp 180-182°. $[\alpha]_D^{22}$ +1.36 (c, 0.6 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*xylopyranoside], 20*-O-*[α*-L-*rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [88480-45-9] ***Gypenoside XVI***
$C_{53}H_{90}O_{21}$ 1063.281
Powder. Mp 195-197°. $[\alpha]_D^{22}$ +0.39 (c, 2.9 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [14197-60-5] ***Ginsenoside Rg$_3$***
$C_{42}H_{72}O_{13}$ 785.023
Isol. from *Panax* spp..

▶ LY9537300

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*α*-L-*arabinopyranoside:* [226712-39-6] ***Vinaginsenoside R17***
$C_{47}H_{80}O_{17}$ 917.139
Constit. of *Panax vietnamensis* (Vietnamese ginseng).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*β*-D-*xylopyranoside:* [226712-51-2] ***Vinaginsenoside R18***
$C_{47}H_{80}O_{17}$ 917.139
Constit. of *Panax vietnamensis* (Vietnamese ginseng).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*β*-D-*glucopyranoside:* [52705-93-8] ***Ginsenoside R$_d$***. *Gypenoside VIII*
$C_{48}H_{82}O_{18}$ 947.165
Constit. of *Panax ginseng* (ginseng). Powder. Mp 206-209°. $[\alpha]_D^{22}$ +19.4 (c, 1 in MeOH).

▶ LZ5858000

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[α*-L-*arabinofuranosyl-(1→6)-β*-D-*glucopyranoside]:* [11021-14-0] ***Ginsenoside R$_c$***
$C_{53}H_{90}O_{22}$ 1079.281
Constit. of *Panax ginseng* (ginseng). Powder. Mp 199-201°. $[\alpha]_D^{22}$ +1.9 (c, 1 in MeOH).

▶ LY9536300

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[α*-L-*arabinopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [11021-13-9] ***Ginsenoside R$_{b2}$***
$C_{53}H_{90}O_{22}$ 1079.281
Constit. of *Panax ginseng* (ginseng). Powder. Mp 200-203°. $[\alpha]_D^{22}$ +3 (c, 1 in MeOH).

▶ LY9536100

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[β*-D-*xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [105214-48-0] ***Gypenoside LVI***
$C_{53}H_{90}O_{22}$ 1079.281
Cryst. + $2.5H_2O$. Mp 212-214°. $[\alpha]_D^{22}$ +7.9 (c, 3.8 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[α*-L-*rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [80321-60-4] ***Gynosaponin E***. *Gypenoside V*
$C_{54}H_{92}O_{22}$ 1093.308
Cryst. + $3H_2O$. Mp 199-201°. $[\alpha]_D^{22}$ +8.61 (c, 1.4 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [41753-43-9] ***Ginsenoside R$_{b1}$***. *Sanchinoside E$_1$*. *Gypenoside III*. *Gynosaponin C*
$C_{54}H_{92}O_{23}$ 1109.307
Constit. of *Panax ginseng* (ginseng). Powder. Mp 197-198°. $[\alpha]_D^{22}$ +12.4 (c, 0.9 in $CHCl_3$).

▶ LD_{50} (mus, ipr) 1110 mg/kg. LZ5856000

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 20*-O-*[β*-D-*xylopyranosyl-(1→2)-α*-L-*arabinofuranosyl-(1→6)-β*-D-*glucopyranoside]:* [83459-42-1] ***Ginsenoside R$_{a2}$***

$C_{58}H_{98}O_{26}$ 1211.397
From root of *Panax ginseng* (ginseng). Powder. $[\alpha]_D^{25}$ -2.4 (c, 1.0 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-xylopyranosyl-(1→4)-α-L-arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [83459-41-0] ***Ginsenoside R_{a1}***
$C_{58}H_{98}O_{26}$ 1211.397
From root of *Panax ginseng* (ginseng). Powder. $[\alpha]_D^{25}$ +12.8 (c, 1.0 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [90985-77-6] ***Ginsenoside Ra_3***
$C_{59}H_{100}O_{27}$ 1241.423
Isol. from *Panax ginseng* (ginseng). Powder + $4H_2O$. $[\alpha]_D^{17}$ +9.8 (c, 0.43 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-xylopyranosyl-(1→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [87741-77-3] ***Notoginsenoside R_4***
$C_{59}H_{100}O_{27}$ 1241.423
Constit. of *Panax notoginseng* (ginseng). Amorph. powder. $[\alpha]_D^{16}$ +8.9 (c, 1 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[α-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [208764-55-0] ***Quinquenoside V***
$C_{60}H_{102}O_{28}$ 1271.449
Constit. of American ginseng (*Panax quinquefolium*). Cryst. (MeOH aq.). Mp 192-194°. $[\alpha]_D^{28}$ +24.4 (c, 0.25 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-6*-O-*acetyl-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [208764-53-8]
$C_{50}H_{84}O_{19}$ 989.202
Constit. of American ginseng (*Panax quinquefolium*). Cryst. (MeOH aq.). Mp 167-169°. $[\alpha]_D^{28}$ +24.3 (c, 0.25 in MeOH).

3-O-*[6*-O-*Acetyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [102805-32-3] ***Pseudoginsenoside R_{c1}***
$C_{50}H_{84}O_{19}$ 989.202
Constit. of *Panax pseudoginseng* (ginseng). Amorph. powder. $[\alpha]_D^{17}$ +20.8 (c, 0.63 in MeOH).

3-O-*[6*-O-*Acetyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[α-L-arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [87733-67-3] ***Ginsenoside Rs_1***
$C_{55}H_{92}O_{23}$ 1121.318
Constit. of *Panax ginseng* (ginseng). Powder + $2H_2O$. $[\alpha]_D^{16}$ +19 (c, 1 in MeOH).

3-O-*[6*-O-*Acetyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [85013-02-1] ***Quinquenoside R_1***
$C_{56}H_{94}O_{24}$ 1151.344
Constit. of American ginseng (*Panax quinquefolium*). Amorph. powder (EtOH/EtOAc). $[\alpha]_D^{16}$ +12 (c, 1 in MeOH).

3-O-*[6*-O-2E-*Butenoyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [208764-50-5] ***Quinquenoside I***
$C_{52}H_{86}O_{19}$ 1015.24
Constit. of American ginseng (*Panax quinquefolium*). Cryst. (MeOH aq.). Mp 172-174°. $[\alpha]_D^{28}$ +34.6 (c, 0.25 in MeOH). λ_{max} 211 (log ϵ 4.3) (MeOH).

3-O-*[6*-O-2E-*Octenoyl-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [208764-52-7] ***Quinquenoside II***
$C_{62}H_{104}O_{24}$ 1233.489
Constit. of American ginseng (*Panax quinquefolium*). Cryst. (MeOH aq.). Mp 168-170°. $[\alpha]_D^{28}$ +22.5 (c, 0.25 in MeOH). λ_{max} 205 (log ϵ 4.5) (MeOH).

3-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [259795-16-9]
$C_{48}H_{82}O_{18}$ 947.165
Constit. of *Panax notoginseng* (ginseng) and *Cyclanthera pedata* (achoccha). Amorph. powder. Mp 190-194°. $[\alpha]_D^{21}$ +13.2 (c, 0.45 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→6)-6*-O-*acetyl-β-D-glucopyranoside], 20*-O-*[α-L-arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [87733-66-2] ***Ginsenoside Rs_2***
$C_{55}H_{92}O_{23}$ 1121.318
Isol. from *Panax ginseng* (ginseng). Powder + $2H_2O$. $[\alpha]_D^{16}$ +2.5 (c, 1 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [156009-83-5] ***Vinaginsenoside R7***
$C_{53}H_{90}O_{22}$ 1079.281
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{25}$ +17.8 (c, 1.07 in MeOH).

3-O-*[β-Xylopyranosyl-(1→2)-β-glucopyranosyl-(1→2)-β-glucopyranoside], 20*-O-*[β-xylopyranosyl-(1→6)-β-glucopyranoside]:* [88122-52-5] ***Notoginsenoside F_c***
$C_{58}H_{98}O_{26}$ 1211.397
Constit. of leaves of *Panax notoginseng* (ginseng). Needles (MeOH). Mp 219-223°. $[\alpha]_D^{18}$ -1.4 (c, 0.67 in H_2O).

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [88100-04-3] ***Notoginsenoside F_a***
$C_{59}H_{100}O_{27}$ 1241.423
Constit. of leaves of *Panax notoginseng* (ginseng). Needles (MeOH). Mp 235-240°. $[\alpha]_D^{17}$ -2 (c, 1.0 in H_2O).

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-xylopyranosyl-(1→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [193895-50-0] ***Notoginsenoside D***
$C_{64}H_{108}O_{31}$ 1373.539
Constit. of *Panax notoginseng* (ginseng). Cryst. (MeOH aq.). Mp 207-210°. $[\alpha]_D$ +6.5 (c, 0.1 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→6)]-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [137348-15-3] ***Chikusetsusaponin VI***
$C_{59}H_{100}O_{27}$ 1241.423
Constit. of *Panax pseudo-ginseng* var. *angustatus*. Powder + $3H_2O$. $[\alpha]_D^{19}$ -10.3 (c, 1 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [80321-73-9] ***Progynospaponin A-AH***
$C_{48}H_{82}O_{17}$ 931.166

3-O-*[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [80321-61-5] ***Gynosaponin F***
$C_{54}H_{92}O_{22}$ 1093.308

3-O-*[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 20*-O-rutinoside: [80321-59-1] ***Gynosaponin B***
$C_{60}H_{102}O_{26}$ 1239.45

3-O-*[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [80325-21-9] ***Gynosaponin A***
$C_{60}H_{102}O_{27}$ 1255.45

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside], 20*-O-*β-D-glucopyranoside:* [85889-23-2] ***Gypenoside VI***
$C_{54}H_{92}O_{22}$ 1093.308
Cryst. + $3H_2O$. Mp 191-193°. $[\alpha]_D^{22}$ +7.76 (c, 1.7 in H_2O).

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside], 20*-O-*[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [85889-22-1] ***Gypenoside II***
$C_{60}H_{102}O_{26}$ 1239.45
Cryst. + $3H_2O$. Mp 196-198°. $[\alpha]_D^{22}$ -3.3 (c, 1.5 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [85889-20-9] ***Gypenoside I***
$C_{60}H_{102}O_{27}$ 1255.45
Cryst. + $3H_2O$. Mp 201-203°. $[\alpha]_D^{22}$ -1.38 (c, 1.5 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-*

glucopyranosyl-(1→6)-β-D-glucopyranoside]: [112722-00-6] ***Ginsenoside RA$_0$***
$C_{60}H_{102}O_{28}$ 1271.449
Isol. from American ginseng (*Panax quinquefolium*).

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside], 20*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [394246-58-3] ***Notoginsenoside L***
$C_{53}H_{90}O_{22}$ 1079.281
Constit. of roots of *Panax notoginseng* (ginseng). Cryst. (MeOH aq.). Mp 195-197°. $[\alpha]_D^{28}$ +20.4 (c, 0.1 in MeOH).

Glycoside (1): ***Panaxoside D***
Isol. from *Panax ginseng* (ginseng). Yellowish powder (EtOH/Me_2CO). Mp 157-160°. $[\alpha]_D^{20}$ +29 (c, 4.82 in MeOH). Struct. unknown. On hydrol. gives panaxadiol and glucose only. C 58.2%, H 8.8%.

Glycoside (2): ***Panaxoside E***
From *Panax ginseng* (ginseng). Mp 185-187°. $[\alpha]_D$ +21.5 (c, 4.18 in MeOH). Struct. unknown. Gives panaxadiol, glucose and arabinose (ratio 4:1) on hydrol. C 58.3% H 8.8%.

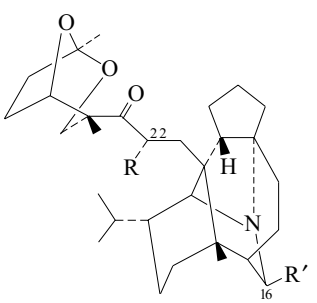
Glycoside (3): ***Panaxoside F***
Glycoside from *Panax ginseng* (ginseng). Mp 185-187°. $[\alpha]_D^{20}$ +20.6 (c, 5.34 in MeOH). Struct. unknown. On hydrol. gives panaxadiol and glucose only C 56.1% H 8.48%.

3-Malonyl, 12-Ac: [152340-18-6] ***Pendulic acid***
$C_{35}H_{56}O_7$ 588.823
Amorph.

Uvarova, N.I. *et al., Khim. Prir. Soedin.*, 1965, **1**, 82-86; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 63-66 (*Panaxosides*)
Elyakov, C.-B. *et al., Khim. Prir. Soedin.*, 1967, **3**, 164-167; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 135-137 (*Panaxosides*)
Nagai, M. *et al., Tet. Lett.*, 1967, 3579-3580 (*Protopanaxadiol, isol*)
Tanaka, O. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1204-1211; 1985, **33**, 2323-2330; 3852-3858 (*Ginsenosides Rc, Rb, Gynosaponin S*)
Sanada, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 421-428; 2407-2412 (*Ginsenosides, isol, struct*)
Lin, T.D. *et al., Chem. Pharm. Bull.*, 1976, **24**, 253-261 (*Chikusetsusaponin Ia*)
Kasai, R. *et al., Chem. Pharm. Bull.*, 1976, **24**, 400-406; 1983, **31**, 2120-2125 (*Protopanaxadiol, synth, Ginsenoside Rs$_1$, Ginsenoside Rs$_2$*)
Yahara, S. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2204-2208 (*Ginsenoside F$_2$*)
Asakawa, J. *et al., Tetrahedron*, 1977, **33**, 1935-1939 (*cmr*)
Besso, H. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2380-2385; 4534-4538 (*Ginsenosides Ra1, Ra2*)
Koizumi, H. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2393-2398 (*Ginsenoside Ra2*)
Matsuura, H. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2281-2287 (*Notoginsenoside R$_4$*)
Yang, T.R. *et al., Phytochemistry*, 1983, **22**, 1473-1478 (*Notoginsenosides*)
Takemoto, T. *et al., Yakugaku Zasshi*, 1983, **103**, 173-185; 1015-1023; 1984, **104**, 1043-1049; 1986, **106**, 664-670; 1987, **107**, 355-360 (*Gypenosides*)
Matsuura, H. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1188-1192 (*Ginsenoside Ra$_3$*)
Namba, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 730-738 (*Pseudoginsenoside R$_{c1}$*)
Xu, S. *et al., Yaoxue Xuebao*, 1987, **22**, 750; *CA*, **108**, 72123 (*Ginsenoside RA$_0$*)
Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 852-854 (*Gypenosides*)
Atopkina, L.N. *et al., Khim. Prir. Soedin.*, 1989, **25**, 813-816; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 690-693 (*synth, Ginsenoside Rh$_2$*)
Kohda, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1588-1590 (*Chikusetsusaponin VI*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1372
Taipale, H.T. *et al., Phytochemistry*, 1993, **34**, 755-758 (*Pendulic acid*)
Rickling, B. *et al., Planta Med.*, 1993, **59**, 76-79 (*isol, pmr, cmr, ms, ir*)
Minh Duc, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 115-122 (*Vinaginsenoside R7*)
Yang, Y.W. *et al., Huaxue Xuebao*, 1994, **52**, 234-242; *CA*, **120**, 299100a (*Ginsenoside Rb$_1$, pmr, cmr*)
Anufriev, V.P. *et al., Carbohydr. Res.*, 1997, **304**, 179-182 (*Ginsenoside Rg$_3$*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1039-1045 (*Notoginsenoside D*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 647-654 (*Quinquenosides*)
De Tommasi, N. *et al., J. Agric. Food Chem.*, 1999, **47**, 4512-4519 (*Cyclanthera pedanta saponin*)
Ma, W.G. *et al., Phytochemistry*, 1999, **52**, 1133-1139 (*Panax notoginseng saponins*)
Elyakov, G.B. *et al., Planta Med.*, 1999, **65**, 30-34 (*activity*)
Minh Duc, N. *et al., Stud. Plant Sci.*, 1999, **6**, 77-82 (*Vinaginsenosides R16-R18*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1452-1456 (*Notoginsenoside L*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAF450

Daphnimacropine D-22

[20249-89-2]



R = H, R′ = OH

$C_{30}H_{47}NO_4$ 485.706

Methiodide:
Mp 306-307°.

Deoxy: [14694-15-6] ***Codaphniphylline***. *Desacetoxydaphniphylline*
$C_{30}H_{47}NO_3$ 469.706
Cryst. ($CHCl_3$/Et_2O)(as hydrochloride). Mp 266-267° (sealed tube)(as hydrochloride). $[\alpha]_D$ +4.2 (c, 2.40 in $CHCl_3$).

16-Deoxy, 22-acetoxy: [15007-67-7] ***Daphniphylline***. *Daphniphyllamine*
$C_{32}H_{49}NO_5$ 527.743
Isol. from the bract of *Hibiscus sabdariffa* (roselle). Noncryst.

16-Deoxy, 22-acetoxy; hydrochloride:
Needles ($CHCl_3$/Et_2O). Mp 238-240° (sealed tube). $[\alpha]_D$ +43.7 (c, 2.18 in $CHCl_3$).

16-Deoxy, 22-acetoxy; hydrobromide:
Cryst. ($CHCl_3$/Et_2O or C_6H_6/hexane). Mp 228-230° Mp 245-246°.

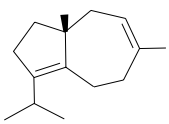
16-Deoxy, 22-acetoxy, methiodide:
Cryst. (Me_2CO/MeOH). Mp 276-279°.

16-Deoxy, 22-acetoxy, N*-oxide:Daphniphylline* N*-oxide.* ***Daphnezomine E***
$C_{32}H_{49}NO_6$ 543.742
Solid. $[\alpha]_D^{24}$ +31 (c, 1.4 in $CHCl_3$).

Sakabe, N. *et al., Tet. Lett.*, 1966, 965 (*Daphniphylline*)
Kamijo, N. *et al., Tet. Lett.*, 1966, 2889 (*cryst struct*)
Nakano, T. *et al., Tet. Lett.*, 1967, 4791 (*ms*)
Irikawa, H. *et al., Tetrahedron*, 1968, **24**, 5691 (*isol, uv, ir, pmr, ms, synth, struct, Codaphniphylline*)
Sasaki, K. *et al., J.C.S.(B)*, 1971, 1565 (*Daphniphylline, abs config*)
Suzuki, K.T. *et al., Tet. Lett.*, 1973, 799 (*biosynth*)
Toda, M. *et al., Tetrahedron*, 1974, **30**, 2683 (*Daphniphylline*)
Yamamura, S. *et al., Alkaloids (N.Y.)*, 1975, **15**, 41 (*struct*)
Yamamura, S. *et al., Chem. Lett.*, 1980, 393 (*Daphniphylline*)
Heathcock, C.H. *et al., J.O.C.*, 1995, **60**, 1120 (*synth, Codaphniphylline*)
Morita, H. *et al., Tetrahedron*, 1999, **55**, 12549-12556 (*Daphnezomine E*)

4,8-Daucadiene D-23

[16661-00-0]
Daucene



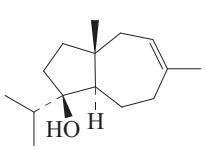
$C_{15}H_{24}$ 204.355
Both enantiomers apparently isol., but data on opt. rotns. and abs. config. is incomplete. Constit. of *Daucus carota* (carrot). Oil. Bp_4 96°. $[\alpha]_D$ +39 (c, 0.3 in $CHCl_3$). n_D^{20} 1.4918.

Bisepoxide:
Cryst. Mp 89°. $[\alpha]_D$ +25 (c, 0.4 in $CHCl_3$).

Enantiomer: [38231-17-3]
$C_{15}H_{24}$ 204.355

De Broissia, H. *et al., Bull. Soc. Chim. Fr.*, 1972, 4314 (*isol, struct*)
Audenaert, F. *et al., Tetrahedron*, 1987, **43**, 5593 (*synth*)
Cool, L.G. *et al., Phytochemistry*, 2001, **58**, 969-972 (*Cupressocyparis leylandii constit*)

8-Daucen-4-ol D-24

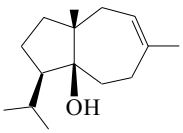


$C_{15}H_{26}O$ 222.37

4β-*form* [255062-40-9]
Constit. of *Daucus carota* (carrot).

Mazzoni, V. *et al., Flavour Fragrance J.*, 1999, **14**, 268-272 (*isol, pmr, cmr*)

8-Daucen-5-ol D-25



$C_{15}H_{26}O$ 222.37

5β-*form* [465-28-1]

Carotol

Constit. of *Daucus carota* (carrot). Oil. $Bp_{2.5}$ 126°. $[\alpha]_D^{20}$ +29.6.

Levisalles, J. *et al., Bull. Soc. Chim. Fr.*, 1967, 2059 (*stereochem*)

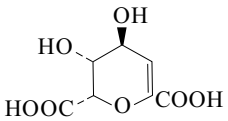
de Broissia, H. *et al., Bull. Soc. Chim. Fr.*, 1972, 4314 (*synth*)

Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*isol, pmr, cmr*)

Daucic acid D-26

[34098-52-7]

2,6-Anhydro-3-deoxy-D-xylo-*hept-2-enaric acid, 9CI*



$C_7H_8O_7$ 204.136

Free acid not obt. pure. Found in wheat, sugar beet and sunflower.

Di-Me ester: [33573-25-0]

Cryst. (EtOAc/petrol). Mp 130-131°. $[\alpha]_D^{24.5}$ -102 (c, 0.9 in Me_2CO).

Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1975, 2069 (*struct, spectra*)

Daucine D-27

$C_{11}H_{18}N_2$ 178.277

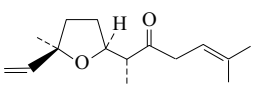
Struct. unknown. Alkaloid from the leaves of *Daucus carota* (carrot). Oil. Bp 240-250°. $[\alpha]_D$ +7.74 (c, 0.645 in Et_2O).

Pictet, A. *et al., Ber.*, 1907, **40**, 3771 (*isol*)

Davanone D-28

[30810-99-2]

2-(5-Ethenyltetrahydro-5-methyl-2-furanyl)-6-methyl-5-hepten-3-one, 9CI



Absolute configuration

$C_{15}H_{24}O_2$ 236.353

Main component of davana oil from *Artemisia pallens*. Davana oil used in food flavouring. $[\alpha]_D^{21}$ +77.7 (neat).

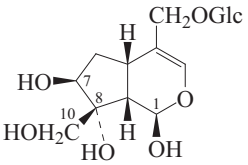
Thomas, A.F. *et al., Helv. Chim. Acta*, 1974, **57**, 2055 (*isol, struct*)

Bartlett, P.A. *et al., Tet. Lett.*, 1983, **24**, 1365 (*synth*)

Honda, Y. *et al., Chem. Lett.*, 1987, 1259-1262 (*synth*)

Molander, G.A. *et al., Tetrahedron*, 1999, 617-624 (*synth*)

Deacylsuspensolide D-29



$C_{16}H_{26}O_{11}$ 394.375

1-O-(3-Methylbutanoyl): [64703-86-2]

Suspensolide F. Kanokoside B

$C_{21}H_{34}O_{12}$ 478.492

Isol. from valerian root. Amorph. powder. Mp 110-111° (as hexa-Ac). $[\alpha]_D$ -25 (c, 0.053 in MeOH).

Endo, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2140 (*isol, Suspensolides*)

Iwagawa, T. *et al., Phytochemistry*, 1990, **29**, 310 (*isol, pmr, cmr, Suspensolides*)

2,4-Decadienal D-30

[2363-88-4]

$H_3C(CH_2)_4CH{=}CHCH{=}CHCHO$

$C_{10}H_{16}O$ 152.236

(*E,E*)-*form* [25152-84-5]

FEMA 3135

Present in apple, bitter orange peel oil, mandarin peel oil, wheat bread, cooked beef, raw cured pork, cooked scented rice, quince, maize, dried bonito, clary sage (*Salvia sclarea*), water yam (*Dioscerea alata*) melon and peas. Flavouring agent. Oily liq. with grapefruit/orange-like taste on dilution. $Bp_{0.05}$ 58-61°.

► HD3000000

Semicarbazone:

Mp 181-182°.

2,4-Dinitrophenylhydrazone:

Mp 141-142°.

4R,5R-Epoxide: [134454-31-2]

[73528-44-6] *3-(3-Pentyloxiranyl)-2-propenal, 9CI. 4,5-Epoxy-2-decenal*

$C_{10}H_{16}O_2$ 168.235

Lipid peroxidation prod. Contributor to warmed-over flavour development in cooked meats and off-flavour in stored soybean oil. Also present in breadcrumb, hop cone and roasted sesame seed odours and pastry products prepared from margarine. Liq. with green hay-like/metallic odour. Odour threshold 0.5 pg/L in air, 1.3 µg/kg in sunflower oil.

(2*E*,4*Z*)-*form* [25152-83-4]

Constit. of numerous plants and food sources. $Bp_{0.05}$ 58-61°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 364B (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 566A (*ir*)

Ohloff, G. *et al., Helv. Chim. Acta*, 1973, **56**, 1176 (*synth, ir, pmr, ms*)

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 753 (*rev, tox*)

Tsuboi, S. *et al., J.O.C.*, 1982, **47**, 4478 (*synth, ir, pmr, cmr*)

Crilley, M.M.L. *et al., J.C.S. Perkin 1*, 1988, 2061 (*synth, ir, pmr, ms*)

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAE450

Guth, M. *et al., Lebensm.-Wiss. Technol.*, 1990, **23**, 59-65; 513-522 (*occur, anal, synth, epoxide*)

Gassenmeier, K. *et al., Lebensm.-Wiss. Technol.*, 1994, **27**, 282 (*occur, epoxide*)

Steinhaus, M. *et al., J. Agric. Food Chem.*, 2000, **48**, 1776-1783 (*occur, epoxide*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

2,8-Decadiene-4,6-diyn-1-ol D-31

[505-98-6]

Matricarianol. Matricariol

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH_2OH$

$C_{10}H_{10}O$ 146.188

(2*E*,8*Z*)-*form* [13894-67-2]

Oil.

3-Methylbutanoyl: [29444-87-9]

Constit. of *Carthamus tinctorius* (safflower). Oil.

[104899-48-1]

Bruun, T. *et al., Acta Chem. Scand.*, 1951, **5**, 1244 (*synth*)

Gardner, J.N. *et al., J.C.S.*, 1960, 691 (*isol, struct*)

Bohlmann, F. *et al., Chem. Ber.*, 1969, **102**, 1679; 1972, **105**, 1919 (*isol, synth, pmr*)

Davies, D.G. *et al., J.C.S. Perkin 1*, 1978, 1602 (*biosynth, isol*)

2,4-Decadienoic acid D-32

[92015-76-4]

$H_3C(CH_2)_4CH{=}CHCH{=}CHCOOH$

$C_{10}H_{16}O_2$ 168.235

(*E,E*)-*form* [30361-33-2]

Mp 49-50°. $Bp_{0.3}$ 121-124°.

Pyrrolidide: [78910-33-5] *1-(1-Oxo-2,4-decadienyl)pyrrolidine, 9CI. 2,4-Decadienoic acid pyrrolidide. 1-(2,4-Decadienoyl)pyrrolidine.* ***Sarmentine***

$C_{14}H_{23}NO$ 221.342

Constit. of fruits of pepper (*Piper nigrum*) and cha-plu (*Piper sarmentosum*) (Piperaceae). Oil.

(2*E*,4*Z*)-*form* [544-48-9]

Phycodioic acid. Stillingic acid

$Bp_{0.5}$ 122°.

Me ester: [4493-42-9] *FEMA 3859*

Found in pears and spineless monkey orange. Flavour for candies etc. Liq. with pear/lemon odour. $Bp_{0.15}$ 71°.

Et ester: [3025-30-7] *Pear ester. FEMA 3148*

Constit. of odoriferous principle of Bartlett pears. Also present in fresh apple, *Vitis* spp., quince and spineless monkey orange (*Strychnos madagasc*). Flavouring agent. $Bp_{0.05}$ 84-86°.

► HD3510900

Propyl ester:

[84788-08-9] *Propyl 2,4-decadienoate. FEMA 3648*

$C_{13}H_{22}O_2$ 210.316

Flavouring ingredient with a Bartlett pear flavour. Coml. product comprises 57% of the (2*E*,4*Z*)-isomer, 35% of the (2*E*,4*E*)-isomer, and 9% other esters.

(2*Z*,4*E*)-*form* [68676-77-7]

$Bp_{0.45}$ 112-114°.

Et ester:
Flavouring material.

Crombie, L. *et al., J.C.S.*, 1955, 1007 (*synth*)
Näf, F. *et al., Helv. Chim. Acta*, 1974, **57**, 1309 (*synth*)
Bestmann, H.J. *et al., Annalen*, 1982, 363 (*synth*)
Likhitwitayawuid, K. *et al., Tetrahedron*, 1987, **43**, 3689 (*Sarmentine*)
Kiuchi, F. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2452 (*pyrrolidide*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 317 (*rev, tox, Pear ester*)
Bari, S.S. *et al., J. Indian Chem. Soc.*, 1990, **67**, 995 (*synth, Sarmentine*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2343 (*propyl ester*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1110-1111; 1537-1538 (*Me ester, propyl ester*)

4,8-Decadienoic acid, 9CI, 8CI D-33

[13159-49-4]
$H_3CCH{=}CHCH_2CH_2CH{=}CHCH_2CH_2COOH$
$C_{10}H_{16}O_2$ 168.235

Me ester: [1191-03-3]
$C_{11}H_{18}O_2$ 182.262
Constit. of essential oil of hops (*Humulus lupulus*).

[94372-21-1]

Buttery, R.G. *et al., Chem. Ind. (London)*, 1963, 1981 (*isol, ir, pmr*)
Buttery, R.G. *et al., J. Chromatogr.*, 1965, **18**, 399 (*chromatog*)
Goliaszewski, A. *et al., Tetrahedron*, 1985, **41**, 5779 (*synth, pmr, ms*)

2,4-Decadienoic isobutylamide D-34

Pellitorine. N-*(2-Methylpropyl)-2,4-decadienamide, 9CI.* N-*Isobutyl-2,4-decadienamide, 8CI. Pyretrin*
$H_3C(CH_2)_4CH{=}CHCH{=}CHCONHCH_2CH(CH_3)_2$
$C_{14}H_{25}NO$ 223.358

(*E*,*E*)-*form* [18836-52-7]
Constit. of *Achillea millefolium* (yarrow). Needles (petrol). Mp 75° (69°) Mp 90-95°.
► Severe irritant.

6-Hydroxy: [133640-43-4] *6-Hydroxy*-N-*(2-methylpropyl)-2,4-decadienamide, 9CI. 6-Hydroxy*-N-*isobutyl-2,4-decadienamide.* ***6-Hydroxypellitorine***
$C_{14}H_{25}NO_2$ 239.357

(2*E*,4*Z*)-*form*
Yellow oil. λ_{max} 257 (MeOH).

Crombie, L. *et al., J.C.S.*, 1955, 1007 (*synth*)
Bowden, K. *et al., J.C.S.*, 1963, 3503 (*isol, uv, ir*)
Loder, J.W. *et al., Aust. J. Chem.*, 1969, **22**, 1531 (*isol, uv, ir, ms, synth*)
Banerji, A. *et al., Experientia*, 1974, **30**, 223 (*isol, struct*)
Mahanta, P.K. *et al., J. Pharm. Sci.*, 1974, **63**, 1160 (*isol, uv, ir*)
Dasgupta, S. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 538 (*isol, uv, ir, pmr, ms*)
Ono, N. *et al., Chem. Lett.*, 1980, 1365 (*synth*)
Nokami, J. *et al., Tet. Lett.*, 1980, **21**, 4455 (*synth*)
Yasusa, I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 564 (*isol, uv, ir, pmr, cmr, ms*)
Tamura, Y. *et al., Tet. Lett.*, 1981, **22**, 1343 (*synth*)
Sato, T. *et al., Tet. Lett.*, 1981, **22**, 2375 (*synth, ir, pmr*)
Bari, S.S. *et al., J. Indian Chem. Soc.*, 1990, **67**, 995 (*synth*)
Ahmed, A. *et al., Pharmazie*, 1990, **45**, 941 (*6-Hydroxypellitorine*)
Kaga, H. *et al., Synlett*, 1994, 607 (*synth*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419 (*synth*)
Abarbri, M. *et al., Synth. Commun.*, 1998, **28**, 239-249 (*synth, ir, pmr, cmr, ms*)
Saadali, B. *et al., Phytochemistry*, 2001, **58**, 1083-1086 (*2E,4Z-isomer*)

2,4-Decadien-1-ol, 9CI D-35

[14507-02-9]
$H_3C(CH_2)_4CH{=}CHCH{=}CHCH_2OH$
$C_{10}H_{18}O$ 154.252

(2*E*,4*E*)-*form* [18409-21-7]
FEMA 3911
Found in blackcurrant buds, malt, peach and Chinese pear. Food flavouring ingredient. Liq. with citrus-like odour. d_4^{23} 0.86. $Bp_{0.5}$ 84° Bp_{10} 112°. n_D^{23} 1.4857.

α-*Naphthylurethane:*
Mp 95°.

(2*E*,4*Z*)-*form* [16195-71-4]
Constit. of *Tordylium apulium* essential oil. d_4^{23} 0.87. $Bp_{0.6}$ 86° Bp_3 78-84°. n_D^{23} 1.4870.

α-*Naphthylurethane:*
Mp 61°.

(2*Z*,4*E*)-*form* [77657-81-9]
d_4^{21} 0.87. $Bp_{0.6}$ 84°. n_D^{21} 1.4892.

(2*Z*,4*Z*)-*form* [77657-76-2]
d_4^{22} 0.87. $Bp_{0.6}$ 87°. n_D^{22} 1.4852.

α-*Naphthylurethane:*
Mp 71°.

Crombie, L. *et al., J.C.S.*, 1955, 1007-1025 (*synth, uv*)
Bosshardt, H. *et al., Helv. Chim. Acta*, 1980, **63**, 2393-2403 (*synth, ir, pmr, ms*)
Furber, M. *et al., J.C.S. Perkin 1*, 1989, 683-690 (*2Z,4E-form, synth, pmr, cmr*)
Horvat, R.J. *et al., J. Agric. Food Chem.*, 1990, **38**, 234-237 (*E,E-form, occur, peach*)
Kofinas, C. *et al., J. Essent. Oil Res.*, 1993, **5**, 33-36 (*Z,E-form, occur*)
Imayoshi, Y. *et al., Koryo*, 1996, **190**, 121-127; *CA*, **125**, 113270y (*E,E-form, occur, chinese pear*)
Zeid, A.H.S. *et al., Egypt. J. Pharm. Sci.*, 1999, **39**, 277-288 (*E,E-form, occur*)

4,7-Decadien-1-ol D-36

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH_2OH$
$C_{10}H_{18}O$ 154.252

(4*Z*,7*E*)-*form*

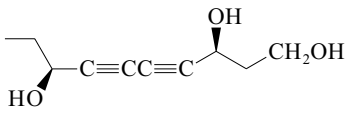
O-*Sulfate:* [160116-62-1]
$C_{10}H_{18}O_4S$ 234.316

(4*Z*,7*Z*)-*form* [104188-11-6]
Constit. of the oil of *Acorus calamus* (sweet flag).

O-*Sulfate:* [160116-61-0]

Van Lier, F.P. *et al., Perfum. Essent. Oil Res.*, 1985, 215; *CA*, **106**, 72677f (*isol, synth*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 1994, **57**, 1606 (*sulfates*)

4,6-Decadiyne-1,3,8-triol D-37



$C_{10}H_{14}O_3$ 182.219

(3*S*,8*S*)-*form* [105304-52-7]
Oil. $Bp_{0.4}$ 122°. $[\alpha]_D^{23}$ -5.8 (c, 1.7 in MeOH). λ_{max} 220 (ϵ 2140); 228 (ϵ 2090); 243 (ϵ 1740); 256 (ϵ 1070) (MeOH) (Derep).

Tri-Ac: [105274-17-7]
$C_{16}H_{20}O_6$ 308.33
Oil. $Bp_{0.4}$ 87°.

Tribenzoyl:
$C_{31}H_{26}O_6$ 494.543
Amorph. solid. Mp 97-102°. $[\alpha]_D^{21}$ +4.7 (c, 1.7 in $CHCl_3$).

Kusano, G. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3465 (*isol*)
Hashimoto, M. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 2751 (*isol, cmr, abs config*)

4,6-Decadiyn-1-ol, 9CI D-38

$H_3CCH_2CH_2C{\equiv}CC{\equiv}CCH_2CH_2CH_2OH$
$C_{10}H_{14}O$ 150.22
Constit. of *Carthamus tinctorius* (safflower). $Bp_{0.001}$ 80-90°.

3-Methylbutanoyl: [29314-16-7] ***4,6-Decadiyn-1-ol isovalerate***
$C_{15}H_{22}O_2$ 234.338
Isol. from *Carthamus tinctorius* (safflower). Oil.

Bohlmann, F. *et al., Chem. Ber.*, 1956, **89**, 1276; 1970, **103**, 2853 (*isol, struct, synth*)

Decanal, 9CI D-39

[112-31-2]
Decyl aldehyde. Capraldehyde. Caprinaldehyde. FEMA 2362
$H_3C(CH_2)_8CHO$
$C_{10}H_{20}O$ 156.267
Constit. of Cassia, Neroli and other oils esp. citrus peel oils. Also present in coriander leaf or seed, caviar, roast turkey, roast filbert, green tea, fish oil, hop oil and beer. Flavouring agent. Liq. with strong orange-peel odour. d_4^{20} 0.85. Mp -5° approx. Bp 208-209° Bp_7 81°. n_D^{20} 1.4887.
► Skin irritant. LD_{50} (rat, orl) 3730 mg/kg. HD6000000

Di-Me acetal: [7779-41-1] *1,1-Dimethoxydecane. FEMA 2363*
$C_{12}H_{26}O_2$ 202.336
Flavouring ingredient. Liq. $d^{15.5}$ 0.83. Bp 218°. n_D^{24} 1.4244.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 469A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 732B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 555C (*ir*)
Pickard, K.J. *et al., J.C.S.*, 1913, **103**, 1947
Mathis, C. *et al., Phytochemistry*, 1964, **3**, 377 (*isol*)
Attaway, J.A. *et al., Phytochemistry*, 1966, **5**, 141 (*isol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 477 (*rev, tox*)

Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir, pmr*)
Stanley, J.B. *et al., J. Food Sci.*, 1975, **40**, 1134 (*ms*)
Org. Synth., 1976, **55**, 84 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAG000; DAG200
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 145 (*di-Me acetal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 772-774 (*props, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAG000; DAG200

Decanedioic acid, 9CI D-40

[111-20-6]
Sebacic acid. Octane-1,8-dicarboxylic acid. Ipomic acid

$HOOC(CH_2)_8COOH$

$C_{10}H_{18}O_4$ 202.25
Leaflets. Spar. sol. H_2O; sol. EtOH, Et_2O. Mp 134.5°. Bp_{100} 294.5° Bp_{15} 243.5°. pK_{a1} 4.58; pK_{a2} 5.54 (25°, 0.1*M* KNO_3).

▶ LD_{50} (rat, orl) 3400 mg/kg. VS0875000

Di-Et ester: [110-40-7] *FEMA 2376*
$C_{14}H_{26}O_4$ 258.357
Flavouring ingredient. Sl. sol. H_2O; sol. Me_2CO, misc. EtOH, Et_2O. d^{15} 0.96. Mp 5°. Bp 305° Bp_{10} 172-174°. n_D^{15} 1.4367.

▶ Fl. p. >71°. VS1180000

Dibutyl ester: [109-43-3] *Dibutyl decanedioate. Dibutyl sebacate. FEMA 2373*
$C_{18}H_{34}O_4$ 314.464
Flavouring ingredient used in fruit food flavouring. Liq. Insol. H_2O. d^{25} 0.93. Mp -11° Mp 12°. Bp 345°. n_D^{20} 1.4433.

[51877-43-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 496D; 619C; 619D; 696C; 742B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 772C; 945C; 1121C; 1253B; 1358A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 645A; 645B; 747B (*ir*)
Sadtler Standard C-13 NMR Spectra, 1046 (*cmr*)
Sadtler Standard PMR Spectra, 9938 (*pmr*)
Gehring, G. *et al., C. R. Hebd. Seances Acad. Sci.*, 1887, **104**, 1289 (*dibutyl ester*)
Kesling, H.S. *et al., ACS Symp. Ser.*, 1987, **328**, 77 (*manuf*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 156; 160
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 809-810; 821-822
Pelter, A. *et al., Synthesis*, 1998, 1793-1802 (*mono-Me ester, Me ester-chloride*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DJY600; SBK000; SBJ500; SBK500

Decanoic acid D-41

[334-48-5]
Capric acid. Caprinic acid. Decylic acid. Decoic acid (obsol.). FEMA 2364

$H_3C(CH_2)_8COOH$

$C_{10}H_{20}O_2$ 172.267
Widespread in plant oils and as glycerides in seed oils. Also present in apple, apricot, banana, morello cherry, citrus fruits, cheese, butter, white wine, Japanese whiskey, peated malt, wort and scallops. Used as a defoamer, lubricant and citrus fruit coating. Salts (Na, K, Mg, Ca, Al) used as binders, emulsifiers and anticaking agents in food manuf.. Needles. Sol. EtOH, Et_2O, Me_2CO, C_6H_6, $CHCl_3$, alkalis; poorly sol. H_2O. d_{40}^{4} 0.89. Mp 31.5°. Bp 268-270° Bp_{11} 148-150°. n_D^{40} 1.4288.

▶ Fl. p. >66°. Skin irritant. LD_{50} (mus, ivn) 129 mg/kg. HD9100000

Me ester: [110-42-9] *Methyl decanoate. Methyl caprate*
$C_{11}H_{22}O_2$ 186.294
Constit. of many plants. Liq. Bp 224° Bp_{15} 114°.

▶ HD9830000

Et ester: [110-38-3] *Ethyl decanoate. Ethyl caprate. FEMA 2432*
$C_{12}H_{24}O_2$ 200.32
Present in sweet and sour cherry, pineapple, blackberry, plum, quince, cape gooseberry, pawpaw, crispbread, wines, spirits, cerimon (*Monstera deliciosa*) and roasted filbert. Flavouring agent. Liq. with fruity odour. $d_4^{15.5}$ 0.87. Bp 243-245° Bp_{13} 122-124°. n_D^{20} 1.4260.

▶ Fl. p. >100°. Skin irritant. HD9420000

Pentyl ester: [5933-87-9] *Pentyl decanoate. Amyl caprate*
$C_{15}H_{30}O_2$ 242.401
Flavouring ingredient.

3-Methylbutyl ester: [2306-91-4] *3-Methylbutyl decanoate. Isoamyl caprate*
$C_{15}H_{30}O_2$ 242.401
Food flavouring. d 0.86. Bp 282°.

[1002-62-6, 13040-18-1, 13747-30-3, 22620-93-5, 30673-38-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 483C; 608A; 730C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 754B; 923B; 923C; 1168B; 1196A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 575D; 626C; 626D (*ir*)
Kao, C.H. *et al., J.C.S.*, 1931, 2046 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 697 (*occur*)
Tsang, C.W. *et al., J.C.S. Perkin 2*, 1975, 1718 (*ms*)
Leovey, E.M.K. *et al., Prostaglandins*, 1975, **10**, 789 (*pmr*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1976, **17**, 1 (*cmr*)
Umemura, J. *et al., J. Chem. Phys.*, 1978, **48**, 42 (*ir, cryst struct*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 735 (*rev, tox*)
Onishenko, T.A. *et al., Zh. Anal. Khim.*, 1987, **42**, 1616 (*use*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAH400; EHE500
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 159-775; 774-775; 963-964 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAH400; EHE500

1-Decanol D-42

[112-30-1]

[36729-58-5]
Decyl alcohol. Paranol. FEMA 2365

$H_3C(CH_2)_8CH_2OH$

$C_{10}H_{22}O$ 158.283
Isol. from plant sources, e.g. citrus oils, apple, coriander, babaco fruit (*Carica pentagonia*), wines, scallop and other foods. Oil, with orange blossom-like odour. Fp 7. Bp_{700} 232-239° Bp_7 107-108°. Isodecanol is a mixture of decanol isomers marketed as a solvent.

▶ Fl. p. 82°, autoignition temp. 288°. Eye and skin irritant. LD_{50} (rat, orl) 4720 mg/kg.. HE4375000

Ac: [112-17-4] *Decyl acetate. FEMA 2367*
$C_{12}H_{24}O_2$ 200.32
Flavouring agent. Present in citrus peels, apple, melon, strawberry, celery and other foodstuffs. Used in apple, orange and rum flavours. Liq. Mp -15°. Bp 272° Bp_{10} 130°.

Propanoyl: [5454-19-3] *Decyl propionate. Decyl propanoate. FEMA 2369*
$C_{13}H_{26}O_2$ 214.347
Flavouring ingredient. Liq. d^{20} 0.86. Bp_{15} 138-139°. n_D^{20} 1.4291.

Butanoyl: [5454-09-1] *Decyl butanoate. FEMA 2368*
$C_{14}H_{28}O_2$ 228.374
Flavouring ingredient. Oil. d^{20} 0.86. Bp 270°. n_D^{20} 1.4308.

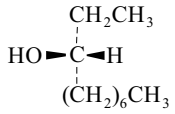
[25339-17-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 111C (*ir*)
Aldrich Atlas of NMR Spectra, **1**, 81B (*pmr*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 166A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 157D (*ir*)
Schrauth, W. *et al., Ber.*, 1931, **64**, 1314 (*synth*)
Komppa, G. *et al., J. Prakt. Chem.*, 1932, **135**, 193 (*synth*)
Craig, B.M. *et al., J. Am. Oil Chem. Soc.*, 1963, **40**, 61 (*use*)
Hoshino, H. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3043 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 105 (*rev, tox*)
Morris, M.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Schnurrenberger, P. *et al., Helv. Chim. Acta*, 1982, **65**, 1197 (*acetate*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1985, **36**, 253 (*cmr*)
Kotsuki, H. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 2684 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAI600
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 775-777; 784-785 (*acyl derivs*)

3-Decanol, 9CI D-43

[1565-81-7]

[36729-58-5]



(*R*)-*form*

$C_{10}H_{22}O$ 158.283

(R)-form [138256-81-2]
Bp_{15} 108°. $[\alpha]_D^{20}$ -10.55 (c, 5 in EtOH).

(±)-form [74683-67-3]
FEMA 3605
Flavouring ingredient. Liq. with an orange, musty odour. d^{20} 0.83. Mp -7.5°. Bp 213° Bp_{12} 101°. n_D^{20} 1.4348.

1-Naphthylurethane:
Mp 60-62°.

Et ether:3-Ethoxydecane
$C_{12}H_{26}O$ 186.337
$Bp_{9.5}$ 89.5°.

Pickard, R.H. *et al., J.C.S.*, 1913, **103**, 1923 (*synth, resoln*)
Woods, G.F. *et al., J.A.C.S.*, 1951, **73**, 2245 (*synth*)
Asinger, F. *et al., Chem. Ber.*, 1959, **92**, 3085 (*synth*)
Godsey, C.E. *et al., Anal. Chem.*, 1966, **38**, 842 (*nmr*)
Remberg, G. *et al., Chem. Ber.*, 1970, **103**, 3640 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 147
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 777-778

2-Decanone, 9CI D-44

[693-54-9]

$H_3C(CH_2)_7COCH_3$

$C_{10}H_{20}O$ 156.267

Constit. of essential oil of rue (*Ruta graveolens*). Needles. d_4^{22} 0.82. Mp 14° (2.5°). Bp_{750} 209° Bp_{12} 95-97°. n_D^{22} 1.4263.

► HE0725000

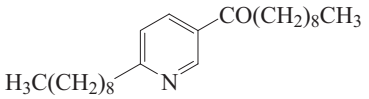
Semicarbazone:
Plates (EtOH). Mp 126° (121°).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 640A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 411C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 496C (*ir*)
Morgan, G.T. *et al., J. Soc. Chem. Ind., London*, 1925, **44**, 108T
Ruzicka, L. *et al., Helv. Chim. Acta*, 1926, **9**, 397 (*synth*)
Murakami, K. *et al., CA*, 1930, **24**, 2426 (*synth*)
Rupe, H. *et al., Helv. Chim. Acta*, 1932, **15**, 845 (*synth*)
Possel, O. *et al., Tet. Lett.*, 1977, 4229 (*synth*)
Sato, F. *et al., Chem. Lett.*, 1979, 167 (*synth*)
McDowell, P.G. *et al., Phytochemistry*, 1988, **27**, 2519
Pena, A. *et al., Entomol. Exp. Appl.*, 1992, **63**, 81
Monflier, E. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 2100 (*synth*)
Yamamoto, H. *et al., Synthesis*, 1994, 1283 (*ir, pmr*)

5-Decanoyl-2-nonylpyridine D-45

[149682-94-0]

1-(6-Nonyl-3-pyridinyl)-1-decanone, 9CI



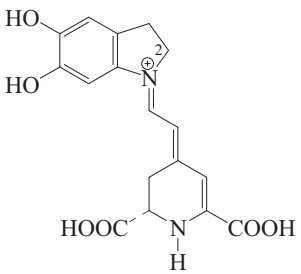
$C_{24}H_{41}NO$ 359.594

Alkaloid from *Houttuynia cordata* (Yu Xing Cao).

Jong, T.T. *et al., J. Chin. Chem. Soc. (Taipei)*, 1993, **40**, 301-303 (*isol*)
Proebstle, A. *et al., Nat. Prod. Lett.*, 1994, **4**, 235-240 (*isol*)

2-Decarboxybetanidin D-46

2-Descarboxybetanidin



$C_{17}H_{17}N_2O_6^{\oplus}$ 345.331

*5-O-β-D-Glucopyranoside:**2-Decarboxybetanin***. *2-Descarboxybetanin*
$C_{23}H_{27}N_2O_{11}^{\oplus}$ 507.473
Constit. of *Beta vulgaris*.

5-O-(6-O-Malonyl-β-D-glucopyranoside):2-Decarboxyphyllocactin. *2-Descarboxyphyllocactin*
$C_{26}H_{29}N_2O_{14}^{\oplus}$ 593.52
Constit. of *Beta vulgaris*.

Kobayashi, N. *et al., Phytochemistry*, 2001, **56**, 429-436 (*isol, pmr, ms*)

2,4,7-Decatrienal, 9CI D-47

[51325-37-2]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH{=}CHCHO$

$C_{10}H_{14}O$ 150.22

(2E,4Z,7Z)-form [43108-49-2]
Component of cooked chicken flavour. $Bp_{0.4}$ 65-67°.

[38664-37-8, 66642-86-2]

Meijboom, P.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 555 (*occur, synth*)
Harkes, P.D. *et al., J. Am. Oil Chem. Soc.*, 1974, **51**, 356 (*occur*)
Seifert, R.M. *et al., J. Agric. Food Chem.*, 1980, **28**, 68 (*synth*)

2,4,7-Decatrienoic acid D-48

[78417-28-4]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH{=}CHCOOH$

$C_{10}H_{14}O_2$ 166.219

(2E,4E,7Z)-form

Et ester: [28290-88-2]

[78417-28-4] *FEMA 3832*
$C_{12}H_{18}O_2$ 194.273
Aroma constit. of fruits incl. pears and durian. Used in food flavouring (as an unspecified mixt. of geom. isomers to which the name FEMA 3832 refers).

(2E,4Z,7Z)-form [244274-82-6]

Et ester: [142676-19-5]

[78417-28-4] *FEMA 3832*
Found as aroma constit. of fruits such as durian and pears. Used in food flavouring (as an unspecified mixt. of geom. isomers to which the name FEMA 3832 refers).

[150922-04-6]

Creveling, R.K. *et al., J. Agric. Food Chem.*, 1970, **18**, 19-24 (*isol, ester*)
Eur. Pat., 1992, 482 385; *CA*, **117**, 76268y (*2E,4Z,7Z-form-Et ester, use*)
Naef, R. *et al., Flavour Fragrance J.*, 1996, **11**, 295-303 (*isol, ester*)
Maier, A. *et al., Pestic. Sci.*, 1999, **55**, 733-739 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 532 (*Et ester*)

2,4,8-Decatrienoic acid D-49

$H_3CCH{=}CHCH_2CH_2CH{=}CHCH{=}CHCOOH$

$C_{10}H_{14}O_2$ 166.219

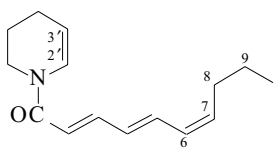
(2E,4E,8Z)-form

2-Methylpropylamide: [52657-13-3] **N-*Isobutyl-2,4,8-decatrienamide***. N-*(2-Methylpropyl)-2,4,8-decatrienamide, 9CI. 2,4,8-Decatrienoic acid isobutylamide*
$C_{14}H_{23}NO$ 221.342
Alkaloid from the roots of *Achillea millefolium* (yarrow). Oil.

Bohlmann, F. *et al., Chem. Ber.*, 1974, **107**, 1038 (*isol, uv, ir, pmr, ms, struct*)

2,4,6-Decatrienoic acid dehydropiperidide D-50

1,2,3,4-Tetrahydro-1-(1-oxo-2,4,6-decatrienyl)pyridine, 9CI



$C_{15}H_{21}NO$ 231.337

(2E,4E,6Z)-form [43110-67-4]
Alkaloid from *Achillea millefolium* (yarrow). Yellow cryst. (Et_2O/petrol). Mp 55°.

6,7-Dihydro: [81427-11-4] ***2,4-Decadienoic acid dehydropiperidide***
$C_{15}H_{23}NO$ 233.353
Gum.

8,9-Didehydro: [43110-68-5] ***2,4,6,8-Decatetraenoic acid dehydropiperidide***
$C_{15}H_{19}NO$ 229.321
Alkaloid from *Achillea millefolium* (yarrow). Yellowish oil. Not. obt. completely pure.

[42997-42-2, 42997-44-4]

Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 1328 (*isol, uv, pmr, struct, synth*)
Greger, H. *et al., Phytochemistry*, 1981, **20**, 2579 (*isol, deriv*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419-432 (*synth, deriv*)

2-Decenal D-51

[3913-71-1]
FEMA 2366
$H_3C(CH_2)_6CH{=}CHCHO$
$C_{10}H_{18}O$ 154.252
Constit. of essential oil of coriander. Also present in French fries, tomato, wheat bread, cooked meats, roasted pecans, roasted filbert and rice. Flavouring agent. Liq. with waxy, orange-like, sweet aldehyde-like odour.
▶ Skin irritant. LD_{50} (rat, orl) 5000 mg/kg. HE2070000

(*E*)-*form* [3913-81-3]
Bp 229-231° $Bp_{11.5}$ 107-107.5°.

Oxime:
$C_{10}H_{19}NO$ 169.266
Mp 55°.

Semicarbazone: [16742-25-9]
Cryst. (EtOH). Mp 168.5°.

(*Z*)-*form*
Bp_{17} 112°. 95% pure.

Romburgh, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1938, **57**, 494 (*isol*)
Swift, C.E. *et al., J.A.C.S.*, 1949, **71**, 1512 (*synth*)
Tschinkel, W.R. *et al., J. Insect Physiol.*, 1975, **21**, 659 (*isol*)
Dirinck, P. *et al., J. Food Sci.*, 1977, **42**, 645 (*isol*)
Selke, E. *et al., Lipids*, 1978, **13**, 511 (*glc, ms*)
Smith, R.M. *et al., N.Z. J. Sci.*, 1978, **21**, 121 (*isol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 761 (*rev, tox*)
Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAI350
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

4-Decenal D-52

[30390-50-2]
$H_3C(CH_2)_4CH{=}CHCH_2CH_2CHO$
$C_{10}H_{18}O$ 154.252

(*E*)-*form* [65405-70-1]
FEMA 3264
Flavouring ingredient. Pale yellow liq. with persistent green-aldehydic-floral odour. Bp_{15} 90-100° Bp_5 90°. n_D^{20} 1.4410.

2,4-Dinitrophenylhydrazone:
Mp 101-103°.

(*Z*)-*form* [21662-09-9]
Bp_{10} 78-80°. n_D^{20} 1.4440.

Ger. Pat., 1970, 2 018 898; *CA*, **74**, 12612s
Nikishin, G.I. *et al., Synthesis*, 1972, 376 (*synth, spectra*)
Bestmann, H.J. *et al., Annalen*, 1981, 1705 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 148
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 779-780

9-Decenal, 9CI D-53

[39770-05-3]
FEMA 3912
$H_2C{=}CH(CH_2)_7CHO$
$C_{10}H_{18}O$ 154.252
Found in coriander leaf. Food flavour component. Oil. Bp_1 61-65°.

Ethylene acetal: [126382-06-7] *2-(8-Nonenyl)dioxolane*
$C_{12}H_{22}O_2$ 198.305
No phys. props. reported.

Hase, T.A. *et al., Synth. Commun.*, 1979, **9**, 63-67 (*synth*)
Jones, T.H. *et al., J. Chem. Ecol.*, 1982, **8**, 285-300 (*synth, pmr, ir*)
Bortolini, O. *et al., J.O.C.*, 1987, **52**, 5467-5469 (*synth*)
Dhillon, R.S. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 757-759 (*ethylene acetal*)
Potter, T.L. *et al., J. Agric. Food Chem.*, 1990, **38**, 2054-2056; 1996, **44**, 1824-1826 (*occur*)
Dickinson, R. *et al., J. Med. Chem.*, 1993, **36**, 111-118 (*synth*)
Yanagisawa, A. *et al., Chem. Comm.*, 1994, 2103-2104 (*synth*)
Sakaguchi, S. *et al., J.O.C.*, 1999, **64**, 5954-5957 (*synth, pmr, cmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 390 (*use*)

8-Decene-4,6-diyn-1-ol D-54

[30339-12-9]
$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH_2CH_2CH_2OH$
$C_{10}H_{12}O$ 148.204

(*Z*)-*form*
Liq. $Bp_{0.05}$ 95°.

3-Methylbutanoyl:
$C_{15}H_{20}O_2$ 232.322
Constit. of *Carthamus tinctorius* (safflower). Oil.

Barrero, A.F. *et al., Phytochemistry*, 1998, **48**, 1237-1240 (*isol, uv, ir, pmr, cmr, ms*)

2-Decene-4,6,8-triynoic acid D-55

Dehydromatricaric acid
$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCOOH$
$C_{10}H_6O_2$ 158.156

(*E*)-*form* [7199-97-5]

Me ester: [692-94-4] *Dehydromatricaria ester*
$C_{11}H_8O_2$ 172.183
Light-yellow cryst. (Et_2O/petrol). Mp 105-106°.

3-Methylbutylamide: [113235-91-9] *2-Decene-4,6,8-triynoic acid isopentylamide*
$C_{15}H_{17}NO$ 227.305
Cryst. Dec. to blue polymers on htg..

2-Phenylethylamide: [113235-93-1] *N-(2-Phenylethyl)-2-decene-4,6,8-triynamide. 2-Decene-4,6,8-triynoic acid 2-phenylethylamide*
$C_{18}H_{15}NO$ 261.323
Cryst. Dec. to blue polymer on htg..

2-Methylpropylamide: [37064-10-1] ***Dehydromatricaric acid isobutylamide***
$C_{14}H_{15}NO$ 213.279
Cryst. (CCl_4). Mp 133-139° Mp 144.5-145.5°.

(*Z*)-*form* [23050-77-3]
Mp 150° dec.

Me ester: [2739-57-3]
Occurs in *Artemisia vulgaris* (mugwort). Light-yellow needles (petrol). Mp 114-115° (112°).

[7329-73-9, 43110-85-6]

Stauholt, K. *et al., Acta Chem. Scand.*, 1950, **4**, 1567 (*isol*)
Christensen, P.K. *et al., Acta Chem. Scand.*, 1952, **6**, 602 (*synth*)
Sorensen, J.S. *et al., Acta Chem. Scand.*, 1954, **8**, 26 (*isol*)
Bell, I. *et al., J.C.S.*, 1958, 1313 (*synth, Me ester*)
Gardner, J.N. *et al., J.C.S.*, 1960, 691 (*isol*)
Bohlmann, F. *et al., Chem. Ber.*, 1962, **95**, 1742; 1973, **106**, 1328 (*isol, struct, synth*)
Hodge, P. *et al., J.C.S.(C)*, 1966, 1216 (*bibl*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 770
Kobayashi, A. *et al., Agric. Biol. Chem.*, 1975, **39**, 911 (*synth*)
Kawazu, K. *et al., Agric. Biol. Chem.*, 1977, **41**, 223
Greger, H. *et al., Phytochemistry*, 1978, **17**, 86; 1982, **21**, 1071 (*isol, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1736; 1980, **19**, 841; 2655 (*isol*)
Greger, H. *et al., J. Nat. Prod.*, 1987, **50**, 1100 (*amides, isol, ir, uv, ms, pmr*)
Japan. Pat., 1991, 03 287532; *CA*, **116**, 181120w (*isol*)
Lu, T. *et al., Phytochemistry*, 1993, **32**, 1483 (*cryst struct*)

2-Decene-4,6,8-triyn-1-ol D-56

[3930-17-4]
Dehydromatricarianol
$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH_2OH$
$C_{10}H_8O$ 144.173

(*E*)-*form* [6071-16-5]
Cryst. (Et_2O/pentane). Mp 129°.

Ac: [52940-10-0]
$C_{12}H_{10}O_2$ 186.21
Cryst. (petrol). Mp 38.2°.

3-Methylbutanoyl:
$C_{15}H_{16}O_2$ 228.29
Oil.

2R,3S**-Epoxide: [155934-76-2] *3-(1,3,5-Heptatriynyl)oxiranemethanol, 9CI. 2,3-Epoxy-4,6,8-decatriyn-1-ol*
$C_{10}H_8O_2$ 160.172
Unstable yellow cryst. Mp 98-102° dec. $[\alpha]_D$ -3 (c, 0.04 in $CHCl_3$). λ_{max} 242 ; 262 ; 270 ; 293 ; 312 (MeOH) (Berdy).

(*Z*)-*form* [6071-46-1]
Metab. of *Fistulina hepatica*.

Ac: [115374-19-1]
Oil. λ_{max} 271 ; 288 ; 317 ; 329 (Et_2O).

Jones, J.B. *et al., J.C.S.*, 1963, 5759 (*synth*)
Jones, E.R.H. *et al., J.C.S.(C)*, 1966, 139 (*isol*)
Hodge, P. *et al., J.C.S.(C)*, 1966, 1216 (*biosynth*)
Bohlmann, F. *et al., Chem. Ber.*, 1974, **107**, 1409 (*isol*)
Hearn, M.T.W. *et al., J.C.S. Perkin 2*, 1976, 1027 (*cmr*)
Zdero, C. *et al., Phytochemistry*, 1988, **27**, 1105 (*isol, struct, uv, ir, ms, acetate*)
Dagne, E. *et al., J. Nat. Prod.*, 1994, **57**, 390 (*2,3-Epoxide*)

2-Decenoic acid D-57

[3913-85-7]
$H_3C(CH_2)_6CH{=}CHCOOH$
$C_{10}H_{18}O_2$ 170.251

(*E*)-*form* [334-49-6]
FEMA 3913
Occurs in pear, capsicum, mutton, pork and black tea. Flavourant for beverages,

baked goods, etc.. Liq. or solid with fresh, sweet fruity-fatty odour. Mp 12°. Bp_{15} 165° $Bp_{4.5}$ 148-149°.

Me ester: [7367-85-3]

[2482-39-5]
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient. Liq. Bp_{15} 130-132°.

Et ester: [7367-88-6]

[37486-72-9] *Ethyl 2-decenoate. FEMA 3641*
$C_{12}H_{22}O_2$ 198.305
Flavouring agent. Liq. Bp_{15} 130-132°. n_D^{20} 1.4442.

Butyl ester: [7492-45-7] *Butyl 2-decenoate. FEMA 2194*
$C_{14}H_{26}O_2$ 226.358
Flavouring agent with a fruity odour and taste. Liq.

Chloride: [110232-46-7]
$C_{10}H_{17}ClO$ 188.696
Bp_{14} 120-122° $Bp_{2.5}$ 95-97°.

Amide:
$C_{10}H_{19}NO$ 169.266
Cryst. (Et_2O). Mp 121-122°.

2-Methylpropylamide: [73785-32-7] N-*(2-Methylpropyl)-2-decenamide.* ***2-Decenoic acid isobutylamide***
$C_{14}H_{27}NO$ 225.373
Solid (EtOAc). Unstable at r.t. Struct. based on ms data only.

(Z)-form [15790-91-7]
$Bp_{0.5}$ 102-103°.

Zaar, B. *et al., Chem. Zentralbl.*, 1930, **1**, 363
v. Romburgh, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1938, **57**, 494 (*isol*)
Skinner, W.A. *et al., Experientia*, 1970, **26**, 728
Quraishi, M.S. *et al., J. Econ. Entomol.*, 1971, **64**, 787
Cahiez, G. *et al., Synthesis*, 1976, 245-248 (*Z-form, synth, ir, pmr*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*occur, bibl*)
Song, J. *et al., Tetrahedron*, 1993, **49**, 6794-6802 (*E-form, synth, ir, pmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 88; 226 (*esters*)
Rosario, S.L. *et al., Planta Med.*, 1996, **62**, 376 (*isobutylamide*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 335-336; 964-965; 1752 (*esters*)
Bellasoued, M. *et al., J.O.C.*, 1998, **63**, 8785-8789 (*E-form, synth, pmr, cmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 391

3-Decenoic acid D-58

[15469-77-9]
$H_3C(CH_2)_5CH{=}CHCH_2COOH$
$C_{10}H_{18}O_2$ 170.251
Occurs in pork and squid oil. Comly. available flavour ingredient. (*E*/*Z*) composition of natural isolates not detd..

(E)-form [53678-20-9]
Liq. Bp_1 110-112°.

Et ester: [82561-67-9]
$C_{12}H_{22}O_2$ 198.305
Liq. $Bp_{0.5}$ 80-82°. n_D^{20} 1.4372.

(Z)-form [2430-93-5]
Liq. or solid with fatty odour. Mp 18°. Bp_{11} 154-163°.

Tulus, R. *et al., CA*, 1940, **40**, 3722 (*synth*)
Gorge, M. *et al., Ann. Chim. (Paris)*, 1951, **6**, 648 (*synth*)
Fukui, H. *et al., Tet. Lett.*, 1974, 3563 (*isol*)
Brown, H.C. *et al., J.O.C.*, 1986, **51**, 3398-3400 (*E-form, Et ester, synth, ir, pmr, cmr*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*occur, bibl*)
Sharma, M.L. *et al., Coll. Czech. Chem. Comm.*, 1991, **56**, 1744 (*synth, ir, pmr*)
Ragoussis, N. *et al., J.C.S. Perkin 1*, 1998, 3529-3533 (*E-form, synth, Et ester, ir, pmr, cmr, ms*)

4-Decenoic acid D-59

[26303-90-2]
FEMA 3914
$H_3C(CH_2)_4CH{=}CHCH_2CH_2COOH$
$C_{10}H_{18}O_2$ 170.251
Occurs in hops and beer. Comly. available flavour ingredient.

(E)-form [57602-94-5]
Liq. with fatty odour. Bp_{13} 145-146°.

Et ester: [76649-16-6] *Ethyl 4-decenoate. FEMA 3642*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. Bp_{10} 112°. n_D^{20} 1.4362.

(Z)-form [505-90-8]
Obtusilic acid
Liq. with fatty/green odour. Bp_{13} 148-150°.

4-Bromophenacyl ester:
Mp 43.3°.

Komori, S. *et al., Bull. Chem. Soc. Jpn.*, 1937, **12**, 226; 433 (*isol*)
Iwakiri, M. *et al., Yakugaku Zasshi*, 1951, **78**, 1460; *CA*, **53**, 1633 (*synth, config*)
Hopkins, C.Y. *et al., Lipids*, 1966, **1**, 118 (*isol*)
Bus, J. *et al., Chem. Phys. Lipids*, 1976, **17**, 501 (*cmr*)
Iwakiri, M. *et al., CA*, 1982, **97**, 20619q (*rev*)
Fujisawa, T. *et al., Tet. Lett.*, 1982, 3583 (*synth*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255 (*synth*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*occur, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 226 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 965-966 (*Et ester*)

5-Decenoic acid, 9CI D-60

[85392-03-6]
$H_3C(CH_2)_3CH{=}CH(CH_2)_3COOH$
$C_{10}H_{18}O_2$ 170.251
Mixt. with 6-Decenoic acid, D-61 is used as a flavouring ingredient (FEMA 3742).

(E)-form [16424-55-8]
Liq. with milky/fatty odour. d_{16} 0.92. Bp_{26} 169°. n_D^{16} 1.4509.

(Z)-form [84168-28-5]
Liq. with fatty/fatty-green odour.

Me ester: [79837-87-9]
$C_{11}H_{20}O_2$ 184.278
Bp_{14} 90-100°.

[84168-29-6, 105986-59-2, 105986-60-5]

Riobe, O. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1967, **264**, 109 (*synth*)
Bestmann, H.J. *et al., Annalen*, 1981, 1705 (*synth*)
Tamaru, Y. *et al., Tet. Lett.*, 1986, **27**, 955 (*synth*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*occur, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 148
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 780

6-Decenoic acid, 9CI D-61

[85392-04-7]
$H_3CCH_2CH_2CH{=}CH(CH_2)_4COOH$
$C_{10}H_{18}O_2$ 170.251
Mixt. with 5-Decenoic acid, D-60 is used as a flavouring ingredient (FEMA 3742).

(E)-form
Liq. (?) with intense milky odour. Not yet found in nature (1986).

[86503-02-8, 86503-03-9, 86503-04-0, 118426-11-2]

Tulloch, A.P. *et al., Chem. Phys. Lipids*, 1985, **37**, 197 (*cmr, Me ester*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*synth, occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 148
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 780-781

9-Decenoic acid D-62

[14436-32-9]
Caproleic acid. FEMA 3660
$H_2C{=}CH(CH_2)_7COOH$
$C_{10}H_{18}O_2$ 170.251
Minor constit. of milk fats. Also detected in beer, wine, clams, Parmesan cheese and snails. Flavouring agent. Liq. with fatty odour. Bp_{21} 158-163°.

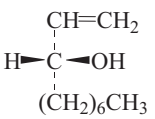
Me ester:
$C_{11}H_{20}O_2$ 184.278
Oil. Bp_{20} 120°.

4-Bromophenacyl ester:
Cryst. (EtOH aq.). Mp 58°.

Black, H.K. *et al., J.C.S.*, 1953, 1785 (*synth*)
Renner, E. *et al., Milchwissenschaft*, 1978, **33**, 489 (*isol*)
Hase, T.A. *et al., Synth. Commun.*, 1979, **9**, 63 (*synth*)
Shirakawa, T. *et al., Dev. Food Sci.*, 1988, **18**, 915 (*occur, props*)
Bartra, M. *et al., J.O.C.*, 1991, **56**, 5132 (*synth, pmr, cmr, ir*)

1-Decen-3-ol D-63

[51100-54-0]
FEMA 3824



(R)-form

$C_{10}H_{20}O$ 156.267

(R)-form [74867-43-9]
Bp_4 70-75°. $[\alpha]_D^{25}$ -14.9 (neat).

(±)-*form* [74824-56-9]
Flavouring ingredient. Bp_{18} 98-103°.

[74867-44-0]

Rinaldi, P.L. *et al., J.O.C.*, 1980, **45**, 4348-4351 (*synth, ir, pmr, ms*)

Janowitz, A. *et al., Helv. Chim. Acta*, 1991, **74**, 1352 (*synth, ir, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 394

3-Decen-2-one, 9CI D-64

[10519-33-2]
FEMA 3532
$H_3C(CH_2)_5CH{=}CHCOCH_3$
$C_{10}H_{18}O$ 154.252

(*E*)-*form* [18402-84-1]
Flavouring ingredient. Bp_{14} 105°.

Semicarbazone:
Cryst. + $1H_2O$ (EtOH aq.). Mp 110-111°. Semicarbazone and 2,4-dinitrophenylhydrazone presumed here to belong to (*E*)-isomer.

2,4-Dinitrophenylhydrazone: [3013-10-3]
Mp 78°.

Sturtz, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 2477 (*synth, ir*)
Sheikh, Y.M. *et al., Org. Mass Spectrom., Suppl.*, 1970, **4**, 273 (*ms*)
Kelleher, R.G. *et al., Chem. Comm.*, 1980, 486 (*synth*)
Loiseau, A.-M. *et al., Bull. Soc. Chim. Fr.*, 1982, 144 (*synth, ir, Raman*)
Hideg, K. *et al., J.C.S. Perkin 1*, 1986, 1431 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 150
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 782

Mytilus Defensin D-65

Peptides. Isol. from the blood of *Mytilus edulis* (blue mussel).

Mytilus defensin A
Contains 37 amino acid residues.

Mytilus defensin B

Charlet, M. *et al., J. Biol. Chem.*, 1996, **271**, 21808-21813

Mytilus galloprovincialis Defensins D-66

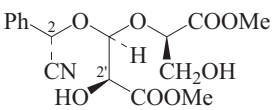
Isol. from the edible Mediterranean mussel *Mytilis galloprovincialis*.

MGD 1
Peptide consisting 39 amino acid residues including 8 cysteines.

MGD 2 An isoform of MGD 1 differing in 5 positions.

Hubert, F. *et al., Eur. J. Biochem.*, 1996, **240**, 302-306 (*MGD 1, isol, struct*)
Mitta, G. *et al., J. Cell Biol.*, 1999, **112**, 4233-4242 (*MGD 2, isol*)
Yang, Y.S. *et al., Biochemistry*, 2000, **39**, 14436-14447 (*MGD 2, synth, pmr, struct*)

Sambucus nigra Degraded cyanogenic glycosides D-67



$C_{16}H_{19}NO_8$ 353.328
Degraded cyanogenic glucoside. Isol. from *Sambucus nigra* (elderberry). $[\alpha]_D$ +15 (c, 0.6 in $CHCl_3$). λ_{max} 221 (ϵ 3150); 278 (ϵ 2170) (EtOH).

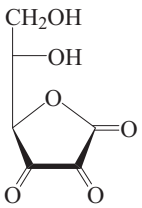
2-Epimer:
$C_{16}H_{19}NO_8$ 353.328
Isol. from *Sambucus nigra* (elderberry). $[\alpha]_D$ -21 (c, 0.3 in $CHCl_3$). λ_{max} 225 (ϵ 3160); 276 (ϵ 2190) (EtOH).

2′-Epimer:
$C_{16}H_{19}NO_8$ 353.328
Isol. from *Sambucus nigra* (elderberry). $[\alpha]_D$ -3 (c, 0.5 in $CHCl_3$). λ_{max} 224 (ϵ 3130); 279 (ϵ 2130) (EtOH).

Della Greca, M. *et al., Tet. Lett.*, 2000, **41**, 6507-6510
Della Greca, M. *et al., J. Periodontal Res.*, 2003, **17**, 177-181 (*synth*)

Dehydroascorbic acid D-68

threo-*2,3-Hexodiulosono-1,4-lactone, 9CI, 8CI*



$C_6H_6O_6$ 174.11

L-*form* [490-83-5]
Widespread in plants, as oxidn. prod. of Ascorbic acid, A-447. Formed reversibly *in vivo* from ascorbic acid and shows similar vitamin function. Mp 225° dec. (196° dec.). $[\alpha]_D^{20}$ +56 → -6 (6d) (c, 1 in phthalate/HCl buffer at pH 3.5). Probably exists in hydrated form as the 2,3-bis-*gem*-diol or as a C-2 hydrated bicyclic form in aq. soln..

2-Phenylhydrazone:
Yellow needles (EtOH). Mp 167-170°.

2,3-Bisphenylhydrazone: [22393-11-9]
Mp 223°.

2,3-Bis(2,4-dinitrophenylhydrazone):
Mp 280° dec.

D-*form*

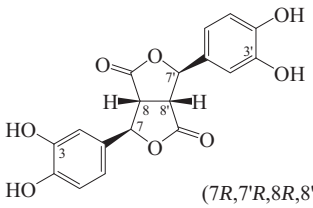
2,3-Bis(2,4-dinitrophenylhydrazone):
[19192-77-9]
Cryst. (EtOH). Mp 252-254°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 702C (*ir*)
Herbert, R.W. *et al., J.C.S.*, 1933, 1270 (*deriv*)
Kenyon, J. *et al., J.C.S.*, 1948, 158 (*synth*)
El Khadem, H. *et al., Carbohydr. Res.*, 1970, **13**, 57; 1972, **21**, 430 (*hydrazones*)
Weiss, W. *et al., Annalen*, 1971, **754**, 152-153 (*deriv*)
Hvoslef, J. *et al., Acta Cryst. B*, 1976, **32**, 448 (*struct*)
Matusch, R. *et al., Z. Naturforsch., B*, 1977, **32**, 562-568 (*cmr*)
Ashny, E.S.H.E. *et al., Chem. Rev.*, 1980, **79**, 151-154 (*ir*)
Tolbert, B.M. *et al., Adv. Chem. Ser.*, 1982, 200 (*rev*)
Ohmuri, W. *et al., Agric. Biol. Chem.*, 1986, **47**, 607-608 (*deriv, synth, ir*)
Kilany, Y.E. *et al., J. Carbohydr. Chem.*, 1988, **7**, 187-198 (*deriv*)
Wolf, G. *et al., Nutr. Rev.*, 1993, **51**, 337-338 (*rev*)
Merck Index, 12th edn., 1996, No. 2920
Kurata, T. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1651-1655 (*props*)

Dehydrodicaffeic acid dilactone D-69

[60804-37-7]

[164201-19-8]
*3,6-Bis(3,4-dihydroxyphenyl)tetrahydro-1*H*,4*H*-furo[3,4-c]furan-1,4-dione, 9CI*



(7*R*,7'*R*,8*R*,8'*R*)-*form*

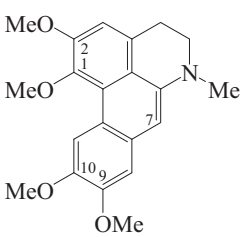
$C_{18}H_{14}O_8$ 358.304

3,3′-Di-Me ether: [13962-76-0] ***Dehydrodiferulic dilactone***
$C_{20}H_{18}O_8$ 386.357
Constit. of the cell walls of wheat and barley. Stereochem. not determined.

Kumada, Y. *et al., J. Antibiot.*, 1976, **29**, 882-889 (*isol*)
Kumada, Y. *et al., Agric. Biol. Chem.*, 1977, **41**, 869-876; 877-885
Quideau, S. *et al., J.C.S. Perkin 1*, 1993, 653-659 (*synth, deriv*)
Turner, L.B. *et al., Phytochemistry*, 1993, **33**, 791-796 (*isol, deriv*)

Dehydroglaucine D-70

[22212-26-6]



$C_{21}H_{23}NO_4$ 353.417
Pale-yellow prisms (EtOH). Mp 133-134°. λ_{max} 260 (ϵ); 332 (ϵ) (MeOH) (Derep). λ_{max} 260 ; 332 (EtOH) (Berdy).

N-*De-Me:6*a*,7-Dehydronorglaucine*
Cryst. (Et_2O/MeOH). Mp 180-183°.

O^1-*De-Me:Dehydrothaliporphine*
Mp 157-160° dec.

O^{10}-*De-Me:Dehydrolirioferine*
Cryst. (EtOAc). Mp 140-142° dec. Unstable.

O^1,O^9-*Di-de-Me:* [53729-86-5] ***Dehydroisoboldine***
$C_{19}H_{19}NO_4$ 325.363

*7-Hydroxy:***7-Hydroxydehydroglaucine**
$C_{21}H_{23}NO_5$ 369.416
Alkaloid from *Annona purpurea* (soncoya). Green needles ($CHCl_3$). Mp 242-243°. λ_{max} 222 ; 260 ; 335 (EtOH).

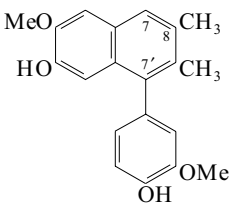
N-*De-Me,* $\Delta^{6,6a}$*-isomer:* [52309-70-3] ***6,6a-Dehydronorglaucine***
$C_{20}H_{21}NO_4$ 339.39First member of a

small subgroup of aporphine-type alkaloids with a conjugated azomethine group.

Kiryakov, H.G. *et al., Chem. Ind. (London)*, 1968, 1807 (*uv, ir, pmr, struct*)
Cava, M.P. *et al., J.O.C.*, 1970, **35**, 175 (*synth, uv*)
Kunimoto, J. *et al., Yakugaku Zasshi*, 1974, **94**, 1149; *CA*, **82**, 14024r (*Dehydroisoboldine*)
Hufford, C.D. *et al., J. Pharm. Sci.*, 1975, **64**, 789 (*isol, uv, pmr*)
Chen, C.-L. *et al., Phytochemistry*, 1976, **15**, 547; 1161 (*isol, pmr, ms*)
Castedo, L. *et al., An. Quim., Ser. C*, 1982, **78**, 103 (*cmr*)
Lenz, G.R. *et al., J.C.S. Perkin 1*, 1984, 1273 (*6,6a-Dehydronorglaucine*)
Gupta, S. *et al., Synth. Commun.*, 1989, **19**, 393 (*synth*)
Chang, F.-R. *et al., J. Nat. Prod.*, 1998, **61**, 1457-1461 (*7-Hydroxydehydroglaucine*)

Dehydroguaiaretic acid D-71

[20601-86-9]
8-(4-Hydroxy-3-methoxyphenyl)-3-methoxy-6,7-dimethyl-2-naphthol. 4,4′-Dihydroxy-3′,5-dimethoxy-2,7′-cycloligna-7,7′-diene



$C_{20}H_{20}O_4$ 324.376
Gum.

Di-Et ether:
Prisms (EtOAc). Mp 162-163°.

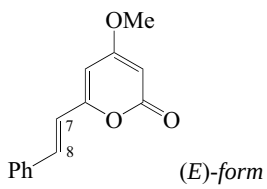
7α,8β-Dihydro: [135962-21-9]

[180470-31-9] ***1,2-Dihydrodehydroguaiaretic acid***. *4,4′-Dihydroxy-3,3′-dimethoxy-2,7′-cyclolign-7-ene. Myrisfragransin*
$C_{20}H_{22}O_4$ 326.391
Constit. of *Myristica fragrans* (nutmeg). Gum. $[\alpha]_D^{25}$ +39.95 (c, 0.39 in $CHCl_3$).

King, F.E. *et al., J.C.S.*, 1964, 4011 (*isol, uv, synth*)
Ayres, D.C. *et al., J.C.S.(C)*, 1971, 1111
Pinto, M.M.M. *et al., Phytochemistry*, 1990, **29**, 1985 (*isol, pmr, cmr, deriv*)
Miyazawa, M. *et al., Nat. Prod. Lett.*, 1996, **8**, 25-26 (*Myrisfragransin*)

5,6-Dehydrokawain D-72

[1952-41-6]
*4-Methoxy-6-(2-phenylethenyl)-2*H*-pyran-2-one. 4-Methoxy-6-styryl-2*H*-pyran-2-one. 12-Demethoxyyangonin*



(*E*)-*form*

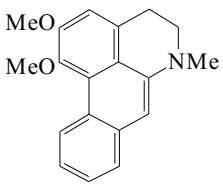
$C_{14}H_{12}O_3$ 228.247

(E)-form [15345-89-8]
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage. Pale yellow cryst. (C_6H_6/petrol). Mp 138-140°.
▶ UQ1240000

Gottlieb, O.R. *et al., J.O.C.*, 1959, **24**, 17; 1614 (*isol, struct*)
Rezende, C.M.A. *et al., Phytochemistry*, 1971, **10**, 3167 (*isol*)
Mascarenhas, Y.P. *et al., Acta Cryst. B*, 1973, **29**, 1361 (*struct*)
Belanger, A. *et al., Can. J. Chem.*, 1975, **53**, 201 (*synth*)
Suzuki, E. *et al., Synthesis*, 1975, 192 (*synth*)
Adityachandbury, N. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 127 (*isol*)
Israeli, Z.H. *et al., J.O.C.*, 1976, **41**, 4070 (*synth, pmr*)
Sirat, H.M. *et al., Planta Med.*, 1996, **62**, 188 (*isol, ir, pmr*)
Ranjith, H. *et al., Phytochemistry*, 2002, **59**, 429-433 (*isol, pmr, cmr, bibl*)

Dehydronuciferine D-73

[7630-74-2]



$C_{19}H_{19}NO_2$ 293.365
Alkaloid from the leaves of *Nelumbo nucifera* (East Indian lotus). Cryst. (EtOH). Mp 130-131°.

N-*De-Me:* [92664-95-4] ***Dehydronornuciferine***
$C_{18}H_{17}NO_2$ 279.338
Off-yellow flakes. Mp 149.5-150.5°.

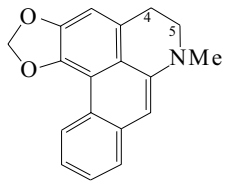
N-*De-Me,* N-*formyl:* [111017-06-2] **N-*De-methyl*-N-*formyldehydronuciferine***
$C_{19}H_{17}NO_3$ 307.348
Needles (MeOH). Mp 140.5°.
▶ Mutagen.

O^1-*De-Me:* ***Dehydrolirinidine***
$C_{18}H_{17}NO_2$ 279.338
Green needles ($CHCl_3$). Mp 189-190°.
λ_{max} 216 ; 253 ; 312 (EtOH).

Cava, M.P. *et al., J.O.C.*, 1970, **35**, 175 (*synth, uv*)
Kunitomo, J. *et al., Phytochemistry*, 1973, **12**, 699 (*occur*)
Guinaudeau, H. *et al., Planta Med.*, 1975, **27**, 304; 1976, **29**, 54; **30**, 201 (*isol*)
Castedo, L. *et al., An. Quim., Ser. C*, 1982, **78**, 103 (*cmr*)
Lenz, G.R. *et al., J.C.S. Perkin 1*, 1984, 1273 (*Dehydronornuciferine, synth, uv, ir, pmr, cmr*)
Cortes, D. *et al., J. Nat. Prod.*, 1986, **49**, 878 (*Dehydronornuciferine, isol*)
Nozaka, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2844 (*N-Demethyl-N-formyldehydronuciferine*)
Atanes, N. *et al., J.O.C.*, 1991, **56**, 2984 (*synth, Dehydronornuciferine*)
Chang, F.R. *et al., J. Nat. Prod.*, 1998, **61**, 1457-1461 (*Dehydrolirinidine*)

Dehydroroemerine D-74

[36285-03-7]
Dehydroaporheine



$C_{18}H_{15}NO_2$ 277.322
Alkaloid from *Nelumbo nucifera* (East India lotus) and *Papaver rhoeas* (corn poppy). Mp 88-89°.

N-*De-Me:* [41679-82-7] ***Dehydroanonaine***
$C_{17}H_{13}NO_2$ 263.295
Alkaloid from the leaves of *Nelumbo nucifera* (East India lotus).

N-*De-Me,* N-*formyl:* [165900-12-9] **N-*Formyldehydroanonaine***
$C_{18}H_{13}NO_3$ 291.306
Cryst. (hexane/EtOAc). Mp 185-186°.

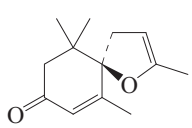
N-*De-Me,* N-*Ac:* [132646-11-8] **N-*Acetyldehydroanonaine***
$C_{19}H_{15}NO_3$ 305.332
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Prisms (MeOH). Mp 151-153°.

4,5-Didehydro: ***Didehydroroemerine***. *Didehydroaporheine*
$C_{18}H_{13}NO_2$ 275.306
Amorph.

Kunitomo, J. *et al., Phytochemistry*, 1973, **12**, 699 (*Dehydroanonaine*)
Preininger, V. *et al., Planta Med.*, 1973, **23**, 233 (*Didehydroroemerine*)
Guinaudeau, H. *et al., Planta Med.*, 1975, **27**, 304; 1976, **30**, 201 (*isol*)
Ziyaev, R. *et al., Khim. Prir. Soedin.*, 1977, **13**, 715; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 602 (*isol, uv, ms*)
Min, Z. *et al., Yaoxue Xuebao*, 1980, **15**, 532; *CA*, **94**, 117773m (*isol*)
Phillipson, J.D. *et al., J. Nat. Prod.*, 1981, **44**, 296 (*occur*)
Sariyar, G. *et al., Plant. Med. Phytother.*, 1981, **15**, 160; *CA*, **96**, 119030g (*isol*)
Kunitomo, J. *et al., Yakugaku Zasshi*, 1981, **101**, 431; *CA*, **95**, 204236c (*isol*)
Min, Z. *et al., Yaoxue Xuebao*, 1981, **16**, 557; *CA*, **97**, 3595m (*isol*)
Atanes, N. *et al., J.O.C.*, 1991, **41**, 1425 (*Dehydroanonaine, synth*)
Menachery, M.D. *et al., Heterocycles*, 1995, **41**, 1425 (*N-Formyldehydroanonaine*)
Chen, I.-S. *et al., Phytochemistry*, 1996, **42**, 217 (*N-Acetyldehydroanonaine*)

8,9-Dehydrotheaspirone D-75

[80722-28-7]
2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one, 9CI



(*R*)-*form*

$C_{13}H_{18}O_2$ 206.284
(R)-form [188745-87-1]

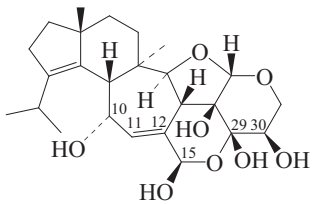
(*S*)-*form* [85248-56-2]

(±)-*form* [80957-74-0]
Cryst. (petrol) with strong woody-flowery odour. Mp 56-57°. Bp_4 99-100°.

(ξ)-*form*
Volatile flavour constit. of white-fleshed nectarines, oranges and Riesling wine.

Shibagaki, M. *et al., Agric. Biol. Chem.*, 1981, **45**, 2911-2913 (*synth, pmr*)
Fujimori, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 2925-2926 (*isol, pmr, ms*)
Enzell, C.R. *et al., Mass Spectrom. Rev.*, 1986, **5**, 39-72 (*ms*)
Winterhalter, P. *et al., J. Agric. Food Chem.*, 1990, **38**, 1041-1048 (*anal*)
Naaf, R. *et al., J. Essent. Oil Res.*, 1996, **8**, 587-595 (*occur*)
Knapp, H. *et al., J. Agric. Food Chem.*, 1997, **45**, 1309-1313 (*occur, cd, abs config*)

O-Demethylstriatin C D-76



$C_{25}H_{36}O_8$ 464.555
Sol. MeOH, EtOAc, $CHCl_3$, EtOH; poorly sol. H_2O, hexane.

▶ LD_{50} (mus, ipr) 150 mg/kg.

O^{15}-*Me:* [62744-74-5] ***Striatin C***
$C_{26}H_{38}O_8$ 478.581
Cryst. (EtOH). Mp 144-145°.

O^{15}-*Me, 30-Ac:* [62744-73-4] ***Striatin B***
$C_{28}H_{40}O_9$ 520.619
Cryst. ($CHCl_3$). Mp 143-144°.

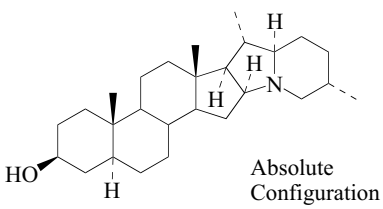
10-Deoxy, O^{15}*-Me, 30-Ac:* [62744-72-3] ***Striatin A***†
$C_{28}H_{40}O_8$ 504.619
Mp 144-145°.

10,29-Dideoxy, 11,12α-dihydro: [178120-48-4]
$C_{25}H_{38}O_6$ 434.572
Constit. of *Hericium erinaceum* (lions mane). Sol. MeOH, Me_2CO, $CHCl_3$.

Anke, T. *et al., J. Antibiot.*, 1977, **30**, 221 (*isol, ms, ir, nmr*)
Hecht, H.-J. *et al., Chem. Comm.*, 1978, 665 (*cryst struct, pmr, cmr, ir*)
Japan. Pat., 1996, 96 73 486; *CA*, **125**, 56399 (*deriv*)
Anke, T. *et al., Z. Naturforsch., C*, 2002, **57**, 263-271 (*biosynth*)

Demissidine D-77

[474-08-8]
Solanidan-3-ol, 9CI. Solanine D. Dihydrosolanidine T



Absolute Configuration

$C_{27}H_{45}NO$ 399.659
Mp 219-220°. $[\alpha]_D^{18}$ +28 (MeOH).

▶ WF0193000

O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [6077-69-6] ***Demissine***
$C_{50}H_{83}NO_{20}$ 1018.2
Alkaloid from *Solanum juzepczukii* (bitter potato) and *Lycopersicon pimpinellifolium* (currant tomato). Mp 305-308° dec. $[\alpha]_D$ -20 (Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [60776-42-3] ***Commersonine***
$C_{51}H_{85}NO_{21}$ 1048.227
Cryst. solid. Mp 230-232°. $[\alpha]_D^{25}$ -17 (Py).

Glycoside: ***β*$_1$*-Demissine***

O-*Ac:*
Mp 194°.

5,6-Didehydro, 3-O-*[β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [65428-74-2] ***Dehydrocommersonine***
$C_{51}H_{83}NO_{21}$ 1046.211

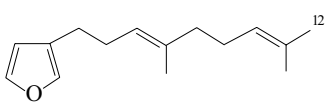
3-Epimer:
$C_{27}H_{45}NO$ 399.659
Alkaloid from *Solanum tuberosum* (potato). Needles (Me_2CO). Mp 215-217° (210-211°). $[\alpha]_D$ +31 ($CHCl_3$).

5-Epimer: [78513-80-1] ***3β-Allosolanidan-3-ol***. *5-Epidemissidine*
$C_{27}H_{45}NO$ 399.659
Alkaloid from *Solanum tuberosum* (potato). Mp 219-220°. $[\alpha]_D$ +26 ($CHCl_3$).

Prelog, V. *et al., Helv. Chim. Acta*, 1944, **27**, 390 (*struct*)
Kuhn, R. *et al., Chem. Ber.*, 1947, **80**, 406; 1957, **90**, 203 (*Demissine*)
Aslanov, K.A. *et al., CA*, 1963, **59**, 6725f (*3-epimer, isol*)
Schreiber, K. *et al., Annalen*, 1964, **672**, 232-235 (*3-epimer, synth*)
Adam, C. *et al., Tetrahedron*, 1964, **20**, 1719 (*synth*)
Wolters, B. *et al., Planta Med.*, 1966, **14**, 1392-1401 (*activity*)
Höhne, E. *et al., Tetrahedron*, 1966, **22**, 673 (*cryst struct*)
Osman, S.F. *et al., Phytochemistry*, 1976, **15**, 1065 (*Commersonine*)
Radeglia, R. *et al., Tet. Lett.*, 1977, 903 (*cmr*)
Shakirov, R. *et al., Khim. Prir. Soedin.*, 1996, **32**, 244; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 234 (*Allosolanidanol*)

Dendrolasin D-78

[23262-34-2]
3-(4,8-Dimethyl-3,7-nonadienyl)furan, 9CI



$C_{15}H_{22}O$ 218.338
Constit. of sweet potato. Oil. Bp_{16} 148-150°. n_D^{20} 1.4860.

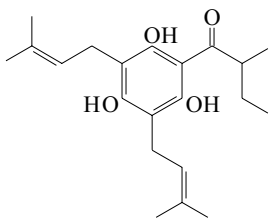
12-Hydroxy: See Neotorreyol in *The Combined Chemical Dictionary.*

9-Oxo: See 9-(3-Furanyl)-2,6-dimethyl-2,6-nonadien-4-one, F-111

Bernadi, R. *et al., Tet. Lett.*, 1967, 3893 (*isol*)
Waldner, E.E. *et al., Helv. Chim. Acta*, 1969, **52**, 15 (*biosynth*)
Kobayashi, M. *et al., J.O.C.*, 1980, **45**, 5225 (*synth*)
Lee, E. *et al., Tet. Lett.*, 1981, **22**, 2671 (*synth*)
Araki, S. *et al., Chem. Lett.*, 1982, 177 (*synth, bibl*)
Janis, S.P. *et al., Tet. Lett.*, 1982, **23**, 3115 (*synth*)
Belardini, M. *et al., J. Nat. Prod.*, 1983, **46**, 481 (*synth, bibl*)
Mandai, T. *et al., J.O.C.*, 1983, **48**, 5183 (*synth*)
Kraus, G.A. *et al., J.O.C.*, 1983, **48**, 5356 (*synth*)
Chakraborty, A. *et al., Tetrahedron*, 1997, **53**, 8513-8518 (*synth*)

4-Deoxyadhumulone D-79

[4374-92-9]
1-[2,4,6-Trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-2-methyl-1-butanone, 9CI



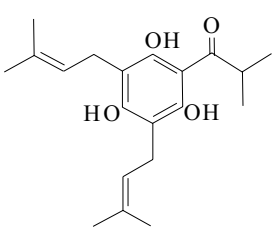
$C_{21}H_{30}O_4$ 346.466
Isol. from hops (*Humulus lupulus*). Oil.

Tribenzoyl:
Solid. Mp 127°.

Huebner, H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1961, **325**, 224 (*isol*)
Collins, E. *et al., J.C.S. Perkin 1*, 1973, 419; 2013 (*synth*)

4-Deoxycohumulone D-80

[5880-42-2]
2,4-Bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-1,3,5-cyclohexanetrione, 9CI. 2′,4′,6′-Trihydroxy-2-methyl-3′,5′-bis(3-methyl-2-butenyl)propiophenone, 8CI. 3,5-Bis(3-methyl-2-butenyl)phlorisobutyrophenone



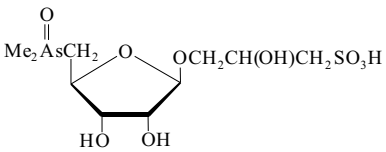
$C_{20}H_{28}O_4$ 332.439
Bitter principle from hops (*Humulus lupulus*). Cryst. (pentane). Pale yellow cryst. ($CHCl_3$/petrol). Mp 88-89°.

[24945-89-9]

Huebner, H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1961, **325**, 224 (*isol*)

Fernandez, C.M. *et al., Chem. Comm.*, 1967, 1212 (*isol*)
Collins, E. *et al., J.C.S. Perkin 1*, 1973, 419; 2013 (*synth*)
Drawert, F. *et al., Phytochemistry*, 1974, **13**, 2149 (*biosynth*)
Zuurbier, K.W.M. *et al., Phytochemistry*, 1995, **38**, 77 (*biosynth*)

3-[5-Deoxy-5-(dimethylarsinyl)ribofuranosyloxy]-2-hydroxy-1-propanesulfonic acid D-81



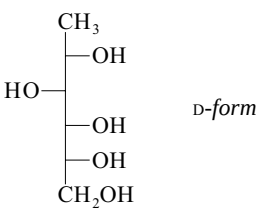
$C_{10}H_{21}AsO_9S$ 392.258

β-D-*form* [77939-92-5]
Isol. from the edible brown seaweeds ishimozuku (*Sphaerotrichia divaricata*), makonbu (*Laminaria japonica*) and hijiki (*Hizikia fusiforme*). Syrup. Possible metab. in formn. of Arsenobetaine, A-420 in marine fauna.

Edmonds, J.S. *et al., Nature (London)*, 1981, **289**, 602 (*isol, pmr, ir*)
Edmonds, J.S. *et al., J.C.S. Perkin 1*, 1983, 2375; 1987, 577 (*isol, pmr, ir, cmr, struct*)
Shibata, Y. *et al., Agric. Biol. Chem.*, 1987, **51**, 391 (*isol, pmr, hplc*)
Jin, K. *et al., Agric. Biol. Chem.*, 1988, **52**, 1965 (*isol, pmr*)
Francesconi, K.A. *et al., J.C.S. Perkin 1*, 1991, 2707; 1992, 1349 (*pmr, struct*)
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421 (*isol, rev*)

1-Deoxyglucitol, 9CI D-82

6-Deoxygulitol. Gulomethylitol



D-*form*

$C_6H_{14}O_5$ 166.174

D-*form* [18545-96-5]
1-Deoxy-D-glucitol. 6-Deoxy-L-gulitol
Constit. of the fruit of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 131-132°. $[\alpha]_D^{25}$ +5 (c, 0.5 in H_2O).

*3,4:5,6-Diisopropylidene:1-Deoxy-3,4:5,6-di-*O*-isopropylidene-D-glucitol. 6-Deoxy-1,2:3,4-di-*O*-isopropylidene-L-gulitol*
$C_{12}H_{22}O_5$ 246.303
Cryst. (EtOH). Mp 134-135° (130-131°). $[\alpha]_D^{20}$ +4 (c, 4 in H_2O).

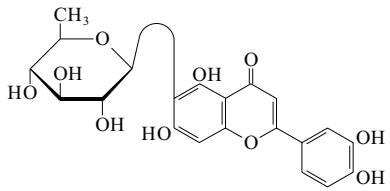
L-*form* *6-Deoxy-D-gulitol. 1-Deoxy-L-glucitol*

*3,4:5,6-Diisopropylidene:1-Deoxy-3,4:5,6-di-*O*-isopropylidene-L-glucitol. 6-Deoxy-1,2:3,4-di-*O*-isopropylidene-D-gulitol*
$C_{12}H_{22}O_5$ 246.303
Light yellow syrup. $[\alpha]_D$ -1 (c, 1.00 in MeOH).

Bollenback, G.N. *et al., Carbohydr. Res.*, 1950, **72**, 741
Wolfrom, M.L. *et al., J.A.C.S.*, 1964, **68**, 1443-1448 (*synth*)
Kuszmann, J. *et al., Carbohydr. Res.*, 1979, **74**, 187-197 (*synth*)
Wiesler, W.T. *et al., J.A.C.S.*, 1989, **111**, 9205-9213 (*synth*)
Lewis, D. *et al., J.C.S. Perkin 2*, 1991, 197-200 (*props, conformn*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)

6-*C*-(6-Deoxyglucopyranosyl)-3′,4′,5,7-tetrahydroxyflavone D-83

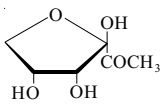
[132368-05-9]
6-C-Chinovosylluteolin. 6-C-Quinovosylluteolin



$C_{21}H_{20}O_{10}$ 432.383
Isol. from *Passiflora edulis* f. *flavicarpa* (yellow passion fruit).

Mareck, U. *et al., Phytochemistry*, 1991, **30**, 3486 (*isol, pmr, cmr*)

1-Deoxy-*erythro*-hexo-2,3-diulose D-84



β-D-3,6-Furanose-*form*

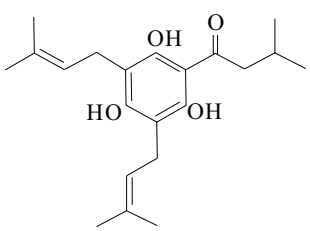
$C_6H_{10}O_5$ 162.142

D-*form*
Postulated common intermed. in the formation of sugar-amine products in food browning and related reactions. Amorph. solid.

Okuda, T. *et al., Carbohydr. Res.*, 1979, **68**, 1
Fisher, B.E. *et al., Carbohydr. Res.*, 1983, **116**, 209

4-Deoxyhumulone D-85

[4374-93-0]
3-Methyl-1-[2,4,6-trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-butanone, 9CI. 3,5-Bis(3-methyl-2-butenyl)phlorisovalerophenone



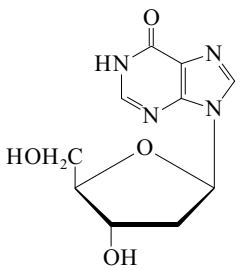
$C_{21}H_{30}O_4$ 346.466
Flavone. Isol. from hops (*Humulus lupulus*). Cryst. (petrol). Mp 83°.
Tribenzoyl:
Shining leaflets (MeOH). Mp 138-139°.

Riedl, W. *et al., Angew. Chem.*, 1958, **70**, 343 (*isol, synth*)
Hübner, H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1961, **325**, 224 (*isol*)
Collins, E. *et al., J.C.S. Perkin 1*, 1973, 419; 2013 (*synth*)
Drawert, F. *et al., Phytochemistry*, 1976, **15**, 1693 (*biosynth*)
Cann, M.R. *et al., Chem. Ind. (London)*, 1982, 779 (*pmr*)
Zuurbier, K.W.M. *et al., Phytochemistry*, 1995, **38**, 77 (*biosynth*)

2′-Deoxyinosine D-86

[29868-32-4]

[890-38-0]
9-(2-Deoxyribofuranosyl)hypoxanthine. Hypoxanthine 2-deoxyriboside



$C_{10}H_{12}N_4O_4$ 252.229
Isol. from *Phaseolus vulgaris* (kidney bean). Needles (MeOH), cryst. (H_2O). Mp 218° dec. $[\alpha]_D^{27}$ +7.92 (c, 0.53 in 0.1*M* NaOH). $[\alpha]_D^{30}$ -21 (c, 1 in H_2O).

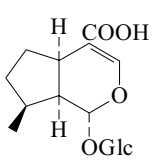
Oxime: [51385-49-0]
Mp 139-140°. $[\alpha]_D$ -21.8 (c, 1 in MeOH). Softens at 110-115° and 130-135°.

3′-Ac: [229326-13-0]
$C_{12}H_{14}N_4O_5$ 294.266
Mp 116°. $[\alpha]_D^{25}$ -22.5 (c, 1 in MeOH).

Brown, D.M. *et al., J.C.S.*, 1950, 1990 (*struct*)
Manson, L.A. *et al., J. Biol. Chem.*, 1951, **191**, 87 (*isol*)
Banhidi, Z.G. *et al., Acta Chem. Scand.*, 1953, **7**, 713 (*isol*)
Venner, H. *et al., Chem. Ber.*, 1960, **93**, 140 (*synth*)
Robins, M.J. *et al., J.A.C.S.*, 1965, **87**, 4934 (*pmr*)
Rousseau, R.J. *et al., J. Het. Chem.*, 1970, **7**, 367 (*synth, uv*)
Robins, M.J. *et al., Can. J. Chem.*, 1973, **51**, 3161 (*synth*)
Yamazaki, A. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1143 (*synth*)
Mengel, R. *et al., Annalen*, 1977, 1585 (*synth*)
Ciuffreda, P. *et al., Tetrahedron*, 2000, **56**, 3239-3243 (*3′-Ac, synth, pmr*)

Deoxyloganic acid D-87

[92842-56-3]
1,5,9-Epideoxyloganic acid



$C_{16}H_{24}O_9$ 360.36

Constit. of *Nepeta cataria* (catnip). Needles. Mp 106° dec. $[\alpha]_D$ +85.1 (c, 1.1 in MeOH). Formerly designated 5-Epideoxyloganic acid. The abs. config. shown appears to be the correct one (see w.r.t. Loganic acid).

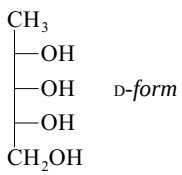
β-D-Glucopyranosyl ester:
$C_{22}H_{34}O_{14}$ 522.502
Amorph. powder. $[\alpha]_D^{27}$ +37.2 (c, 0.98 in MeOH). λ_{max} 240 (log ϵ 4.01) (MeOH).

1,5,8,9-Tetraepimer: [88668-99-9] ***8-Epideoxyloganic acid***
$C_{16}H_{24}O_9$ 360.36
Cryst. Mp 213-214°. $[\alpha]_D$ -122 (c, 0.29 in MeOH).

Damtoft, S. *et al., Phytochemistry*, 1983, **22**, 1929-1930 (*8-Epideoxyloganic acid*)
Murai, F. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2809
Takeda, Y. *et al., Phytochemistry*, 1998, **48**, 787-791 (*glucosyl ester*)
Nakamura, M. *et al., Phytochemistry*, 2000, **53**, 253-256 (*8-Epideoxyloganic acid*)

1-Deoxyribitol D-88

[62137-55-7]
5-Deoxyribitol



D-*form*

$C_5H_{12}O_4$ 136.147

D-*form* [13046-76-9]
1-Deoxy-D-ribitol. 5-Deoxy-L-ribitol
Constit. of the fruit of *Foeniculum vulgare* (fennel). Cryst. (MeCN). Mp 69°. $[\alpha]_D^{21}$ +15 (c, 0.9 in H_2O). The CAS no. was originally applied erroneously to the L-enantiomer.

Tetra-Ac: [7260-90-4] *Tetra*-O-*acetyl-1-deoxy-D-ribitol*
$C_{13}H_{20}O_8$ 304.296No phys. props. reported.

L-*form* [67968-45-0]
1-Deoxy-L-ribitol. 5-Deoxy-D-ribitol
Cryst. (EtOAc/MeOH). Mp 80-85°. $[\alpha]_D^{23}$ -11.2 (c, 1.4 in MeOH).

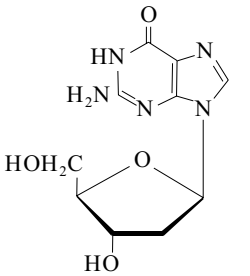
*3,4-Isopropylidene:5-Deoxy-2,3-*O*-isopropylidene-D-ribitol. 1-Deoxy-3,4-*O*-isopropylidene-L-ribitol*
$C_8H_{16}O_4$ 176.212
Syrup. $[\alpha]_D^{27}$ -15.5 (c, 2.7 in EtOH). n_D^{20} 1.4510.

[25289-19-4]

Hough, L. *et al., Can. J. Chem.*, 1958, **36**, 1720 (*synth, L-form*)
Buck, K.W. *et al., Carbohydr. Res.*, 1966, **2**, 115 (*synth*)
Sepulchre, A.-M. *et al., Carbohydr. Res.*, 1972, **24**, 311 (*synth, D-form*)
Fischer, J.-C. *et al., Can. J. Chem.*, 1977, **55**, 4078 (*synth, ms*)
Takai, K. *et al., J.O.C.*, 1985, **50**, 3247 (*synth, pmr, cmr, tetra-Ac*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)

2′-Deoxyribofuranosylguanine D-89

2-Amino-9-(2-deoxy-erythro-*pentofuranosyl)-6-purinone*



β-D-*form*

$C_{10}H_{13}N_5O_4$ 267.244

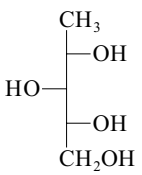
β-D-*form* [961-07-9]
2′-Deoxyguanosine. Guanine deoxyriboside
Isol. from plants, e.g. *Phaseolus vulgaris* (kidney bean). Cryst. + $1H_2O$. Mp 300° (also said to be indefinite). $[\alpha]_D^{26}$ -20.3 (c, 1.2 in DMF). $[\alpha]_D^{19}$ -47.7 (0.1*M* NaOH). $[\alpha]_D^{24}$ -30.2 (H_2O). λ_{max} 254 (ϵ 10700); 274 (ϵ 7710) (HCl) (Berdy). λ_{max} 259 (ϵ 9960) (NaOH) (Berdy). λ_{max} 252 (ϵ 13700) (H_2O) (pH 7). λ_{max} 255 (ϵ 12100); 272 (sh) (ϵ 8460) (H_2O) (pH 1). λ_{max} 262 (ϵ 12000) (H_2O) (pH 11).
► MF8760000

[102783-74-4]

Montgomery, J.A. *et al., Adv. Carbohydr. Chem.*, 1962, **17**, 301 (*rev*)
Ulbricht, T.L.V. *et al., Tet. Lett.*, 1964, 695 (*ord*)
Robins, M.J. *et al., J.O.C.*, 1969, **34**, 2160; 1970, **35**, 636 (*α-D-form, β-D-form, α-D-2N-Me, α-L-form, β-L-form*)
Jones, A.J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1970, **65**, 27; *CA*, **72**, 96682j (*cmr*)
Davies, D.B. *et al., J.C.S. Perkin 2*, 1975, 1703 (*pmr*)

1-Deoxyxylitol D-90

[62137-56-8]
5-Deoxyxylitol



D-*form*

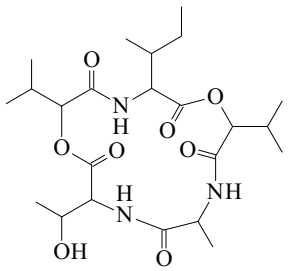
$C_5H_{12}O_4$ 136.147

D-*form* [68832-17-7]
1-Deoxy-D-xylitol. 5-Deoxy-L-xylitol
Constit. of the fruit of *Foeniculum vulgare* (fennel). Cryst. (EtOH aq). Mp 77-78°. $[\alpha]_D$ 0 (H_2O).

[25289-19-4]

Zissis, E. *et al., J.A.C.S.*, 1953, **75**, 129 (*D-form*)
Ness, A.T. *et al., J.A.C.S.*, 1953, **75**, 132 (*L-form, DL-form*)
David, S. *et al., J.C.S. Perkin 1*, 1982, 2131-2137 (*synth*)
Lewis, D. *et al., J.C.S. Perkin 2*, 1991, 197-200 (*conformn*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)

Sarcodon scabrosus Depsipeptide D-91

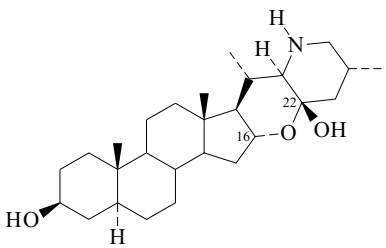


$C_{23}H_{39}N_3O_8$ 485.576
Isol. from the mushroom *Sarcodon scabrosus* of unknown palatability.

Tomida, I. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2300-2302 (*struct*)

3-Desamino-3-hydroxysolanocapsine D-92

16,23-Epoxy-16,28-secosolanidane-3,23-diol, 9CI



$C_{27}H_{45}NO_3$ 431.657
Needles (MeOH aq.). Mp 204°. $[\alpha]_D^{25}$ +20.1 (c, 1 in $CHCl_3$).

O^{22}-*Me:* [91377-17-2] ***Aculeamine***
$C_{28}H_{47}NO_3$ 445.684
Needles (MeOH aq.). Mp 205-207°. $[\alpha]_D^{24}$ +50.8 (c, 0.9 in $CHCl_3$).

O^{22}-*Et:* [92070-74-1] ***3-Desamino-O^{22}-ethyl-3-hydroxysolanocapsine***
$C_{29}H_{49}NO_3$ 459.711
Needles (Me_2CO aq.). Mp 183-185°. $[\alpha]_D^{23}$ +45.2 (c, 0.4 in $CHCl_3$). Artifact.

16-Epimer: [138665-46-0] ***Solanocardinol. Pimpifolidine***
$C_{27}H_{45}NO_3$ 431.657
Alkaloid from *Lycopersicon pimpinellifolium* (currant tomato). Cryst. (Me_2CO aq.). Mp 200-203°. $[\alpha]_D^{20}$ -1.9 (c, 1.05 in Py). Solanocardinol and Pimpifolidine not compared. Phys. props. refer to Pimpifolidine.

16,22-Diepimer: [152322-51-5] ***22-Isopimpifolidine***
$C_{27}H_{45}NO_3$ 431.657
Alkaloid from roots of *Lycopersicon pimpinellifolium* (currant tomato). Needles (Me_2CO). Mp 200-204°. $[\alpha]_D^{20}$ -13.6 (c, 0.77 in Py).

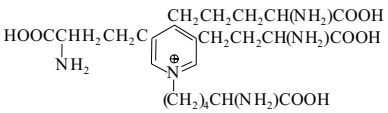
Coll, F. *et al., Phytochemistry*, 1983, **22**, 2099; 1984, **23**, 883 (*isol, struct, cmr, pmr*)
Kubschabsky, L. *et al., CA*, 1984, **101**, 111265p (*cryst struct*)
Osman, S.F. *et al., Phytochemistry*, 1991, **30**, 3161 (*Solanocardinol*)

Ripperger, H. *et al., Phytochemistry*, 1994, **35**, 813 (*Pimpifolidine, Isopimpifolidine*)

Desmosine D-93

[11003-57-9]

4-(4-Amino-4-carboxybutyl)-1-(5-amino-5-carboxypentyl)-3,5-bis(3-amino-3-carboxypropyl)pyridinium, 9CI



$C_{24}H_{40}N_5O_8^{\oplus}$ 526.609

Degradn. prod. of Elastin. pK_{a1} 1.7; pK_{a2} 2.4; pK_{a3} 8.8; pK_{a4} 9.9; pK_{a5} 11.5.

Thomas, J. *et al., Nature (London)*, 1963, **200**, 651 (*struct*)

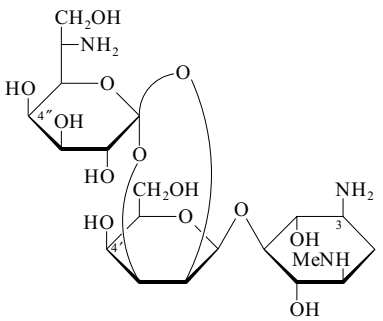
Anwar, R.A. *et al., Nature (London)*, 1966, **210**, 1254 (*struct*)

Anwar, R.A. *et al., Adv. Exp. Med. Biol.*, 1977, **86B**, 709 (*rev*)

Destomycin A D-94

[14918-35-5]

XK 33FI. Antibiotic XK 33FI. Anthelmin. Destonate 20



$C_{20}H_{37}N_3O_{13}$ 527.525

Aminoglycoside antibiotics.Powder. Sol. H_2O, MeOH; poorly sol. butanol, hexane. Mp 180-190° dec. $[\alpha]_D^{22}$ +7 (c, 2 in H_2O).

▶ LD_{50} (mus, orl) 50 mg/kg. LD_{50} (mus, ivn) 5 mg/kg. WK2129900

N^3-*Me:* [55651-94-0] ***Destomycin C***. N-*Methylhygromycin A. AB 74. Antibiotic AB 74*

$C_{21}H_{39}N_3O_{13}$ 541.551

Hygroscopic powder. Mp 182-190° dec. $[\alpha]_D^{22}$ +9 (c, 1 in H_2O). Log P -7.68 (uncertain value) (calc).

▶ LD_{50} (mus, ivn) 6.25 mg/kg. WK2129000

N-*De-Me:* [31357-30-9] ***Antibiotic SS 56D***. *A 396I. SS 56D. Antibiotic A 396I*

$C_{19}H_{35}N_3O_{13}$ 513.498

Amorph. powder. Sol. H_2O, MeOH; fairly sol. EtOH, butanol; poorly sol. Me_2CO, hexane. Mp 185-190° dec. $[\alpha]_D^{25}$ +12.7 (c, 1.08 in H_2O).

▶ LD_{50} (mus, ivn) 12.5 mg/kg. CB9198000

N-*De-Me,* N^3-*Me:* [31282-04-9] ***Hygromycin B***. *Hygrovetine. Hyanthelmix*

$C_{20}H_{37}N_3O_{13}$ 527.525

FDA approved antibiotic food additive for swine and poultry. Amorph. Mp 160-180° dec. $[\alpha]_D^{26}$ +20.2 (c, 1 in H_2O). pK_{a2} 8.8.

▶ WK2130000

2S-*Hydroxy,* N-*de-Me:* [39471-55-1]

[40980-50-5] ***Antibiotic SS 56C***. *SS 56C*

$C_{19}H_{35}N_3O_{14}$ 529.497

Amorph. powder. Sol. H_2O; poorly sol. butanol, hexane. Mp 201-203° dec. $[\alpha]_D^{25}$ +12 (c, 1.08 in H_2O). Related to Destomycin A, D-94 and Hygromycin B.

2S-*Hydroxy,* N-*de-Me,* N^1-*amidino:* [96479-74-2] ***1-N-Amidino-1-N-demethyl-2-hydroxydestomycin A***

$C_{20}H_{37}N_5O_{14}$ 571.537

Powder +1H_2O (as trihydrochloride). Sol. H_2O; fairly sol. MeOH; poorly sol. Me_2CO, hexane. $[\alpha]_D^{25}$ +7.7 (c, 1 in H_2O). Hydrochloride dec. at 172-183°.

▶ LD_{50} (mus, ivn) 6.25 - 12.5 mg/kg. WK2128700

4′-*Epimer,* N-*de-Me,* N^3-*Me:* [83378-70-5] ***Antibiotic RH 5012C***. *RH 5012C*

$C_{20}H_{37}N_3O_{13}$ 527.525

Powder + 2H_2O. Sol. H_2O; poorly sol. EtOH, hexane, Et_2O. Mp 191-194° dec. $[\alpha]_D^{20}$ +12.9 (c, 1 in H_2O).

▶ LD_{50} (mus, orl) 100 - 300 mg/kg , LD_{50} (mus, ipr) 6.5 - 11.5 mg/kg. WK2128350

4′,4″-*Diepimer,* N^3-*Me:* [11005-98-4] ***Destomycin B***. *A 16316C. Antibiotic A 16316C*

$C_{21}H_{39}N_3O_{13}$ 541.551

Powder. Mp 140-200° dec., 175-185° dec. $[\alpha]_D^{21}$ +6 (c, 1 in H_2O). Log P -7.68 (uncertain value) (calc).

▶ LD_{50} (mus, orl) 50 mg/kg. LD_{50} (mus, ivn) 5 mg/kg. HH1330000

[59794-19-3]

Mann, R.L. *et al., J.A.C.S.*, 1958, **80**, 2714-2716 (*Hygromycin B, isol*)

Wiley, P.F. *et al., J.O.C.*, 1962, **27**, 2793-2796 (*Hygromycin B*)

Kondo, S. *et al., J. Antibiot., Ser. A*, 1965, **18**, 38-42; 1966, **19**, 139-140 (*isol, struct, ir, ms, pmr*)

Neuss, N. *et al., Helv. Chim. Acta*, 1970, **53**, 2314-2319 (*struct*)

Shoji, J. *et al., J. Antibiot.*, 1970, **23**, 391 (*SS56, isol*)

Inouye, S. *et al., J. Antibiot.*, 1973, **26**, 374-385 (*SS 56C, SS 56D*)

Shimura, M. *et al., J. Antibiot.*, 1975, **28**, 83-84 (*Destomycins A-C*)

Shimura, M. *et al., Agric. Biol. Chem.*, 1976, **40**, 611-618 (*Destomycin B*)

Tamura, A. *et al., J. Antibiot.*, 1976, **29**, 590-591; 592-594 (*Destomycin A, AB 74, isol*)

Japan. Pat., 1976, 76 82 793, (*Dainippon*); *CA*, **86**, 15201n (*Destomycin B*)

Wright, D.E. *et al., Tetrahedron*, 1979, **35**, 1207 (*Hygromycin B, Destomycins, rev*)

Horito, S. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 2147-2150 (*cryst struct*)

Yoshimura, J. *et al., CA*, 1981, **96**, 181549; 1986, **105**, 97853 (*rev, synth*)

Japan. Pat., 1982, 82 95 995; *CA*, **97**, 198514 (*RH 5012C*)

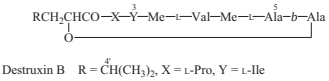
Ikeda, Y. *et al., J. Antibiot.*, 1985, **38**, 436 (*1-Amidino-1-demethyl-2-hydroxydestomycin A*)

Tamura, J. *et al., Carbohydr. Res.*, 1988, **174**, 181-199 (*Destomycin C, synth, pmr*)

Kamps-Holtzapple, C. *et al., J. Agric. Food Chem.*, 1994, **42**, 822-827 (*Hygromycin B, anal*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DBB400

Destruxins D-95



Destruxin B R = $CH(CH_3)_2$, X = L-Pro, Y = L-Ile

B_1 R = $CH(CH_3)_2$, X = L-Piperidinecarboxylic acid, Y = L-Ile

B_2 R = $CH(CH_3)_2$, X = L-Pro, Y = L-Val

Cyclic depsipeptide antibiotic complex.

Destruxin B, 9CI [2503-26-6]

$C_{30}H_{51}N_5O_7$ 593.762

Cryst. (C_6H_6/hexane). Mp 238°. $[\alpha]_D^{20}$ -241 (c, 0.5 in MeOH).

▶ HH1500100

4′-*Hydroxy:* ***Hydroxydestruxin B***

$C_{30}H_{51}N_5O_8$ 609.762

Constit. of the leaves of *Sinapis alba* (white mustard). $[\alpha]_D^{25}$ -255 (c, 0.1 in MeOH).

4′-*β-D-Glucopyranosyloxy:* ***β-D-Glucosyloxydestruxin B***

$C_{36}H_{61}N_5O_{13}$ 771.904

Constit. of the leaves of *Brassica napus* (rape).

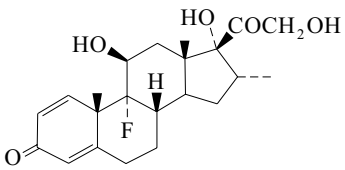
Pedras, M.S.C. *et al., Org. Lett.*, 1999, **1**, 1655-1658 (*Hydroxydestruxin B*)

Pedras, M.S.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2001, **98**, 747-752 (*Glucosyloxydestruxin B*)

Dexamethasone, BAN, INN D-96

[50-02-2]

9-Fluoro-11,17,21-trihydroxy-16-methylpregna-1,4-diene-3,20-dione. 9-Fluoro-16-methylprednisolone. Decaderm. Deltafluorene. Desametasone. Dexadeltone. Dexametasone. Dexamethazone. Hexadecadrol. Hexadrol. Millicorten. Superprednol. MK 125. NSC 34521



$C_{22}H_{29}FO_5$ 392.466

Glucocorticoid with potent antiinflammatory props. Not FDA approved for use in food-producing animals, but may be used illegally. Cryst. (Et_2O). Mp 262-264°. $[\alpha]_D^{25}$ +77.5 (dioxan). Log P 1.49 (uncertain value) (calc). Stereochem. is (9α,11β,16α,17αOH).

▶ TU3980000

[1879-72-7, 55812-90-3]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 585C (*nmr*)

Oliveto, E.P. *et al., J.A.C.S.*, 1958, **80**, 4431 (*synth*)

McAleer, W.J. *et al., J.O.C.*, 1958, **23**, 508 (*synth*)

Cohen, E.M. *et al., Anal. Profiles Drug Subst.*, 1973, **2**, 163 (*rev*)

Fiegel, G. *et al., Arzneim.-Forsch.*, 1975, **25**, 560 (*props*)

Rohrer, D.C. *et al., Cryst. Struct. Commun.*, 1977, **6**, 123 (*struct*)

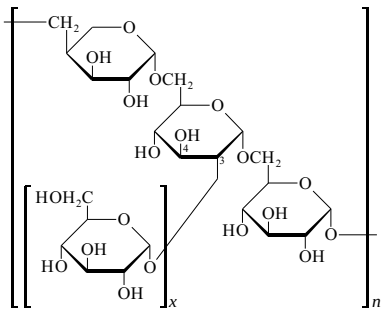
Hickey, J.P. *et al., J. Magn. Reson.*, 1980, **38**, 501 (*cmr*)

Crowe, D.F. *et al., Tetrahedron*, 1983, **39**, 3083 (*synth, C-13*)

Grinenko, G.S. *et al., Khim.-Farm. Zh.*, 1987, **21**, 373 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 6644; 6675; 7130 (*synonyms*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 728
Mallinson, E.T. *et al., J. Agric. Food Chem.*, 1995, **43**, 140-145 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BFW325; SOW000; DBC510; DAE525; DBC525; DBC550; DBC575

Dextran, 9CI, 8CI, BAN, INN D-97

[9004-54-0]
Hemodex. Hyskon. Infucoll. Intradex. Macrose



Bacterial polysaccharides of α-(1-6)-D-Glcp units differing only in chain length and degree of branching which occurs through α(1→3) (illus.) and α(1→4) branch points. M40000 (average for Dextran 40). Indirect food additive produced by bacterial fermentation of sucrose. Chem. and phys. props. differ depending on mode of prodn. Native dextrans have a high Mw, clinical dextrans prod. by synth. or by depolymerisation of native dextrans have a low Mw.

▶ Adverse human systemic effects when used therapeutically. Exp. reprod. and teratogenic effects (large doses) (Dextran 70). LD_{50} (rat, scu) 10700 mg/kg. HH9247500

Na salt, Al complex: [37209-31-7] ***Detralfate, INN***
$[\alpha]_D^{20}$ +83.2 (c, 5 in 1*M* HCl).

▶ LD_{50} (rat, ipr) 200 mg/kg. LD_{50} (rat, scu) 1600 mg/kg. HH2860000

Poly-O-*sulfate:* [9042-14-2]

[9011-18-1]
Powder. Heparin-like polysaccharide containing up to three sulfate groups per glucose molecule with a molecular weight range of 4000-500,000 Da.

Poly-O-*2-(diethylaminoethyl):* [9015-73-0] ***Colextran, INN***

▶ HH9250000

Poly-O-*(carboxymethyl):* [9044-05-7]
Powder. Sol. MeOH, H_2O, insol. Me_2CO.

Poly(2,3-dihydroxypropyl-2-hydroxy-1,3-propanediyl) ether: [56087-11-7] ***Dextranomer, BAN, INN***. *Debrisan*

▶ HH9255000

[9011-18-1, 39422-86-1]

Jeanes, A. *et al., J.A.C.S.*, 1954, **76**, 5041
Neely, W. *et al., Adv. Carbohydr. Chem.*, 1960, **15**, 341 (*struct, synth, rev*)
Jeanes, A. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 118; 127 (*synth*)
Ger. Pat., 1969, 1 916 535, (*Meito Sangyo*); *CA*, **72**, 35780 (*Detralfate*)
Murphy, P.T. *et al., Ind. Gums*, (Whistler, R.L., Ed.), 2nd Ed., Academic Press, 1973, 513 (*struct, manuf, rev*)
Sidebotham, R.L. *et al., Adv. Carbohydr. Chem. Biochem.*, 1974, **30**, 371 (*rev*)
Friebolin, H. *et al., Makromol. Chem.*, 1976, **177**, 845 (*cmr*)
Weetman, D.F. *et al., Drugs of Today (Barcelona)*, 1978, **14**, 360 (*pharmacol, Dextranomer*)
Walker, G.J. *et al., Int. Rev. Biochem.*, 1978, **16**, 75 (*rev*)
Seymour, F.R. *et al., Carbohydr. Res.*, 1979, **74**, 77-92 (*pmr*)
Kennedy, J.F. *et al., Compr. Org. Chem.*, (Drayton, C.J., Ed.), Pergamon Press, Oxford, Part 26, 1979, **5**, 790 (*rev*)
Heel, R.C. *et al., Drugs*, 1979, **18**, 89 (*rev, pharmacol, Dextranomer*)
Alsop, R.M. *et al., Prog. Ind. Microbiol.*, 1983, **18**, 1 (*rev, manuf, fermn*)
Guizard, C. *et al., Macromolecules*, 1984, **17**, 100 (*cryst struct*)
Forsgren, M. *et al., J.C.S. Perkin 1*, 1985, **11**, 2383 (*pmr*)
Encyclopaedia of Polymer Science and Engineering, 1986, **4**, 752 (*rev*)
Peterson, E.A. *et al., Methods Enzymol.*, 1987, **138**, 429-442 (*carboxymethyl ether*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 650; 651; 652
Merck Index, 12th edn., 1996, 500 (*sulfate*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 792-793
Mähner, C. *et al., Carbohydr. Res.*, 2001, **331**, 203-208 (*sulfate, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DBB500; DBD000; DBD200; DBD400; DBD600; DHW600; DBD700; DBC800

Dextranase, 9CI D-98

[9025-70-1]
1,6-α-D-Glucan 6-glucanohydrolase. Dextron hydrolase. Endodextranase. E.C. 3.2.1.11

Enzyme. Used to improve purifn. of sugar cane by eliminating filtration and crystallisation problems. Hydrolyses the 1,6-α-D-glucosidic linkages in dextran.

Bailey, R.W. *et al., Biochem. J.*, 1959, **72**, 49-54 (*isol*)
Sidebottom, R.L. *et al., Adv. Carbohydr. Chem. Biochem.*, 1974, **30**, 371-444 (*rev*)
Madhu, G.L. *et al., Int. Sugar J.*, 1984, **86**, 136-138 (*use*)
Merck Index, 12th edn., 1996, 2990

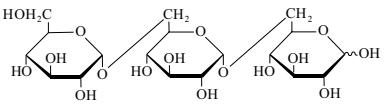
Dextranicin 24 D-99

Polypeptide. Prod. by *Leuconostoc mesenteroides* ssp. *dextranicum* J24. Bacteriocin.

Revul-Junelles, A.M. *et al., Curr. Microbiol.*, 1996, **33**, 136-137 (*isol*)

Dextrantriose D-100

[3371-50-4]
O-α-D-*Glucopyranosyl-(1→6)*-O-α-D-*glucopyranosyl-(1→6)*-D-*glucose, 9CI. 6-α-Isomaltosyl-*D-*glucose. Isomaltotriose*



$C_{18}H_{32}O_{16}$ 504.441
Occurs in Saké. $[\alpha]_D$ +134 (c, 0.5 in H_2O).

Undecabenzoyl:
$C_{95}H_{76}O_{27}$ 1649.629
Mp 226-227°. $[\alpha]_D$ +131 ($CHCl_3$).

Pazur, J.H. *et al., J. Biol. Chem.*, 1952, **196**, 265 (*isol*)
Jeans, A. *et al., J.A.C.S.*, 1953, **75**, 5911
Takiura, K. *et al., Chem. Pharm. Bull.*, 1973, **21**, 523 (*synth*)
Friebolin, H. *et al., Makromol. Chem.*, 1976, **177**, 845 (*conformn, cmr*)

Dextrin, 9CI, 8CI, BAN D-101

[9004-53-9]
Icodextrin, BAN. Adept. AmylinStarch gum. British gum. Amylodextrin. Dextrid. Icodial. Starch gum

$(C_6H_{10}O_5)_n.xH_2O$. A mixture of polymerised glucosans. Gives a reddish-brown colour with iodine and does not reduce Fehling's soln. Commercial dextrin is less pure and usually contains sol. starch and glucose. Treatment with dil. acids gives maltose and finally glucose.. Binder, colloid stabiliser and other uses in food, oral dietary supplement. Approved for clinical use in the European Union (1999). White or yellow, amorph. powder. Insol. EtOH, Et_2O; sol. in boiling water to give a gummy soln.

▶ HH9450000

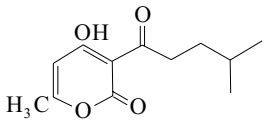
Mixt. with iron(III) hydroxide: [8063-26-1] ***Dextriferron, BAN, INN***. *Astrafer. Haemigron*

[9004-51-7, 9005-84-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 199C (*ir*)
Satterthwaite, R.W. *et al., Ind. Gums*, 2nd Ed., Academic Press, New York, 1973, 577 (*rev*)
Usui, T. *et al., J.C.S. Perkin 1*, 1973, 2425 (*cmr*)
Umeki, K. *et al., J. Biochem. (Tokyo)*, 1975, **78**, 897 (*struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DBD800
Biotechnol. Amylodextrin Oligosaccharides, Friedman, R.B. (ed.), Amer. Chem. Soc., 1991, (*book*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 151-153
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1359
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 793-796 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DBD800; IGT000

Dhelwangin D-102

[23800-56-8]
*4-Hydroxy-6-methyl-3-(4-methyl-1-oxopentyl)-2*H*-pyran-2-one, 9CI. Pogostone*



$C_{12}H_{16}O_4$ 224.256
Isol. from leaves of *Pogostemon cablin* (patchouli). Cryst. Sol. $CHCl_3$, bases; fairly sol. C_6H_6; poorly sol. H_2O. Mp 41-41.6°. Log P 2.98 (calc). λ_{max} 225 (ϵ 10300); 310 (ϵ 12630) (EtOH) (Berdy).

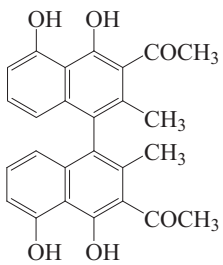
Klein, E. *et al., Tet. Lett.*, 1969, 2279 (*synth*)
Anon, *et al., CA*, 1977, **87**, 172771 (*isol, struct*)

Diacetin B D-103

[169277-12-7]
Peptide containing 37 amino acid residues. Isol. from *Lactococcus lactis* ssp. *diacetylactis* UL720. Bacteriocin.

Ali, D. *et al., Can. J. Microbiol.*, 1995, **41**, 832-841 (*isol*)

3,3′-Diacetyl-4,4′,5,5′-tetrahydroxy-2,2′-dimethyl-1,1′-binaphthalene D-104

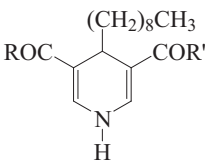


$C_{26}H_{22}O_6$ 430.456

5,5′-Di-O-*β*-D-*glucopyranoside:* ***Labadoside***
$C_{38}H_{42}O_{16}$ 754.74
Constit. of the roots of *Rumex patientia* (patience dock). Amorph. λ_{max} 230 ; 314 ; 337 (MeOH).

Demirezer, O. *et al., Phytochemistry*, 2001, **56**, 399-402

3,5-Diacyl-1,4-dihydro-4-nonylpyridines D-105



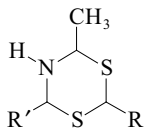
3,5-Didecanoyl-1,4-dihydro-4-nonylpyridine [158528-00-8]
1,1′-(1,4-Dihydro-4-nonyl-3,5-pyridinediyl)bis[1-decanone], 9CI
$C_{34}H_{61}NO_2$ 515.861
Alkaloid from *Houttuynia cordata* (Yu Xing Cao).

3-Decanoyl-5-dodecanoyl-1,4-dihydro-4-nonylpyridine [158528-01-9]
1-[1,4-Dihydro-4-nonyl-5-(1-oxodecyl)-3-pyridinyl]-1-dodecanone, 9CI
$C_{36}H_{65}NO_2$ 543.915
Alkaloid from *Houttuynia cordata* (Yu Xing Cao).

3,5-Didodecanoyl-1,4-dihydro-4-nonylpyridine [158528-02-0]
1,1′-(1,4-Dihydro-4-nonyl-3,5-pyridinediyl)bis[1-dodecanone], 9CI
$C_{38}H_{69}NO_2$ 571.969
Alkaloid from *Houttuynia cordata* (Yu Xing Cao).

Proebstle, A. *et al., Nat. Prod. Lett.*, 1994, **4**, 235-240

2,6-Dialkyl-4-methyl-4*H*-1,3,5-dithiazines D-106



R = CH_3, R′ = $CH(CH_3)_2$
R = $CH(CH_3)_2$, R′ = CH_3
R = CH_3, R′ = $CH_2CH(CH_3)_2$
R = $CH_2CH(CH_3)_2$, R′ = CH_3
R = CH_3, R′ = $CH(CH_3)CH_2CH_3$
R = $CH(CH_3)CH_2CH_3$, R′ = CH_3

Dihydro-6-isopropyl-2,4-dimethyl-4*H*-1,3,5-dithiazine [104691-41-0]
Dihydro-2,4-dimethyl-6-(1-methylethyl)-4H-1,3,5-dithiazine, 9CI
$C_8H_{17}NS_2$ 191.361
Isol. from dried squid aroma. Flavouring ingredient.

Dihydro-2-isopropyl-4,6-dimethyl-4*H*-1,3,5-dithiazine [104691-40-9]
Dihydro-4,6-dimethyl-2-(1-methylethyl)-4H-1,3,5-dithiazine, 9CI
$C_8H_{17}NS_2$ 191.361
Isol. from dried squid aroma. Flavouring ingredient.

Dihydro-2,4-dimethyl-6-(2-methylpropyl)-4*H*-1,3,5-dithiazine, 9CI [101517-86-6]
$C_9H_{19}NS_2$ 205.388
Isol. from dried squid aroma.

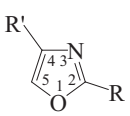
Dihydro-4,6-dimethyl-2-(2-methylpropyl)-4*H*-1,3,5-dithiazine, 9CI [101517-87-7]
$C_9H_{19}NS_2$ 205.388
Isol. from dried squid aroma.

Dihydro-2,4-dimethyl-6-(1-methylpropyl)-4*H*-1,3,5-dithiazine, 9CI [104691-37-4]
$C_9H_{19}NS_2$ 205.388
Isol. from dried squid aroma.

Dihydro-4,6-dimethyl-2-(1-methylpropyl)-4*H*-1,3,5-dithiazine, 9CI [104691-36-3]
$C_9H_{19}NS_2$ 205.388
Isol. from dried squid aroma.

Ger. Pat., 1986, 3 447 209; *CA*, **105**, 172518c
Kawai, T. *et al., J. Agric. Food Chem.*, 1989, **37**, 1026-1031; 1991, **39**, 770-777 (*occur*)

2,4-Dialkyloxazoles D-107



See also 2,4-Dimethyloxazole, D-861.
Odorants/flavorants with actual or potential food use.

2-Ethyl-4-methyloxazole, 9CI [24667-03-6]
C_6H_9NO 111.143
Constit. of Arabica coffee aroma. Bp 127°.

4-Ethyl-2-methyloxazole, 9CI [53833-20-8]
C_6H_9NO 111.143
Constit. of Arabica coffee aroma and French fries. Characterised spectroscopically.

2,4-Diethyloxazole [84027-83-8]
$C_7H_{11}NO$ 125.17
Acidic smoky aroma. Characterised spectroscopically.

2-Methyl-4-propyloxazole, 9CI [126484-99-9]
$C_7H_{11}NO$ 125.17
Constit. of boiled shrimp (*Panaeus brevistoris*) aroma.

4-Methyl-2-propyloxazole, 9CI [24667-04-7]
$C_7H_{11}NO$ 125.17
Constit. of boiled shrimp (*Panaeus brevistoris*) aroma. Bp_{20} 57°. n_D^{20} 1.4421.

4-Ethyl-2-isopropyloxazole, 8CI [84027-90-7]
4-Ethyl-2-(1-methylethyl)oxazole, 9CI
$C_8H_{13}NO$ 139.197Characterised spectroscopically.

2-Butyl-4-methyloxazole, 9CI [24667-15-0]
$C_8H_{18}NO$ 144.236
Sweet, spicy, nutmeg, butter-like odour. Characterised spectroscopically.

4-Butyl-2-methyloxazole, 9CI [84027-87-2]
$C_8H_{13}NO$ 139.197
Constit. of roasted peanut and French fried potato aroma. Green, floral odour. Characterised spectroscopically.

2-Methyl-4-pentyloxazole, 9CI [102586-52-7]
$C_9H_{15}NO$ 153.224
Constit. of French fries. Characterised spectroscopically.

4-Methyl-2-pentyloxazole, 9CI [52713-58-3]
$C_9H_{15}NO$ 153.224
Volatile constit. of French fried potato. Liq. with very sweet, herbal odour. Bp_{22} 88°. n_D^{20} 1.4452.

2,4-Dipropyloxazole [84027-95-2]
$C_9H_{15}NO$ 153.224
Acidic, green, spicy, cheesy odour. Characterised spectroscopically.

2-Butyl-4-propyloxazole, 9CI [84028-04-6]
$C_{10}H_{17}NO$ 167.25Characterised spectroscopically.

4-Butyl-2-propyloxazole, 9CI [84028-01-3]
$C_{10}H_{17}NO$ 167.25Characterised spectroscopically.

2-Pentyl-4-propyloxazole, 9CI [94794-10-2]
$C_{11}H_{19}NO$ 181.277
Sweet, sl. herbal, acidic odour. No phys. props. reported.

4-Pentyl-2-propyloxazole, 9CI [84028-12-6]
$C_{11}H_{19}NO$ 181.277Characterised spectroscopically.

4-Butyl-2-pentyloxazole, 9CI [84028-18-2]
$C_{12}H_{21}NO$ 195.304
Cocoa, sweet, nutty odour. Characterised spectroscopically.

4-Methyl-2-octyloxazole, 9CI [84028-23-9]

$C_{12}H_{21}NO$ 195.304
Waxy, shortening-like, sl. sweet odour. No phys. props. reported.

4-Ethyl-2-hexyloxazole, 9CI [84028-15-9]
$C_{11}H_{19}NO$ 181.277
Fatty, sweet, sl. floral odour. Characterised spectroscopically.

4-Ethyl-2-heptyloxazole, 9CI [84028-22-8]
$C_{12}H_{21}NO$ 195.304
Weak herbal odour. Characterised spectroscopically.

2-Hexyl-4-methyloxazole [84028-07-9]
$C_{10}H_{17}NO$ 167.25
Very sweet, floral, herbal odour. Characterised spectroscopically.

2-Hexyl-4-propyloxazole [84028-21-7]
$C_{12}H_{21}NO$ 195.304
Very fatty, deep-fat fried, little green odour. Characterised spectroscopically.

2-Heptyl-4-methyloxazole [84028-16-0]
$C_{11}H_{19}NO$ 181.277
Sweet, floral odour. Characterised spectroscopically.

Ger. Pat., 1969, 1 915 232; *CA*, **72**, 21679e (*2-Et-4-Me, synth*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, coffee*)
Terentiev, P.B. *et al., Org. Prep. Proced. Int.*, 1974, **6**, 145-147 (*4-Me-2-propyl, 4-Me-2-pentyl, synth*)
Ho, C.-T. *et al., J. Agric. Food Chem.*, 1983, **31**, 180-181; 1384-1386 (*occur, synth, ms*)
Jin, Q.Z. *et al., Perfum. Flavor.*, 1984, **9(4)**, 25-28 (*synth, aroma*)
Carlin, J.T. *et al., J. Agric. Food Chem.*, 1986, **34**, 621-623 (*occur*)
Golovnya, R.V. *et al., J. Chromatogr.*, 1991, **552**, 1-12 (*glc*)
Shenderyuk, V.V. *et al., CA*, **112**, 177182t (*occur, shrimp*)

2,5-Dialkyloxazoles D-108

See also 2,5-Dimethyloxazole, D-862. Odorants/flavourants with potential food uses.

2-Ethyl-5-methyloxazole, 9CI [42463-54-7]
C_6H_9NO 111.143
Constit. of Arabica coffee aroma. Characterised spectroscopically.

5-Ethyl-2-methyloxazole, 9CI [53833-29-7]
C_6H_9NO 111.143
Constit. of Arabica coffee aroma and roasted cashew nuts. Characterised spectroscopically.

2-Methyl-5-propyloxazole, 9CI [80935-99-5]
$C_7H_{11}NO$ 125.17
Constit. of roasted peanut. Sweet, fruity, nutty odour. Characterised spectroscopically.

5-Methyl-2-propyloxazole, 9CI [53833-31-1]
$C_7H_{11}NO$ 125.17
Constit. of Arabica coffee aroma. Characterised spectroscopically.

5-Butyl-2-methyloxazole, 9CI [84027-85-0]
$C_8H_{13}NO$ 139.197Characterised spectroscopically.

5-Butyl-2-ethyloxazole, 9CI [77311-04-7]
$C_9H_{15}NO$ 153.224
Volatile constit. of roasted peanuts. Green, fatty, sweet odour. Characterised spectroscopically.

2-Methyl-5-pentyloxazole [84027-91-8]
$C_9H_{15}NO$ 153.224
Sweet, strong floral, fatty waxy odour. Characterised spectroscopically.

2-Ethyl-5-pentyloxazole [84027-99-6]
$C_{10}H_{17}NO$ 167.25Characterised spectroscopically.

Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, coffee*)
Lee, M.-H. *et al., J. Agric. Food Chem.*, 1981, **29**, 684-686 (*occur, synth, ms*)
Ho, C.-T. *et al., J. Food Sci.*, 1981, **47**, 127-133 (*occur, ms*)
Ho, C.-T. *et al., J. Agric. Food Chem.*, 1983, **31**, 180-181 (*synth, ms*)
Jin, Q.Z. *et al., Perfum. Flavor.*, 1984, **9**, 25-28 (*synth, aroma*)
Jayalekshmy, A. *et al., ACS Symp. Ser.*, 1989, **409**, 355-365 (*occur, ms, cashew nut*)

4,5-Dialkyloxazoles D-109

See also 4,5-Dimethyloxazole, D-863. Odorants/flavourants with potential food use. Mostly not reported in nature.

5-Ethyl-4-methyloxazole, 9CI [29584-92-7]
C_6H_9NO 111.143
Constit. of Arabica coffee and yeast extract aromas.

4-Methyl-5-propyloxazole, 9CI [27744-95-2]
$C_7H_{11}NO$ 125.17
Liq. with vegetable-like, green odour. Bp 150-152°. n_D^{20} 1.4444.

5-Methyl-4-propyloxazole [79886-35-4]
$C_7H_{11}NO$ 125.17
Green, weak bell pepper-like odour. Characterised spectroscopically.

4,5-Diethyloxazole, 9CI [54026-91-4]
$C_7H_{11}NO$ 125.17
Green, vegetable-like odour. Characterised spectroscopically.

4-Ethyl-5-propyloxazole, 9CI [79886-38-7]
$C_8H_{13}NO$ 139.197
Vegetable-like, green odour. Characterised spectroscopically.

5-Ethyl-4-propyloxazole
$C_8H_{13}NO$ 139.197
Celery-like, green odour. Characterised spectroscopically.

4-Butyl-5-methyloxazole, 9CI [79886-39-8]
$C_8H_{13}NO$ 139.197
Bell pepper-like odour. Characterised spectroscopically.

5-Butyl-4-methyloxazole, 9CI [52713-55-0]
$C_8H_{13}NO$ 139.197
Liq. with vegetable-like, green odour. Bp_7 49-51°. n_D^{20} 1.4468.

5-Butyl-4-ethyloxazole, 9CI [79886-40-1]
$C_9H_{15}NO$ 153.224
Vegetable-like, green odour. Characterised spectroscopically.

5-Methyl-4-pentyloxazole [79886-41-2]
$C_9H_{15}NO$ 153.224
Bell pepper-like odour. Characterised spectroscopically.

4-Ethyl-5-pentyloxazole, 9CI [79886-43-4]
$C_{10}H_{17}NO$ 167.25
Constit. of ripe tomato. Vegetable-like, green odour. Characterised spectroscopically.

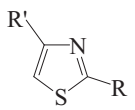
4-Butyl-5-propyloxazole, 9CI [79886-42-3]
$C_{10}H_{17}NO$ 167.25
Bell pepper-like odour. Characterised spectroscopically.

4-Hexyl-5-methyloxazole, 9CI [76162-84-0]
$C_{10}H_{17}NO$ 167.25
Vegetable-like, green odour. Characterised spectroscopically.

5-Hexyl-4-methyloxazole [52713-56-1]
$C_{10}H_{17}NO$ 167.25
Liq. with vegetable-green odour. Bp_8 73-75°. n_D^{20} 1.4480.

Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, coffee*)
Terentiev, P.B. *et al., Org. Prep. Proced. Int.*, 1974, **6**, 145-147 (*synth*)
Ho, C.-T. *et al., J. Agric. Food Chem.*, 1981, **29**, 1306-1308; 1983, **31**, 180-181 (*synth, ms, odour*)
Ho, C.-T. *et al., Lebensm.-Wiss. Technol.*, 1982, **15**, 340-342 (*occur, 4-ethyl-5-pentyl*)
Ames, J.M. *et al., Flavour Fragrance J.*, 1992, **7**, 89-103 (*occur, yeast*)

2,4-Dialkylthiazoles D-110



See also 2,4-Dimethylthiazole, D-908. Maillard prods. present in cooked food volatiles.

2-Isopropyl-4-methylthiazole [15679-13-7]
4-Methyl-2-(1-methylethyl)thiazole, 9CI. FEMA 3555
$C_7H_{11}NS$ 141.237
Fruit flavour intensifier. Present in Indonesian durian fruit (*Durio zibethinus*), cocoa butter/roasted beans, red tomatoes, yeast extract, coriander seed oil and roast meats. Off-flavour component in fortified juice-containing beverages. Liq. with camphorous, nutty odour. d_4^{20} 1.01. Bp_{10} 59-62°. n_D^{20} 1.4989.

4-Isopropyl-2-methylthiazole [32272-52-9]
2-Methyl-4-(1-methylethyl)thiazole, 9CI
$C_7H_{11}NS$ 141.237
Aroma component of yeast extract.

2,4-Diethylthiazole, 9CI [32272-49-4]
$C_7H_{11}NS$ 141.237
Volatile flavour component of coffee aroma and yeast extract.

2-Butyl-4-methylthiazole, 9CI [76572-47-9]
$C_8H_{13}NS$ 155.263

4-Butyl-2-methylthiazole, 9CI [41981-69-5]
$C_8H_{13}NS$ 155.263
Claimed food uses are not well documented.

2-Ethyl-4-propylthiazole, 9CI [41981-67-3]
$C_8H_{13}NS$ 155.263
Claimed food uses are not well documented. Liq. Mp 96° (as picrate). Bp_{15} 97.5-98°.

4-Ethyl-2-propylthiazole, 9CI [41981-68-4]
$C_8H_{13}NS$ 155.263
Claimed food uses are not well documented.

4-Methyl-2-pentylthiazole, 9CI [96693-92-4]
$C_9H_{15}NS$ 169.29

2,4-Dipropylthiazole, 9CI [41981-74-2]
$C_9H_{15}NS$ 169.29
Claimed food uses are not well documented.

2-Isopropyl-4-propylthiazole [87116-69-6]
2-(1-Methylethyl)-4-propylthiazole, 9CI
$C_9H_{15}NS$ 169.29
Component of roast peanut flavour.

4-Ethyl-2-pentylthiazole, 9CI [96693-88-8]
$C_{10}H_{17}NS$ 183.317

2-Butyl-4-propylthiazole, 9CI [96693-89-9]
$C_{10}H_{17}NS$ 183.317
Claimed food uses are not well documented.

4-Ethyl-2-hexylthiazole, 9CI [96693-85-5]
$C_{11}H_{19}NS$ 197.344

2-Pentyl-4-propylthiazole, 9CI [96693-86-6]
$C_{11}H_{19}NS$ 197.344
Claimed food uses are not well documented.

4-Ethyl-2-heptylthiazole, 9CI [96693-84-4]
$C_{12}H_{21}NS$ 211.371

4-Ethyl-2-octylthiazole, 9CI [96693-83-3]
$C_{13}H_{23}NS$ 225.397
Maillard product.

2-Octyl-4-propylthiazole, 9CI [96693-82-2]
$C_{14}H_{25}NS$ 239.424
Claimed food uses are not well documented.

Beraud, J. *et al., Bull. Soc. Chim. Fr.*, 1962, 2072-2074 (*synth*)
Asinger, F. *et al., Annalen*, 1964, **672**, 156-178 (*synth*)
Vincent, E.J. *et al., Bull. Soc. Chim. Fr.*, 1966, 3524-3530 (*pmr*)
Babadjamian, A. *et al., Bull. Soc. Chim. Fr.*, 1968, 4878-4880 (*synth*)
Roussel, C. *et al., Bull. Soc. Chim. Fr.*, 1971, 1087-1092 (*synth*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1973, **21**, 488-490 (*synth, ms*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*occur, coffee*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511-524 (*ms*)
Loser, B. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-70 (*tox*)
Ger. Pat., 1978, 2 804 077; *CA*, **76**, 163587s (*use*)
Ho, C.T. *et al., Lebensm.-Wiss. Technol.*, 1982, **15**, 340-342 (*glc, occur, tomato*)
Ho, C.T. *et al., J. Agric. Food Chem.*, 1983, **31**, 1384-1386 (*synth, ms, occur, peanut*)
Ho, C.T. *et al., J. Food Sci.*, 1983, **48**, 1570-1571 (*synth, props, ms*)
Ho, C.T. *et al., Perfum. Flavor.*, 1984, **9**, 15-18 (*synth, odour*)
Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur*)
Lamparsky, D. *et al., Perfum. Flavor.*, 1988, **13**, 17-25 (*occur, coriander*)
Ames, J.M. *et al., Flavour Fragrance J.*, 1992, **7**, 89-103 (*occur, yeast*)
ACS Symp. Ser., 1995, 147-159 (*occur, yeast extract*)
Weenan, H. *et al., J. Agric. Food Chem.*, 1996, **44**, 3291-3293 (*glc, occur, durian*)
Elmore, J.S. *et al., J. Agric. Food Chem.*, 1997, **45**, 3595-3602 (*occur*)
Swaine, R.L. *et al., Perfum. Flavor.*, 1997, **22**, 57-58; **22(5)**, 60; 62; 64 (*occur*)

2,5-Dialkylthiazoles D-111

See also 2,5-Dimethylthiazole, D-909.
Maillard prods. present in cooked food volatiles.

5-Ethyl-2-methylthiazole, 9CI [19961-52-5]
C_6H_9NS 127.21
Volatile component of coffee aroma, fried chicken, cooked pork and yeast extract. d^{25} 1.02. Mp 124° (as picrate). Bp_{750} 167-168°. n_D^{25} 1.5048.

2,5-Diethylthiazole, 9CI [15729-76-7]
$C_7H_{11}NS$ 141.237
Component of coffee aroma. Liq. d^{25} 1, Mp 104° (as picrate). Bp_{735} 186-188°. n_D^{25} 1.5002.

2,5-Dipropylthiazole, 9CI [41981-73-1]
$C_9H_{15}NS$ 169.29
Claimed food uses are not well documented.

5-Methyl-2-pentylthiazole, 9CI [86290-21-3]
$C_9H_{15}NS$ 169.29
Volatile flavour component of roast beef.

Thiel, M. *et al., Annalen*, 1958, **611**, 121-131 (*2,5-di-Et, synth*)
Chouteau, J. *et al., Bull. Soc. Chim. Fr.*, 1962, 1794-1804 (*ir*)
Poite, M. *et al., Bull. Soc. Chim. Fr.*, 1962, 2078-2085 (*synth*)
Vincent, E.J. *et al., Bull. Soc. Chim. Fr.*, 1966, 3524-3530 (*2,5-di-Et, pmr*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1973, **21**, 488-490 (*synth, ms*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*occur, coffee*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511-524 (*ms*)
Hartman, G.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1030-1033 (*occur, beef*)
Tang, J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1287-1292 (*occur, chicken*)
Ho, C.T. *et al., Perfum. Flavor.*, 1984, **9**, 15-18 (*synth, odour*)
Mottram, D.S. *et al., J. Sci. Food Agric.*, 1985, **36**, 377-382 (*occur, pork*)
Ames, J.M. *et al., ACS Symp. Ser.*, 1995, **564**, 147-159 (*occur, yeast extract*)

4,5-Dialkylthiazoles D-112

See also 4,5-Dimethylthiazole, D-910.
Organoleptic Maillard products.

4-Ethyl-5-methylthiazole, 9CI [52414-91-2]
C_6H_9NS 127.21
Volatile component of coffee and cooked pork. Liq. d^{20} 1.035. Mp 127-129° (as picrate). Bp 169-171°. n_D^{20} 1.5129.

4-Butyl-5-methylthiazole, 9CI [57246-60-3]
$C_8H_{13}NS$ 155.263
Bell-pepper odour; claimed food uses are not well documented.

4-Ethyl-5-propylthiazole, 9CI [57246-61-4]
Bell-pepper odour; claimed food uses are not well documented. Liq. Mp 108° (as picrate). Bp_{15} 82-83°.

4-Butyl-5-ethylthiazole, 9CI [57246-62-5]
$C_9H_{15}NS$ 169.29
Bell-pepper aroma; claimed food uses not well documented.

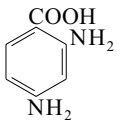
5-Butyl-4-ethylthiazole, 9CI [57246-63-6]
$C_9H_{15}NS$ 169.29
Bell-pepper aroma; claimed food uses not well documented.

4-Butyl-5-propylthiazole, 9CI [57246-59-0]
$C_{10}H_{17}NS$ 183.317
Bell-pepper odour; claimed food uses not well documented.

Metzger, J. *et al., Bull. Soc. Chim. Fr.*, 1953, 702-707 (*synth*)
Asinger, F. *et al., Annalen*, 1957, **610**, 49-56; 1959, **634**, 131-144; 1961, **648**, 83-95 (*synth*)
Haag, A. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*ms*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*occur, coffee*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1976, **24**, 1-3 (*synth, pmr, ms*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511-524 (*ms*)
Mottram, D.S. *et al., J. Sci. Food Agric.*, 1985, **36**, 377-382 (*occur, pork*)

2,4-Diaminobenzoic acid D-113

[611-03-0]
4-Aminoanthranilic acid



$C_7H_8N_2O_2$ 152.152
Mp *ca.* 140. Unstable.

Hydrochloride: [61566-58-3]
Needles. Mp 270° dec.

2-N-*Ac:* [59156-43-3]
$C_9H_{10}N_2O_3$ 194.19
Needles (EtOH). Mp 217°.

4-N-*Ac:* [43134-76-5]
$C_9H_{10}N_2O_3$ 194.19
Needles (EtOH). Mp 207° dec.

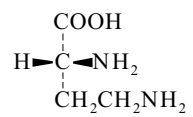
2,4-N-*Di-Ac:* [73748-78-4]
$C_{11}H_{12}N_2O_4$ 236.227
Needles. Mp 261° (248°).

4-N-*(4-Aminobenzoyl):2-Amino-4-(4-aminobenzoylamino)benzoic acid.* ***Carotamine***
$C_{14}H_{13}N_3O_3$ 271.275
Isol. from carrots. Amorph. yellow powder.

Ullmann, F. *et al., Ber.*, 1903, **36**, 1803 (*synth*)
Lesiak, T. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1957, **31**, 1033; *CA*, **52**, 8086 (*synth*)
Franc, J. *et al., J. Chromatogr.*, 1961, **6**, 396 (*glc*)
Stevenson, P.E. *et al., J. Mol. Spectrosc.*, 1965, **15**, 220 (*uv*)
Mori, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4859 (*synth, pmr, ir, derivs*)
Gould, S.J. *et al., J. Antibiot.*, 1988, **41**, 688 (*isol*)
Eldahshan, O.A. *et al., Molecules*, 2002, **7**, 501-506 (*isol, pmr, cmr, Carotamine*)

2,4-Diaminobutanoic acid, 9CI D-114

[305-62-4]



(R)-form

$C_4H_{10}N_2O_2$ 118.135
► EK7769000

(S)-form [1758-80-1]
L-form

Found in free state in seeds of legumes.

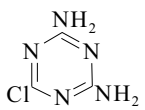
N^4-*Ac:* [1190-46-1] *4-Acetamido-2-aminobutanoic acid*. N-*γ-Acetyldiaminobutyric acid*
$C_6H_{12}N_2O_3$ 160.172
Found in sugar beet. Needles (propanol). Mp 220-222° (208-211°). $[\alpha]_D^{20}$ +43 (c, 0.6 ion 5M HCl).

4-(2-Hydroxypropanoyl): [38710-35-9] *2-Amino-4-[(2-hydroxy-1-oxopropyl)amino]butanoic acid, 9CI. 2-Amino-4-(lactoylamino)butyric acid*
$C_7H_{14}N_2O_4$ 190.199
Isol. from sugarbeet. $[\alpha]_D^{20}$ +12 (c, 5 in H_2O). Stereochem. of lactyl residue not determined.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 586C (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 494A (*nmr*)
Fischer, E. *et al., Ber.*, 1901, **34**, 2900 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1926, **9**, 301 (*synth*)
Paulus, H. *et al., J. Biol. Chem.*, 1964, **239**, 865 (*abs config*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Bell, E.A. *et al., Phytochemistry*, 1966, **5**, 1211 (*occur*)
Hinazumi, F. *et al., Acta Cryst. B*, 1971, **27**, 2152 (*cryst struct*)
Fowden, L. *et al., Phytochemistry*, 1972, **11**, 2271 (*rev, deriv*)
Effenberger, F. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 474 (*synth*)
Solladié-Cavallo, A. *et al., Tet. Lett.*, 1989, **30**, 6011 (*optically pure synth, bibl*)

2,4-Diamino-6-chloro-1,3,5-triazine D-115

[3397-62-4]
6-Chloro-1,3,5-triazine-2,4-diamine, 9CI



$C_3H_4ClN_5$ 145.551
Needles (DMF aq.). Evolves NH_3 on heating, forming polymer.

N-*Et:* [1007-28-9]
$C_5H_8ClN_5$ 173.604
Cryst. (H_2O). Mp 177-179°.

2,4-N-*Di-Et:* [122-34-9] ***Simazine, ANSI, BSI, ISO, WSSA***. *CAT, JMAF. Aquazine. Azotop. Gesatop. Herbatoxol S. Herbazin. Herbex. Hungazin DT. Primatol*†. *Tafazine. Yrodazin. Weedex*
$C_7H_{12}ClN_5$ 201.658
Cryst. Mp 228-229°. pK_a 1.7 (21°,basic).
▶ LD_{50} (rat, orl) >5000 mg/kg. XY5250000

2,2,4-N-*Tri-Et:* [1912-26-1] ***Trietazine, ANSI, BSI, ISO, JMAF***. *Aventox. Bronox. Remtal*
$C_9H_{16}ClN_5$ 229.712
Cryst. solid. Mp 100-101°.
▶ LD_{50} (rat, orl) 594 mg/kg. XY5425000

2,2,4,4-N-*Tetra-Et:* [580-48-3] *2-Chloro-4,6-bis(diethylamino)-1,3,5-triazine. 6-Chloro*-N,N,N′,N′-*tetraethyl-1,3,5-triazine-2,4-diamine, 9CI.* ***Chlorazine, BSI, WSSA***
$C_{11}H_{20}ClN_5$ 257.765
Mp 27°. $Bp_{0.05}$ 104-106°.
▶ LD_{50} (rat, orl) 850 mg/kg. XY5075000

N-*Isopropyl:* [6190-65-4] *6-Chloro*-N-*(1-methylethyl)-1,3,5-triazine-2,4-diamine, 9CI. 2-Amino-4-chloro-6-(isopropylamino)-1,3,5-triazine. Deethyatrazine. Desethylatrazine*
$C_6H_{10}ClN_5$ 187.631
Major soil metab. of Atrazine. Environmental pollutant of soil and water. Mp 135-137°.

N^2-*Et*, N^4-*isopropyl:* See Atrazine in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 850C (*ir*)
Aldrich Library of ^{13}C *and* ^1H *FT NMR Spectra*, 1992, **3**, 419A (*nmr*)
Pearlman, W.M. *et al., J.A.C.S.*, 1948, **70**, 3726-3728 (*N-alkylderivs*)
Thurston, J. *et al., J.A.C.S.*, 1951, **73**, 2981-2983 (*synth*)
Gast, D. *et al., Experientia*, 1955, **11**, 107
Grisley, D.W. *et al., J.O.C.*, 1958, **23**, 1802
Bieling, H. *et al., J. Prakt. Chem.*, 1965, **28**, 513 (*synth*)
Shimakukuro, R.H. *et al., J. Agric. Food Chem.*, 1966, **14**, 392-395 (*N-isopropyl*)
Morimoto, G. *et al., Nippon Kagaku Zasshi*, 1966, **87**, 785; *CA*, **66**, 37197h (*uv*)
Ross, J.A. *et al., Org. Mass Spectrom.*, 1970, **3**, 219 (*ms*)
Leclercq, P.A. *et al., J. Chromatogr.*, 1979, **178**, 193 (*gc, ms*)
Dufek, P. *et al., J. Chromatogr.*, 1979, **178**, 193; 1980, **187**, 341 (*gc, ms, hplc*)
Dangerous Prop. Ind. Mater. Rep., 1987, **7**, 109 (*rev, tox, Simazine*)
Suprock, J.F. *et al., J. Assoc. Off. Anal. Chem.*, 1987, **70**, 1014 (*detn, Simazine*)
Pacakova, V. *et al., J. Chromatogr.*, 1988, **442**, 147 (*hplc, Trietazine*)
IARC Monog., 1991, **53**, 495 (*rev, tox*)
Pesticide Manual, 9th edn., 1991, Nos. 2200; 10740; 12060
Gardyan, C. *et al., Z. Lebensm.-Unters. -Forsch.*, 1991, **192**, 40 (*hplc, Simazine*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A369; A410
Kruger, E.L. *et al., J. Agric. Food Chem.*, 1996, **44**, 1144-1149 (*bibl, Deethylatraxine*)
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1385
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BJP000; CDQ325; TJL500

4,4′-Diaminodibutylamine, 8CI D-116

[4427-76-3]
N-*(4-Aminobutyl)-1,4-butanediamine, 9CI.* sym-*Homospermidine. 1,9-Diamino-5-azanonane*
$H_2NCH_2(CH_2)_3NH(CH_2)_3CH_2NH_2$
$C_8H_{21}N_3$ 159.274
Constit. of the famine food *Santalum album* (sandalwood). Flavouring.

Hydrochloride (1:2):
Mp 283-285° dec.

Hydrochloride (1:3): [189340-78-1]
Cryst. (EtOH aq.).

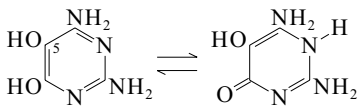
N^1-*(3-Aminopropyl):* [86812-44-4] N^1-*(3-Aminopropyl)homospermidine*
$C_{11}H_{28}N_4$ 216.369

[138656-54-9]

Kuttan, R. *et al., Biochemistry*, 1971, **10**, 361 (*isol, synth*)
Yamamoto, S. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3315 (*isol*)
Samejima, K. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3428 (*Aminopropylhomospermidine*)
Hamana, K. *et al., Can. J. Microbiol.*, 1990, **36**, 567; 1991, **37**, 350 (*Aminopropylhomospermidine*)
Ramaswamy, S. *et al., CA*, 1992, **116**, 55605v (*cryst struct*)
Bergeron, R.J. *et al., J. Med. Chem.*, 1997, **40**, 1475-1494 (*synth, pmr*)

2,4-Diamino-5,6-dihydroxypyrimidine D-117

[60337-65-7]
*2,6-Diamino-5-hydroxy-4(1*H*)-pyrimidinone, 9CI. Divicine*



$C_4H_6N_4O_2$ 142.117
Pale yellow microcryst. Mp 300° dec.

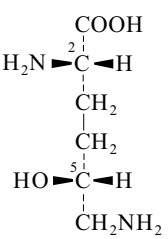
5-O-*Arabinopyranoside:* [165171-52-8]
Charine
$C_9H_{14}N_4O_6$ 274.233
Alkaloid from the unripe fruit of *Momordica charantia* (bitter melon). Needles (MeOH). Mp 180-182°. λ_{max} 239 (no solvent reported).

5-O-*β-D-Glucopyranoside:* [152-93-2]
Vicine†. *Vicioside*
$C_{10}H_{16}N_4O_7$ 304.259
Isol. from *Vicia faba* and other legumes. Mp 243-244° dec. $[\alpha]_D^{26}$ -11.7 (0.2*M* NaOH).

Bendich, A. *et al., Biochim. Biophys. Acta*, 1953, **12**, 462 (*isol, struct*)
Davoll, J. *et al., J.C.S.*, 1956, 2124 (*synth*)
Chesterfield, J.H. *et al., J.C.S.*, 1964, 1001 (*synth*)
Brown, E.G. *et al., Phytochemistry*, 1972, **11**, 3203
Dutta, P.K. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 669 (*isol, pmr, cmr*)
Kunesch, N. *et al., Annalen*, 1994, 1059 (*synth, Vicine*)
El-Gengaihi, S. *et al., Pharmazie*, 1995, **50**, 361-362 (*Charine*)

2,6-Diamino-5-hydroxyhexanoic acid D-118

[504-91-6]
5-Hydroxylysine, 9CI. α,ε-Diamino-δ-hydroxycaproic acid



(2*S*,5*R*)-*form*

$C_6H_{14}N_2O_3$ 162.188
(2*S*,5*R*)-*form* [1190-94-9]
L-erythro-*form*
One of the natural protein-bound amino acids. Occurs free in plant tissues,

e.g. *Medicago sativa* (alfalfa). $[\alpha]_D^{25}$ +17.8 (c, 2 in 6*M* HCl).

β-D-Galactopyranoside: [32448-36-5]
$C_{12}H_{24}N_2O_8$ 324.33
Component of collagen. $[\alpha]_D^{23}$ -1.4 (c, 0.18 in MeOH).

(2*S*,5*S*)-*form* [18899-29-1]
L-threo-*form*. *L*-allo-*form*

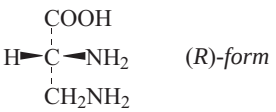
N^6-*Ac:*
Prod. by *Beta vulgaris* (sugar beet).

[6000-08-4, 18899-30-4, 18899-31-5, 78088-29-6]

Sheehan, J.C. *et al., J.A.C.S.*, 1950, **72**, 2472-2474 (*synth*)
Biochem. Prep., 1961, **8**, 55-62; 62-69 (*isol, resoln, purifn*)
Wilding, M.D. *et al., Phytochemistry*, 1962, **1**, 263-265 (*isol*)
Lindstedt, S. *et al., J.O.C.*, 1963, **28**, 251-252 (*abs config*)
Kakimoto, Y. *et al., J. Biol. Chem.*, 1970, **245**, 5751-5758 (*isol, galactoside*)
Rohr, B. *et al., Synlett*, 1999, 1139-1141 (*synth*)
Van den Nieuwendijk, A.M. *et al., Eur. J. Org. Chem.*, 2000, 3683-3691 (*synth*)
Adamczyk, M. *et al., Synth. Commun.*, 2000, **30**, 3281-3290 (*β-D-galactosyl*)
Allevi, P. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 3151-3160 (*2S,5R-form, 2S,5S-form, synth, pmr, cmr*)

2,3-Diaminopropanoic acid D-119

[515-94-6]
3-Aminoalanine, 9CI



(*R*)-*form*

$C_3H_8N_2O_2$ 104.108

(*R*)-*form*
D-form

Hydrochloride (1:2):
$[\alpha]_D^{25}$ -25.2 (1*N* HCl).

N,N′-*Dibenzoyl:*
$C_{17}H_{16}N_2O_4$ 312.324
Mp 156-157°. $[\alpha]_D^{16}$ -23.9 (MeOH).

N,N′-*Dibenzoyl, Me ester:*
$C_{18}H_{18}N_2O_4$ 326.351
Mp 153-154°. $[\alpha]_D^{16}$ -21.58 (MeOH).

N,N′-*Dibenzoyl, Et ester:*
$C_{19}H_{20}N_2O_4$ 340.378
Mp 151°. $[\alpha]_D^{18}$ -13.3 (EtOH).

N^3-*Me:* [20790-80-1]
$C_4H_{10}N_2O_2$ 118.135
Mp 168°. $[\alpha]_D^{20}$ -35 (c, 1.2 in 5*M* HCl).

(*S*)-*form* [4033-39-0] *L-form*
Mp 237° dec.

Hydrochloride (1:2): [28843-13-2]
Mp 237° dec. $[\alpha]_D^{25}$ +25.2 (1*M* HCl).

N^3-*Ac:* [20584-70-7] *3-Acetamido-2-aminopropanoic acid. β-Acetamidoalanine*
$C_5H_{10}N_2O_3$ 146.146
$[\alpha]_D^{20}$ -81 (c, 8 in H_2O). $[\alpha]_D^{20}$ -33 (c, 4 in 6*M* HCl).

N^2-tert-*Butyloxycarbonyl:*
$C_8H_{16}N_2O_4$ 204.225
Mp 202° (197-199°).

N^3-*Me:* [15920-93-1] *2-Amino-3-(methylamino)propanoic acid*
Cryst. (as hydrochloride). Mp 168° dec. (hydrochloride). $[\alpha]_D^{25}$ +35 (c, 1.15 in 5*M* HCl).

▶ Toxic, exp. carcinogen.

N^3-*Nitro:* [58130-89-5] *(3-Nitroamino)alanine, 9CI. 2-Amino-3-nitraminopropionic acid*
$C_3H_7N_3O_4$ 149.106
Isol. from *Agaricus silvaticus* (red staining mushroom). Cryst. (EtOH aq.).

(±)-*form* [6018-54-8]
Mp 110-120° (softens at 97°). pK_{a2} 6.79; pK_{a3} 9.51 (25°, 0.1*M* KCl). Hygroscopic. Absorbs CO_2.

Hydrochloride: [54897-59-5]
Cryst. (EtOH aq.). Mp 232° dec.

Hydrobromide: [18635-45-5]
Cryst. (H_2O). Mp 235° dec.

Oxalate:
Cryst. + $2H_2O$. Mp 175-178° dec.

Tc complex: See 2,3-Diaminopropanoic acid technetium complex in *The Combined Chemical Dictionary.*

Me ester:
$C_4H_{10}N_2O_2$ 118.135
Solid (as dihydrochloride). Mp 172° (dihydrochloride).

Et ester:
$C_5H_{12}N_2O_2$ 132.162
Mp 142-144° dec.

N,N′-*Di-Ac:*
$C_7H_{12}N_2O_4$ 188.183
Mp 181-182°.

(ξ)-*form*

Nitrile, N^2-*α-L-arabinosyl,* N^3-*β-D-glucopyranoside:* [26401-22-9] *2-(Arabinosylamino)-3-(glucosylamino)propanenitrile*
$C_{14}H_{25}N_3O_9$ 379.366
Constit. of the seeds of *Lathyrus sativus* (chickling pea). Pale yellow cryst. + $1H_2O$. Tentative struct. Config. not known.

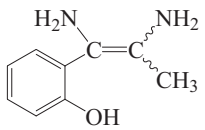
N^3-*Benzoyl:* [116480-11-6] *3-(Benzoylamino)alanine. 2-Amino-3-(benzoylamino)propanoic acid*
$C_{10}H_{12}N_2O_3$ 208.216
Sol. H_2O.

[1482-97-9, 6018-55-9, 61049-68-1, 69531-11-9]

Karrer, P. *et al., Helv. Chim. Acta*, 1926, **9**, 314 (*synth*)
Schneider, F. *et al., Annalen*, 1937, **529**, 1 (*abs config*)
Birnbaum, S.M. *et al., J. Biol. Chem.*, 1952, **198**, 335 (*resoln*)
Hellmann, H. *et al., Chem. Ber.*, 1954, **87**, 1690 (*synth*)
Bohme, M. *et al., Chem. Ber.*, 1959, **92**, 1258 (*synth*)
Gmelin, R. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1959, **314**, 28 (*isol*)
Vega, A. *et al., Phytochemistry*, 1967, **6**, 759; 1968, **77**, 1885 (N^3-*Me*)
Rukmini, C. *et al., Indian J. Chem.*, 1969, **7**, 1062 (*nitrile diglycoside*)
Chilton, W.S. *et al., Phytochemistry*, 1975, **14**, 2291 (*derivs*)
Evans, C.S. *et al., Phytochemistry*, 1979, **18**, 1807 (*isol*)
Nilsson, L. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 929 (*synth, pmr, ms*)
van der Baan, J.L. *et al., J.C.S. Perkin 1*, 1984, 2809 (*biosynth*)
Japan. Pat., 1988, 88 60 959; *CA*, **109**, 134966 (*3-(Benzoylamino)alanine*)
Merck Index, 11th edn., 1989, 2962
Kucharczyk, N. *et al., Synth. Commun.*, 1989, **19**, 1603 (N^2-*tert-butyloxycarbonyl*)
Andruszkiewicz, R. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1995, **69**, 1615 (*rev, occur, derivs*)
Jones, P. *et al., J. Med. Chem.*, 1998, **41**, 3062-3077 (*Me ester, synth, ir, pmr, cmr*)

2-(1,2-Diamino-1-propenyl)-phenol, 9CI D-120

[173559-57-4]
1,2-Diamino-1-(2-hydroxyphenyl)propene



$C_9H_{12}N_2O$ 164.207
Present in shrimp shell (*Pandalus jordani*) waste. Antioxidant. Characterised spectroscopically.

Seymour, T.A. *et al., J. Agric. Food Chem.*, 1996, **44**, 682-685 (*isol, ms, uv, pmr*)

Diammonium sulfite, 9CI D-121

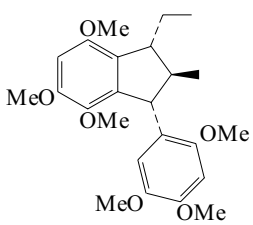
[10196-04-0]
Ammonium sulfite
$(NH_4)_2SO_3$
$H_8N_2O_3S$ 116.141
Food Additive listed in the EAFUS Food Additive Database (Jan 2001). V. deliquescent cryst. Subl. 150.

Monohydrate: [7783-11-1]
Efflorescent cryst. Sol. H_2O; insol, EtOH, Me_2CO.

Divers, E. *et al., J.C.S.*, 1900, **77**, 336-340 (*synth*)
Miller, F.A. *et al., Spectrochim. Acta A*, 1960, **16**, 135-235 (*ir*)
Durand, J. *et al., Acta Cryst. B*, 1977, **33**, 1414-1417 (*cryst struct, monohydrate*)
Cooper, D. *et al., Eur. J. Solid State Inorg. Chem.*, 1989, **26**, 129-136 (*synth, ir, cryst struct*)
Degen, I.A. *et al., Spectrochim. Acta A*, 1993, **49**, 859-887 (*Raman*)

Diasarone 2 D-122

[80434-33-9]
1-Ethyl-2,3-dihydro-4,5,7-trimethoxy-2-methyl-3-(2,4,5-trimethoxyphenyl)-1H-indene, 9CI. γ-Diasarone



$C_{24}H_{32}O_6$ 416.513
Isol. from rhizomes of *Acorus calamus* (sweet flag). Prisms. Mp 99-100° (84°).

[101910-59-2, 130746-43-9, 137490-15-4]

Lemini, C. *et al., Org. Prep. Proced. Int.*, 1981, **13**, 374 (*synth*)

Bohlmann, F. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1982, **315**, 474 (*struct*)
Saxena, D.B. *et al., Phytochemistry*, 1986, **25**, 553 (*isol, struct, ir, pmr, cmr*)
Lemini, C. *et al., Acta Cryst. C*, 1990, **46**, 1542 (*cryst struct*)
Al-Farhan, E. *et al., J. Chem. Res., Synop.*, 1992, 36 (*synth, struct, pmr*)

Diazenedicarboxylic acid, 9CI D-123

[504-89-2]
Azoformic acid. Azodicarboxylic acid. Azodiformic acid. $\Delta^{2,2'}$-Bicarbamic acid. Azobisformic acid

HOOCN=NCOOH

$C_2H_2N_2O_4$ 118.049

Free acid unknown. Known in the form of unstable salts and stable esters.

Diamide: [123-77-3] *Azoformamide. Azodicarbonamide. Azodicarboxamide. Diazenedicarboxamide. AZM 2S. Azobis CA 110B. Azobis CA 51C. Azocel. Azoform A. Azoplastone. Celogen AZ. Evipor. Genitron EPC. Paramid K1. Vinyfor*

$C_2H_4N_4O_2$ 116.079

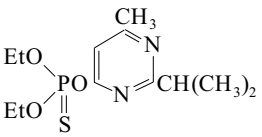
Bleaching agent for flour. Orange cryst. Sol. hot H_2O. Mp 225° (180°).

► LQ1040000

Picard, J.P. *et al., Can. J. Chem.*, 1951, **29**, 223 (*amide*)
Moriarty, R.M. *et al., Synth. Commun.*, 1987, **17**, 409 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 220-222 (*amide*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1412; 2278
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 99
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ASM270; ASM300; DIT300; DQH509

Diazinon, ANSI, BAN, BSI, ISO, JMAF D-124

[333-41-5]
O,O-*Diethyl* O-*[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] phosphorothioate, 9CI.* O,O′-*Diethyl 2-isopropyl-6-methyl-4-pyrimidinyl phosphorothioate.* ***Dimpylate, INN.*** *Basudin. Diazitol. Spertacide. Many other names*



$C_{12}H_{21}N_2O_3PS$ 304.349

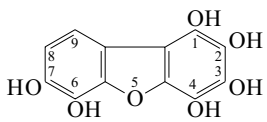
Nonsystemic insecticide for rice and fruit trees. Cholinesterase inhibitor. Used against animal ectoparasites. Liq. d^{20} 1.12. $Bp_{0.002}$ 83-84°. Log P 3.5 (calc). Slowly dec. by H_2O and dil. acids. Component of Neocidol.

► OES: long-term 0.1 mg m^{-3}; short-term 0.3 mg m^{-3} (Sk). Skin and severe eye irritant. Fatal human dose *ca*. 90-444 mg/kg. LD_{50} (rat, orl) 66 mg/kg. LD_{50} (rat, skn) 180 mg/kg. TF3325000

Gasser, R. *et al., Z. Naturforsch., B*, 1953, **8**, 225-232 (*rev, use*)
Gysin, H. *et al., Chimia*, 1954, **8**, 205-210; 221-228 (*rev*)
Shvetsova-Shilovskaya, K.D. *et al., Zh. Obshch. Khim.*, 1956, **26**, 808-810; *CA*, **50**, 14769 (*synth*)
Mortland, M.M. *et al., J. Agric. Food Chem.*, 1967, **15**, 163 (*uv, complexes*)
Keith, L.H. *et al., J. Assoc. Off. Anal. Chem.*, 1968, **51**, 1063-1094 (*pmr*)
Ross, R.T. *et al., Anal. Chim. Acta*, 1970, **52**, 139-141 (*P-31 nmr*)
Pardue, J. *et al., J. Agric. Food Chem.*, 1970, **18**, 405-408 (*metab, ir, ms, glc*)
Gore, R.C. *et al., J. Assoc. Off. Anal. Chem.*, 1971, **54**, 1040-1082 (*ir, uv*)
Stan, H.-J. *et al., Fresenius' Z. Anal. Chem.*, 1977, **287**, 271-285 (*glc, ms*)
Stan, H.-J. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 483-492 (*ms*)
Stan, H.-J. *et al., J. Chromatogr.*, 1983, **279**, 173-187 (*glc*)
Hummel, S.V. *et al., Org. Mass Spectrom.*, 1986, **21**, 785-791 (*ms*)
Dangerous Prop. Ind. Mater. Rep., 1987, **7**, 36-43 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2568
Miles, C.J. *et al., J. Agric. Food Chem.*, 1990, **38**, 986-989 (*glc*)
Res. Discl., 1990, **310**, 165 (*synth*)
Liao, W. *et al., J. Assoc. Off. Anal. Chem.*, 1991, **74**, 554-565 (*glc-ms*)
Pesticide Manual, 9th edn., 1991, No. 4030
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A131
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1125
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1049
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DCM750

1,2,3,4,6,7-Dibenzofuranhexol D-125

1,2,3,4,6,7-Hexahydroxydibenzofuran



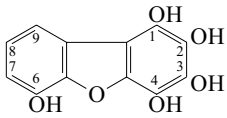
$C_{12}H_8O_7$ 264.191

1,3,4,6-Tetra-Me ether: [167278-45-7] *1,3,4,6-Tetramethoxy-2,7-dibenzofurandiol. 2,7-Dihydroxy-1,3,4,6-tetramethoxydibenzofuran.* ***7-Hydroxy-6-methoxy-α-pyrufuran***
$C_{16}H_{16}O_7$ 320.298
Constit. of the sapwood of *Mespilus germanica* (European medlar). λ_{max} 238 (ε 21380); 267 (ε 15800); 295 (ε 16300) (MeOH) (Berdy). λ_{max} 235 ; 278 ; 316 (MeOH-NAOH) (Berdy).

Kokubun, T. *et al., Phytochemistry*, 1995, **39**, 1039 (*isol, uv, pmr, cmr, ms*)

1,2,3,4,6-Dibenzofuranpentol D-126

1,2,3,4,6-Pentahydroxydibenzofuran



$C_{12}H_8O_6$ 248.192

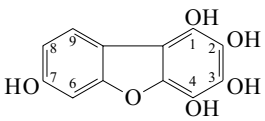
1,3,4-Tri-Me ether: [167278-43-5] *1,3,4-Trimethoxy-2,6-dibenzofurandiol. 2,6-Dihydroxy-1,3,4-trimethoxydibenzofuran.* ***6-Hydroxy-α-pyrufuran***
$C_{15}H_{14}O_6$ 290.272
Constit. of the sapwood of *Mespilus germanica* (European medlar). λ_{max} 238 (ε 14790); 268 (ε 12300); 286 (ε 10715); 310 (ε 4073); 321 (ε 4570) (MeOH) (Berdy). λ_{max} 244 ; 340 (MeOH-NaOH) (Berdy).

1,3,4,6-Tetra-Me ether: [167278-44-6] *1,3,4,6-Tetramethoxy-2-dibenzofuranol. 2-Hydroxy-1,3,4,6-tetramethoxydibenzofuran.* ***6-Methoxy-α-pyrufuran***
$C_{16}H_{16}O_6$ 304.299
Constit. of the sapwood of *Mespilus germanica* (European medlar). λ_{max} 262 (ε 9900); 285 (ε 8800); 306 (ε 5120); 318 (ε 4990) (MeOH) (Berdy). λ_{max} 234 ; 286 ; 322 (MeOH-NaOH) (Berdy).

Kokubun, T. *et al., Phytochemistry*, 1995, **39**, 1039 (*isol, uv, pmr, cmr, ms*)

1,2,3,4,7-Dibenzofuranpentol D-127

1,2,3,4,7-Pentahydroxydibenzofuran



$C_{12}H_8O_6$ 248.192

1,3,4-Tri-Me ether: [93973-18-3] *2,7-Dihydroxy-1,3,4-trimethoxydibenzofuran.* ***γ-Pyrufuran***
$C_{15}H_{14}O_6$ 290.272
Constit. of *Pyrus communis* (pear) infected with *Chondrostereum purpureum*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 210 (ε 25800); 227 (ε 27900); 262 (ε 15500); 297 (ε 15800) (EtOH) (Berdy).

Kemp, M.S. *et al., J.C.S. Perkin 1*, 1984, 1441

2,3,4,6,7-Dibenzofuranpentol D-128

2,3,4,6,7-Pentahydroxydibenzofuran

$C_{12}H_8O_6$ 248.192

3,4,6-Tri-Me ether: [93973-22-9] *2,7-Trihydroxy-3,4,6-trimethoxydibenzofuran.* ***α-Cotonefuran***
$C_{15}H_{14}O_6$ 290.272
Constit. of *Mespilus germanica* (European medlar). Cryst. (EtOAc/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 150-151°. λ_{max} 221 (ε 37153); 264 (ε 17782); 304 (ε 16596) (MeOH) (Berdy). λ_{max} 226 (ε 35200); 266 (ε 17000); 306 (ε 15300) (EtOH) (Berdy). λ_{max} 273 ; 330 (MeOH-NAOH) (Berdy).

3,4,7-Tri-Me ether: [161748-49-8] *2,6-Dihydroxy-3,4,7-trimethoxydibenzofuran.* ***ϵ-Cotonefuran***

$C_{15}H_{14}O_6$ 290.272

2,3,4,6-Tetra-Me ether: [161748-46-5] *7-Hydroxy-2,3,4,6-tetramethoxydibenzofuran.* ***β-Cotonefuran***

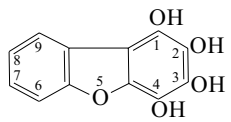
$C_{16}H_{16}O_6$ 304.299

λ_{max} 224 (ϵ 15500); 264 (ϵ 7585); 304 (ϵ 7244) (MeOH) (Berdy). λ_{max} 268 ; 320 (MeOH-NAOH) (Berdy).

Burden, R.S. *et al., J.C.S. Perkin 1*, 1984, 1445
Kokubun, T. *et al., Phytochemistry*, 1995, **38**, 57; **39**, 1033 (*isol, pmr, cmr*)

1,2,3,4-Dibenzofurantetrol D-129

1,2,3,4-Tetrahydroxydibenzofuran



$C_{12}H_8O_5$ 232.192

1,2,4-Tri-Me ether: [88256-04-6] *1,2,4-Trimethoxy-3-dibenzofuranol, 9CI.* ***β-Pyrufuran***

$C_{15}H_{14}O_5$ 274.273

Phytoalexin from *Pyrus communis* (pear). Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 217 (ϵ 32500); 227 (ϵ 31000); 261 (ϵ 10500); 289 (ϵ 15200) (EtOH) (Berdy).

1,3,4-Tri-Me ether: [88256-05-7] *1,3,4-Trimethoxy-2-dibenzofuranol, 9CI.* ***α-Pyrufuran***

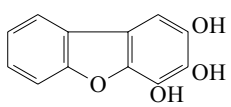
$C_{15}H_{14}O_5$ 274.273

Phytoalexin from *Pyrus communis* (pear). Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 224 (ϵ 27700); 259 (ϵ 11700); 287 (ϵ 17000) (EtOH) (Berdy).

Kemp, M.S. *et al., J.C.S. Perkin 1*, 1983, 2267 (*isol, struct, synth*)
Carvalho, C.F. *et al., Aust. J. Chem.*, 1985, **38**, 777 (*synth*)

2,3,4-Dibenzofurantriol D-130

2,3,4-Trihydroxydibenzofuran



$C_{12}H_8O_4$ 216.193

2,4-Di-Me ether: [97218-06-9] *2,4-Dimethoxy-3-dibenzofuranol, 9CI. 3-Hydroxy-2,4-dimethoxydibenzofuran.* ***Eriobofuran***

$C_{14}H_{12}O_4$ 244.246

Phytoalexin from the leaves of *Eriobotrya japonica* (loquat). Cryst. Mp 157-158°. λ_{max} 260 ; 294 ; 302 (MeOH) (Berdy). λ_{max} 333 (MeOH-NaOH) (Berdy).

Miyakado, M. *et al., Nippon Noyaku Gakkaishi*, 1985, **10**, 101; *CA*, **103**, 66221z (*Eriobofuran*)

Dibenzoyl peroxide, 9CI D-131

[94-36-0]

Benzoyl peroxide, USAN. *Benzoyl superoxide. Benoxyl. Benzac. Eloxyl. Persadox. NSC 675. Many other names*

PhCO-O-O-OCPh

$C_{14}H_{10}O_4$ 242.231

Added to bread and cheese as bleaching agent. Prisms. Mp 106-108° dec. Component of Benzamycin and Vanoxide.

▶ Explodes on heating. Can explode spontaneously when dry. Eye, skin, and respiratory tract irritant. Can cause contact dermatitis. Exp. skin tumour promoter. OES: long-term 5 mg m^{-3}. DM8576200

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 315B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 331B (*ir*)
Aldrich Library of NMR Spectra, **7**, 49B (*pmr*)
Gambarjan, S. *et al., Ber.*, 1909, **42**, 4003 (*synth*)
Hey, D.H. *et al., J.C.S.*, 1948, 2213 (*synth*)
Cadogan, J.I.G. *et al., J.C.S.*, 1959, 2844 (*synth*)
Sax, M. *et al., Acta Cryst.*, 1967, **22**, 281 (*cryst struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 196 (*use*)
Food Chemicals Codex, 2nd Ed., 1972, **2**, 82 (*anal*)
Burguera, J.L. *et al., Talanta*, 1979, **26**, 795 (*use*)
Aganov, A.V. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1982, 271; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1982, 247 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BDS000
Hill, C.L. *et al., Inorg. Chem.*, 1989, **28**, 2511 (*uv*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1082
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 256-259
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 3380
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 109
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 387
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDS000

Dibenzyl disulfide D-132

[150-60-7]

Bis(phenylmethyl) disulfide, 9CI. Benzyl disulfide, 8CI. FEMA 3617

$PhCH_2$-S-S-CH_2Ph

$C_{14}H_{14}S_2$ 246.397

Flavouring ingredient. Pale yellow leaflets (EtOH) with burnt caramel odour. Mp 71-72°. Exposure to sunlight causes conversion to a second form, Mp 69-70° λ_{max} 239 (ϵ 9200); 279 (ϵ 340) (MeOH).

▶ Skin and eye irritant. LD_{50} (rat, orl) 3780 mg/kg. JO1750000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1184D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 445A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1104C (*ir*)
Cumper, C.W.N. *et al., J.C.S.*, 1965, 5323 (*synth*)
Bowie, J.H. *et al., J.C.S.(B)*, 1966, 946 (*ms*)
Voronkov, M.G. *et al., Zh. Strukt. Khim.*, 1968, **9**, 627 (*pmr*)
Reiter, G.F. *et al., J. Appl. Phys.*, 1970, **41**, 1368 (*uv*)
Srinivasan, R. *et al., Acta Cryst. B*, 1972, **28**, 2615 (*cryst struct*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Subrahmanyan, B. *et al., Chem. Age India*, 1975, **26**, 333 (*synth, use*)
Meshram, H.M. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 232 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 59
Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **113**, 499-502 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 267
Benevides, P.J.C. *et al., Phytochemistry*, 2001, **57**, 743-747 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXH200

Dibenzyl ether D-133

[103-50-4]

1,1'-[Oxybis(methylene)]bisbenzene, 9CI. Benzyl ether, 8CI. FEMA 2371

$PhCH_2OCH_2Ph$

$C_{14}H_{14}O$ 198.264

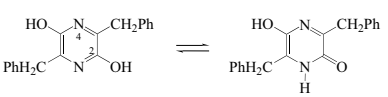
Flavouring ingredient. Insol. H_2O, misc. EtOH, Et_2O. d^{16} 1.06 d^{20} 1.04. Mp 3-4°. Bp 298° Bp_{22} 182-183°. n_D^{20} 1.5610.

▶ Fl. p. 135°. Explodes with $AlCl_2H$ diethyl etherate. Eye and skin irritant. LD_{50} (rat, orl) 2500 mg/kg. DQ6125000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1059A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 214B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 991D (*ir*)
McKillop, A. *et al., Tetrahedron*, 1974, **30**, 2467-2475 (*synth*)
Egorochkin, A.N. *et al., Zh. Obshch. Khim.*, 1974, **44**, 1062-1068 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 703 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 155
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 806-807
Nishiyama, T. *et al., Can. J. Chem.*, 1999, **77**, 258-262 (*synth, pmr, cmr, ms*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 3395
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEO250

3,6-Dibenzyl-2,5-dihydroxypyrazine D-134

3,6-Bis(phenylmethyl)-2,5-pyrazinediol. 3,6-Dibenzyl-5-hydroxy-2(1H)-pyrazinone



$C_{18}H_{16}N_2O_2$ 292.337

Mono-Me ether: [132213-65-1] *5-Methoxy-3,6-bis(phenylmethyl)-2(1H)-pyrazinone, 9CI. 2,5-Dibenzyl-3-hydroxy-6-methoxypyrazine*

$C_{19}H_{18}N_2O_2$ 306.363
Isol. from fruiting bodies of the mushroom *Albatrellus confluens* (edibility unknown). Needles. Mp 159-161°.

2-Me ether, N^4-oxide: [117333-12-7] *5-Methoxy-3,6-bis(phenylmethyl)-2(1H)-pyrazinone 4-oxide, 9CI. 2,5-Dibenzyl-3-hydroxy-6-methoxypyrazine 1-oxide.* ***Emeheterone***
$C_{19}H_{18}N_2O_3$ 322.363
Needles (C_6H_6). Sol. MeOH, $CHCl_3$. Mp 215-217°. Struct. revised in 1990 λ_{max} 228 (ϵ 28200); 276 (ϵ 7000); 352 (ϵ 9800) (MeOH) (Berdy).

Kawahara, N. *et al., Phytochemistry*, 1988, **27**, 3022 (*isol, uv, ir, pmr, cmr, ms, Emeheterone*)
Ohta, A. *et al., Heterocycles*, 1990, **31**, 1655 (*synth, struct, Emeheterone*)
Kawagishi, H. *et al., Phytochemistry*, 1996, **42**, 547 (*isol, pmr, cmr, cryst struct, Me ether*)

1,1-Dibromo-1-chloro-2-propanone, 9CI, 8CI D-135

[30957-55-2]
1,1-Dibromo-1-chloroacetone
$H_3CCOCClBr_2$
$C_3H_3Br_2ClO$ 250.317
Minor component of the essential oil of the edible Hawaiian red alga (*Asparagopsis taxiformis*). Liq. Bp 164-165° Bp_1 41-42°. n_D^{20} 1.5370.

► Lachrymator.

Barrett, G.C. *et al., J.C.S.(C)*, 1971, 279 (*synth, ir*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*synth, pmr, ms, glc*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

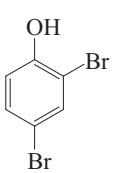
1,1-Dibromo-3-iodo-2-propanone, 9CI D-136

[59227-99-5]
1,1-Dibromo-3-iodoacetone
$Br_2CHCOCH_2I$
$C_3H_3Br_2IO$ 341.769
Minor component of the essential oil of the edible Hawaiian red algae, *Asparagopsis taxiformis* and *Asparagopsis armata*.

Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol, glc, ms*)
McConnell, O. *et al., Phytochemistry*, 1977, **16**, 367 (*isol, glc, ms*)

2,4-Dibromophenol, 9CI, 8CI D-137

[615-58-7]



$C_6H_4Br_2O$ 251.905
Commonly found in molluscs and crustaceans. Mp 40°. Bp_{11} 154°. pK_a 7.79 (25°).

► LD_{50} (mus, orl) 282 mg/kg. SK8010000

Ac: [36914-79-1]
$C_8H_6Br_2O_2$ 293.942
Mp 36°.

Benzoyl:
$C_{13}H_8Br_2O_2$ 356.013
Mp 97.5°.

Me ether: [21702-84-1] *2,4-Dibromo-1-methoxybenzene. 2,4-Dibromoanisole*
$C_7H_6Br_2O$ 265.932
Mp 61.5°. Bp 272°.

Et ether: [38751-57-4] *2,4-Dibromo-1-ethoxybenzene. 2,4-Dibromophenetole*
$C_8H_8Br_2O$ 279.959
Mp 53.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1090B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 197A; 276A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 978C; 1026C (*ir*)
Hashimoto, T. *et al., Yakugaku Zasshi*, 1960, **80**, 1399; *CA*, **55**, 5393 (*synth*)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2059 (*uv*)
Rowbotham, J.B. *et al., Can. J. Chem.*, 1974, **52**, 3037 (*pmr*)
Tashiro, M. *et al., Org. Prep. Proced. Int.*, 1974, **6**, 107 (*synth*)
Higa, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1980, **65**, 525-530 (*isol*)
Kajigaeshi, S. *et al., J.C.S. Perkin 1*, 1990, 897 (*Me ether, synth*)
Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)
Flodin, C. *et al., Phytochemistry*, 2000, **53**, 77-80 (*isol*)

2,6-Dibromophenol, 9CI, 8CI D-138

[608-33-3]
$C_6H_4Br_2O$ 251.905
Important flavour component of marine fish, molluses and crustaceans. Needles (H_2O). Sol. EtOH, Et_2O. Mp 56-57°. Bp_{21} 162°. pK_a 6.67 (25°). Sublimes λ_{max} 279 (ϵ 2180); 286 (ϵ 2130) (EtOH) (Berdy). λ_{max} 305 (EtOH/NaOH) (Berdy).

Ac: [28165-72-2]
$C_8H_6Br_2O_2$ 293.942
Mp 46°.

Benzoyl:
$C_{13}H_8Br_2O_2$ 356.013
Mp 68°.

Me ether:1,3-Dibromo-2-methoxybenzene. 2,6-Dibromoanisole
$C_7H_6Br_2O$ 265.932
Mp 13°. Bp_{34} 143-145°.

Et ether:1,3-Dibromo-2-ethoxybenzene. 2,6-Dibromophenetole
$C_8H_8Br_2O$ 279.959
Mp 40.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1083C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 261A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1016D (*ir*)
Pope, F.G. *et al., J.C.S.*, 1912, **101**, 1826 (*synth*)
Ashworth, R.B. *et al., Science (Washington, D.C.)*, 1967, **155**, 1558 (*isol*)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2509 (*uv*)
Dwivedi, B.K. *et al., Indian J. Pure Appl. Phys.*, 1974, **12**, 597 (*ir*)
Tashiro, M. *et al., Org. Prep. Proced. Int.*, 1975, **7**, 189 (*synth*)
Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)
Whitfield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405 (*occur*)

Dibromopropanedioic acid, 9CI D-139

[595-45-9]
Dibromomalonic acid
$Br_2C(COOH)_2$
$C_3H_2Br_2O_4$ 261.854
Needles or prisms. Sol. H_2O, EtOH, Et_2O; spar. sol. C_6H_6, petrol. Mp 136-137° (130-131°).

Di-Me ester: [37167-59-2]
$C_5H_6Br_2O_4$ 289.908
Needles. Mod. sol. EtOH. Mp 67° (64°).

Me-Et ester: [107607-10-3]
$C_6H_8Br_2O_4$ 303.935
Liq. Bp_2 108°.

Di-Et ester: [631-22-1]
$C_7H_{10}Br_2O_4$ 317.962
Bp_4 108-110°.

Dichloride: [74539-43-8]
$C_3Br_2Cl_2O_2$ 298.745
Bp_{15} 75-77°.

Diamide: [73003-80-2]
$C_3H_4Br_2N_2O_2$ 259.885
Needles. Spar. sol. EtOH, hot H_2O. Mp 200° (206°) dec.

Nitrile-amide: [10222-01-2] *2,2-Dibromo-2-cyanoacetamide, 9CI*
$C_3H_2Br_2N_2O$ 241.87
Antimicrobial agent used in sugar mills. Cryst. (C_6H_6). Mp 126°.

Dinitrile: [1885-23-0] *Dibromopropanedinitrile. Dibromomalononitrile. Dibromodicyanomethane*
$C_3Br_2N_2$ 223.854
Oil. Mp 3°. Bp_{11} 49.2°. Dec. on standing.

Willstätter, R. *et al., Ber.*, 1902, **35**, 1374 (*synth*)
Prüsse, A. *et al., Annalen*, 1918, **416**, 233 (*synth*)
Gupta, B.M. *et al., J.C.S.*, 1922, **121**, 1896-1904 (*amide-nitrile*)
Ott, E. *et al., Ber.*, 1937, **70**, 1829 (*deriv*)
Teichmann, B. *et al., Z. Chem.*, 1965, **5**, 106 (*synth*)
van Haverbeke, L. *et al., Bull. Soc. Chim. Belg.*, 1973, **82**, 133 (*nitrile, synth*)
Van der Wolf, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1977, **96**, 72 (*di-Et ester, synth*)
Beelitz, K. *et al., Z. Naturforsch., B*, 1978, **33**, 417 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 169 (*use*)
Freeman, F. *et al., Synthesis*, 1981, 925 (*rev, nitrile*)
Prosyanik, A.V. *et al., Khim. Geterotsikl. Soedin.*, 1986, 525; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1986, 431 (*esters, synth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1811 (*di-Et ester, use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 807-808 (*amide-nitrile*)

1,1-Dibromo-2-propanone, 9CI D-140

[867-54-9]
1,1-Dibromoacetone
$H_3CCOCHBr_2$
$C_3H_4Br_2O$ 215.872
Minor component of the essential oil of the edible Hawaiian red alga *Asparagopsis*

taxiformis and of *Falkenbergia rufolanosa*. Liq. Bp_{13} 55-57°. n_D^{25} 1.5237. pK_a 11.9 (25°, H_2O).

Hughes, E.D. *et al., J.C.S.*, 1931, 3318 (*synth*)
Rappe, C. *et al., Ark. Kemi*, 1964, **21**, 503; *CA*, **59**, 431b (*synth, pmr, ir*)
Takahashi, K. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 963 (*pmr*)
Burreson, B.J. *et al., J. Agric. Food Chem.*, 1976, **24**, 856 (*isol, glc*)
Combaut, G. *et al., Phytochemistry*, 1978, **17**, 1661 (*isol, glc*)
Geigert, J. *et al., J. Biol. Chem.*, 1983, **258**, 2273 (*glc, ms*)
Guthrie, J.P. *et al., J.A.C.S.*, 1984, **106**, 1351 (*pKa*)
Bostroem, G.O. *et al., J. Mol. Struct.*, 1987, **158**, 23 (*conformn*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)

Dibutyl disulfide, 9CI D-141

[629-45-8]
Butyl disulfide

$H_3C(CH_2)_3–S–S–(CH_2)_3CH_3$

$C_8H_{18}S_2$ 178.362
Constit. of *Ferula assa-foetida* (asafoetida). Oil. d_4^{20} 0.94. Bp 226° Bp_6 94°. n_D^{20} 1.4923.

▶ Fl. p. 93°.

S-*Oxide:* [111698-31-8] S-*Butyl 1-butanesulfinothioate*
$C_8H_{18}OS_2$ 194.362
Viscous yellow oil. Known as racemate and as opt. active preparation of unknown opt. purity λ_{max} 206 (log ϵ 3.56); 250 (log ϵ 3.35) (EtOH).

S,S′-*Dioxide:Dibutyl disulfoxide*
$C_8H_{18}O_2S_2$ 210.361
Obt. as a mixt. of diastereoisomers; characterised by low temp. cmr.

S,S-*Dioxide:* [1118-40-7] S-*Butyl 1-butanesulfonothioate*
$C_8H_{18}O_2S_2$ 210.361
$Bp_{0.13}$ 128-130°.

S,S,S′-*Trioxide, (±)-form:* [78186-29-5] *1-[(Butylsulfinyl)sulfonyl]butane*
$C_8H_{18}O_3S_2$ 226.36
Cryst. (Et_2O). Mp 31°.

S,S,S′,S′-*Tetraoxide:* [7559-57-1] *Dibutyl disulfone*
$C_8H_{18}O_4S_2$ 242.36
Mp 56-57°.

[7559-55-9, 85085-02-5, 85085-03-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 266D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 429A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 350C (*ir*)
Birch, S.F. *et al., J. Inst. Pet.*, 1953, **39**, 206 (*synth*)
Kice, J.L. *et al., J.A.C.S.*, 1968, **90**, 7378 (*synth, trioxide*)
Olah, G.A. *et al., Synthesis*, 1979, 721 (*synth*)
Freeman, F. *et al., J.O.C.*, 1982, **47**, 4194 (*oxides, synth, cmr*)
Freeman, F. *et al., Synthesis*, 1983, 913 (*S,S-dioxide, synth, ms, ir*)
Rajanikanth, B. *et al., Indian J. Chem., Sect. B*, 1985, 824 (*oxide, synth*)
Nemecek, C. *et al., Nouv. J. Chim.*, 1986, **10**, 761 (*oxide, synth*)
Harpp, D.N. *et al., Sulfur Lett.*, 1988, **7**, 73; *CA*, **109**, 210477 (*S,S-dioxide, synth*)
Noleau, I. *et al., J. Essent. Oil Res.*, 1991, **3**, 241-256 (*isol*)
Meshram, H.M. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 232 (*synth*)
Noureldin, N.A. *et al., Synthesis*, 1998, 1587-1589 (*synth, ir, pmr, ms*)
Kubec, R. *et al., J. Nat. Prod.*, 2002, **65**, 960-964 (*S-oxide, isol*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 446

Dibutyl sulfide, 8CI D-142

[544-40-1]
1,1′-Thiobisbutane, 9CI. Butyl sulfide. 5-Thianonane. FEMA 2215

$H_3C(CH_2)_3S(CH_2)_3CH_3$

$C_8H_{18}S$ 146.296
Present in raw cabbage, boiled and cooked beef, and some varieties of mushroom. Flavouring ingredient. Liq. Insol. H_2O, sol. Et_2O. d^{20} 0.84. Mp -80°. Bp 185-185.5°. n_D^{20} 1.4926.

▶ Skin irritant. LD_{50} (rat, orl) 2220 mg/kg. ER6417000

S-*Oxide:* [2168-93-6] *1,1′-Sulfinylbisbutane, 9CI. Dibutyl sulfoxide*
$C_8H_{18}OS$ 162.296
Needles. Mp 31°. Bp_3 102-105°.

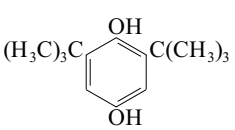
▶ EK5700000

S,S-*Dioxide:* [598-04-9] *1,1′-Sulfonylbisbutane, 9CI. Dibutyl sulfone*
$C_8H_{18}O_2S$ 178.295
Plates (H_2O). Mp 44°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 266C; 879B; 881C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 428C; 1417B; 1419C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 350B (*ir*)
Mann, F.G. *et al., J.C.S.*, 1935, 1556 (*synth*)
Vaughan, W.E. *et al., J.O.C.*, 1942, **7**, 472 (*synth*)
Aplin, R.T. *et al., J.C.S.(B)*, 1967, 513 (*ms*)
Hardy, F.E. *et al., J.C.S.(C)*, 1969, 2334 (*dioxide*)
Calo, V. *et al., Int. J. Sulfur Chem., Part A*, 1971, **1**, 130 (*oxide*)
Reich, H.J. *et al., Synthesis*, 1978, 299 (*dioxide*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 769 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 96
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 356-357
Ali, M.H. *et al., Synthesis*, 1997, 764-768 (*oxide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSM125

2,6-Di-*tert*-butyl-1,4-benzenediol D-143

[2444-28-2]
*2,6-Bis(1,1-dimethylethyl)-1,4-benzenediol, 9CI. 2,6-Di-*tert*-butylhydroquinone*



$C_{14}H_{22}O_2$ 222.327
Isol. from ginseng roots. Cryst. (petrol). Mp 117-118°. V. prob. a contaminant.

Di-Ac: [739-92-4]
$C_{18}H_{26}O_4$ 306.401
Cryst. Mp 102.5-103.5°.

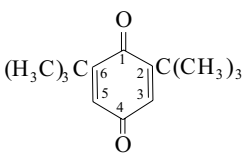
1-Me ether: [24289-65-4] *3,5-Di-*tert*-butyl-4-methoxyphenol*
$C_{15}H_{24}O_2$ 236.353
Cryst. (hexane). Mp 91-93°.

4-Me ether: [489-01-0] *2,6-Di-*tert*-butyl-4-methoxyphenol. 2,6-Bis(1,1-dimethylethyl)-4-methoxyphenol, 9CI*
$C_{15}H_{24}O_2$ 236.353
Cryst. (petrol). Mp 105-106°. Fieser and Fieser (1992) refer to this compd. incorrectly as BHA which is a mixt. of 2- and 3-*tert*-butyl-4-methoxyphenol (see Butylated hydroxyanisole, B-241).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1095A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 285B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1031D (*ir*)
Cook, C.D. *et al., J.A.C.S.*, 1955, **77**, 1672-1673 (*4-Me ether*)
Stroh, R. *et al., Angew. Chem.*, 1957, **69**, 699-706 (*synth*)
Cohen, L.A. *et al., J.A.C.S.*, 1963, **85**, 3397-3402 (*4-Me ether, uv*)
Popisil, J. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 98 (*4-Me ether, synth*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1971, 1206-1212 (*synth*)
Karhu, M. *et al., J.C.S. Perkin 1*, 1981, 303 (*di-Ac, synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 94; 1992, **16**, 110 (*4-Me ether, synth, use*)
Lu, Q. *et al., CA*, 1990, **113**, 55845 (*isol*)
Omura, K. *et al., Synth. Commun.*, 2000, **30**, 877-885 (*1-Me ether*)

2,6-Di-*tert*-butyl-1,4-benzoquinone D-144

[719-22-2]
2,6-Bis(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione, 9CI



$C_{14}H_{20}O_2$ 220.311
Detected in tapwater as presumed oxidant of 2,6-Di-*tert*-butyl-4-methylphenol, D-148. Formed as dec. prod. of 2,6-Di-*tert*-butyl-4-methylphenol D-148 in fat frying. Yellow cryst. (MeOH). Mp 68°. Subl.0.01 60.

▶ LD_{50} (mus, ipr) 2270 mg/kg. DK3970000

4-Oxime: [15052-28-5]
$C_{14}H_{21}NO_2$ 235.325
Yellow plates (C_6H_6). Mp 221-222°.

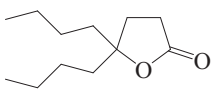
4-(2,4-Dinitrophenylhydrazone):
Red cryst. Mp 198-200°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 453A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 714B (*nmr*)
Metro, S.J. *et al., J.A.C.S.*, 1955, **77**, 2901 (*synth, deriv*)

Ley, K. *et al., Chem. Ber.*, 1956, **89**, 1402 (*synth*)
Kharasch, M.S. *et al., J.O.C.*, 1962, **27**, 651 (*synth, deriv*)
Heiss, J. *et al., Org. Mass Spectrom.*, 1969, **2**, 1325 (*ms*)
Rieker, A. *et al., Z. Naturforsch., B*, 1969, **24**, 547 (*pmr, uv, ir*)
Berger, S. *et al., Tetrahedron*, 1972, **28**, 3123 (*cmr*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 659 (*isol*)
Barton, D.H.R. *et al., Synth. Commun.*, 1997, **27**, 3625-3630 (*synth, pmr, cmr*)

5,5-Dibutyl-4,5-dihydro-2(3*H*)furanone, 9CI D-145

[7774-47-2]
4,4-Dibutyl-γ-butyrolactone. FEMA 2372

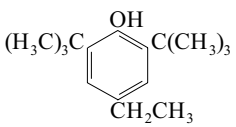


$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. with creamy, coconut-like flavour. $Bp_{1.7}$ 111-112°.

Nakamura, E. *et al., J.A.C.S.*, 1986, **108**, 3745-3755 (*synth*)
Lehman, J. *et al., Synthesis*, 1987, 1064-1067 (*synth, pmr*)
Adams, T.B. *et al., Food Chem. Toxicol.*, 1998, **36**, 249-278 (*tox*)

2,6-Di-*tert*-butyl-4-ethylphenol, 8CI D-146

[4130-42-1]
2,6-Bis(1,1-dimethylethyl)-4-ethylphenol, 9CI. Nocrac M17. Yoshinox 250



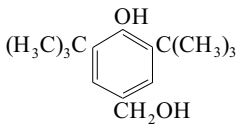
$C_{16}H_{26}O$ 234.381
Reported as a constit. of mango and green tea leaves. Cryst. (EtOH aq.). Mp 43.5-45°. Bp_{10} 134°. Isol. poorly documented. Given its use as a coml. antioxidant the claimed occurrence is presumably as a contaminant.

Benzoyl:
$C_{23}H_{30}O_2$ 338.489
Mp 161°.

Stillson, G.H. *et al., J.A.C.S.*, 1945, **67**, 303 (*synth*)
Cook, C.D. *et al., J.A.C.S.*, 1959, **81**, 1176 (*synth*)
Kornblum, N. *et al., J.A.C.S.*, 1961, **83**, 3668 (*synth*)
Afanasiev, I.D. *et al., CA*, 1967, **67**, 32392 (*synth*)
Ng, S. *et al., J.C.S. Perkin 2*, 1972, 1514 (*pmr*)
U.S. Pat., 1975, 3 919 333; *CA*, **84**, 43611 (*synth*)
Koutek, B. *et al., Coll. Czech. Chem. Comm.*, 1976, **41**, 2250 (*synth*)
Pang, X. *et al., Chin. Chem. Lett.*, 1991, **2**, 387 (*occur*)

2,6-Di-*tert*-butyl-4-hydroxymethylphenol D-147

[88-26-6]
3,5-Bis(1,1-dimethylethyl)-4-hydroxybenzenemethanol, 9CI. 3,5-Di-tert-*butyl-4-hydroxybenzyl alcohol, 8CI. 4-Hydroxymethyl-2,6-di*-tert-*butylphenol. Ionox 100. Butylated hydroxymethylphenol*



$C_{15}H_{24}O_2$ 236.353
Antioxidant used in foods. Cryst. (Et_2O/petrol). Mp 141°. $Bp_{2.6}$ 162°.
▶ Low oral acute toxicity. DO0750000

1′-O-Ac: [14387-17-8]
$C_{17}H_{26}O_3$ 278.391
Mp 105-106° (98.5°).

Di-Ac: [13154-59-1]
$C_{19}H_{28}O_4$ 320.428
Bp_7 166-168°.

1′-Me ether: [87-97-8] *2,6-Di*-tert-*butyl-4-(methoxymethyl)phenol. Ionol 4*
$C_{16}H_{26}O_2$ 250.38
Mp 99.5°.
▶ SK8350000

1′-Et ether: [3080-84-0] *2,6-Di*-tert-*butyl-4-(ethoxymethyl)phenol. 2,6-Di*-tert-*butyl-α-ethoxy*-p-*cresol, 8CI*
$C_{17}H_{28}O_2$ 264.407
Needles (petrol). Bp_{11} 162-163°.

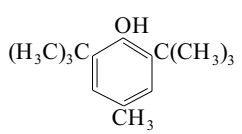
3,5-Di-tert-*butyl-4-hydroxybenzyl ether:* [6922-60-7]
$C_{30}H_{46}O_3$ 454.692
Cryst. (MeOH aq.). Mp 135-136°.

Starnes, W.H. *et al., J.O.C.*, 1966, **31**, 3164 (*synth, pmr*)
Lounasmaa, H. *et al., Acta Chem. Scand.*, 1967, **21**, 2807 (*synth, ir, pmr*)
Teuber, H.J. *et al., Annalen*, 1978, 757 (*synth, ir*)
Davis, B.R. *et al., J.C.S. Perkin 1*, 1982, 1499 (*3,5-tert-butyl-4-hydroxybenzyl ether, uv, ms, pmr*)
Thompson, J.A. *et al., Drug Metab. Dispos.*, 1987, **15**, 833 (*metab*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 1377
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IFX200

2,6-Di-*tert*-butyl-4-methylphenol D-148

[128-37-0]

[30587-81-6]
2,6-Bis(1,1-dimethylethyl)-4-methylphenol, 9CI. 2,6-Di-tert-*butyl*-p-*cresol, 8CI. Butylated hydroxytoluene. Ionol. BHT. Popol. FEMA 2184. E321*



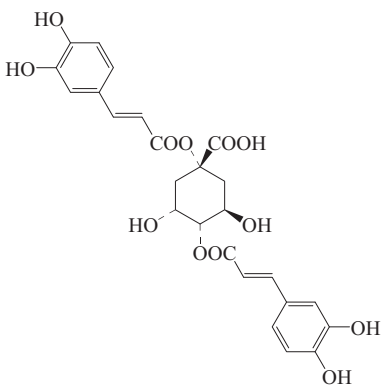
$C_{15}H_{24}O$ 220.354
Antioxidant, used in cosmetics, foods and pharmaceuticals. Cryst. Insol. H_2O; sol. most org. solvs. Mp 71°. Bp 265°.
▶ Fl. p. 127°. Mod. toxic, exp. teratogen. OES: long-term 100 ppm. GO7875000

[6858-01-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1094D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 285A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1031C (*ir*)
U.S. Pat., 1948, 2 428 745; *CA*, **42**, 354
Adv. Chem. Ser., 1955, **15**, 313 (***props***)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2059 (*uv*)
Kalinowski, H.O. *et al., Org. Magn. Reson.*, 1975, **7**, 128 (*cmr*)
Iimura, Y. *et al., Acta Cryst. C*, 1983, **39**, 778 (*cryst struct*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 359 (*361*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 47-48
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1121
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 326-330 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BFW750

1,4-Di-*O*-caffeoylquinic acid D-149

[1182-34-9]
NSC 91529. 1,4-Bis-(3,4-dihydroxycinnamoyl)quinic acid



$C_{25}H_{24}O_{12}$ 516.457
The CAS no. [1182-34-9] has been erroneously used in CA for 1,5-Di-*O*-caffeoylquinic acid. Isol. from flowers and leaves of *Helichrysum italicum* (curry plant). Mp 228-231° (218-220°). $[\alpha]_D^{18}$ -30 (c, 0.5 in MeOH).

[1884-23-7]

Panizzi, L. *et al., Gazz. Chim. Ital.*, 1965, **95**, 71-82 (*synth*)
Gumenyuk, L.A. *et al., Khim. Prir. Soedin.*, 1971, **6**, 525; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **6**, 503 (*isol*)
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1992, **28**, 50-55; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 40-44 (*isol, pmr, hplc*)

3,4-Di-*O*-caffeoylquinic acid D-150

[14534-61-3]
Isochlorogenic acid b

$C_{25}H_{24}O_{12}$ 516.457

Numbering systems vary. Isol. from coffee and maté. Powder. Mp 234-238° dec. $[\alpha]_D^{28}$ -225 (MeOH).

Me ester: [114637-83-1] ***Macroantoin F.*** *Macranthoin F*
$C_{26}H_{26}O_{12}$ 530.484
Light yellow powder. Mp 115-116°.

5-O-(3-Hydroxy-3-methylglutaroyl):
[103744-76-9]
$C_{31}H_{32}O_{16}$ 660.584
$[\alpha]_D^{18}$ -169.8 (c, 0.95 in MeOH).

3′-Me ether: [96990-65-7]

[102851-10-5] ***4-O-Caffeoyl-3-O-feruloylquinic acid***
$C_{26}H_{26}O_{12}$ 530.484
Constit. of coffee beans.

3″-Me ether: [125132-81-2] ***3-Caffeoyl-4-feruloylquinic acid***
$C_{26}H_{26}O_{12}$ 530.484
Constit. of the peel *Citrus reticulata* (mandarin). Amorph. yellow solid. $[\alpha]_D^{29}$ -24.7 (c, 0.1 in MeOH). λ_{max} 206 ; 216 ; 233 ; 328 (EtOH).

3″-Me ether, Me ester: [345642-66-2]
$C_{27}H_{28}O_{12}$ 544.511
Constit. of the peel of *Citrus reticulata* (mandarin). Amorph. solid. $[\alpha]_D^{29}$ -171 (c, 0.1 in MeOH). λ_{max} 219 ; 236 ; 328 (EtOH).

5″-Methoxy, 3″-Me ether: [110241-35-5] ***3-O-Caffeoyl-4-O-sinapoylquinic acid***
$C_{27}H_{28}O_{13}$ 560.51
Amorph. powder. $[\alpha]_D^{20}$ -252 (c, 0.54 in MeOH). Log P -0.19 (calc).

[2271-12-7]

Scarpati, M.L. *et al., Tet. Lett.*, 1964, 2851-2853 (*isol*)
Taylor, A.O. *et al., Phytochemistry*, 1968, **7**, 63-71 (*isol*)
Timmermann, B.N. *et al., J. Nat. Prod.*, 1983, **46**, 365-368 (*isol, pmr, cmr, ms*)
Iwahashi, H. *et al., Phytochemistry*, 1985, **24**, 630-632 (*Caffeoylferuloylquinic acid*)
Nishizawa, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1419-1421; 1987, **35**, 2133-2135 (*derivs*)
Chen, M. *et al., Yaoxue Xuebao*, 1994, **29**, 617-620 (*Macroantoin F*)
Lin, L.-C. *et al., J. Nat. Prod.*, 1999, **62**, 405-408 (*isol, pmr, cmr*)
Choi, E.M. *et al., Phytochemistry*, 2001, **56**, 733-739 (*3-Caffeoyl-4-feruloylquinic acid*)

3,5-Di-*O*-caffeoylquinic acid D-151

[2450-53-5]
3,5-Bis-(3,4-dihydroxycinnamoyl)quinic acid. Isochlorogenic acid a

$C_{25}H_{24}O_{12}$ 516.457

Care needed with numbering. Positions 3 and 5 frequently interchanged. Isol. from coffee and maté, globe artichoke (*Cynara scolymus*) and Caucasian whortleberry (*Vaccinium arctostaphylos*). Cryst. Mp 170-172° dec. $[\alpha]_D$ -198 (MeOH).

Me ester: [159934-13-1] ***Macroantoin G.*** *Macranthoin G*
$C_{26}H_{26}O_{12}$ 530.484
Light yellow powder. Mp 123-124°.

Butyl ester:
$C_{29}H_{32}O_{12}$ 572.565

1-O-(2-Methylpropanoyl): ***3,5-Dicaffeoyl-1-isobutyrylquinic acid***
$C_{29}H_{30}O_{13}$ 586.548
Amorph. pale yellow powder. λ_{max} 242 ; 300 (sh) ; 328 (MeOH).

4-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl): [114637-82-0] ***3,5-Dicaffeoyl-4-O-(3-hydroxy-3-methylglutaroyl)quinic acid***
$C_{31}H_{32}O_{16}$ 660.584
Amorph. powder + ½H_2O. $[\alpha]_D^{20}$ -170 (c, 0.95 in MeOH). λ_{max} 216 (ϵ 26600); 242 (ϵ 17600); 304 (sh) ; 329 (ϵ 30800) (MeOH).

4-O-Succinoyl: [179761-31-0] ***3,5-Dicaffeoyl-4-succinoylquinic acid***
$C_{29}H_{28}O_{15}$ 616.531
Constit. of *Chrysanthemum coronarium* (chop-suey greens).

1-Me ether, Me ester:
$C_{27}H_{28}O_{12}$ 544.511
Mp 132-134°. $[\alpha]_D^{20}$ -34.7 (MeOH).

3-Epimer: ***3,5-Di-O-caffeoyl-muco-quinic acid***
$C_{25}H_{24}O_{12}$ 516.457
Yellowish gum. $[\alpha]_D$ -153.8 (c, 0.78 in MeOH). λ_{max} 219 (log ϵ 4.43); 244 (log ϵ 4.28); 300 (sh) (log ϵ 4.4); 328 (log ϵ 4.52) (EtOH).

Haslam, E. *et al., J.C.S.*, 1964, 2137 (*isol*)
Corse, J. *et al., Phytochemistry*, 1965, **4**, 527 (*uv, pmr*)
Nichiforescu, E.A. *et al., Plant. Med. Phytother.*, 1970, **4**, 56 (*isol*)
Mzhavanadze, V.V. *et al., CA*, 1972, **76**, 124113c
Timmermann, B.N. *et al., J. Nat. Prod.*, 1983, **46**, 365 (*isol, pmr, cmr, ms*)
Nishizawa, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 87-95 (*4-3-hydroxy-3-methylglutarate*)
Chen, M. *et al., Yaoxue Xuebao*, 1994, **29**, 617 (*Macroantoin G*)
Tatefuji, T. *et al., Biol. Pharm. Bull.*, 1996, **19**, 966-970 (*isol, props*)
Chudo, Y. *et al., J. Agric. Food Chem.*, 1996, **44**, 2037 (*4-succinate*)
Kodoma, M. *et al., Phytochemistry*, 1998, **47**, 371-373 (*isol, pmr, cmr*)
Miketova, P. *et al., J. Mass Spectrom.*, 1999, **34**, 1240-1252 (*ms*)
Heilmann, J. *et al., Phytochemistry*, 1999, **51**, 713-718 (*Dicaffeoyl-1-isobutyrylquinic acid*)
Kwon, H.C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1796-1798 (*3,5-Dicaffeoylmucoquinic acid, isol, activity, pmr*)
Peng, L.Y. *et al., Fitoterapia*, 2000, **71**, 713-715 (*butyl ester, isol*)
Zhang, W.-D. *et al., Yaoxue Xuebao*, 2001, **36**, 360-363 (*1-Me ether Me ester*)

4,5-Di-*O*-caffeoylquinic acid D-152

[57378-72-0]
4,5-Bis(3,4-dihydroxycinnamoyl)quinic acid. Isochlorogenic acid c

$C_{25}H_{24}O_{12}$ 516.457

Numbering systems vary. Isol. from coffee, Brazilian propolis and maté. Cryst. Mp 140° dec. $[\alpha]_D^{28}$ -170 (MeOH).

[32451-88-0]

Scarpati, M.L. *et al., Tet. Lett.*, 1964, 2851 (*isol*)
Timmermann, B.N. *et al., J. Nat. Prod.*, 1983, **46**, 365-368 (*isol, pmr, cmr*)
Tatefuji, T. *et al., Biol. Pharm. Bull.*, 1996, **19**, 966-970 (*isol, pmr, cmr*)
Miketova, P. *et al., J. Mass Spectrom.*, 1999, **34**, 1240-1252 (*ms*)

Dicarbonic acid, 9CI D-153

[503-81-1]
Oxydiformic acid, 8CI. Pyrocarbonic acid. Oxybisformic acid

HOOC–O–COOH

$C_2H_2O_5$ 106.035

Di-Me ester: [4525-33-1] *Dimethyl dicarbonate. Dimethyl pyrocarbonate. Velcorin*
$C_4H_6O_5$ 134.088
Yeast inhibitor and preservative for alcoholic beverages esp. low alcohol wines. d_4^{20} 1.25. Mp 15-17°. Bp_5 44-47°. n_D^{20} 1.3948.

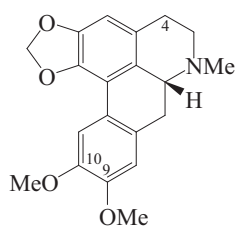
Di-Et ester: [1609-47-8] *Diethyl dicarbonate. Diethyl pyrocarbonate. Baycovin*
$C_6H_{10}O_5$ 162.142
Formerly used as a fermentation inhibitor and preservative for wines, soft drinks and fruit juices. No longer permitted as a food additive. d_4^{20} 1.12. Bp_3 58.5-62°. n_D^{25} 1.3975.

▶ Poss. protocarcinogen (forms carcinogenic ethyl carbamate with dietary $NH_4^{\oplus}$). Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 850 mg/kg. LQ9350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 611B (*ir*)
Rosnati, L. *et al., Chem. Ber.*, 1963, **96**, 3098 (*synth, di-Et ester*)
Fr. Pat., 1968, 1 542 382; *CA*, **71**, 123555h (*manuf, di-Me ester*)
Gejvall, T. *et al., J. Chromatogr.*, 1974, **90**, 157 (*use, Et ester*)
Brysova, V.P. *et al., J.O.C., USSR*, 1974, **10**, 2551 (*synth, di-Me ester*)
Turczan, J.W. *et al., J. Agric. Food Chem.*, 1977, **25**, 594 (*pmr, di-Et ester*)
Pauli, G.H. *et al., J. Chem. Educ.*, 1984, **61**, 332 (*rev, di-Et ester*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DRJ850
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 821; 853 (*diesters, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DIZ100

Dicentrine D-154

9,10-Dimethoxy-1,2-methylenedioxyaporphine. N,O-*Dimethylactinodaphnine. Eximine*†



(*R*)-*form*

$C_{20}H_{21}NO_4$ 339.39Log P 2.86 (uncertain value) (calc).

(S)-form [517-66-8]
Mp 168-169°. $[\alpha]_D$ +57 (c, 1 in EtOH). λ_{max} 281 (log ε 4.18); 305 (log ε 4.23) (95% EtOH).

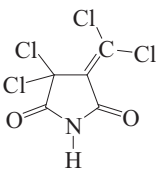
▶ CE0455000

O^9-*De-Me:* [5890-28-8] *9-Hydroxy-10-methoxy-1,2-methylenedioxyaporphine.* ***Cassythicine.*** N-*Methylactinodaphnine*
$C_{19}H_{19}NO_4$ 325.363
Alkaloid from *Laurus nobilis* (bay laurel). Cryst. + $1CHCl_3$ ($CHCl_3$). Mp 210-212°. $[\alpha]_D$ +62 (c, 0.43 in $CHCl_3$). λ_{max} 283 (log ε 4.23); 307 (log ε 4.27) (95% EtOH).

Johns, S.R. *et al., Aust. J. Chem.*, 1966, **19**, 2339-2345 (*Actinodaphnine, Cassythicine*)
Nakasato, T. *et al., Yakugaku Zasshi*, 1966, **86**, 129-134 (*Cassythicine*)
Cava, M.P. *et al., J.O.C.*, 1968, **33**, 2443-2446 (*Actinodaphnine, Cassythicine, uv*)
Yang, T.H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1971, **18**, 133-136; *CA*, **77**, 16567r (*(-)-Cassythicine*)
Hara, H. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1946-1949 (*Dicentrine, Cassythicine, synth, pmr*)
Soicke, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 149-152 (*(±)-Cassythicine*)
Likhitwitayawuid, K. *et al., J. Nat. Prod.*, 1993, **56**, 1468-1478 (*(-)-Nordicentrine, (-)-Cassythicine*)

3,3-Dichloro-4-(dichloromethylene)-2,5-pyrrolidinedione, 9CI D-155

[165606-93-9]



$C_5HCl_4NO_2$ 248.879
Bacterial mutagen produced by chlorination of simulated poultry chiller water.

▶ Mutagenic.

Stevens, K.L. *et al., J. Agric. Food Chem.*, 1995, **43**, 2424-2427; 1996, **44**, 256-263 (*synth, cryst struct*)

Dichlorodifluoromethane, 9CI D-156

[75-71-8]
Arcton 12. CFC 12. Fluorocarbon 12. Forane 12. Freon 12. Frigen 12. Fron 12. Genetron 12

CCl_2F_2

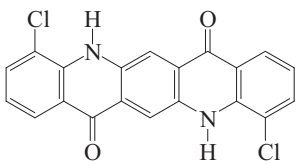
CCl_2F_2 120.913
Direct contact freezing agent for foods. Refrigerant, aerosol propellant. Almost odourless gas. Fp -158. Bp -29.8° Bp 42.4°.

▶ Can react violently with Al or Mg. Dec. to toxic carbonyl halides if strongly heated in air. Production controlled by environmental legislation. V. high conc. can cause conjunctiva irritation, fibrosing alveolitis, and adverse hepatic effects. OES: long-term 1000 ppm; short-term 1250 ppm. PA8200000

Henne, A.L. *et al., Org. React. (N.Y.)*, 1944, **2**, 49 (*rev*)
Hamilton, J.M. *et al., Adv. Fluorine Chem.*, 1963, **3**, 117 (*manuf, use*)
Abraham, R.J. *et al., J.C.S. Perkin 2*, 1973, 1027 (*F-19 nmr*)
Gilbert, R. *et al., J. Chem. Phys.*, 1974, **60**, 4820 (*uv*)
Beattie, W.H. *et al., Appl. Spectrosc.*, 1975, **29**, 334 (*ms*)
Le Blanc, L.M. *et al., J. Raman Spectrosc.*, 1991, **22**, 255 (*Raman*)
Hall, C.D. *et al., Mol. Phys.*, 1991, **74**, 27 (*ed*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 160-162
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1188
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 810
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 187
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0310
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 416
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DFA600

4,11-Dichloro-5,12-dihydroquino[2,3-*b*]acridine-7,14-dione, 9CI D-157

[3089-16-5]

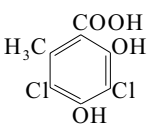


$C_{20}H_{10}Cl_2N_2O_2$ 381.217
FDA approved colourant for food contact polymers. Red-orange or red solid.

Labana, S.S. *et al., Chem. Rev.*, 1967, **67**, 1-18 (*rev, synth, props*)
Altiparmakian, R.H. *et al., Helv. Chim. Acta*, 1972, **55**, 85-100 (*pmr*)
Lincke, G. *et al., Chem.-Ztg.*, 1982, **106**, 365-369 (*cryst struct*)
Osvath, R. *et al., Food Chem. News*, 2001, **43**, 6 (*use*)

3,5-Dichloro-2,4-dihydroxy-6-methylbenzoic acid D-158

[5859-25-6]



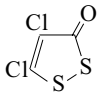
$C_8H_6Cl_2O_4$ 237.038
Needles (MeOH aq.). Mp 202-203°.

2-Me ether: [4101-80-8] *3,5-Dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid. Dichloroisoeverninic acid*
$C_9H_8Cl_2O_4$ 251.065
Food additive; residue present in orthomycin antibiotics. Cryst. (H_2O). Mp 129-130°. Slowly decarboxylates on standing in soln..

Galmarini, O.L. *et al., Tetrahedron*, 1961, **15**, 76 (*2-Me ether*)
Buzzetti, F. *et al., Experientia*, 1968, **24**, 320 (*2-Me ether*)
Dornhagen, J. *et al., Tetrahedron*, 1985, **41**, 173 (*2-Me ether, synth, ir, pmr, cmr, bibl*)

4,5-Dichloro-3*H*-1,3-dithiol-2-one, 9CI D-159

[1192-52-5]
4,5-Dichloro-1,2-dithiol-2-one. 4,5-Dichloro-1,2-dithia-4-cyclopenten-3-one. Dichlorodithiolone



$C_3Cl_2OS_2$ 187.07
FDA approved slimicide for use in food-contact paper and paperboard. Cryst. (petrol). Mp 61°. $Bp_{0.11}$ 125° $Bp_{0.05}$ 87°.

▶ JP1290000

Boberg, F. *et al., Annalen*, 1964, **679**, 109 (*synth, uv*)
Anon, *et al., Food Chem. News*, 1991, **41**, 29 (*use*)

1,2-Dichloroethane, 9CI D-160

[107-06-2]

[1300-21-6]
Ethylene dichloride, BSI, ISO. Ethylene chloride. Dutch oil. R 150. EDC, JMAF. Granosan

$ClCH_2CH_2Cl$

$C_2H_4Cl_2$ 98.959
Solvent used in food processing. Liq. Sl. sol. H_2O; misc. most org. solvs. d_4^{20} 1.25. Fp -35.3. Bp 83-84°. n_D^{20} 1.4443.

▶ Highly flammable, fl. p. 13°, autoignition temp. 413/438°. Eye, skin and respiratory tract irritant. High vapour conc. cause CNS depression and adverse gastrointestinal effects, and the symptoms incl. mental confusion, dizziness, nausea, vomiting. Liver, kidney and adrenal injury may occur at sub-acute levels and from prolonged or repeated exp. Exp. carcinogen and teratogen. MEL: long-term 5 ppm (Sk). KI0525000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 72A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 107A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 103D (*ir*)
Bahr, H.A. *et al., Angew. Chem.*, 1930, **43**, 233; *CA*, **24**, 2717 (*synth*)
Simeral, L. *et al., J. Phys. Chem.*, 1973, **77**, 1590 (*cmr*)
Stahl-Larivière, H. *et al., Org. Magn. Reson.*, 1974, **6**, 170 (*pmr*)
IARC Monog., 1979, **20**, 429; *Suppl.* 7, 62 (*rev, tox*)
Hanner, A.W. *et al., Org. Mass Spectrom.*, 1982, **17**, 19 (*ms*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A6**, 263 (*rev*)
Organo-chlorine Solvents, Royal Society of Chemistry, London, 1986, 73 (*tox, rev*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 12 (*rev*)
Pesticide Manual, 9th edn., 1991, No. 5810
Durig, J.R. *et al., Vib. Spectrosc.*, 1992, **3**, 9 (*ir*)
Boese, R. *et al., Z. Kristallogr.*, 1992, **198**, 311 (*cryst struct*)

Kropp, P.J. *et al., J.O.C.*, 1994, **59**, 3102 (*synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 970-972
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3491
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 419
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EIY600

Dichloromethane, 9CI D-161

[75-09-2]
Methylene chloride. Methane dichloride. R 30

CH_2Cl_2

CH_2Cl_2 84.932
Used as an extraction solv. in the preparation of decaffeinated coffee, hop extracts and spice oleoresins. Diluent for colour additives and inks for marking fruit and vegetables. Volatile liq. d_4^{15} 1.34. Fp -96.8. Bp 40.1°. n_D^{20} 1.4246. Much more reactive than commonly supposed. Use as solvent in basic conds. should be avoided (see Souquet, *et al*).

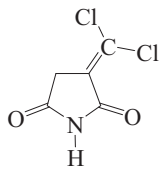
▶ Autoignition temp. 605°. Gives explosive mixts. with various materials and reacts exothermically with amines in conc. soln. Vapour can ignite or explode if heated. Possible human carcinogen. Eye, skin and respiratory tract irritant. De-fats the skin. High vapour conc. depress CNS and cause headache, dizziness and coma. Prolonged or repeated exposure can cause carboxyhaemoglobinaemia, gastrointestinal disturbances plus the symptoms of acute exposure. Exp. carcinogen. Exp. reprod. and teratogenic effects. MEL: long-term 100 ppm; short-term 300 ppm (proposed). PA8050000

[1665-00-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 70D (*ir*)
Aldrich Atlas of NMR Spectra, **1**, 57A (*pmr*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 105A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 102A (*ir*)
Panizzon, L. *et al., Helv. Chim. Acta*, 1932, **15**, 1191 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 273; **7**, 239
Kawaguchi, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 62 (*cryst struct*)
Russell, B.R. *et al., J.A.C.S.*, 1973, **95**, 2129 (*uv*)
Illing, H.P.A. *et al., HSE Toxicity Review 12: Dichloromethane (Methylene Chloride)*, HMSO, London, 1985,
IARC Monog., 1986, **41**, 43; *Suppl*. 7, 194; *Suppl*. 6, 228 (*rev, tox*)
Dostovalova, V.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1986, 2467; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1986, 2282 (*cmr*)
Duncan, J.L. *et al., J. Mol. Spectrosc.*, 1986, **118**, 145 (*ir*)
Organo-chlorine Solvents, Health Risks to Workers, Royal Society of Chemistry, 1986, 147 (*tox, rev*)
Bretherick, L. *et al., Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **5**, 1041 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1105
Souquet, F. *et al., Synth. Commun.*, 1993, **23**, 817 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Chem. Eng. News, (Jan. 13), 1997, 7 (*tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0379
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 425
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MJP450

3-(Dichloromethylene)-2,5-pyrrolidinedione, 9CI D-162

[170660-62-5]

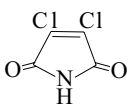


$C_5H_3Cl_2NO_2$ 179.99
Bacterial mutagen produced by chlorination of simulated poultry chiller water. Cryst. (Et_2O/CCl_4). Mp 192-192.5°.

Haddon, W.F. *et al., J. Agric. Food Chem.*, 1996, **44**, 256-263 (*formn, synth, nmr, uv*)

3,4-Dichloro-2,5-pyrrolidinedione D-163

[1193-54-0]
Dichloromaleimide



$C_4HCl_2NO_2$ 165.963
Bacterial mutagen produced by chlorination of simulated poultry chiller water. Mp 175°.

▶ LD_{50} (mus, ipr) 31 mg/kg. Mutagen. ON5150000

Dunlap, F.L. *et al., J.A.C.S.*, 1896, **18**, 332 (*synth*)
Bonse, G. *et al., Annalen*, 1981, 1658 (*synth*)
Haddon, W.F. *et al., J. Agric. Food Chem.*, 1996, **44**, 256-263 (*occur, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DFN800

Dichlorvos, BAN, BSI, INN, ISO D-164

[62-73-7]
O-*(2,2-Dichloroethenyl)* O,O-*dimethyl phosphate, 9CI. 2,2-Dichlorovinyl dimethyl phosphate, 8CI. Dichlorophos. DDVP, JMAF. Aquaguard. Brevinyl. Chlorvinphos. Dederap. Dichlorvos. Estrosol. Fecama. Insectigas D. Nefafros. Novotox. Nogos. Nuvan. Panaplate. Vapona. Vaponite. Vinylofos. Winylophos. NSC 6738*

$(MeO)_2P(O)OCH{=}CCl_2$

$C_4H_7Cl_2O_4P$ 220.976
Used as a household and public health fumigant, for crop protection and as an anthelmintic in animal feeds. Liq. with aromatic odour. Mod. sol. H_2O (1% w/v), misc. EtOH. d_4^{25} 1.42. Bp_{14} 120° Bp_3 88°. n_D^{20} 1.4550. Log P 1.72 (uncertain value) (calc). Hydrolysed rel. slowly by H_2O, more quickly by alkalis.

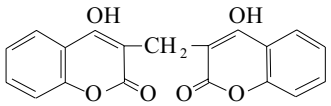
▶ Cholinesterase inhibitor, rapidly metabolised and excreted. LD_{50} (rat, orl) 46-80 mg/kg. Neurotoxic symptoms from acute human exposure. OES: long-term 0.1 ppm; short-term 0.3 ppm (Sk). TC0350000

Barthel, W.F. *et al., J.A.C.S.*, 1955, **77**, 2424-2427 (*synth*)
Keith, L.H. *et al., J. Assoc. Off. Anal. Chem.*, 1968, **51**, 1063-1094 (*pmr*)
Ross, R.T. *et al., Anal. Chim. Acta*, 1970, **52**, 139-141 (*P nmr*)
Gore, R.C. *et al., J. Assoc. Off. Anal. Chem.*, 1971, **54**, 1040-1082 (*ir, uv*)
Betteridge, D. *et al., Anal. Chem.*, 1972, **44**, 2005-2010 (*pe*)
Gillett, J.W. *et al., Residue Rev.*, 1972, **44**, 115-160; 161-184 (*tox, rev*)
Gaydou, E.M. *et al., Bull. Soc. Chim. Fr.*, 1973, 2275-2278 (*synth, props*)
Gaydou, E.M. *et al., Org. Mass Spectrom.*, 1974, **9**, 157-171 (*ms*)
Nikonorov, K.V. *et al., Zh. Obshch. Khim.*, 1974, **44**, 1267-1272; *J. Gen. Chem. USSR (Engl. Transl.)*, 1974, **44**, 1245-1250 (*synth*)
Nicholas, M.L. *et al., J. Assoc. Off. Anal. Chem.*, 1976, **59**, 1071-1080 (*Raman*)
Szalontai, G. *et al., J. Chromatogr.*, 1976, **124**, 9-16 (*hplc*)
Stan, H.-J. *et al., Fresenius' Z. Anal. Chem.*, 1977, **287**, 271-285 (*glc, ms*)
Szalontai, G. *et al., Org. Magn. Reson.*, 1977, **10**, 63-69 (*cmr*)
Wright, A.S. *et al., Arch. Toxicol.*, 1979, **42**, 1-18 (*metab, props, bibl*)
Ramel, C. *et al., Mutat. Res.*, 1980, **76**, 297-309 (*rev, tox*)
Johnson, M.K. *et al., Acta Pharmacol. Toxicol.*, Suppl., 1981, **49**, 87-98 (*rev, tox*)
Reuber, M.D. *et al., Clin. Toxicol.*, 1981, **18**, 47-84 (*rev, props*)
Prinsloo, S.M. *et al., J. Assoc. Off. Anal. Chem.*, 1985, **68**, 1100-1108 (*glc*)
Santodonato, J. *et al., CA*, 1986, **105**, 231583 (*rev, haz*)
Singh, A.K. *et al., J. Chem. Res.*, 1986, **369**, 83-96 (*gc-ms*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 201 (*synonyms*)
Betowski, L.D. *et al., Environ. Sci. Technol.*, 1988, **22**, 1430-1434 (*hplc-ms*)
Dangerous Prop. Ind. Mater. Rep., 1989, **9**, 2-18 (*rev*)
Sharma, V.K. *et al., Forensic Sci. Int.*, 1990, **48**, 21-25 (*hplc*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A141
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1126
Pharmaceutical Manufacturing Encyclopaedia, 1997, No. 218
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 194
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 990
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DGP900

Dicoumarol, INN D-165

[66-76-2]

*3,3′-Methylenebis[4-hydroxy-2*H*-1-benzopyran-2-one], 9CI. 3,3′-Methylenebis-4-hydroxycoumarin, 8CI. Bishydroxycoumarin. Dicoumarin. Cumid. Dicumarol. Dufalone. Melitoxin. Many other names*



$C_{19}H_{12}O_6$ 336.3

Isol. from *Melilotus alba* (white melilot). Cryst. (cyclohexanone). Sol. bases, Py; fairly sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 288-289°. Log P 3.73 (calc). λ_{max} 289 (ϵ 21200); 310 (ϵ 23460); 325 (ϵ 19320) ($CHCl_3$) (Berdy).

► Adverse effects reported (similar to Warfarin) when used therapeutically. Human and exp. reprod. effects. Exp. teratogen. LD_{50} (rat, orl) 250 mg/kg ; LD_{50} (mus, scu) 200 - 300 mg/kg. GN7875000

Di-Ac:

Cryst. (C_6H_6). Mp 250-252° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 325A (*ir*)

Stahmann, M.A. *et al., J. Biol. Chem.*, 1941, **138**, 21; 513; 529 (*isol, synth, uv*)

Wittmann, H. *et al., Monatsh. Chem.*, 1965, **96**, 1200 (*synth*)

Korenmann, I.M. *et al., Zh. Anal. Khim.*, 1967, **22**, 1305 (*use*)

Hutchinson, D.W. *et al., Tetrahedron*, 1969, **25**, 2531 (*ir, pmr, struct*)

Levy, G. *et al., J. Pharmacokinet. Biopharm.*, 1973, **1**, 541 (*rev*)

Owen, C.A. *et al., Mayo Clin. Proc.*, 1974, **49**, 912 (*rev, pharmacol*)

Kirkiacharian, B.S. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 697 (*cmr*)

Alcock, N.W. *et al., Acta Cryst. B*, 1978, **28**, 1957 (*cryst struct*)

Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, 271 (*biochem*)

Hayward, R.C. *et al., J. Chem. Educ.*, 1984, **61**, 87 (*synth*)

Griminger, P. *et al., J. Nutr.*, 1987, **117**, 1325 (*rev*)

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 5099

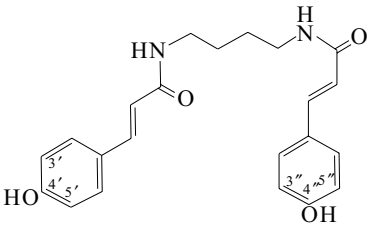
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 225

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BJZ000

Di-4-coumaroylputrescine D-166

[37946-59-1]

N,N′*-1,4-Butanediylbis[3-(4-hydroxyphenyl)-2-propenamide], 9CI.* N,N′*-Bis(4-hydroxycinnamoyl)-1,4-butanediamine*



$C_{22}H_{24}N_2O_4$ 380.443

Alkaloid from *Helianthus annuus* (sunflower), *Pyrus communis* (pear), *Rubus idaeus* (raspberry) and *Vicia faba*.

3′,3″-Dihydroxy: [60422-23-3] ***Dicaffeoylputrescine.*** N,N′*-Bis(3,4-dihydroxycinnamoyl)-1,4-butanediamine*

$C_{22}H_{24}N_2O_6$ 412.441

Alkaloid from *Helianthus annuus* (sunflower) and *Pyrus communis* (pear).

3,3′-Dimethoxy: [42369-86-8] ***Diferuloylputrescine.*** N,N′*-Bis(4-hydroxy-3-methoxycinnamoyl)-1,4-butanediamine*

$C_{24}H_{28}N_2O_6$ 440.495

Alkaloid from *Ananas comosus* (pineapple), *Vicia faba and Lycopersicon esculentum* (tomato).

3′,3″,5′,5″-Tetramethoxy: [70185-58-9] ***Disinapoylputrescine.*** N,N′*-Bis(4-hydroxy-3,5-dimethoxycinnamoyl)-1,4-butanediamine*

$C_{26}H_{32}N_2O_8$ 500.547

Martin-Tanguy, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1973, **276**, 1433 (*uv, struct, synth, Diferuloylputrescine*)

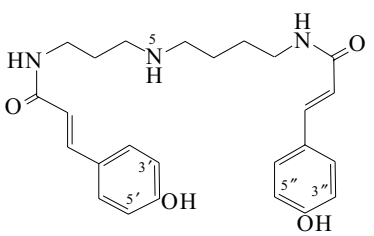
Cabanne, F. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1976, **282**, 1959 (*uv, struct, Dicaffeoylputrescine*)

Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*occur, derivs*)

N^1,N^{10}-Dicoumaroylspermidine D-167

[65715-79-9]

N^1,N^{10}*-Bis(4-hydroxycinnamoyl)spermidine*



$C_{25}H_{31}N_3O_4$ 437.538

Alkaloid from *Helianthus annuus* (sunflower), *Vicia faba and Pyrus communis* (pear).

3′,3″-Dihydroxy: [59001-33-1] ***Dicaffeoylspermidine***

$C_{25}H_{31}N_3O_6$ 469.536

3′ or 3″-Hydroxy, 3″ or 3′-methoxy: ***Caffeoylferuloylspermidine***

$C_{26}H_{33}N_3O_6$ 483.563

Alkaloid from the pollen of *Corylus avellana* (filbert).

3′,3″-Dimethoxy: [70185-61-4] ***N^1,N^{10}-Diferuloylspermidine***

$C_{27}H_{35}N_3O_6$ 497.59

Alkaloid from the pollen of *Corylus avellana* (filbert), also from *Ananas comosus* (pineapple) and *Vicia faba*. Only the alkaloid from *C. avellana* has been shown to have the exact struct. shown. The other isolates are diferuloylspermidine with undefined regioisomerism (i.e. could be N^5-substituted).

3′,3″,5′,5″-Tetramethoxy: [70185-63-6] ***Disinapoylspermidine***

$C_{29}H_{39}N_3O_8$ 557.642

Regioisomerism not rigorously established.

[101330-61-4]

Delétang, J. *et al., Ann. Tab., Sect. 2*, 1974, **11**, 123; *CA*, **84**, 147656m (*uv, pmr, struct, Dicaffeoylspermidine*)

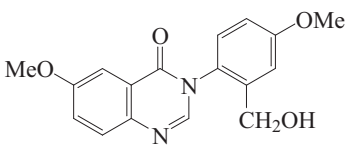
Cabanne, F. *et al., Physiol. Veg.*, 1977, **15**, 429; *CA*, **88**, 86095m (*uv, struct*)

Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*occur*)

Meurer, B. *et al., Phytochemistry*, 1986, **25**, 433 (*Caffeoylferuloylspermidine, Diferuloylspermidine*)

Dictyoquinazol A D-168

*3-(2-Hydroxymethyl-4-methoxyphenyl)-6-methoxy-4(3*H*)-quinazolinone*



$C_{17}H_{16}N_2O_4$ 312.324

Alkaloid from the edible mushroom *Dictyophora indusiata*. Pale yellow oil. λ_{max} 224 (log ϵ 3.9); 274 (log ϵ 3.43); 319 (log ϵ 2.78) (MeOH).

N^1*,2-Dihydro,* N^1*-formyl:1-Formyl-2,3-dihydro-3-(2-hydroxymethyl-4-methoxyphenyl)-6-methoxy-4(1*H*)-quinazolinone.* ***Dictyoquinazol C***

$C_{18}H_{18}N_2O_5$ 342.351

Alkaloid from *Dictyophora indusiata*. Pale yellow oil. $[\alpha]_D$ +60 (c, 0.03 in MeOH). Exists as a mixt. of rotamers λ_{max} 228 (log ϵ 3.9); 319 (log ϵ 2.9) (MeOH).

4-Deoxo, N^1*,2-dihydro,* N^1*-formyl:1-Formyl-1,2,3,4-tetrahydro-3-(2-hydroxymethyl-4-methoxyphenyl)-6-methoxyquinazoline.* ***Dictyoquinazol B***

$C_{18}H_{20}N_2O_4$ 328.367

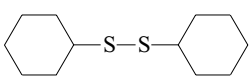
Alkaloid from *Dictyophora indusiata*. Pale yellow oil. $[\alpha]_D$ -80 (c, 0.05 in MeOH). Exists as a mixt. of rotamers λ_{max} 206 (log ϵ 3.7); 239 (log ϵ 3.85); 290 (log ϵ 3.2) (MeOH).

Lee, I.-K. *et al., J. Nat. Prod.*, 2002, **65**, 1769-1772 (*isol, pmr, cmr*)

Dicyclohexyl disulfide, 9CI D-169

[2550-40-5]

FEMA 3448

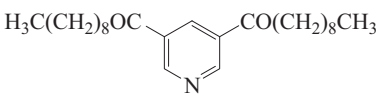


$C_{12}H_{22}S_2$ 230.438
Flavouring ingredient. Liq. Bp_{20} 195°. n_D^{20} 1.5430.

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 157
Tanner, D.D. *et al., J.O.C.*, 1995, **60**, 4481 (*synth, pmr, ir, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 811

3,5-Didecanoylpyridine D-170

[149682-93-9]
1,1′-(3,5-Pyridinediyl)bis-1-decanone, 9CI

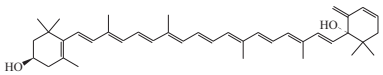


$C_{25}H_{41}NO_2$ 387.604
Alkaloid from *Houttuynia cordata* (Yu Xing Cao).

Jong, T.T. *et al., J. Chin. Chem. Soc. (Taipei)*, 1993, **40**, 301-303 (*isol*)
Proebstle, A. *et al., Nat. Prod. Lett.*, 1994, **4**, 235-240 (*isol*)

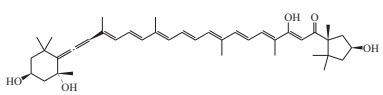
3′,4′-Didehydro-β,γ-carotene-3,6′-diol D-171

3′,18′-Didehydro-β,ε-carotene-3,6′-diol



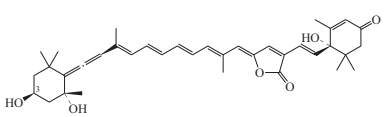
$C_{40}H_{54}O_2$ 566.865
(3*R*,6′*S*)-*form* [158312-69-7]
Nigroxanthin
Constit. of the ripe pods of red paprika *Capsicum annuum* var. *longum*.
Deli, J. *et al., Chimia*, 1995, **48**, 102-104 (*isol, pmr, cmr*)
Deli, J. *et al., Tet. Lett.*, 2001, **42**, 1395-1397 (*abs config*)

6,7-Didehydro-5,6-dihydro-3,3′,5,8′-tetrahydroxy-β,κ-caroten-6′-one D-172



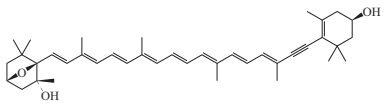
$C_{40}H_{56}O_5$ 616.879
(3*S*,3′*S*,5*R*,5′*R*,6*R*)-*form* [256505-54-1]
Constit. of the oyster *Crassostrea gigas*. Red amorph. solid. λ_{max} 468 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr*)

6,7-Didehydro-5,6-dihydro-3,5,6′-trihydroxy-13,14,20-trinor-3′-oxo-β,ε-caroten-19′,11′-olide D-173



$C_{37}H_{46}O_6$ 586.767
(3*S*,5*R*,6*R*,6′*S*)-*form*
3-Ac: [256505-50-7]
$C_{39}H_{48}O_7$ 628.804
Constit. of the oyster *Crassostrea gigas*. Red amorph. solid. λ_{max} 457 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr, cmr*)

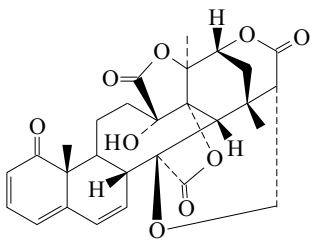
7′,8′-Didehydro-3,6-epoxy-5,6-dihydro-β,β-carotene-3′,5-diol D-174



$C_{40}H_{54}O_3$ 582.865
(3*S*,3′*R*,5*R*,6*R*)-*form* [256505-52-9]
Constit. of the oyster *Crassostrea gigas*. Orange amorph. solid. λ_{max} 446 ; 476 (Et_2O).
Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr*)

4,7-Didehydroneophysalin B D-175

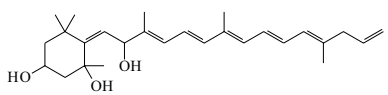
[134461-76-0]



$C_{28}H_{28}O_9$ 508.524
Constit. of *Physalis alkekengi* (winter cherry). Yellow prisms. Mp 299-300° (synth). $[\alpha]_D$ +21 (c, 0.26 in MeOH).
Kawai, M. *et al., Tetrahedron*, 1991, **47**, 2103 (*cryst struct*)
Sunayama, R. *et al., Phytochemistry*, 1993, **34**, 529 (*isol, pmr, cmr*)

10′,11′-Didehydro-5,8,11′,12′-tetrahydro-10′-apo-β-carotene-3,5,8-triol D-176

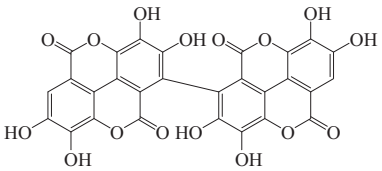
[53905-14-9]
Unknown 370



$C_{27}H_{40}O_3$ 412.611
Struct. assignment is tentative. CA name appears to be defective. Isol. from the avocado fruit (*Persea americana*). λ_{max} 350 ; 370 ; 393 (petrol).
Gross, J. *et al., J. Food Sci.*, 1972, **37**, 589
Gross, J. *et al., Phytochemistry*, 1974, **13**, 1917

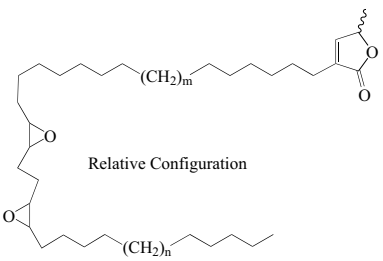
Diellagilactone D-177

[153816-55-8]
2,2′,3,3′,7,7′,8,8′-Octahydroxy-[1,1′-bi[1]-benzopyrano[5,4,3-cde][1]benzopyran]-5,5′,10,10′-tetrone, 9CI. 3,3′-Diellagic acid



$C_{28}H_{10}O_{16}$ 602.377
Constit. of the pericarp of pomegranate (*Punica granatum*).
Japan. Pat., 1993, 93 310 745; *CA*, **120**, 226939w

Dieporeticanin D-178



Dieporeticanin 1 m=1, n=3
" 2 m=3, n=1

Constit. of *Annona reticulata* (custard apple). Amorph. solid. $[\alpha]_D$ +12 (c, 1 in $CHCl_3$). Isol. as a 1:1 mixture of Dieporeticanin 1 and 2.

Dieporeticanin 1 [160525-55-3]

[129196-64-1]
Epoxyrollin A

$C_{37}H_{66}O_4$ 574.926
Identity of Epoxyrollin A and Dieporeticanin 1 not certain. Konno *et al* (1996) suggest that the struct. of Epoxyrollin A needs revision.

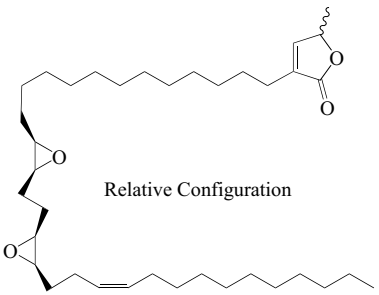
Dieporeticanin 2 [160525-56-4]

$C_{37}H_{66}O_4$ 574.926

Laprevote, O. *et al., Tet. Lett.*, 1990, **31**, 2283-2286 (*Epoxyrollin A*)
Vu Thi Tam, *et al., Nat. Prod. Lett.*, 1994, **4**, 255-262 (*isol, uv, ir, pmr, cmr, ms*)
Konno, H. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2355 (*pmr, cmr, ms*)
Konno, H. *et al., Tetrahedron*, 1996, **37**, 9399 (*synth*)

Dieporeticenin D-179

[160544-67-2]

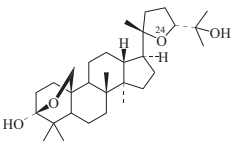


$C_{37}H_{64}O_4$ 572.91

Constit. of *Annona reticulata* (custard apple). Wax. $[\alpha]_D$ +11 (c, 1 in $CHCl_3$). λ_{max} 208 (MeOH).

Vu Thi Tam, *et al., Nat. Prod. Lett.*, 1994, **4**, 255-262 (*isol, uv, ir, pmr, cmr, ms*)

3,19:20,24-Diepoxydammarane-3,25-diol D-180



(3α*OH*,20*S*,24*R*)-*form*

$C_{30}H_{50}O_4$ 474.723

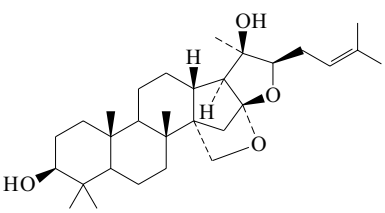
(3α*OH*,20*S*,24*R*)-*form* [149172-44-1]
Cryst. (EtOH). Mp 100°.

(3α*OH*,20*S*,24*S*)-*form* [189031-58-1]
Constit. of *Cleome gynandra* (cat's whiskers). Cryst. Mp 108-110°. $[\alpha]_D^{25}$ +115.4 (c, 0.35 in EtOH).

Tsichritzis, F. *et al., Phytochemistry*, 1993, **33**, 423 (*isol, pmr, cmr*)

Das, P.C. *et al., J. Nat. Prod.*, 1999, **62**, 616-618 (*isol, pmr, cmr*)

16,18;16,22-Diepoxydammar-24-ene-3,20-diol D-181



$C_{30}H_{48}O_4$ 472.707

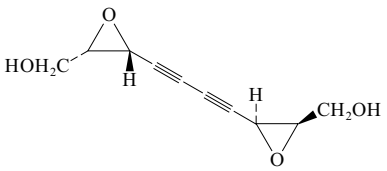
(3β,20*R*,22*S*)-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-galactopyranoside]:* [146445-93-4] ***Jujubasaponin IV***
$C_{48}H_{78}O_{18}$ 943.133
Constit. of *Zizyphus jujuba* (Chinese date). Amorph. powder. Mp 185-187°. $[\alpha]_D$ -3.64 (c, 5 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]:* [146503-31-3] ***Jujubasaponin V***
$C_{48}H_{78}O_{18}$ 943.133
Constit. of *Zizyphus jujuba* (Chinese date). Amorph. powder. Mp 210-212°. $[\alpha]_D$ -14.2 (c, 4.3 in MeOH).

Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2275 (*isol, pmr, cmr*)

2,3:8,9-Diepoxy-4,6-decadiyne-1,10-diol D-182



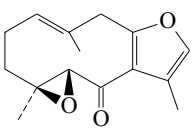
$C_{10}H_{10}O_4$ 194.187

(2*R*,3*R*,8*R*,9*R*)-*form* [147921-90-2]
Repandiol
Constit. of the edible mushrooms *Hydnum repandum* and *Hydnum repandum* var. *album*. Leaflets (MeOH). Mp 168-169°. $[\alpha]_D^{19}$ +40 (c, 0.12 in MeOH). λ_{max} 203 (ϵ 28900); 229 (ϵ 4460); 241 (ϵ 6200); 255 (ϵ 7250); 269 (ϵ 5550) (MeOH) (Berdy).
▶ Cytotoxic.

Di-Ac:
Amorph. powder. $[\alpha]_D^{26}$ +63.4 (c, 0.12 in $CHCl_3$).

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1992, **40**, 3181 (*isol, pmr, cmr, synth, struct*)

4,5:8,12-Diepoxy-1(10),7,11-germacratrien-6-one D-183



$C_{15}H_{18}O_3$ 246.305

The incorrect abs. config. was assigned in 1971.

(1(10)*E*,4β,5β)-*form* [7727-79-9]
Zederone
Constit. of the rhizome of *Curcuma zedoaria* (zedoary). Cryst. (EtOAc). Mp 153.5-154°. $[\alpha]_D$ +265.8 (c, 0.5 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1081 (*isol, struct*)

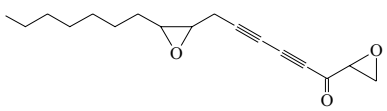
Shibuya, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 924 (*abs config, cryst struct*)

Phan, M.G. *et al., Tap Chi Hoa Hoc*, 2000, **38**, 91-94 (*activity*)

Pant, N. *et al., Indian J. Chem., Sect. B*, 2001, 87-88 (*cmr*)

1,2:9,10-Diepoxy-4,6-heptadecadiyn-8-one D-184

[145427-82-3]
Panaquinquecol 4. *PQ 4*



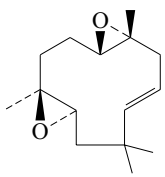
$C_{17}H_{22}O_3$ 274.359

Constit. of *Panax quinquefolium* (American ginseng). Oil. $[\alpha]_D$ -55.5 (c, 0.6 in $CHCl_3$).

Fujimoto, Y. *et al., Phytochemistry*, 1992, **31**, 3499 (*isol, pmr, cmr*)

2,3:6,7-Diepoxy-9-humulene D-185

[118899-63-1]
Humulene diepoxide A



$C_{15}H_{24}O_2$ 236.353

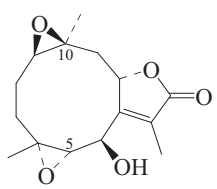
Constit. of hops, *Zingiber zerumbet* (wild ginger). Needles ($CHCl_3$). Mp 106-107°. $[\alpha]_D$ -83.5 ($CHCl_3$).

Peacock, V.E. *et al., J. Am. Soc. Brew. Chem.*, 1989, **47**, 4 (*isol, cryst struct*)

Takeda, S. *et al., Chem. Lett.*, 1990, 155 (*abs config*)

Heymann, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 138 (*isol, pmr, cmr*)

1,10:4,5-Diepoxy-6-hydroxy-7(11)-germacren-12,8-olide D-186

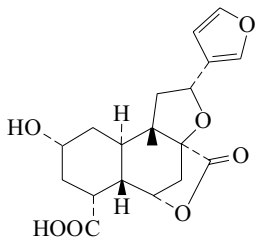


$C_{15}H_{20}O_5$ 280.32

(1β,4α,5α,6β,8α,10β)-*form* [366494-94-2]
Constit. of *Smyrnium olusatrum* (alexanders). Cryst. (MeOH). Mp 165-168°. λ_{max} 217 (MeOH).

El-Gamal, A.A. *et al., Phytochemistry*, 2001, **57**, 1197-1200 (*isol, pmr, cmr*)

8,12:15,16-Diepoxy-2-hydroxy-19-nor-13(16),14-clerodadien-17,6-olid-18-oic acid D-187



$C_{19}H_{22}O_7$ 362.379

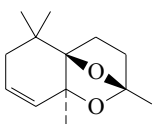
(2α,4β*H*,5β,6α,8β,12β*H*)-*form* [20086-07-1]
Diosbulbin C
Constit. of *Dioscorea bulbifera* (air potato). Cryst. (Me_2CO). Mp 247-250° dec. $[\alpha]_D^{20}$ +64.7 (c, 0.35 in Py).

Me ester: [20086-05-9] ***Diosbulbin A***
$C_{20}H_{24}O_7$ 376.405
Constit. of *Dioscorea bulbifera* (air potato). Cryst. Mp 265° dec.

Kawasaki, T. *et al., Chem. Pharm. Bull.*, 1968, **16**, 2430 (*isol*)
Kamiya, K. *et al., Tet. Lett.*, 1972, 1869 (*cryst struct*)
Komori, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1701 (*abs config*)

5,9:6,9-Diepoxy-3-megastigmene D-188

2,2,6,8-Tetramethyl-7,11-dioxatricyclo[6.2.1.0^{1,6}]undec-4-ene

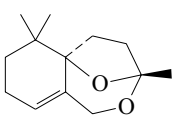


$C_{13}H_{20}O_2$ 208.3
Constit. of quince fruit (*Cydonia oblonga*) brandy and Riesling wine.

Näf, R. *et al., Tet. Lett.*, 1991, **32**, 753 (*struct, synth*)

5,9:6,9-Diepoxy-4-megastigmene D-189

[133661-30-0]
2,2,9-Trimethyl-8,12-dioxatricyclo[7.2.1.0^{1,6}]dodec-5-ene

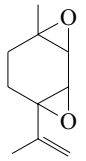


$C_{13}H_{20}O_2$ 208.3
Constit. of quince fruit (*Cydonia oblonga*) brandy.

Näf, R. *et al., Tet. Lett.*, 1991, **32**, 753 (*struct, synth*)

1,2:3,4-Diepoxy-*p*-menth-8-ene D-190

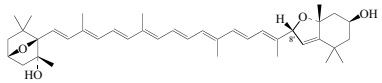
[120749-18-0]
1,2:3,4-Bisepoxy-p-*menth-8-ene*



$C_{10}H_{14}O_2$ 166.219
Constit. of parsley leaves (*Petroselinum crispum*).

Nitz, S. *et al., Phytochemistry*, 1989, **28**, 3051 (*isol, pmr, ms, ir*)

3,6:5′,8′-Diepoxy-5,5′,6,8′-tetrahydro-β,β-carotene-3′,5-diol D-191



(3S,3'S,5R,5'R,6R,8'R)-form

$C_{40}H_{56}O_4$ 600.88

(3*S*,3′*S*,5*R*,5′*R*,6*R*,8′*R*)-*form* [181229-73-2]
Cucurbitachrome 1
Constit. of ripe pods of red paprika (*Capsicum annuum* var. *longum*).

(3*S*,3′*S*,5*R*,5′*R*,6*R*,8′*S*)-*form* [181229-74-3]
Cucurbitachrome 2
Constit. of ripe pods of red paprika (*Capsicum annuum* var. *longum*). Yellow cryst. Mp 182-184°.

Deli, J. *et al., Helv. Chim. Acta*, 1996, **79**, 1435-1443 (*isol, pmr, cmr, cd*)

1,1-Diethoxyethane, 9CI D-192

[105-57-7]
Acetal. Acetaldehyde diethyl acetal. Ethylidene diethyl ether. FEMA 2002
$H_3CCH(OEt)_2$
$C_6H_{14}O_2$ 118.175
Acetal of Acetaldehyde, A-20. Flavouring ingredient used in fruit, rum and whisky flavours. Liq. Mod. sol. H_2O, misc. EtOH. Bp 103.2° Bp_{22} 21°. n_D^{20} 1.3805.
▶ Highly flammable, fl. p. -21°. Peroxidizable. Eye and skin irritant. High vapour conc. prob. narcotic. AB2800000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 214B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 349A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 282C (*ir*)
Aldrich Library of NMR Spectra, **1**, 137A (*pmr*)
Org. Synth., Coll. Vol., 1, 1932, 1 (*synth*)
Vericat, J.B. *et al., CA*, 1945, **39**, 3784 (*synth*)
Borisova, I.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1981, 1518; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1981, 1518 (*ms*)
Dostovalova, V.I. *et al., Magn. Reson. Chem.*, 1987, **25**, 1 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 3
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 7-8
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2391
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 445
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAG000

Diethyl disulfide, 9CI D-193

[110-81-6]
Ethyl disulfide. 3,4-Dithiahexane
Et–S–S–Et
$C_4H_{10}S_2$ 122.255
Present in durian fruit. Oil with garlic odour. Spar. sol. H_2O. d_4^{20} 0.99. Bp 154° Bp_{11} 46°. n_D^{20} 1.5063.
▶ Flammable, fl. p. 42°. Skin and eye irritant. LD_{50} (rat , orl) 2030 mg/kg. JO1925000

S,S′-Dioxide:Diethyl disulfoxide
$C_4H_{10}O_2S_2$ 154.254
Liq. with garlic odour. $d^{19.5}$ 1.2. Bp_{11} 123-124°. Prob. a mixt. of diastereoisomers.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 266A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 427B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 348D (*ir*)
Otto, R. *et al., Ber.*, 1882, **15**, 125 (*dioxide*)
Haines, W.E. *et al., J. Phys. Chem.*, 1954, **58**, 270 (*props, ir, uv*)
Baldry, J. *et al., Phytochemistry*, 1972, **11**, 2081-2087 (*isol*)
Cohen, V.I. *et al., Helv. Chim. Acta*, 1976, **59**, 840 (*synth*)
Drabowicz, J. *et al., Synthesis*, 1980, 32 (*synth*)
Rybin, A.G. *et al., Zh. Obshch. Khim.*, 1983, **53**, 1863 (*synth*)
Meshram, H.M. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 232 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DJC600

Diethyl malonate D-194

[105-53-3]
Diethyl propanedioate, 9CI. Malonic ester. Ethyl malonate. FEMA 2375
$H_2C(COOEt)_2$
$C_7H_{12}O_4$ 160.169
Flavour ingredient. Present in guava fruit, melon, concord grape, pineapple, blackberry and many wines and spirits. Liq. with aromatic odour. Sl. sol. H_2O; sol. EtOH, Et_2O, $CHCl_3$, C_6H_6. d_4^{20} 1.06. Mp -50°. Bp 198.9° Bp_{20} 85°. n_D^{20} 1.4143.
▶ Low oral toxicity. OO0700000

Na deriv: [996-82-7]
$C_7H_{11}NaO_4$ 182.151
Needles (EtOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 614B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 935B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 637A (*ir*)
Conrad, M. *et al., Annalen*, 1880, **204**, 121-203 (*Na deriv*)
Lux, H. *et al., Ber.*, 1929, **62**, 1824 (*synth*)
Shaw, J.E. *et al., J.O.C.*, 1974, **39**, 1968 (*synth*)
Large, R. *et al., Org. Mass Spectrom.*, 1976, **11**, 582 (*ms*)
Yamashita, M. *et al., Chem. Lett.*, 1977, 1355 (*synth*)
Ono, N. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 2401 (*synth*)
Kiyooka, S. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 2318 (*pmr*)

Bauer, S.H. *et al., J. Phys. Chem.*, 1983, **87**, 2411 (*cmr*)
Shim, S.C. *et al., Synthesis*, 1987, 59 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EMA500
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **15**, 930 (*props*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1822-1825 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EMA500

Diethyl sulfide D-195

[352-93-2]
1,1′-Thiobisethane, 9CI. Ethyl sulfide, 8CI. 3-Thiapentane. Diethyl thioether. Ethyl thioether. FEMA 3825

EtSEt

$C_4H_{10}S$ 90.189
Food additive listed in the EAFUS Food Additive Database (Jan 2001). Found in various foods and brandies. Food flavour ingredient. Liq. with garlic/ethereal odour. Insol. H_2O. d_4^{20} 0.84. Fp -102.05. Bp 92°. n_D^{20} 1.4423.

▶ Highly flammable, fl. p. -10°. Eye and skin irritant. Evolves H_2S on contact with acids. LC7200000

S-*Oxide:* See Diethyl sulfoxide in *The Combined Chemical Dictionary.*

S,S-*Dioxide:* See Diethyl sulfone in *The Combined Chemical Dictionary.*

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 427A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 265B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 348C (*ir*)
Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1963, **82**, 68 (*synth*)
Drefahl, G. *et al., Z. Chem.*, 1964, **4**, 347 (*synth*)
Cumper, C.W.N. *et al., J.C.S.(A)*, 1966, 239 (*uv*)
Wilson, G. *et al., Tet. Lett.*, 1972, 379 (*synth*)
Fujisawa, T. *et al., Chem. Lett.*, 1973, 1241 (*synth*)
Barbarella, G. *et al., Org. Magn. Reson.*, 1976, **8**, 108 (*cmr*)
Hamada, K. *et al., Spectrosc. Lett.*, 1977, **10**, 357 (*pmr, ir*)
Wagner, W. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1980, **36**, 125 (*ms*)
Mizhiritskii, M.D. *et al., Zh. Obshch. Khim.*, 1986, **56**, 1547; *J. Gen. Chem. USSR (Engl. Transl.)*, 1986, **56**, 1373 (*synth*)
Christesen, S.D. *et al., J. Raman Spectrosc.*, 1991, **22**, 459 (*ir, Raman*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EPH000

Diethyl trisulfide, 9CI D-196

[3600-24-6]
Ethyl trisulfide, 8CI. 3,4,5-Trithiaheptane

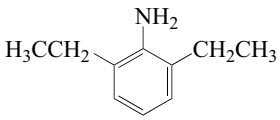
Et-S-S-S-Et

$C_4H_{10}S_3$ 154.321
Cystine thermal degradation product. Aroma constit. of salted pork, cooked beef and durian fruit (*Durio zibethinus*). Bp_3 81-83°.

Golovnya, R.V. *et al., Nahrung*, 1980, **24**, 141-154; 1982, **26**, 89-96 (*occur, pork, beef*)
Shu, C.-K. *et al., J. Agric. Food Chem.*, 1985, **33**, 438-442 (*occur*)
Capozzi, G. *et al., Tet. Lett.*, 1989, **30**, 2991-2994 (*synth*)
Naef, R. *et al., Flavour Fragrance J.*, 1996, **11**, 295-303 (*occur, durian*)

2,6-Diethylaniline, 8CI D-197

[579-66-8]
2,6-Diethylbenzenamine, 9CI



$C_{10}H_{15}N$ 149.235
Terminal metab. of Alachlor, A-150 in soil and animals. Liq. d 0.96. Fp 3-4. Bp 235-236° Bp_{10} 111°. n_D^{20} 1.5460. Light-sensitive.

Hydrochloride: [71477-82-2]
Cryst. (HCl aq.). Mp 175-179° dec.

N-*Ac:* [16665-89-7]
$C_{12}H_{17}NO$ 191.272
Soil degradn. prod. of Alachlor, A-150. Cryst. Mp 141-142° (130-131°).

N-*Benzoyl:*
$C_{17}H_{19}NO$ 253.343
Cryst. Mp 232-233°.

N-*Chloroacetyl:* [6967-29-9]
$C_{12}H_{16}ClNO$ 225.717
Soil degradn. prod. of Alachlor, A-150. Cryst. (H_2O). Mp 135-136°.

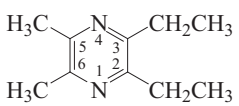
▶ Bacterial mutagen.

N-*(4-Methylbenzenesulfonyl):* [4703-16-6]
$C_{17}H_{21}NO_2S$ 303.424
Cryst. (C_6H_6). Mp 132-133°.

U.S. Pat., 1954, 2 762 845; *CA*, **51**, 5116i (*synth*)
Stroh, R. *et al., Angew. Chem.*, 1957, **69**, 124-131 (*synth, N-Ac, N-benzoyl*)
Ecke, G.G. *et al., J.O.C.*, 1957, **22**, 639-642 (*synth*)
Bavin, P.M.G. *et al., Can. J. Chem.*, 1958, **36**, 1284-1288 (*derivs*)
Tiedje, J.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 77-81 (*occur, derivs*)
U.S. Pat., 1979, 4 169 106; *CA*, **91**, 39160f (*N-chloroacetyl*)
Eur. Pat., 1980, 8 057; *CA*, **93**, 114508x (*N-chloroacetyl*)
Rolls, W.A. *et al., J. Chromatogr.*, 1990, **504**, 97 (*hplc*)
Tessier, D.M. *et al., J. Agric. Food Chem.*, 1995, **43**, 2504-2512 (*occur, props, bibl*)

2,3-Diethyl-5,6-dimethylpyrazine D-198

[106060-96-2]



$C_{10}H_{16}N_2$ 164.25
Roast coffee aroma constit.. Characterised spectroscopically.

Baltes, W. *et al., J. Agric. Food Chem.*, 1987, **35**, 340-346 (*occur, coffee, ms*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1988, **36**, 349-352 (*occur, ms, uv*)

2,5-Diethyl-3,6-dimethylpyrazine D-199

[18903-30-5]

$C_{10}H_{16}N_2$ 164.25
Constit. of cooked beef and roast coffee aroma. Maillard product. Liq. Bp 214-217° Bp_2 65°.

Octahydrate:
Mp 48-50°.

Asinger, F. *et al., Monatsh. Chem.*, 1959, **90**, 402-416 (*synth*)
Baltes, W. *et al., J. Agric. Food Chem.*, 1987, **35**, 340-346 (*occur, coffee, ms*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1988, **36**, 349-352 (*synth, ms, pmr, uv*)
Silwar, R. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 112-119 (*occur*)

2,6-Diethyl-3,5-dimethylpyrazine D-200

[18940-74-4]

$C_{10}H_{16}N_2$ 164.25
Constit. of roast coffee aroma. Maillard product. Characterised spectroscopically.

Baltes, W. *et al., J. Agric. Food Chem.*, 1987, **35**, 340-346 (*occur, coffee, ms*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1988, **36**, 349-352 (*occur, ms, uv*)
Silwar, R. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 112-119 (*occur*)

Diethylenetriamine, 8CI D-201

[111-40-0]
N-*(2-Aminoethyl)-1,2-ethanediamine, 9CI. Di(2-aminoethyl)amine. 2,2′-Diaminodiethylamine. Bis(2-aminoethyl)amine. 3-Aza-1,5-pentanediamine. 3-Aza-1,5-diaminopentane. 2,2′-Iminobisethylamine. 2,2′-Iminodi(ethylamine). 1,4,7-Triazaheptane*

$H_2NCH_2CH_2N'HCH_2CH_2N''H_2$

$C_4H_{13}N_3$ 103.167
Constituent of ion-exchange resins for use in food processing, e.g. in the production of grapefruit juice. Viscous liq. with an ammoniacal odour. Misc. H_2O, EtOH. d_4^{20} 0.95. Mp -39°. Bp 208° Bp_3 82-83°. n_D^{20} 1.4826. pK_{a1} 10.1; pK_{a2} 9.1; pK_{a3} 3.9 (25°). Vp 0.37 mmHg (20°).

▶ Corrosive and irritating to skin, eyes and respiratory tract. Skin and pulmonary sensitiser. LD_{50} (rat, orl) 1080 mg/kg. LD_{50} (rbt, skn) 1090 mg/kg. Fl. p. 98° (oc), autoignition temp. 358°. OES: long-term 1 ppm (Sk). IE1225000

Hydrochloride (1:3): [4109-20-0]
Needles (EtOH/HCl). Mp 228-230° dec.

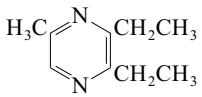
[37296-80-3, 52601-80-6, 56187-04-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 308C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 499B; 499C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 396A (*ir*)
Fargher, R.G. *et al., J.C.S.*, 1920, **117**, 1351 (*synth, derivs*)
Sudmeier, J.L. *et al., Anal. Chem.*, 1964, **36**, 1698 (*pmr*)
Hague, D.N. *et al., J.C.S. Dalton*, 1987, 2889 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **8**, 74 (*rev*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 814-815
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 60
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 711
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DJG600; PBG500

2,3-Diethyl-5-methylpyrazine, 8CI D-202

[18138-04-0]
FEMA 3336



$C_9H_{14}N_2$ 150.223
Aroma constit. of Parmesan cheese, roasted filbert, roasted peanut, baked or chipped potato, cooked chicken, beef, lamb, mutton and pork. Present in galbanum oil. Flavouring agent. Bp_{12} 79-80°. n_D^{20} 1.4980.

U.S. Pat., 1975, 3 924 015; *CA*, **84**, 164364g (*synth*)
Masuda, H. *et al., J. Agric. Food Chem.*, 1981, **29**, 944 (*occur*)
Mihara, S. *et al., J. Chromatogr.*, 1987, **402**, 309 (*glc*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 819-820 (*use, occur*)

2,5-Diethyl-3-methylpyrazine, 9CI D-203

[32736-91-7]
FEMA 3915

$C_9H_{14}N_2$ 150.223
Present in coffee aroma; flavouring ingredient. Present in various cooked foods, e.g. potato, beef, pork, cocoa, coffee, bread, sesame seed, soyabean etc.. No phys. props. reported.

Gianturco, M.A. *et al., J. Agric. Food Chem.*, 1971, **19**, 530-532 (*occur*)
Friedel, P. *et al., J. Agric. Food Chem.*, 1971, **19**, 530-532 (*occur, coffee, ir, ms*)
U.S. Pat., 1975, 3 924 015; *CA*, **84**, 164364g (*synth, use*)
Ohta, A. *et al., Heterocycles*, 1984, **22**, 2317-2321 (*synth*)
Macleod, G.A. *et al., Flavour Fragrance J.*, 1986, **1**, 91-104 (*occur, beef*)
Fadel, H.H.M. *et al., Nahrung*, 1993, **37**, 386-394 (*occur, bread*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 411 (*use, occur*)

3,5-Diethyl-2-methylpyrazine D-204

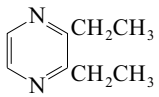
[18138-05-1]
FEMA 3916

$C_9H_{14}N_2$ 150.223
Found in potato, chicken, beef and pork, tea, coffee, galbanum oil and other foods. Flavouring agent.

Kato, S. *et al., Agric. Biol. Chem.*, 1970, **34**, 1826 (*synth*)
Burrell, J.W.K. *et al., Chem. Ind. (London)*, 1970, 1409 (*isol*)
Shigematsu, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 1631 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 410

2,3-Diethylpyrazine, 9CI, 8CI D-205

[15707-24-1]
FEMA 3136



$C_8H_{12}N_2$ 136.196
Flavour component in cooked foods, e.g. baked potato, wheat bread and roasted filbert. Flavouring ingredient. Bp 180-182°. n_D^{20} 1.5000.

Rizzi, G.P. *et al., J.O.C.*, 1968, **33**, 1333 (*synth*)
Gianturco, M.A. *et al., J. Agric. Food Chem.*, 1971, **19**, 530 (*ms, ir*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 126 (*ir*)
Tsai, S. *et al., CA*, 1984, **104**, 168437 (*synth*)
Stanton, D.T. *et al., Anal. Chem.*, 1989, **61**, 1328 (*glc*)

2,5-Diethylpyrazine, 9CI, 8CI D-206

[13238-84-1]

$C_8H_{12}N_2$ 136.196
Constit. of roasted coffee beans. Used in food flavouring. Bp 187-188°.

Picrate:
Mp 93°.
N^1*-Oxide:* [65257-55-8]
$C_8H_{12}N_2O$ 152.196
Oil. Bp_{10} 135-140°.
N^1,N^4*-Dioxide:* [65257-59-2]
$C_8H_{12}N_2O_2$ 168.195
Mp 208-209°.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694 (*isol, glc, ms*)
U.S. Pat., 1969, 3 453 278; *CA*, **71**, 91526 (*manuf*)
Ohta, A. *et al., Chem. Pharm. Bull.*, 1979, **27**, 2027 (*synth, oxides*)

2,6-Diethylpyrazine, 9CI, 8CI D-207

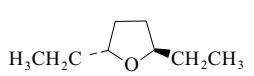
[13067-27-1]

$C_8H_{12}N_2$ 136.196
Constit. of roasted coffee beans. Used in food flavouring. Bp_{10} 70°.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694 (*isol, glc, ms*)
U.S. Pat., 1976, 3 952 026; *CA*, **85**, 94216e (*synth, use*)
Tsai, S. *et al., CA*, 1986, **104**, 168437n (*synth*)

2,5-Diethyltetrahydrofuran, 9CI D-208

[41239-48-9]
FEMA 3743



(2*R*,5*R*)-*form*

$C_8H_{16}O$ 128.214
Used in flavour compositions. Present in Spanish origanum (*Coridothymus capitatus*) and lemon balm (*Melissa officinalis*). Liq. with fruity-herbal odour.
▶ LU0650000

(2*R*,5*R*)-*form* [32101-31-8]
(-)-trans-*form*
Constit. of the essential oil of *Mentha* spp.. Bp 143-144°. $[\alpha]_D^{24}$ -9.9 (c, 2 in EtOH).

(2*S*,5*S*)-*form*
(+)-trans-*form*
Bp 142-144°. $[\alpha]_D^{24}$ +4.4 (c, 1.2 in EtOH).

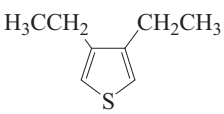
(2*RS*,5*RS*)-*form*
(±)-trans-*form*
Bp 142-144°. n_D^{24} 1.4222.

(2*RS*,5*SR*)-*form* [5921-97-1]
cis-*form*
Bp 140-142°. n_D^{24} 1.4168.

Mihailovic, M.L. *et al., Tetrahedron*, 1967, **23**, 215 (*synth, abs config*)
Itahara, Y. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 3947 (*isol, synth*)

3,4-Diethylthiophene D-209

[35686-14-7]



$C_8H_{12}S$ 140.249
Flavour component of various cooked meats. Bp_{12} 70°. n_D^{20} 1.5160.

Boelens, H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1972, **91**, 141-145 (*synth, pmr*)
Werkhoff, P. *et al., CA*, 1995, **122**, 313271g (*occur*)

Diflubenzuron, ANSI, BSI, ISO D-210

[35367-38-5]
N-[[(4-Chlorophenyl)amino]carbonyl]-2,6-difluorobenzamide, 9CI. 1-(4-Chlorophenyl)-3-(2,6-difluorobenzoyl)urea. Dimilin



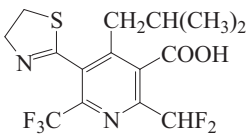
$C_{14}H_9ClF_2N_2O_2$ 310.687
Insecticide, interfering with chitin deposition by oral absorption. Used on soya beans, citrus, tea, vegetables and mushrooms. Also used as an insecticide in feed for poultry and pigs and as a controlled release bolus in cattle. Cryst. Mp 230-232° dec. pK_a 13.92.
▶ LD_{50} (rat, orl) 4640 mg/kg; LD_{50} (rbt, skn) 2000 mg/kg. YS6200000

U.K. Pat., 1970, 1 324 293; *CA*, **76**, 85578m
Cruse, W.B.T. *et al., Acta Cryst. B*, 1978, **34**, 2904 (*cryst struct*)
Rabenort, B. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1978, **10**, 57 (*rev, props*)
Riley, W.C. *et al., Cryst. Struct. Commun.*, 1981, **10**, 1341 (*cryst struct*)

Marks, E.P. *et al., Insectic. Mode Action*, (Coats, J.R. Ed.), Academic Press, N.Y., 1982, 281 (*biochem*)
Nakagawa, Y. *et al., Pestic. Biochem. Physiol.*, 1984, **21**, 309 (*synth, activity*)
Kavalek, J. *et al., Coll. Czech. Chem. Comm.*, 1989, **54**, 1363 (*synth*)
Howbert, J.J. *et al., J. Med. Chem.*, 1990, **33**, 2393 (*activity*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A148
Pesticide Manual, 11th edn., 1997, No. 231
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CJV250

2-(Difluoromethyl)-5-(4,5-dihydro-2-thiazolyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-3-pyridinecarboxylic acid, 9CI D-211

[117717-36-9]



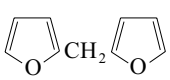
$C_{15}H_{15}F_5N_2O_2S$ 382.354

Me ester: [117718-60-2] ***Thiazopyr, ANSI, BSI***. *Methyl 2-(difluoromethyl)-5-(4,5-dihydro-2-thiazolyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-3-pyridinecarboxylate. Visor. MON 13200. RH 123652*
$C_{16}H_{17}F_5N_2O_2S$ 396.381
Pre-emergence control herbicide, inhibitor of cell division. Used on fruit trees, vines sugar cane, pineapples and citrus fruits. Pale orange cryst. (hexane). Mp 79-81° Mp 77-79°.
► LD_{50} (rat, orl) >5000 mg/kg.

Eur. Pat., (Monsanto), 1988, 278 944; *CA*, **109**, 230818w (*Me ester, synth, activity*)
Armbruster, B.L. *et al., Pestic. Biochem. Physiol.*, 1991, **39**, 110-120 (*Me ester, activity*)
U.S. Pat., 1991, 4 988 384; *CA*, **109**, 230818w (*Me ester, synth, use*)
Feng, P.C.C. *et al., Xenobiotica*, 1994, **24**, 729-734; 1995, **25**, 27-35 (*Me ester, metab*)
Warner, H.L. *et al., Brighton Crop Prot. Conf. - Weeds*, 1995, 942-946 (*activity*)
Feng, P.C.C. *et al., Pestic. Sci.*, 1995, **45**, 203-207 (*metab*)
Pesticide Manual, 12th edn., 2000, No. 752

Di-2-furanylmethane D-212

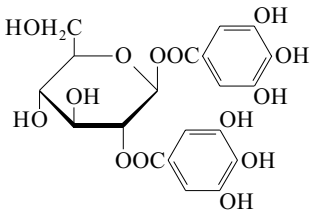
[1197-40-6]
2,2′-Methylenebisfuran, 9CI



$C_9H_8O_2$ 148.161
Minor constit. of coffee. Liq. Mp -26°. Bp_{13} 75°. n_D^{22} 1.5038.

Gilman, H. *et al., J.A.C.S.*, 1933, **55**, 3302
Cairns, T.L. *et al., J.A.C.S.*, 1951, **73**, 1270
Takano, K. *et al., Nippon Kagaku Zasshi*, 1961, **82**, 373; *CA*, **56**, 10071b (*ir*)
Gianturco, M.A. *et al., Tetrahedron*, 1964, **20**, 2951 (*synth, isol*)
Ferretti, A. *et al., Org. Mass Spectrom.*, 1974, **8**, 403 (*ms*)
Stibor, I. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 987 (*pmr, cmr*)
Schwenter, M.-E. *et al., Chem. Eur. J.*, 2000, **6**, 4091-4103 (*synth*)

1,2-Digalloylglucose D-213

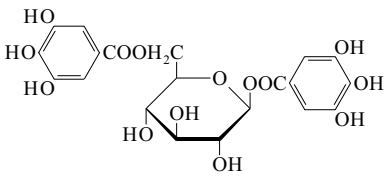


$C_{20}H_{20}O_{14}$ 484.37

β-D-Pyranose-*form* [115713-50-3]
Isol. from *Rheum* sp.. Needles + $2H_2O$ (H_2O). Mp 169-170°. $[\alpha]_D^{17}$ -79.1 (c, 0.64 in Me_2CO).

Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1473 (*struct, pmr, cmr*)
Lee, S.H. *et al., Phytochemistry*, 1989, **28**, 3469 (*pmr*)

1,6-Digalloylglucose D-214



$C_{20}H_{20}O_{14}$ 484.37

β-D-Pyranose-*form* [23363-08-8]
Present in commercial rhubarb. Needles + $\frac{1}{2}H_2O$ (H_2O). Mp 204-206°. $[\alpha]_D^{20}$ -20 (c, 0.4 in Me_2CO).

Haddock, E.A. *et al., J.C.S. Perkin 1*, 1982, 2515 (*struct, pmr*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1652 (*pmr, cmr*)
Saijo, R. *et al., Phytochemistry*, 1990, **29**, 267 (*pmr*)

2,6-Digalloylglucose D-215

[94356-20-4]

$C_{20}H_{20}O_{14}$ 484.37

Exists as an equilibrated mixt. of α- and β-anomers. Isol. from *Rheum* sp.. Needles + $2H_2O$ (H_2O). Mp 184-186°. $[\alpha]_D$ -18.5 (c, 0.62 in Me_2CO).

Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461 (*struct, pmr, cmr*)
Nawwar, M.A.M. *et al., Phytochemistry*, 1994, **36**, 1035 (*isol, pmr, cmr*)

4,6-Digalloylglucose D-216

$C_{20}H_{20}O_{14}$ 484.37

Exists as an equilibrated mixt. of α- and β-anomers.

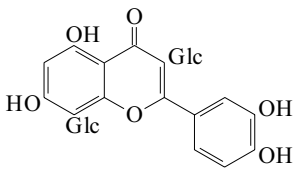
D-*form*
Light brown amorph. powder. $[\alpha]_D^{25}$ +49.3 (c, 1.1 in MeOH).

β-D-Pyranose-*form*
Me glycoside: [88847-08-9] *Methyl 4,6-di-O-galloyl-β-D-glucopyranoside*
$C_{21}H_{22}O_{14}$ 498.396
Gallotannin from *Sanguisorba officinalis* (burnet bloodwort). Tan amorph. powder. $[\alpha]_D^{24}$ +22 (c, 0.4 in Me_2CO).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1176
Lee, M.-W. *et al., Phytochemistry*, 1992, **31**, 2835

3,8-Diglucopyranosyl-3′,4′,5,7-tetrahydroxyflavone D-217

2-(3,4-Dihydroxyphenyl)-3,8-di-β-D-glucopyranosyl-5,7-dihydroxy-4H-1-benzopyran-4-one



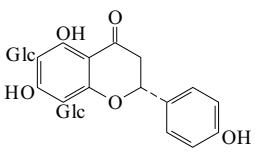
$C_{27}H_{30}O_{16}$ 610.524

4′-Me ether: [97218-32-1] *3,8-Diglucopyranosyl-3′,5,7-trihydroxy-4′-methoxyflavone. 3,8-Diglucopyranosyldiosmetin. 3,8-Diglucosyldiosmetin*
$C_{28}H_{32}O_{16}$ 624.551
Isol. from peelings of *Citrus sinensis* (orange).

Matsubara, Y. *et al., CA*, 1985, **103**, 42455
Kumamoto, H. *et al., Agric. Biol. Chem.*, 1986, **50**, 781

6,8-Diglucopyranosyl-4′,5,7-trihydroxyflavanone D-218

6,8-Di-β-D-glucopyranosyl-2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. 6,8-Diglucopyranosylnaringenin. 6,8-Diglucosylnaringenin



(*R*)-*form*

$C_{27}H_{32}O_{15}$ 596.541

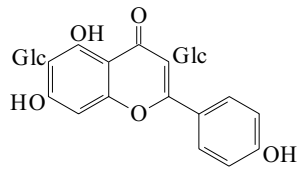
(2*R*)-*form* [81446-26-6]
Constit. of *Zizyphus jujuba* (Chinese date). Powder (as per-Ac). $[\alpha]_D^{21}$ -43.1 (c, 1.48 in $CHCl_3$) (per-Ac).

(2*S*)-*form* [81426-09-7]
Constit. of *Zizyphus jujuba* (Chinese date). Powder (as per-Ac). $[\alpha]_D^{21}$ -40.8 (c, 2.05 in $CHCl_3$) (per-Ac).

Okamura, N. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3507 (*isol*)

3,6-Diglucopyranosyl-4′,5,7-trihydroxyflavone D-219

[90456-55-6]
3,6-Di-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. 3,6-Diglucopyranosylapigenin. 3,6-Diglucosylapigenin



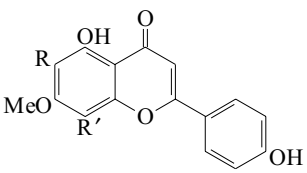
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Citrus unshiu* (satsuma mandarin). No phys. props. reported.

4′-Me ether: [98891-91-9] ***3,6-Diglucopyranosyl-5,7-dihydroxy-4′-methoxyflavone.*** *3,6-Diglucopyranosylacacetin. 3,6-Diglucosylacacetin*
$C_{28}H_{32}O_{15}$ 608.552
Isol. from *Fortunella japonica* (round kumquat). Yellow needles. Mp 210° dec.

Matsubara, Y. *et al., Agric. Biol. Chem.*, 1985, **49**, 909 (*isol*)
Kumamoto, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 2613 (*deriv*)

6,8-Dihexosyl-4′,5-dihydroxy-7-methoxyflavone D-220

6,8-Di-C-hexosylgenkwanin



R,R′ = Hexosyl residues

$C_{28}H_{30}O_{15}$ 606.536
Isol. from roots of *Glycine max* (soybean). No phys. props. reported.

Jay, M. *et al., Phytochemistry*, 1984, **23**, 1153

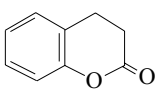
1,1-Dihexyloxyethane D-221

[5405-58-3]
1,1′-[Ethylidenebis(oxy)]bis[hexane], 9CI. Acetaldehyde dihexyl acetal
$H_3CCH(OCH_2CH_2CH_2CH_2CH_2CH_3)_2$
$C_{14}H_{30}O_2$ 230.39
Present in strawberry volatiles. Liq. d_4^{20} 0.83. Bp_{24} 152-154° $Bp_{2.2}$ 95-100°. n_D^{20} 1.4223.

Friedel, R.A. *et al., Anal. Chem.*, 1956, **28**, 940 (*ms*)
McFadden, W.H. *et al., J. Chromatogr.*, 1965, **18**, 10 (*isol*)
Barot, B.C. *et al., J.O.C.*, 1981, **46**, 2981 (*synth*)

3,4-Dihydro-2*H*-1-benzopyran-2-one, 9CI D-222

[119-84-6]
Hydrocoumarin, 8CI. 3,4-Dihydrocoumarin. 2-Hydroxyhydrocinnamic lactone. 2-Chromanone. Benzodihydropyrone. Melilotin†. Melilotol. Melilotic lactone. 2-Oxochroman. FEMA 2381

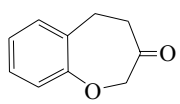


$C_9H_8O_2$ 148.161
Isol. from *Melilotus officinalis* (sweet clover). Flavouring ingredient. Cryst. or liq. Sl. sol H_2O, sol. EtOH, Et_2O, $CHCl_3$. Mp 25°. Bp 272° Bp_{13} 145°.
► Skin irritant. LD_{50} (rat, orl) 1460 mg/kg.
MW5775000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 322A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1311A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1386B (*ir*)
Aldrich Library of NMR Spectra, **7**, 45B (*pmr*)
Palfray, C.L. *et al., Bull. Soc. Chim. Fr.*, 1938, **5**, 1423 (*synth*)
de Benneville, H. *et al., J.A.C.S.*, 1940, **62**, 283 (*isol*)
Barnes, C.S. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
Appleton, R.A. *et al., Phytochemistry*, 1971, **10**, 447 (*isol*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 521 (*rev, tox*)
Usynina, R.V. *et al., Khim. Prir. Soedin.*, 1976, 810; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, 726 (*isol*)
Chatterjee, A. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 214 (*synth*)
Collins, D.J. *et al., Aust. J. Chem.*, 1989, **42**, 1235 (*synth, cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HHR500
Pickett, J.E. *et al., Tet. Lett.*, 1992, **33**, 1161 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 164
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 829-830
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HHR500

4,5-Dihydro-1-benzoxepin-3(2*H*)-one D-223

[35783-10-9]



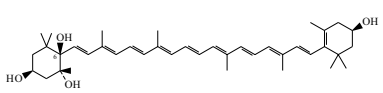
$C_{10}H_{10}O_2$ 162.188
Compd. and derivs. are flavorants with watermelon like taste and odour. Pale yellow liq. $Bp_{0.5}$ 100-105° (lit. gives a pressure range). n_D^{25} 1.5410.

Oxime: [38824-40-7]
$C_{10}H_{11}NO_2$ 177.202
$Bp_{1.5}$ 145-147°.

Huckle, D. *et al., J.C.S. Perkin 1*, 1972, 2425 (*synth*)

5,6-Dihydro-β,β-carotene-3,3′,5,6-tetrol D-224

5,6-Dihydro-5,6-dihydroxyzeaxanthin



(1*R*,3*S*,3′*R*,6*R*)-*form*

$C_{40}H_{58}O_4$ 602.896

(3*S*,3′*R*,5*R*,6*R*)-*form* [99664-48-9]
Karpoxanthin. *Carpoxanthin*
Constit. of *Capsicum annuum* (red paprika pods). Orange cryst. (Et_2O/hexane/MeOH). Mp 182-183° (174°).

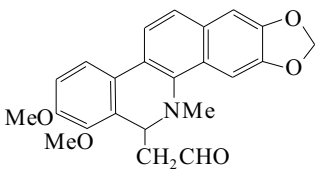
(3*S*,3′*R*,5*R*,6*S*)-*form* [99664-49-0]
6-Epikarpoxanthin
Constit. of *Capsicum annuum* (red paprika pods). Red cryst.(C_6H_6/hexane). Mp 145-147°.

(3*S*,3′*R*,5*S*,6*S*)-*form* [104012-90-0]
5,6-Diepikarpoxanthin
Isol. from *Capsicum annuum* (red paprika pods). Red cryst.(C_6H_6/hexane). Mp 150°.

Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1985, **68**, 1704; 1708
Parkes, K.E.B. *et al., Tet. Lett.*, 1986, **27**, 2535
Deli, J. *et al., Helv. Chim. Acta*, 1998, **81**, 1233-1241 (*isol, cd, pmr, cmr, ms*)

Dihydrochelerythrinyl-8-acetaldehyde D-225

[51876-09-6]
12,13-Dihydro-1,2-dimethoxy-12-methyl[1,3]benzodioxolo[5,6-c]phenanthridine-13-acetaldehyde, 9CI. Alkaloid ZT_2



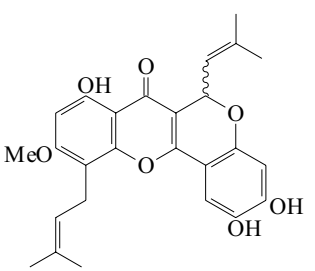
$C_{23}H_{21}NO_5$ 391.423
Various numbering schemes used. Probably an artifact.Cryst. ($CHCl_3$/MeOH). Mp 206-210°. Opt. inactive.

2′-Carboxylic acid: ***8-Carboxymethyldihydrochelerythrine***
$C_{23}H_{21}NO_6$ 407.422
Alkaloid reported to occur in *Zanthoxylum simulans* (Szechuan pepper).

Decaudain, N. *et al., Phytochemistry*, 1974, **13**, 505 (*uv, ir, pmr, struct*)
Castedo, L. *et al., Heterocycles*, 1981, **16**, 533 (*occur*)
Ng, K.M. *et al., Phytochemistry*, 1984, **26**, 3251 (*8-Carboxymethyldihydrochelerythrine*)

Dihydrocycloartomunin D-226

[135023-16-4]
*2,3,8-Trihydroxy-10-methoxy-11-(3-methyl-2-butenyl)-6-(2-methyl-1-propenyl)-6*H,7H-*[1]benzopyrano[4,3-b][1]benzopyran-7-one, 9CI*

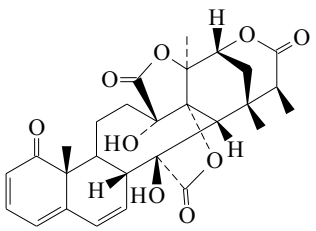


$C_{26}H_{26}O_7$ 450.487
Isol. from the root bark of *Artocarpus communis* (breadfruit). Yellow needles (Me_2CO). Mp 229-231°.

Lin, C.-N. *et al., Phytochemistry*, 1991, **30**, 1669 (*isol*)

25,27-Dihydro-4,7-didehydro-7-deoxyphysalin A D-227

[134434-71-2]

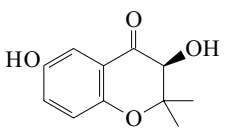


$C_{28}H_{30}O_9$ 510.54
Constit. of *Physalis alkekengi* (winter cherry). Yellow needles (Me_2CO) (synth). Mp 273-275° (synth). $[\alpha]_D$ -67 (c, 0.24 in MeOH).

Kawai, M. *et al., Tetrahedron*, 1991, **47**, 2103 (*ir, pmr, cmr, ms*)
Sunayama, R. *et al., Phytochemistry*, 1993, **34**, 529 (*isol, pmr, cmr*)

2,3-Dihydro-3,6-dihydroxy-2,2-dimethyl-4*H*-1-benzopyran-4-one D-228

3,6-Dihydroxy-2,2-dimethyl-4-chromanone



$C_{11}H_{12}O_4$ 208.213

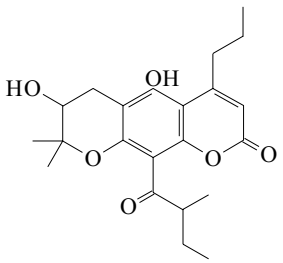
(*S*)-*form*

6-Me ether: [31298-69-8] *2,3-Dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-4*H*-1-benzopyran-4-one. 3-Hydroxy-6-methoxy-2,2-dimethyl-4-chromanone*
$C_{12}H_{14}O_4$ 222.24
Isol. from the mushroom *Lentinus crinitus* (palatability uncertain). Yellowish oil. $[\alpha]_D^{27}$ +32 (c, 0.5 in $CHCl_3$).

Abraham, W.-R. *et al., Z. Naturforsch., C*, 1995, **50**, 748-750 (*isol, pmr, cmr*)

7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(2-methyl-1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one D-229

Mammea B/BB cyclo E

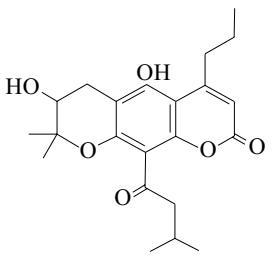


$C_{22}H_{28}O_6$ 388.46
Constit. of *Mammea americana* (mamey). Cryst. Mp 213-217°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2241; 1987, 317 (*synth*)

7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(3-methyl-1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, 9CI D-230

[30390-05-7]
M9. Mammea B/BA cyclo E

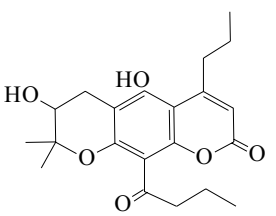


$C_{22}H_{28}O_6$ 388.46
Constit. of *Mammea americana* (mamey). Cryst. Mp 209-212°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2241; 1987, 317 (*isol, struct, synth*)

7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, 9CI D-231

[30390-07-9]
Mammea B/BC cyclo E

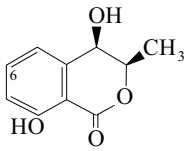


$C_{21}H_{26}O_6$ 374.433
Constit. of *Mammea americana* (mamey). Mp 213-217°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2241; 1987, 317 (*isol, struct, synth*)

3,4-Dihydro-4,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one, 9CI D-232

[33788-22-6]
3,4-Dihydro-4,8-dihydroxy-3-methylisocoumarin. 4-Hydroxymellein. 4-Hydroxyochracin



(3*R*,4*R*)-*form*

$C_{10}H_{10}O_4$ 194.187
λ_{max} 244 (ε 7820); 312 (ε 4370) (MeOH) (Derep).

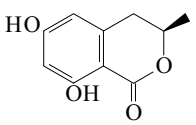
▶ NQ7830050

(3*R,4*S**)-*form*** [70287-70-6]
(-)-trans-*form*
Isol. from *Moringa oleifera* (horseradish tree). Mp 131-132°. $[\alpha]_D$ -29 (MeOH).

Cole, R.J. *et al., J. Agric. Food Chem.*, 1971, **19**, 909 (*isol*)
Aldridge, D.C. *et al., J.C.S.(C)*, 1971, 1623 (*isol*)
Camarda, L. *et al., Phytochemistry*, 1976, **15**, 537 (*abs config*)
Saluja, M.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1044 (*isol*)
Devys, M. *et al., Z. Naturforsch., C*, 1992, **47**, 779 (*isol, pmr, abs config*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 133

3,4-Dihydro-6,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one D-233

[19314-92-2]
*3,4-Dihydro-6,8-dihydroxy-3-methylisocoumarin. **6-Hydroxymellein***



(*R*)-*form*

$C_{10}H_{10}O_4$ 194.187
λ_{max} 243 (ε 3800); 308 (ε 10000) (neutral solvent not reported) (Derep). λ_{max} 216 (ε); 270 (ε 12900); 303 (ε 5750) (MeOH) (Derep).

(*R*)-*form* [70901-60-9]
Prisms (Me_2CO/petrol). Mp 214-217°. $[\alpha]_D^{20}$ -63 (c, 0.6 in EtOH). λ_{max} 216 (log ε 4.12); 269 (log ε 3.97); 304 (log ε 3.61) (EtOH) (Berdy).

6-Me ether: [13410-15-6] *3,4-Dihydro-8-hydroxy-6-methoxy-3-methyl-1*H*-2-benzopyran-1-one. **6-Methoxymellein**. LL-N313α. Antibiotic LL-N313α*
$C_{11}H_{12}O_4$ 208.213
Isol. from *Aspergillus caespitosus*, *Aspergillus variecolor* and *Sporormia bipartis*. Reaches fungitoxic levels in stored infected carrot. Shows broad antimicrobial action. Needles (petrol). Sol. MeOH, $CHCl_3$, bases; poorly sol. hexane, H_2O. Mp 75-76°. $[\alpha]_D^{27}$ -52.7 (c, 1.135 in MeOH). λ_{max} 216 (ε 196860); 267 (ε 12580); 302 (ε 4890) (MeOH) (Berdy). λ_{max} 216 (ε 22500); 267 (ε

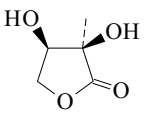
14000); 302 (ϵ 5600) (EtOH) (Berdy). λ_{max} 267 (ϵ 8900); 334 (ϵ 7800) (EtOH/NaOH) (Berdy).

[6803-02-7]

Sondheimer, E. *et al., J.A.C.S.*, 1957, **79**, 5036 (*isol, 6-Me ether, 6-Me ether 8-Ac*)
Dunn, A.W. *et al., J.C.S. Perkin 1*, 1979, 2113 (*6-Methoxymellein*)
Rama, N.H. *et al., J. Chem. Soc. Pak.*, 1992, **14**, 138 (*synth, 6-Methoxymellein*)

4,5-Dihydro-3,4-dihydroxy-3-methyl-2(3*H*)-furanone D-234

[63700-30-1]
2,3,4-Trihydroxy-2-methylbutanoic acid, 1,4-lactone. 2,3-Dihydroxy-2-methylbutanolide. 2,3-Dihydroxy-2-methylbutyrolactone



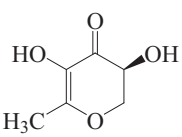
$C_5H_8O_4$ 132.116

(2ξ,3ξ)-*form*
Isol. from chickpea *Cicer arietinum*. Syrup. $[\alpha]_D$ -29 (c, 0.8 in MeOH). $[\alpha]_D^{23}$ -3.5 (c, 1.2 in $CHCl_3$).

Ford, C.W. *et al., Phytochemistry*, 1981, **20**, 2019 (*isol*)
Opletal, L. *et al., &hCesk. Farm.*, 1986, **35**, 127 (*isol, pmr, cmr, ir, struct*)
Budesinsky, M. *et al., Pharmazie*, 1994, **49**, 607 (*abs config*)
Ahmed, A.A. *et al., Phytochemistry*, 1995, **39**, 1127 (*isol, pmr, cmr*)

2,3-Dihydro-3,5-dihydroxy-6-methyl-4*H*-pyran-4-one D-235

[28564-83-2]



(*S*)-*form*

$C_6H_8O_4$ 144.127

(*S*)-*form*
Me ether: [121043-40-1] *2,3-Dihydro-3-hydroxy-5-methoxy-6-methyl-4*H*-pyran-4-one, 9CI.* ***Streptopyrone***
$C_7H_{10}O_4$ 158.154
Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{25}$ +52.2 (c, 0.97 in MeOH). λ_{max} 282 (ϵ 8900) (MeOH) (Berdy).

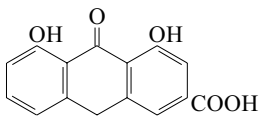
(±)-*form*
Cryst. (Et_2O/pentane). Mp 70-72°.

(ξ)-*form*
Found in numerous cooked or stored foods such as cooked vegetables, bread crust, caramelised sugar products and dehydrated orange juice powder. Intermed. prod. in Maillard reaction; formed in non-enzymic browning reactions; synth. from aldohexoses and secondary amines. Struct. of food prod. revised in 1971.

Severin, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1968, **137**, 4-6 (*synth, pmr, uv*)
Van den Ouweland, G.A.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1970, **89**, 750-754 (*Me ether, synth, ir, uv, pmr, ms*)
Mills, F.D. *et al., Tet. Lett.*, 1970, 1243-1246 (*Me ether, synth, ir, pmr*)
Shaw, P.E. *et al., Carbohydr. Res.*, 1971, **16**, 207-211 (*struct*)
Ledl, F. *et al., Z. Lebensm.-Unters. -Forsch.*, 1976, **160**, 367-370 (*occur*)
Kobayashi, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 889 (*Me ether, isol, struct*)
Kim, M.O. *et al., J. Agric. Food Chem.*, 1996, **44**, 282-289 (*occur, synth, ms*)
Torres, J.A. *et al., Biochem. Syst. Ecol.*, 2001, **29**, 673-680 (*isol*)

9,10-Dihydro-4,5-dihydroxy-10-oxo-2-anthracenecarboxylic acid D-236

[480-09-1]
9,10-Dihydro-4,5-dihydroxy-10-oxo-2-anthroic acid, 8CI. ***Rheinanthrone***



$C_{15}H_{10}O_5$ 270.241
Prod. from *Rheum* spp.. Mp 250-280° dec.

O-*Glucoside:* [54003-18-8]
$C_{21}H_{20}O_{10}$ 432.383

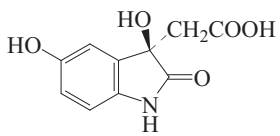
O-*Diglucoside:* [57077-57-3]
$C_{27}H_{30}O_{15}$ 594.525

[30201-14-0, 57077-55-1, 117639-10-8]

Lemli, J. *et al., Phytochemistry*, 1975, **14**, 1397 (*glucoside*)
Evans, F.J. *et al., Biomed. Mass Spectrom.*, 1979, **6**, 374 (*ms*)
De Witte, P. *et al., Pharmacology*, suppl. 1, 1988, **36**, 152 (*metab*)

2,3-Dihydro-3,5-dihydroxy-2-oxo-1*H*-indole-3-acetic acid D-237

3,5-Dihydroxy-2-indolinone-3-acetic acid



(*R*)-*form*

$C_{10}H_9NO_5$ 223.185
Tentative stereochem. assigned.

(*R*)-*form*
5-O-β-D-Glucopyranoside: [218604-37-6]
$C_{16}H_{19}NO_{10}$ 385.327
Isol. from rice bran. $[\alpha]_D^{20}$ -25.8 (c, 0.2 in H_2O). λ_{max} 210 (ϵ 16400); 259 (ϵ 6600); 305 (ϵ 1200) (MeOH).

5-O-[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]: [218604-48-9]
$C_{22}H_{29}NO_{15}$ 547.469
Isol. from rice bran. $[\alpha]_D^{20}$ -30.7 (c, 0.3 in H_2O). λ_{max} 210 (ϵ 19000); 259 (ϵ 7400); 305 (ϵ 1300) (MeOH).

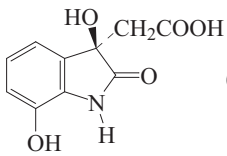
(*S*)-*form*
5-O-β-D-Glucopyranoside: [218604-43-4]
Isol. from rice bran. $[\alpha]_D^{20}$ -44.1 (c, 1.2 in H_2O). λ_{max} 210 (ϵ 16400); 259 (ϵ 6600); 305 (ϵ 1200) (MeOH).

5-O-[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]: [218604-54-7]
Isol. from rice bran. $[\alpha]_D^{20}$ -46.5 (c, 1.3 in H_2O). λ_{max} 210 (ϵ 19000); 259 (ϵ 7400); 305 (ϵ 1300) (MeOH).

Tateishi, K. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1870-1874 (*isol, uv, ir, pmr, cmr*)

2,3-Dihydro-3,7-dihydroxy-2-oxo-1*H*-indole-3-acetic acid D-238

3,7-Dihydroxy-2-indolinone-3-acetic acid



(*R*)-*form*

$C_{10}H_9NO_5$ 223.185

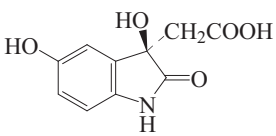
(*R*)-*form*
7-O-β-D-Glucopyranoside: [120293-55-2]
Zeanoside C
$C_{16}H_{19}NO_{10}$ 385.327
Isol. from immature sweet corn kernels *Zea mays* (Gramineae). Fine cryst. (EtOH). Mp 162-163°. $[\alpha]_D^{19}$ -162.1 (c, 0.1 in H_2O).

(*S*)-*form*
7-O-β-D-Glucopyranoside: [113202-68-9]
Zeanoside A
$C_{16}H_{19}NO_{10}$ 385.327
Isol. from sweet corn kernels *Zea mays* (Gramineae). Fine needles (EtOH). Mp 197-198°. $[\alpha]_D$ -36.8 (c, 0.1 in H_2O).

Tateishi, K. *et al., Agric. Biol. Chem.*, 1987, **51**, 3445; 1988, **52**, 3231; 1989, **53**, 2545 (*isol, uv, ir, pmr, cmr, ms, struct*)

2,3-Dihydro-3,5-dihydroxy-2-oxo-3-indoleacetic acid D-239

[61935-03-3]
5-Hydroxydioxindole-3-acetic acid



(*R*)-*form*

$C_{10}H_9NO_5$ 223.185

(*R*)-*form*
Constit. of rice bran. $[\alpha]_D^{21}$ +6 (c, 1 in MeOH).

5-O-β-D-Glucopyranoside:
$C_{16}H_{19}NO_{10}$ 385.327
Constit. of rice bran. Powder. $[\alpha]_D^{20}$ -25.8 (c, 0.2 in H_2O). λ_{max} 210 (ϵ 16400); 259 (ϵ 6600); 305 (ϵ 1200) (MeOH).

5-O-[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]:
$C_{22}H_{29}NO_{15}$ 547.469
Constit. of rice bran. Powder. $[\alpha]_D^{20}$ -30.7 (c, 0.3 in H_2O). λ_{max} 210 (ϵ 19000); 259 (ϵ 7400); 305 (ϵ 1300) (MeOH).

(*S*)-*form*
5-O-β-D-Glucopyranoside:
Constit. of rice bran. Powder. $[\alpha]_D^{20}$ -44.1 (c, 1.2 in H_2O). λ_{max} 210 (ϵ 16400); 259

(ϵ 6600); 305 (ϵ 1200) (MeOH).

5-O-[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]:
Constit. of rice bran. Powder. $[\alpha]_D^{20}$ -46.5 (c, 1.3 in H_2O). λ_{max} 210 (ϵ 19000); 259 (ϵ 7400); 305 (ϵ 1300) (MeOH).

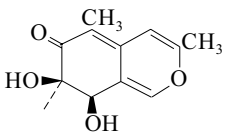
(±)-*form* [63389-29-7]
Pale yellow powder.

Me ester: [57061-18-4]
$C_{11}H_{11}NO_5$ 237.212
Constit. of rice bran. Needles. Mp 78-80°. Possibly an artifact.

Kinashi, H. *et al., Agric. Biol. Chem.*, 1976, **40**, 2465 (*isol*)
Suzuki, Y. *et al., Phytochemistry*, 1977, **16**, 635 (*isol*)
Tateishi, K. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1870-1874 (*glycosides*)

7,8-Dihydro-7,8-dihydroxy-3,5,7-trimethyl-6*H*-2-benzopyran-6-one, 9CI D-240

[58957-07-6]
Dihydrodeoxy-8-epiaustdiol

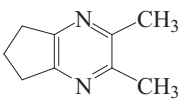


$C_{12}H_{14}O_4$ 222.24
Mycotoxin prod. by the food storage mould (*Aspergillus ustus*). Cryst. (Me_2CO/hexane). Mp 208-210°. $[\alpha]_D^{23}$ +250 (c, 0.64 in $CHCl_3$).

Steyn, P.S. *et al., J.C.S. Perkin 1*, 1976, 204 (*isol*)

6,7-Dihydro-2,3-dimethyl-5*H*-cyclopentapyrazine, 9CI D-241

[38917-63-4]
FEMA 3917



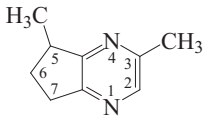
$C_9H_{12}N_2$ 148.207
Formed from cysteine and rhamnose under roasting conditions. Found in beef, coffee, cocoa, earth almond (*Cyperus esulentus*), roast almonds, walnut and hazelnut. Flavouring ingredient. Mp 25-27°. Bp_{10} 102-104°.

N-*Oxide:* [61928-81-2]
$C_9H_{12}N_2O$ 164.207
Hygroscopic cryst. Mp 36-39°. $Bp_{0.001}$ 85°.

Flament, I. *et al., Helv. Chim. Acta*, 1973, **56**, 610-619; 1976, **59**, 2308-2313; 2314-2326 (*synth, occur, pmr, ms, 1-oxide*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 273-279 (*synth*)
Flament, I. *et al., Bull. Soc. Chim. Belg.*, 1979, **88**, 941-950 (*synth, pmr, ms*)
Silwar, R. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 112-119 (*N-oxide*)
Cantelejo, M.J. *et al., J. Agric. Food Chem.*, 1997, **45**, 1853-1860 (*occur, Cyperus esculentus*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 421 (*occur, use*)

6,7-Dihydro-2,5-dimethyl-5*H*-cyclopentapyrazine, 9CI D-242

[38917-61-2]



$C_9H_{12}N_2$ 148.207
Analytical methods may not always distinguish between the 2,5-dimethyl and 2,7-dimethyl isomers which have very similar spectra. Maillard product. Present in roasted Earth almond (*Cyperus esculentus*), fermented wild rice (*Zizania aquatica*), cooked pork, cooked beef, roasted filberts, coffee and cocoa butter. Bp_{12} 90-91°. Bp data refers to a synthetic mixt. with the 2,7-dimethyl isomer.

Flament, I. *et al., Helv. Chim. Acta*, 1973, **56**, 610-619 (*synth, ms*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 273-279 (*synth, uv, ir, ms*)
Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur, cocoa*)
Cantelego, M.J. *et al., J. Agric. Food Chem.*, 1997, **45**, 1853-1860 (*occur, earth almond*)
Ames, J.M. *et al., J. Agric. Food Chem.*, 2001, **49**, 4315-4323 (*glc*)

6,7-Dihydro-2,6-dimethyl-5*H*-cyclopentapyrazine D-243

[61928-63-0]

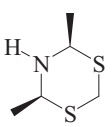
$C_9H_{12}N_2$ 148.207
Maillard product. Component of roasted coffee bean volatiles. Liq. Bp_{10} 90-93°.

Flament, I. *et al., Helv. Chim. Acta*, 1976, **59**, 2314-2326 (*synth, ms, ir, pmr*)
Baltes, W. *et al., J. Agric. Food Chem.*, 1987, **35**, 340-346 (*occur, ms*)

Dihydro-4,6-dimethyl-4*H*-1,3,5-dithiazine D-244

[51647-36-0]

[82989-67-1, 82989-68-2]



$C_5H_{11}NS_2$ 149.281
Present in meat aromas.

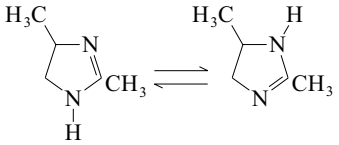
(3*R*,5*S*)-*form* [82989-67-1]
cis-*form*

Kruse, H.P. *et al., Nahrung*, 1982, **26**, 369-376 (*occur*)
Peerzada, N. *et al., Sulfur Lett.*, 2000, **23**, 185-192 (*isol, synth*)

4,5-Dihydro-2,4(5)-dimethyl-1*H*-imidazole, 9CI D-245

[930-61-0]

2,4-Dimethyl-2-imidazoline, 8CI



$C_5H_{10}N_2$ 98.147

(±)-*form*
Liq. Bp_{15} 107.5-108°. Irritant.

Picrate:
Solid. Mp 141-141.5°.

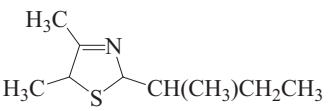
(ξ)-*form*
Volatile component of rainbow trout tissue.

[73006-98-1]

Ohashi, M. *et al., Org. Mass Spectrom.*, 1968, **1**, 703 (*ms*)
Hiatt, M.H. *et al., Anal. Chem.*, 1983, **55**, 506 (*isol, glc*)
Butler, R.N. *et al., J.C.S. Perkin 1*, 1989, 155 (*synth*)

2,5-Dihydro-4,5-dimethyl-2-(1-methylpropyl)thiazole, 9CI D-246

[65894-82-8]
2-(2-Butyl)-4,5-dimethyl-3-thiazoline.
FEMA 3619



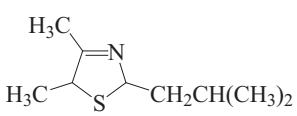
$C_9H_{17}NS$ 171.306
Flavouring ingredient. Reported in hydrolysed vegetable protein. Liq. with sweet, green, nutty, bread-like aroma. Insol. H_2O. d 0.952. Bp_4 71° (60:40 mixt. of *cis*/*trans* racemates).

U.S. Pat., 1978, 4 067 344; *CA*, **88**, 118019h (*synth, pmr, ms, ir*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 196 (*use, props*)

2,5-Dihydro-4,5-dimethyl-2-(2-methylpropyl)thiazole, 9CI D-247

[65894-83-9]

[64383-84-2, 64383-85-3]
2-Isobutyl-4,5-dimethyl-3-thiazoline.
FEMA 3621



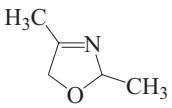
$C_9H_{17}NS$ 171.306
Component of cooked beef aroma. Flavouring ingredient. Liq. with meat, spice, vegetable odour. Bp_4 71°. n_D^{20} 1.4855. Bp data is for a 60:40 mixture of *cis*/*trans* isomers.

Japan. Pat., 1978, 78 47 543; *CA*, **89**, 146894d (*synth, use*)

U.S. Pat., 1978, 4 040 987; *CA*, **89**, 146894d (*synth, use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Werkhoff, P. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1991, **13**, 30-57 (*occur, props, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 181 (*use, props*)
Elmore, J.S. *et al., J. Agric. Food Chem.*, 1997, **45**, 3595-3602; 3603-3607 (*occur, beef*)

2,5-Dihydro-2,4-dimethyloxazole D-248

[77311-02-5]
2,4-Dimethyl-3-oxazoline

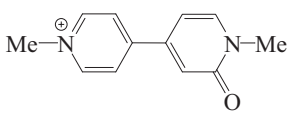


C_5H_9NO 99.132

(ξ)-*form*
Aroma constit. of cooked beef, fried bacon, fried chicken and roasted peanuts.
Mussinan, C.J. *et al., ACS Symp. Ser.*, 1976, **26**, 133-145 (*occur, ms*)
Galt, A.M. *et al., J. Agric. Food Chem.*, 1984, **32**, 59-64 (*occur*)

1′,2′-Dihydro-1,1′-dimethyl-2′-oxo-4,4′-bipyridinium(1+), 9CI D-249

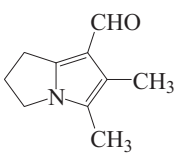
[197645-02-6]



$C_{12}H_{13}N_2O^{\oplus}$ 201.248
Metab. of 1,1′-Dimethyl-4,4′-bipyridinium(2+), D-768 produced by plant residue microorganisms and rat liver homogenates, also formed by photolysis. Yellow cryst. (EtOH aq.) (as iodide). Mp 280-290° dec. (iodide).
Calderbank, A. *et al., J.C.S. Perkin 1*, 1972, 139-142 (*synth, pmr, uv*)
Mau, A.W. *et al., J.C.S. Faraday 2*, 1986, **82**, 869-876 (*occur*)
Fuke, C. *et al., Nippon Hoigaku Zasshi*, 1993, **47**, 33-45; *CA*, **119**, 88572x (*metab*)
Lee, S.J. *et al., J. Agric. Food Chem.*, 1995, **43**, 1343-1347 (*metab*)

2,3-Dihydro-5,6-dimethyl-1*H*-pyrrolizine-7-carboxaldehyde D-250

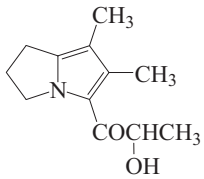
[97073-05-7]
*7-Formyl-2,3-dihydro-5,6-dimethyl-1*H*-pyrrolizine*



$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product. Characterised spectroscopically.
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr, ir*)

1-(2,3-Dihydro-6,7-dimethyl-1*H*-pyrrolizin-5-yl)-2-hydroxy-1-propanone D-251

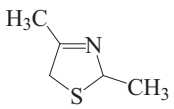
[97073-12-6]
*2,3-Dihydro-6,7-dimethyl-5-(2-hydroxypropionyl)-1*H*-pyrrolizine*



$C_{12}H_{17}NO_2$ 207.272
Proline-derived Maillard product. Characterised spectroscopically.
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr, ir*)

2,5-Dihydro-2,4-dimethylthiazole, 9CI D-252

[60755-05-7]
2,4-Dimethyl-3-thiazoline



C_5H_9NS 115.199

(±)-*form*
Liq. Mp 129° (as picrate). Bp_{11} 52°.

(ξ)-*form*
Volatile component of roasted peanuts and fried chicken.
Asinger, F. *et al., Annalen*, 1964, **672**, 156-178 (*synth*)
Buckholz, L.L. *et al., ACS Symp. Ser.*, 1981, **170**, 163-181 (*occur, peanuts*)
Tang, J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1287-1292 (*occur, chicken*)

Dihydro-2(3*H*)-furanone, 9CI D-253

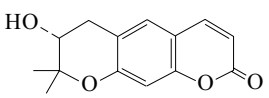
[96-48-0]
γ-Butyrolactone. 4-Hydroxybutyric acid lactone. 2-Oxotetrahydrofuran. FEMA 3291



$C_4H_6O_2$ 86.09
Present in morello cherry, melon, pineapple, blackberry, quince, strawberry jam, wine, soybeans, black tea, Bourbon vanilla, wheat bread, crispbread and other breads. Flavour ingredient. Liq. Misc. H_2O. d^0 1.44. Bp 203-204° Bp_{12} 89°. Steam-volatile.
▶ LD_{50} (rat, orl) 1540 mg/kg. Exp. reprod. and teratogenic effects. LU3500000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 697D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1127A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 749A (*ir*)
Aldrich Library of NMR Spectra, **3**, 72B (*pmr*)
Sircar, S.S.G. *et al., J.C.S.*, 1928, 898 (*synth*)
Bakassian, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 2643 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 101
Koshland, D.E. *et al., J.A.C.S.*, 1972, **94**, 5805 (*cmr*)
Kamiya, Y. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1401 (*synth*)
IARC Monog., 1976, **11**, 231; *Suppl.* 7, 59 (*rev, tox*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A4**, 495 (*rev*)
Kajigaeshi, S. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 747 (*synth*)
McDermott, D.P. *et al., J. Phys. Chem.*, 1986, **90**, 2569 (*ir, Raman*)
Heusinger, H. *et al., Org. Mass Spectrom.*, 1987, **22**, 235 (*ms*)
Alonso, J.L. *et al., J. Chem. Soc., Faraday Trans.*, 1990, **86**, 453; 459 (*conformn*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 211 (*rev*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 955-958 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1360-1362 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BOV000

7,8-Dihydro-7-hydroxy-8,8-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, 9CI D-254

[5993-18-0]



(*R*)-*form*

$C_{14}H_{14}O_4$ 246.262

(*R*)-*form* [21860-31-1]
Aegelinol
Obt. from *Aegle marmelos* (bael fruit). Cryst. (C_6H_6). Mp 181.5°. $[\alpha]_D^{23}$ -107 (c, 0.1 in Py).

Ac: ***Acetylaegelinol***
$C_{16}H_{16}O_5$ 288.299
Needles. Mp 174-176°. $[\alpha]_D$ -4.1 (c, 0.5 in $CHCl_3$). λ_{max} 255 (log ε 3.49); 332 (log ε 4.18) (MeOH).

Angeloyl: [23402-19-9] ***Agasyllin***
$C_{19}H_{20}O_5$ 328.364
Cryst. Mp 78-80°. $[\alpha]_D^{24}$ -44 (c, 0.91 in $CHCl_3$).

O-*(3-Methyl-2-butenoyl):* [63100-57-2] ***Grandivittin***. *Grandivitin*
$C_{19}H_{20}O_5$ 328.364
Oil. $[\alpha]_D^{20}$ -154.9 (c, 1.44 in $CHCl_3$).

O-*Benzoyl:Aegelinol benzoate*
$C_{21}H_{18}O_5$ 350.37
$[\alpha]_D^{20}$ -95.6 ($CHCl_3$).

(*S*)-*form* [23458-02-8] ***Decursinol***
Cryst. (EtOH). Mp 177°. $[\alpha]_D^{17}$ +104.2 (c, 0.7 in EtOH).

Ac:
Mp 138-139°. $[\alpha]_D^{17}$ +45.7.

O-*(3-Methyl-2-butenoyl):* [5928-25-6] ***De-***

cursin
$C_{19}H_{20}O_5$ 328.364
Prisms (EtOH). Mp 110-111°. $[\alpha]_D^{15}$ +172.9 ($CHCl_3$). λ_{max} 220 (MeOH) (Berdy).

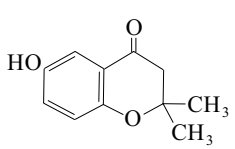
2-Methyl-2-butenoyl(Z-): [130848-06-5]
Acutilobin. *Decursinol angelate*
$C_{19}H_{20}O_5$ 328.364
Constit. of *Angelica acutiloba* (Dong Dang Gui). Prisms (MeOH). Mp 94-95°. $[\alpha]_D^{15}$ +172.9 (c, 1.3 in $CHCl_3$).

(±)-*form* [15575-65-2]
Needles (petrol/EtOAc). Mp 167.5-168.5°.

Lemmich, J. *et al., Acta Chem. Scand.*, 1966, **20**, 2497 (*Agasyllin, isol*)
Hata, K. *et al., Tet. Lett.*, 1966, 1461 (*Decursinol, isol*)
Nikonov, G.K. *et al., Khim. Prir. Soedin.*, 1969, **5**, 119; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 102 (*struct, Agasyllin*)
Lemmich, J. *et al., Tet. Lett.*, 1969, 3 (*struct*)
Hata, K. *et al., Yakugaku Zasshi*, 1969, **89**, 549 (*isol*)
Steck, W. *et al., Can. J. Chem.*, 1971, **49**, 2297 (*synth, pmr*)
Perel'son, M.E. *et al., Khim. Prir. Soedin.*, 1971, **7**, 712; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 692 (*pmr, Agasyllin, Decursin*)
Murray, R.D.H. *et al., Tetrahedron*, 1971, **27**, 4901 (*struct, pmr, ms*)
Sano, K. *et al., Chem. Pharm. Bull.*, 1975, **23**, 20 (*abs config*)
Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1977, **13**, 640; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 531 (*Grandivittin*)
Lemmich, J. *et al., Phytochemistry*, 1978, **17**, 139-141 (*synth*)
Chatterjee, A. *et al., Phytochemistry*, 1978, **17**, 328-329 (*Aegelinol, isol, ir, pmr, ms, uv, struct*)
Erdelmeier, C.A.J. *et al., Planta Med.*, 1985, 407 (*deriv*)
Ceccherelli, P. *et al., J. Nat. Prod.*, 1989, **52**, 888; 1990, **53**, 536 (*Grandivittin*)
Ahn, K.S. *et al., Planta Med.*, 1996, **62**, 7 (*Decursin*)
Ahn, K.-S. *et al., Planta Med.*, 1997, **63**, 360-361 (*Acutilobin*)
Pat. Coop. Treaty (WIPO), 2000, 23 074; *CA*, **132**, 288766u
Lim, J. *et al., Tet. Lett.*, 2001, **42**, 4001-4003 (*Acutilobin, Decursin, synth*)
Kim, S. *et al., Tet. Lett.*, 2001, **42**, 7641-7643 (*synth*)
Kong, L.-Y. *et al., Heterocycles*, 2003, **60**, 599-606 (*Acetylaegelinol*)

2,3-Dihydro-6-hydroxy-2,2-dimethyl-4*H*-1-benzopyran-4-one, 9CI D-255

[31366-85-5]
6-Hydroxy-2,2-dimethyl-4-chromanone



$C_{11}H_{12}O_3$ 192.214
Cryst. (CCl_4). Mp 154-156°.

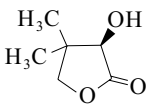
Me ether: [13229-59-9] *2,3-Dihydro-6-methoxy-2,2-dimethyl-4*H*-1-benzopyran-4-one. 6-Methoxy-2,2-dimethyl-4-chromanone*
$C_{12}H_{14}O_3$ 206.241
Isol. from the mushroom *Lentinus crinitus* (palatability not certain). Plates. Mp 75°.

4-Alcohol, Me ether: [65383-71-3] *3,4-Dihydro-6-methoxy-2,2-dimethyl-2*H*-1-benzopyran-4-ol. 6-Methoxy-2,2-dimethyl-4-chromanol*
$C_{12}H_{16}O_3$ 208.257
Isol. from mushroom *Lentinus crinitus*. Yellowish oil. $[\alpha]_D^{27}$ +16 (c, 0.2 in $CHCl_3$).

Closse, A. *et al., Helv. Chim. Acta*, 1970, **53**, 1577 (*isol*)
Lourenco, T.O. *et al., Phytochemistry*, 1981, **20**, 773 (*isol, uv, ir, pmr, ms*)
Abraham, W.-R. *et al., Z. Naturforsch., C*, 1995, **50**, 748 (*derivs, isol, pmr, cmr*)

Dihydro-3-hydroxy-4,4-dimethyl-2(3*H*)-furanone, 9CI D-256

[52126-90-6]
2,4-Dihydroxy-3,3-dimethylbutyric acid γ-lactone. α-Hydroxy-β,β-dimethyl-γ-butyrolactone. Pantolactone. Pantoyl lactone. Pantoic lactone



(*R*)-*form*

$C_6H_{10}O_3$ 130.143

(*R*)-*form* [599-04-2]
Hygroscopic cryst. (C_6H_6/petrol or by subl.). Mp 92°. $[\alpha]_D^{25}$ -50.7 (c, 2.05 in H_2O). Shows plastic crystal behaviour.

O-*β*-D-*Glucopyranoside:*
$C_{12}H_{20}O_8$ 292.285
Isol. from rice seedlings (*Oryza sativa*).

O-*[β*-D-*Xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [307003-33-4] *Pantoyl lactone primeveroside*
$C_{17}H_{28}O_{12}$ 424.401

4-Nitrobenzoyl:
Cryst. (EtOH aq.). Mp 112°.

(*S*)-*form* [5405-40-3]
Hygroscopic cryst. (C_6H_6). Mp 91°. $[\alpha]_D^{25}$ +50 (c, 2.00 in H_2O).

4-Nitrobenzoyl:
Cryst. (EtOH aq.). Mp 114°.

(±)-*form* [79-50-5]
Hygroscopic rosettes or prisms. Sol. H_2O, EtOH, Et_2O, $CHCl_3$, C_6H_6, CS_2.

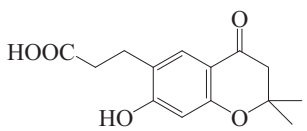
4-Nitrobenzoyl:
Long needles (EtOH). Mp 137-138°.

Benzyl ether:
$C_{13}H_{16}O_3$ 220.268
Solid. Mp 48.1°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 700B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1134C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 753C; 753D (*ir*)
Reichstein, T. *et al., Helv. Chim. Acta*, 1940, **23**, 650 (*synth*)
Stiller, E.T. *et al., J.A.C.S.*, 1940, **62**, 1785 (*synth*)
Carter, H.E. *et al., J.A.C.S.*, 1941, **63**, 312 (*synth*)
Hill, R.K. *et al., Biochem. Biophys. Res. Commun.*, 1970, **38**, 181 (*abs config*)
Dillon, J. *et al., J.A.C.S.*, 1974, **46**, 4055 (*config*)
Achiwa, K. *et al., Tet. Lett.*, 1977, 4431 (*synth*)
Panst, J. *et al., Annalen*, 1978, 1024 (*synth*)
Achiwa, K. *et al., Chem. Lett.*, 1978, 297 (*synth*)
Ojima, I. *et al., J.O.C.*, 1978, **43**, 3444 (*synth, use*)
Wasmuth, D. *et al., Helv. Chim. Acta*, 1982, **65**, 344 (*synth, biosynth*)
Nakai, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3549 (*cmr, props*)
Fizet, C. *et al., Helv. Chim. Acta*, 1986, **69**, 404 (*resoln, bibl*)
Larsen, R.D. *et al., J.A.C.S.*, 1989, **111**, 7650 (*use*)
Kinoshita, T. *et al., J. Het. Chem.*, 1991, **28**, 619 (*synth, pmr, cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1992, **16**, 269 (*use*)
Paetow, M. *et al., Tet. Lett.*, 1992, **33**, 5323 (*synth*)
Rao, A.V.R. *et al., Tet. Lett.*, 1994, **35**, 5735 (*synth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3893-3896 (*use*)
Calmes, M. *et al., Org. Prep. Proced. Int.*, 1995, **27**, 107 (*synth, S-form*)
Menegus, F. *et al., Phytochemistry*, 1995, **40**, 1617 (*glycoside*)
Scaglioni, L. *et al., Nat. Prod. Lett.*, 2000, **14**, 159-166 (*6-xylosylglucoside, Pantoyl lactone primeveroside*)
Pansare, S.V. *et al., Org. Lett.*, 2000, **2**, 175-177 (*synth*)
Akkari, R. *et al., J.O.C.*, 2001, **66**, 5859-5865 (*benzyl ether, ir, pmr, cmr, ms*)

2,3-Dihydro-7-hydroxy-2,2-dimethyl-4-oxo-4*H*-1-benzopyran-6-propanoic acid D-257

6-(2-Carboxyethyl)-7-hydroxy-2,2-dimethyl-4-chromanone



$C_{14}H_{16}O_5$ 264.277

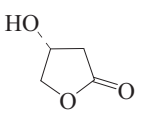
O-*β*-D-*Glucopyranoside:*
$C_{20}H_{26}O_{10}$ 426.419
Constit. of fennel, *Foeniculum vulgare*. Amorph. powder. $[\alpha]_D^{22}$ -68 (c, 0.8 in MeOH).

Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1448-1450

Dihydro-4-hydroxy-2(3*H*)-furanone, 9CI D-258

[5469-16-9]

[131432-37-6]
3-Hydroxy-4-butanolide. 3,4-Dihydroxybutanoic acid γ-lactone. 3-Hydroxy-γ-butyrolactone



(*R*)-*form*

$C_4H_6O_3$ 102.09

(*R*)-*form* [58081-05-3]
Viscous oil. $Bp_{0.4}$ 103-105° $Bp_{0.1}$ 90-95°. $[\alpha]_D^{23}$ +86 (c, 2 in EtOH).

O-*β*-D-*Glucopyranoside:* [151870-74-5]
Kinsenoside
$C_{10}H_{16}O_8$ 264.232
Oil. $[\alpha]_D^{16}$ +48.4 (c, 2.07 in EtOH).

Me ether: [137008-54-9] *Dihydro-4-methoxy-2(3H)-furanone*
$C_5H_8O_3$ 116.116
Oil. $[\alpha]_D^{23}$ +34.2 (c, 0.92 in $CHCl_3$).

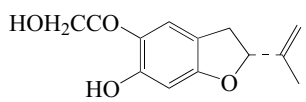
(*S*)-*form* [7331-52-4]
$Bp_{0.1}$ 120°. $[\alpha]_D$ -86.1 (c, 3.1 in EtOH).

O-*β*-D-*Glucopyranoside:* [211107-44-7]
Constit. of *Crocus sativus* (saffron). Needles (EtOH). Mp 156-157°. $[\alpha]_D^{25}$ -71.2 (c, 0.55 in H_2O) (tetra-Ac).

Mori, K. *et al., Tetrahedron*, 1979, **35**, 933-940 (*synth, ir, pmr*)
Saito, S. *et al., Chem. Lett.*, 1984, 1389-1392 (*synth*)
Moore, R.E. *et al., J.O.C.*, 1984, **49**, 2484-2489 (*synth, isol*)
Ainslie, R.D. *et al., Phytochemistry*, 1986, **25**, 2654-2655 (*isol, pmr*)
Henrot, S. *et al., Synth. Commun.*, 1986, **16**, 183-190 (*synth*)
Seebach, D. *et al., Synthesis*, 1986, 37-40 (*synth*)
Tanaka, A. *et al., Synthesis*, 1987, 570-572 (*synth*)
Uchikawa, O. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 2025-2029 (*synth, ir, pmr, cmr, bibl*)
Luk, K.-C. *et al., Synthesis*, 1988, 226-227 (*synth, ir, pmr, ms*)
Sugita, Y. *et al., J.C.S. Perkin 1*, 1992, 2855-2861 (*S-form*)
Ito, A. *et al., Phytochemistry*, 1993, **33**, 1133-1137 (*synth, Kinsenoside*)
Yuasa, Y. *et al., Liebigs Ann./Recl.*, 1997, 1877-1879 (*synth, pmr, cmr, ms*)
Masse, C.E. *et al., J.A.C.S.*, 1998, **120**, 4123-4134 (*synth, ir, pmr, cmr*)
Du, X.-M. *et al., Phytochemistry*, 1998, **49**, 1925-1928 (*Kinsenoside*)
Huang, G. *et al., Tetrahedron*, 1998, **54**, 1355-1360 (*synth, ir, pmr, cmr*)
Gao, W.-Y. *et al., Planta Med.*, 1999, **65**, 425-427 (*S-form glucoside*)
Du, X.-M. *et al., Biol. Pharm. Bull.*, 2000, **23**, 731-734 (*S-form glucoside*)

2,3-Dihydro-6-hydroxy-5-(hydroxyacetyl)-2-isopropenylbenzofuran D-259

1-[2,3-Dihydro-6-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-2-hydroxyethanone, 9CI

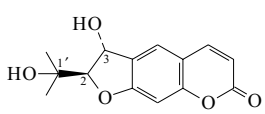


$C_{13}H_{14}O_4$ 234.251

(*S*)-*form* [83218-05-7]
Constit. of *Madia sativa* (Chile tarweed). Gum.

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1103 (*isol, ir, pmr, ms*)

2,3-Dihydro-3-hydroxy-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI D-260



(2*R*,3*R*)-*form*

$C_{14}H_{14}O_5$ 262.262

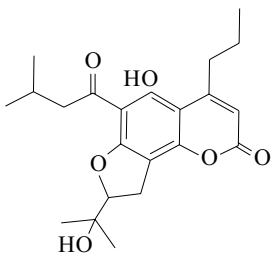
(2*S*,3*R*)-*form* [87725-60-8]
3R-Hydroxymarmesin
Mp 176° (softens at 159°). $[\alpha]_D^{20}$ +43 (c, 0.2 in MeOH).

1′-O-*β*-D-*Glucopyranoside:* [87592-77-6]
$C_{20}H_{24}O_{10}$ 424.404
Constit. of *Angelica archangelica* (angelica). Needles (MeOH). Mp 267-269°. $[\alpha]_D^{22}$ -18 (c, 0.8 in Py).

Perel'son, M.E. *et al., Khim. Prir. Soedin.*, 1971, **7**, 712-721; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 692-699 (*pmr, derivs*)
Lemmich, J. *et al., Phytochemistry*, 1995, **38**, 427-432 (*1′-glucoside*)

8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9CI D-261

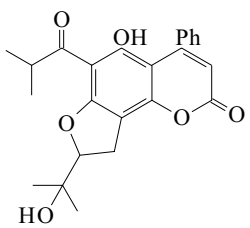
[30390-14-8]
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-isovaleryl-4-propylfuro[2,3-h]coumarin. Mammea B/AA cyclo F



$C_{22}H_{28}O_6$ 388.46
Obt. from seeds of *Mammea americana* (mamey). Cryst. ($CHCl_3$/hexane). Mp 72-77°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248; 1987, 317 (*isol, ir, uv, pmr, synth*)

8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxopropyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one D-262

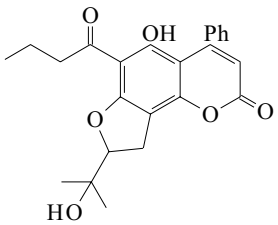


$C_{24}H_{24}O_6$ 408.45
Isol. from *Mammea americana* (mamey) seeds. Closely related to MAB 3, M-4.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248

8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one D-263

[233764-88-0]
Mammea A/AC cyclo F

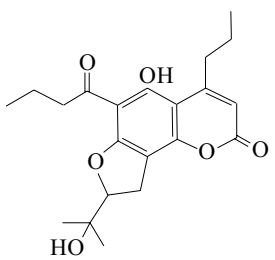


$C_{24}H_{24}O_6$ 408.45
Constit. of *Mammea americana* (mamey). Yellow prisms (hexane/EtOAc). Mp 119°. $[\alpha]_D$ -2.6 (c, 4.5 in $CHCl_3$).

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248-2254 (*occur*)
Morel, C. *et al., Phytochemistry*, 1999, **50**, 1243-1247 (*isol, uv, ir, pmr, cmr, ms*)

8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(1-oxobutyl)-4-propyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9CI D-264

[38537-82-5]
6-Butyryl-8,9-dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-4-propylfuro[2,3-h]coumarin. Mammea B/AC cyclo F

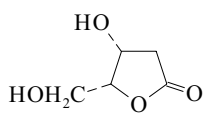


$C_{21}H_{26}O_6$ 374.433
Constit. of *Mammea americana* (mamey). Yellow cryst. ($CHCl_3$/hexane). Mp 75-81°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248; 1987, 317 (*isol, struct, synth*)

4,5-Dihydro-4-hydroxy-5-(hydroxymethyl)-2(3*H*)-furanone D-265

3-Hydroxy-4-hydroxymethyl-4-butanolide. 3,4,5-Trihydroxypentanoic acid 1,4-lactone. 2-Deoxypentono-1,4-lactone



(4*R*,5*R*)-*form*

$C_5H_8O_4$ 132.116

(4*R*,5*R*)-*form* [78185-08-7]
D-threo-*form. 2-Deoxy-D-xylono-1,4-lactone*
Oil. $[\alpha]_D^{24}$ +67.3 (c, 1.01 in MeOH) (+49.3).

(4*R*,5*S*)-*form* [38996-14-4]
L-erythro-*form. 2-Deoxy-L-ribono-1,4-lactone*
Constit. of the fruit of *Foeniculum vulgare* (fennel). Oil. $[\alpha]_D^{22}$ +3.5 (c, 0.8 in MeOH). $[\alpha]_D$ +13.5 (c, 0.8 in H_2O).

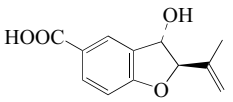
(4*S*,5*R*)-*form* [34371-14-7]
D-erythro-*form. 2-Deoxy-D-ribono-1,4-lactone*

$[\alpha]_D^{24}$ -4.5 (c, 1.44 in EtOH) (-1.5).

(4*R,5*S**)-*form***

Fernández, M.V. *et al., Tetrahedron*, 1990, **46**, 7911-7922 (*synth, pmr, cmr*)
Matsumoto, K. *et al., Bull. Chem. Soc. Jpn.*, 1995, **68**, 670-672 (*synth*)
Kita, Y. *et al., J.O.C.*, 1998, **53**, 554-561 (*synth*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)
Doyle, M.P. *et al., J.O.C.*, 1999, **64**, 8907-8915 (*synth, bibl, pmr*)
He, M. *et al., Yaoxue Xuebao*, 2001, **36**, 278-280 (*isol*)

2,3-Dihydro-3-hydroxy-2-isopropenyl-5-benzofurancarboxylic acid D-266



(2*R**,3*S**)-*form*

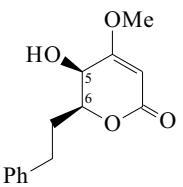
$C_{12}H_{12}O_4$ 220.224

(2*R*,3*S*)-*form*

Me ester:
$C_{13}H_{14}O_4$ 234.251
Constit. of the famine food *Pandanus odoratissimus*. Oil. λ_{max} 220 (sh) ; 258 ; 290 (sh) (no solvent reported).
Jong, T.-T. *et al., Phytochemistry*, 1998, **49**, 2145-2148 (*isol, uv, pmr, cmr*)

5,6-Dihydro-5-hydroxy-4-methoxy-6-(2-phenylethyl)-2*H*-pyran-2-one, 9CI D-267

Dihydrokawain-5-ol



(5*R*,6*S*)-*form*

$C_{14}H_{16}O_4$ 248.278

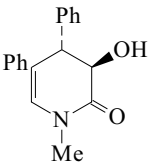
(5*R*,6*S*)-*form* [52247-81-1]
(+)-cis-*form*
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Mp 92°. $[\alpha]_D^{25}$ +73 ($CHCl_3$).

(5*RS*,6*SR*)-*form* [41002-32-8]
(±)-cis-*form*
Cryst. (Et_2O). Mp 77-78°.

(5*RS*,6*RS*)-*form* [41002-33-9]
(±)-trans-*form*
Cryst. (Et_2O). Mp 77-78°.

Achenbach, H. *et al., Tet. Lett.*, 1970, 3259; 1974, 119 (*synth*)
Haensel, R. *et al., Chem. Ber.*, 1973, **106**, 570 (*synth, spectra*)
Arai, Y. *et al., J.O.C.*, 2000, **65**, 258-262 (*synth*)

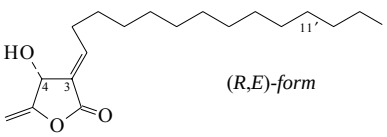
3,4-Dihydro-3-hydroxy-1-methyl-4,5-diphenyl-2(1*H*)-pyridinone, 9CI D-268



$C_{18}H_{17}NO_2$ 279.338

(3*R*,4*S*)-*form* [136112-76-0]
Homoclausenamide
Alkaloid from *Clausena lansium* (wampee).
Yang, M. *et al., Chin. Chem. Lett.*, 1991, **2**, 291; *CA*, **115**, 155059t (*isol, struct*)

Dihydro-4-hydroxy-5-methylene-3-tetradecylidene-2(3*H*)-furanone D-269



(*R*,*E*)-*form*

$C_{19}H_{32}O_3$ 308.46

(*R*,*E*)-*form* [170212-29-0]
Isolinderanolide B
Oil. $[\alpha]_D^{20}$ +40.8 (c, 0.1 in $CHCl_3$).

11′,12′-Didehydro: [170129-22-3] *Dihydro-4-hydroxy-5-methylene-3-(11-tetradecenylidene)-3(2*H*)-furanone.* ***Isolinderanolide A***
$C_{19}H_{30}O_3$ 306.444
Oil. $[\alpha]_D^{20}$ +45.7 (c, 0.1 in $CHCl_3$).

(*R*,*Z*)-*form* [170212-27-8] ***Linderanolide B***
Oil. $[\alpha]_D^{20}$ +39.7 (c, 0.1 in $CHCl_3$).

11′,12′-Didehydro: [170129-20-1] ***Linderanolide A***
$C_{19}H_{30}O_3$ 306.444
Oil. $[\alpha]_D^{20}$ +34.9 (c, 0.1 in $CHCl_3$).

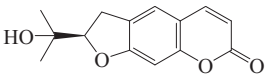
(*S*,*E*)-*form* [56522-16-8] ***Isoobtusilactone A***. *Borbonol 2*
Isol. from *Persea borbonia* (red bay) and other *Persea* spp.. Viscous liq. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{23}$ -54 (c, 0.50 in $CHCl_3$). λ_{max} 225 (MeOH) (Berdy).

(*S*,*Z*)-*form* [56522-15-7] ***Obtusilactone A***. *Borbonol*
Constit. of *Persea borbonia* (red bay). Viscous liq. $[\alpha]_D^{23}$ -46 (c, 0.45 in $CHCl_3$). Stereochem. identity of Borbonol with Obtusilactone A is not certain λ_{max} 224 (MeOH) (Berdy).

[71242-34-7]

Niwa, M. *et al., Chem. Lett.*, 1975, 655 (*Obtusilactones*)
Zaki, A.I. *et al., Physiol. Plant Pathol.*, 1980, **16**, 205 (*Borbonols*)
Rollinson, S.W. *et al., J.A.C.S.*, 1981, **103**, 4114 (*synth*)
Seki, K. *et al., Phytochemistry*, 1995, **40**, 1175-1181 (*Linderanolides, Isolinderanolides*)

2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI D-270



(*R*)-*form*

$C_{14}H_{14}O_4$ 246.262

(*R*)-*form* [495-32-9]
Nodakenetin. *Prangeferol*
Constit. of *Angelica* spp.. Mp 186.5°. $[\alpha]_D$ -22.4.

O-*β*-D-*Glucopyranoside:* [495-31-8] ***Nodakenin***
$C_{20}H_{24}O_9$ 408.404
Platelets (EtOH), prisms (H_2O). Mp 215-219° Mp 259-260° dec. $[\alpha]_D^{30}$ +56.6 (H_2O).

O-*[(2*E*-Butenoyl)-(→6)-β-D-glucopyranoside]:6′-*O-*(2*-trans-*Butenoyl)nodakenin*. ***Decuroside VI***
$C_{24}H_{28}O_{10}$ 476.479
Yellow powder. λ_{max} 203 ; 334 (no solvent reporetd).

O-*[(4-Hydroxy-3-methoxy*-E-*cinnamoyl)-(→6)-β-D-glucopyranoside]:* [131623-14-8] ***6′*-O-trans-*Feruloylnodakenin***
$C_{30}H_{32}O_{12}$ 584.576
Needles (MeOH aq.). Mp 138-140°. $[\alpha]_D$ +49.8 (c, 0.5 in 50% EtOH aq.).

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [96627-80-4] ***Decuroside IV***
$C_{25}H_{32}O_{13}$ 540.52
Powder (MeCN aq.). Mp 236.5-239°. $[\alpha]_D^{24}$ -14.9 (c, 2.96 in DMSO).

O-*[α-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]:* [96638-81-2] ***Decuroside III***. *Nodakenetin 4′*-O-*β-maltoside*
$C_{26}H_{34}O_{14}$ 570.546
Powder. Mp 143.5-146.5° dec. $[\alpha]_D^{24}$ +85.5 (c, 1.00 in MeOH).

O-*[α-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [96638-80-1] ***Decuroside II***. *Nodakenetin 4′*-O-*β-isomaltoside*
$C_{26}H_{34}O_{14}$ 570.546
Powder. Mp 139.5-142° dec. $[\alpha]_D^{24}$ +69.7 (c, 1.00 in MeOH).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [96638-79-8] ***Decuroside I***. *Nodakenetin 4′*-O-*β-gentiobioside*
$C_{26}H_{34}O_{14}$ 570.546
Powder. Mp 147-151.5° dec. $[\alpha]_D^{24}$ +17.5 (c, 1.00 in MeOH).

Ac: ***Nodakenetin acetate***
$C_{16}H_{16}O_5$ 288.299
Cryst. ($CHCl_3$/petrol). Mp 134-135°. $[\alpha]_D$ -13.7 (c, 0.8 in $CHCl_3$).

O-*(4-Hydroxyphenylglyoxylyl):* [39380-09-1] ***Tschuin***. *Chuin*
$C_{22}H_{18}O_7$ 394.38
Cryst. Mp 212-213.5°. $[\alpha]_D^{26}$ -225 (c, 0.2 in EtOH).

O-*(4-Hydroxycinnamoyl):* [53106-45-9] ***Secorin***
$C_{23}H_{20}O_6$ 392.407
Cryst. Mp 212-213°. $[\alpha]_D^{20}$ -220 (c, 1.0 in EtOH).

(*S*)-*form* [13849-08-6] ***Marmesin***

Occurs in Bael bark (*Aegle marmelos*). Plates (Me_2CO, EtOH, C_6H_6 or EtOAc). Mp 189.5°. $[\alpha]_D^{34}$ +26.8 ($CHCl_3$). λ_{max} 217 (ε 7420); 338 (ε 17700) (MeOH) (Berdy). λ_{max} 332 (EtOH) (Berdy).

▶ LV1045500

O-*α-L-Arabinopyranoside:* [192935-76-5]
$C_{19}H_{22}O_8$ 378.378
Mp 128-130°. λ_{max} 217 ; 230 ; 240 ; 260 ; 315 (No solvent reported).

O-*α-L-Rhamnopyranoside:* [142347-99-7]
$C_{20}H_{24}O_8$ 392.405
Isol. from the stem bark of *Aegle marmelos* (bael fruit). Mp 140-142°.

O-*β-D-Galactopyranoside:* [156363-69-8]
$C_{20}H_{24}O_9$ 408.404
Constit. of *Murraya koenigii* (curry leaf tree).

O-*β-D-Glucopyranoside:* [495-30-7] ***Ammajin***. *Marmesinin*
$C_{20}H_{24}O_9$ 408.404
Plates (H_2O). Mp 259-260° dec. $[\alpha]_D$ -60 (EtOH aq.).

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{25}H_{32}O_{13}$ 540.52
Amorph. powder. $[\alpha]_D^{22}$ -45.8 (c, 0.5 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [159650-11-0] ***Marmesin rutinoside***
$C_{26}H_{34}O_{13}$ 554.547
Constit. of the roots of *Murraya koenigii* (curry leaf tree). Mp 190-191°.

Ac: ***Marmesin acetate***
Cryst. (H_2O). Mp 130° (135-136°). $[\alpha]_D$ +25 ($CHCl_3$).

O-*(3-Methylbutanoyl):* ***Marmesin isovalerate***
$C_{19}H_{22}O_5$ 330.38
Cryst. Mp 115-116°. $[\alpha]_D$ -10.5 (c, 0.7 in $CHCl_3$).

O-*(3-Methyl-2-butenoyl):* [13209-79-5] ***Prantschimgin***. *Pranchimgin*
$C_{19}H_{20}O_5$ 328.364
Cryst. Mp 138-140°. $[\alpha]_D^{20}$ -23 (c, 0.87 in $CHCl_3$).

▶ LD_{50} (mus, scu) 73 mg/kg. GQ5730000

O-*Angeloyl:* [19662-71-6] ***Deltoin***
$C_{19}H_{20}O_5$ 328.364
Cryst. (Et_2O/petrol). Mp 105-105.5°. $[\alpha]_D^{18}$ -38.5 (c, 0.8 in $CHCl_3$).

O-*Tigloyl:*
$C_{19}H_{20}O_5$ 328.364
Cryst. (hexane). Mp 111.5-113°. $[\alpha]_D^{23}$ -33 (c, 1 in $CHCl_3$).

O-*Benzoyl:* [17559-85-2] ***Felamidin***. *Benzoylmarmesin*. *Felamedin*
$C_{21}H_{18}O_5$ 350.37
Cryst. Mp 132-134°. $[\alpha]_D^{20}$ -98.9 ($CHCl_3$).

O-*(3-Methylthio-2-propenoyl(Z-)):* [31002-17-2] ***Seseliflorin***
$C_{18}H_{18}O_5S$ 346.403
Mp 143-144°. $[\alpha]_D^{19}$ -58.4 (c, 0.85 in $CHCl_3$).

(ξ)-*form*

O-*(2,3-Dihydroxy-2-methylbutanoyl):* [55747-77-8] ***Lindiol***
$C_{19}H_{22}O_7$ 362.379
Cryst. (C_6H_6). Mp 112°. Abs. config. not detd..

(±)-*form* [13928-55-7]
Plates (C_6H_6). Mp 153-154°.

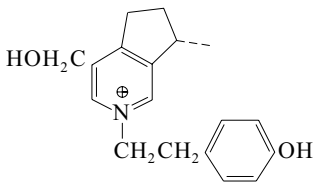
O-*Angeloyl:* [89827-11-2] ***Tortuosinin***
$C_{19}H_{20}O_5$ 328.364
Cryst. Mp 109°.

O-*Tigloyl:* [36706-20-4] ***Sprengelianin***
$C_{19}H_{20}O_5$ 328.364
Cryst. (MeOH). Mp 105°.

Späth, E. *et al., Ber.*, 1939, **72**, 2089 (*Nodakenin*)
Chatterjee, A. *et al., J.A.C.S.*, 1949, **71**, 606 (*struct*)
Abu-Mustafa, E.A. *et al., J.O.C.*, 1961, **26**, 161 (*isol, uv, deriv*)
Kuznetsova, G.A. *et al., Khim. Prir. Soedin.*, 1966, **2**, 235; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 190 (*Prantschimgin*)
Abu-Mustafa, E.A. *et al., Can. J. Chem.*, 1967, **45**, 325 (*pmr*)
Ognyanov, I. *et al., Z. Naturforsch., B*, 1967, **22**, 1231 (*isol*)
Harada, I. *et al., Tet. Lett.*, 1968, 5463 (*synth, abs config*)
Nielsen, B.E. *et al., Acta Chem. Scand.*, 1970, **24**, 2863 (*isol*)
Savina, A.A. *et al., Khim. Prir. Soedin.*, 1970, **6**, 522; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 540 (*Seseliflorin*)
Krivut, B.A. *et al., Khim. Prir. Soedin.*, 1970, **6**, 526; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 545 (*synth*)
Steck, W. *et al., Can. J. Chem.*, 1971, **49**, 2297 (*synth, pmr*)
Murray, R.D.H. *et al., Tetrahedron*, 1971, **27**, 4901 (*synth, ir, pmr, ms*)
Molho, D. *et al., Bull. Soc. Chim. Fr.*, 1972, 208 (*isol*)
Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1972, **8**, 114; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 107 (*isol, ir, uv, pmr*)
Aminov, A.M. *et al., Khim. Prir. Soedin.*, 1972, **8**, 799; 1973, **9**, 487; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 779; 1973, **9**, 459 (*isol*)
Dukhovlinova, L.J. *et al., Khim. Prir. Soedin.*, 1973, **9**, 663; 1974, **10**, 785; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 626; 1974, **10**, 806 (*isol*)
Talapatra, S.K. *et al., Phytochemistry*, 1973, **12**, 2312 (*isol*)
Innocenti, G. *et al., Planta Med.*, 1978, **34**, 167 (*biosynth*)
De Pascual Teresa, J. *et al., An. Quim.*, 1979, **75**, 175 (*isol*)
Elgamal, M.H.A. *et al., Phytochemistry*, 1979, **18**, 139 (*cmr*)
Burke, B.A. *et al., Heterocycles*, 1981, **16**, 897 (*isol*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, (*book*)
Asahara, T. *et al., Planta Med.*, 1984, **50**, 488 (*Decuroside IV*)
Grande, M. *et al., Phytochemistry*, 1986, **25**, 505
Matano, Y. *et al., Planta Med.*, 1986, 135 (*Decurosides I-III*)
Jain, R.K. *et al., Proc. Natl. Acad. Sci., India*, 1992, **62**, 5 (*galactoside*)
Srivastava, S.K. *et al., J. Indian Chem. Soc.*, 1993, **70**, 655 (*rutinoside*)
Srivastava, S.D. *et al., J. Indian Chem. Soc.*, 1996, **73**, 666-668 (*arabinoside*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1404-1407 (*Marmesin apiosylglucoside*)
Kong, L.Y. *et al., Chin. Chem. Lett.*, 2000, **11**, 315-318 (*Decuroside VI*)
Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, 2002, **83**, 1-619 (*rev*)

6,7-Dihydro-4-(hydroxymethyl)-2-(*p*-hydroxyphenethyl)-7-methyl-5*H*-2-pyrindinium D-271

[15794-93-1]



$C_{18}H_{22}NO_2^{\oplus}$ 284.377
Minor alkaloid from the roots of *Valeriana officinalis* (valerian).

Chloride:
$C_{18}H_{22}ClNO_2$ 319.83
Mp 220-223° dec.

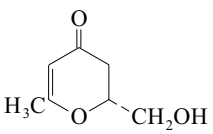
Picrate:
Mp 60-65° (resolidifies and melts at ca. 113°).

Trifluoroacetate:
Mp 145-147°. $[\alpha]_D^{22}$ +19.3 (MeOH).

Torssell, K. *et al., Acta Chem. Scand.*, 1967, **21**, 53 (*isol, ir, pmr, ms, struct*)

2,3-Dihydro-2-(hydroxymethyl)-6-methyl-4*H*-pyran-4-one, 9CI D-272

[146064-67-7]
Erinapyrone B

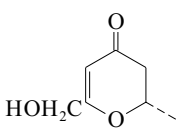


$C_7H_{10}O_3$ 142.154
Isol. from *Hericium erinaceum* (lions mane). Oil.

Kawagishi, H. *et al., Chem. Lett.*, 1992, 2475 (*isol, cd, pmr, cmr*)
Noda, Y. *et al., Heterocycles*, 1996, **43**, 271 (*synth*)

2,3-Dihydro-6-(hydroxymethyl)-2-methyl-4*H*-pyran-4-one, 9CI D-273

[146064-66-6]
Erinapyrone A

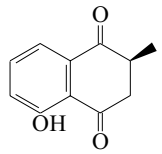


$C_7H_{10}O_3$ 142.154
Isol. from *Hericium erinaceum* (lions mane). Oil.

Kawagishi, H. *et al., Chem. Lett.*, 1992, 2475 (*isol, cd, pmr, cmr*)
Noda, Y. *et al., Heterocycles*, 1996, **43**, 271 (*synth*)

2,3-Dihydro-5-hydroxy-2-methyl-1,4-naphthoquinone D-274

[74413-19-7]
Dihydroplumbagin. β-Hydroplumbagin



(*S*)-*form*

$C_{11}H_{10}O_3$ 190.198

(*S*)-*form* [76372-21-9]
Constit. of *Juglans nigra* (black walnut). Cryst. (pentane). Mp 89-91°. $[\alpha]_D^{18}$ -115 (c, 0.5 in $CHCl_3$).

O-*β*-D-*Glucopyranoside:* [155569-76-9] ***Plumbaside C***
$C_{17}H_{20}O_8$ 352.34
Amorph. powder.

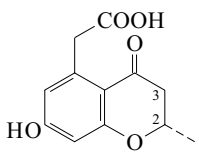
(±)-*form*
Yellow cryst. (petrol). Mp 83-85°.

[79516-55-5]

Sankaram, A.V.B. *et al., Tetrahedron*, 1979, **35**, 1777 (*synth*)
Lavault, M. *et al., Planta Med.*, *Suppl*., 1980, 17 (*isol*)
Hanson, S.W. *et al., Phytochemistry*, 1981, **20**, 1162 (*synth, pmr*)
Binder, R.G. *et al., Phytochemistry*, 1989, **28**, 2799 (*isol, pmr*)
Yue, J. *et al., Phytochemistry*, 1994, **35**, 1023 (*Plumbaside C*)

2,3-Dihydro-7-hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-acetic acid, 9CI D-275

5-(Carboxymethyl)-7-hydroxy-2-methyl-4-chromanone



$C_{12}H_{12}O_5$ 236.224

(*S*)-*form* [94356-37-3]
Constit. of *Rheum* sp. (rhubarb). Needles + ½H_2O (MeOH aq.). Mp 205-207°. $[\alpha]_D^{24}$ -9.1 (c, 0.23 in MeOH).

2,3-Didehydro: [94356-34-0] ***7-Hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-acetic acid, 9CI***. *5-(Carboxymethyl)-7-hydroxy-2-methylchromone*
$C_{12}H_{10}O_5$ 234.208
Constit. of *Rheum* sp.. Needles (MeOH aq.). Mp 263.5-265°.

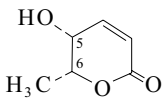
2,3-Didehydro, Me ether: [124793-06-2]
Needles (MeOH). Mp 237-239°.

2,3-Didehydro, Me ester, Me ether: [124793-05-1]
Needles (Et_2O/hexane). Mp 140-142°.

Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3493 (*isol, pmr, cmr, ir*)
Takeuchi, N. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2012 (*synth*)

5,6-Dihydro-5-hydroxy-6-methyl-2*H*-pyran-2-one, 9CI D-276

[54826-92-5]
4-Hydroxy-2-hexen-5-olide



(5*R*,6*R*)-*form*

$C_6H_8O_3$ 128.127

(5*R*,6*R*)-*form*
O-*β*-D-*Glucopyranoside:* [80433-52-9] ***Angiopteroside***
$C_{12}H_{18}O_8$ 290.269
Cryst. ($CHCl_3$/MeOH).

Ac: [54621-88-4]
$C_8H_{10}O_4$ 170.165
Oil. $Bp_{0.1}$ 130°. $[\alpha]_D^{20}$ -179 (c, 1 in $CHCl_3$).

(5*R*,6*S*)-*form* [69308-39-0] ***Osmundalactone***
Constit. of *Osmunda japonica* (zenmai). Plates (C_6H_6) or needles. Mp 82-82.5°. $[\alpha]_D^{22}$ -70.6 (c, 2.0 in H_2O).

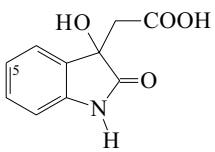
O-*β*-D-*Glucopyranoside:* [54835-71-1] ***Osmundalin***
$C_{12}H_{18}O_8$ 290.269
Isol. from ferns *Osmunda japonica* (zenmai). Syrup; needles (MeOH) as tetra-Ac. Mp 172.5-173.5° (tetra-Ac).

(5*S*,6*R*)-*form*
Cryst. (EtOAc). Mp 81.5-82.5°. $[\alpha]_D$ +70.9 (c, 1.3 in H_2O).

Hollenbeak, K.H. *et al., Tetrahedron*, 1974, **30**, 2307 (*isol, synth*)
Torssell, K. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 297; 1978, **32**, 457 (*synth*)
Yamagiwa, S. *et al., J.C.S. Perkin 1*, 1979, 570 (*synth*)
Hseu, T.H. *et al., Acta Cryst. B*, 1981, **37**, 2095 (*cryst struct*)
Numata, A. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2815
Murayama, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 2347 (*synth*)
Lichtenthaler, F.W. *et al., Annalen*, 1989, 1153 (*synth, pmr, acetate*)
Buchanan, M.S. *et al., Phytochemistry*, 1995, **40**, 1251 (*isol, pmr, cmr*)
Ono, M. *et al., Heterocycles*, 1999, **51**, 1503-1508 (*synth*)
Yonghang, G. *et al., J. Chem. Res., Synop.*, 1999, 488-489 (*synth*)
Carda, M. *et al., Eur. J. Org. Chem.*, 2002, 2649-2655 (*synth*)

2,3-Dihydro-3-hydroxy-2-oxo-1*H*-indole-3-acetic acid, 9CI D-277

Dioxindole-3-acetic acid



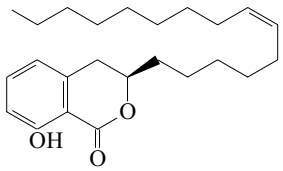
$C_{10}H_9NO_4$ 207.185

Me ester:
$C_{11}H_{11}NO_4$ 221.212
Isol. from rice bran. Amorph. powder.

Kinashi, H. *et al., Agric. Biol. Chem.*, 1976, **40**, 2465

3,4-Dihydro-8-hydroxy-3-(6-pentadecenyl)-1*H*-2-benzopyran-1-one D-278

3,4-Dihydro-8-hydroxy-3-(6-pentadecenyl)isocoumarin



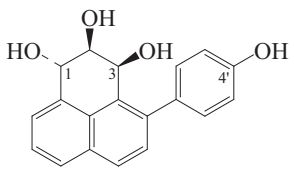
$C_{24}H_{36}O_3$ 372.547

(3*R*, 6′*Z*)-*form* [158627-94-2]
Constit. of the fruit of *Ginkgo biloba* (ginkgo). $[\alpha]_D^{25}$ -23 (c, 0.8 in $CHCl_3$). Probable config..

Choukchou-Braham, N. *et al., Tet. Lett.*, 1994, **35**, 3949 (*isol, ir, pmr, cmr, synth*)

2,3-Dihydro-4-(4-hydroxyphenyl)-1*H*-phenalene-1,2,3-triol D-279

*2,3-Dihydro-1,2,3-trihydroxy-4-(4-hydroxyphenyl)-1*H*-phenalene*



(1*S*,2*R*,3*S*)-*form*

$C_{19}H_{16}O_4$ 308.333

(1*S*,2*R*,3*S*)-*form*
Isol. from *Musa acuminata* (dwarf banana) infected with *Colletotrichum musae*. Powder. $[\alpha]_D^{25}$ -5 (c, 0.5 in MeOH). λ_{max} 231 (ε 24000); 259 (ε 15000); 290 (ε 6800) (MeOH).

4′-Me ether: [163811-78-7] *2,3-Dihydro-4-(4-methoxyphenyl)-1*H*-phenalene-1,2,3-triol*
$C_{20}H_{18}O_4$ 322.36
Isol. from the rhizomes of *Musa acuminata* (dwarf banana) infected with *Fusarium oxysporum*. Cryst. (C_6H_6/hexane). Mp 104-106° (92-96°). $[\alpha]_D^{25}$ -35 (c, 0.3 in $CHCl_3$) ((-15.4)). λ_{max} 268 ; 284 ; 352 ; 388 (EtOH).

1-Ketone: ***2,3-Dihydro-2,3-dihydroxy-4-(4-hydroxyphenyl)-1*H*-phenalen-1-one***
$C_{19}H_{14}O_4$ 306.317
Constit. of *Musa acuminata* (dwarf banana) infected with *Colletotrichum musae*. Powder. $[\alpha]_D^{25}$ +44 (c, 0.2 in MeOH). (2*S*,3*S*)- Config. owing to change in Cahn-Ingold-Prelog priorities λ_{max} 219 (ε 24000); 229 (ε 25000); 245 (ε 17000); 273 (ε 11000); 325 (ε 4600) (MeOH).

1-Ketone, 4′-Me ether: [159853-37-9] ***2,3-Dihydro-2,3-dihydroxy-4-(4-methoxyphenyl)-1*H*-phenalen-1-one***
$C_{20}H_{16}O_4$ 320.344
Constit. of *Musa acuminata* (dwarf banana) infected with *Colletotrichum*

musae. Needles. Mp 175-177°. $[\alpha]_D^{25}$ +65 (c, 0.7 in $CHCl_3$) ((+40.9)). λ_{max} 276 ; 312 ; 340 ; 386 (EtOH) (Berdy).

3-Ketone: [173560-63-9] *2,3-Dihydro-2,3-dihydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one.* ***Musanolone C***
$C_{19}H_{14}O_4$ 306.317
Constit. of *Musa acuminata* (dwarf banana) infected with *Colletotrichum musae*. Yellowish solid. Mp 258-261°. λ_{max} 265 ; 280 ; 323 ; 377 (EtOH).

*3′-Hydroxy, 1-ketone:4-(3,4-Dihydroxyphenyl)-2,3-dihydro-2,3-dihydroxy-1*H*-phenalen-1-one*
$C_{19}H_{14}O_5$ 322.317
Constit. of *Musa acuminata* (dwarf banana) infected with *Colletotrichum musae*. Powder. $[\alpha]_D^{25}$ +31 (c, 0.03 in MeOH). (2*S*,3*S*)- Config. owing to change in Cahn-Ingold-Prelog priorities λ_{max} 268 (ϵ 23000); 282 (ϵ 13000) (MeOH).

*4′-Deoxy, 3-ketone:****2,3-Dihydro-2,3-dihydroxy-9-phenyl-1*H*-phenalen-1-one***
$C_{19}H_{14}O_3$ 290.318
Constit. of *Musa acuminata* (dwarf banana) infected with *Colletotrichum musae*. Powder. $[\alpha]_D^{26}$ -142 (c, 0.1 in MeOH).

3′-Methoxy, 3-ketone: [173560-64-0] *2,3-Dihydro-2,3-dihydroxy-9-(4-hydroxy-3-methoxyphenyl)-1*H*-phenalen-1-one.* ***Musanolone D***
$C_{20}H_{16}O_5$ 336.343
Constit. of *Musa acuminata* (dwarf banana) (Musaceae). Solid. Mp 248-250°. λ_{max} 266 ; 352 ; 384 (EtOH).

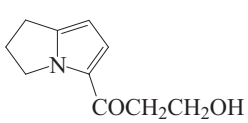
(1*R*,2*R*,3*R*)-*form*

3-Ketone:
Constit. of *Musa acuminata* (dwarf banana) infected with *Colletotrichum musae*. Powder. $[\alpha]_D^{25}$ -106 (c, 0.06 in MeOH). λ_{max} 246 (ϵ 23000); 287 (ϵ 9800); 320 (ϵ 6100) (MeOH).

Luis, J.G. *et al., Tetrahedron*, 1995, **51**, 4117-4130 (*4′-Me ether*)
Luis, J.G. *et al., Phytochemistry*, 1996, **41**, 753-757 (*Musanolones*)
Kamo, T. *et al., Tetrahedron*, 2001, **57**, 7649-7656 (*isol, uv, pmr, cmr, ms, abs config*)

2,3-Dihydro-5-(3-hydroxypropanoyl)-1*H*-pyrrolizine D-280

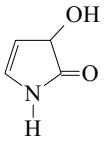
[97073-09-1]
*1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-3-hydroxy-1-propanone*



$C_{10}H_{13}NO_2$ 179.218
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr*)
Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

1,3-Dihydro-3-hydroxy-2*H*-pyrrol-2-one, 9CI D-281



$C_4H_5NO_2$ 99.089

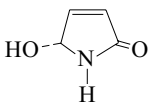
O-*β*-D-*Glucopyranoside:* [18814-39-6] ***Pisatoside***
$C_{10}H_{15}NO_7$ 261.231
Isol. from seedlings of *Pisum sativum* (peas). Mp 104-107°. $[\alpha]_D^{20}$ -4.9.

[18814-40-9]

Kocourek, J. *et al., Arch. Biochem. Biophys.*, 1967, **121**, 531 (*isol, struct*)

1,5-Dihydro-5-hydroxy-2*H*-pyrrol-2-one, 9CI D-282

[34085-09-1]
Dihydromaleimide*. Isosuccinimide*



$C_4H_5NO_2$ 99.089
No evidence for tautomerism from form shown.

(*R*)-*form* [87710-47-2]
Alkaloid from the shoots of dwarf pea (*Pisum sativum*). Prisms. Mp 103-105°. $[\alpha]_D^{23}$ -12.6.

O-*β*-D-*Glucopyranoside:* [26696-59-3] ***Dihydromaleimide β-D-glucoside****. Isosuccinimide β-D-glucoside*
$C_{10}H_{15}NO_7$ 261.231
Alkaloid from *Pisum sativum* (peas). Prisms. Mp 185-188°. $[\alpha]_D^{22.5}$ -73.7. The identity (structural and stereochemical) of the various isolates of this glucoside is not certain. May be identical with Pisatoside.

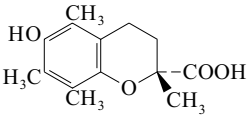
(±)-*form*
Cryst. (Me_2CO). Mp 102°.

Me ether: [34128-18-2] *1,5-Dihydro-5-methoxy-2*H*-pyrrol-2-one, 9CI*
$C_5H_7NO_2$ 113.116
Mp 38°. Bp_9 95°.

de Mayo, P. *et al., Chem. Ind. (London)*, 1962, 1576 (*synth*)
Liu, T.-Y. *et al., Plant Physiol.*, 1970, **45**, 424 (*isol, glucoside*)
Farina, F. *et al., Synthesis*, 1973, 167 (*synth, glucoside*)
Masuko, M. *et al., Phytochemistry*, 1983, **22**, 1278 (*isol, uv, ir, pmr, cmr, cd, struct*)

3,4-Dihydro-6-hydroxy-2,5,7,8-tetramethyl-2*H*-1-benzopyran-2-carboxylic acid, 9CI D-283

[56305-04-5]
6-Hydroxy-2,5,7,8-tetramethyl-2-chromancarboxylic acid. Trolox C



(*R*)-*form*

$C_{14}H_{18}O_4$ 250.294
Antioxidant used in food industry.
▶ DJ2273000

(*R*)-*form* [53101-49-8]
Cryst. (Et_2O/petrol). Mp 159-161° dec. $[\alpha]_D^{25}$ +66.1 (c, 1 in EtOH).

Me ester: [70897-16-4]
$C_{15}H_{20}O_4$ 264.321
Cryst. (MeOH aq.). Mp 132-134.5°. $[\alpha]_D^{25}$ +61.4 (c, 4.91 in MeOH).

(*S*)-*form* [53174-06-4]
Cryst. (Et_2O/pentane). Mp 161°. $[\alpha]_D^{20}$ -64.8 (c, 1.01 in EtOH).

Me ester: [70897-17-5]
$[\alpha]_D^{24}$ -60.5 (c, 1.02 in MeOH).

Me ether: [135806-59-6] *6-Methoxy-2,5,7,8-tetramethyl-2-chromancarboxylic acid*
$C_{15}H_{20}O_4$ 264.321
Cryst. (Et_2O/hexane). Mp 144-145°. $[\alpha]_D^{20}$ -69.2.

(±)-*form* [53188-07-1]
Cryst. (H_2O). Mp 190-192°.

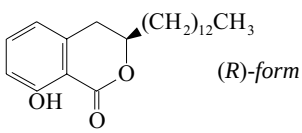
Me ester: [53101-52-3]
Cryst. (Me_2CO/Et_2O). Mp 158.5-161.5°.

Et ester: [53174-07-5]
$C_{16}H_{22}O_4$ 278.347
Cryst. (Et_2O). Mp 124-126°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1176B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 245B (*ir*)
Scott, J.W. *et al., J. Am. Oil Chem. Soc.*, 1974, **51**, 200; 1975, **52**, 174 (*synth, antioxidant*)
Yoda, H. *et al., Chem. Lett.*, 1989, 465 (*synth*)
Walther, W. *et al., Chimia*, 1991, **45**, 121 (*synth, use, Me ether*)
Netscher, T. *et al., Annalen*, 1992, 543 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TNR625

3,4-Dihydro-8-hydroxy-3-tridecyl-1*H*-2-benzopyran-1-one D-284

3,4-Dihydro-8-hydroxy-3-tridecylisocoumarin



(*R*)-*form*

$C_{22}H_{34}O_3$ 346.509

(*R*)-*form* [158627-93-1]
Constit. of the fruit of *Ginkgo biloba* (ginkgo).

Me ether: [158627-99-7] *3,4-Dihydro-8-methoxy-3-tridecylisocoumarin*
$C_{23}H_{36}O_3$ 360.536
Cryst. Mp 77-78°. $[\alpha]_D^{23}$ -106 (c, 1 in $CHCl_3$).

(±)-*form*

Me ether:
Cryst. Mp 73-74°.

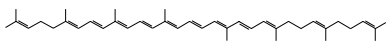
[158628-00-3, 158628-01-4]

Choukchou-Braham, N. *et al., Tet. Lett.*, 1994, **35**, 3949 (*isol, uv, ir, pmr, cmr, synth*)

7,8-Dihydrolycopene D-285

[502-64-7]

7,8-Dihydro-ψ,ψ-carotene, 9CI. ***Neurosporene****. Neurosporin. Flavorhodin. Proneurosporene*



$C_{40}H_{58}$ 538.898

Present in higher plants, e.g. pineapple (*Ananas sativus*). Yellow-orange cryst. (EtOH). Mp 124° (115-116°).

(9Z,7′Z,9′Z)-form [10467-46-6]

Isol. from tomato (*Lycopersicon esculentum* var. 'Tangella'). Dark red viscous oil. λ_{max} 410 ; 433 (hexane).

Davis, J.B. *et al., J.C.S.(C)*, 1966, 2154 (*synth, pmr*)

Suzue, G. *et al., Biochim. Biophys. Acta*, 1969, **176**, 653 (*biosynth*)

Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1817b (*occur*)

Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*cmr, ms*)

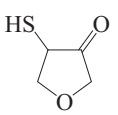
Frecknell, E.A. *et al., Phytochemistry*, 1984, **23**, 1707 (*isol, occur*)

Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 34 (*bibl*)

Dihydro-4-mercapto-3(2*H*)-furanone D-286

[56078-98-9]

4-Mercapto-3-oxotetrahydrofuran



$C_4H_6O_2S$ 118.156

Component of meat aroma model systems with green, meaty-hydrolysed vegetable aroma. Characterised spectroscopically.

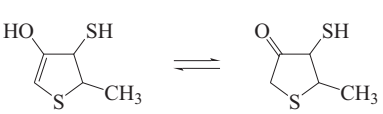
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*formn, isol, ms, ir*)

Dihydro-4-mercapto-5-methyl-3(2*H*)-thiophenone, 10CI D-287

[65936-90-5]

[56079-01-7]

4,5-Dihydro-4-mercapto-5-methylthiophene-3-ol, 9CI. 3-Mercapto-4-hydroxy-2-methyl-2,3-dihydrothiophene



$C_5H_8OS_2$ 148.25

Component of meat aroma models. Possesses a roasted meat aroma. Characterised spectroscopically.

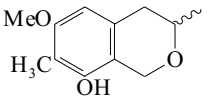
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms, ir*)

Misharina, T.A. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1992, **14**, 27-32 (*occur*)

3,4-Dihydro-6-methoxy-3,7-dimethyl-1*H*-2-benzopyran-8-ol, 9CI D-288

[70080-82-9]

8-Hydroxy-6-methoxy-3,7-dimethylisochroman



$C_{12}H_{16}O_3$ 208.257

Mycotoxin prod. by *Penicillium corylophilum* and *Penicillium steckii*. Isol. from *P. steckii* infected millet hay. Mp 122°.

► NQ7185000

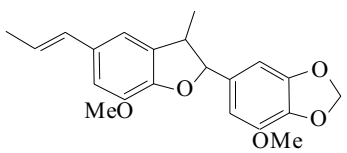
Cox, R.H. *et al., J. Agric. Food Chem.*, 1979, **27**, 999-1001 (*isol*)

Cutler, H.G. *et al., Agric. Biol. Chem.*, 1989, **53**, 1975 (*isol*)

Malmstrom, J. *et al., Phytochemistry*, 2000, **54**, 301-309 (*occur*)

2,3-Dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(1-propenyl)benzofuran D-289

[50354-06-8]



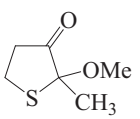
$C_{21}H_{22}O_5$ 354.402

Isol. from the seed kernels of *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D^{23}$ +43.5 (c, 1.65 in $CHCl_3$).

Isogai, A. *et al., Agric. Biol. Chem.*, 1973, **37**, 889; 1479 (*isol*)

Dihydro-2-methoxy-2-methyl-3(2*H*)-thiophenone D-290

[129314-86-9]



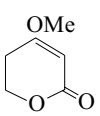
$C_6H_{10}O_2S$ 146.21

Component of meat aroma model systems. Characterised spectroscopically.

Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, ms, pmr*)

5,6-Dihydro-4-methoxy-2*H*-pyran-2-one D-291

[83920-64-3]



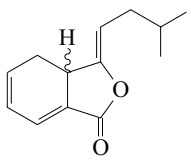
$C_6H_8O_3$ 128.127

Mycotoxin prod. by *Penicillium italicum*. Pale yellow cryst. ($CHCl_3$/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 77°. λ_{max} 232 (ϵ 11200) (MeOH) (Berdy).

Gorst-Allman, C.P. *et al., S. Afr. J. Chem.*, 1982, **35**, 102; 1983, **36**, 83 (*isol, struct, props, biosynth*)

3*a*,4-Dihydro-3-(3-methylbutylidene)-1(3*H*)-isobenzofuranone D-292

*3-Isovalidene-3*a*,4-dihydrophthalide*



$C_{13}H_{16}O_2$ 204.268

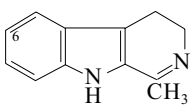
Odorous constit. of celery stem and leaf (*Apium graveolens*). Light-yellow oil. Bp_{10} 175°. $n_D^{27.5}$ 1.5172. λ_{max} 197 (log ϵ 5.08); 227 (log ϵ 4.6); 273 (log ϵ 4.14); 282 (log ϵ 4.12) (no solvent reported).

Gold, H.J. *et al., J.O.C.*, 1963, **28**, 985 (*isol, ir, uv*)

3,4-Dihydro-1-methyl-β-carboline D-293

[525-41-7]

*4,9-Dihydro-1-methyl-3*H*-pyrido[3,4-*b*]indole, 9CI.* ***Harmalan****. Dihydroharman*



$C_{12}H_{12}N_2$ 184.24

Alkaloid from *Elaeagnus angustifolia* (Russian olive). Cream needles (Me_2CO). Mp 183-185° dec.

Picrate:

Yellow needles ($CHCl_3$/MeOH). Mp 245° dec. (234-235° dec.).

6-Methoxy: [3589-73-9] ***6-Methoxyharmalan***

$C_{13}H_{14}N_2O$ 214.266

► UU9802000

Manske, R.H.F. *et al., J.C.S.*, 1927, 1 (*synth*)

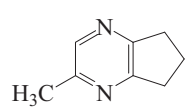
Kanaoka, Y. *et al., Chem. Pharm. Bull.*, 1967, **15**, 101 (*synth, uv, ir*)

Cassady, J.M. *et al., J. Nat. Prod.*, 1971, **34**, 161 (*isol, uv, struct, 6-Methoxyharmalan*)

Picker, K. *et al., Aust. J. Chem.*, 1976, **29**, 2023 (*isol, uv, ir, pmr, ms*)

6,7-Dihydro-2-methyl-5*H*-cyclopenta[*b*]pyrazine, 9CI D-294

[23747-46-8]



$C_8H_{10}N_2$ 134.18

Maillard prod. Present in sesame seed oil, green tea, coffee, roast oats, wheat bread,

cocoa bean, roast coconut, fried chicken, yeast extract, cooked beef and roast filbert. Bp_{10} 125-130°.

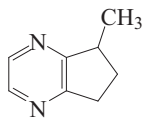
1-Oxide: [61928-78-7]
$C_8H_{10}N_2O$ 150.18
Mp 74°.

Flament, I. *et al., Helv. Chim. Acta*, 1973, **56**, 610-619; 1976, **59**, 2314-2326 (*synth, 1-oxide, ms, ir, pmr*)
Vitzthum, O.G. *et al., J. Agric. Food Chem.*, 1975, **23**, 510-516 (*pmr, ms*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*glc, anal*)
Jayalekshmy, A. *et al., J. Am. Oil Chem. Soc.*, 1991, **68**, 873-880 (*glc, occur, coconut*)
Ames, J.M. *et al., Flavour Fragrance J.*, 1992, **7**, 89-103 (*occur, yeast*)

6,7-Dihydro-5-methyl-5*H*-cyclopenta[*b*]pyrazine, 9CI D-295

[23747-48-0]

[149403-32-7, 149403-33-8]
FEMA 3306



$C_8H_{10}N_2$ 134.18
Flavouring ingredient. Present in coffee aroma, asparagus, wheat bread, rye bread, cocoa, green tea, roasted barley, roasted filbert, roasted peanut, fried chicken, wild rice, roast almond, baked potato, earth-almond (*Cyperus esculentus*) and other foodstuffs.

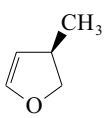
(±)-*form* [149310-63-4]
Bp_{10} 78-80°.

1-Oxide: [61928-79-8]
$C_8H_{10}N_2O$ 150.18
$Bp_{0.002}$ 90-95°.

Flament, I. *et al., Helv. Chim. Acta*, 1973, **56**, 610-619; 1976, **59**, 2314-2316 (*synth, 1-oxide, ms, pmr*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **23**, 273-279 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1752-1753 (*occur, props*)
Cantalego, M.J. *et al., J. Agric. Food Chem.*, 1997, **45**, 1853-1860 (*glc, occur*)
Deibler, K.D. *et al., Dev. Food Sci.*, 1998, **40**, 69-78 (*glc, occur, coffee*)
Farouk, A. *et al., Nahrung*, 2000, **44**, 188-192 (*formn*)

2,3-Dihydro-3-methylfuran, 9CI D-296

[1708-27-6]



(*R*)-*form*

C_5H_8O 84.118

(*R*)-*form* [56717-99-8]
Bp 69-70°. $[\alpha]_D^{25}$ -19.93 (c, 5.1 in heptane).

(±)-*form*
Bp 68°. n_D^{25} 1.4161.

(ξ)-*form*
Constit. of licorice root (*Glycyrrhiza glabra*).

Parham, W. *et al., J.A.C.S.*, 1951, **73**, 913 (*synth, props*)
Botteghi, C. *et al., J.O.C.*, 1972, **37**, 1835 (*pmr, ms, synth*)
Botteghi, C. *et al., Gazz. Chim. Ital.*, 1975, **105**, 233 (*R-form, synth*)
Sakagami, H. *et al., CA*, 1993, **118**, 232572w (*occur*)

2,3-Dihydro-4-methylfuran D-297

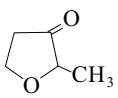
[34314-83-5]

C_5H_8O 84.118
Constit. of volatiles from cooked ham and beef and of oil from licorice roots (*Glycyrrhiza glabra*). Liq. Bp_{20} 63-64°. n_D^{20} 1.4425.

Botteghi, C. *et al., J.O.C.*, 1972, **37**, 1835-1837 (*synth, pmr, ms*)
Hiatt, M.H. *et al., Anal. Chem.*, 1983, **55**, 506 (*glc, ms*)
McLeod, G. *et al., J. Food Sci.*, 1986, **51**, 1427 (*occur*)
Kameoka, H. *et al., Nippon Kagaku Kaishi*, 1987, **61**, 119 (*isol*)
Balog, D.W. *et al., J. Agric. Food Chem.*, 1990, **38**, 2021 (*occur*)
Liang, B. *et al., CA*, 1993, **118**, 143402y (*isol*)
Temme, O. *et al., J.O.C.*, 1998, **63**, 6007-6015 (*synth*)

Dihydro-2-methyl-3(2*H*)-furanone, 9CI D-298

[3188-00-9]
Tetrahydro-2-methyl-3-furanone. FEMA 3373



$C_5H_8O_2$ 100.117
►LU3579000

(±)-*form*
Liq. d_4^{25} 1.02. Bp 139°. n_D^{25} 1.4278.

2,4-Dinitrophenylhydrazone:
Yellow-orange cryst. (EtOH). Mp 179-181°.

(ξ)-*form*
Volatile constit. of coffee. Present in many foods. Flavouring ingredient.

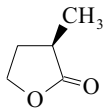
[36541-25-0]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 548D (*ir*)
Giauturco, M.A. *et al., Tetrahedron*, 1964, **20**, 1763 (*synth, ir*)
Colovray, G. *et al., Bull. Soc. Chim. Fr.*, 1965, 1985 (*synth*)
Decor, J.P. *et al., Bull. Soc. Chim. Fr.*, 1970, 2370 (*synth, ms*)
Ferretti, A. *et al., J. Agric. Food Chem.*, 1971, **19**, 245 (*glc, ms*)
Tarnchompoo, B. *et al., Tet. Lett.*, 1984, **25**, 5567 (*synth*)
Ragoussis, V. *et al., Synth. Commun.*, 1998, **28**, 4273-4278 (*synth, pmr, ms*)

Dihydro-3-methyl-2(3*H*)-furanone, 9CI D-299

[1679-47-6]

α-Methyl-γ-butyrolactone. 2-Methyl-4-butanolide



(*R*)-*form*

$C_5H_8O_2$ 100.117
Present in *Mangifera indica* (mango).

(*R*)-*form* [55254-35-8]
Liq. Bp_{22} 93-95°. $[\alpha]_D^{23}$ +13.8 (c, 10.0 in EtOH).

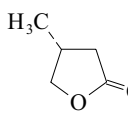
(*S*)-*form* [65527-79-9]
Bp_{20} 94-95°. $[\alpha]_D^{24}$ -14.7 (c, 6.3 in EtOH).

(±)-*form* [69010-09-9]
Bp_{20} 92.5°. n_D^{20} 1.4332.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1127C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 698B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 749D (*ir*)
Kaneko, T. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 1149 (*synth, resoln, pmr, ms*)
Marion, J.P. *et al., Helv. Chim. Acta*, 1967, **50**, 1509 (*synth*)
Timmer, R. *et al., J. Agric. Food Chem.*, 1975, **23**, 53 (*isol, ms, chromatogr*)
Meyers, A.I. *et al., J.O.C.*, 1980, **45**, 2792 (*synth, cd*)
Evans, D.A. *et al., J.A.C.S.*, 1982, **104**, 1737 (*synth*)
Polonski, T. *et al., Tetrahedron*, 1983, **39**, 3131 (*cd*)
Midland, M.M. *et al., Tetrahedron*, 1984, **40**, 1371 (*synth. pmr, cmr, ir*)
Fuji, K. *et al., Tet. Lett.*, 1986, **27**, 5381 (*resoln*)
Bock, K. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 13 (*synth, pmr*)
Jedlinski, Z. *et al., J.O.C.*, 1987, **52**, 4601 (*synth, ir, ms, pmr*)
Ishii, Y. *et al., J.O.C.*, 1988, **53**, 5549 (*synth, cmr, pmr, ir*)
Gerlach, U. *et al., Annalen*, 1989, 103 (*hplc, uv*)
Ozegowski, R. *et al., Annalen*, 1995, 1699 (*R-form, synth, pmr, cmr*)

Dihydro-4-methyl-2(3*H*)-furanone D-300

[1679-49-8]
3-Methyl-4-butanolide. 3-Methyl-γ-butyrolactone



(*R*)-*form*

$C_5H_8O_2$ 100.117

(*R*)-*form* [65284-00-6]
Bp_{45} 120°. $[\alpha]_D^{20}$ +24 (c, 3.32 in Et_2O).

(*S*)-*form* [64190-48-3]
Bp_{15} 87-89°. $[\alpha]_D$ -24.6 (neat).

(±)-*form* [70470-05-2]
d_4^{20} 1.06. Bp_{11} 76-76.5°. n_D^{20} 1.4339.

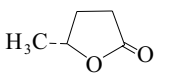
(ξ)-*form*
Volatile flavour component of dried beans, e.g. soy beans.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1128A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 750A (*ir*)
Seidel, C.F. *et al., Helv. Chim. Acta*, 1959, **42**, 1830 (*synth, ir*)

Leuenberger, H.G.W. *et al., Helv. Chim. Acta*, 1979, **62**, 455 (*synth, pmr*)
Mukaiyama, T. *et al., Chem. Lett.*, 1980, 635 (*synth*)
Nikishin, G.I. *et al., J.C.S. Perkin 2*, 1983, 595 (*synth, ir, pmr, ms*)
Mori, K. *et al., Tetrahedron*, 1983, **39**, 3107 (*synth, ir, pmr*)
Midland, M.M. *et al., Tetrahedron*, 1984, **40**, 1371 (*synth, pmr, cmr, ir*)
Mattes, H. *et al., J. Med. Chem.*, 1987, **30**, 1948 (*synth, pmr, ir*)
Fuganti, C. *et al., J.C.S. Perkin 1*, 1988, 3061 (*synth*)
Ferraboschi, P. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 371 (***synth***)
Takeda, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2706 (*synth*)
Berens, U. *et al., Synthesis*, 1991, 832 (*synth, pmr, cmr*)
Trybulski, E.J. *et al., J. Med. Chem.*, 1993, **36**, 3533 (*synth, pmr, ir*)
Ozegowski, R. *et al., Annalen*, 1995, 1699 (*S-form, synth, pmr, cmr*)
Pemp, A. *et al., J. Prakt. Chem.*, 1999, **341**, 65-68 (*R-form, synth, ir, pmr, cmr, ms*)
Buszek, K.R. *et al., Org. Prep. Proced. Int.*, 2000, **32**, 491-492 (*R-form, synth, pmr*)

Dihydro-5-methyl-2(3*H*)-furanone, 9CI D-301

[108-29-2]
Tetrahydro-5-methyl-2-furanone. γ-Valerolactone. γ-Methylbutyrolactone. 4-Hydroxypentanoic acid γ-lactone. FEMA 3103



(*R*)-*form*

$C_5H_8O_2$ 100.117
Flavouring agent. Present in peach, strawberry jam, tomato, wheat bread, Swiss cheese, Gruyere de Comte cheese, heated butter, cooked beef, white wine, red wine, coffee, black tea, roasted filbert, roasted peanut and Bourbon vanilla. Liq. with sweet herbaceous odour.

► Skin irritant. LD_{50} (rat, orl) 8800 mg/kg.
LU3580000

(*R*)-*form* [58917-25-2]
Bp_{35} 105°. $[\alpha]_D^{23}$ +30.1.

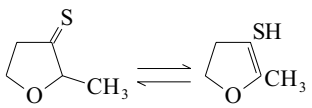
(*S*)-*form* [19041-15-7]
Bp_{39} 110°. $[\alpha]_D^{23}$ -29.6.

(±)-*form* [57129-69-8]
Constit. of crude pyroligneous acid. Used in smoke flavours. Leaflets. Fp -31. Bp 205-207° Bp_{13} 83-84°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 698A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1128B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 749C (*ir*)
Boldt, P. *et al., Chem. Ber.*, 1969, **102**, 4157 (*synth*)
Pyysalo, H. *et al., Finn. Chem. Lett.*, 1975, 136 (*cmr*)
Mori, K. *et al., Tetrahedron*, 1975, **31**, 3011 (*synth*)
Hullot, P. *et al., Can. J. Chem.*, 1977, **55**, 266 (*synth*)
Pirkle, W.M. *et al., J.O.C.*, 1977, **42**, 384 (*abs config*)
Ojima, I. *et al., J.O.C.*, 1977, **42**, 1671 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 847 (*rev, tox*)
Papageorgiou, C. *et al., Tet. Lett.*, 1984, **25**, 6041 (*synth*)
Gutman, A.L. *et al., Tet. Lett.*, 1987, **28**, 3861 (*synth*)
Ortuña, R.M. *et al., Tetrahedron*, 1987, **43**, 2191 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, VAV000
Jacobs, H. *et al., Synth. Commun.*, 1990, **20**, 999 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2888-2889 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VAV000

Dihydro-2-methyl-3(2*H*)-furanthione, 9CI D-302

[65936-86-9]
4,5-Dihydro-2-methyl-3-furanthiol, 9CI. 4,5-Dihydro-3-mercapto-2-methylfuran



C_5H_8OS 116.184
Component of roasted meat aroma. Food flavouring agent. Liq. with roasted meat aroma.

***SH*-form** [26486-13-5]

S-*Ac:* [26486-14-6] S-*(4,5-Dihydro-2-methyl-3-furanyl) ethanethioate, 9CI. 2-Methyl-3-(thioacetoxy)-4,5-dihydrofuran. FEMA 3636*
$C_7H_{10}O_2S$ 158.221
Synthetic meat flavouring agent. Food flavour, not reported to occur in nature. Liq. $Bp_{0.6}$ 57-59°. n_D^{20} 1.5188.

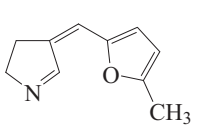
S-*Me:* [22929-45-9] *2,3-Dihydro-5-methyl-4-(methylthio)furan, 8CI*
$C_6H_{10}OS$ 130.21
Liq. Bp_{13} 60°. n_D^{20} 1.5101.

[145206-67-3]

Hoff, S. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 609 (*deriv, synth, pmr, ir*)
Ger. Pat., 1970, 1 932 800; *CA*, **72**, 90265d (*S-Ac, use*)
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501 (*synth, ir, glc, ms*)
Austrian Pat., 1977, 340 748, (*Unilever*); *CA*, **88**, 120972g (*synth*)
U.S. Pat., 1977, 4 020 170; *CA*, **72**, 90265d (*S-Ac, synth, ms, ir, use*)
Hartman, G.J. *et al., J. Agric. Food Chem.*, 1984, **32**, 1015 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 567

3,4-Dihydro-4-[(5-methyl-2-furanyl)methylene]-2*H*-pyrrole D-303

[118248-30-9, 118248-31-0]
3-(5-Methylfurfurylidene)-1-pyrroline

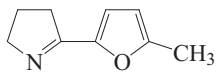


$C_{10}H_{11}NO$ 161.203
Putative proline-derived Maillard product formed in model reactions with proline or 1-pyrroline and 5-methylfurfural. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, ms, ir, pmr*)

3,4-Dihydro-5-(5-methyl-2-furanyl)-2*H*-pyrrole D-304

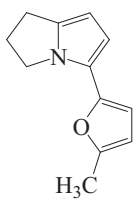
[118248-26-3]
2-(5-Methyl-2-furyl)-1-pyrroline



$C_9H_{11}NO$ 149.192
Putative proline-derived Maillard product formed in model reactions with 1-pyrroline and ascorbic acid. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*synth, occur, ms, pmr, ir*)

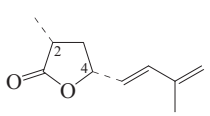
2,3-Dihydro-5-(5-methyl-2-furanyl)-1*H*-pyrrolizine D-305



$C_{12}H_{13}NO$ 187.241
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr*)

4,5-Dihydro-3-methyl-5-(3-methyl-1,3-butadienyl)-2(3*H*)-furanone D-306



(2*R*,4*R*)-*form*

$C_{10}H_{14}O_2$ 166.219

(2*R*,4*R*)-*form* [74183-60-1]
Marmelolactone B
From quince (*Cydonia oblonga*). Syrup. $[\alpha]_D^{23}$ +21.8 (c, 0.11 in MeOH).

(2*R*,4*S*)-*form* [74133-35-0]
Marmelolactone A
Contributes to the flavour of ripe quince fruit (*Cydonia oblonga*). Syrup. $[\alpha]_D^{23}$ +93.6 (c, 0.09 in MeOH).

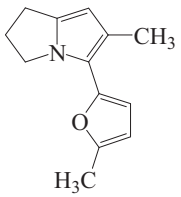
[88269-65-2, 89016-29-5, 125949-14-6, 125949-15-7]

Tsuneya, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 957 (*isol*)
Ishihara, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 2121 (*abs config*)

Nishida, Y. *et al., Agric. Biol. Chem.*, 1983, **47**, 2123; 1986, **50**, 191; 813; 1665 (*synth, cmr, cd*)
Escher, S. *et al., Helv. Chim. Acta*, 1991, **74**, 179

2,3-Dihydro-6-methyl-5-(5-methyl-2-furanyl)-1*H*-pyrrolizine D-307

[97073-02-4]

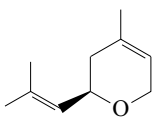


$C_{13}H_{15}NO$ 201.268
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)

3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2*H*-pyran, 9CI D-308

[1786-08-9]
4,8-Epoxy-2,6-dimethyl-2,6-octadiene.
***Nerol oxide**. FEMA 3661*



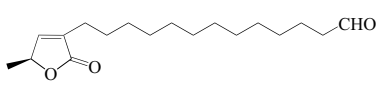
(*R*)-*form*

$C_{10}H_{16}O$ 152.236
► UP7965000
(*R*)-*form* [76936-33-9]
$[\alpha]_D^{20}$ +106 (c, 9.7 in $CHCl_3$).
(*S*)-*form* [76936-31-7]
$[\alpha]_D^{20}$ -105.1 (c, 10.3 in $CHCl_3$).
(ξ)-*form*
Present in grapefruit (*Citrus paradisi*), grapes and other fruit and in wine. Flavouring ingredient.

[76985-28-9]

Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1980, **63**, 1582 (*isol, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 166
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 833-834
Wuest, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3145-3150 (*synth, biosynth, abs config*)

2,5-Dihydro-5-methyl-2-oxo-3-furantridecanal, 9CI D-309

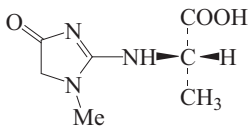


$C_{18}H_{30}O_3$ 294.433
(*S*)-*form* [156764-90-8]
Squamostanal A
Acetogenin isol. from the seeds of *Annona squamosa* (sugar apple). Wax. Mp 66-68°. $[\alpha]_D^{22}$ +21.1 (c, 0.6 in $CHCl_3$).

Araya, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1146-1147 (*isol, struct, pmr, abs config*)
Konno, H. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 526 (*synth, ir, pmr*)
Franck, X. *et al., Tet. Lett.*, 1996, **37**, 1593 (*synth*)

N-(4,5-Dihydro-1-methyl-4-oxo-1*H*-imidazol-2-yl)alanine, 9CI D-310

N-*(1-Methyl-4-hydroxy-3-imidazolin-2-ylidene)alanine*

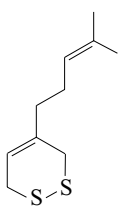


$C_7H_{11}N_3O_3$ 185.182
(*S*)-*form* [176698-63-8]
Isol. from beef broth. No phys. props. reported. Intense meaty flavour.

Eur. Pat., 1996, 699 667; *CA*, **124**, 344129m (*synth, isol, use*)
Shima, K. *et al., J. Agric. Food Chem.*, 1998, **46**, 1465-1468 (*isol, cmr, pmr*)

3,6-Dihydro-4-(4-methyl-3-pentenyl)-1,2-dithiin, 9CI D-311

[73188-23-5]
4-(4-Methyl-3-pentenyl)-1,2-dithia-4-cyclohexene

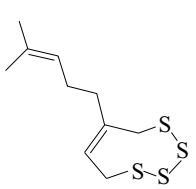


$C_{10}H_{16}S_2$ 200.368
Constit. of hops. Bright yellow oil.

Peppard, T.L. *et al., Chem. Ind. (London)*, 1979, 552 (*isol, struct*)
Elvidge, J.A. *et al., J.C.S. Perkin 1*, 1982, 1089 (*isol, synth*)
Schmidt, M. *et al., Angew. Chem., Int. Ed.*, 1987, **26**, 887 (*synth*)
Steliou, K. *et al., J.A.C.S.*, 1987, **109**, 926 (*synth*)
Omata, A. *et al., Dev. Food Sci.*, 1988, **18**, 707 (*isol*)
Sato, R. *et al., Chem. Lett.*, 1990, 139 (*synth*)

5,8-Dihydro-6-(4-methyl-3-pentenyl)-1,2,3,4-tetrathiocin, 9CI D-312

[82203-03-0]
6-(4-Methyl-3-pentenyl)-1,2,3,4-tetrathia-6-cyclooctene

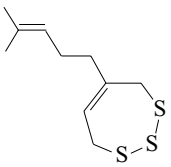


$C_{10}H_{16}S_4$ 264.5
Constit. of hops. Yellow oil.

Elvidge, J.A. *et al., J.C.S. Perkin 1*, 1982, 1089

4,7-Dihydro-5-(4-methyl-3-pentenyl)-1,2,3-trithiepin, 9CI D-313

[73188-26-8]
5-(4-Methyl-3-pentenyl)-1,2,3-trithia-5-cycloheptene

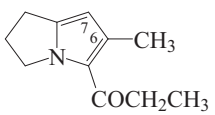


$C_{10}H_{16}S_3$ 232.434
Constit. of hops. Yellow oil.

Elvidge, J.A. *et al., J.C.S. Perkin 1*, 1982, 1089

2,3-Dihydro-6-methyl-5-propanoyl-1*H*-pyrrolizine D-314

[97073-08-0]
*1-(2,3-Dihydro-6-methyl-1*H*-pyrrolizin-5-yl)-1-propanone*



$C_{11}H_{15}NO$ 177.246
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr*)

2,3-Dihydro-7-methyl-5-propanoyl-1*H*-pyrrolizine D-315

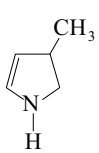
[97072-98-5]
*1-(2,3-Dihydro-7-methyl-1*H*-pyrrolizin-5-yl)-1-propanone*

$C_{11}H_{15}NO$ 177.246
Proline- or lysine-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)
Ames, J.M. *et al., Food Chem.*, 1993, **48**, 271-277 (*occur*)

2,3-Dihydro-3-methyl-1*H*-pyrrole D-316

4-Methyl-2-pyrroline

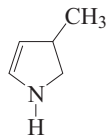


C_5H_9N 83.133
Present in small quantities in the fruit of *Piper nigrum* (pepper).
(±)-*form*
Picrate:
Mp 216-217°.

Pictet, A. *et al., Helv. Chim. Acta*, 1927, **10**, 594 (*synth*)

2,3-Dihydro-3-methylpyrrole D-317

β-Methylpyrroline



C_5H_9N 83.133

(+)(HCl)-*form*

Alkaloid from black pepper (*Piper nigrum* Piperaceae).

Hydrochloride:

V. hygroscopic, long needles. $[\alpha]_D$ +2.77.

Picrate:

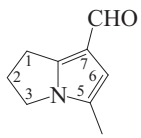
Yellow powder or prisms. Mp 165°.

Pictet, A. *et al., Helv. Chim. Acta*, 1927, **10**, 593 (*isol, struct*)

2,3-Dihydro-5-methyl-1*H*-pyrrolizine-7-carboxaldehyde D-318

[97073-07-9]

*7-Formyl-2,3-dihydro-5-methyl-1*H*-pyrrolizine*



$C_9H_{11}NO$ 149.192

Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr, ir*)

2,3-Dihydro-6-methyl-1*H*-pyrrolizine-5-carboxaldehyde, 9CI D-319

[55041-87-7]

*5-Formyl-2,3-dihydro-6-methyl-1*H*-pyrrolizine*

$C_9H_{11}NO$ 149.192

Proline-derived Maillard product. Volatile constit. of beer and cooked asparagus. Characterised spectroscopically.

Shigematsu, H. *et al., J. Agric. Food Chem.*, 1975, **23**, 233-237 (*occur, ms, pmr*)

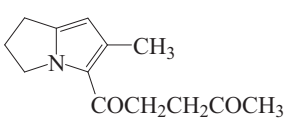
Tressl, R. *et al., J. Agric. Food Chem.*, 1977, **25**, 459-463 (*occur, asparagus, ms*)

Hill, V.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3675-3681 (*occur*)

1-(2,3-Dihydro-6-methyl-1*H*-pyrrolizin-5-yl)-1,4-pentanedione D-320

[97073-01-3]

*2,3-Dihydro-6-methyl-5-(4-oxopentanoyl)-1*H*-pyrrolizine*



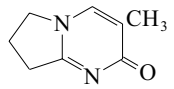
$C_{13}H_{17}NO_2$ 219.283

Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)

7,8-Dihydro-3-methylpyrrolo[1,2-*a*]pyrimidin-2(6*H*)-one, 9CI D-321

[76884-47-4]



$C_8H_{10}N_2O$ 150.18

Alkaloid from the roots of *Glycyrrhiza uralensis* (Chinese licorice).

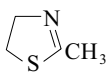
Ger. Pat., 1980, 3 017 625; *CA*, **94**, 121592 (*synth*)

Han, Y.N. *et al., Arch. Pharmacal Res.*, 1990, **13**, 103; *CA*, **113**, 227985 (*isol*)

4,5-Dihydro-2-methylthiazole, 9CI D-322

[2346-00-1]

2-Methyl-2-thiazoline, 8CI



C_4H_7NS 101.172

Constit. of various cooked foods. Pale yellow liq. Mp -101°. Bp 144.5-145°.

▶ XJ4261470

Picrate: [5243-50-5]

Yellow needles (EtOH). Mp 171-172°.

N-*Me:4,5-Dihydro-2,3-dimethylthiazolium(1+)*

$C_5H_{10}NS^{\oplus}$ 116.207

Needles (EtOH) (as iodide). Mp 235-237° (iodide).

N-*Et:* [54654-71-6] *3-Ethyl-4,5-dihydro-2-methylthiazolium(1+)*

$C_6H_{12}NS^{\oplus}$ 130.234

Needles (MeOH/Me_2CO) (as iodide). Mp 191-193° (iodide). CAS no. refers to iodide.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 824A (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1333A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 793C (*ir*)

Wenker, H. *et al., J.A.C.S.*, 1935, **57**, 1079 (*synth*)

Brooker, L.G.S. *et al., J.A.C.S.*, 1936, **58**, 662 (*N-Et, synth*)

Kuhn, R. *et al., Annalen*, 1954, **590**, 55 (*synth*)

Meyers, A.I. *et al., J.O.C.*, 1975, **40**, 2021 (*use*)

Suzuki, N. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3155 (*synth, ir, pmr*)

Mille, G. *et al., J. Mol. Struct.*, 1978, **50**, 247 (*ir, Raman*)

Chen, B.C. *et al., Helv. Chim. Acta*, 1983, **66**, 1537 (*N-15 nmr*)

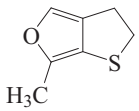
Laduranty, J. *et al., Bull. Soc. Chim. Fr.*, 1989, 850 (*synth*)

Sirugue, D. *et al., J. Chem. Ecol.*, 1992, **18**, 2261 (*occur*)

2,3-Dihydro-6-methylthieno[2,3-*c*]furan, 8CI D-323

[26693-24-3]

4-Methyl-3-oxa-6-thiabicyclo[3.3.0]octa-1,4-diene. ***Kahweofuran***



C_7H_8OS 140.206

Constit. of the aroma of roasted coffee. Oil. Bp_{22} 105-107°. λ_{max} 245 (ε 3100) (EtOH).

Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*isol*)

Büchi, G. *et al., J.O.C.*, 1971, **36**, 199 (*struct, synth, uv, pmr*)

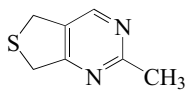
Gorzynski, M. *et al., Annalen*, 1986, 625 (*synth, pmr, ms*)

Brenna, E. *et al., J. Chem. Res., Synop.*, 1998, 74-75 (*synth*)

5,7-Dihydro-2-methylthieno[3,4-*d*]pyrimidine, 9CI D-324

[36267-71-7]

FEMA 3338



$C_7H_8N_2S$ 152.22

Cystine-derived Maillard prod. Flavouring ingredient. Sweetness enhancer at low conc. (10 ppm), at higher conc. enhances root vegetable flavour in chicken broth base. Needles. Mp 64.5-65°.

S,S-*Dioxide:* [154697-85-5]

$C_7H_8N_2O_2S$ 184.218

Cryst. (CH_2Cl_2/hexane). Mp 134-136°.

U.S. Pat., 1973, 3 726 692; *CA*, **79**, 17226g (*synth, use*)

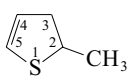
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*formn*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 167 (*use*)

Tomé, A.C. *et al., Tetrahedron*, 1996, **52**, 1735 (*synth, ir, pmr, cmr, ms*)

2,3-Dihydro-2-methylthiophene D-325

[129763-90-2]



C_5H_8S 100.184

Maillard product.

(±)-*form*

S,S-*Dioxide:*

$C_5H_8O_2S$ 132.183

d_4^{20} 1.25. Mp 25-26°. Bp_1 75-77.5°. n_D^{20} 1.4949.

Krug, R.C. *et al., J.O.C.*, 1958, **23**, 1697 (*deriv, synth, ir*)

2,3-Dihydro-5-methylthiophene D-326

[4610-02-0]

C_5H_8S 100.184

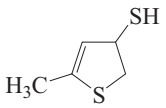
Maillard product; present in meaty aromas. Bp 127-128° Bp_{18} 35-36°.

S,S-*Dioxide:*
$C_5H_8O_2S$ 132.183
Needles (EtOH). Mp 128-128.5°.

Birch, F.F. *et al., J.C.S.*, 1951, 3411 (*synth*)
Bacchetti, T. *et al., Gazz. Chim. Ital.*, 1953, **83**, 1037 (*synth*)
Krug, R.C. *et al., J.O.C.*, 1958, **23**, 1697 (*deriv, synth*)

2,3-Dihydro-5-methyl-3-thiophenethiol, 9CI D-327

[56079-02-8]
4-Mercapto-2-methyl-4,5-dihydrothiophene

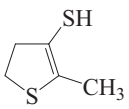


$C_5H_8S_2$ 132.25
Component of roast meat aroma models. Possesses a rubbery, meaty aroma. Characterised spectroscopically.

Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms, ir*)
Hincelin, O. *et al., Food Chem.*, 1992, **44**, 381-389 (*occur*)

4,5-Dihydro-2-methyl-3-thiophenethiol, 9CI, 8CI D-328

[26486-23-7]
3-Mercapto-2-methyl-4,5-dihydrothiophene

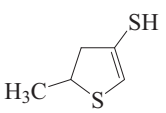


$C_5H_8S_2$ 132.25
Constit. of meat odour model systems. Possesses a roasted meat aroma. Characterised spectroscopically.

Ger. Pat., 1970, 1 932 800; *CA*, **72**, 90265d (*occur, use*)
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms, ir*)
Hincelin, O. *et al., Food Chem.*, 1992, **44**, 381-389 (*occur*)

4,5-Dihydro-5-methyl-3-thiophenethiol, 9CI, 8CI D-329

[26486-15-7]
4-Mercapto-2-methyl-2,3-dihydrothiophene

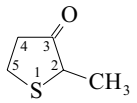


$C_5H_8S_2$ 132.25
Component of meat odour models. Possesses a roasted meat aroma. Characterised spectroscopically.

Ger. Pat., 1970, 1 932 800; *CA*, **72**, 90265d (*occur, use*)
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*occur, anal, ms, ir*)
Hincelin, O. *et al., Food Chem.*, 1992, **44**, 381-389 (*occur*)

Dihydro-2-methyl-3(2*H*)-thiophenone, 9CI D-330

[13679-85-1]
FEMA 3512



C_5H_8OS 116.184

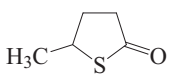
(±)-*form* [74015-70-6]
Flavouring ingredient. Liq. Bp_{17} 66°.

(ξ)-*form*
Present in beer, coffee, roasted peanut and cooked beef as flavour constituent.

Karrer, P. *et al., Helv. Chim. Acta*, 1944, **27**, 124 (*synth*)
Buchmann, E.R. *et al., J.A.C.S.*, 1944, **66**, 847 (*synth*)
Hatanaka, M. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2515 (*synth, ir*)
Nootens, C. *et al., Bull. Soc. Chim. Belg.*, 1988, **97**, 1045 (*synth, ir, pmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 564
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1861

Dihydro-5-methyl-2(3*H*)-thiophenone, 9CI D-331

[5650-74-8]
4-Mercaptopentanoic acid γ-lactone. 5-Methyl-γ-thiobutyrolactone



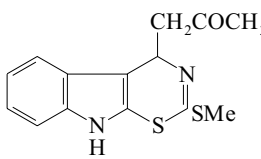
C_5H_8OS 116.184
Maillard product.

(±)-*form*
Bp_{18} 90°.

Holmquist, H.E. *et al., J.O.C.*, 1960, **25**, 2240 (*synth*)
Korte, F. *et al., Chem. Ber.*, 1961, **94**, 1956 (*synth*)
Rioult, P. *et al., Bull. Soc. Chim. Fr.*, 1968, 4477 (*synth*)
Chua, Y.T. *et al., J.C.S. Perkin 2*, 1996, 577 (*synth, pmr, ir, ms*)

1-[4,9-Dihydro-2-(methylthio)-1,3-thiazino[6,5-*b*]indol-4-yl]-2-propanone, 9CI D-332

[113866-43-6]



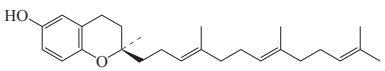
$C_{14}H_{14}N_2OS_2$ 290.409
Isol. from Chinese cabbage (*Brassica campestris* ssp. *pekinensis,* Cruciferae) inoculated with the bacterium *Pseudomonas cichorii*. Amorph. solid. λ_{max} 202 (ε 18900); 227 (ε 28000); 282 (ε 6490); 294 (ε 6690) (MeOH) (Berdy).

Takasugi, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 285 (*isol, uv, ir, pmr, cmr, ms, struct*)

3,4-Dihydro-2-methyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2*H*-1-benzopyran-6-ol, 9CI D-333

[6829-55-6]

[97530-73-9, 136774-61-3, 136774-62-4]
2-Methyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-6-chromanol, 8CI. Demethyl-δ-tocotrienol



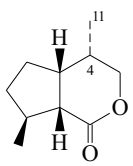
$C_{26}H_{38}O_2$ 382.585Basic nucleus of the tocotrienols: see α-Tocotrienol, T-415, β-Tocotrienol, T-416, δ-Tocotrienol, T-417, γ-Tocotrienol, T-418.

(*R*)-*form*
Isol. from rice bran.

Cimino, G. *et al., Tetrahedron*, 1985, **41**, 1093-1100 (*synth*)
Eur. Pat., 1991, 421 419; *CA*, **115**, 198523g (*synth, ir, pmr*)
Pearce, B.C. *et al., J. Med. Chem.*, 1992, **35**, 3595-3606; 1994, **37**, 526-541 (*synth, ir, pmr, use*)
Qureshi, A.A. *et al., J. Agric. Food Chem.*, 2000, **48**, 3130-3140 (*isol*)

Dihydronepetalactone D-334

[17672-81-0]



$C_{10}H_{16}O_2$ 168.235
Constit. of *Nepeta cataria* (catnip). Oil. Bp_1 107-110°. $[\alpha]_D^{25}$ +72.

4-Epimer: [17672-96-7] ***Isodihydronepetalactone***
$C_{10}H_{16}O_2$ 168.235
Constit. of *Nepeta cataria* (catnip). Oil. $[\alpha]_D^{25}$ +2.73.

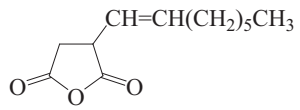
4,11-Didehydro: [60419-56-9] ***Dolicholactone***
$C_{10}H_{14}O_2$ 166.219
$Bp_{0.5}$ 80-82°.

8,9-Didehydro: See Neonepetalactone in *The Combined Chemical Dictionary.*

Sakan, T. *et al., Tet. Lett.*, 1965, 4097 (*isol*)
Wolinsky, J. *et al., J.O.C.*, 1972, **37**, 3376 (*synth*)
Pagnoni, U.M. *et al., Aust. J. Chem.*, 1976, **29**, 1375 (*Dolicholactone*)
Ficini, J. *et al., Tet. Lett.*, 1976, 687 (*synth*)
Grandi, R. *et al., Phytochemistry*, 1983, **22**, 2723 (*biosynth, deriv*)
Fleming, J. *et al., Tet. Lett.*, 1984, **25**, 5103 (*synth*)
Tanimori, S. *et al., Agric. Biol. Chem.*, 1991, **55**, 1181 (*synth*)
Kigawa, M. *et al., Heterocycles*, 1992, **33**, 117 (*synth*)
Lee, E. *et al., Chem. Comm.*, 1994, 479 (*synth*)
Nangia, A. *et al., Tetrahedron*, 1997, **53**, 14507-14545 (*rev, synth*)

Dihydro-3-(1-octenyl)-2,5-furandione, 9CI D-335

[7757-96-2]
1-Octenylsuccinic anhydride, 8CI



$C_{12}H_{18}O_3$ 210.272
Starch modifier (esterification agent) for use in beverages and beverage bases as a stabiliser or emulsifier. Pale yellow viscous liq.

Fed. Regist., 1993, **58**, 21099-21100; *CA*, **119**, 7504b (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2026 (*use*)
U.S. Pat., 4 012 438; *CA*, **87**, 202577a (*synth*)

Dihydro-3-(2-octenyl)-2,5-furandione, 9CI D-336

[42482-06-4]

[81949-83-9, 81949-84-0]
2-Octenylsuccinic anhydride, 8CI. OSA

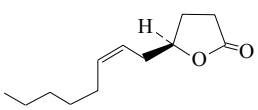
$C_{12}H_{18}O_3$ 210.272
Reactant for manuf. of octenylsuccinoyl starches, which are used as emulsifiers in foods and pharmaceutical products. Moisture-sensitive liq. d 1. Mp 8-12°. Bp_{10} 168°. n_D^{20} 1.4694. Phys. props. are for an unspecified mixt. of *E*- and *Z*-isomers.
► Fl p. >110°. Irritant.

[26680-54-6]

U.S. Pat., 1953, 2 661 349; *CA*, **48**, 1720d (*use*)
Fed. Regist., 1961, **26**, 6583; *CA*, **55**, 20245i (*use*)
Koenig, N.H. *et al., Text. Res. J.*, 1965, **35**, 708-715; *CA*, **63**, 13472a (*use*)
Pliev, T.N. *et al., Zh. Prikl. Spektrosk.*, 1973, **18**, 94-100; *CA*, **78**, 148415v (*ir, anal*)
U.S. Pat., 1988, 4 785 036; *CA*, **110**, 214180x (*use*)
Jung, J.C. *et al., Angew. Makromol. Chem.*, 1991, **185-186**, 129-131 (*synth, pmr*)
Park, P.W. *et al., J. Agric. Food Chem.*, 1995, **43**, 2580-2584 (*anal*)
Jönsson, B.A.G. *et al., Analyst (London)*, 1996, **121**, 1279-1284; 1285-1290 (*anal*)
Patten, T.E. *et al., Macromolecules*, 1996, **29**, 5882-5892 (*synth, pmr, cmr*)
Trubiano, P.C. *et al., Modif. Starches: Prop. Uses. 1987*, (ed. Wurzburg, O.B.), CRC Press, 131-147 (*use*)

Dihydro-5-(2-octenyl)-2(3*H*)-furanone, 9CI D-337

[15456-69-6]
5-(2-Octenyl)tetrahydrofuran-2-one. 6-Dodecen-4-olide



(*R*,*Z*)-*form*

$C_{12}H_{20}O_2$ 196.289
Isol. from butterfat. Flavouring ingredient.

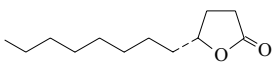
(*R,Z*)-*form* [63357-99-3]
$[\alpha]_D^{20}$ -16.1 (c, 0.3 in MeOH).
(*S,Z*)-*form* [63357-98-2]
$[\alpha]_D^{20}$ +15 (c, 0.1 in MeOH).

[18679-18-0, 60551-23-7, 127127-84-8]

Brownlee, R.G. *et al., Nature (London)*, 1969, **221**, 284 (*isol*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 3518 (*synth*)
Meuller-Schwarze, D. *et al., J. Chem. Ecol.*, 1976, **2**, 389; 1978, **4**, 247
Burger, B.V. *et al., Z. Naturforsch., C*, 1977, **32**, 49 (*synth*)
Ravid, U. *et al., Tetrahedron*, 1978, **34**, 1449 (*synth*)
Dormán, G. *et al., J.C.S. Perkin 1*, 1989, 1543 (*use*)
Lee, S.-L. *et al., J. Ferment. Bioeng.*, 1994, **78**, 114 (*isol*)

Dihydro-5-octyl-2(3*H*)-furanone, 9CI D-338

[2305-05-7]
4-Hydroxydodecanoic acid γ-lactone. 4-Dodecanolide. γ-Dodecalactone. γ-Dodecanolactone. FEMA 2400



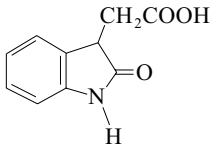
(*R*)-*form*

$C_{12}H_{22}O_2$ 198.305
► Skin irritant. LU3600000
(*R*)-*form* [69830-91-7]
$[\alpha]_D$ +37.7 (c, 1 in MeOH).
(*S*)-*form* [69830-92-8]
$[\alpha]_D$ -32.8 (c, 1.6 in MeOH).
(±)-*form* [57084-18-1]
Used in perfumery and flavour industries. Oil. Bp_{11} 170-171°.
(ξ)-*form*
Present in orange peel oil, various fruits, kumquat peel oil, milk, cooked beef, raw cured pork, roasted peanut, coriander leaf, cheeses and unprocessed rice. Flavouring ingredient.

Muys, G.T. *et al., Nature (London)*, 1962, **194**, 995
Wheeler, J.M. *et al., Tet. Lett.*, 1972, 4635 (*isol*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 3518 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 751 (*rev, tox*)
Nakamura, E. *et al., J.A.C.S.*, 1977, **99**, 7360 (*synth*)
Vigneron, J.P. *et al., Tet. Lett.*, 1980, **21**, 1735
Solladie, G. *et al., J.O.C.*, 1982, **47**, 91
Chattopadhyay, S. *et al., Tetrahedron*, 1990, **46**, 3667 (*synth*)
Fronza, G. *et al., J.C.S. Perkin 1*, 1991, 2977 (*synth*)
Cardillo, R. *et al., J.O.C.*, 1991, **56**, 5237 (*synth*)
Cere, V. *et al., J.O.C.*, 1993, **58**, 4567 (*synth*)
Bhalerao, U.T. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 266 (*synth*)
Schoettler, M. *et al., Helv. Chim. Acta*, 1995, **78**, 847; 1996, **79**, 1488 (*biosynth*)
Bonini, C. *et al., J.O.C.*, 1995, **60**, 4803 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 904-905 (*occur, use*)
Parker, S.R. *et al., J. Agric. Food Chem.*, 1997, **45**, 2774-2776 (*activity*)

2,3-Dihydro-2-oxo-1*H*-indole-3-acetic acid, 9CI D-339

[2971-31-5]
*2-Hydroxy-1*H*-indole-3-acetic acid. Oxindole-3-acetic acid. 2-(2-Oxo-3-indolinyl)acetic acid*

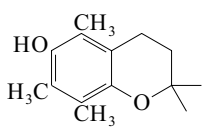


$C_{10}H_9NO_3$ 191.186
(±)-*form* [99102-28-0]
Needles (Me_2CO/C_6H_6). Mp 146°.
Me ester: [110425-83-7]
$C_{11}H_{11}NO_3$ 205.213
Needles (MeOH). Mp 164-167°.
Et ester: [40940-16-7]
$C_{12}H_{13}NO_3$ 219.24
Cryst. (petrol). Mp 94-98°.
(ξ)-*form*
Isol. from *Ribes rubrum* (currant), *Brassica* spp. and *Helianthus annuus* (sunflower). Prod. of catabolism of 1*H*-Indole-3-acetic acid, I-25 in *Zea mays* (sweetcorn).
Me ester: [61989-29-5]
Isol. from rice bran. Prob. intermed. in biosynth. of 2,6-Dihydroxy-4-quinolinecarboxylic acid, D-681 from 1*H*-Indole-3-acetic acid, I-25. Needles. Mp 170-172°.

Julian, P.L. *et al., J.A.C.S.*, 1953, **75**, 5305 (*synth*)
Hinman, R.L. *et al., J.O.C.*, 1964, **29**, 1206 (*synth*)
Kinashi, H. *et al., Agric. Biol. Chem.*, 1976, **40**, 2465 (*isol*)
Nonhebel, H.M. *et al., J. Biol. Chem.*, 1985, **260**, 12685 (*biosynth*)
Takase, S. *et al., Tetrahedron*, 1986, **42**, 5879 (*synth, ir, pmr*)
Lower, P. *et al., J.C.S. Perkin 1*, 1987, 753 (*synth, pmr*)

3,4-Dihydro-2,2,5,7,8-pentamethyl-2*H*-1-benzopyran-6-ol D-340

[950-99-2]
*2,2,5,7,8-Pentamethyl-6-chromanol, 8CI. 3,4-Dihydro-6-hydroxy-2,2,5,7,8-pentamethyl-2*H*-1-benzopyran. PMHC. Chromane C_1*



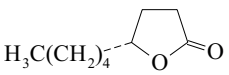
$C_{14}H_{20}O_2$ 220.311
Analogue of α-Tocopherol, T-406. Antioxidant for edible oils and fats. Cryst. (hexane or EtOH aq.). Mp 94°.
Ac: [57721-81-0]
$C_{16}H_{22}O_3$ 262.348
Cryst. Mp 92.5-93.5°.

Smith, L.I. *et al., J.O.C.*, 1939, **4**, 311 (*synth*)
Nilsson, J.L.G. *et al., Acta Chem. Scand.*, 1968, **22**, 3160 (*synth*)
Matsuo, M. *et al., Tetrahedron*, 1976, **32**, 229 (*cmr*)
Bolzoni, L. *et al., Angew. Chem., Int. Ed.*, 1978, **17**, 684 (*synth*)

Doba, T. *et al., J.A.C.S.*, 1983, **105**, 6505 (*cryst struct, epr*)
Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1987, 487 (*synth*)
Sow, M. *et al., J. Photochem. Photobiol., A*, 1990, **54**, 349 (*spectra, props*)

Dihydro-5-pentyl-2(3*H*)-furanone, 9CI, 8CI D-341

[104-61-0]
*γ-Nonalactone. 4-Hydroxynonanoic acid γ-lactone. γ-Amylbutyrolactone. 1,4-Nonanolide. 5-Pentyldihydro-2(3*H*)-furanone. γ-Pelargonolactone. Apricolin. Prunolide. Cocos aldehyde (misleading). Aldehyde C_{18} (misleading). FEMA 2781*



(*R*)-*form*

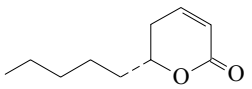
$C_9H_{16}O_2$ 156.224
Present in blackcurrant buds and berries, melon, papaya, pineapple, peaches, apricot, wheat bread, crispbread, wines, black tea and other foodstuffs. Flavouring agent. Liq. with coconut odour and fatty taste.
►Skin irritant. LU3675000
(*R*)-*form* [63357-96-0]
Oil. Bp_{12} 108°. $[\alpha]_D^{24}$ +47.5 (c, 1.82 in MeOH). ν_{max} 1770 cm^{-1}.
(*S*)-*form* [63357-97-1]
$[\alpha]_D^{24}$ -47.9 (c, 1.70 in MeOH).
(±)-*form* [57084-16-9]
Flavouring ingredient. Used in coconut flavours. Bp_{12} 134-134.5° $Bp_{1.5}$ 93-94°.

[82373-92-0]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1130A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 751B (*ir*)
Terai, Y. *et al., Bull. Chem. Soc. Jpn.*, 1956, **29**, 822 (*synth*)
Sakai, T. *et al., CA*, 1962, **58**, 8845 (*isol*)
Goldwhite, H. *et al., Tetrahedron*, 1964, **20**, 1657 (*synth, ir*)
Honkanen, E. *et al., Acta Chem. Scand.*, 1965, **19**, 370 (*ms*)
Oser, B.L. *et al., Food Cosmet. Toxicol.*, 1965, **3**, 563 (*rev*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 889 (*rev, tox*)
Sataro, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 770 (*synth*)
Miyashita, Y. *et al., Agric. Biol. Chem.*, 1981, **45**, 2521 (*synth*)
Cardellach, J. *et al., J. Het. Chem.*, 1984, **21**, 377 (*synth, cmr, bibl*)
Ballini, R. *et al., Synthesis*, 1987, 711 (*synth, ir, pmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CNF250
Cardillo, R. *et al., J.O.C.*, 1991, **56**, 5237 (*synth*)
Yadav, J.S. *et al., Synth. Commun.*, 1993, **23**, 2731 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1969-1971 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNF250

5,6-Dihydro-6-pentyl-2*H*-pyran-2-one, 9CI D-342

[54814-64-1]
2-Decen-5-olide. Massoia lactone. Massoy lactone. Massoilactone. 5-Hydroxy-2-decenoic acid δ-lactone. FEMA 3744



(*R*)-*form*

$C_{10}H_{16}O_2$ 168.235
Present in blackberries and cane molasses. Flavouring ingredient.
►Skin irritant.
(*R*)-*form* [51154-96-2]
Oil. $Bp_{0.5}$ 103-104°. $[\alpha]_D^{20}$ -99.4 (c, 1 in $CHCl_3$).
►UQ0550000
(±)-*form* [501-23-5]
$Bp_{0.07}$ 85-86°.

Crombie, L. *et al., J.C.S.*, 1955, 2535 (*synth*)
Hashizume, T. *et al., Agric. Biol. Chem.*, 1968, **32**, 1306 (*isol*)
Cavill, G.W.K. *et al., Aust. J. Chem.*, 1968, **21**, 2819 (*isol*)
Crombie, L. *et al., J.C.S.(C)*, 1968, 2852 (*config*)
Urbach, G. *et al., Agric. Biol. Chem.*, 1972, **36**, 1217 (*ms*)
Fehr, C. *et al., Helv. Chim. Acta*, 1981, **64**, 1247 (*synth*)
Hoffmann, R.W. *et al., Tet. Lett.*, 1983, **24**, 3209 (*synth*)
Stevenson, R. *et al., J. Nat. Prod.*, 1988, **51**, 1215 (*synth*)
Bennett, F. *et al., Heterocycles*, 1989, **29**, 639 (*synth*)
Romeyke, Y. *et al., Tetrahedron*, 1991, **47**, 3335 (*synth*)
Takano, S. *et al., Tetrahedron: Asymmetry*, 1992, **3**, 533
Yu, L. *et al., Chin. Chem. Lett.*, 1993, **4**, 1 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 361
Zhang, C. *et al., Chin. Chem. Lett.*, 1997, **8**, 13-14 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1367-1368
Parker, S.R. *et al., J. Agric. Food Chem.*, 1997, **45**, 2774-2776 (*activity*)
Pais, G.C. *et al., Tetrahedron*, 1999, **55**, 13445-13450 (*synth*)
Ramachandran, P.V. *et al., Tet. Lett.*, 2000, **41**, 583-586 (*synth*)
Sadayori, N. *et al., Heterocycles*, 2002, **58**, 191-202 (*synth*)

2,2-Dihydroperoxypropane D-343

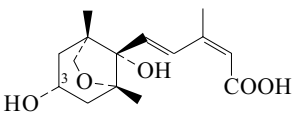
[2614-76-8]
(1-Methylethylidene)bis[hydroperoxide], 9CI. Isopropylidene hydroperoxide, 8CI. Peroxyacetone
$(H_3C)_2C(OOH)_2$
$C_3H_8O_4$ 108.094
A mixture of acetone peroxides (usually supplied adsorbed onto an inert carrier such as cornstarch) is added to foods as a bleaching agent and dough conditioner. Liq. Peroxidn. of Acetone, A-25 also produces a linear peroxide dimer and a cyclic trimer, both extremely shock-sensitive solids.
►V. shock-sensitive explosive. Strong oxidising agent.

[1336-17-0]

Milas, N.A. *et al., J.A.C.S.*, 1959, **81**, 6461 (*synth*)
Hine, J. *et al., J.O.C.*, 1970, **35**, 2769 (*synth*)
Sauer, M.C.V. *et al., J. Phys. Chem.*, 1972, **76**, 1283 (*synth*)
Hutton, W. *et al., Chem. Eng. News*, Sept. 17, 1984, 4 (*haz*)
Schwoegler, E.J. *et al., Chem. Eng. News*, Jan. 7, 1985, 6 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BJY825
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1210

Dihydrophaseic acid D-344

[41756-77-8]
5-(3,8-Dihydroxy-1,5-dimethyl-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl-2,4-pentadienoic acid, 9CI



$C_{15}H_{22}O_5$ 282.336
Isol. from French beans. Amorph.

Me ester:
$C_{16}H_{24}O_5$ 296.363
Isol. from French beans. λ_{max} 267 (log ϵ 1.99) (MeOH).

3-O-β-D-Glucopyranoside: [78914-56-4]
$C_{21}H_{32}O_{10}$ 444.478
λ_{max} 268 (MeOH).

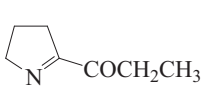
3-Epimer: [60102-38-7] ***Epidihydrophaseic acid***
$C_{15}H_{22}O_5$ 282.336
Isol. from French beans. Amorph.

[60102-40-1, 128821-82-9, 128821-83-0, 128821-85-2, 128821-86-3]

Takasugi, M. *et al., Chem. Lett.*, 1973, 245 (*isol*)
Walton, D.C. *et al., Planta*, 1973, **112**, 87 (*isol, ester*)
Beeley, L.J. *et al., Phytochemistry*, 1975, **14**, 779 (*occur*)
Milborrow, B.V. *et al., Phytochemistry*, 1975, **14**, 1045 (*abs config*)
Zeevaart, J.A.D. *et al., Phytochemistry*, 1976, **15**, 493 (*Epidihydrophaseic acid*)
Takeda, N. *et al., Agric. Biol. Chem.*, 1984, **48**, 685 (*ms*)
Champavier, Y. *et al., Phytochemistry*, 1999, **50**, 1219-1223 (*3-glucoside*)

3,4-Dihydro-5-propanoyl-2*H*-pyrrole D-345

[133447-37-7]
*1-(3,4-Dihydro-2*H*-pyrrol-5-yl)-1-propanone, 9CI. 2-Propionyl-1-pyrroline*

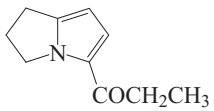


$C_7H_{11}NO$ 125.17
Formed by thermal treatment of proline and glucose mixtures. Constit. of freshly popped corn aroma. No phys. props. reported. Odour threshold 0.02 ng/L in air.

Schieberle, P. *et al., J. Agric. Food Chem.*, 1991, **39**, 1141-1144 (*detn, synth, pmr, ms*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 2721-2726 (*occur, ms*)

2,3-Dihydro-5-propanoyl-1*H*-pyrrolizine D-346

[80933-76-2]
*1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-1-propanone*

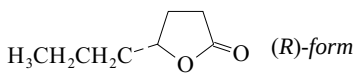


$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr, ir*)
Chen, W.-C. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

Dihydro-5-propyl-2(3*H*)-furanone, 9CI D-347

[105-21-5]
4-Hydroxyheptanoic acid lactone. γ-Propyl-γ-butyrolactone. FEMA 2539

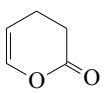


$C_7H_{12}O_2$ 128.171
►Skin irritant. LU3697000
(*R*)-*form* [88270-38-6]
$[\alpha]_D$ +56.2 (c, 1.56 in THF).
(*S*)-*form* [31323-51-0]
Bp_{20} 145-150°. $[\alpha]_D^{25}$ -55.9 (c, 1.54 in THF).
(±)-*form* [57129-71-2]
Flavouring agent. Bp_5 123-124°.
(ξ)-*form*
Present in papaya, peach, pineapple, mango, nectarine, cape gooseberry, asparagus, licorice, black tea, wines and canned beef.

Ono, M. *et al., J.A.C.S.*, 1971, **93**, 1285 (*synth*)
Nakamura, E. *et al., J.A.C.S.*, 1977, **99**, 7360 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HBA550
Brown, H.C. *et al., J.O.C.*, 1994, **59**, 365 (*synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1261-1262 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBA550

3,4-Dihydro-2*H*-pyran-2-one D-348

[26638-97-1]
5-Hydroxy-4-pentenoic acid δ-lactone. 4,5-Dehydrovalerolactone



$C_5H_6O_2$ 98.101
Constit. of roasted peanut flavour. No phys. props. reported.

Plouin, D. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 343 (*synth*)
Ger. Pat., 1982, 3 045 555; *CA*, **97**, 127501 (*synth, pmr*)
U.S. Pat., 1984, 4 424 369; *CA*, **100**, 120886 (*synth*)
Jimenez-Tenorio, M. *et al., Chem. Comm.*, 2001, 2324-2325 (*synth*)

2,3-Dihydro-1*H*-pyrrole, 9CI D-349

[638-31-3]
2-Pyrroline, 8CI



C_4H_7N 69.106

N-*Ac:* [23105-58-0]
C_6H_9NO 111.143
Odorous constit. of cooked rice and of pandan rampeh (*Pandanus amaryllifolius*). Oil.

N-*Ph:2,3-Dihydro-1-phenyl-1*H*-pyrrole. 1-Phenyl-2-pyrroline*
$C_{10}H_{11}N$ 145.204
Cryst. Mp 166-167.5°.

Wittig, G. *et al., Annalen*, 1955, **594**, 1 (*N-Ph*)
Sato, S. *et al., CA*, 1969, **71**, 21828 (*deriv*)
Leblanc, R. *et al., Tet. Lett.*, 1969, 2441 (*deriv*)
Westheimer, F.H. *et al., J.O.C.*, 1971, **36**, 1570 (*deriv*)
Buttery, R.G. *et al., Chem. Ind. (London)*, 1983, 478 (*isol, deriv*)
Marais, W. *et al., Synth. Commun.*, 1998, **28**, 3681-3691 (*N-Ac, N-benzoyl*)

3,4-Dihydro-2*H*-pyrrole, 9CI D-350

[5724-81-2]
1-Pyrroline. FEMA 3898



C_4H_7N 69.106
Present in clam and squid. Flavouring agent for fish products and other foods. Stable in dil. soln., trimerises readily.

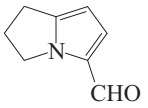
N-*Oxide:* [24423-88-9]
C_4H_7NO 85.105
$Bp_{0.1}$ 74-76°.

Trimer: See Dodecahydrotripyrrolo[1,2-*a*:1′,2′-*c*:1″,2″-*e*][1,3,5]triazine in *The Combined Chemical Dictionary.*

Amoore, J.E. *et al., J. Chem. Ecol.*, 1975, **1**, 299
Poisel, H. *et al., Monatsh. Chem.*, 1978, **109**, 925 (*synth, pmr*)
Baker, R. *et al., Chem. Comm.*, 1985, 824
Bock, H. *et al., Chem. Ber.*, 1987, **120**, 1961 (*synth, pe, bibl*)
Guillemin, J.-C. *et al., Tetrahedron*, 1988, **44**, 4447 (*synth, pmr*)
Murahashi, S. *et al., J.O.C.*, 1990, **55**, 1736-1744 (*N-oxide, synth, ir, pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4389-4390 (*N-oxide, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 1568

2,3-Dihydro-1*H*-pyrrolizine-5-carboxaldehyde, 9CI D-351

[6225-59-8]
*5-Formyl-2,3-dihydro-1*H*-pyrrolizine*

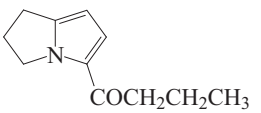


C_8H_9NO 135.165
Proline-derived Maillard product. Yellow oil. d_4^{20} 1.13. $Bp_{4.5}$ 108-109°. n_D^{20} 1.5902.

Ponomarev, A.A. *et al., CA*, 1969, **70**, 114924e (*synth*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)
Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)
Aldabbagh, F. *et al., Tetrahedron*, 1999, **55**, 8111-8128 (*synth, pmr, cmr, ms*)

1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-1-butanone D-352

[97072-99-6]
*5-Butanoyl-2,3-dihydro-1*H*-pyrrolizine*

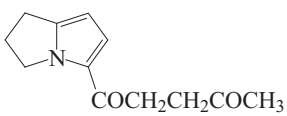


$C_{11}H_{15}NO$ 177.246
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)

1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-1,4-pentanedione D-353

[97073-10-4]
*2,3-Dihydro-5-(4-oxopentanoyl)-1*H*-pyrrolizine*

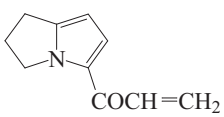


$C_{12}H_{15}NO_2$ 205.256
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr, ir*)

1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-2-propen-1-one D-354

[97073-00-2]
*5-Acryloyl-2,3-dihydro-1*H*-pyrrolizine*

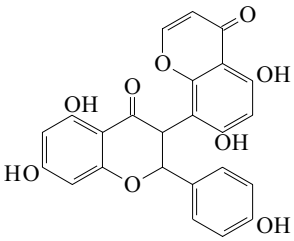


$C_{10}H_{11}NO$ 161.203
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)

2,3-Dihydro-5,5′,7,7′-tetrahydroxy-2-(4-hydroxyphenyl)[3,8′-bi-4*H*-1-benzopyran]-4,4′-dione, 9CI D-355

[60857-34-3]
4″,5,5′,7,7′-Pentahydroxyflavanone-(3,8)-chromone

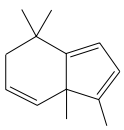


$C_{24}H_{16}O_9$ 448.385
Isol. from leaves of *Garcinia dulcis* (mundu). Yellow cryst. ($CHCl_3$/EtOAc). Mp 300°.

Ansari, W.H. *et al., J.C.S. Perkin 1*, 1976, 1458 (*isol*)

5,7*a*-Dihydro-1,4,4,7*a*-tetramethyl-4*H*-indene, 9CI D-356

[99901-21-0]
2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4,7-triene



$C_{13}H_{18}$ 174.285
Constit. of quince fruit flavour (*Cydonia oblonga*). Oil.

Ishihara, M. *et al., J.O.C.*, 1986, **51**, 491

2,3-Dihydrothiophene D-357

[1120-59-8]



C_4H_6S 86.157
Maillard product. Bp_{100} 48° Bp_{40} 37°.

S-*Oxide:* [14852-21-2]
C_4H_6OS 102.157
$Bp_{1.6}$ 78-80°. n_D^{20} 1.5321.

S,S-*Dioxide:* [1192-16-1]

[28452-93-9] *2,3-Dihydrothiophene 1,1-dioxide. 2-Sulfolene*
$C_4H_6O_2S$ 118.156
Cryst. (C_6H_6/petrol). Mp 48-49°.

▶ XM8825000

Birch, S.F. *et al., J.C.S.*, 1951, 2556 (*synth*)
Krug, R.C. *et al., J.O.C.*, 1958, **23**, 212 (*oxides*)
Sosnovsky, G. *et al., Tetrahedron*, 1962, **18**, 903 (*synth*)
Cohen, L.E. *et al., J. Org. Chem. USSR (Engl. Transl.)*, 1966, **31**, 2334 (*synth, uv*)
Krug, R.C. *et al., J. Het. Chem.*, 1967, **4**, 309 (*oxides*)
Weinberg, D.S. *et al., Tetrahedron*, 1968, **24**, 5409 (*dioxide, ms*)
Delaney, P.A. *et al., J.C.S. Perkin 1*, 1986, 1861 (*synth*)
Trahanovsky, W.S. *et al., J.O.C.*, 1986, **51**, 113 (*synth, pmr, cmr*)
Rozhenko, A.B. *et al., Zh. Org. Khim.*, 1991, **27**, 2254; *J. Org. Chem. USSR (Engl. Transl.)*, 1991, **27**, 1996 (*cmr, O-17 nmr, S-33 nmr*)
Aitken, R.A. *et al., J.C.S. Perkin 1*, 1994, 927 (*dioxide*)

Dihydro-2(3*H*)-thiophenone, 9CI D-358

[1003-10-7]
2-Thiolanone. 4-Mercaptobutanoic acid γ-thiolactone. γ-Thiobutyrolactone



C_4H_6OS 102.157
Component of roasted coffee beans. Liq. d_4^{20} 1.18. Bp_{20} 90-92° Bp_1 45-46°. n_D^{20} 1.5230.

▶ LD_{50} (mus, orl) 1860 mg/kg. XN1930000

Oxime: [4781-84-4]
C_4H_7NOS 117.171
Cryst. Mp 115-116°.

Ethylene dithioketal: [121921-84-4] *1,4,6-Trithiaspiro[4.4]nonane, 9CI*
$C_6H_{10}S_3$ 178.343
Cryst. (pentane). Mp 43-45°. $Bp_{0.25}$ 90-91°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1127B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 699C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 752B (*ir*)
Aldrich Library of NMR Spectra, **3**, 73C (*pmr*)
Stevens, M. *et al., J.O.C.*, 1954, **19**, 1996 (*synth, uv*)
Kharasch, N. *et al., J.O.C.*, 1963, **28**, 1901 (*synth*)
Stoffelsma, J. *et al., J. Agric. Food Chem.*, 1968, **16**, 1000 (*glc, ms*)
Hawkins, R.T. *et al., J. Het. Chem.*, 1974, **11**, 291 (*synth*)
Fukui, K. *et al., J. Phys. Chem.*, 1980, **84**, 98 (*uv*)
Delaney, P.A. *et al., J.C.S. Perkin 1*, 1991, 285 (*ethylenedithioketal*)
Alonso, J.L. *et al., Z. Naturforsch., A*, 1992, **47**, 588 (*struct, microwave*)

Dihydro-3(2*H*)-thiophenone, 9CI D-359

[1003-04-9]
3-Thiolanone. 3-Thiophanone. FEMA 3266

C_4H_6OS 102.157
Present in cooked beef, coffee, roast filbert and roasted peanut. Food flavouring agent. Bp 175° Bp_7 58°.

Oxime: [24030-02-2]
C_4H_7NOS 117.171
Cryst. (EtOH). Mp 36°.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 209-212°.

S,S-*Dioxide:* [17115-51-4]
$C_4H_6O_3S$ 134.156
Cryst. (2-propanol aq.).

Ethylene ketal: [176-35-2] *1,4-Dioxa-7-thiaspiro[4.4]nonane*
$C_6H_{10}O_2S$ 146.21
Liq. Bp_{15} 92-96°.

Ethylene ketal, S-*oxide:* [110431-53-3]
$C_6H_{10}O_3S$ 162.209
Liq. $Bp_{0.18}$ 103-106°.

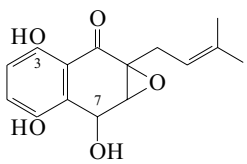
Ethylene ketal, S,S-*dioxide:* [110431-52-2]
$C_6H_{10}O_4S$ 178.209
Needles ($CHCl_3$/petrol). Mp 56-57°.

Ethylene dithioketal: [176-41-0] *1,4,7-Trithiaspiro[4.4]nonane, 9CI*
$C_6H_{10}S_3$ 178.343
Oil. d_4^{20} 1.3. $Bp_{0.15}$ 89-91°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 725C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 548B (*ir*)
Woodward, R.B. *et al., J.A.C.S.*, 1946, **28**, 2229 (*synth*)
Korobitsyna, I.K. *et al., Zh. Obshch. Khim.*, 1955, **25**, 1571; *J. Gen. Chem. USSR (Engl. Transl.)*, 1955, **25**, 1531 (*ethylene dithioketal*)
Wynberg, H. *et al., J.A.C.S.*, 1957, **79**, 1972 (*synth*)
Gianturco, M.A. *et al., Tetrahedron*, 1964, **20**, 1763 (*synth*)
Prochazka, M. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 3744 (*synth, uv*)
Herzschuh, R. *et al., Org. Mass Spectrom.*, 1974, **9**, 665 (*ms*)
Borsdorf, R. *et al., J. Prakt. Chem.*, 1980, **322**, 152 (*ir*)
Miklos, P. *et al., Tetrahedron*, 1987, **43**, 249 (*deriv, synth, pmr, ir, ms*)
Delaney, P.A. *et al., J.C.S. Perkin 1*, 1991, 285 (*ethylene dithioketal*)

7,7*a*-Dihydro-3,6,7-trihydroxy-1*a*-(3-methyl-2-butenyl)-naphth[2,3-*b*]oxiren-2(1*aH*)-one, 9CI D-360

[111261-13-3]
2,3-Epoxy-4,5,8-trihydroxy-2-prenyl-1-tetralone



$C_{15}H_{16}O_5$ 276.288
λ_{max} 205 (ε 14400); 242 (ε 9800); 268 (ε 6100); 379 (ε 4600) (MeOH) (Berdy).

3-O-β-D-Glucopyranoside: [111261-15-5]
$C_{21}H_{26}O_{10}$ 438.43

7-Ketone: [111261-12-2] *3,6-Dihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]-2,7(1*aH*,7*aH*)-dione. 2,3-Epoxy-2-prenylnaphthazarin.* ***2,3-Epoxysesamone***
$C_{15}H_{14}O_5$ 274.273
Constit. of *Sesamum indicum* (sesame). Pale yellow cryst. (MeOH). Mp 85-86°. $[\alpha]_D^{25}$ -43 (c, 0.34 in $CHCl_3$). λ_{max} 209 (ε 18800); 271 (ε 5600); 413 (ε 6800) (MeOH) (Berdy).

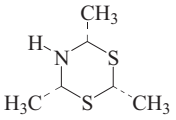
7-Ketone, 3-O-β-D-glucopyranoside: [111261-14-4]
$C_{21}H_{24}O_{10}$ 436.415
λ_{max} 208 (ε 22100); 235 (ε 10700); 261 (ε 7600); 387 (ε 5400) (MeOH) (Berdy).

Potterat, O. *et al., Helv. Chim. Acta*, 1987, **70**,

1551-1557
Ogasawara, T. *et al., Phytochemistry*, 1993, **33**, 1095-1098 (*isol*)
Feroj Hasan, A.F.M. *et al., Phytochemistry*, 2001, **58**, 1225-1228 (*2,3-Epoxysesamone*)

Dihydro-2,4,6-trimethyl-4*H*-1,3,5-dithiazine, 9CI D-361

[86241-90-9]
Thialdine



(2α,4α,6α)-*form*

$C_6H_{13}NS_2$ 163.307
Occurs in a variety of foods and flavours and in food pyrolysis products.

(2α,4α,6α)-*form* [638-17-5]
Flavourant with chicken aroma. Volatile component of roasted shrimp. Cryst. V. sol. Et_2O; sol. EtOH; spar. sol. H_2O. Mp 43°. Steam-volatile, dec. on boiling.
► LD_{50} (mus, ipr) 265 mg/kg, fl. p. 93° (oc). JO6430000

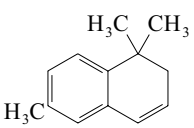
N-*Nitroso:* [114375-58-5]
$C_6H_{12}N_2OS_2$ 192.306
Potential dietary carcinogen. Yellow needles. V. sol. Et_2O; spar. sol. EtOH; insol. H_2O. Mp 79°.
► Potent exp. carcinogen.

N-*Me:* [37434-57-4]
$C_7H_{15}NS_2$ 177.334
Needles (EtOH). Mp 79°.

Marckwald, W. *et al., Ber.*, 1886, **19**, 2378 (*synth*)
U.S. Pat., 1976, 3 966 988; *CA*, **85**, 92425y
Hansen, T.J. *et al., Tetrahedron*, 1981, **37**, 4143 (*deriv, bibl*)
Lijinsky, W. *et al., Food Chem. Toxicol.*, 1988, **26**, 3 (*N-nitroso, tox*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 1027

1,2-Dihydro-1,1,6-trimethylnaphthalene D-362

3,4-Dehydroionene. TDN

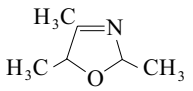


$C_{13}H_{16}$ 172.269
Isol. from strawberry oil, peaches, tobacco and wines. Component of wine off-flavour on ageing. Bp_{18} 115°.

Stoltz, L.P. *et al., Phytochemistry*, 1970, **9**, 1157 (*isol*)
Stevens, K.L. *et al., Tetrahedron*, 1975, **31**, 2749 (*synth*)
Simpson, R.F. *et al., Chem. Ind. (London)*, 1978, 37 (*biol*)
Migniac, P. *et al., Synth. Commun.*, 1990, **20**, 1853 (*synth, pmr, cmr*)
Winterhalter, P. *et al., J. Agric. Food Chem.*, 1991, **39**, 1825-1829 (*formn in wine, ms*)

2,5-Dihydro-2,4,5-trimethyloxazole, 9CI D-363

[22694-96-8]
2,4,5-Trimethyl-3-oxazoline, 8CI. FEMA 3525

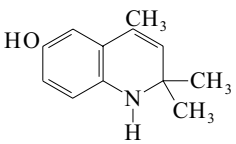


$C_6H_{11}NO$ 113.159
Volatile flavour constit. of boiled beef and roasted peanuts. Used as flavour enhancer in fish products. Oil with characteristic odour. Bp 96.6° Bp_{12} 45-47°.
► LD_{50} (mus, orl) 4840 mg/kg. RQ5665000

Chang, S.S. *et al., Chem. Ind. (London)*, 1968, 1639 (*isol, ir, ms*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249 (*tox*)
Lee, M.-S. *et al., J. Agric. Food Chem.*, 1981, **29**, 684 (*isol*)
Ho, C.T. *et al., J. Agric. Food Chem.*, 1982, **30**, 793
Hartman, G.J. *et al., Lebensm.-Wiss. Technol.*, 1984, **17**, 171 (*use*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TLX800
U.S. Pat., 1990, 4 960 6903; *CA*, **114**, 162797q (*use*)

1,2-Dihydro-2,2,4-trimethyl-6-quinolinol, 9CI D-364

[72107-05-2]
1,2-Dihydro-6-hydroxy-2,2,4-trimethylquinoline



$C_{12}H_{15}NO$ 189.257
Mp 180-181°.

O-*Ac:* [71043-64-6]
$C_{14}H_{17}NO_2$ 231.294
Plates (petrol). Mp 60-61°.

Et ether: [91-53-2] *6-Ethoxy-1,2-dihydro-2,2,4-trimethylquinoline, 9CI, 8CI.* ***Ethoxyquin****. EMQ. Santoquin*
$C_{14}H_{19}NO$ 217.31
Antioxidant used in animal feeds and for the preservation of colour in the production of chilli powder, paprika and ground chilli. Formerly used as an agricultural pesticide/herbicide, now superseded . Also used as a post-harvest dip for apples and pears to prevent scald. Yellow liq. d_{25}^{25} 1.03. Bp_{12} 169° Bp_2 123-125°.
► LD_{50} (rat, orl) 800 mg/kg. Exp. nephrotoxic. VB8225000

Et ether, hydrochloride: [3659-01-6]
Cryst. Mp 192-193°.

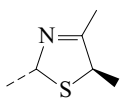
Et ether, N-*oxide:* [14362-24-4] *Ethoxyquinnitroxide*
$C_{14}H_{19}NO_2$ 233.31
Viscous red oil.

[3659-01-6]

Knoevenagel, E. *et al., Ber.*, 1921, **54**, 1722 (*synth, Ethoxyquin*)
Tung, C.C. *et al., Tetrahedron*, 1963, **19**, 1685 (*synth, uv, pmr*)
Chaffard, M. *et al., Def. Veg.*, 1970, **24**, 235; *CA*, **74**, 98246 (*rev*)
Skaare, J.U. *et al., Xenobiotica*, 1970, **9**, 649
Lin, J.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 798 (*Ethoxyquinnitroxide, synth*)
Skaare, J.U. *et al., J. Agric. Food Chem.*, 1975, **23**, 1091 (*metab, chromatog, ms*)
Bonnett, R. *et al., J.C.S. Perkin 1*, 1979, 488 (*cryst struct, synth, ir, uv, pmr, deriv*)
Welch, S.C. *et al., J. Med. Chem.*, 1982, **25**, 81 (*synth, ir, pmr*)
Kahl, R. *et al., Toxicology*, 1984, **33**, 185 (*rev, props*)
Kim, H.L. *et al., J. Toxicol. Environ. Health*, 1985, **15**, 663 (*hydrochloride, synth*)
Merck Index, 11th edn., 1989, No. 3710 (*synth, bibl*)
Taimr, L. *et al., Angew. Makromol. Chem.*, 1991, **190**, 53 (*synth, activity, Ethoxyquin*)
Gunstone, F.D. *et al., J.C.S. Perkin 2*, 1991, 1955 (*epr, Ethoxyquin*)
Thorisson, S. *et al., Chem. Phys. Lipids*, 1992, **60**, 263 (*autoxid*)
Hard, G.C. *et al., Fundam. Appl. Toxicol.*, 1992, **18**, 278 (*tox*)
Hayes, J.D. *et al., Cancer Res.*, 1993, **53**, 3887 (*chemoprotectant*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1367
Reyes, J.L. *et al., Biochem. Pharmacol.*, 1995, **49**, 283 (*Ethoxyquin, pharmacol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 938-939 (*Ethoxyquin, use*)
Pesticide Manual, 11th edn., 1997, No. S1025
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SAV000

2,5-Dihydro-2,4,5-trimethylthiazole, 9CI D-365

[60633-24-1]
2,4,5-Trimethyl-3-thiazoline, 8CI



(2*R*,5*R*)-*form*

$C_6H_{11}NS$ 129.226
Flavour constit. of cooked meats. Bp_{12} 57°.

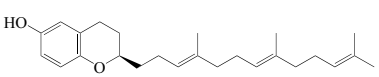
Picrate:
Cryst. (MeOH). Mp 117-118°.

[134281-36-0, 134281-37-1]

Thiel, M. *et al., Annalen*, 1960, **638**, 174 (*synth*)
Mussinan, C.J. *et al., ACS Symp. Ser.*, 1976, **26**, 133 (*occur*)
Hwang, S.S. *et al., J. Agric. Food Chem.*, 1986, **34**, 538 (*synth, occur*)
Sullivan, T.P. *et al., J. Chem. Ecol.*, 1988, **14**, 363; 379 (*isol*)

3,4-Dihydro-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2*H*-1-benzopyran-6-ol D-366

2-(4,8,12-Trimethyl-3,7,11-tridecatrienyl)-6-chromanol. Didemethyl-δ-tocotrienol



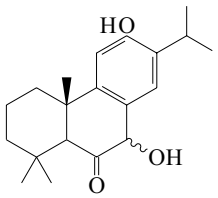
$C_{25}H_{36}O_2$ 368.558

(R)-form

Isol. from rice bran. Antitumour agent and antioxidant.

Qureshi, A.A. *et al., J. Agric. Food Chem.*, 2000, **48**, 3130-3140

7,12-Dihydroxy-8,11,13-abietatrien-6-one D-367



$C_{20}H_{28}O_3$ 316.439

(7ξ)-form [128741-29-7]

Trilobinone

Constit. of *Salvia triloba* (Greek sage). Light yellow powder.

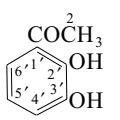
Ulubelen, A. *et al., Planta Med.*, 1990, **56**, 82 (*isol, pmr, cmr*)

2′,3′-Dihydroxyacetophenone, 8CI D-368

[13494-10-5]

[28631-86-9]

1-(2,3-Dihydroxyphenyl)ethanone, 9CI. 3-Acetylcatechol



$C_8H_8O_3$ 152.149

Potential component of FEMA 3662. Flavouring ingredient. Dark-yellow prisms (C_6H_6/petrol). Mp 97-98°. pK_a -6.96. pK_{a1} 8.96; pK_{a2} 13.4 (25°).

2-Ac:

$C_{10}H_{10}O_4$ 194.187

Needles. Mp 53-55°.

Di-Ac:

$C_{12}H_{12}O_5$ 236.224

Leaflets (C_6H_6). Mp 109°.

Di-Me ether: [38480-94-3] *2′,3′-Dimethoxyacetophenone*

$C_{10}H_{12}O_3$ 180.203

Bp_{14} 143-144°.

Methylene ether: [33842-14-7] *2′,3′-Methylenedioxyacetophenone, 8CI. 1-(1,3-Benzodioxol-4-yl)ethanone*

$C_9H_8O_3$ 164.16

Cryst. (cyclohexane). Mp 92.5°.

Methylene ether, 2,4-dinitrophenylhydrazone: [33842-34-1]

Carmine-red cryst. Mp 232°.

v. Krannichfeldt, H. *et al., Ber.*, 1913, **46**, 4016 (*synth*)
Awad, W.I. *et al., J.A.C.S.*, 1959, **80**, 6057 (*ir*)
Bruce, J.M. *et al., J.C.S.*, 1960, 360
Arnaud, R. *et al., Bull. Soc. Chim. Fr.*, 1967, 4541
Dallacker, F. *et al., Chem. Ber.*, 1971, **104**, 2347 (*methylene ether*)
Wu, E.S.C. *et al., J. Med. Chem.*, 1989, **32**, 183 (*synth*)
Adam, W. *et al., Chem. Ber.*, 1992, **125**, 2455 (*2-Ac*)
Ahmad, T. *et al., Carbohydr. Res.*, 1993, **247**, 211 (*formation*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 834-835 (*use*)

2′,4′-Dihydroxyacetophenone, 8CI D-369

[89-84-9]

[28631-86-9]

1-(2,4-Dihydroxyphenyl)ethanone, 9CI. Resacetophenone. 4-Acetylresorcinol. Resoacetophenone

$C_8H_8O_3$ 152.149

Potential component of FEMA 3662. Flavouring ingredient. Leaflets or needles. Mp 147°. pK_a -5.11. pK_{a1} 7.42; pK_{a2} 12 (25°).

▶ Eye irritant. LD_{50} (rat, orl) 2830 mg/kg. Exp. reprod. effects. AM7525000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 34C; 41B; 43D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 848B; 857A; 859A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1254A; 1260C (*ir*)
Robinson, R. *et al., J.C.S.*, 1934, 1491 (*synth*)
Gumprecht, D.L. *et al., J. Chromatogr.*, 1967, **30**, 528 (*chromatog*)
Lutskii, A.E. *et al., Zh. Prikl. Spektrosk.*, 1970, **13**, 298 (*uv*)
Rao, K.V.K. *et al., Curr. Sci.*, 1975, **44**, 547; *CA*, **83**, 130838d (*props*)
Lutskii, A.E. *et al., Zh. Obshch. Khim.*, 1977, **47**, 905 (*nmr*)
Patra, A. *et al., Magn. Reson. Chem.*, 1987, **25**, 734 (*cmr*)
Boykin, D.W. *et al., J.O.C.*, 1991, **56**, 1969 (*O-17 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 834-835 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DMG400; PAC250

2,4′-Dihydroxyacetophenone, 8CI D-370

[5706-85-4]

[28631-86-9]

2-Hydroxy-1-(4-hydroxyphenyl)ethanone, 9CI. p-*Hydroxyphenacyl alcohol.* p-*Hydroxybenzoylcarbinol. Hydroxymethyl* p-*hydroxyphenyl ketone*

$C_8H_8O_3$ 152.149

Potential component of FEMA 3662. Flavouring ingredient.

2-O-β-D-Glucopyranoside:4′-Hydroxyphenacyl β-D-glucoside

$C_{14}H_{18}O_8$ 314.291

$[\alpha]_D$ -33 (c, 0.2 in MeOH).

2-Ac: [20816-46-0]

$C_{10}H_{10}O_4$ 194.187

Mp 59°.

2-Me ether: [32136-81-5] *4′-Hydroxy-2-methoxyacetophenone*

$C_9H_{10}O_3$ 166.176

Yellow needles (C_6H_6). Mp 128-130°.

4′-Me ether: [4136-21-4] *2-Hydroxy-4′-methoxyacetophenone. Anisoylmethanol*

$C_9H_{10}O_3$ 166.176

Mp 104°.

4′-Me ether, 2-O-β-D-glucopyranoside: [135743-08-7] ***Icariside D_3***

$C_{15}H_{20}O_8$ 328.318

Amorph. powder. $[\alpha]_D^{23}$ -116.7 (c, 0.81 in MeOH).

Stoermer, R. *et al., Ber.*, 1902, **35**, 3549 (*synth*)
Robertson, A. *et al., J.C.S.*, 1928, 1460 (*synth*)
Kondo, K. *et al., Yakugaku Zasshi*, 1930, **50**, 928 (*synth*)
Shetty, H.O. *et al., J. Med. Chem.*, 1988, **31**, 55 (*Me ether*)
Matsushita, H. *et al., Phytochemistry*, 1991, **30**, 2025 (*Icariside D_3*)
Pan, H. *et al., Phytochemistry*, 1995, **39**, 1423 (*Hydroxyphenacyl glucoside*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 834-835 (*use*)

2′,5′-Dihydroxyacetophenone, 8CI D-371

[490-78-8]

1-(2,5-Dihydroxyphenyl)ethanone, 9CI. Acetylquinol. Acetylhydroquinone. Quinacetophenone

$C_8H_8O_3$ 152.149

A mixt. of dihydroxyacetophenone isomers is used in food flavouring. Potential component of FEMA 3662. Green needles (H_2O). Mp 202-203°. pK_{a1} 9.48; pK_{a2} 12.9 (25°).

▶ AM7700000

[28631-86-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 34D; 41C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 848C; 857B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1254B; 1260D (*ir*)
Klinger, H. *et al., Ber.*, 1898, **31**, 1214 (*synth*)
Org. Synth., 1948, **28**, 42 (*synth*)
Patra, A. *et al., Magn. Reson. Chem.*, 1987, **25**, 734 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 834 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DMG600

2′,6′-Dihydroxyacetophenone, 8CI D-372

[699-83-2]

[28631-86-9]

1-(2,6-Dihydroxyphenyl)ethanone, 9CI. 2-Acetylresorcinol

$C_8H_8O_3$ 152.149

Potential component of FEMA 3662. Flavouring ingredient. Yellow needles. Mp 155-156°. pK_a -5.35. pK_{a1} 7.94; pK_{a2} 12.35 (25°).

Me ether: [703-23-1] *2′-Hydroxy-6′-methoxyacetophenone*

$C_9H_{10}O_3$ 166.176

Cryst. (EtOH). Mp 59-60°.

Di-Me ether: [2040-04-2] *2′,6′-Dimethoxyacetophenone*

$C_{10}H_{12}O_3$ 180.203

Mp 72-73°.

▶ AM8400000

2-O-Benzyl: [4047-24-9] *2′-Benzyloxy-6′-hydroxyacetophenone. Populneol*
$C_{15}H_{14}O_3$ 242.274
Cryst. (MeOH). Mp 109-110°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 42B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 848A; 856C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1254C; 1261A (*ir*)
Forbes, W.F. *et al., Can. J. Chem.*, 1957, **35**, 1049 (*uv*)
Allport, D. *et al., J.C.S.*, 1960, 654 (*synth*)
Arnaud, R. *et al., Bull. Soc. Chim. Fr.*, 1967, 4541
Gumprecht, D.L. *et al., J. Chromatogr.*, 1967, **30**, 528 (*chromatog*)
Moses, P. *et al., Acta Chem. Scand.*, 1970, **24**, 312
Datta, S.C. *et al., Indian J. Chem.*, 1971, **9**, 286 (*isol, deriv*)
Ternai, B. *et al., Tetrahedron*, 1976, **32**, 565 (*cmr*)
Bobik, A. *et al., J. Med. Chem.*, 1977, **20**, 1194 (*synth*)
Lau, C.K. *et al., J.O.C.*, 1987, **52**, 1670 (*deriv, synth, pmr*)
Boireau, G. *et al., Synth. Commun.*, 1995, **25**, 149 (*Me ether, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 834-835 (*use*)

3′,4′-Dihydroxyacetophenone, 8CI D-373

[1197-09-7]
1-(3,4-Dihydroxyphenyl)ethanone, 9CI. 4-Acetocatechol. Acetylpyrocatechol

$C_8H_8O_3$ 152.149
Extracted from coffee residues. Potential component of FEMA 3662. A mixt. of dihydroxyacetophenone isomers is used in food flavouring. Needles (H_2O). Mp 116°.
▶ KM5775200

[16522-48-8, 28631-86-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 46A; 46B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 864A; 864B; 1293A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1261D; 1262A (*ir*)
Stephen, H. *et al., J.C.S.*, 1914, **105**, 1046 (*synth*)
Lange, R.G. *et al., J.O.C.*, 1962, **27**, 2037 (*synth*)
Kovacik, V. *et al., Chem. Ber.*, 1969, **102**, 1513 (*ms*)
Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 2418; 1972, **37**, 1825 (*uv*)
Nishina, A. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 293 (*isol, props, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 834 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HLQ500

3′,5′-Dihydroxyacetophenone, 8CI D-374

[51863-60-6]

[28631-86-9]
1-(3,5-Dihydroxyphenyl)ethanone, 9CI. 5-Acetylresorcinol

$C_8H_8O_3$ 152.149
A mixt. of dihydroxyacetophenone isomers is used in food flavouring. Potential component of FEMA 3662. Cryst. (H_2O). Mp 147-148°.

Semicarbazone:
Needles (EtOH). Mp 205-206°.

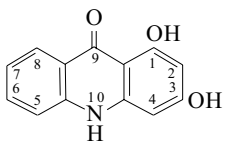
Di-Ac: [35086-59-0]
$C_{12}H_{12}O_5$ 236.224
Needles (petrol). Mp 91-92°.

Di-Me ether: [39151-19-4] *3′,5′-Dimethoxyacetophenone*
$C_{10}H_{12}O_3$ 180.203
Needles (petrol). Mp 42-43°. Bp_{10} 151-152°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 35B; 36A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 850B; 864C; 1296B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1254D (*ir*)
Mauthner, F. *et al., J. Prakt. Chem.*, 1927, **115**, 274 (*synth*)
Valyashko, A. *et al., Zh. Obshch. Khim.*, 1951, **21**, 1069 (*uv*)
Huls, R. *et al., Bull. Soc. Chim. Belg.*, 1956, **65**, 596 (*synth*)
Masse, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1976, **282**, 473
Busch-Petersen, J. *et al., J. Med. Chem.*, 1996, **39**, 3790-3796 (*di-Me ether, synth, ir, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 834-835 (*use*)

1,3-Dihydroxyacridone D-375

[20324-10-1]
1,3-Dihydroxy-9(10H)-acridinone, 9CI



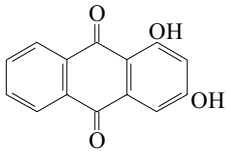
$C_{13}H_9NO_3$ 227.219
Yellow needles (Me_2CO/EtOH). Mp 345° dec. (355° dec., 370°).

3-Me ether, N-*Me:* [13161-83-6] ***1-Hydroxy-3-methoxy-10-methylacridone***
$C_{15}H_{13}NO_3$ 255.273
Alkaloid from the roots *Ruta graveolens* (rue). Yellow cryst. (EtOAc/petrol or EtOAc/C_6H_6). Mp 164-165° Mp 174-176°.

Fish, F. *et al., Phytochemistry*, 1971, **10**, 3322-3324 (*3-Me ether N-Me, isol, uv, ir*)
Scharlemann, W. *et al., Z. Naturforsch., B*, 1972, **27**, 806-808 (*3-Me ether N-Me, isol, uv*)
Bahar, M.H. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 782-783 (*3-Me ether N-Me, synth, uv, ir, pmr, ms*)
Reisch, J. *et al., Annalen*, 1991, 685-689 (*N-Me, 3-Me ether N-Me, 1,3-di-Me ether N-Me, synth, ir, pmr, cmr*)

1,3-Dihydroxyanthraquinone, 8CI D-376

[518-83-2]
*1,3-Dihydroxy-9,10-anthracenedione, 9CI. **Xanthopurpurin**. Purpuroxanthin*



$C_{14}H_8O_4$ 240.215
Obt. from *Asperula odorata* (sweet woodruff). Yellow leaflets (C_6H_6), orange needles by subl. Mp 268-270°.
▶ CB6590000

Di-Me ether: [1989-42-0] *1,3-Dimethoxyanthraquinone*
$C_{16}H_{12}O_4$ 268.268
Isol. from *Asperula odorata* (sweet woodruff). Yellow needles. Mp 154-155°.

Perkin, A.G. *et al., J.C.S.*, 1893, **63**, 1159; 1929, 1399 (*isol, synth*)
Kido, H. *et al., Anal. Chim. Acta*, 1960, **23**, 116 (*ir*)
Davies, D.G. *et al., Chem. Comm.*, 1968, 953
Murti, V.V.S. *et al., Indian J. Chem.*, 1970, **8**, 779 (*synth*)
Castonguay, A. *et al., Can. J. Chem.*, 1977, **55**, 1324 (*synth*)
Khanapure, S.P. *et al., J.O.C.*, 1987, **52**, 5685 (*deriv, synth, pmr, cmr, ir*)
El-Gamal, A.A. *et al., Phytochemistry*, 1995, **40**, 245 (*cmr*)

1,8-Dihydroxyanthraquinone, 8CI D-377

[117-10-2]
*1,8-Dihydroxy-9,10-anthracenedione, 9CI. Chrysazin. **Dantron, INN**. Danthron, BAN. Istizin. Danivac. Dorbane. Many other names*

$C_{14}H_8O_4$ 240.215
Occurs in roots of *Rheum palmatum* (Turkey rhubarb). Square orange plates (Me_2CO), metastable fine fibres by rapid cryst. Sol. EtOH, alkalis; insol. H_2O. Mp 193°. pK_{a1} 8.3; pK_{a2} 12.46 (25°). Log P 1.92 (calc). It has been suggested that the 1,10-dioxo tautomer is present in the crystal state but there is no spectroscopic evidence for this.
▶ Can discolour urine when used therapeutically. Exp. carcinogen.
CB6650000

Di-Ac: [1963-82-2]
$C_{18}H_{12}O_6$ 324.289
Yellow needles. Mp 231-232°.
▶ CB6690000

Mono-Me ether: [5539-66-2] *1-Hydroxy-8-methoxyanthraquinone*
$C_{15}H_{10}O_4$ 254.242
Orange-red needles (EtOH). Mp 197-198°.

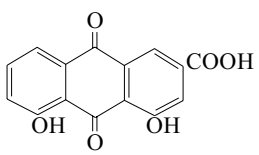
Di-Me ether: [6407-55-2] *1,8-Dimethoxyanthraquinone*
$C_{16}H_{12}O_4$ 268.268
Yellow cryst. Mp 219°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 87D (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 91B (*nmr*)
Naylor, C.A. *et al., J.A.C.S.*, 1931, **53**, 4112
Aoyama, S. *et al., Yakugaku Zasshi*, 1932, **52**, 17
Lish, P.M. *et al., J. Am. Pharm. Assoc.*, 1958, **47**, 371 (*pharmacol*)

Kido, H. *et al., Anal. Chim. Acta*, 1960, **23**, 116 (*ir*)
Beynon, J.H. *et al., Appl. Spectrosc.*, 1960, **14**, 156 (*ms*)
Ruggieri, R. *et al., Anal. Chim. Acta*, 1961, **25**, 145 (*use*)
Prakesh, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1965, **122**, 272 (*cryst struct*)
Fairbairn, J.W. *et al., J. Pharm. Pharmacol.*, 1970, **22**, 584 (*pharmacol*)
Idris, K.A. *et al., Egypt. J. Chem.*, 1973, 67 (*uv*)
Morley, J.O. *et al., J.C.S. Perkin 2*, 1973, 1626 (*pmr*)
Fournier, G. *et al., Phytochemistry*, 1975, **14**, 2099 (*isol*)
Breimer, D.D. *et al., Pharmacology*, 1976, **14**, 30 (*metab*)
Case, M.T. *et al., Drug Chem. Toxicol.*, 1978, **1**, 89 (*tox*)
Berger, Y. *et al., Org. Magn. Reson.*, 1978, **11**, 375 (*cmr*)
Cameron, A.W. *et al., Aust. J. Chem.*, 1982, **35**, 2095 (*synth*)
Howard, D.F. *et al., Naturwissenschaften*, 1982, **69**, 91 (*isol*)
Roman Ceba, M. *et al., Mikrochim. Acta*, 1983, **2**, 85 (*detn, Mg*)
Mueller, K. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1984, **317**, 120 (*synth*)
Gattuso, J.M. *et al., Drug Saf.*, 1984, **10**, 47 (*rev*)
Khanapure, S.P. *et al., J.O.C.*, 1987, **52**, 5685 (*deriv, synth, pmr, ir*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2970 (*synonyms*)
IARC Monog., 1990, **50**, 265 (*rev, tox*)
Grunwell, J.R. *et al., J.O.C.*, 1991, **56**, 91 (*synth, pmr*)
Kahr, B. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1 (*tautom*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1215
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DMH400

4,5-Dihydroxyanthraquinone-2-carboxylic acid D-378

[478-43-3]
9,10-Dihydro-4,5-dihydroxy-9,10-dioxo-2-anthracenecarboxylic acid, 9CI. Chrysazin-3-carboxylic acid. ***Rhein****. Monorhein. Cassic acid*



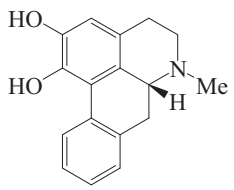
$C_{15}H_8O_6$ 284.225
Present in *Rheum palmatum* (Chinese rhubarb). Yellow needles (MeOH). Sol. bases; fairly sol. MeOH, Et_2O; poorly sol. H_2O, hexane, acids. Mp 321° (310°). Log P 1.7 (calc). λ_{max} 229 (ϵ 36800); 258 (ϵ 20100); 435 (ϵ 11100) (MeOH) (Berdy). λ_{max} 270 ; 425 (EtOH) (Berdy).

►CA9516000

5-O-β-D-Glucopyranoside: [34298-86-7]
Glucorhein*. Glucorein*
$C_{21}H_{18}O_{11}$ 446.367
Isol. from *Rheum palmatum* (Chinese rhubarb). Mp 260-266°.

Hauptmann, H. *et al., J.A.C.S.*, 1950, **72**, 1492 (*occur*)
Nawa, H. *et al., J.O.C.*, 1961, **26**, 979 (*struct*)
Romanova, A.S. *et al., Khim. Prir. Soedin.*, 1966, **2**, 143; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 113 (*isol, glucosides*)
Murty, V.K. *et al., Tetrahedron*, 1967, **23**, 515 (*synth, deriv*)
Romonova, A.S. *et al., CA*, 1969, **70**, 9366 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1297 (*occur*)
Ger. Pat., 1977, 2 711 493; *CA*, **88**, 37504k (*synth*)
Hauser, F.M. *et al., J.O.C.*, 1982, **47**, 383 (*synth*)
Gallagher, P.T. *et al., Tet. Lett.*, 1994, **35**, 289 (*synth*)
Dahms, M. *et al., Drug Metab. Dispos.*, 1997, **25**, 442 (*metab, bibl*)

1,2-Dihydroxyaporphine D-379



(*R*)-*form*

$C_{17}H_{17}NO_2$ 267.327

(R)-form

O^1*-Me:* [3153-55-7] *2-Hydroxy-1-methoxyaporphine.* ***Floribundine****.* N-*Methylasimilobine.* O-*Nornuciferine*
$C_{18}H_{19}NO_2$ 281.354
Alkaloid from *Nelumbo nucifera* (East India lotus). Mp 195-196°. $[\alpha]_D^{20}$ -220 (c, 0.40 in $CHCl_3$). λ_{max} 231 (log ϵ 4.07); 272 (log ϵ 4); 314 (log ϵ 3.29) (no solvent reported).

O^1*-Me,* N-*de-Me,* N-*methoxycarbonyl:* [356048-23-2] ***Romucosine A***
$C_{19}H_{19}NO_4$ 325.363
Alkaloid from *Rollinia mucosa* (biriba). Amorph. brown powder. $[\alpha]_D^{25}$ -105 (c, 0.1 in $CHCl_3$). λ_{max} 237 (log ϵ 4.4); 285 (log ϵ 4.22); 307 (log ϵ 4.05) (MeOH).

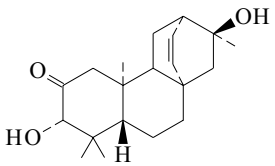
(S)-form

Di-Me ether, N-*de-Me,* N-*methoxycarbonyl:* [356042-11-0] **N-*Methoxycarbonyl*-N-*nornuciferine***
$C_{20}H_{21}NO_4$ 339.39
Alkaloid from *Rollinia mucosa* (biriba). Amorph. powder. $[\alpha]_D^{25}$ +165 (c, 0.05 in $CHCl_3$). λ_{max} 235 (log ϵ 4.23); 285 (log ϵ 4.2); 307 (log ϵ 3.36) (MeOH).

3-Chloro, O^1*-Me,* N-*de-Me,* N-*methoxycarbonyl:* [356048-24-3] ***Romucosine B***
$C_{19}H_{18}ClNO_4$ 359.808
Alkaloid from *Rollinia mucosa* (biriba). Amorph. powder. $[\alpha]_D^{25}$ +153 (c, 0.05 in $CHCl_3$). Opposite abs. config. to Romucosine A λ_{max} 245 (log ϵ 4.43); 285 (log ϵ 4.25) (MeOH).

Gulland, J.M. *et al., J.C.S.*, 1928, 581-591 (*Nuciferine, synth*)
Konvalova, R. *et al., Ber.*, 1935, **68**, 2277-2282 (*Floribundine, isol*)
Arthur, H.R. *et al., J.C.S.*, 1959, 2306 (*Nuciferine, isol*)
Tomita, M. *et al., Yakugaku Zasshi*, 1961, **81**, 469-473; 1965, **85**, 77-82 (*Floribundine, Asimilobine*)
Kunimoto, J.I. *et al., Yakugaku Zasshi*, 1964, **84**, 1141-1142 (*Floribundine, Nuciferine, isol*)
Kupchan, S.M. *et al., J.O.C.*, 1971, **36**, 2413-2418 (*Nuciferine, synth, uv*)
Guinaudeau, H. *et al., Phytochemistry*, 1971, **10**, 1963-1966 (*Nuciferine, isol, ir, pmr, ms*)
Mitscher, L.A. *et al., J. Nat. Prod.*, 1972, **35**, 157-176 (*activity*)
Guinaudeau, H. *et al., Planta Med.*, 1975, **27**, 304-318 (*Floribundine*)
Jackman, L.M. *et al., J. Nat. Prod.*, 1979, **42**, 437-449 (*cmr*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80-85 (*cd*)
Villar, A. *et al., Planta Med.*, 1986, **57**, 556-557 (*activity*)
Ramana, M.M.V. *et al., Tet. Lett.*, 1996, **37**, 1671-1674 (*N-Nornuciferine, synth*)
Kuo, R.-Y. *et al., Phytochemistry*, 2001, **57**, 421-425 (*Romucosines, N-Methoxycarbonylnornuciferine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NOE500

3,16-Dihydroxy-13-atisen-2-one D-380



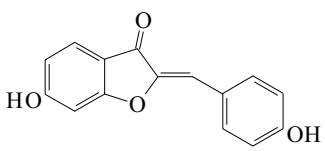
$C_{20}H_{30}O_3$ 318.455

(ent-3β,16α)-form [119642-83-0]
Yucalexin A19
Constit. of cassava roots (*Manihot esculenta*). $[\alpha]_D^{23}$ +8.28 (c, 0.35 in $CHCl_3$).

Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769

4′,6-Dihydroxyaurone D-381

*6-Hydroxy-2-[(4-hydroxyphenyl)methylene]-3(2*H*)-benzofuranone, 9CI. 6-Hydroxy-2-(*p*-hydroxybenzylidene)-3(2*H*)-benzofuranone, 8CI.* ***Hispidol***†



$C_{15}H_{10}O_4$ 254.242

(Z)-form [5786-54-9]
Isol. from seedlings of *Glycine max* (soybean) *(Soja hispida)*. Yellow needles (EtOH aq.). Mp 288° dec.

Di-Ac:
Pale-yellow needles (MeOH/AcOH). Mp 162-163°.

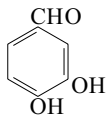
6-O-β-D-Glucopyranosyl: [20550-08-7]
$C_{21}H_{20}O_9$ 416.384
Isol. from seedlings of *Glycine max* (soybean). Yellow cryst. or cubes (MeOH aq. or H_2O). Mp 211-212° (191-192°).

Geissman, T.A. *et al., J.A.C.S.*, 1956, **78**, 832

(*synth, uv*)
Wong, E. *et al., Phytochemistry*, 1966, **5**, 463 (*isol*)
Farkas, L. *et al., Tetrahedron*, 1968, **24**, 4213 (*synth*)
Huke, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1969, **302**, 401; 423 (*uv, pmr*)
El Sherbeiny, A.E.A. *et al., Planta Med.*, 1978, **34**, 335 (*isol*)
Breytenbach, J.C. *et al., J.C.S. Perkin 1*, 1982, 1157 (*synth*)

3,4-Dihydroxybenzaldehyde D-382

[139-85-5]
Protocatechualdehyde, 8CI. Protocatechuic aldehyde. Rancinamycin IV



$C_7H_6O_3$ 138.123
Cryst. (toluene). Sol. EtOH, H_2O, Et_2O. Mp 153-154°. pK_{a1} 7.27; pK_{a2} 11.4 (25°). λ_{max} 220 (ϵ 9500) (95% EtOH) (Derep).
▶ LD_{50} (mus, ipr) 205 mg/kg. UL0380000

3-Me ether: [121-33-5] *4-Hydroxy-3-methoxybenzaldehyde.* ***Vanillin, USAN****. Zimco. Vanillaldehyde. FEMA 3107*
$C_8H_8O_3$ 152.149
Constit. of vanilla (*Vanilla* spp.) and many other plants, e.g. Peru balsam, clove bud oil. Widely used flavouring agent esp. in cocoa products. Obt. from spent wood-pulp liquors. Needles or tetragonal cryst. with characteristic pleasant odour (H_2O). Spar. sol. cold H_2O; mod. sol. hot. Mp 81-82° Mp 77-79° (dimorph.). Bp_{15} 170°. pK_{a1} 7.4 (25°). Slowly oxid. in air. 3 Cryst. modifications exist λ_{max} 232 (ϵ 15500); 279 (ϵ 10500); 309 (ϵ 1030) (MeOH) (Berdy). λ_{max} 251 (ϵ 8330); 319 (ϵ 25200) (MeOH-NaOH) (Berdy).
▶ LD_{50} (rat, orl) 1580 mg/kg. LD_{50} (mus, ipr) 721 mg/kg. Exp. reprod. effects. YW5775000

3-Me ether, 4-O-β-D-glucopyranoside: [494-08-6] ***Vanilloside****. Glucovanillin. Avenein*
$C_{14}H_{18}O_8$ 314.291
Isol. from oats. Needles (EtOH aq.). Mp 188-192°. $[\alpha]_D^{20}$ -88.7 (H_2O).

3-Me ether, Ac: [881-68-5] *Vanillin acetate. FEMA 3108*
$C_{10}H_{10}O_4$ 194.187
Flavouring material. Present in fermented soya hydrolysate (shoyu). Needles (Et_2O) with mild balsamic, floral odour. Mp 77-79° Mp 102-103°.

3-Me ether, 4-O-(2-methylpropanoyl): [20665-85-4] *Vanillin isobutyrate. Isobutavan. FEMA 3754*
$C_{12}H_{14}O_4$ 222.24
Flavouring ingredient. Liq. d^{20} 0.99. $Bp_{5.5}$ 155°. n_D^{20} 1.5219.

3-Et ether: [121-32-4] *3-Ethoxy-4-hydroxybenzaldehyde. Vanillal. Bourbonal.* ***Ethyl vanillin, USAN****†. Aethylvanillin. Vanirom. FEMA 2464*
$C_9H_{10}O_3$ 166.176
Flavouring agent with flavouring power 2-4 times greater than vanillin. Used esp. in cocoa products. Cryst. (EtOH) with intense vanilla odour and sweet taste. Mp 76-78°. Bp 285°. Log P 1.8 (calc).
▶ Human skin irritant. LD_{50} (rat, orl) 1590 mg/kg. CU6125000

3-Et ether, 4-O-β-D-glucopyranoside: [122397-96-0] *Ethylvanillin glucoside*
$C_{15}H_{20}O_8$ 328.318
Flavouring ingredient with vanilla aroma.

3-Et ether, 4-O-(2-methylpropanoyl): [188417-26-7] *Ethyl vanillin isobutyrate*
$C_{13}H_{16}O_4$ 236.267
Flavouring ingredient.

4-Et, 3-Me ether: [120-25-2] *4-Ethoxy-3-methoxybenzaldehyde. Ethylvanillin†*
Isol. from storax. Flavouring. Stabiliser. Prisms. Mp 64-65°.

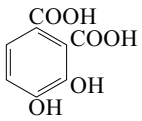
4-O-(3,7-Dimethyl-2,6-octadienyl), 3-Me ether: [151455-08-2] **O-*Geranylvanillin***
$C_{18}H_{24}O_3$ 288.386
Constit. of rock samphire (*Crithmum maritimum*). Oil. λ_{max} 230 (ϵ 19000); 264 (ϵ 18500); 300 (ϵ 16850) (hexane) (Berdy).

[2169-98-4]

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **15**, 633 (*rev, tox, Vanillin*)
Slabbert, N.P. *et al., Tetrahedron*, 1977, **33**, 821 (*props*)
Blanchflower, W.J. *et al., Analyst (London)*, 1985, **110**, 1283 (*deriv, use*)
Burger, B.V. *et al., Z. Naturforsch., C*, 1985, **40**, 847 (*Vanillin, isol*)
Gannett, P.M. *et al., J.O.C.*, 1988, **53**, 1064 (*Vanillin, derivs, ir, pmr, cmr, ms, uv*)
Pat. Coop. Treaty (WIPO), 1988, 88 09 133; *CA*, **111**, 112377u (*3-Et ether glucoside, synth, use*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EQF000; VFK000
Loupy, A. *et al., Org. Prep. Proced. Int.*, 1990, **22**, 99 (*synth, derivs*)
Cunsolo, F. *et al., J. Nat. Prod.*, 1993, **56**, 1598 (*O-Geranylvanillin*)
Liu, J. *et al., Neuropharmacology*, 1993, **32**, 659 (*Vanillin, pharmacol*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 184-185; 542-543
Velavan, R. *et al., Acta Cryst. C*, 1995, **51**, 1131 (*cryst struct, polymorphism, Vanillin*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1704; 1766
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1048; 2899; 2901 (*Vanillin, derivs, occur, use*)
Hocking, M.B. *et al., J. Chem. Educ.*, 1997, **74**, 1055-1059 (*Vanillin, rev*)
Ger. Pat., 1998, 19 714 826; *CA*, **129**, 302444j (*Et vanillin isobutyrate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EQF000; FNM000; VFK000

3,4-Dihydroxy-1,2-benzenedicarboxylic acid, 9CI D-383

3,4-Dihydroxyphthalic acid, 8CI. Catechol-3,4-dicarboxylic acid. Norhemipinic acid



$C_8H_6O_6$ 198.132
Plates + $1H_2O$ (H_2O). Mp 210-212° (→ anhydride).

Di-Me ether: [518-90-1] *3,4-Dimethoxy-1,2-benzenedicarboxylic acid. 3,4-Dimethoxyphthalic acid. Hemipinic acid. Hemipic acid*
$C_{10}H_{10}O_6$ 226.185
Isol. from poppy straw (*Papaver somniferum*). Cryst. + $2H_2O$. Mp 124-126° Mp 165-166° Mp 181°.

Reisch, J. *et al., Annalen*, 1990, 1047 (*di-Me ether, synth, ir, pmr, cmr*)

4,5-Dihydroxy-1,2-benzenedicarboxylic acid, 9CI D-384

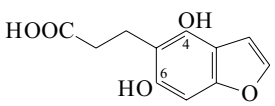
[63958-66-7]
4,5-Dihydroxyphthalic acid, 8CI. Catechol-4,5-dicarboxylic acid. Normetahemipinic acid

$C_8H_6O_6$ 198.132
Prisms (H_2O). Mp 175° (→ anhydride).

Di-Me ether: [577-68-4] *4,5-Dimethoxy-1,2-benzenedicarboxylic acid. 4,5-Dimethoxyphthalic acid. Veratrole-4,5-dicarboxylic acid. Metahemipic acid.* m-*Hemipinic acid*
$C_{10}H_{10}O_6$ 226.185
Degradn. prod. of many alkaloids. Isol. from poppy straw (*Papaver somniferum*). Needles (H_2O). Mp 174-175°.

Schmid, H. *et al., Helv. Chim. Acta*, 1945, **28**, 722-740 (*isol, di-Me ether*)

4,6-Dihydroxy-5-benzofuranpropanoic acid D-385



$C_{11}H_{10}O_5$ 222.197

4-Me ether, 6-O-β-D-glucopyranoside: [169312-28-1] ***Picraquassioside A***
$C_{18}H_{22}O_{10}$ 398.366
Constit. of *Ruta graveolens* (rue). Amorph. powder. $[\alpha]_D^{20}$ -32 (c, 1 in MeOH).

4-Me ether, 6-O-β-D-glucopyranoside, Me ester: ***Methylpicraquassioside A***
$C_{19}H_{24}O_{10}$ 412.393
Constit. of *Ruta graveolens* (rue). Glassy powder. Mp 67-69°. $[\alpha]_D^{25}$ -58.8 (c, 0.34 in MeOH). λ_{max} 214 (log ϵ 4.59); 251 (log ϵ 4.08); 278 (log ϵ 3.37) (MeOH).

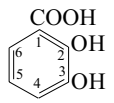
Yoshikawa, K. *et al., Phytochemistry*, 1995, **40**, 253-256 (*isol, uv, ir, pmr, cmr, ms*)

Chen, C.C. *et al., J. Nat. Prod.*, 2001, **64**, 990-992 (*Methylpicraquassiolide A*)

2,3-Dihydroxybenzoic acid, 9CI D-386

[303-38-8]

Pyrocatechuic acid, 8CI. Catechol-3-carboxylic acid. o-*Pyrocatechuic acid*



$C_7H_6O_4$ 154.122

Occurs in *Gentiana lutea* (yellow gentian). Cryst. + $1H_2O$ (H_2O). Mp 204° (anhyd.). pK_a 2.91. Log P 1.06 (calc). λ_{max} 241 ; 307 (H_2O) (Berdy). λ_{max} 244 ; 316 (HCl) (Berdy). λ_{max} 254 ; 326 (NaOH) (Berdy).

▶ DG8576490

[13189-89-4, 66168-85-2, 67984-81-0]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1096B; 1096C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 205B; 205C (*ir*)
Rodionov, V.M. *et al., CA*, 1941, **35**, 5101 (*synth*)
Cason, J. *et al., J.A.C.S.*, 1950, **72**, 621 (*synth*)
King, F.E. *et al., J.C.S.*, 1955, 4206 (*synth*)
Polukordas, M.R. *et al., Farmakol. Toksikol. (Moscow)*, 1966, **29**, 594 (*pharmacol*)
Coward, R.F. *et al., J. Chromatogr.*, 1969, **45**, 311 (*glc*)
Scott, K.N. *et al., J. Magn. Reson.*, 1970, **2**, 361 (*pmr*)
Scott, K.N. *et al., J.A.C.S.*, 1972, **92**, 8564 (*cmr*)
Kamath, B.V. *et al., J. Appl. Chem. Biotechnol.*, 1975, **25**, 743 (*uv*)
De Koster, C.G. *et al., Fresenius' Z. Anal. Chem.*, 1986, **323**, 321 (*ms*)
Al-Tel, T.H. *et al., Phytochemistry*, 1991, **30**, 3081 (*isol, deriv*)
Hayashi, K. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 319 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HJB500

2,4-Dihydroxybenzoic acid, 9CI D-387

[89-86-1]

β-Resorcylic acid, 8CI. Resorcinol-4-carboxylic acid. FEMA 3798

$C_7H_6O_4$ 154.122

Found in avocado, beer, wine and coffee. Food flavour ingredient and flavour modifier. Solid ($CHCl_3$). Mp 152° subl Mp 175° Mp 218-219° (213° rapid heat). pK_{a1} 3.11; pK_{a2} 8.55; pK_{a3} 14 (25°).

▶ Exp. teratogenic effects. VH3708050

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 215C; 216D; 299A; 300A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1115B; 1117A; 1258A; 1259C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1369C (*ir*)
Org. Synth., 1930, **10**, 94 (*synth*)
Robinson, R. *et al., J.C.S.*, 1934, 1491 (*synth*)
King, L.C. *et al., J.A.C.S.*, 1945, **67**, 2089 (*synth*)
Idris Jones, J. *et al., Chem. Ind. (London)*, 1958, 228 (*synth*)
Coward, R.F. *et al., J. Chromatogr.*, 1969, **45**, 311 (*glc*)
Scott, K.N. *et al., J. Magn. Reson.*, 1970, **2**, 361 (*pmr*)
Scott, K.N. *et al., J.A.C.S.*, 1972, **92**, 8564 (*cmr*)
Kamath, B.V. *et al., J. Appl. Chem. Biotechnol.*, 1975, **25**, 743 (*uv*)
Scriven, F.M. *et al., J. Liq. Chromatogr.*, 1979, **2**, 125 (*hplc*)
Venkataramaiah, V. *et al., Indian J. Exp. Biol.*, 1980, **18**, 887; *CA*, **93**, 164513r (*occur*)
de Koster, C.G. *et al., Fresenius' Z. Anal. Chem.*, 1986, **323**, 321 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 428
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HOE600

2,5-Dihydroxybenzoic acid, 9CI D-388

[490-79-9]

Gentisic acid, 8CI, INN. *Hydroquinonecarboxylic acid. 5-Hydroxysalicylic acid. Gentisinic acid. Hydroxyquinonecarboxylic acid*

$C_7H_6O_4$ 154.122

Needles or prisms (H_2O). Sol. H_2O, Et_2O, EtOH. Mp 204.5-205°. pK_a 2.95 (25°). Log P 1.62 (calc).

▶ LD_{50} (rat, orl) 800 mg/kg. Exp. reprod. and teratogenic effects. LY3850000

5-Me ether: [2612-02-4] *2-Hydroxy-5-methoxybenzoic acid. 5-Methoxysalicylic acid*
Isol. from *Primula veris* (cowslip). Mp 145-146°.

[1084-96-4, 6245-34-7, 21715-15-1, 52405-73-9]

Ibrahim, R.K. *et al., Arch. Biochem. Biophys.*, 1960, **87**, 125 (*isol, 5-Me ether*)

2,6-Dihydroxybenzoic acid, 9CI D-389

[303-07-1]

γ-Resorcylic acid, 8CI. Resorcinol-2-carboxylic acid

$C_7H_6O_4$ 154.122

Cryst. + $1H_2O$ (H_2O). Mp 150° (variable acc. to rate of heating) dec. pK_a 1.08. V. strong acid. In soln. exists in intramol. H-bonded form with CO of COOH H bonded to one OH and O of COOH H bonded to the other.

▶ DG8578000

Benzyl ester, 2-O-β-D-glucopyranoside:
$C_{20}H_{22}O_9$ 406.388
Constit. of *Sambucus nigra* (elderberry). Oil.

[3144-59-0, 3147-50-0, 57764-46-2]

D'Abrosca, B. *et al., Phytochemistry*, 2001, **58**, 1073-1081 (*benzyl ester glucoside*)

3,4-Dihydroxybenzoic acid D-390

[99-50-3]

Protocatechuic acid, 8CI. Carbohydroquinonic acid. Catechol-4-carboxylic acid. Hypogallic acid

$C_7H_6O_4$ 154.122

Present in red wine and plant sources. Needles + $1H_2O$ (H_2O). Mp 195-196° (anhyd.). pK_{a1} 4.49; pK_{a2} 8.64; pK_{a3} 1 (25°).

▶ UL0560000

β-D-Xylopyranosyl ester: [143986-30-5] *3,4-Dihydroxybenzoyl β-D-xylopyranoside.* ***Uralenneoside***
$C_{12}H_{14}O_8$ 286.238
Constit. of the leaves of *Glycyrrhiza uralensis* (Chinese licorice). Cryst. Mp 185-187°.

3-Me ether: [121-34-6] *4-Hydroxy-3-methoxybenzoic acid. Vanillic acid*
$C_8H_8O_4$ 168.149
Needles (H_2O). Mp 210°. pK_{a2} 9.39 (25°). Sublimes.

▶ YW5300000

[58534-64-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 212B; 215D; 216A; 216B; 299B; 300B; 457A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1110C; 1115C; 1116A; 1116B; 1258C; 1260A; 1533B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1368D; 1418C (*ir*)
Ewins, A.J. *et al., J.C.S.*, 1909, 1482-1488 (*synth*)
Pratt, D.S. *et al., J.A.C.S.*, 1918, **40**, 198 (*synth*)
Pearl, J.A. *et al., J.A.C.S.*, 1946, **68**, 2180 (*synth*)
Schwarz, R. *et al., Monatsh. Chem.*, 1952, **83**, 883 (*deriv*)
Coward, R.F. *et al., J. Chromatogr.*, 1969, **45**, 311 (*glc*)
Scott, K.N. *et al., J. Magn. Reson.*, 1970, **2**, 361 (*pmr*)
Scott, K.N. *et al., J.A.C.S.*, 1972, **92**, 8564 (*cmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 895; 896
Kamath, B.V. *et al., J. Appl. Chem. Biotechnol.*, 1975, **25**, 743 (*uv*)
Jia, S.S. *et al., Yaoxue Xuebao*, 1992, **27**, 441-444 (*Uralenneoside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HJC000; VFF000

3,5-Dihydroxybenzoic acid, 9CI D-391

[99-10-5]

α-Resorcylic acid, 8CI. Resorcinol-5-carboxylic acid

$C_7H_6O_4$ 154.122

Constit. of *Arachis hypogaea* (peanuts) and *Cicer arietinum* (chickpea). Cryst. + $1^1/_2$ H_2O (H_2O). Sol. H_2O. Mp 232-233° (anhyd.). pK_a 4.04.

▶ VH3708000

Me ester: [2150-44-9]
$C_8H_8O_4$ 168.149
Leaflets. Mp 168-170° (163-165°). pK_{a2} 10.66 (20°).

Et ester: [4142-98-7]
$C_9H_{10}O_4$ 182.176
Cryst. (EtOH aq.). Mp 128-129°.

▶ DG8576840

Ph ester: [133551-50-5]
$C_{13}H_{10}O_4$ 230.22
Cryst. (MeOH aq.). Mp 174-176°.

Amide: [3147-62-4]
$C_7H_7NO_3$ 153.137
Tan solid (EtOH). Mp 285-287° dec.

Di-Ac: [35354-29-1]
$C_{11}H_{10}O_6$ 238.196
Mp 161-162°.

Mono-Me ether: [19520-75-3] *3-Hydroxy-5-methoxybenzoic acid*
$C_8H_8O_4$ 168.149
Cryst. ($CHCl_3$/petrol). Mp 202°.

Mono-Me ether, Me ester: [19520-74-2]
$C_9H_{10}O_4$ 182.176
Needles ($CHCl_3$/MeOH). Mp 99°.

Di-Me ether: See 3,5-Dimethoxybenzoic acid in *The Combined Chemical Dictionary.*

Dibenzyl ether: [28917-43-3] *3,5-Dibenzyloxybenzoic acid*
$C_{21}H_{18}O_4$ 334.371
Cryst. (EtOH or EtOAc). Mp 214-216° (210-211°).

Dibenzyl ether, Me ester: [58605-10-0]
$C_{22}H_{20}O_4$ 348.398
Mp 65-66°.

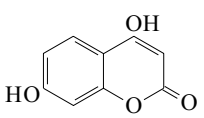
Mono-Me ether, nitrile: [124993-53-9] *3-Hydroxy-5-methoxybenzonitrile, 9CI. 3-Cyano-5-methoxyphenol*
$C_8H_7NO_2$ 149.149
Solid.

[41696-97-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 227A; 300C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1137C (*nmr*)
Suter, C.M. *et al., J.A.C.S.*, 1939, **61**, 232 (*synth*)
Birkenshaw, J.H. *et al., J.C.S.*, 1942, 368 (*synth*)
Curtis, R.F. *et al., J.C.S.(C)*, 1968, 1807 (*deriv*)
Coward, R.F. *et al., J. Chromatogr.*, 1969, **45**, 311 (*glc*)
Scott, K.N. *et al., J. Magn. Reson.*, 1970, **2**, 361 (*pmr*)
Desai, M.N. *et al., Mikrochim. Acta*, 1970, 190 (*detn, Fe*)
Scott, K.N. *et al., J.A.C.S.*, 1972, **92**, 8564 (*cmr*)
Belg. Pat., 1975, 833 181; *CA*, **86**, 72210 (*manuf*)
Kamath, B.V. *et al., J. Appl. Chem. Biotechnol.*, 1975, **25**, 743 (*uv*)
Reddy, S.B. *et al., Curr. Sci.*, 1977, **46**, 236 (*occur*)
Kumar, N.R. *et al., Indian J. Exp. Biol.*, 1979, **17**, 114; *CA*, **90**, 118113a
Settine, R.L. *et al., Org. Prep. Proced. Int.*, 1979, **11**, 87 (*amide*)
de Koster, C.G. *et al., Fresenius' Z. Anal. Chem.*, 1986, **323**, 321 (*ms*)
Hawker, C.J. *et al., J.A.C.S.*, 1991, **113**, 4583 (*Ph ester, dibenzyl ether, synth, ir, pmr, cmr, ms*)
Hawker, C.J. *et al., J.C.S. Perkin 1*, 1992, 2459 (*dendritic polyesters*)
Chakraborty, T.K. *et al., J.O.C.*, 1992, **57**, 5462 (*Me esters*)
Walpole, C.S.J. *et al., J. Med. Chem.*, 1993, **36**, 2362 (*Mono-Me ether, nitrile*)
Zhu, J. *et al., J.O.C.*, 1995, **60**, 6389 (*derivs, synth, pmr, cmr*)
McElhanon, J.R. *et al., J.O.C.*, 1997, **62**, 908-915 (*Dibenzyl ether Me ester*)

4,7-Dihydroxy-2*H*-1-benzopyran-2-one, 9CI D-392

[1983-81-9]
4,7-Dihydroxycoumarin



$C_9H_6O_4$ 178.144

Constit. of the seeds of *Corchorus olitorius* (Jew's mallow). Needles (H_2O). Mp 265° dec Mp 282°.

7-Ac: [19225-18-4]
$C_{11}H_8O_5$ 220.181
Cryst. (H_2O). Mp 223°.

Di-Ac: [42520-59-2]
$C_{13}H_{10}O_6$ 262.218
Prisms. Mp 145.5°.

Dibenzoyl:
$C_{23}H_{14}O_6$ 386.36
Mp 136-137°.

Di-Me ether: [17575-27-8] *4,7-Dimethoxy-2*H*-1-benzopyran-2-one. 4,7-Dimethoxycoumarin*
$C_{11}H_{10}O_4$ 206.198
Needles (H_2O). Mp 162° (155-156°).

Sonn, A. *et al., Ber.*, 1917, **50**, 1292-1305 (*synth*)
Heilbron, I.M. *et al., J.C.S.*, 1927, 1705-1708 (*di-Me ether*)
Lefeuvre, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1962, **255**, 2611-2613 (*synth*)
Pelter, A. *et al., J. Het. Chem.*, 1965, **2**, 262-271 (*ms*)
Mehta, M.J. *et al., J. Appl. Chem.*, 1969, **19**, 29-30 (*uv*)
Buckle, D.R. *et al., J. Med. Chem.*, 1975, **18**, 391-394 (*synth*)
Mizuno, T. *et al., Synthesis*, 1988, 257-259 (*synth, pmr*)
Pandey, G. *et al., Tetrahedron*, 1989, **45**, 6867-6874 (*synth, ir, pmr*)
Traven, V.F. *et al., Can. J. Chem.*, 1997, **75**, 365-376; 377-383 (*uv, pmr, cmr*)
Mukherjee, K.K. *et al., Nat. Prod. Sci.*, 1998, **4**, 51-52 (*isol*)

5,7-Dihydroxy-2*H*-1-benzopyran-2-one, 9CI D-393

[2732-18-5]
5,7-Dihydroxycoumarin

$C_9H_6O_4$ 178.144
Prisms (AcOH aq.), yellow needles (H_2O). Mp 285-286°.

Di-Me ether: [487-06-9] *5,7-Dimethoxy-2*H*-1-benzopyran-2-one. 5,7-Dimethoxycoumarin.* ***Citropten****. Limettin. Citraptene. Limetin*
$C_{11}H_{10}O_4$ 206.198
Found in lime and bergamot oils. Prisms (MeOH). Mp 147°. Fluorescent in EtOH λ_{max} 222 (ϵ 10715); 247 (ϵ 6918); 250 (ϵ 6918); 324 (ϵ 15135) (MeOH) (Berdy).

▶ GN6530000

5-O-(3-Methyl-2-butenyl), 7-Me ether: [35590-41-1] *7-Methoxy-5-prenyloxycoumarin*
$C_{15}H_{16}O_4$ 260.289
Isol. from lemon oil (*Citrus limon*). Mp 90-92°.

5-O-(3,7-Dimethyl-2,6-octadienyl), 7-O-Me: [7380-39-4] ***5-Geranyloxy-7-methoxycoumarin***
$C_{20}H_{24}O_4$ 328.407
Isol. from lime oil (*Citrus aurantifolia*). Mp 86-87°.

5-O-(6-Hydroxy-3,7-dimethyl-2,7-octadienyl), 7-O-Me: [40520-59-0]
$C_{20}H_{24}O_5$ 344.407
Isol. from lime oil (*Citrus aurantifolia*).

Heyes, R.G. *et al., J.C.S.*, 1936, 1831 (*Citropten, synth*)

5,7-Dihydroxy-4*H*-1-benzopyran-4-one, 9CI D-394

[31721-94-5]
5,7-Dihydroxychromone

$C_9H_6O_4$ 178.144
Isol. from peanut shells. Pale yellow plates (EtOH). Mp 272-273°.

7-O-β-Glucopyranoside: [60444-96-4]
$C_{15}H_{16}O_9$ 340.286

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [84575-25-7]
$C_{21}H_{26}O_{13}$ 486.429
Needles (MeOH). Mp 227-228° (152-155°). $[\alpha]_D$ -57.2 (c, 1 in MeOH).

7-Me ether: [59887-92-2] *5-Hydroxy-7-methoxy-4*H*-1-benzopyran-4-one. 5-Hydroxy-7-methoxychromone*
$C_{10}H_8O_4$ 192.171
Mp 98-101°.

Di-Me ether: [59887-91-1] *5,7-Dimethoxy-4*H*-1-benzopyran-4-one. 5,7-Dimethoxychromone*
$C_{11}H_{10}O_4$ 206.198
Mp 133-134°.

Pendse, R. *et al., Phytochemistry*, 1973, **12**, 2033 (*isol*)
Stocker, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 946 (*synth, uv, pmr*)
Romussi, G. *et al., J. Het. Chem.*, 1976, **13**, 211 (*ir, pmr, uv*)
Bhardwaj, D.K. *et al., Phytochemistry*, 1982, **21**, 2154 (*7-neohesperidoside*)
Jain, A.C. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 1036 (*synth*)
Spencer, G.F. *et al., Org. Prep. Proced. Int.*, 1991, **23**, 390 (*synth*)
Kosuge, K. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1669 (*7-neohesperidoside*)
Simon, A. *et al., Phytochemistry*, 1994, **36**, 1043 (*7-glucoside*)
Vasconcelos, J.M.J. *et al., Phytochemistry*, 1998, **49**, 1421-1424 (*isol, pmr, cmr*)

6,7-Dihydroxy-2*H*-1-benzopyran-2-one, 9CI D-395

[305-01-1]
6,7-Dihydroxycoumarin, 8CI. ***Aesculetin****. Esculetin. Cichorigenin. Esculetol*

$C_9H_6O_4$ 178.144
Metab. of infected sweet potato. Cryst. (EtOH). Mp 270°. Log P 1.21 (calc). λ_{max} 230 (ϵ 14125); 260 (ϵ 5320); 302 (ϵ 5890); 353 (ϵ 12000) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 1500 mg/kg. GN6382500

6-O-β-D-Glucopyranoside: [531-75-9] ***Aesculin****. Esculin. Crataegin. Bicolorin. Polychrome. Vitamin C_2. Esculoside*
$C_{15}H_{16}O_9$ 340.286
Vitamin C_2 is generally considered a bioflavonoid, related to vitamin P. Mp 205°. $[\alpha]_D$ -77.5 (c, 3 in aq. dioxan). Log P -2.07 (calc).

7-O-β-D-Glucopyranoside: [531-58-8] ***Cichoriin****. 6-Hydroxyskimmin. Cichoriioside*
$C_{15}H_{16}O_9$ 340.286
Isol. from chicory (*Cichorium intybus*). Mp 213-214°. $[\alpha]_D^{20}$ -104 (dioxan).

Di-Me ether: [120-08-1] *6,7-Dimethoxy-2*H*-1-benzopyran-2-one. 6,7-Dimethoxycoumarin.* ***Scoparone****. Escoparone. Scoparin*†

$C_{11}H_{10}O_4$ 206.198
Found in several citrus oils. Needles (H_2O). Mp 144°.
▶ LD_{50} (rat, orl) 292 mg/kg. Exp. reprod. effects. GN6550000

Head, F.S.H. *et al., J.C.S.*, 1939, 1266 (*synth*)
Bohlmann, F. *et al., Chem. Ber.*, 1957, **90**, 1512 (*synth*)
Bursey, M.M. *et al., Chem. Comm.*, 1967, 712 (*ms*)
Khan, M.A.S. *et al., Anal. Chim. Acta*, 1968, **43**, 153 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1325-1327 (*occur*)
Sato, M. *et al., Phytochemistry*, 1972, **11**, 657 (*biosynth*)
Günther, H. *et al., Org. Magn. Reson.*, 1975, **7**, 339 (*cmr, deriv*)
Cussans, N.J. *et al., Tetrahedron*, 1975, **31**, 2719 (*cmr*)
Ashwood-Smith, M.J. *et al., Experientia*, 1982, **39**, 262 (*physiol, tox, deriv*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, (*occur, rev*)
Kelkar, S.L. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 458 (*synth*)
Joseph-Nathan, P. *et al., J. Het. Chem.*, 1984, **21**, 1141 (*pmr, deriv*)
Abu-Eittah, R.H. *et al., Can. J. Chem.*, 1985, **63**, 1173 (*uv*)
Jackson, Y.A. *et al., Heterocycles*, 1995, **41**, 1979 (*synth*)

7,8-Dihydroxy-2*H*-1-benzopyran-2-one D-396

[486-35-1]
7,8-Dihydroxycoumarin, 8CI. ***Daphnetin****. Daphnetol*

$C_9H_6O_4$ 178.144
Pale yellow needles (MeOH). Sol. H_2O, bases. Mp 255-256°. Log P 1.21 (calc).
▶ GN6382600

7-Me ether: [19492-03-6] *8-Hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, 9CI. 8-Hydroxy-7-methoxycoumarin, 8CI*
$C_{10}H_8O_4$ 192.171
From *Artemisia dracunculoides* (Russian tarragon). Prisms (C_6H_6/MeOH). Mp 173-174°.

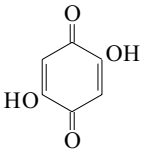
Methylene ether: [4361-93-7] *8*H*-1,3-Dioxolo[4,5-*h*][1]benzopyran-8-one, 9CI. 7,8-Methylenedioxycoumarin*
$C_{10}H_6O_4$ 190.155
Constit. of *Apium graveolens*. Cryst. Mp 187-189°.

[62190-05-0, 99787-85-6, 148812-48-0, 168110-95-0]

Günther, H. *et al., Org. Magn. Reson.*, 1975, **7**, 339 (*cmr, deriv*)
Shimomura, H. *et al., Chem. Pharm. Bull.*, 1980, 347 (*deriv*)
Barua, N.C. *et al., Phytochemistry*, 1980, **19**, 2217 (*deriv*)
Gray, A.I. *et al., Phytochemistry*, 1981, **26**, 1171; 1987, 257 (*derivs*)
Joseph-Nathan, P. *et al., J. Het. Chem.*, 1984, **21**, 1141 (*pmr, deriv*)

2,5-Dihydroxy-1,4-benzoquinone D-397

[615-94-1]
2,5-Dihydroxy-2,5-cyclohexadiene-1,4-dione, 9CI



$C_6H_4O_4$ 140.095
Tautomeric with 4,5-Dihydroxy-1,2-benzoquinone.Golden-orange cryst. (EtOH), dark-yellow needles (EtOAc). Sol. EtOH, Me_2CO; sl. sol. H_2O. Mp 210° dec. (215-220° subl.). pK_{a1} 2.73; pK_{a2} 5.18 (25°).

Di-Ac: [16523-32-3]
$C_{10}H_8O_6$ 224.17
Yellow plates or prisms (C_6H_6). Mp 150-152°.

Dibenzoyl: [51767-59-0]
$C_{20}H_{12}O_6$ 348.311
Gold plates (AcOH). Mp 174°.

Di-Me ether: [3117-03-1] *2,5-Dimethoxy-1,4-benzoquinone.* ***Thermophillin****. Thermophyllin*
$C_8H_8O_4$ 168.149
Isol. from *Acorus calamus* (sweet flag). Yellow prisms (MeOH). Mp 250° dec. (300° dec.).

Di-Et ether: [20765-04-2] *2,5-Diethoxy-1,4-benzoquinone*
$C_{10}H_{12}O_4$ 196.202
Cryst. (EtOH). Mp 184°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 716A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 451A (*ir*)
Knoevenagel, E. *et al., Ber.*, 1901, **34**, 3993 (*synth*)
Jones, R.G. *et al., J.A.C.S.*, 1945, **67**, 1034 (*synth*)
Huisman, H.O. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1950, **69**, 1133 (*isol*)
Ungnade, H.E. *et al., J.O.C.*, 1951, **16**, 64 (*deriv*)
Davidge, H. *et al., J.C.S.*, 1958, 4569 (*synth*)
Singhal, S.P. *et al., Anal. Chim. Acta*, 1966, **35**, 195 (*use*)
Bowie, J.H. *et al., J.C.S.(B)*, 1966, 335 (*ms*)
Wanzlick, H.W. *et al., Chem. Ber.*, 1968, **101**, 3744 (*synth*)
Stille, J.K. *et al., Macromolecules*, 1968, **1**, 36 (*polymers*)
Donnelly, B.J. *et al., Tetrahedron*, 1969, **25**, 4409 (*isol*)
Le Blanc, G.D. *et al., Can. J. Microbiol.*, 1972, **18**, 261 (*isol*)
Nakajima, S. *et al., Agric. Biol. Chem.*, 1976, **40**, 811 (*isol*)
Höfle, G. *et al., Tetrahedron*, 1976, **32**, 1431 (*cmr*)
Semmingsen, D. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 11 (*cryst struct*)
Patra, A. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 412 (*isol*)
Tindale, C.R. *et al., Aust. J. Chem.*, 1984, **37**, 611 (*synth, ir*)
Matsumoto, M. *et al., Synth. Commun.*, 1985, **15**, 515 (*synth*)
Kitanaka, S. *et al., Yakugaku Zasshi*, 1986, **106**, 302 (*isol*)
Orita, H. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 1652 (*synth*)

2,6-Dihydroxy-1,4-benzoquinone D-398

[35069-70-6]
2,6-Dihydroxy-2,5-cyclohexadiene-1,4-dione, 9CI

$C_6H_4O_4$ 140.095
Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 286 (ϵ 15100); 287 (ϵ 22200); 376 (ϵ 1020); 385 (ϵ 600) (MeOH) (Berdy). λ_{max} 283 (ϵ 14500); 287 (ϵ 19050); 375 (ϵ 560); 377 (ϵ 602) ($CHCl_3$) (Berdy). λ_{max} 287 (ϵ 19200); 377 (ϵ 630) (EtOH) (Berdy).

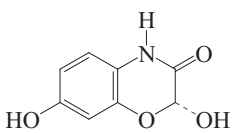
Di-Me ether: [530-55-2] *2,6-Dimethoxy-1,4-benzoquinone*
$C_8H_8O_4$ 168.149
Constit. of bark of *Phyllostachys heterocycla* var. *pubescens* (moso bamboo). Yellow cryst. (AcOH). Mp 252°. λ_{max} 288 (ϵ 12600) (MeOH) (Derep).
▶ Causes dermatitis. Mutagenic props.. DK4750000

Di-Me ether, 4-oxime: [22867-29-4]
$C_8H_9NO_4$ 183.163
Yellow plates (H_2O). Mp 218.8° dec.

Polonsky, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 1157; 1962, 1715 (*isol, deriv*)
Horner, L. *et al., Chem. Ber.*, 1961, **94**, 1291 (*synth*)
Bolker, H.I. *et al., Can. J. Chem.*, 1969, **47**, 2109 (*deriv*)
Schmalle, H. *et al., Naturwissenschaften*, 1977, **64**, 534 (*cryst struct, deriv*)
Org. Synth., 1977, **57**, 78 (*synth*)
Nishina, A. *et al., J. Agric. Food Chem.*, 1991, **39**, 266 (*isol, deriv*)
Frick, E. *et al., Nat. Prod. Lett.*, 1996, **9**, 153-159 (*synth*)
Omura, K. *et al., Synthesis*, 1998, 1145-1148 (*synth*)
Villemin, D. *et al., Synth. Commun.*, 2002, **32**, 1501-1515 (*di-Me ether, synth*)

2,7-Dihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, 9CI D-399

[69804-59-7]



$C_8H_7NO_4$ 181.148

(R)-form
Identified in sweet corn extracts. Sol. MeOH, H_2O, $CHCl_3$. λ_{max} 254 ; 281 (MeOH) (Berdy). λ_{max} 253 ; 279 (H_2O) (Berdy).

2-O-β-D-Glucopyranoside: [28512-70-1] *DHBOA-Glc*
$C_{14}H_{17}NO_9$ 343.29
Constit. of the roots of *Coix lachryma-jobi* (Job's tears). Cryst. (MeOH). Mp 267-269°. $[\alpha]_D^{24}$ +22.3 (c, 0.6 in Py). λ_{max} 263 (log ϵ 4); 286 (sh) (log ϵ 3.84) (EtOH).

7-Me ether: [17359-53-4] *2-Hydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one*
$C_9H_9NO_4$ 195.174
Constit. of *Coix lachryma-jobi* (Job's tears), wheat and sweet corn (*Zea mays*). Cryst. Mp 198-199.5°. λ_{max} 258 (log ϵ 4.06); 286 (sh) (log ϵ 3.78) (EtOH).

7-Me ether, 2-O-β-D-glucopyranoside: [17622-26-3] *HMBOA-Glc*

$C_{15}H_{19}NO_9$ 357.316
Constit. of the roots of *Coix lachryma-jobi* (Job's tears). Cryst. (MeOH). Mp 250-251° (230-235°). $[\alpha]_D^{24}$ +31.4 (c, 0.8 in Py). λ_{max} 205 (ϵ 12340); 259 (ϵ 9141); 282 (sh) (ϵ 7100) (MeOH).

Di-Me ether: [131761-45-0] *2,7-Dimethoxy-2*H*-1,4-benzoxazin-3(4*H*)-one*
$C_{10}H_{11}NO_4$ 209.201
Cryst. Mp 149-150°.

N-*Hydroxy,* O^7*-Me:* [15893-52-4]

[147802-15-1, 147802-16-2, 157194-49-5] *2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one. DIMBOA*
$C_9H_9NO_5$ 211.174
Isol. from wheat, in which it is present mainly as glucoside. Appears to be a natural aphicide, insecticide and fungicide. Involved in the *in vivo* detoxification of herbicides , e.g. Simazine. Pink needles. Mp 168-169° (138°).

N-*Hydroxy,* O^7*-Me, 2-O-β-D-glucopyranoside:* [113565-32-5]

[18607-79-9, 157241-65-1] *DIMBOA-Glc*
$C_{15}H_{19}NO_{10}$ 373.316
Isol. from sweet corn (*Zea mays*). Needles (EtOH). Mp 262-263° dec.

N-*Methoxy, 7-Me ether:* [149182-67-2] *2-Hydroxy-4,7-dimethoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, 9CI. HDMBOA*
$C_{10}H_{11}NO_5$ 225.201
Isol. from sweet corn (*Zea mays*).

N-*Methoxy, 7-Me ether. 2-O-β-D-glucopyranoside:* [113565-33-6]

[29845-81-6] *HDMBOA-Glc*
$C_{16}H_{21}NO_{10}$ 387.343
Constit. of the roots of *Coix lachryma-joba* (Job's tears) and from wheat and sweet corn (*Zea mays*). Pale yellow cryst. Mp 143-145°. $[\alpha]_D^{21}$ +22 (c, 0.25 in H_2O). λ_{max} 262 (log ϵ 3.97); 285 (sh) (log ϵ 3.84) (EtOH).

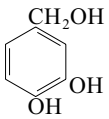
8-Methoxy, 7-Me ether, 2-O-β-D-glucopyranoside: [40246-09-1]
$C_{16}H_{21}NO_{10}$ 387.343
Isol. from sweet corn (*Zea mays*).

Wahlroos, O. *et al., Acta Chem. Scand.*, 1959, **13**, 1906 (*isol, struct*)
Reimann, J.E. *et al., Biochemistry*, 1964, **3**, 847 (*biosynth*)
Hofman, J. *et al., Tet. Lett.*, 1969, 5001 (*isol, uv, glucoside*)
Woodward, M.D. *et al., Plant Physiol.*, 1979, **63**, 9; *CA*, **90**, 147969q (*isol*)
Argandoă, V.H. *et al., Phytochemistry*, 1980, **19**, 1665; 1981, **20**, 673 (*isol*)
Nagao, T. *et al., Phytochemistry*, 1985, **24**, 2959-2962 (*isol, uv, pmr, abs config*)
Atkinson, J. *et al., J.O.C.*, 1991, **56**, 1788 (*deriv, synth, pmr, ms, ir*)
Kluge, M. *et al., Tetrahedron*, 1996, **52**, 10389-10398 (*synth*)
Kluge, M. *et al., Carbohydr. Res.*, 1997, **298**, 147 (*synth*)
Glawischnig, E. *et al., Phytochemistry*, 1997, **45**, 715 (*biosynth*)
Baumeler, A. *et al., Phytochemistry*, 2000, **53**, 213-222

3,4-Dihydroxybenzyl alcohol, 8CI D-400

[3897-89-0]

3,4-Dihydroxybenzenemethanol, 9CI. α,3,4-Trihydroxytoluene. Protocatechuyl alcohol. 3,4-Dihydroxyphenylcarbinol. 4-(Hydroxymethyl)-1,2-benzenediol



$C_7H_8O_3$ 140.138
Highly air-sensitive prisms (H_2O). Mp 137-138°.

3-Me ether: [498-00-0] *4-Hydroxy-3-methoxybenzenemethanol, 9CI. α,4-Dihydroxy-3-methoxytoluene. Vanillyl alcohol. FEMA 3737*
$C_8H_{10}O_3$ 154.165
Constit. of *Capsicum* spp.; flavouring ingredient. Cryst. (H_2O) with mild, sweet balsamic vanilla odour. Mp 114-115°.

3-Me ether, 4-O-β-D-glucopyranoside: ***Vanilloloside****. Glucovanillyl alcohol*
$C_{14}H_{20}O_8$ 316.307
Isol. from unripe vanilla pods. Needles (EtOH). Mp 120°.

3-Me ether, 1′-O-(7-methyloctanoyl):4-Hydroxy-3-methoxybenzyl 7-methyloctanoate. ***Nordihydrocapsiate***
$C_{17}H_{26}O_4$ 294.39
Constit. of fruits of *Capsicum annuum*. Oil. λ_{max} 231 (ϵ 6800); 281 (ϵ 2400) (MeOH).

3-Me ether, 1′-O-(8-methylnonanoyl):4-Hydroxy-3-methoxybenzyl 8-methylnonanoate. ***Dihydrocapsiate***
$C_{18}H_{28}O_4$ 308.417
Constit. of fruits of *Capsicum annuum*. Oil. λ_{max} 231 (ϵ 8700); 279 (ϵ 3700) (MeOH).

*3-Me ether, 1′-O-(8-methyl-6-nonenoyl)(*E*-):4-Hydroxy-3-methoxybenzyl 8-methyl-6-nonenoate.* ***Capsiate***
$C_{18}H_{26}O_4$ 306.401
Constit. of fruits of *Capsicum annuum*. Oil. λ_{max} 231 (ϵ 6200); 280 (ϵ 2400) (MeOH).

1′-Et, 3-Me diether: [13184-86-6] *4-(Ethoxymethyl)-2-methoxyphenol, 9CI. Vanillyl ethyl ether*
$C_{10}H_{14}O_3$ 182.219
Food additive listed in the EAFUS Food Additive Database (Jan 2001). Bp_4 124-125°. n_D^{20} 1.5297.

3-Et, 1′-Me diether: [5595-79-9] *2-Ethoxy-4-(methoxymethyl)phenol, 9CI. Methyl diantilis*
$C_{10}H_{14}O_3$ 182.219
Fragrance ingredient with a vanilla odour. Bp_3 112-115°.

1′-Butyl, 3-Me diether: [82654-98-6] *4-(Butoxymethyl)-2-methoxyphenol, 9CI. Vanillyl butyl ether*
$C_{12}H_{18}O_3$ 210.272
Cooling agent used in confectionery etc..

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1140C; 1142B (*ir*)
Aldrich Library of ^{13}C *and* ^1H *FT NMR Spectra*, 1992, **2**, 362A; 364C (*nmr*)
Rosenmund, K.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1926, **264**, 458
Eur. Pat., 1985, 137 419; *CA*, **103**, 11244d (*3-Et 1-Me ether*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 793 (*3-Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2903 (*3-Me ether*)
Kobata, K. *et al., J. Agric. Food Chem.*, 1998, **46**, 1695-1697 (*Capsiate, Dihydrocapsiate*)
Kobata, K. *et al., J. Nat. Prod.*, 1999, **62**, 335-336 (*Nordihydrocapsiate*)

3,5-Dihydroxybenzyl alcohol, 8CI D-401

[29654-55-5]
3,5-Dihydroxybenzenemethanol, 9CI. 5-(Hydroxymethyl)-1,3-benzenediol

$C_7H_8O_3$ 140.138
Cryst. (H_2O). Mp 189-190°.
▶ DO1400000

3-Me ether: [30891-29-3] *3-Hydroxy-5-methoxybenzyl alcohol.* ***Sylvopinol***
$C_8H_{10}O_3$ 154.165
Constit. of *Pinus sylvestris* (Scotch pine). Mp 85-86°.

3-Me ether, 1′-Ac:
$C_{10}H_{12}O_4$ 196.202
Mp 87-88°.

3,5-Di-Me ether: [705-76-0] *3,5-Dimethoxybenzyl alcohol, 8CI. 3,5-Dimethoxybenzenemethanol, 9CI. α-Hydroxy-3,5-dimethoxytoluene*
$C_9H_{12}O_3$ 168.192
Mp 48-48.5°.

3,5-Di-Me ether, 1′-Ac:
$C_{11}H_{14}O_4$ 210.229
Oil.

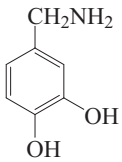
3,5-Dibenzyl ether: [24131-31-5]
$C_{21}H_{20}O_3$ 320.387
Solid. Mp 78-80°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1143B (*ir*)
Aldrich Library of ^{13}C *and* ^1H *FT NMR Spectra*, 1992, **2**, 366A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1068D (*ir*)
Lightowler, J.E. *et al., J. Pharm. Pharmacol.*, 1963, **15**, 633 (*synth*)
Ridley, D.D. *et al., Aust. J. Chem.*, 1968, **21**, 2979 (*di-Me*)
Bovodina, N.M. *et al., Khim. Prir. Soedin.*, 1970, **6**, 204; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 199 (*isol, deriv*)
Reimann, E. *et al., Annalen*, 1971, **750**, 109 (*synth*)
Kingston, J.F. *et al., Can. J. Chem.*, 1977, **55**, 785 (*di-Me*)
Elix, J.A. *et al., Aust. J. Chem.*, 1978, **31**, 1041 (*synth*)
Halton, D.D. *et al., J. Chem. Res., Synop.*, 1979, 4 (*synth*)
Pitt, C.G. *et al., J.O.C.*, 1979, **44**, 677 (*synth, pmr*)
Swindell, C.S. *et al., J.O.C.*, 1996, **61**, 1101 (*deriv, synth, pmr*)
McElhanon, J.R. *et al., J.O.C.*, 1997, **62**, 908-915 (*dibenzyl ether, synth, pmr*)
Combes, S. *et al., Synth. Commun.*, 1997, **27**, 3769-3778 (*di-Me ether*)

3,4-Dihydroxybenzylamine D-402

[37491-68-2]
4-(Aminomethyl)-1,2-benzenediol, 9CI.

(3,4-Dihydroxyphenyl)methylamine



$C_7H_9NO_2$ 139.154

▶ CZ8725000

3-Me ether, N-*(6-methyl-4*E*-heptenoyl):* [61229-09-2] N-*[(4-Hydroxy-3-methoxyphenyl)methyl]-6-methyl-4-heptenamide.* ***Dinorcapsaicin****. Nornorcapsaicin*
$C_{16}H_{23}NO_3$ 277.363
Constit. of red pepper (*Capsicum annuum*).

3-Me ether, N-*octanoyl:* [58493-47-3] N-*[(4-Hydroxy-3-methoxyphenyl)methyl]octanamide, 9CI*
$C_{16}H_{25}NO_3$ 279.378
Constit. of red pepper (*Capsicum annuum*).

3-Me ether, N-*(7-methyloctanoyl):* [28789-35-7] N-*[(4-Hydroxy-3-methoxyphenyl)methyl]-7-methyloctanamide, 9CI.* ***Nordihydrocapsaicin***
$C_{17}H_{27}NO_3$ 293.405
Isol. from the pungent principle of red pepper (*Capsicum annuum*). Cryst. (Et_2O/petrol). Mp 60-61°.

3-Me ether, N-*(7-methyl-5*E*-octenoyl):* [61229-08-1]

[62356-06-3, 112375-60-7] N-*[(4-Hydroxy-3-methoxyphenyl)methyl]-7-methyl-5-octenamide, 9CI.* ***Norcapsaicin****. 7-Methyl*-N-*vanillyl-5-octenamide*
$C_{17}H_{25}NO_3$ 291.389
Isol. from the pungent principle of red pepper (*Capsicum annuum*). Cryst. (Et_2O/hexane). Mp 42.5-44°.

3-Me ether, N-*(9-methyldecanoyl):* [20279-06-5] N-*[(4-Hydroxy-3-methoxyphenyl)methyl]-9-methyldecanamide, 9CI.* ***Homodihydrocapsaicin***
$C_{19}H_{31}NO_3$ 321.459
Isol. from the pungent principle of red pepper (*Capsicum annuum*). Cryst. (Et_2O/petrol). Mp 70-71°.

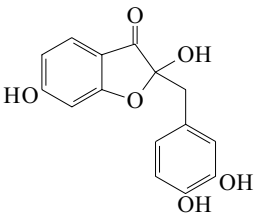
3-Me ether, N-*(9-methyl-7*E*-decenoyl):* [58493-48-4]

[62356-07-4, 112375-61-8] N-*[(4-Hydroxy-3-methoxyphenyl)methyl]-9-methyl-7-decenamide, 9CI.* ***Homocapsaicin****. 9-Methyl*-N-*vanillyl-7-decenamide*
$C_{19}H_{29}NO_3$ 319.443
Isol. from the pungent principle of red pepper (*Capsicum annuum*). Cryst, (Et_2O/hexane). Mp 64.5-65.5°.

Jentzsch, K. *et al., Monatsh. Chem.*, 1968, **99**, 661-663 (*Homodihydrocapsaicin*)
Kosuge, S. *et al., Agric. Biol. Chem.*, 1970, **34**, 248-256 (*Nordihydrocapsaicin, Homodihydrocapsaicin*)
Jurenitsch, J. *et al., Planta Med.*, 1979, **36**, 61-67 (*N-Octanoylcapsaicin, Homocapsaicin*)
Gannett, P.M. *et al., J.O.C.*, 1988, **53**, 1064-1071; 6162 (*Capsaicins, synth, ir, pmr, cmr, ms*)
Kaga, H. *et al., Synthesis*, 1989, 864-866 (*Nordihydrocapsaicin, Homodihydrocapsaicin, synth, ir*)
Kaga, H. *et al., Tetrahedron*, 1996, **52**, 8451-8470 (*Nordihydrocapsaicin, Homocapsaicin, synth, ir, pmr, cmr, ms*)

2-(3,4-Dihydroxybenzyl)-2,6-dihydroxy-3(2*H*)-benzofuranone D-403

[38681-22-0]
*2-[(3,4-Dihydroxyphenyl)methyl]-2,6-dihydroxy-3(2*H*)-benzofuranone, 9CI. 2-Benzyl-2,3′,4′,6-tetrahydroxycoumaran-3-one*



$C_{15}H_{12}O_6$ 288.256

(+)-*form* [89984-19-0]
Mp 105°.

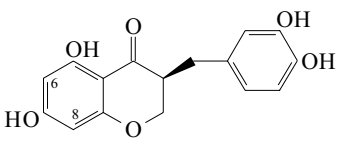
4′-Me ether:2,3′,6-Trihydroxy-4′-methoxybenzylcoumaranone
$C_{16}H_{14}O_6$ 302.283
Isol. from quebracho. Cryst. (H_2O). Mp 196°. $[\alpha]_D^{23}$ -1.2 (50% Me_2CO aq.).

(±)-*form* [54352-62-4]

King, H.G.C. *et al., J.C.S.*, 1961, 3231 (*isol, synth, deriv*)
Ferreira, D. *et al., J.C.S. Perkin 1*, 1974, 1492 (*isol*)
Burger, A.P.N. *et al., Phytochemistry*, 1983, **22**, 2813 (*isol*)
Bezuidenhout, S.C. *et al., Phytochemistry*, 1988, **27**, 2329 (*isol*)

3-(3,4-Dihydroxybenzyl)-5,7-dihydroxy-4-chromanone D-404

[107585-71-7]
*3-[(3,4-Dihydroxyphenyl)methyl]-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one*



$C_{16}H_{14}O_6$ 302.283
Oil.

5-Me ether: [107585-72-8] *3-(3,4-Dihydroxybenzyl)-7-hydroxy-5-methoxy-4-chromanone*
$C_{17}H_{16}O_6$ 316.31
Constit. of *Muscari* spp.. Vitreous solid. $[\alpha]_D$ -59 (c, 0.6 in MeOH).

4′-Me ether: [107585-75-1] *5,7-Dihydroxy-3-(3-hydroxy-4-methoxybenzyl)-4-chromanone. 3′-Hydroxy-3,9-dihydroeucomin*
$C_{17}H_{16}O_6$ 316.31
From *Muscari comosum* (tassel hyacinth). Cryst. ($CHCl_3$). Mp 140-142° (136-138°). $[\alpha]_D$ -51 (c, 0.7 in MeOH).

3′,4′-Di-Me ether:3-(3,4-Dimethoxybenzyl)-5,7-dihydroxy-4-chromanone
$C_{18}H_{18}O_6$ 330.337
Powder. Mp 183-185°. $[\alpha]_D^{25}$ -74.7 (c, 0.39 in MeOH). λ_{max} 214 (log ε 4.38); 288 (log ε 4.35) (MeOH).

3′,7-Di-Me ether:5-Hydroxy-3-(4-hydroxy-3-methoxybenzyl)-7-methoxy-4-chromanone
$C_{18}H_{18}O_6$ 330.337
Oil. λ_{max} 202 (log ε 3.93); 288 (log ε 3.56) (MeOH).

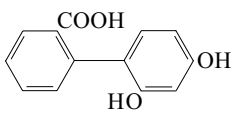
4′,5-Di-Me ether: [107585-73-9] *7-Hydroxy-3-(3-hydroxy-4-methoxybenzyl)-5-methoxy-4-chromanone*
$C_{18}H_{18}O_6$ 330.337
Constit. of *Muscari* spp.. Powder.

4′,7-Di-Me ether:5-Hydroxy-3-(3-hydroxy-4-methoxybenzyl)-7-methoxy-4-chromanone
$C_{18}H_{18}O_6$ 330.337
Pale yellow cryst. Mp 115-117°. $[\alpha]_D$ -36 (c, 0.55 in MeOH). λ_{max} 288 (log ε 4.34) (no solvent reported).

[96910-99-5, 120185-49-1]

Adinolfi, M. *et al., Phytochemistry*, 1985, **24**, 624; 1987, **26**, 285
Bangani, V. *et al., Phytochemistry*, 1999, **51**, 947-951 (*4′,7-di-Me ether*)
Silayo, A. *et al., Phytochemistry*, 1999, **52**, 947-955

2′,4′-Dihydroxy-2-biphenylcarboxylic acid D-405



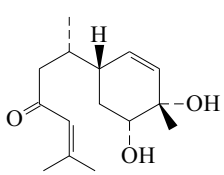
$C_{13}H_{10}O_4$ 230.22
Constit. of *Trifolium repens* (white clover) (isol. as the permethyl deriv.).

Di-Me ether, Me ester: [116107-12-1]
$C_{16}H_{16}O_4$ 272.3
Straw-coloured microcryst. (MeOH). Mp 144-146°.

Lactone: See 3-Hydroxy-6*H*-dibenzo[*b,d*]pyran-6-one in *The Combined Chemical Dictionary.*

Ghosal, S. *et al., J. Chem. Res., Synop.*, 1988, 196 (*isol*)
Ghosal, S. *et al., Pure Appl. Chem.*, 1990, **62**, 1285 (*isol*)

3,4-Dihydroxy-1,10-bisaboladien-9-one D-406



(3α,4α)-*form*

$C_{15}H_{24}O_3$ 252.353

(3α,4α)-*form* [127214-85-1]
Bisacurone B

Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ +9.5 (c, 0.89 in MeOH).

(3α,4β)-*form* [120681-81-4]
Bisacurone
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ -19.2 (c, 0.15 in MeOH). λ_{max} 239 (ε 8000) (MeOH) (Derep).

1α,2α-Epoxide: [127214-83-9] *1,2-Epoxy-3,4-dihydroxy-10-bisabolen-9-one.* ***Bisacurone epoxide***
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ -11.6 (c, 0.61 in MeOH).

3-Me ether: ***4-Hydroxy-3-methoxy-2,10-bisaboladien-9-one***
$C_{16}H_{26}O_3$ 266.38
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Viscous oil. $[\alpha]_D$ -7.4 (c, 0.11 in MeOH).

(3β,4α)-*form* [127214-86-2]
Bisacurone C
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ -24.8 (c, 0.37 in MeOH).

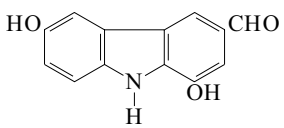
(3β,4β)-*form* [127214-84-0]
Bisacurone A
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ -35.9 (c, 0.9 in MeOH).

Uehara, S. *et al., Chem. Pharm. Bull.*, 1989, **37**, 237; 1990, **38**, 261 (*isol, cryst struct, abs config*)

Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201-2205 (*Me ether*)

1,6-Dihydroxy-9*H*-carbazole-3-carboxaldehyde D-407

3-Formyl-1,6-dihydroxycarbazole



$C_{13}H_9NO_3$ 227.219

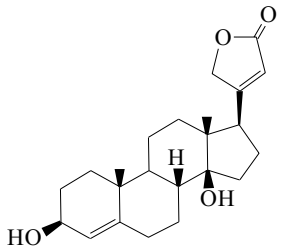
Di-Me ether: [132922-59-9] *1,6-Dimethoxy-9*H*-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-1,6-dimethoxy-9*H*-carbazole*
$C_{15}H_{13}NO_3$ 255.273
Alkaloid from the roots of *Clausena lansium* (wampee). Prisms (Me_2CO/hexane). Mp 231-233°.

Carboxylic acid, 6-Me ether, Me ester: [186002-62-0] *3-Carbomethoxy-1-hydroxy-6-methoxycarbazole.* ***Clausine G***
$C_{15}H_{13}NO_4$ 271.272
Granules (Me_2CO). Mp >280° λ_{max} 224 ; 272 ; 282 ; 316 (sh) ; 353 (sh) (MeOH).

Li, W.-S. *et al., Phytochemistry*, 1991, **30**, 343 (*isol, deriv*)

Wu, T.-S. *et al., Phytochemistry*, 1996, **43**, 1427-1429 (*Clausine G*)

3,14-Dihydroxycarda-4,20(22)-dienolide D-408



$C_{23}H_{32}O_4$ 372.503

(3α,14β)-*form*
3-Epicanarigenin
Mp 207-215°. $[\alpha]_D^{23}$ +105 (c, 1.38 in $CHCl_3$).

(3β,14β)-*form* [1778-88-7]
Canarigenin. *Canariengenin*
Cryst. (Me_2CO/hexane). Mp 260-262°. $[\alpha]_D^{23}$ +59 ($CHCl_3$). Stated not to be identical with Canarygenin, Mp. 207-208°, which was isol. from the same plant (A. González *et al*, 1956) and assigned the same gross struct..

3-O-α-L-Rhamnopyranoside: [35536-76-6] ***Corchoroside B***
$C_{29}H_{42}O_8$ 518.646
Constit. of *Corchorus olitorius* (Jew's mallow). Cryst. Mp 222-224°. $[\alpha]_D^{20}$ -68.

► FH4450000

3-(3-O-Methyl-L-rhamnoside): [20248-01-5] ***Acofrioside L***
$C_{30}H_{44}O_8$ 532.673
Cryst. (MeOH). Mp 248-253°. $[\alpha]_D^{17}$ -54.1 (MeOH).

*3-O-(2,6-Dideoxy-β-D-*ribo*-hexopyranoside):* ***Canaridigitoxoside***. *Canarigenin 3-digitoxoside*
$C_{29}H_{42}O_7$ 502.647
Prismatic plates (MeOH/Et_2O); needles + ½H_2O (Me_2CO/Et_2O). Mp 135-142° (plates) Mp 190-201° (hydrate). $[\alpha]_D$ -11.4 ($CHCl_3$).

*3-O-(2,6-Dideoxy-*xylo*-hexopyranoside):-* ***Canariboivinoside***
$C_{29}H_{42}O_7$ 502.647
Needles (MeOH aq.). Mp 192-196°. $[\alpha]_D^{21}$ -10 (c, 0.65 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→4)-6-deoxy-β-D-allopyranoside]: [229319-08-8]
$C_{35}H_{52}O_{13}$ 680.788
Constit. of *Corchorus olitorius* (Jew's mallow).

Tschesche, R. *et al., Annalen*, 1963, **663**, 157 (*Canariboivinoside*)

Studer, P. *et al., Helv. Chim. Acta*, 1963, **46**, 23 (*3-Epicanarigenin, Canaridigitoxoside*)

Hauschild-Rogat, P. *et al., Helv. Chim. Acta*, 1967, **50**, 2299 (*deriv*)

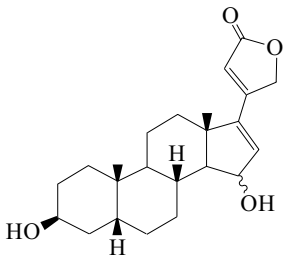
Albrecht, H.P. *et al., Annalen*, 1975, 2211 (*synth*)

Kamano, Y. *et al., J.C.S. Perkin 1*, 1975, 1972 (*synth*)

Rao, D.V. *et al., Phytochemistry*, 1975, **14**, 533 (*deriv*)

Goda, Y. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1998, **40**, 371-376; *CA*, **131**, 85493j (*Corchorus olitorius constit*)

3,15-Dihydroxycarda-16,20(22)-dienolide D-409



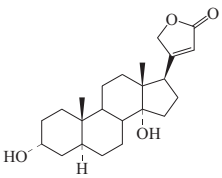
$C_{23}H_{32}O_4$ 372.503

(3β,5β,15ξ)-*form*
Neriantogenin
Hydrol. prod. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Cryst. (EtOH). Mp 255-259°.

3-O-L-Oleandroside: ***Neriantin***
$C_{30}H_{44}O_7$ 516.673
Cryst. (MeOH/$CHCl_3$). Mp 206-208°. $[\alpha]_D$ 0 ($CHCl_3$).

Tschesche, R. *et al., Chem. Ber.*, 1955, **88**, 511 (*isol*)

3,14-Dihydroxycard-20(22)-enolide D-410



(3α,5α,14α,17β)-*form*

$C_{23}H_{34}O_4$ 374.519

► FH4975000

(3β,5α,14β,17β)-*form* [466-09-1]
Uzarigenin. *Odorigenin B*
Cryst. (MeOH/CH_2Cl_2). Mp 246-249°. $[\alpha]_D$ +14 ($CHCl_3$). Log P 2.48 (uncertain value) (calc). λ_{max} 217 (ε 19500) (MeOH) (Berdy).

► YV1950000

3-O-[β-D-Xylopyranosyl-(1→2)-α-L-rhamnopyranoside]: [255861-29-1]
$C_{34}H_{52}O_{12}$ 652.778
Constit. of *Tamarindus indica* (tamarind).

(3β,5β,14β,17β)-*form* [143-62-4]
Digitoxigenin. *Thevetigenin*. *Cerberigenin*. *Echujetin*
Cryst. (EtOH aq.). Mp 253°. $[\alpha]_D^{17}$ +19.1 (c, 1.4 in MeOH).

► LD_{50} (mus, orl) 26.2 mg/kg.

*3-O-(2,6-Dideoxy-β-D-*xylo*-hexopyranoside):* [57361-72-5] ***Desglucocoroloside***. *Digitoxigenin boivinoside. Deglucocoroloside*
$C_{29}H_{44}O_7$ 504.662
From *Corchorus olitorius* (Jew's mallow). Cryst. Mp 190-192°. $[\alpha]_D^{20}$ -22.9 (c, 1.66 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-α-L-rhamnopyranoside]: [79435-42-0] ***Evobioside***
$C_{35}H_{54}O_{13}$ 682.804

Constit. of the seeds of *Descurainia sophia* (flixweed). Needles. Mp 228-230°. λ_{max} 267 (MeOH).

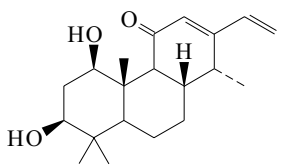
3-O-*[β-D-Glucopyranosyl-(1→4)-2,6-dideoxy*-xylo-*hexopyranoside]:* [57361-71-4] ***Coroloside***
$C_{35}H_{54}O_{12}$ 666.804
Constit. of *Corchorus olitorius* (Jew's mallow). Cryst. Mp 235-237°. $[\alpha]_D^{20}$ -46.7 (MeOH).

3-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→4)-2,6-dideoxy-β-D*-ribo-*hexopyranoside]:* [220710-06-5]
$C_{41}H_{64}O_{17}$ 828.946
Constit. of *Corchorus olitorius* (Jew's mallow). Amorph. powder. $[\alpha]_D^{22}$ -1.3 (c, 0.4 in MeOH).

[17598-65-1]

Maslennikova, V.A. *et al., Khim. Prir. Soedin.*, 1975, **11**, 525-526; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 553-554 (*Corolosides*)
Chen, Y.-Q. *et al., Yao Hsueh Hsueh Pao*, 1981, **16**, 62-64; *CA*, **95**, 209447 (*Evobioside*)
Nakamura, T. *et al., Phytochemistry*, 1998, **49**, 2097-2101 (*Coroloside, Glucoevatromonoside, Deglucocoroloside, Evatromonoside, pmr, cmr*)
Goda, Y. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1998, **40**, 371-376; *CA*, **131**, 85493j (*Corchorus olitorius constit*)
Yadava, R.N. *et al., Fitoterapia*, 1999, **70**, 284-286 (*Evobioside*)
Yadava, R.N. *et al., J. Asian Nat. Prod. Res.*, 1999, **1**, 245-249 (*Tamarindus indica constit*)

1,3-Dihydroxy-12,15-cassadien-11-one D-411



$C_{20}H_{30}O_3$ 318.455

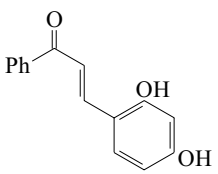
(1β,3β)-*form* [166547-23-5]
Phytocassane C
Phytoalexin from *Oryza sativa* (rice). Gum. λ_{max} 274 (MeOH) (Berdy).

3-Ketone: [181524-78-7] *1-Hydroxy-12,15-cassadiene-3,11-dione.* ***Phytocassane E***
$C_{20}H_{28}O_3$ 316.439
Phytoalexin from *Oryza sativa* (rice). Gum. λ_{max} 273 (EtOH).

Koga, J. *et al., Tetrahedron*, 1995, **51**, 7907-7918 (*isol, pmr, cmr*)
Koga, J. *et al., Phytochemistry*, 1997, **44**, 249-253 (*Phytocassane E*)

2,4-Dihydroxychalcone D-412

[92496-59-8]
3-(2,4-Dihydroxyphenyl)-1-phenyl-2-propen-1-one

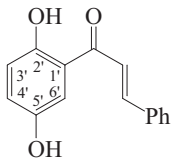


$C_{15}H_{12}O_3$ 240.258
Constit. of the fruit of *Litchi chinensis* (lychee).

Jaiswal, B.P. *et al., Indian J. Exp. Biol.*, 1987, **25**, 66 (*occur*)

2′,5′-Dihydroxychalcone, 8CI D-413

[19312-13-1]
1-(2,5-Dihydroxyphenyl)-3-phenyl-2-propen-1-one. 2,5-Dihydroxyphenyl styryl ketone



$C_{15}H_{12}O_3$ 240.258
Antioxidant for edible oils and fats. Red needles (C_6H_6). Mp 170° Mp 215°.

Obara, H. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 560 (*synth, ir, uv*)

3′,4′-Dihydroxychalcone, 8CI D-414

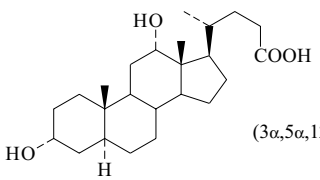
[88596-30-9]

[88191-20-2]
1-(3,4-Dihydroxyphenyl)-3-phenyl-2-propen-1-one, 9CI. 3,4-Dihydroxyphenyl styryl ketone

$C_{15}H_{12}O_3$ 240.258
Antioxidant for edible oils and fats. Yellow needles. Mp 187°. pK_a 8.2.

Klinke, P. *et al., Chem. Ber.*, 1961, **94**, 26 (*synth, uv*)

3,12-Dihydroxycholan-24-oic acid D-415



$C_{24}H_{40}O_4$ 392.578

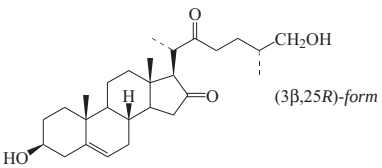
(3α,5β,12α)-*form* [83-44-3]

[302-95-4]
Deoxycholic acid. *Choleic acid. Cholorebic acid. Droxolan. Pyrochol. Septochol*
Emulsifying agent used in foods. Cryst. (EtOH). Mp 187-189°. $[\alpha]_D^{19}$ +47.7 (c, 1.7 in dioxan). $[\alpha]_D$ +53 ($CHCl_3$). Log P 4.47 (uncertain value) (calc). Adduct with menthol is marketed as Degalol.

▶ LD_{50} (rat, orl) 1000 mg/kg. LD_{50} (mus, orl) 1000 mg/kg. FZ2100000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1056D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 593A (*nmr*)
Reichstein, T. *et al., Helv. Chim. Acta*, 1942, **25**, 797 (*synth*)
Bergström, S. *et al., Acta Chem. Scand.*, 1953, **7**, 481 (*synth*)
Fieser, L.F. *et al., Steroids*, Reinhold, N.Y., 1959, (*rev*)
Danielsson, H. *et al., J. Biol. Chem.*, 1963, **238**, 3846 (*isol*)
Chang, F.C. *et al., J.O.C.*, 1965, **30**, 1718 (*synth*)
Leibfritz, D. *et al., J.A.C.S.*, 1973, **95**, 4996 (*cmr*)
Inoue, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1949 (*ms*)
Coiro, V.M. *et al., Acta Cryst. B*, 1979, **35**, 2941 (*cryst struct*)
Iida, T. *et al., J. Lipid Res.*, 1985, **26**, 874 (*synth*)
Limmatvapirat, S. *et al., Acta Cryst. C*, 1997, **53**, 803-805 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 790-791
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAQ400

3,26-Dihydroxycholest-5-ene-16,22-dione D-416



$C_{27}H_{42}O_4$ 430.626

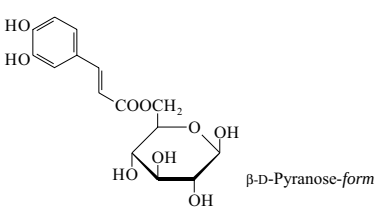
(3β,25*R*)-*form* [468-99-5]
Cryptogenin. *Kryptogenin*
Constit. of *Balanites aegyptiaca* (soapberry tree fruits). Cryst. (Me_2CO). Mp 187-189°.

(3β,25*S*)-*form* [64161-55-3]
Barogenin
Isol. from *Solanum tuberosum* (potato). Needles (Me_2CO). Mp 196-199°. $[\alpha]_D^{18}$ -88.8 (c, 0.36 in $CHCl_3$).

Marker, R.E. *et al., J.A.C.S.*, 1947, **69**, 2167 (*isol*)
Takeda, K. *et al., Chem. Pharm. Bull.*, 1965, **13**, 691
Kessar, S.V. *et al., Tetrahedron*, 1968, **24**, 899 (*synth*)
Faul, W.H. *et al., J.O.C.*, 1970, **35**, 2571 (*pmr*)
Kaneko, K. *et al., Phytochemistry*, 1977, **16**, 791 (*Barogenin*)
Kadkade, P.G. *et al., Biochem. Physiol. Pflanz.*, 1979, **34**, 357 (*isol*)

6-*O*-(3,4-Dihydroxycinnamoyl)glucose D-417

[10066-92-9]
6-O-*Caffeoylglucose*



$C_{15}H_{18}O_9$ 342.302

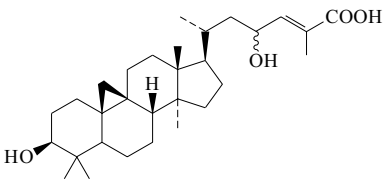
β-D-Pyranose-*form*

3′-Me ether, 2,3,4-trihydroxy-3-methylbutyl glycoside: [257939-69-8]
$C_{21}H_{30}O_{12}$ 474.461
Constit. of sage (*Salvia officinalis*) leaf. Powder.

[114297-66-4]

Wang, M. *et al., J. Agric. Food Chem.*, 2000, **48**, 235-238 (*Me ether trihydroxymethylbutyl glycoside*)

3,23-Dihydroxycycloart-24-en-26-oic acid D-418



$C_{30}H_{48}O_4$ 472.707

(3β,23ξ)-*form* [123563-63-3]
Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 279-281°. $[\alpha]_D^{30}$ +49 (c, 0.52 in MeOH).

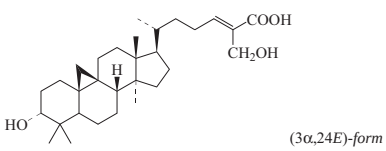
3-Ketone: ***23-Hydroxy-3-oxocycloart-24-en-26-oic acid***
$C_{30}H_{46}O_4$ 470.691
Constit. of *Mangifera indica* (mango).

23-Epimer:
$C_{30}H_{48}O_4$ 472.707
Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 240-242°. λ_{max} 218 (EtOH).

Anjaneyulu, V. *et al., Phytochemistry*, 1989, **28**, 1471

Anjaneyulu, V. *et al., Phytochemistry*, 1999, **50**, 1229-1236 (*23-epimer, 3-ketone*)

3,27-Dihydroxycycloart-24-en-26-oic acid D-419



(3α,24*E*)-*form*

$C_{30}H_{48}O_4$ 472.707

(3α,24*E*)-*form* [123563-64-4]
27-Hydroxyisomangiferolic acid
Constit. of *Mangifera indica* (mango). Cryst. (C_6H_6/EtOAc). Mp 207-209°. $[\alpha]_D^{30}$ +21.5 (c, 0.8 in $CHCl_3$).

(3β,24*E*)-*form* [17983-82-3]
27-Hydroxymangiferolic acid
Constit. of the stem bark of *Mangifera indica* (mango). Mp 201-204°. $[\alpha]_D$ +39 (c, 0.4 in $CHCl_3$).

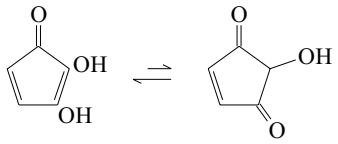
Corsano, S. *et al., Ann. Chim. (Rome)*, 1967, **57**, 508-521

Anjaneyulu, V. *et al., Phytochemistry*, 1989, **28**, 1471-1477 (*isol*)

Sharma, S.K. *et al., J. Indian Chem. Soc.*, 1995, **72**, 339-342 (*isol*)

2,3-Dihydroxy-2,4-cyclopentadien-1-one, 9CI D-420

[124902-00-7]

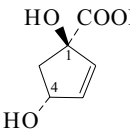


$C_5H_4O_3$ 112.085
Constit. of the seeds of *Trifolium repens* (white clover). Powder. Sol. MeOH, hexane; poorly sol. H_2O. Mp 208° dec. λ_{max} 218 (ϵ 2440); 258 (ϵ 3400) (MeOH) (Berdy).

Di-Me ether:2,3-Dimethoxy-2,4-cyclopentadien-1-one
$C_7H_8O_3$ 140.138
Mp 123-125°.

Nakatani, M. *et al., Phytochemistry*, 1989, **28**, 2499 (*isol*)

1,4-Dihydroxy-2-cyclopentene-1-carboxylic acid D-421



(1*R*,4*R*)-*form*

$C_6H_8O_4$ 144.127

(1*S*,4*S*)-*form*
*Nitrile, 1-*O*-β-D-glucopyranoside:* [34323-07-4] ***Tetraphyllin B****. Barterin*
Isol. from dried damiana leaves (*Turnera diffusa*). Needles (MeOH/EtOAc). Mp 169-170°. $[\alpha]_D^{26}$ -75 (c, 0.5 in MeOH). $[\alpha]_D^{25}$ -35.6 (c, 1 in H_2O).

*Nitrile, 1-*O*-β-glucopyranoside, 4-*O*-sulfate:* [85758-30-1] ***Tetraphyllin B sulfate***
$C_{12}H_{17}NO_{10}S$ 367.333
Isol. from *Passiflora caerulea* (blue passion flower) and other *Passiflora* spp.. Glassy syrup.

[85758-31-2, 85799-11-7, 97564-59-5, 99694-23-2, 109906-27-6, 121783-15-1, 133576-30-4]

Russell, G.B. *et al., Phytochemistry*, 1971, **10**, 1373 (*Tetraphyllin B*)

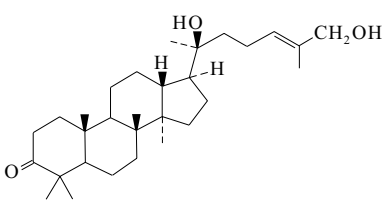
Spencer, K.C. *et al., Planta Med.*, 1981, **43**, 175-178 (*Tetraphyllin B*)

Siegler, D.S. *et al., Phytochemistry*, 1982, **21**, 2277 (*Tetraphyllin B sulfate*)

Jaroszewski, J.W. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 410 (*Volkenin, Tetraphyllin B*)

20,26-Dihydroxy-24-dammaren-3-one D-422

3-Keto-24-dammarene-20,26-diol



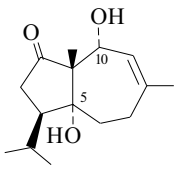
$C_{30}H_{50}O_3$ 458.723

(20*S*,24*E*)-*form* [99891-80-2]
Constit. of *Mangifera indica* (mango). Cryst. (C_6H_6/hexane). Mp 116-118°. $[\alpha]_D^{30}$ +30.6 (c, 0.6 in $CHCl_3$).

Anjaneyulu, V. *et al., Phytochemistry*, 1985, **24**, 2359

5,10-Dihydroxy-8-daucen-2-one D-423

1,6-Dihydroxy-2-caroten-9-one



$C_{15}H_{24}O_3$ 252.353

(5α,10α)-*form*
10-Ac: [94595-16-1]
$C_{17}H_{26}O_4$ 294.39
Cryst. ($CHCl_3$/hexane). Mp 129-130°. $[\alpha]_D^{30}$ -232.5 (c, 2.37 in $CHCl_3$).

(5β,10α)-*form* [87860-27-3] *Siol*
10-Ac: ***Siol acetate***
$C_{17}H_{26}O_4$ 294.39
Cryst. Mp 130-131°. $[\alpha]_D^{20}$ -252 (c, 0.28 in $CHCl_3$).

10-Angeloyl: [11053-21-7] ***Vaginatin***†. *Crispane*
$C_{20}H_{30}O_4$ 334.455
Constit. of *Petroselinum crispum* (parsley). Cryst. (petrol). Mp 77-78° (68-69°). $[\alpha]_D$ -266.7 (c, 4.32 in $CHCl_3$). Struct. of Crispane revised in 1998.

10-(4-Methoxybenzoyl): [104758-20-5] ***Fercomin***
$C_{23}H_{30}O_5$ 386.487
Cryst. (Et_2O/hexane). Mp 130-132°. λ_{max} 261 (ϵ 11000) (MeOH) (Derep).

[87746-59-6]

Casinovi, C.G. *et al., Coll. Czech. Chem. Comm.*, 1983, **48**, 2411 (*cryst struct, Siol acetate*)

Pandita, K. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 956

Appendino, G. *et al., J.C.S. Perkin 1*, 1986, 1363 (*Vaginatin*)

Miski, M. *et al., Phytochemistry*, 1986, **25**, 1673 (*Vaginatin, Fercomin*)

Spraul, M.H. *et al., Phytochemistry*, 1992, **31**, 3109 (*Crispane*)

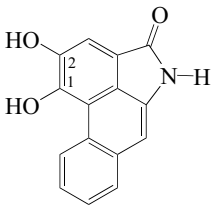
Appendino, G. *et al., Phytochemistry*, 1998, **49**, 1719-1722 (*Crispane, struct*)

2,3-Dihydroxy-4-decynoic acid D-424

Matsutakic acid A
$H_3C(CH_2)_4C{\equiv}CCH(OH)CH(OH)COOH$
$C_{10}H_{16}O_4$ 200.234
Isol. from the fungus *Laetiporus sulphureus* var. *miniatus*. Amorph. powder. $[\alpha]_D$ -13.2 (c, 0.7 in MeOH).

Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 327-329

1,2-Dihydroxydibenz[*cd*,*f*]indol-4(5*H*)-one, 9CI D-425



$C_{15}H_9NO_3$ 251.241

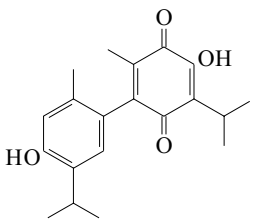
CAS numbering shown. Alternative (phenanthrene) numbering frequently encountered, in which 1,2- are 4,3- respectively.

2-Me ether: [112501-42-5] *1-Hydroxy-2-methoxydibenz[*cd,f*]indol-4(5*H*)-one, 9CI.* ***Piperolactam A****. Aristolactam F1*
$C_{16}H_{11}NO_3$ 265.268
Alkaloid from roots of *Piper longum* (long pepper). Cryst. (C_6H_6/MeOH). Mp 303-306° dec. (271-273°).

Achari, B. *et al., Heterocycles*, 1982, **19**, 1203 (*occur*)
Priestap, H.A. *et al., Phytochemistry*, 1985, **24**, 849 (*pmr, cmr*)
Sun, N.J. *et al., J. Nat. Prod.*, ', 1987, **50**, 843 (*Piperolactam A*)
Desai, S.J. *et al., Phytochemistry*, 1988, **27**, 1511 (*Piperolactam A*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1006-1009 (*activity*)
Chia, Y.-C. *et al., J. Nat. Prod.*, 2000, **63**, 1160-1163 (*isol, activity*)

4,4′-Dihydroxy-5,5′-diisopropyl-2,2′-dimethyl-3,6-biphenyldione D-426

[120866-14-0]

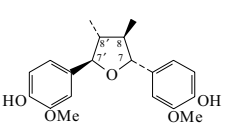


$C_{20}H_{24}O_4$ 328.407
Constit. of the leaves of thyme *Thymus vulgaris*. Shows antioxidant activity. Red semi-solid. Mp 67°. $[\alpha]_D^{25}$ -7.9 (c, 0.42 in $CHCl_3$).

Nakatani, N. *et al., Agric. Biol. Chem.*, 1989, 53; 1375 (*isol, pmr, cmr*)

4,4′-Dihydroxy-3,3′-dimethoxy-7,7′-epoxylignan D-427

4,4′-(Tetrahydro-3,4-dimethyl-2,5-furandiyl)bis[2-methoxyphenol], 9CI. Tetrahydro-2,5-bis(4-hydroxy-3-methoxyphenyl)-3,4-dimethylfuran



(7*R**,7′*R**,8*R**,8′*R**)-

$C_{20}H_{24}O_5$ 344.407
A common lignan various stereoisomers of which have been repeatedly isol. under different names. The abs. configs. require clarification however.

(7*R,7′*R**,8*R**,8′*R**)-*form*** [112652-46-7]
(2α,3β,4α,5β)-form. ***Fragransin A₂***
Isol. from arils of *Myristica fragrans* (nutmeg). Cryst. Mp 200-202°. $[\alpha]_D$ +79 ($CHCl_3$).

(7*R,7′*R**,8*R**,8′*S**)-*form*** [114422-21-8]
(2α,3α,4α,5β)-form. Machilin I. 3,3′-Dimethoxylarreatricin
Gum or oil. $[\alpha]_D^{25}$ -93 (c, 0.13 in $CHCl_3$). CD $[\theta]_{203}$ +10,600.

(7*R,7′*S**,8*R**,8′*R**)-*form*** [83198-63-4]
(2α,3α,4β,5α)-form. ***Verrucosin****. Epimachilin A*
Oil. $[\alpha]_D^{22}$ +38 (c, 0.25 in $CHCl_3$). Props. refer to Verrucosin. Epimachilin A incompletely characterised.

(7*R,7′*S**,8*R**,8′*S**)-*form*** [74683-16-2]
(2α,3β,4β,5α)-form. ***Malabaricanol****. Tetrahydrofuroguaiacin A. Calophyllin. Nectandrin B*
Isol. from *Myristica fragrans*. Oil. Opt. inactive (*meso*-).

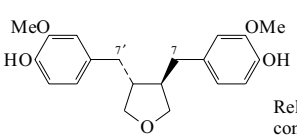
(7*R,7′*S**,8*S**,8′*R**)-*form*** [131829-51-1]
(2α,3α,4α,5α)-form. ***Tetrahydrofuroguaiacin B****. Isonectandrin B*
Opt. inactive (*meso*-).

[128524-98-1]

Hughes, G.K. *et al., Aust. J. Chem.*, 1954, **7**, 104 (*isol*)
Blears, J.G. *et al., J.C.S.*, 1958, 1985 (*synth*)
Birch, A.J. *et al., J.C.S.*, 1958, 4471 (*stereochem*)
King, F.E. *et al., J.C.S.*, 1964, 4011 (*isol, struct*)
Sarkanen, K.V. *et al., J.C.S. Perkin 1*, 1973, 1869 (*synth*)
Le Quesne, P.W. *et al., J. Nat. Prod.*, 1980, **43**, 353 (*Machilin I*)
Dias, A. de F. *et al., Phytochemistry*, 1982, **21**, 1137 (*Verrucosin*)
Puroshothaman, K.K. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 46 (*isol*)
Hattori, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3315 (*Fragransin A₂*)
Alvarez, V. *et al., CA*, 1988, **108**, 183594 (*Calophyllin*)
Shimomura, H. *et al., Phytochemistry*, 1988, **27**, 634 (*Nectandrin B*)
Konno, C. *et al., J. Nat. Prod.*, 1990, **53**, 396 (*3,3′-Dimethoxylarreatricin*)
Schmeda-Hirschmann, G. *et al., Phytochemistry*, 1992, **31**, 1731 (*Epimachilin A*)
Herath, H.M.T.B. *et al., Phytochemistry*, 1997, **44**, 699 (*isol, pmr, cmr*)

4,4′-Dihydroxy-3,3′-dimethoxy-9,9′-epoxylignan D-428

[34730-78-4]
*4,4′-[(Tetrahydro-3,4-furandiyl)bis(methylene)]bis[2-methoxyphenol], 9CI. α,α′-[Tetrahydro-3,4-furandiyl]bis[2-methoxy-*p*-cresol], 8CI. Divanillyltetrahydrofuran. Shonanin. Anhydrosecoisolariciresinol*



Relative configuration

$C_{20}H_{24}O_5$ 344.407
The recently descr. Shonanin appears to be identical to prev. known isolates.Prisms, cryst. (EtOAc/hexane). Mp 116-117° (136-137°). $[\alpha]_D^{25}$ -52.2 (c, 1.4 in THF).

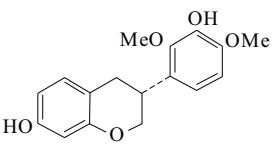
*4-O-(4-Hydroxy-3-methoxycinnamoyl)(*E*-):* [96917-11-2] ***Divanillyltetrahydrofuran ferulate***
$C_{30}H_{32}O_8$ 520.578
Constit. of *Diospyros kaki* (Japanese persimmon). Needles (EtOAc). Mp 184-185°. $[\alpha]_D^{25}$ -58.3 (c, 0.1 in THF). λ_{max} 233 (log ϵ 4.3); 290 (log ϵ 4.2); 327 (log ϵ 4.3) (MeOH).

[15429-99-9, 29388-32-7, 29388-33-8]

Freudenberg, K. *et al., Chem. Ber.*, 1957, **90**, 2857
Lapteva, K.I. *et al., Khim. Prir. Soedin.*, 1971, **7**, 829; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 802 (*isol*)
Modonova, L.D. *et al., Khim. Prir. Soedin.*, 1972, **8**, 165; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 170 (*isol*)
Leont'eva, V.G. *et al., Khim. Prir. Soedin.*, 1974, **10**, 399; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 399 (*isol*)
Luedemann, H.D. *et al., Makromol. Chem.*, 1974, **175**, 2393 (*cmr*)
Matsuura, S. *et al., Phytochemistry*, 1985, **24**, 626-628 (*ferulate*)
Fang, J.-M. *et al., Phytochemistry*, 1989, **28**, 3553 (*isol, pmr, cmr, cryst struct*)
Daugan, H. *et al., J. Nat. Prod.*, 1991, **54**, 110 (*synth*)
Pan, H. *et al., Phytochemistry*, 1995, **39**, 1425 (*isol, pmr, cmr*)

3′,7-Dihydroxy-2′,4′-dimethoxyisoflavan D-429

[27213-18-9]
*3,4-Dihydro-3-(3-hydroxy-2,4-dimethoxyphenyl)-*2*H-1-benzopyran-7-ol, 9CI.* ***Mucronulatol***



(*R*)-*form*

$C_{17}H_{18}O_5$ 302.326

(*R*)-*form* [57128-11-7]
Constit. of *Pterocarpus soyauxii*. Cream-coloured cryst. (EtOH). Mp 147-149°. $[\alpha]_D$ -18.5 (Me_2CO).

(*S*)-*form* [20878-97-1]
Mp 145°.

7-O-β-D-Glucopyranoside: [131749-60-5]
$C_{23}H_{28}O_{10}$ 464.468
Cryst. Mp 167-169°.

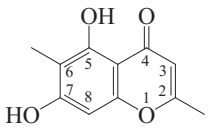
(±)-*form* [20878-98-2]
Isol. from *Astragalus gummifer* (tragacanth). Cryst. (MeOH). Mp 227-229°.

Braga de Oliveira, A. *et al., Chem. Comm.*, 1968, 1263 (*struct*)
Gottlieb, O.R. *et al., Chem. Comm.*, 1968, 1265 (*abs config*)
Antus, S. *et al., J.C.S. Perkin 1*, 1974, 305 (*synth*)
Gottlieb, O.R. *et al., Phytochemistry*, 1975, **14**, 1452 (*isol, struct*)
Kurosawa, K. *et al., Phytochemistry*, 1978, **17**, 1405; 1423 (*isol, abs config, ord*)

Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
He, Z.Q. *et al., Yaoxue Xuebao*, 1990, **25**, 694-696 (*7-glucoside*)
Sreenivasulu, B. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 1217-1218 (*isol, pmr*)

5,7-Dihydroxy-2,6-dimethyl-4*H*-1-benzopyran-4-one, 9CI D-430

[491-48-5]
5,7-Dihydroxy-2,6-dimethylchromone. ***Eugenitol***



$C_{11}H_{10}O_4$ 206.198
Constit. of the flowers of *Eugenia caryophyllata* (clove). Prisms (EtOH or Me_2CO). Mp 290-292°.

*7-*O*-(2-*O*-Acetyl-β-D-glucopyranoside):* [39387-36-5] ***Mollin***
$C_{19}H_{22}O_{10}$ 410.377
Mp 270-271°.

*7-*O*-(2,6-Di-*O*-acetyl-β-D-glucopyranoside):* [41666-57-3] ***Roccellin***
$C_{21}H_{24}O_{11}$ 452.414
Needles. Mp 206-207°.

7-Me ether: [480-12-6] *5-Hydroxy-7-methoxy-2,6-dimethyl-4*H*-1-benzopyran-4-one.* ***Eugenitin***
$C_{12}H_{12}O_4$ 220.224
From *Eugenia caryophyllata* (clove). Prisms (EtOH or Me_2CO). Sol. MeOH. Mp 162°.

7-Me ether, 5-Ac:
$C_{14}H_{14}O_5$ 262.262
Cryst. (EtOH). Mp 176-177°.

Schmid, H. *et al., Helv. Chim. Acta*, 1949, **32**, 813; 1950, **33**, 917 (*isol, synth*)
Schönberg, A. *et al., J.A.C.S.*, 1953, **75**, 4992 (*synth*)
Mukerjee, S.K. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1953, **38**, 207 (*synth*)
Mukerjee, S.K. *et al., Chem. Ind. (London)*, 1955, 1009
Murata, A. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1970, **119**, 1346 (*synth*)
Coombe, R.G. *et al., Aust. J. Chem.*, 1972, **25**, 875 (*isol*)
Ito, T. *et al., Anal. Chim. Acta*, 1980, **113**, 343 (*detn, Ti*)
Sekita, K. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2428 (*deriv*)
Huneck, S. *et al., Z. Naturforsch., B*, 1992, **47**, 449 (*Roccellin, Mollin*)
Sawada, S. *et al., Bull. Kyoto Univ. Educ., Ser. B*, 2000, **95/96**, 1-9; *CA*, **134**, 113013j (*Eugenitin, isol, activity, struct*)

5,7-Dihydroxy-2,8-dimethyl-4*H*-1-benzopyran-4-one, 9CI D-431

[479-06-1]
5,7-Dihydroxy-2,8-dimethylchromone. ***Isoeugenitol***

$C_{11}H_{10}O_4$ 206.198
Present in *Eugenia caryophyllata* (clove). Mp 229-230°.

*7-(2,3,6-Tri-*O*-acetyl-β-D-glucopyranoside):* [50816-68-7] ***Lobodirin***
$C_{23}H_{26}O_{12}$ 494.451
Mp 247-249°. $[\alpha]_D^{24}$ -63 (c, 0.74 in EtOH/Py). Struct. revised in 1992.

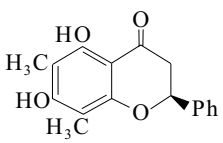
7-Me ether: [519-18-6] *5-Hydroxy-7-methoxy-2,8-dimethyl-4*H*-1-benzopyran-4-one.* ***Isoeugenitin***
$C_{12}H_{12}O_4$ 220.224
Constit. of *Eugenia caryophyllata* (clove). Golden needles. Mp 147.5-148°.

Di-Me ether: [211751-31-4] *5,7-Dimethoxy-2,8-dimethyl-4*H*-1-benzopyran-4-one, 9CI.* ***Isoeugenitin methyl ether***
$C_{13}H_{14}O_4$ 234.251
Yellowish needles (C_6H_6/hexane) (synthetic). Mp 173.5-174.5° (synthetic). Originally given the incorrect isomeric struct. 4,6-Dimethoxy-3,7-dimethylcoumarin.

Schmid, H. *et al., Helv. Chim. Acta*, 1949, **32**, 1358-1360; 1950, **33**, 917-922; 1770-1772 (*isol, Isoeugenitin, synth*)
Huneck, S. *et al., Phytochemistry*, 1973, **12**, 2497-2500 (*Lobodirin*)
Huneck, S. *et al., Z. Naturforsch., B*, 1992, **47**, 449-451 (*Lobodirin, struct, pmr, cmr*)
Fudo, R. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 183-184 (*Isoeugenitin, uv, ir, pmr, cmr, activity*)
Kalinin, A.V. *et al., Tet. Lett.*, 1998, **39**, 4999-5002 (*Isoeugenitin methyl ether*)

5,7-Dihydroxy-6,8-dimethylflavanone D-432

[27593-80-2]
*2,3-Dihydro-5,7-dihydroxy-6,8-dimethyl-2-phenyl-4*H*-1-benzopyran-4-one, 9CI.* ***Demethoxymatteucinol****. Desmethoxymatteucinol. 6,8-Dimethylpinocembrin*



$C_{17}H_{16}O_4$ 284.311
(*S*)-*form* [56297-79-1]
Isol. from *Eugenia javanica* (Java apple). Pale-yellow needles (EtOH). Mp 202-204°. $[\alpha]_D^{22}$ -48 (c, 3.8 in Me_2CO).

*7-*O*-β-D-Glucopyranoside:*
$C_{23}H_{26}O_9$ 446.453

5-Me ether: [83247-72-7] *7-Hydroxy-5-methoxy-6,8-dimethylflavanone*
$C_{18}H_{18}O_4$ 298.338
Constit. of *Eugenia javanica* (Java apple). Pale-yellow needles (MeOH). Mp 207-209°.

7-Me ether: [55820-35-4] *5-Hydroxy-7-methoxy-6,8-dimethylflavanone*
$C_{18}H_{18}O_4$ 298.338
Cryst. (hexane). Mp 130°.

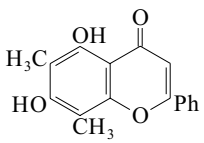
*7-O-[6-*O*-(3-Hydroxy-3-methylglutaroyl)-β-D-glucopyranoside]:* ***Matteuorienate B***
$C_{29}H_{34}O_{13}$ 590.58
Pale yellow amorph. solid.

[51621-50-2, 51621-52-4, 81703-17-5]

Fujise, S. *et al., Ber.*, 1933, **66**, 929; 1936, **69**, 1893 (*synth, struct, resoln*)
Arakawa, H. *et al., Annalen*, 1960, **636**, 114 (*abs config*)
Mitscher, L.A. *et al., J. Nat. Prod.*, 1973, **36**, 422 (*isol*)
Joshi, B.S. *et al., Indian J. Chem., Sect. B*, 1974, **12**, 1033 (*7-Me ether*)
Cannon, J.R. *et al., Aust. J. Chem.*, 1977, **30**, 2099 (*isol, bibl*)
Hiraoka, A. *et al., Biochem. Syst. Ecol.*, 1978, **6**, 171 (*glucoside*)
Wollenweber, E. *et al., CA*, 1979, **91**, 120332k (*isol*)
Hufford, C.D. *et al., J.O.C.*, 1981, **46**, 3073 (*isol*)
Tanrisever, N. *et al., Phytochemistry*, 1987, **26**, 175-179 (*isol, pmr, cryst struct*)
Kadota, S. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1712 (*Matteuorienate B*)

5,7-Dihydroxy-6,8-dimethylflavone D-433

[171439-53-5]
*5,7-Dihydroxy-6,8-dimethyl-2-phenyl-4*H*-1-benzopyran-4-one, 9CI.* ***Matteuorien***



$C_{17}H_{14}O_4$ 282.295
Yellow powder. Mp 290° (dec.).

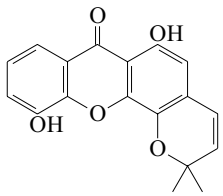
7-Me ether: [14004-56-9] *5-Hydroxy-7-methoxy-6,8-dimethylflavone.* ***Desmosflavone***
$C_{18}H_{16}O_4$ 296.322
Constit. of *Leptospermum scoparium* (red tea). Yellow cryst. (Et_2O). Mp 212-214°.

7-O-[6-O-(3-Hydroxy-3-methylglutaroyl)-β-D-glucopyranoside]: [171439-54-6] ***Matteuorienate C***
$C_{29}H_{32}O_{13}$ 588.564
Light yellow powder. $[\alpha]_D$ -54 (c, 0.1 in MeOH).

Mayer, R. *et al., Phytochemistry*, 1990, **29**, 1340 (*isol, cmr, pmr, uv*)
Wu, J. *et al., Chin. Chem. Lett.*, 1994, **5**, 211 (*Desmosflavone*)
Basnet, P. *et al., Chem. Pharm. Bull.*, 1995, **59**, 1559 (*isol, pmr, cmr*)
Hauteville, M. *et al., Annalen*, 1996, 1217 (*synth, pmr, cmr, ms*)

6,11-Dihydroxy-2,2-dimethylpyrano[3,2-*c*]xanthen-7(2*H*)-one, 9CI D-434

[136364-53-9]

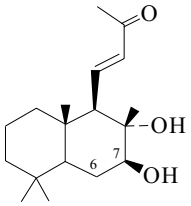


$C_{18}H_{14}O_5$ 310.306
Constit. of the root bark of *Garcinia livingstonei* (imbe). Yellow solid. Mp 217-219°. λ_{max} 245 (ε 28200); 280 (ε 14800); 291 (ε 15600); 330 (ε 13800); 420 (ε 4400) (MeOH) (Berdy).

Sordat-Diserens, I. *et al., Phytochemistry*, 1992,

31, 313 (*isol, pmr, cmr*)

7,8-Dihydroxy-14,15-dinor-11-labden-13-one D-435



$C_{18}H_{30}O_3$ 294.433

(7β,8α,11*E*)-*form*
Sterebin D
Constit. of *Stevia rebaudiana* (stevia). Powder. $[\alpha]_D$ +22.8 (c, 0.05 in MeOH).

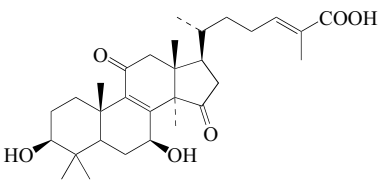
6α-Hydroxy: [107647-14-3] *6α,7β,8α-Trihydroxy-14,15-dinor-11-labden-13-one.*
Sterebin A
$C_{18}H_{30}O_4$ 310.433
Isol. from leaves of *Stevia rebaudiana* (stevia). Needles (Me_2CO). Mp 157-158°. $[\alpha]_D$ +39.6 (c, 0.63 in Me_2CO).

*6α-Acetoxy:****Sterebin B***
$C_{20}H_{32}O_5$ 352.47
Constit. of *Stevia rebaudiana* (stevia). Powder. $[\alpha]_D$ +15.9 (c, 0.11 in MeOH).

*6α-Hydroxy, 7-Ac:****Sterebin C***
$C_{20}H_{32}O_5$ 352.47
Constit. of *Stevia rebaudiana* (stevia). Powder. $[\alpha]_D$ +34.8 (c, 0.07 in MeOH).

Oshima, Y. *et al., Tetrahedron*, 1986, **42**, 6443

3,7-Dihydroxy-11,15-dioxolanosta-8,24-dien-26-oic acid D-436

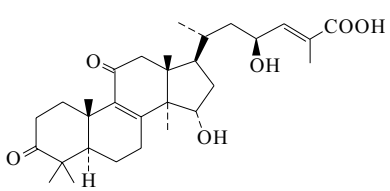


$C_{30}H_{44}O_6$ 500.674

(3β,7β,24*E*)-*form* [217476-76-1]
Ganoderic acid β
Constit. of *Ganoderma lucidum* (reishi). Needles (EtOH/MeOH aq.). Mp 187-189°. $[\alpha]_D$ +60 (c, 0.1 in MeOH). λ_{max} 215 (ε 12590); 252 (ε 6310) (MeOH) (Berdy).

Min, B.-S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1607-1612 (*isol, pmr, cmr*)

15,23-Dihydroxy-3,11-dioxolanosta-8,24-dien-26-oic acid D-437

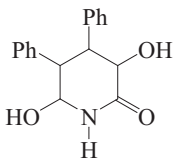


$C_{30}H_{44}O_6$ 500.674

(15α,23*S*,24*E*)-*form* [102607-22-7]
Ganolucidic acid D
Metab. of *Ganoderma lucidum* (reishi). $[\alpha]_D^{27}$ +192 (c, 0.1 in EtOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 809; 1988, **52**, 367

3,6-Dihydroxy-4,5-diphenyl-2-piperidinone D-438



$C_{17}H_{17}NO_3$ 283.326

N-*Me:* [211504-98-2] *3,6-Dihydroxy-1-methyl-4,5-diphenyl-2-piperidinone.* ***Lansimide 3****. Lansamide 3*
$C_{18}H_{19}NO_3$ 297.353
Constit. of *Clausena lansium* (wampee). Needles. Mp 236-237°. Racemic. It appears that this is a struct. revision for the compound formerly assigned a pyrrolidinone struct. and isol. from a sp. referred to as *Clausena lansium*. However this is not clear from the paper. See, Lansimide 3, C-302.

N,O^6-*Di-Me:* [211505-00-9] *3-Hydroxy-6-methoxy-1-methyl-4,5-diphenyl-2-piperidinone.* ***Lansimide 4****. Lansamide 4*
$C_{19}H_{21}NO_3$ 311.38
Constit. of *Clausena lansium* (wampee). Needles. Mp 187-188°. Racemic.

Lakshmi, V. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 422-424

2,3-Dihydroxy-1,3-diphenyl-1-propanone D-439

[82105-21-3, 82105-22-4, 153617-30-2]
1-Benzoyl-2-phenyl-1,2-ethanediol. α,β-Dihydroxydihydrochalcone

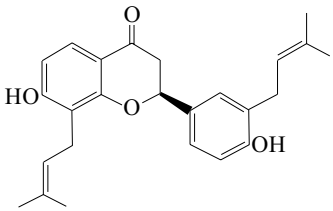
PhCH(OH)CH(OH)COPh

$C_{15}H_{14}O_3$ 242.274
Constit. of peanut oil.

Mukaiyama, T. *et al., Chem. Lett.*, 1982, 509-512 (*synth*)
Clerici, A. *et al., J.O.C.*, 1989, **54**, 3872-3878 (*synth*)
Traditional Chinese Medicines, (ed. Milne, G.A.), Ashgate, 1999, 1963

4′,7-Dihydroxy-3′,8-diprenylflavanone D-440

*2,3-Dihydro-7-hydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.*
Glabrol



$C_{25}H_{28}O_4$ 392.494Log P 6.35 (uncertain value) (calc).
λ_{max} 286 (ε 22500); 312 (ε 11500) (EtOH) (Berdy).

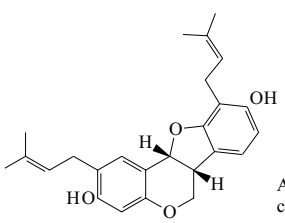
(*S*)-*form* [59870-65-4]
Constit. of roots of *Glycyrrhiza glabra* (licorice). Needles (MeOH aq.). Mp 90°. $[\alpha]_D^{22}$ -44.2 (c, 0.91 in MeOH). Pharmacol. active isomer.

*3*R*-Hydroxy:* [74148-41-7] ***3-Hydroxyglabrol***
$C_{25}H_{28}O_5$ 408.493
From *Glycyrrhiza glabra* (licorice). Mp 117-119°. $[\alpha]_D^{20}$ -17.65 (c, 1.02 in $CHCl_3$). λ_{max} 282 (ε 16600); 312 (ε 8300) (MeOH) (Berdy). λ_{max} 247 (ε 20000); 284 (ε 11200); 338 (ε 15800) (MeOH-NAOH) (Berdy).

Saitoh, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 752 (*isol, ir, pmr, uv, ms*)
Mitscher, L.A. *et al., Heterocycles*, 1978, **9**, 1533 (*pmr, uv*)
Birecka, H. *et al., J. Nat. Prod.*, 1980, **43**, 259 (*isol*)
Mizuno, M. *et al., Phytochemistry*, 1990, **29**, 2738 (*isol*)

3,9-Dihydroxy-2,10-diprenylpterocarpan D-441

[77263-06-0]
Erythrabyssin II



Absolute configuration

$C_{25}H_{28}O_4$ 392.494
Isol. from *Phaseolus lunatus* (butter bean). Sol. MeOH, Et_2O. λ_{max} 220 (ε 18000); 287 (ε 8130) (MeOH) (Berdy).

Kamat, V.S. *et al., Heterocycles*, 1981, **15**, 1163 (*isol, uv, pmr, struct, abs config*)
O'Neill, M.J. *et al., Phytochemistry*, 1986, **25**, 1315 (*isol*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2749 (*isol*)

3,9-Dihydroxy-4,10-diprenylpterocarpan D-442

[119269-76-0]

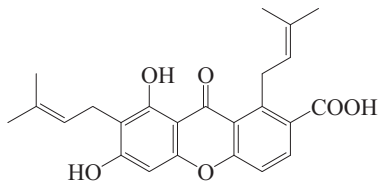
6a,11a-Dihydro-4,10-bis(3-methyl-2-butenyl)-6H-benzofuro[3,2-c][1]benzopyran-3,9-diol, 9CI. ***Erybraedin A***

$C_{25}H_{28}O_4$ 392.494
Isol. from *Phaseolus lunatus* (butter bean). Cryst. (CH_2Cl_2/hexane). Mp 69-71°. $[\alpha]_D^{25}$ -40.67 (c, 0.5 in MeOH).

O'Neill, M.J. *et al., Phytochemistry*, 1986, **25**, 1315 (*isol, pmr, cmr*)
Mitscher, L.A. *et al., Phytochemistry*, 1988, **27**, 3449; 1989, **28**, 1789 (*isol, pmr, cmr*)

6,8-Dihydroxy-1,7-diprenylxanthone-2-carboxylic acid D-443

6,8-Dihydroxy-1,7-bis(3-methyl-2-butenyl)-9-oxo-9H-xanthene-2-carboxylic acid

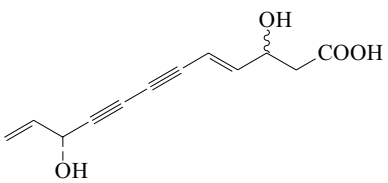


$C_{24}H_{24}O_6$ 408.45
Constit. of the fruit hulls of *Garcinia mangostana* (mangosteen). Mp 204-206°.

Gopalakrishnan, G. *et al., Fitoterapia*, 2000, **71**, 607-609

3,10-Dihydroxy-4,11-dodecadiene-6,8-diynoic acid D-444

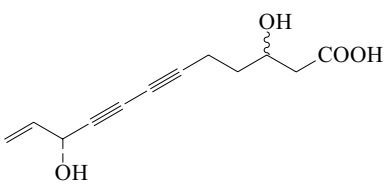
[152340-31-3]
Helianthenic acid E



$C_{12}H_{12}O_4$ 220.224
(3ξ,4*E*,10*R*)-*form*
10-O-β-D-Glucopyranoside, Me ester:
[142449-85-2]
$C_{19}H_{24}O_9$ 396.393
Constit. of *Helianthus tuberosus* (Jerusalem artichoke). Amorph. solid. $[\alpha]_D^{23}$ -166 (c, 0.02 in MeOH).
Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1492

3,10-Dihydroxy-11-dodecene-6,8-diynoic acid D-445

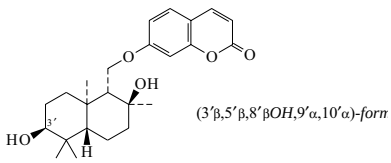
[152340-29-9]
Helianthenic acid C



$C_{12}H_{14}O_4$ 222.24
(3ξ,10*R*)-*form*
10-O-β-D-Glucopyranoside, Me ester:
[152141-43-0]
$C_{19}H_{26}O_9$ 398.409
Constit. of *Helianthus tuberosus* (Jerusalem artichoke). Amorph. solid. $[\alpha]_D^{23}$ -98 (c, 0.2 in MeOH).
Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1492

O-(3,8-Dihydroxydriman-11-yl)umbelliferone D-446

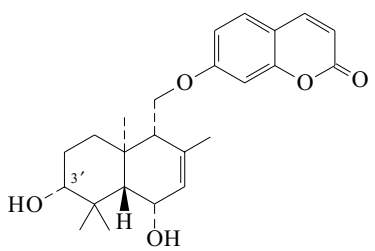
[28699-16-3]
Samarkandin



(3′β,5′β,8′β*OH*,9′α,10′α)-*form*

$C_{24}H_{32}O_5$ 400.514
(3′α,5′β,8′α*OH*,9′α,10′α)-*form* [61490-17-3]
Nevskin. *Episamarcandin*
Constit. of *Ferula assa-foetida* (asafoetida). Cryst. Mp 193-194°. $[\alpha]_D^{26}$ -79 (Py).
3′-O-Ac: [61490-18-4] ***3-O-Acetylepisamarcandin***
$C_{26}H_{34}O_6$ 442.551
Isol. from *Ferula assa-foetida* (asafoetida). Orange oil.
Bagirov, V.Y. *et al., Khim. Prir. Soedin.*, 1976, **12**, 450; 1978, **14**, 652; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 397; 1978, **14**, 562 (*Nevskin, Nevskone*)
Nassar, M.I. *et al., Fitoterapia*, 1998, **69**, 41-42 (*3′-Acetylsamarcandin, 3′-Acetylepisamarcandin*)

O-(3,6-Dihydroxy-7-drimen-11-yl)umbelliferone D-447



(3′α,5′β,6′α,9′α,10′α)-*form*

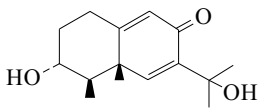
$C_{24}H_{30}O_5$ 398.498
(3′ξ,5′α,9′ξ,10′β)-*form*
6′-Ketone:
$C_{24}H_{28}O_5$ 396.482
Constit. of *Ferula galbaniflua* (galbanum). Cryst. Mp 93-94°.
3′-Deoxy, 6′-ketone:
$C_{24}H_{28}O_4$ 380.483
Constit. of *Ferula galbaniflua* (galbanum). Cryst. Mp 157°.
Vandyshev, V.V. *et al., Khim. Prir. Soedin.*, 1972, **8**, 669; 670; 1974, **10**, 658; 1975, **11**, 420; 1978, **14**, 707; 1979, **15**, 574; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 653; 654; 1974, **10**, 670; 1975, **11**, 432; 1978, **14**, 601; 1979, **15**, 500 (*config*)
Kadyrov, A.Sh. *et al., Khim. Prir. Soedin.*, 1974, **10**, 400; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 401
Borisov, V.N. *et al., Khim. Prir. Soedin.*, 1974, **10**, 515; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 519
Kuliev, Z.A. *et al., Khim. Prir. Soedin.*, 1977, **13**, 477; 1978, **14**, 322; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 267
Graf, E. *et al., Planta Med.*, 1985, 428

10,20-Dihydroxyeicosanoic acid D-448

[120727-26-6]
$HOCH_2(CH_2)_9CH(OH)(CH_2)_8COOH$
$C_{20}H_{40}O_4$ 344.534
Isol. from the leaf cutin of *Limonia acidissima* (wood apple).

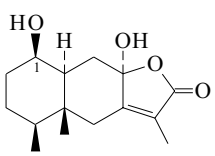
Das, S. *et al., Phytochemistry*, 1989, **28**, 509-511 (*isol*)

3,11-Dihydroxy-6,9-eremophiladien-8-one D-449



$C_{15}H_{22}O_3$ 250.337
3α-*form* [19887-91-3]
Petasitol
Cryst. (EtOAc/petrol). Mp 110-113°. $[\alpha]_D^{21}$ -1.2 (c, 1.1 in $CHCl_3$).
3-Angeloyl: [19887-90-2] ***Petasitin***
$C_{20}H_{28}O_4$ 332.439
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{22}$ -26.
3-(3-Methylthio-2-propenoyl) (Z-):
[211691-00-8] **S-*Petasitin***
$C_{19}H_{26}O_4S$ 350.478
Needles (EtOH). Mp 143-144°. $[\alpha]_D^{25}$ -15 (c, 1 in MeOH). λ_{max} 240 (log ε 4.43) (MeOH).
Takagi, I. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 3320
Lin, Y.-L. *et al., J. Nat. Prod.*, 1998, **61**, 887-890 (S-*Petasitin*)

1,8-Dihydroxy-7(11)-eremophilen-12,8-olide D-450

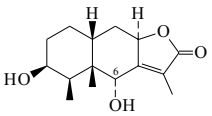


(1β,8α*OH*)-*form*

$C_{15}H_{22}O_4$ 266.336
(4α,5α,8β*OH*,10β)-*form*
1-Ketone: [35481-83-5] ent-*8α-Hydroxy-1-oxo-7(11)-eremophilen-12,8-olide.* ***Istanbulin A***
$C_{15}H_{20}O_4$ 264.321
Isol. from *Smyrnium olusatrum* (alexanders). Cryst. Mp 246°. $[\alpha]_D^{20}$ +81.5 (MeOH). λ_{max} 285 (ε 158) (MeOH) (Berdy). λ_{max} 221 (log ε 4.16); 285 (log ε 2.2) (EtOH).

Ulubelen, A. *et al., Tet. Lett.*, 1971, **12**, 4455-4456 (*Istanbulin A*)
Buděšinský, M. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1311-1317 (*abs config, Istanbulin A*)
Dupré, S. *et al., Phytochemistry*, 1991, **30**, 1211-1220 (*isol, pmr*)

3,6-Dihydroxy-7(11)-eremophilen-12,8-olide D-451



(3β,6α,8β,10β)-*form*

$C_{15}H_{22}O_4$ 266.336

(3β,6α,8β,10β)-*form*

6-Angeloyl, 3-(3-methylsulfinyl-2-propenoyl) (R,E-)*:* [182127-79-3] ***Eremosulphoxinolide A***
$C_{24}H_{32}O_7S$ 464.579
Constit. of *Petasites japonicus* (sweet coltsfoot). Pale yellow oil. $[\alpha]_D^{24}$ -13.2 (c, 0.4 in $CHCl_3$).

6-Angeloyl, 3-(3-methylsulfinyl-2-propenoyl) (S,E-)*:* [182266-16-6] ***Eremosulphoxinolide B***
$C_{24}H_{32}O_7S$ 464.579
Constit. of *Petasites japonicus* (sweet coltsfoot). Pale yellow oil. $[\alpha]_D^{24}$ -77.6 (c, 0.5 in $CHCl_3$).

6-Me ether: [171595-26-9] *3-Hydroxy-6-methoxy-7(11)-eremophilen-12,8-olide*
$C_{16}H_{24}O_4$ 280.363
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{26}$ -54.4 (c, 0.2 in $CHCl_3$).

(3β,6β,8β,10β)-*form*

6-Angeloyl: [149475-45-6]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Gum. $[\alpha]_D^{22}$ -100.3 (c, 3 in $CHCl_3$).

6-Tigloyl: [149475-46-7]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Gum. $[\alpha]_D^{22}$ -105.5 (c, 0.2 in $CHCl_3$).

3,6-Diangeloyl: [149475-47-8]
$C_{25}H_{34}O_6$ 430.54
Constit. of *Petasites japonicus* (sweet coltsfoot). Gum. $[\alpha]_D^{22}$ -120.3 (c, 0.3 in $CHCl_3$).

6-Me ether: [162613-64-1]
Constit. of *Petasites japonicus* (sweet coltsfoot). Needles (Et_2O/EtOAc). Mp 180-181°. $[\alpha]_D^{23}$ -189.6 (c, 0.9 in $CHCl_3$).

(3β,6β,8α,10β)-*form*

6-Angeloyl: [199675-13-3]
$C_{20}H_{28}O_5$ 348.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{23}$ +26.3 (c, 0.04 in $CHCl_3$). λ_{max} 225 (log ϵ 4) (MeOH).

6-Me ether: [171595-27-0]
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{25}$ +95.7 (c, 0.2 in $CHCl_3$).

3-Ketone, 6-angeloyl: [199675-14-4]
$C_{20}H_{26}O_5$ 346.422
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{20}$ +90.4 (c, 0.2 in $CHCl_3$). λ_{max} 222 (log ϵ 4.2) (MeOH).

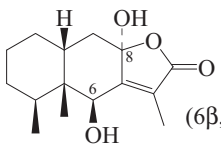
(3β,6β,8β,10β)-*form*

6-(3-Chloro-2-hydroxy-2-methylbutanoyl): [171422-90-5]
$C_{20}H_{29}ClO_6$ 400.898
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{21}$ -55.6 (c, 0.1 in $CHCl_3$).

6-(2,3-Epoxy-2-methylbutanoyl): [171422-91-6]
$C_{20}H_{28}O_6$ 364.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{20}$ -96.2 (c, 0.05 in $CHCl_3$).

Sugama, K. *et al., Phytochemistry*, 1985, **24**, 1531 (*isol, pmr, cmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 3277; 1994, **42**, 1944; 1995, **43**, 1738 (*isol, pmr, cmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1731 (*Eremosulphoxinolides*)
Yaoita, Y. *et al., Nat. Med. (Tokyo)*, 1997, **51**, 372-375; *CA*, **128**, 32374c (*isol, pmr, cmr*)

6,8-Dihydroxy-7(11)-eremophilen-12,8-olide D-452



(6β,8α*OH*)-*form*

$C_{15}H_{22}O_4$ 266.336

(6β,8α*OH*)-*form* [98204-90-1]
Constit. of *Petasites japonicus* (sweet coltsfoot).

Di-Ac:
Cryst. (EtOAc/hexane). Mp 150-151°. $[\alpha]_D$ -103 (c, 0.52 in $CHCl_3$).

6-Angeloyl: [244779-32-6] ***Ligusongaricanolide A***
$C_{20}H_{28}O_5$ 348.438
Needles. Mp 182-183°. $[\alpha]_D$ -89.9 (c, 0.63 in $CHCl_3$).

8-Me ether: [58848-44-5] ***6-Hydroxy-8-methoxy-7(11)-eremophilen-12,8-olide***
$C_{16}H_{24}O_4$ 280.363
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (Me_2CO/hexane). Mp 160-162°. $[\alpha]_D$ -154 (c, 1 in $CHCl_3$).

(6β,8β*OH*)-*form* [58848-38-7]
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. ($CHCl_3$/C_6H_6). Mp 217-218°. $[\alpha]_D$ +82 (c, 1 in EtOH).

Di-Ac:
Cryst. (Me_2CO/hexane). Mp 119-122°. $[\alpha]_D$ +62.6 (c, 1 in $CHCl_3$).

6-Me ether: [259528-61-5] ***8-Hydroxy-6-methoxy-7(11)-eremophilen-12,8-olide***
$C_{16}H_{24}O_4$ 280.363
Cryst. (petrol). Mp 148-150°.

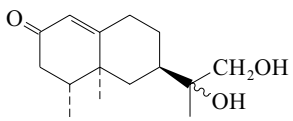
8-Me ether: [58848-45-6]
$C_{16}H_{24}O_4$ 280.363
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (EtOAc/hexane). Mp 128-129.5°. $[\alpha]_D$ +194 (c, 0.63 in $CHCl_3$).

6-Ketone: [259528-62-6] ***8-Hydroxy-6-oxo-7(11)-eremophilen-12,8-olide***
$C_{15}H_{20}O_4$ 264.321
Cryst. (petrol). Mp 216-218°.

[65349-94-2]

Moriyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3196-3199 (*6β,8βOH-form*)
Sugama, K. *et al., Phytochemistry*, 1985, **24**, 1531-1535 (*8-Me ether*)
Wang, W.S. *et al., Chin. Chem. Lett.*, 1999, **10**, 571-572 (*6-Me ether, 6-ketone*)
Fu, B. *et al., Pharmazie*, 1999, **54**, 620-624 (*Ligusongaricanolide A*)

11,12-Dihydroxy-1(10)eremophilen-2-one D-453



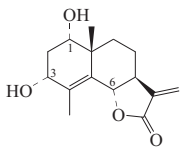
$C_{15}H_{24}O_3$ 252.353

(11ξ)-*form*

Urodiolenone
Found in grapefruit. Oil.

Chayen, R. *et al., Phytochemistry*, 1988, **27**, 369

1,3-Dihydroxy-4,11(13)-eudesmadien-12,6-olide D-454



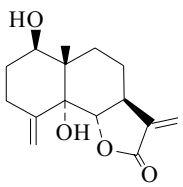
(1α,3α,6α)-*form*

$C_{15}H_{20}O_4$ 264.321

(1β,3β,6α)-*form* [293313-26-5]
3-Epiarmefolin
Constit. of *Tanacetum vulgare* (tansy).

Todorova, M. *et al., Dokl. Bolg. Akad. Nauk*, 1999, **52**, 41-44; *CA*, **133**, 235127a (*3-Epiarmefolin*)

1,5-Dihydroxy-4(15),11(13)-eudesmadien-12,6-olide D-455



(1β,5α,6α)-*form*

$C_{15}H_{20}O_4$ 264.321

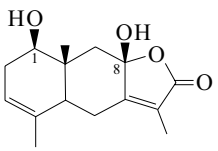
(1β,5α,6α)-*form* [1401-54-3]
Tanacetin
Constit. of *Tanacetum vulgare* (tansy). Cryst. ($CHCl_3$/Me_2CO). Mp 205-206°. $[\alpha]_D^{25}$ +154 (c, 0.15 in EtOH).

11β,13-Dihydro: [22149-38-8] *(11α)-1β,5α-Dihydroxy-4(15)-eudesmen-12,6α-olide.* ***Artemin***
$C_{15}H_{22}O_4$ 266.336
Constit. of *Artemisia* spp.. Cryst. (EtOAc/petrol). Mp 238-240°. $[\alpha]_D$ +167 (c, 0.5 in $CHCl_3$).

Samek, Z. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 1971 (*isol, struct*)

El-Feraly, F.S. *et al., J.C.S. Perkin 1*, 1983, 355 (*synth*)
Ahmed, A.A. *et al., Phytochemistry*, 1990, **29**, 3661 (*deriv*)
Marco, J.A. *et al., Phytochemistry*, 1994, **37**, 477 (*11,13-Dihydro derivs, pmr, cmr*)

1,8-Dihydroxy-3,7(11)-eudesmadien-12,8-olide D-456



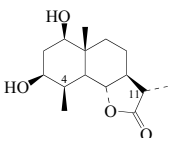
$C_{15}H_{20}O_4$ 264.321

(1β,8β)-*form* [366494-92-0]
Constit. of *Smyrnium olusatrum* (alexanders). Cryst. (MeOH). Mp 193-195°. λ_{max} 215 (MeOH).

1-Ac: [108044-19-5] *1β-Acetoxy-8β-hydroxy-3,7(11)-eudesmadien-12,8-olide*
$C_{17}H_{22}O_5$ 306.358
Amorph.

Ulubelen, A. *et al., J. Nat. Prod.*, 1986, **49**, 1104
El-Gamal, A.A. *et al., Phytochemistry*, 2001, **57**, 1197-1200 (*Smyrnium olusatrum constit*)

1,3-Dihydroxy-12,6-eudesmanolide D-457



(1β,3β,4β,6α,11α*H*)-*form*

$C_{15}H_{24}O_4$ 268.352

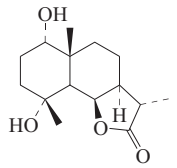
(1β,3β,4β,6α,11α*H*)-*form* [75991-58-1]
4,11,13,15-Tetrahydroridentin B
Constit. of *Taraxacum officinale* (dandelion). Cryst. (Et_2O/petrol). Mp 141-142°.

(1β,4α,6α,11α*H*)-*form*

3-Ketone, 1-O-*β*-D-*glucopyranoside:* [75911-12-5]
$C_{21}H_{32}O_9$ 428.478
Constit. of *Taraxacum officinale* (dandelion). Amorph., cryst. (as tetra-Ac). Mp 192° (tetra-Ac).

Moiseeva, G.P. *et al., Khim. Prir. Soedin.*, 1973, **9**, 167; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 162 (*struct*)
Yamakawa, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2810 (*synth*)
Haensel, R. *et al., Phytochemistry*, 1980, **19**, 837; 857-861 (*Tetrahydroridentin B, Arsanin glucoside*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **43**, 4761 (*synth, rev*)
Yang, D.S. *et al., Arch. Pharmacal Res.*, 1996, **19**, 507-513; *CA*, **126**, 190812g (*glucosides*)
Zielińska, K. *et al., Phytochemistry*, 2000, **54**, 791-794 (*pmr*)

1,4-Dihydroxy-12,6-eudesmanolide D-458



(1α,4α,6β,11β*H*)-*form*

$C_{15}H_{24}O_4$ 268.352

(1α,4α,6β,11β*H*)-*form* [246231-47-0]
1α-Hydroxycolartin
Oil. $[\alpha]_D^{25}$ +31 (c, 0.5 in $CHCl_3$).

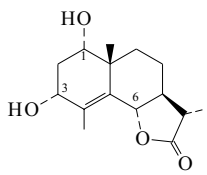
(1β,4α,6α,11β*H*)-*form* [66428-35-1]
1β-Hydroxycolartin
Constit. of *Tanacetum vulgare* (tansy). Prisms (EtOH). Mp 200-201° (194-196°).

(1β,4α,6β,11α*H*)-*form*
1β-Hydroxy-11-epicolartin
Cubes (EtOAc). Mp 250-251°.

(1β,4β,6β,11α*H*)-*form*
1β-Hydroxy-4,11-diepicolartin
Cubes (EtOAc). Mp 198-200°.

Samek, E. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 1971 (*isol, pmr, ir, ms, cd*)
Ando, M. *et al., Tetrahedron*, 1977, **33**, 2785 (*synth, ir, pmr*)
Gonzalez, A.G. *et al., Tetrahedron*, 1980, **36**, 2015 (*synth, pmr, ir*)
Sanz, J.F. *et al., Phytochemistry*, 1990, **29**, 541 (*isol, pmr, cmr, ir, ms*)
Tan, R.X. *et al., Phytochemistry*, 1990, **29**, 1209 (*isol, pmr*)
Mansilla, H. *et al., Phytochemistry*, 1999, **51**, 995-997 (*1α-Hydroxycolartin*)

1,3-Dihydroxy-4-eudesmen-12,6-olide D-459



(1α,3α,6α,11α)-*for*

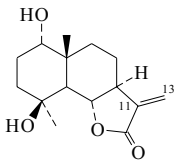
$C_{15}H_{22}O_4$ 266.336

(1α,3α,6α,11α)-*form* [71241-93-5]
Alkhanol. *Isoerivanin. Alhanol. Alkanol*
Constit. of *Balsamita major* (costmary). Cryst. Mp 179-181° (172-174°).

3-Ketone: [71327-31-6] *1α-Hydroxy-3-oxo-4-eudesmen-12,6α-olide. Dehydroisoerivanin.* ***Alkhanin***
$C_{15}H_{20}O_4$ 264.321
Isol. from *Balsamita major* (costmary). Cryst. Mp 201-203° (189-191°).

Samek, Z. *et al., Coll. Czech. Chem. Comm.*, 1979, **44**, 1468 (*isol, struct*)
Serkerov, S.V. *et al., Khim. Prir. Soedin.*, 1979, **15**, 326; 488; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 282; 424 (*isol, struct*)
Khafagy, S.M. *et al., Phytochemistry*, 1988, **23**, 1125
Bruno, M. *et al., Phytochemistry*, 1988, **27**, 1201 (*isol*)
Sanz, J.F. *et al., J. Nat. Prod.*, 1990, **53**, 940 (*deriv*)
Sanz, J.F. *et al., Planta Med.*, 1991, **57**, 74 (*deriv*)
Blay, G. *et al., Can. J. Chem.*, 1992, **70**, 817 (*synth*)
Marco, J.A. *et al., J. Nat. Prod.*, 1992, **55**, 476 (*cryst struct*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)
Marco, J.A. *et al., Phytochemistry*, 1994, **37**, 477 (*deriv, pmr, cmr*)
Suzuki, T. *et al., Heterocycles*, 2001, **54**, 865-870 (*synth*)

1,4-Dihydroxy-11(13)-eudesmen-12,6-olide D-460



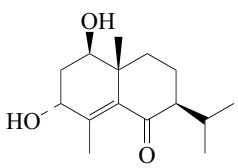
(1α,4β*OH*,6α)-*form*

$C_{15}H_{22}O_4$ 266.336

(1α,4β*OH*,6α)-*form* [50301-94-5]
1α-Hydroxyarbusculin A
Isol. from *Tanacetum vulgare* (tansy). Cryst. Mp 194-196°.

Samek, Z. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 1971 (*Hydroxyarbusculin A*)
Ando, M. *et al., Tetrahedron*, 1977, **33**, 2785 (*synth*)
Bohlmann, F. *et al., J. Nat. Prod.*, 1984, **47**, 663 (*isol, pmr*)
García-Grandos, A. *et al., Tetrahedron*, 1993, **49**, 1091 (*synth*)

1,3-Dihydroxy-4-eudesmen-6-one D-461

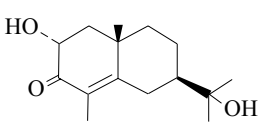


$C_{15}H_{24}O_3$ 252.353

(1β,3α)-*form* [185307-44-2]
Acorusdiol
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D$ -67 (c, 0.03 in MeOH). λ_{max} 240 (ϵ 6260) (MeOH).

Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175-1182 (*isol, pmr, cmr*)

2,11-Dihydroxy-4-eudesmen-3-one D-462



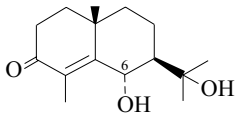
$C_{15}H_{24}O_3$ 252.353

2α-*form* [99957-09-2]
α-Carissanol
Constit. of *Carissa edulis* (agam). Oil. $[\alpha]_D^{20}$ +124 (c, 0.07 in $CHCl_3$).

Achenbach, H. *et al., Phytochemistry*, 1985, **24**, 2325

6,11-Dihydroxy-4-eudesmen-3-one D-463

Carissanol



$C_{15}H_{24}O_3$ 252.353

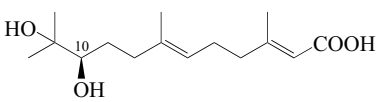
6α-*form* [99957-10-5]
Constit. of *Carissa edulis* (agam). Oil. $[\alpha]_D^{20}$ +66.4 (c, 0.25 in $CHCl_3$).

6β-*form* [99957-11-6]
From *Carissa edulis* (agam). Cryst. Mp 115-118°. $[\alpha]_D^{20}$ +10 (c, 0.3 in $CHCl_3$).

Achenbach, H. *et al., Phytochemistry*, 1985, **24**, 2325

10,11-Dihydroxy-2,6-farnesadien-1-oic acid D-464

[113932-58-4]
10,11-Dihydroxy-3,7,11-trimethyl-2,6-dodecadienoic acid. JH III diol



(2*E*,6*E*,10*R*)-*form*

$C_{15}H_{26}O_4$ 270.368

(2*E*,6*E*,10*R*)-*form* [129785-21-3]
Me ester: [60209-33-8]
$C_{16}H_{28}O_4$ 284.395
Oil. $[\alpha]_D$ +17.4 (c, 2.6 in $CHCl_3$).

(2*E*,6*E*,10*S*)-*form* [40202-97-9]
Oil (as Me ester). $[\alpha]_D$ -12.1 ($CHCl_3$) (Me ester).

Me ester: [37133-77-0]
Viscous oil. $[\alpha]_D^{25}$ -20.1 (c, 0.6 in MeOH) (92% ee). $[\alpha]_D$ -12.1 ($CHCl_3$).

(2*E*,6*E*,10*RS*)-*form* [153379-82-9]
Me ester: [38227-48-4]
Oil. $Bp_{0.03}$ 85° (bath).

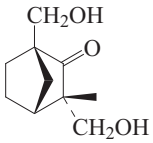
(2*E*,6*E*,10ξ)-*form*
β-D-Glucopyranosyl ester: [204927-92-4]
$C_{21}H_{36}O_9$ 432.51
Present in Riesling wine.

[36999-94-7, 96848-62-3]

Anderson, R.J. *et al., J.A.C.S.*, 1972, **94**, 5379 (*synth*)
Kuhnz, W. *et al., Org. Magn. Reson.*, 1981, **16**, 138 (*cmr*)
Waterman, P.G. *et al., Phytochemistry*, 1985, **24**, 523-527 (*isol*)
Jacobs, H. *et al., J. Nat. Prod.*, 1987, **50**, 507 (*isol*)
Mori, K. *et al., Tetrahedron*, 1987, **43**, 4097 (*synth*)
Etse, J.T. *et al., J. Nat. Prod.*, 1988, **51**, 314 (*isol*)
Crispino, G.A. *et al., Synthesis*, 1993, 777 (*synth*)
Bonnlander, B. *et al., J. Agric. Food Chem.*, 1998, **46**, 1474-1478 (*glucosyl ester*)

9,10-Dihydroxy-2-fenchanone D-465

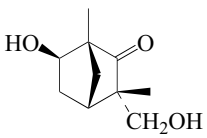
[240495-77-6]
1,3-Bis(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one. 9,10-Dihydroxyfenchone



$C_{10}H_{16}O_3$ 184.235
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ +4.6 (c, 0.4 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 805-808 (*isol, pmr, cmr*)

6,9-Dihydroxyfenchone D-466

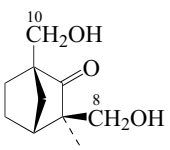


$C_{10}H_{16}O_3$ 184.235

(1*R*,3*S*,4*S*,6*R*)-*form*
6-O-β-D-Glucopyranoside: [217960-73-1]
$C_{16}H_{26}O_8$ 346.377
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -64.5 (c, 0.7 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

8,10-Dihydroxyfenchone D-467

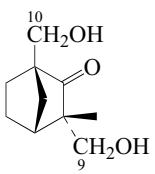


$C_{10}H_{16}O_3$ 184.235

(1*S*,3*R*,4*R*)-*form*
10-O-β-D-Glucopyranoside: [217960-79-7]
$C_{16}H_{26}O_8$ 346.377
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 86-88°. $[\alpha]_D^{23}$ +12.7 (c, 0.3 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

9,10-Dihydroxyfenchone D-468



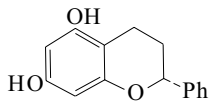
$C_{10}H_{16}O_3$ 184.235

(1*S*,3*S*,4*R*)-*form*
10-O-β-D-Glucopyranoside: [217960-77-5]
$C_{16}H_{26}O_8$ 346.377
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 167-169°. $[\alpha]_D^{26}$ -13.8 (c, 1.4 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

5,7-Dihydroxyflavan D-469

3,4-Dihydro-2-phenyl-2H-1-benzopyran-5,7-diol, 9CI. 5,7-Dihydroxy-2-phenylchroman



(*R*)-*form*

$C_{15}H_{14}O_3$ 242.274

(*R*)-*form*
7-O-β-D-Glucopyranoside: [30984-77-1] ***Koaburanin***
$C_{21}H_{24}O_8$ 404.416
$[\alpha]_D$ -64.2 (EtOH).

(*S*)-*form*
5-Me ether: [35290-20-1] ***7-Hydroxy-5-methoxyflavan***
$C_{16}H_{16}O_3$ 256.301
Isol. from the pith of sago palm. Mp 96-97° (85-87°). $[\alpha]_D^{24}$ -8.22 (c, 1.08 in $CHCl_3$).

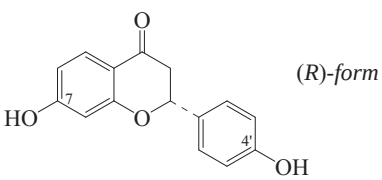
5,7-Di-Me ether: [97640-83-0] *5,7-Dimethoxyflavan*. ***Tephrowatsin E***
$C_{17}H_{18}O_3$ 270.327
Oil.

[39828-25-6]

Ogawa, M. *et al., Yakugaku Zasshi*, 1970, **90**, 1081 (*Koaburanin*)
Cardillo, G. *et al., J.C.S.(C)*, 1971, 3967 (*7-Hydroxy-5-methoxyflavan*)
Gomez, F. *et al., Phytochemistry*, 1985, **24**, 1057
Okamoto, A. *et al., Agric. Biol. Chem.*, 1986, **50**, 1655 (*7-Hydroxy-5-methoxyflavan*)

4′,7-Dihydroxyflavanone D-470

2,3-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. ***Liquiritigenin***



(*R*)-*form*

$C_{15}H_{12}O_4$ 256.257
Log P 2.35 (uncertain value) (calc).

(*R*)-*form*
4′-O-[4-Hydroxycinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]: ***Licorice glycoside D1***
$C_{35}H_{36}O_{15}$ 696.66
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. pale yellow powder. $[\alpha]_D$ -42.9 (c, 1 in MeOH). λ_{max} 218 (log ε 4.54); 228 (log ε 4.44); 280 (log ε 4.34); 314 (log ε 4.4) (MeOH).

4′-O-[4-Hydroxy-3-methoxycinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]: ***Licorice glycoside C1***
$C_{36}H_{38}O_{16}$ 726.687
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow powder + $2H_2O$. $[\alpha]_D$ -9.9 (c, 1 in MeOH). λ_{max}

205 (log ϵ 4.41); 218 (log ϵ 4.33); 231 (log ϵ 4.28); 279 (log ϵ 4.11); 322 (log ϵ 4.17) (MeOH).

(*S*)-*form* [578-86-9]
Isol. from *Glycyrrhiza, Medicago, Myroxylon, Cicer* and all Leguminosae spp. Several glycosides, particularly the rutinoside and neohesperidoside, are important in influencing citrus fruit flavour. Cryst. Mp 203-205°. $[\alpha]_D^{25}$ -36.2 (c, 0.09 in MeOH). Pharmacol. active isomer.

7-O-*β-D-Apiofuranoside, 4′*-O-*β-D-glucopyranoside:* [199796-12-8]
$C_{26}H_{30}O_{13}$ 550.515
Powder. Mp 214-215°.

7-O-*(3*-O-*Acetyl-β-D-apiofuranoside), 4′*-O-*β-D-glucopyranoside:* [199796-13-9]
$C_{28}H_{32}O_{14}$ 592.552
Powder. Mp 201-202°.

4′-O-*β-D-Glucopyranoside:* [551-15-5] ***Liquiritin***. *Liquiritoside*
$C_{21}H_{22}O_9$ 418.399
Isol. from *Glycyrrhiza glabra* (licorice) and *Glycyrrhiza uralensis* (Chinese licorice). Cryst. + $1H_2O$ (EtOH aq.). Mp 212°. Log P -0.47 (uncertain value) (calc).

4′-O-*(6*-O-*Acetyl-β-D-glucopyranoside):* [166531-17-5] ***6′′-Acetylliquiritin***
$C_{23}H_{24}O_{10}$ 460.437
Constit. of *Glycyrrhiza uralensis* (Chinese licorice).

7-O-*β-D-Glucopyranoside:* [5088-75-5] ***Neoliquiritin***. *Glucoliquiritigenin*
$C_{21}H_{22}O_9$ 418.399
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Mp 164-166°. $[\alpha]_D^{18}$ -60.2 (AcOH aq.). Log P -0.75 (uncertain value) (calc).

4′,7-Di-O-*β-D-glucopyranoside:* [93446-18-5] *Liquiritigenin 4′,7-diglucoside.* ***Glucoliquiritin***
$C_{27}H_{32}O_{14}$ 580.541
Isol. from the roots of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. powder + $1H_2O$. $[\alpha]_D^{19}$ -94.9 (c, 1.1 in MeOH).

4′-O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [74639-14-8] *Liquiritin apioside*
$C_{26}H_{30}O_{13}$ 550.515
Found in *Glycyrrhiza uralensis* (Chinese licorice) and *Glycyrrhiza glabra* (licorice). Powder. $[\alpha]_D^{19}$ -79.6 (c, 1.37 in MeOH).

4′-O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside], 7*-O-*β-D-glucopyranoside:* [157226-47-6] ***Glucoliquiritin apioside***
$C_{32}H_{40}O_{18}$ 712.657
Constit. of *Glycyrrhiza glabra* (licorice). Pale yellow prisms ($CHCl_3$/MeOH aq.). Mp 157-158°. $[\alpha]_D^{20}$ -80 (c, 0.35 in MeOH).

7-O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [135432-48-3]
$C_{26}H_{30}O_{13}$ 550.515
Constit. of *Glycyrrhiza glabra* (licorice).

4′-O-*[3*-O-*Acetyl-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [226946-10-7]
$C_{28}H_{32}O_{14}$ 592.552
Constit. of the roots of *Glycyrrhiza uralensis* (Chinese licorice).

4′-O-*[4-Hydroxycinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Licorice glycoside D2***
$C_{35}H_{36}O_{15}$ 696.66
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. pale yellow powder. $[\alpha]_D$ -23.4 (c, 1 in MeOH). λ_{max} 218 (log ϵ 4.66); 228 (log ϵ 4.56); 280 (log ϵ 4.46); 314 (log ϵ 4.54) (MeOH).

4′-O-*[4-Hydroxy-3-methoxycinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Licorice glycoside C2***
$C_{36}H_{38}O_{16}$ 726.687
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. pale yellow powder + $3H_2O$. $[\alpha]_D$ -31.1 (c, 1 in MeOH). λ_{max} 205 (log ϵ 4.59); 217 (log ϵ 4.62); 230 (log ϵ 4.47); 280 (log ϵ 4.31); 322 (log ϵ 4.37) (MeOH).

4′-O-*[1*H-*Indole-3-ylcarbonyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Licorice glycoside E***
$C_{35}H_{35}NO_{14}$ 693.66
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. pale yellow powder. $[\alpha]_D$ -52.9 (c, 1 in MeOH). λ_{max} 206 (log ϵ 4.68); 223 (log ϵ 4.22); 280 (log ϵ 3.83); 285 (log ϵ 3.8) (MeOH).

4′-O-*[α-L-Rhamnopyranosyl-(1→?)-β-D-glucopyranoside]:* [31512-05-7] ***Rhamnoliquiritin***
$C_{27}H_{32}O_{13}$ 564.542
Isol. from *Glycyrrhiza glabra* (licorice). Mp 131°.

7-O-*[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:*
$C_{27}H_{32}O_4$ 420.547

7-Me ether: [61504-06-1] *4′-Hydroxy-7-methoxyflavanone*
$C_{16}H_{14}O_4$ 270.284
Cryst. (C_6H_6/petrol). Mp 150-152° (147°). $[\alpha]_D^{20}$ -53 (c, 0.24 in MeOH).

4′-Me ether: [116384-18-0] *7-Hydroxy-4′-methoxyflavanone*
$C_{16}H_{14}O_4$ 270.284
Cryst. Mp 175-178°. $[\alpha]_D^{21}$ -29 (c, 0.07 in MeOH).

4′-Me ether, 7-O-*α-L-rhamnopyranoside:* [83697-43-2]
$C_{22}H_{24}O_8$ 416.427
Constit. of *Prunus cerasoides* (wild Himalayan cherry). Yellow needles (MeOH aq.). Mp 300° dec.

4′-Me ether, 7-O-*β-D-glucopyranoside:* ***4′-O-Methylglucoliquiritigenin***
$C_{22}H_{24}O_9$ 432.426
Constit. of the roots of *Glycyrrhiza uralensis* (Chinese licorice). Cryst. (EtOH). Mp 173-175°. $[\alpha]_D$ -42.5 (c, 0.8 in MeOH). λ_{max} 215 (log ϵ 4.24); 230 (log ϵ 3.74); 276 (log ϵ 3.39); 314 (log ϵ 3.42); 335 (log ϵ 2.76) (EtOH).

Di-Me ether: [95753-46-1] *4′,7-Dimethoxyflavanone*
$C_{17}H_{16}O_4$ 284.311

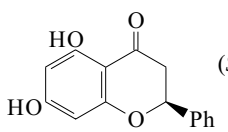
(±)-*form* [41680-09-5]
Cryst. Mp 197-198°.

[25826-69-1, 32274-71-8]

Shinoda, S. *et al., Ber.*, 1934, **67**, 434 (*isol*)
Nordström, C.G. *et al., Arch. Biochem. Biophys.*, 1956, **60**, 329 (*7-glycosides*)
Arakawa, H. *et al., Annalen*, 1961, **636**, 113 (*abs config*)
Kovalev, I.P. *et al., Zh. Obshch. Khim.*, 1963, **33**, 1670 (*ir*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
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Wong, E. *et al., Biochim. Biophys. Acta*, 1965, **111**, 358 (*biosynth*)
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Van Hulle, C. *et al., Planta Med.*, 1971, **20**, 278 (*Rhamnoliquiritin*)
de Oliveira, A.B. *et al., Phytochemistry*, 1972, **11**, 3515 (*isol*)
Donnelly, D.M.X. *et al., J.C.S. Perkin 1*, 1973, 1737 (*isol*)
Parthasarathy, M.R. *et al., Phytochemistry*, 1976, **15**, 226 (*isol*)
Camarda, L. *et al., Aust. J. Chem.*, 1977, **30**, 873 (*deriv*)
Ingham, J.L. *et al., Biochem. Syst. Ecol.*, 1979, **7**, 29 (*isol*)
Shrivastava, S.P. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 604 (*4′-Me ether 7-rhamnoside*)
Shrivastava, S.P. *et al., Phytochemistry*, 1982, **21**, 1464 (*4′-Me ether 7-xyloside*)
Yahara, S. *et al., Phytochemistry*, 1984, **23**, 2108 (*4′,7-diglucoside*)
Nakanishi, T. *et al., Phytochemistry*, 1985, **24**, 339 (*apiofuranosylglucoside*)
Crins, W.J. *et al., Phytochemistry*, 1987, **26**, 2128 (*isol*)
Achenbach, H. *et al., Phytochemistry*, 1988, **27**, 1835 (*derivs*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1056 (*Glucoliquiritin apioside*)
Wang, B. *et al., Yaoxue Xuebao*, 1997, **32**, 199-202 (*7-apioside 4′-glucosides*)
Hatano, T. *et al., Phytochemistry*, 1998, **47**, 287-293 (*Licorice glycosides*)
Youssef, D.T.A. *et al., Phytochemistry*, 1998, **49**, 2579-2583 (*isol, ir, pmr, cmr*)
Yin, S. *et al., CA*, 1999, **131**, 29799b (*4′-3-Acetylapiosylglucoside*)
Shults, E.E. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2000, **36**, 362-368 (*4′-O-Methylglucoliquiritigenin*)

5,7-Dihydroxyflavanone D-471

[68745-38-0]
*2,3-Dihydro-5,7-dihydroxy-2-phenyl-4*H-*1-benzopyran-4-one, 9CI.* ***Pinocembrin***



(*S*)-*form*

$C_{15}H_{12}O_4$ 256.257
λ_{max} 229 (ϵ 14800); 290 (ϵ 28800) (MeOH/HCl) (Derep). λ_{max} 246 (ϵ 7410); 324 (ϵ 25700) (MeOH/NaOH) (Derep). λ_{max} 246 (ϵ 5130); 323 (ϵ 28800) (MeOH) (Derep). λ_{max} 246 (ϵ 5100); 287 (ϵ 15500); 320 (ϵ 7460); 323 (ϵ 29000) (MeOH) (Berdy). λ_{max} 211 ; 290 ; 324 (EtOH) (Berdy). λ_{max} 245 ; 246 (ϵ 7400); 324 (ϵ 25500); 325 (MeOH/NaOH) (Berdy).

(*R*)-*form*

7-O-*Benzoyl:* [153653-38-4] *7*-O-*Benzoyloxy-5-hydroxyflavanone. Pinocembrin 7-benzoate*

$C_{22}H_{16}O_5$ 360.365

7-Me ether: ***(+)-Pinostrobin***
$C_{16}H_{14}O_4$ 270.284
Cryst. Mp 100-101°. $[\alpha]_D^{25}$ +5 (c, 0.05 in MeOH).

(S)-form [480-39-7]
Isol. from many plants incl. food plants. Cryst. (MeOH). Mp 192-193°. $[\alpha]_D^{15}$ -45.3 (c, 0.9 in Me_2CO). The abs. config. of isolates is not very clear: opt. rotns. not reported in most cases.

7-O-α-L-Rhamnopyranoside: Pinocembrin 7-rhamnoside
$C_{21}H_{22}O_8$ 402.4

5-O-β-D-Glucopyranoside: Pinocembrin 5-glucoside. ***Verecundin***
$C_{21}H_{22}O_9$ 418.399
Cryst. + $2H_2O$. Mp 135°. $[\alpha]_D^{14}$ -71.1 (60% Me_2CO aq.).

7-O-β-D-Glucopyranoside: [75829-43-5] *Pinocembrin 7-glucoside.* ***Pinocembroside***
$C_{21}H_{22}O_9$ 418.399
Needles (MeOH). Mp 139-141°. $[\alpha]_D^{15}$ -89 (c, 0.2 in MeOH).

7-O-β-D-Glucuronopyranoside: [117160-67-5] *Pinocembrin 7-glucuronide*
$C_{21}H_{20}O_{10}$ 432.383

7-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [117160-68-6] *Pinocembrin 7-gentiobioside*
$C_{27}H_{32}O_{14}$ 580.541

7-O-[β-D-Glucopyranosyl-(1→6)-2-O-acetyl-β-D-glucopyranoside]: [79541-04-1]
$C_{29}H_{34}O_{14}$ 606.579
Mp 130-135°. $[\alpha]_D^{25}$ -62 (c, 0.2 in Py).

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [13241-31-1] ***Sarotanoside.*** *Isosarotanoside. Onychin. Pinocembrin 7-neohesperidoside*
$C_{27}H_{32}O_{13}$ 564.542
Cryst. (EtOH). Mp 277-280° (274-276°). $[\alpha]_D$ -119.6 (c, 2 in Py). λ_{max} 213 (ε 28840); 286 (ε 18200); 330 (ε 3162) (MeOH) (Berdy).

7-O-[α-L-Rhamnopyranosyl-(1→2)-6-O-acetyl-β-D-glucopyranoside]: [82206-45-9] *6-′′O-Acetylsarotanoside*
$C_{29}H_{34}O_{15}$ 622.579

7-O-[3-O-Acetyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [82206-44-8] ***3′′′-O-Acetylsarotanoside***
$C_{29}H_{34}O_{14}$ 606.579
No phys. props. reported.

7-O-[4-O-Acetyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [80443-11-4] ***4′′′-O-Acetylsarotanoside***
$C_{29}H_{34}O_{14}$ 606.579
Cryst. (MeOH). Mp 220-225°. $[\alpha]_D^{20}$ -103.1 (c, 0.75 in Py).

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [118985-31-2] *Pinocembrin 7-rutinoside*
$C_{27}H_{32}O_{13}$ 564.542

7-O-[β-D-Apiofuranosyl-(1→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:
$C_{31}H_{38}O_{17}$ 682.631
Amorph. solid. $[\alpha]_D$ -119 (c, 0.3 in MeOH). λ_{max} 284 (log ε 4.54); 326 (sh) (log ε 3.78) (MeOH).

5-Me ether: [36052-37-6] *7-Hydroxy-5-methoxyflavanone.* ***Alpinetin***
$C_{16}H_{14}O_4$ 270.284
Cryst. (Me_2CO). Mp 218-220°. $[\alpha]_D^{15}$ -46 (c, 0.9 in $CHCl_3$).

7-Me ether: [480-37-5] *5-Hydroxy-7-methoxyflavanone.* ***Pinostrobin.*** *Glyyunnanin*
$C_{16}H_{14}O_4$ 270.284
Needles (MeOH). Mp 112-113° (100-101°). $[\alpha]_D^{20}$ -56 ($CHCl_3$). Config. of Glyunnanin not detd..

7-Me ether, 5-O-β-D-glucopyranoside: [115799-14-9] *Pinostrobin 5-glucoside*
$C_{22}H_{24}O_9$ 432.426
Isol. from bark of morello cherry. Powder.

Di-Me ether: [36052-66-1] *5,7-Dimethoxyflavanone*
$C_{17}H_{16}O_4$ 284.311
Cryst. (Me_2CO). Mp 159-160°. $[\alpha]_D^{15}$ -45.8 (1:1 $Me_2CO/CHCl_3$).

7-O-(3-Methyl-2-butenyl): [94393-10-9] *5-Hydroxy-7-prenyloxyflavanone.* ***7-O-Prenylpinocembrin***
$C_{20}H_{20}O_4$ 324.376
Oil.

7-O-(3-Methyl-2-butenyl), 5-Me ether: [96386-73-1] *5-Methoxy-7-prenyloxyflavanone*
$C_{21}H_{22}O_4$ 338.402
Oil.

7-O-(2,3-Epoxy-3-methylbutyl): [117611-69-5]
$C_{20}H_{20}O_5$ 340.375
No phys. props. reported.

7-O-[4-(1-Hydroxyethyl)phenyl] ether: [108544-83-8] *5-Hydroxy-7-[4-(1-hydroxyethyl)phenoxy]flavanone*
$C_{23}H_{20}O_5$ 376.408
Cryst. Mp 107°.

7-O-(3,7-Dimethyl-2,6-octadienyl)(Z-): [140158-56-1] *5-Hydroxy-7-neryloxyflavanone*
$C_{25}H_{28}O_4$ 392.494

7-O-[4,6-[(S)-4,4′,5,5′,6,6′-Hexahydroxydiphenoyl]-β-D-glucopyranoside]:
$C_{35}H_{28}O_{17}$ 720.596
Yellow powder. $[\alpha]_D^{25}$ -122 (c, 0.5 in MeOH). λ_{max} 212 (log ε 4.6); 281 (log ε 4.37) (MeOH).

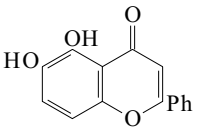
7-O-[4,6-[(S)-4,4′,5,5′,6,6′-Hexahydroxydiphenoyl]-3-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranoside]:
$C_{42}H_{32}O_{21}$ 872.702
Yellow powder. $[\alpha]_D^{25}$ -56 (c, 0.6 in MeOH). λ_{max} 215 (log ε 4.94); 282 (log ε 4.67) (MeOH).

[1225-38-3, 30784-66-8, 61490-55-9, 163660-09-1]

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Hasegawa, M. *et al., J.A.C.S.*, 1957, **79**, 450; 1738 (*Verecundin*)
Arakawa, H. *et al., Annalen*, 1960, **636**, 114 (*abs config*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
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Audier, H. *et al., Bull. Soc. Chim. Fr.*, 1966, 2892 (*ms*)
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Asakawa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 271 (*isol*)
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Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2058 (*isol*)
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Miyakado, M. *et al., Phytochemistry*, 1976, **15**, 846 (*isol*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799 (*nmr*)
Pomilio, A.B. *et al., Phytochemistry*, 1979, **18**, 1410 (*Sarotanoside*)
Tanaka, N. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2843 (*Pinocembroside*)
Gonzalez, M.D. *et al., Phytochemistry*, 1981, **20**, 1174; 1982, **21**, 757 (*isol, deriv*)
Jaipetch, T. *et al., Aust. J. Chem.*, 1982, **35**, 351 (*isol*)
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Bohlmann, F. *et al., Phytochemistry*, 1984, **23**, 1338 (*7-O-Prenylpinocembrin*)
Norbedo, C. *et al., Phytochemistry*, 1984, **23**, 2698 (*7-O-2,3-epoxy-3-methylbutanoyl*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 271 (*5-Methoxy-7-prenyloxyflavanone*)
Talapatra, B. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 561 (*isol, synth*)
Kaoujadi, M. *et al., J. Nat. Prod.*, 1986, **49**, 153 (*7-O-Prenylpinocembrin*)
Jakupovic, J. *et al., Phytochemistry*, 1987, **26**, 803 (*hydroxyethylphenyl ether*)
Kapetanidis, J. *et al., Pharm. Acta Helv.*, 1988, **63**, 206 (*7-rutinoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988, 358 (*occur*)
Gonzalez, A.G. *et al., Phytochemistry*, 1989, **28**, 2871
Shoja, M. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1989, **189**, 89 (*cryst struct, Pinostrobin*)
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Randriaminahy, M. *et al., Z. Naturforsch., C*, 1992, **47**, 10 (*neryl ether*)
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Bilia, A.R. *et al., Phytochemistry*, 1993, **33**, 1449 (*7-Me ether 5-glucoside*)
Hoeneisen, M. *et al., Phytochemistry*, 1993, **34**, 1653 (*7-benzoyl*)
Hounghton, P.J. *et al., Pharm. Pharmacol. Lett.*, 1997, **7**, 96-98 (*activity*)
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Yuldashev, M.P. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2001, **37**, 224-225 (*Pinocembroside*)
Hodgetts, K.J. *et al., Tet. Lett.*, 2001, **42**, 3763-3766 (*Pinostrobin, synth*)
Lin, J.-H. *et al., J. Nat. Prod.*, 2002, **65**, 638-640 (*7-apiosylapiosylglucoside*)

5,6-Dihydroxyflavone, 8CI D-472

[6665-66-3]
5,6-Dihydroxy-2-phenyl-4H-1-benzopyran-4-one, 9CI



$C_{15}H_{10}O_4$ 254.242
Yellow cryst. (EtOH). Mp 190°.

Di-Ac:
Cryst. (EtOH). Mp 167°.

5-Me ether:6-Hydroxy-5-methoxyflavone
$C_{16}H_{12}O_4$ 268.268
Cryst. (MeOH). Mp 185°.

6-Me ether: [85395-95-5] *5-Hydroxy-6-methoxyflavone*
$C_{16}H_{12}O_4$ 268.268
Yellow cryst. (EtOH). Mp 129-130°.

Di-Me ether: [33554-48-2] *5,6-Dimethoxyflavone*
$C_{17}H_{14}O_4$ 282.295
Isol. from bark of *Casimiroa edulis* (Mexican apple). Cryst. (MeOH). Mp 199°.

Baker, W. *et al., J.C.S.*, 1939, 956 (*synth*)
Iyer, R.N. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1953, **37**, 629 (*synth*)
Iriarte, J. *et al., J.C.S.*, 1956, 4170 (*isol, uv*)
Looker, J.H. *et al., J. Het. Chem.*, 1966, **3**, 55 (*ir*)
Dominguez, X.A. *et al., Phytochemistry*, 1972, **11**, 2648 (*5,6-Dimethoxyflavone*)
Wollenweber, E. *et al., Biochem. Physiol. Pflanz.*, 1986, **181**, 667 (*5-Hydroxy-6-methoxyflavone*)

5,7-Dihydroxyflavone D-473

[480-40-0]
*5,7-Dihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI*. ***Chrysin***. *Chrysinic acid. Ois 3*

$C_{15}H_{10}O_4$ 254.242
Yellowish plates. Sol. Et_2O, bases; fairly sol. $CHCl_3$, EtOH; poorly sol. H_2O. Mp 290-291° (275°). pK_{a1} 9.05; pK_{a2} 7.42 (20°,50% EtOH). pK_{a1} 12.37; pK_{a2} 8.37 (25°,50% dioxan). λ_{max} 249 ; 272 ; 316 (MeOH) (Berdy). λ_{max} 252 ; 282 ; 332 ; 382 (MeOH/NaOH) (Berdy). λ_{max} 212 ; 269 ; 318 (EtOH) (Berdy).

► LK8329050

5-O-β-D-Glucopyranoside: [1329-10-8] ***Toringin***
$C_{21}H_{20}O_9$ 416.384
Occurs in *Malus* spp.. Needles (MeOH). Mp 240°. $[\alpha]_D^{25}$ -71.3 (Py). Originally descr. as the 7-glycoside.

7-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:
$C_{27}H_{30}O_{13}$ 562.526
Constit. of the fruit of *Cyclanthera pedata* (achoccha). Amorph. yellow powder. $[\alpha]_D^{25}$ -41.2 (c, 0.1 in MeOH). λ_{max} 210 ; 275 ; 330 (MeOH).

Di-Me ether: [21392-57-4] *5,7-Dimethoxyflavone*
$C_{17}H_{14}O_4$ 282.295
Constit. of *Leptospermum scoparium* (red tea). Cryst. ($CHCl_3$/hexane). Mp 154° (149-150°). λ_{max} 263 ; 305 (MeOH) (Berdy). λ_{max} 263 ; 305 (MeOH/NaOH) (Berdy).

Marsh, C.A. *et al., Biochem. J.*, 1955, **59**, 58 (*isol, deriv*)
Dev, B. *et al., Fresenius' Z. Anal. Chem.*, 1963, **196**, 178 (*synth, use, deriv*)
Jain, P.K. *et al., Synthesis*, 1982, 221 (*synth, 5,7-Dimethoxyflavone*)
Mayer, R. *et al., Planta Med.*, 1993, **59**, 269 (*5,7-Dimethoxyflavone*)
Montoro, P. *et al., J. Agric. Food Chem.*, 2002, **49**, 5156-5160 (*7-4-rhamnosylglucoside*)

6,7-Dihydroxyflavone, 8CI D-474

[38183-04-9]
*6,7-Dihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{10}O_4$ 254.242
Cream needles (AcOH aq.). Mp 254°.

Di-Ac:
$C_{19}H_{14}O_6$ 338.316
Needles (EtOH). Mp 201°.

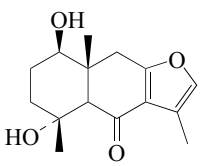
6-Me ether: [38070-97-2] *7-Hydroxy-6-methoxyflavone*. ***Trigraecum***
$C_{16}H_{12}O_4$ 268.268
Isol. from *Trigonella foenum-graecum* (fenugreek). Needles (EtOH/MeOH). Mp 246-247° (149-151°).

7-Me ether: [30797-59-2] *6-Hydroxy-7-methoxyflavone. Isotrigraecum*
$C_{16}H_{12}O_4$ 268.268
Prisms (EtOH aq.). Mp 203-204°.

Di-Me ether: [26964-27-2] *6,7-Dimethoxyflavone*
$C_{17}H_{14}O_4$ 282.295
Needles (EtOH aq.). Mp 189°.

Hattori, S. *et al., Acta Phytochim.*, 1932, **6**, 131 (*synth*)
Chadha, T.C. *et al., J.C.S.*, 1933, 1073 (*synth*)
Bhardwaj, D.K. *et al., Proc. Indian Natl. Sci. Acad., Part A*, 1987, **53**, 463; 1988, **54**, 638 (*Trigraecum*)
Pathak, V. *et al., Phytochemistry*, 1997, **46**, 1219-1223 (*Trigraecum*)

1,4-Dihydroxyfuranoeremophilan-6-one D-475

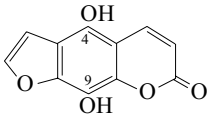


$C_{15}H_{20}O_4$ 264.321
(1β,4α)-*form* [217817-09-9] ***Curcolonol***
Constit. of *Curcuma zedoaria* (zedoary). Cryst. (Me_2CO). Mp 183-184°. $[\alpha]_D^{25}$ 0 (c, 2 in EtOH).

Syu, W.-J. *et al., J. Nat. Prod.*, 1998, **61**, 1531-1534 (*isol, pmr, cmr*)

4,9-Dihydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI D-476

[14348-23-3]
4,9-Dihydroxypsoralen. 8-Hydroxybergaptol. 5,9-Dihydroxypsoralen. Psoralen hydroquinone



$C_{11}H_6O_5$ 218.165
9CI numbering shown. Other systems have been used.Green cryst. Mp 270° dec.

4-O-β-D-Glucopyranoside:
$C_{17}H_{16}O_{10}$ 380.307
Light brown powder. Mp 290° dec. $[\alpha]_D^{25}$ -25 (c, 0.04 in Py) (approximate value). λ_{max} 199 (log ε 4.4); 221 (log ε 4.6); 244 (log ε 4.3); 269 (log ε 4.4); 282 (log ε 4.2); 313 (log ε 4.2) (H_2O).

4-Me ether: [1603-47-0] *9-Hydroxy-4-methoxyfuro[3,2-g][1]benzopyran-7-one, 9CI*. ***9-Hydroxy-4-methoxypsoralen***. *9-Hydroxy-5-methoxypsoralen. 8-Hydroxy-5-methoxypsoralen. 8-Hydroxybergapten. 9-Hydroxybergapten*
$C_{12}H_8O_5$ 232.192
Isol. from *Casimiroa edulis* (Mexican apple). Yellow cryst. Mp 222.5-223°.

4-Me ether, 9-O-β-D-glucopyranoside: [115356-06-4]
$C_{18}H_{18}O_{10}$ 394.334
Constit. of *Apium graveolens*. Needles ($CHCl_3$/MeOH). Mp 230°.

Di-Me ether: See Isopimpinellin, I-113

4-O-Isopropyl, 9-Me ether: [39262-34-5] ***Tederin***
$C_{15}H_{14}O_5$ 274.273
Cryst. (EtOH). Mp 126-127°.

4-O-(3-Methyl-2-butenyl), 9-Me ether: [14348-22-2] ***Cnidilin***. *Isophellopterin. Knidilin*
$C_{17}H_{16}O_5$ 300.31
Cryst. (EtOH). Mp 117-118°.

9-O-(3-Methyl-2-butenyl), 4-Me ether: See Phellopterin in *The Combined Chemical Dictionary.*

9-O-(2,3-Epoxy-3-methylbutyl), 4-Me ether: See Byakangelicol in *The Combined Chemical Dictionary.*

9-O-(2,3-Dihydroxy-3-methylbutyl), 4-Me ether: See Byakangelicin, B-264

Bis-O-(3-methyl-2-butenyl): [14348-21-1] ***Cnidicin***. *Knidicin*
$C_{21}H_{22}O_5$ 354.402
Cryst. (EtOH). Mp 78-79°.

Bis-O-(2,3-epoxy-3-methylbutyl): [77063-74-2] ***Sen-byakangelicol***
$C_{21}H_{22}O_7$ 386.401
Cryst. Mp 102-103°. $[\alpha]_D^{25}$ +10 ($CHCl_3$).

Bis-O-(2,3-dihydroxy-3-methylbutyl): [188818-25-9]
$C_{21}H_{26}O_9$ 422.431
$[\alpha]_D^{30}$ +34 (c, 0.1 in MeOH). λ_{max} 218 (log ε 2.03); 242 (log ε 2.68); 249 (log ε 2.69); 267 (log ε 2.73); 312 (log ε 2.79) (MeOH).

9-O-(1,1-Dimethyl-2-propenyl), 4-Me ether: [57419-90-6] ***8-(1,1-Dimethylallyloxy)bergapten***
$C_{17}H_{16}O_5$ 300.31
Cryst. (Et_2O/petrol). Mp 90°.

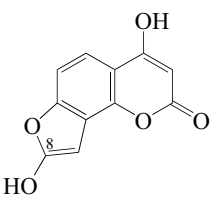
9-O-(3,7-Dimethyl-2,6-octadienyl), 4-Me ether: [17182-52-4] ***9-Geranyloxy-4-methoxypsoralen***. *5-Methoxy-8-gerany-*

loxypsoralen
$C_{22}H_{24}O_5$ 368.429
Yellow cryst. (EtOAc). Mp 53-54°.

4-O-*(3,7-Dimethyl-2,6-octadienyl), 4-Me ether:* [69239-53-8]
$C_{22}H_{24}O_5$ 368.429
Constit. of *Citrus medica* (citron). Cryst. Mp 74.5-75.5°.

Briggs, L.H. *et al., Tetrahedron*, 1958, **2**, 256 (*isol, deriv*)
Brokke, M.E. *et al., J.O.C.*, 1959, **24**, 523 (*synth*)
Komissarenko, N.F. *et al., Khim. Prir. Soedin.*, 1966, **2**, 375; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 307 (*Cnidilin*)
Stanley, W.L. *et al., Phytochemistry*, 1967, **6**, 585 (*deriv*)
González, A.G. *et al., An. Quim.*, 1972, **68**, 425 (*Tederin*)
Abu-Mustafa, G.A. *et al., J. Het. Chem.*, 1973, **10**, 443 (*bibl*)
Bohlmann, F. *et al., Chem. Ber.*, 1975, **108**, 2955 (*deriv*)
Sokolova, A.I. *et al., Khim. Prir. Soedin.*, 1976, **12**, 166; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 150 (*4-Methoxy-9-gernanyloxypsoralen*)
Fujiwara, H. *et al., Yakugaku Zasshi*, 1980, **100**, 1258 (*deriv*)
Reed, M.W. *et al., J.O.C.*, 1988, **53**, 4166 (*synth*)
Ahluwalia, V.K. *et al., Phytochemistry*, 1988, **27**, 1181 (*deriv*)
Kwon, Y.-S. *et al., Phytochemistry*, 1997, **44**, 887 (*bis-dihydroxymethylbutyl*)
Xiao, Y.-Q. *et al., Yaoxue Xuebao*, 2001, **36**, 519-522 (*4-glucoside*)
Niu, X.-M. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 33-41 (*4-glucoside*)

4,8-Dihydroxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one D-477

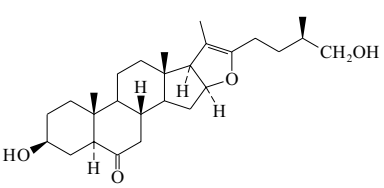


$C_{11}H_6O_5$ 218.165

8-Me ether: [196503-96-5] *4-Hydroxy-8-methoxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9CI*
$C_{12}H_8O_5$ 232.192
Constit. of the leaves of *Camellia sinensis* (Japanese tea). Mp 212°.

Banerjee, J. *et al., Nat. Prod. Sci.*, 1997, **3**, 11-13 (*isol, pmr, cmr, ms*)

3,26-Dihydroxyfurost-20(22)-en-6-one D-478

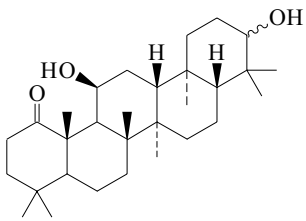


$C_{27}H_{42}O_4$ 430.626
(3β,5α,25*R*)-*form*
26-O-*β*-D-*Glucopyranoside, 3*-O-*[β*-D-*xylopyranosyl-(1→4)-[α*-L-*arabinopyranosyl-(1→6)]-β*-D-*glucopyranoside]:* [172589-64-9] ***Chinenoside II***
$C_{49}H_{78}O_{22}$ 1019.142
Constit. of *Allium chinense* (rakkyo). Amorph. powder. $[\alpha]_D$ -63.1 (c, 0.43 in Py).

26-O-*β*-D-*Glucopyranoside, 3*-O-*[α*-L-*arabinopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [172519-52-7] ***Chinenoside III***
$C_{44}H_{70}O_{18}$ 887.026
Constit. of *Allium chinense* (rakkyo). Amorph. powder. $[\alpha]_D$ -42.8 (c, 0.6 in Py).

Peng, J.-P. *et al., Phytochemistry*, 1996, **41**, 283 (*isol, pmr, cmr*)
Zhang, Y.W. *et al., Planta Med.*, 2000, **66**, 114-118; 119-126 (*activity, Chinenoside II*)

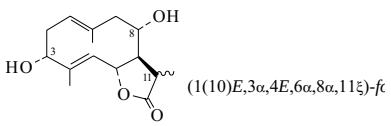
11,21-Dihydroxy-1-gamma-ceranone D-479



$C_{30}H_{50}O_3$ 458.723
(11β,21ξ)-*form* [87018-23-3] ***Coriandrinonediol***
Constit. of *Coriandrum sativum* (coriander). Cryst. Mp 285-290°. $[\alpha]_D$ +38.3.

Naik, C.G. *et al., Curr. Sci.*, 1983, **52**, 598 (*isol*)

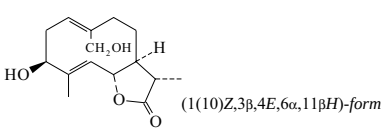
3,8-Dihydroxy-1(10),4-germacradien-12,6-olide D-480



$C_{15}H_{22}O_4$ 266.336
(1(10)*E*,3α,4*E*,6α,8α,11ξ)-*form*
Di-Ac: [39262-27-6] ***Millefin***
$C_{19}H_{26}O_6$ 350.411
Constit. of *Achillea millefolium* (yarrow). Cryst. Mp 209-210°.

Kasymov, Sh.Z. *et al., Khim. Prir. Soedin.*, 1972, **8**, 247; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 246 (*Millefin*)

3,14-Dihydroxy-1(10),4-germacradien-12,6-olide D-481



$C_{15}H_{22}O_4$ 266.336
(1(10)*Z*,3β,4*E*,6α,11β*H*)-*form* [102518-83-2] ***3,14-Dihydroxy-11,13-dihydrocostunolide***
Constit. of *Lactuca sativa* (lettuce). Cryst. Mp 110°. $[\alpha]_D^{24}$ +110 (c, 0.1 in MeOH).

3-O-*β*-D-*Glucopyranoside:*
$C_{21}H_{32}O_9$ 428.478
Gum.

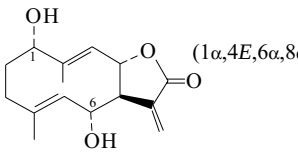
(1(10)*E*,3β,4*E*,6α,11β*H*)-*form*
3-O-*β*-D-*Glucopyranoside:* ***Lactuside B***
$C_{21}H_{32}O_9$ 428.478
Amorph. $[\alpha]_D^{22}$ +21.9 (c, 0.98 in MeOH).

14-Aldehyde: [102488-14-2] *3-Hydroxy-14-oxo-1(10),4-germacradien-12,6-olide.* ***Lactulide A***
$C_{15}H_{20}O_4$ 264.321
Cryst. (MeOH). Mp 191.5-195°. $[\alpha]_D^{25}$ -82.1 (c, 0.95 in Py).

14-Aldehyde, 3-O-*β*-D-*glucopyranoside:* [106009-43-2] ***Lactuside A***
$C_{21}H_{30}O_9$ 426.463
Amorph. $[\alpha]_D^{25}$ -73.8 (c, 0.84 in MeOH).

Mahmoud, Z.F. *et al., Phytochemistry*, 1986, **25**, 747
Nishimura, K. *et al., Phytochemistry*, 1986, **25**, 2375
Kisiel, W. *et al., Phytochemistry*, 1997, **46**, 1241-1243 (*Lactuca virosa glucoside*)

1,6-Dihydroxy-4,9,11(13)-germacratrien-12,8-olide D-482



$C_{15}H_{20}O_4$ 264.321
(1α,4*E*,6α,8α,9*E*)-*form* [71030-09-6] ***Tavulin***. *Tabulin*
Constit. of *Tanacetum vulgare* (tansy). Cryst. Mp 160-161°.

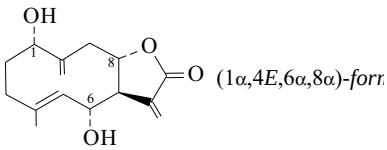
(1β,4*E*,6α,8α,9*Z*)-*form*
6-Ac: [72811-84-8] ***Tulirinol***
$C_{17}H_{22}O_5$ 306.358
Cryst. ($Et_2O/CHCl_3$). Mp 204-206°. $[\alpha]_D^{23}$ -51 (c, 0.3 in MeOH). λ_{max} 208 (ε 21400) (MeOH) (Berdy).

(1β,4*E*,6α,8β,9*Z*)-*form*
6-(2-Methylpropanoyl): [111625-64-0] ***Subcordatolide D***
$C_{19}H_{26}O_5$ 334.411
Cryst. ($CHCl_3$/hexane). Mp 246° dec.

El-Feraly, F.S. *et al., J.C.S. Perkin 1*, 1973, 355 (*synth*)
Yunusov, A.I. *et al., Khim. Prir. Soedin.*, 1979, **15**, 101; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 88 (*Tavulin*)
Doskotch, R.W. *et al., J.O.C.*, 1980, **45**, 1441 (*Tulirinol*)
Ober, A.G. *et al., J. Nat. Prod.*, 1987, **50**, 604 (*Subcordatolide D*)

1,6-Dihydroxy-4,10(14),11(13)-germacratrien-12,8-olide D-483

[119875-15-9]



(1α,4*E*,6α,8α)-*form*

$C_{15}H_{20}O_4$ 264.321

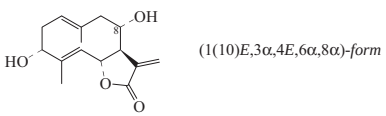
(1β,4*E*,6α,8α)-*form* [41653-76-3]
Tatridin B. *1β-Hydroxy-1-desoxotamirin*
Isol. from *Tanacetum vulgare* (tansy). Gum. $[\alpha]_D^{24}$ +38 (c, 0.2 in $CHCl_3$).

[88243-75-8, 88243-76-9]

Appendino, G. *et al., Gazz. Chim. Ital.*, 1986, **116**, 57 (*cryst struct, Tatridin B*)

3,8-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide D-484

3,8-Dihydroxycostunolide



(1(10)*E*,3α,4*E*,6α,8α)-*form*

$C_{15}H_{20}O_4$ 264.321

(1(10)*E*,3α,4*Z*,6α,8α)-*form*

8-Angeloyl: ***3-Epinobilin***
$C_{20}H_{26}O_5$ 346.422
Isol. from *Anthemis nobilis* (Roman chamomile) flowers. Mp 137°.

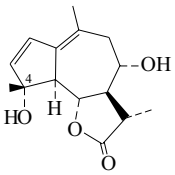
(1(10)*E*,3β,4*Z*,6α,8α)-*form*

8-Angeloyl: [31824-11-0] ***Nobilin***
$C_{20}H_{26}O_5$ 346.422
Constit. of *Anthemis nobilis* (Roman chamomile). Cryst. (EtOH). Mp 177-178°. $[\alpha]_D$ 0.

3-Ketone, 8-angeloyl: [63529-14-6] ***3-Dehydronobilin***
$C_{20}H_{24}O_5$ 344.407
Isol. from *Anthemis nobilis* (Roman chamomile). Cryst. (EtOH/$CHCl_3$). Mp 205°. $[\alpha]_D^{20}$ +136.6 (c, 0.526 in MeOH).

Benesova, V. *et al., Tet. Lett.*, 1970, 5017 (*Nobilin*)
Holub, M. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 1053 (*Nobilin, Epinobilin, Dehydronobilin*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 471-474; 1979, **18**, 847; 1981, **20**, 1613; 2431; 1985, **24**, 1319-1321 (*3-Acetoxy-8-tigloyloxycostunolide, 3-Hydroxyliacylindrolide, Deacetylprovincialin, Hydroxydeoxyprovincialin, other esters*)
Bohlmann, F. *et al., Annalen*, 1984, 250
Gil, R.R. *et al., Phytochemistry*, 1992, **31**, 593 (*deriv*)
Jakupovic, J. *et al., Phytochemistry*, 1992, **31**, 863 (*derivs*)

4,8-Dihydroxy-1(10),2-guaiadien-12,6-olide D-485



(4α,5α,6α,8α,11α)-*for*

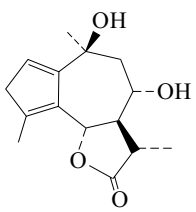
$C_{15}H_{20}O_4$ 264.321

(4α,5α,6α,8α,11α)-*form*

8-Ac: [29041-35-8] ***Matricin***. *Prochamazulene*
$C_{17}H_{22}O_5$ 306.358
Constit. of *Matricaria chamomilla* (German chamomile). Cryst. Mp 158-160°. $[\alpha]_D^{20}$ -131 (c, 1.96 in $CHCl_3$). Log P -0.52 (calc). Component of commercially available chamomile extracts.

Goeters, S. *et al., Planta Med.*, 2001, **67**, 292-294 (*Matricin, abs config*)

8,10-Dihydroxy-1,4-guaiadien-12,6-olide D-486



$C_{15}H_{20}O_4$ 264.321

(6α,8α,10β,11β*H*)-*form*

8-Ac: [71616-00-7] ***Achillicin***. *8-Acetoxyartabsin*
$C_{17}H_{22}O_5$ 306.358
Constit. of *Achillea millefolium* (yarrow). Cryst.

8-Angeloyl: ***8-Angeloyloxyartabsin***
$C_{20}H_{26}O_5$ 346.422

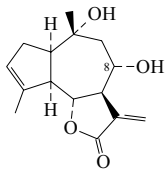
8-Tigloyl: ***8-Tigloyloxyartabsin***
$C_{20}H_{26}O_5$ 346.422

1β,2β;4β,5β-Diepoxide:1,2:4,5-Diepoxy-8,10-dihydroxy-12,6-guaianolide
$C_{15}H_{20}O_6$ 296.319

1β,2β;4β,5β-Diepoxide, 8-angeloyl: [393860-80-5]
$C_{20}H_{26}O_7$ 378.421
$[\alpha]_D^{20}$ +2.7 (c, 0.16 in $CHCl_3$). λ_{max} 222 (MeOH aq.).

Banh-Nhu, C. *et al., Phytochemistry*, 1979, **18**, 331 (*isol*)
Schröder, H. *et al., Phytochemistry*, 1994, **36**, 1449 (*struct, bibl*)
Glasl, S. *et al., Phytochemistry*, 2001, **58**, 1189-1194 (*diepoxide angeloyl*)

8,10-Dihydroxy-3,11(13)-guaiadien-12,6-olide D-487



(1α,5α,6α,8α,10α)-*form*

$C_{15}H_{20}O_4$ 264.321

(1α,5α,6α,8α,10α)-*form* [21982-83-2]
Cumambrin B. *8-Hydroxycumambranolide. Artenovin*
Cryst. (EtOAc/Et_2O). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 178-180°. $[\alpha]_D$ +92.5 (c, 5.58 in $CHCl_3$). λ_{max} 212 (ε 12200) (EtOH) (Berdy).
▶ ME6360000

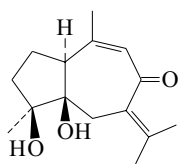
11β,13-Dihydro, 8-Ac: [20482-39-7] ***Dihydrocumambrin A***
$C_{17}H_{24}O_5$ 308.374
From *Chrysanthemum coronarium* (chop-suey greens). Cryst. Mp 174°. $[\alpha]_D^{24}$ +44 (c, 0.08 in $CHCl_3$).

(1α,5α,6α,8β,10β)-*form*

8-Angeloyl: ***Annuolide G***
$C_{20}H_{26}O_5$ 346.422
Constit. of *Helianthus annuus* (sunflower). Oil.

El-Nasry, S. *et al., Phytochemistry*, 1984, **23**, 2953 (*Dihydrocumambrin A*)
Macias, F.A. *et al., Phytochemistry*, 1996, **43**, 1205 (*Annuolide G*)

4,5-Dihydroxy-7(11),9-guaiadien-8-one D-488

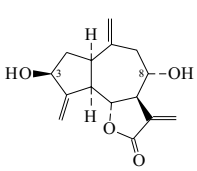


$C_{15}H_{22}O_3$ 250.337

(4β,5β)-*form* [129673-90-1]
Procurcumadiol
Constit. of *Curcuma longa* (turmeric). Needles (C_6H_6). Mp 150-150.5°. λ_{max} 254 (log ε 3.95); 280 (log ε 3.85) (MeOH).

Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201-2205 (*isol, pmr, cmr*)

3,8-Dihydroxy-4(15),10(14),11(13)-guaiatrien-12,6-olide D-489



(1α,3β,5α,6α,8α)-*form*

$C_{15}H_{18}O_4$ 262.305

(1α,3β,5α,6α,8α)-*form* [31565-50-1]
8-Hydroxyzaluzanin C. *Eleganin*†

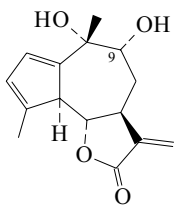
Cryst. Mp 150-151.5°. $[\alpha]_D^{20}$ +119.7. The name Eleganin is unchecked and may refer to Integrifolin below; its description in CA is defective λ_{max} 216 (EtOH) (Berdy).

8-(2-Hydroxymethylpropenoyl): [35730-78-0] ***Cynaropicrin***
$C_{19}H_{22}O_6$ 346.379
Constit. of *Cynara scolymus* (artichoke). Noncryst. $[\alpha]_D^{20}$ +108.6.

3-Ketone, 8-O-(2-hydroxymethylpropenoyl): [35821-02-4] ***Dehydrocyanaropicrin***
$C_{19}H_{20}O_6$ 344.363
Constit. of *Cynara scolymus* (artichoke). Cryst. Mp 126°. $[\alpha]_D^{20}$ +60.

Corbella, A. *et al., Chem. Comm.*, 1972, 386-387 (*Cynaropicrin*)
González, A.G. *et al., An. Quim.*, 1973, **69**, 1333
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 475-482; 1981, **20**, 2379-2382; 1982, **21**, 1171-1172; 1799-1800 (*3-ketones, Pseudostiffia Kingii esters*)
Zdero, C. *et al., Phytochemistry*, 1991, **30**, 3810-3811 (*isol, pmr, cmr*)

9,10-Dihydroxy-1,3,11(13)-guaiatrien-12,6-olide D-490

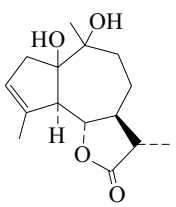


$C_{15}H_{18}O_4$ 262.305
(5α,6α,9α,10α)-*form*

9-Tigloyl: ***Isoachifolidiene***
$C_{20}H_{24}O_5$ 344.407
Constit. of *Achillea millefolium* (yarrow). Cryst. Mp 153°.

Rücker, G. *et al., Planta Med.*, 1992, **58**, 293 (*isol, pmr, cmr*)

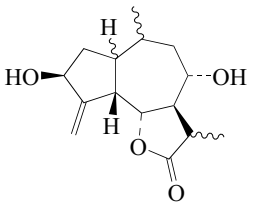
1,10-Dihydroxy-3-guaien-12,6-olide D-491



$C_{15}H_{22}O_4$ 266.336
(1ξ,5α,6α,10ξ,11α)-*form* [93552-69-3] ***Arlatin***
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOH). Mp 203-205°.

Kasamov, Sh.Z. *et al., Khim. Prir. Soedin.*, 1984, **20**, 794; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 754 (*isol*)
Adekenov, S.M. *et al., Khim. Prir. Soedin.*, 1984, **20**, 795; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 755 (*isol*)

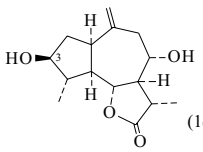
3,8-Dihydroxy-4(15)-guaien-12,6-olide D-492



$C_{15}H_{22}O_4$ 266.336
(1ξ,3β,5β,6α,8α,10ξ,11ξ)-*form* [213198-34-6] ***Absindiol***
Constit. of *Artemisia absinthium* (wormwood). Cryst. ($CHCl_3$/petrol). Mp 161-163°.

Safarova, A.G. *et al., Khim. Prir. Soedin.*, 1997, **33**, 834-836; *Chem. Nat. Compd. (Engl. Transl.)*, 1997, **33**, 653-654 (*isol*)

3,8-Dihydroxy-10(14)-guaien-12,6-olide D-493



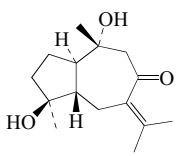
(1α,3β,4α,5α,6α,8α,11α)-*for*

$C_{15}H_{22}O_4$ 266.336
(1α,3β,4α,5α,6α,8α,11α)-*form* [30825-68-4] ***Isolipidiol***
Prisms (Me_2CO). Mp 167-168.5°. $[\alpha]_D$ +41.3.

3-Ketone: [30825-69-5] ***Isoamberboin***. *Maximolide*
$C_{15}H_{20}O_4$ 264.321
Constit. of *Cynara scolymus* (artichoke). Cryst. (EtOAc/petrol). Mp 183°. $[\alpha]_D^{20}$ +138 ($CHCl_3$).

Corbella, A. *et al., Chem. Comm.*, 1972, 386 (*Amberboin, Isoamberboin*)
Zakerov, S.Kh. *et al., Khim. Prir. Soedin.*, 1975, **11**, 261; 1976, **12**, 398; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 273; 1976, **12**, 350 (*Jurmolide, Isoamberoin*)

4,10-Dihydroxy-7(11)-guaien-8-one D-494



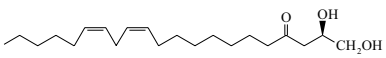
(1α,4β,5β,10α)-*form*

$C_{15}H_{24}O_3$ 252.353
(1α,4β,5β,10α)-*form* [108887-68-9] ***Isozedoarondiol***
Needles ($CHCl_3$). Mp 150-156°. $[\alpha]_D^{23}$ -147.2 (c, 0.8 in MeOH).
(1α,4β,5β,10β)-*form* [98644-24-7] ***Zedoarondiol***
Constit. of *Curcuma zedoaria* (zedoary). Needles ($CHCl_3$). Mp 133-134°. $[\alpha]_D^{23}$ -44 (c, 1.0 in MeOH).

10-Me ether: ***Methylzedoarondiol***
$C_{16}H_{26}O_3$ 266.38
Needles (hexane). Mp 83-85°. $[\alpha]_D^{23}$ -43.1 (c, 0.2 in MeOH).
(1β,4β,5β,10β)-*form* [116425-34-4]

Kouno, I. *et al., Phytochemistry*, 1985, **24**, 1845 (*isol*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 53 (*cryst struct*)
Takano, I. *et al., Phytochemistry*, 1995, **40**, 1197 (*pmr, cmr*)

1,2-Dihydroxy-12,15-heneicosadien-4-one D-495



(2*R*,12*Z*,15*Z*)-*form*

$C_{21}H_{38}O_3$ 338.529
(2*R*,12*Z*,15*Z*)-*form*

1-Ac: [56164-07-9] *2-Hydroxy-4-oxo-12,15-heneicosadien-1-yl acetate.* ***Persin***
$C_{23}H_{40}O_4$ 380.567
Constit. of avocado leaves. Oil. $[\alpha]_D^{24}$ +11.3 (c, 4.5 in $CHCl_3$).

2-Ac:1-Hydroxy-4-oxo-12,15-heneicosadien-2-yl acetate. ***Isopersin***
$C_{23}H_{40}O_4$ 380.567
Constit. of avocado (*Persea americana*). Unstable. Readily isomerises to, 1-Ac.

12,13,15,16-Tetrahydro, 1-Ac: [163955-67-7]

[160030-66-0] *2-Hydroxy-4-oxoheneicos-1-yl acetate.* ***Tetrahydropersin***
$C_{23}H_{44}O_4$ 384.598
Constit. of avocado (*Persea americana*). Yellow cryst. Mp 65.5-66°. $[\alpha]_D$ +2 (c, 4 in $CHCl_3$).

5,6-Didehydro(E-), 1-Ac:2-Hydroxy-4-oxo-5,12,15-heneicosatrien-1-yl acetate
$C_{23}H_{38}O_4$ 378.551
Constit. of avocado (*Persea americana*). Oil. $[\alpha]_D^{22}$ +17.6 (c, 0.48 in $CHCl_3$).

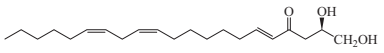
5,6-Didehydro(E-), 15,16-dihydro, 1-Ac:2-Hydroxy-4-oxo-5,12-heneicosadien-1-yl acetate
$C_{23}H_{40}O_4$ 380.567
Constit. of avocado (*Persea americana*). Oil. $[\alpha]_D^{23}$ +9 (c, 1 in $CHCl_3$).
(2*S*,12*Z*,15*Z*)-*form*

1-Ac: [160167-29-3]
Oil. $[\alpha]_D$ -9 (c, 1 in $CHCl_3$).

[60640-59-7, 86535-60-6, 160030-67-1]

Chang, C.-F. *et al., Agric. Biol. Chem.*, 1975, **39**, 1167 (*isol, ir, pmr*)
Sivanathan, S. *et al., J. Phytopathol.*, 1989, **125**, 97 (*props*)
Prusky, D. *et al., Plant Pathol.*, 1991, **40**, 45
Bull, S.D. *et al., Aust. J. Chem.*, 1994, **47**, 1661 (*synth, abs config, pmr, cmr*)
Carman, R.M. *et al., Tet. Lett.*, 1995, **36**, 2119 (*synth*)
Rodriguez-Saona, C. *et al., J. Nat. Prod.*, 1998, **61**, 1168-1170 (*Isopersin*)
Carman, R.M. *et al., Aust. J. Chem.*, 2000, **53**, 191-194 (*Tetrahydropersin*)
Paramashivappa, R. *et al., J. Agric. Food Chem.*, 2001, **49**, 2548-2551

1,2-Dihydroxy-5,12,15-heneicosatrien-4-one D-496



(2*R*,5*E*,12*Z*,15*Z*)-*form*

$C_{21}H_{36}O_3$ 336.514

(2*R*,5*E*,12*Z*,15*Z*)-*form*

1-Ac:1-Acetoxy-2-hydroxy-5,12,15-heneicosatrien-4-one. 2-Hydroxy-4-oxo-5,12,15-heneicosatrien-1-yl acetate
$C_{23}H_{38}O_4$ 378.551
Constit. of avocado (*Persea americana*). $[\alpha]_D^{22}$ +11.7 (c, 0.22 in $CHCl_3$).

(2ξ,5*E*,12*Z*,15*Z*)-*form*

1-Ac:5,6-Didehydropersin. ***Persenone A***
$C_{23}H_{38}O_4$ 378.551
Constit. of the fruit of avocado (*Persea americana*). Oil. $[\alpha]_D^{22}$ +17.6 (c, 0.48 in $CHCl_3$). λ_{max} 224 (ϵ 9000) (MeCN).

Kim, O.K. *et al., J. Agric. Food Chem.*, 2000, **48**, 1557-1563 (*Persenone A*)
Domergue, F. *et al., Phytochemistry*, 2000, **54**, 183-189

1,2-Dihydroxy-5-heneicosen-4-one D-497

$H_3C(CH_2)_{14}CH$
$=CHCOCH_2CH(OH)CH_2OH$

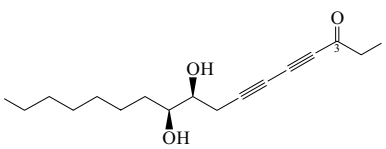
$C_{21}H_{40}O_3$ 340.545

(2ξ,5*E*)-*form*

*1-Ac:****Persenone B***
$C_{23}H_{42}O_4$ 382.582
Constit. of the fruit of *Persea americana* (avocado). Oil. $[\alpha]_D^{22}$ +8.3 (c, 0.33 in $CHCl_3$). λ_{max} 222 (ϵ 3200) (MeCN).

Kim, O.K. *et al., J. Agric. Food Chem.*, 2000, **48**, 1557-1563 (*Persenone B*)

9,10-Dihydroxy-4,6-heptadecadiyn-3-one D-498



$C_{17}H_{26}O_3$ 278.391

(9*S*,10*S*)-*form* [106828-96-0]
Panaxacol
Present in ginseng. $[\alpha]_D$ +18.3 (c, 1.0 in MeOH). λ_{max} 205 (ϵ); 245 (sh) (ϵ); 255 (ϵ); 270 (ϵ); 286 (ϵ) (MeOH) (Derep). λ_{max} 205 ; 255 ; 270 ; 286 ; 540 ; 570 (MeOH) (Berdy). λ_{max} 254 (ϵ 4000); 268 (ϵ 5100); 284 (ϵ 4200) (EtOH) (Berdy).

3S(?)-Alcohol: [113122-25-1] *4,6-Heptadecadiyne-3,9,10-triol*. ***Dihydropanaxacol***
$C_{17}H_{28}O_3$ 280.406
Present in ginseng. Sol. EtOAc, Et_2O.

[114687-50-2]

Fujimoto, Y. *et al., Phytochemistry*, 1987, **26**, 2850
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1447 (*synth, abs config*)

1,2-Dihydroxy-16-heptadecen-4-one D-499

Avocadenone
$H_2C=CH(CH_2)_{11}COCH_2CH(OH)CH_2OH$
$C_{17}H_{32}O_3$ 284.438

1-Ac: [25346-18-3]
$C_{19}H_{34}O_4$ 326.475
Constit. of avocado (*Persea americana*). Mp 47°. $[\alpha]_D^{25}$ +20 ($CHCl_3$).

Kashman, Y. *et al., Isr. J. Chem.*, 1969, **7**, 173
Kashman, Y. *et al., Tetrahedron*, 1969, **25**, 4617 (*isol*)
Alves, H.M. *et al., Ann. Acad. Bras. Ci&eenc.*, 1970, **42S**, 45 (*isol*)
Neeman, L. *et al., Appl. Microbiol.*, 1970, **19**, 470 (*isol*)

1,2-Dihydroxy-16-heptadecyn-4-one D-500

Avocadynone
$HC\equiv C(CH_2)_{11}COCH_2CH(OH)CH_2OH$
$C_{17}H_{30}O_3$ 282.422

1-Ac: [24607-10-1]
$C_{19}H_{32}O_4$ 324.459
Constit. of avocado (*Persea americana*). Mp 47°. $[\alpha]_D^{25}$ +26 ($CHCl_3$).

Kashman, Y. *et al., Isr. J. Chem.*, 1969, **7**, 173
Kashman, Y. *et al., Tetrahedron*, 1969, **25**, 4617 (*isol, nmr*)
Alves, H.M. *et al., Ann. Acad. Bras. Cienc.*, 1970, **42S**, 45 (*isol*)

10,16-Dihydroxyhexadecanoic acid D-501

[3233-90-7]
10,16-Dihydroxypalmitic acid
$HOH_2C(CH_2)_5CH(OH)(CH_2)_8COOH$
$C_{16}H_{32}O_4$ 288.426

(*S*)-*form* [69232-67-3]
Constit. of numerous plant cutins incl. apple and tomato. Mp 74-75°. $[\alpha]_D$ +3.1 (c, 0.5 in $MeOH/CHCl_3$). Partial dec. at 64-65°.

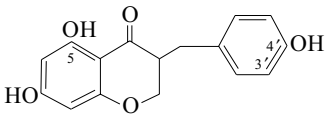
10-Ketone: [53833-25-3] *16-Hydroxy-10-oxohexadecanoic acid*
$C_{16}H_{30}O_4$ 286.411
Constit. of the fruit cutin of lemon *Citrus limon*.

[77441-79-3, 77441-82-8]

Eglinton, G. *et al., Phytochemistry*, 1968, **7**, 313 (*isol*)
Deas, A.H.B. *et al., Phytochemistry*, 1974, **13**, 1901-1905
Espelie, K.E. *et al., Lipids*, 1978, **13**, 832 (*isol, cd*)
Ray, A.K. *et al., Phytochemistry*, 1995, **38**, 1361-1369 (*isol, ms*)
Ahmed, A. *et al., Phytochemistry*, 2003, **63**, 47-52 (*synth, abs config*)

5,7-Dihydroxy-3-(4-hydroxybenzyl)-4-chromanone D-502

[96911-00-1]
2,3-Dihydro-5,7-dihydroxy-3-[(4-hydroxyphenyl)methyl]-4H-1-benzopyran-4-one, 9CI. 4′-Demethyl-3,9-dihydroeucomin



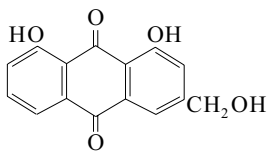
$C_{16}H_{14}O_5$ 286.284

(-)-*form*
Constit. of *Muscari comosum* (tassel hyacinth). Cryst. (C_6H_6/MeOH). Mp 103-104°. $[\alpha]_D$ -34 (c, 0.4 in MeOH).

Finckh, R.E. *et al., Experientia*, 1970, **26**, 472
Farkas, L. *et al., Tetrahedron*, 1971, **27**, 5049
Tamm, C. *et al., Arzneim.-Forsch.*, 1972, **22**, 1776
Adinolfi, M. *et al., Phytochemistry*, 1985, **24**, 624-626 (*isol, pmr, cmr*)

1,8-Dihydroxy-3-hydroxymethylanthraquinone, 8CI D-503

[481-72-1]
1,8-Dihydroxy-3-hydroxymethyl-9,10-anthracenedione, 9CI. 3-(Hydroxymethyl)-chrysazin. ***Aloeemodin***. *Rottlerin*†



$C_{15}H_{10}O_5$ 270.241
Found in aloes, also bark of cascara sagrada *Rhamnus purshiana*, Chinese rhubarb *Rheum palmatum* and *Rheum undulatum* (rhubarb). Orange needles (toluene). Mp 221-223°. pK_a 10.17 (25°, H_2O). Log P 0.88 (calc).

▶ CB6712200

1-O-*β*-D-*Glucopyranoside:****1*-O-*β*-D-*Glucopyranosylaloeemodin***
$C_{21}H_{20}O_{10}$ 432.383
Constit. of the rhizomes of *Rheum undulatum* (rhubarb). Yellow needles (MeOH). Mp 174-177°. $[\alpha]_D^{24}$ -56.4 (c, 0.1 in MeOH).

1′-O-*β*-D-*Glucopyranoside:* [50488-89-6] ***ω*-O-*β*-D-*Glucopyranosylaloeemodin***
$C_{21}H_{20}O_{10}$ 432.383
Isol. from Chinese rhubarb. Orange needles (MeOH). Mp 187-189°.

8-O-*β*-D-*Glucopyranoside:* [33037-46-6]
$C_{21}H_{20}O_{10}$ 432.383
Found in Chinese rhubarb (*Rheum palmatum*), cascara sagrada (*Rhamnus purshiana*) and Alexandria senna (*Cassia acutifolia*). Yellow needles + ½ H_2O ($CHCl_3$). Mp 237-238°.

1,8-Di-O-*β*-D-*glucopyranoside:*
$C_{27}H_{30}O_{15}$ 594.525
Found in Chinese rhubarb (*Rheum palmatum*). Yellow cryst. (MeOH). Mp 229°. $[\alpha]_D^{20}$ -115 (c, 0.085 in 85% Me_2CO aq.).

1′-Ac: [65615-58-9] *3-(Acetoxymethyl)-1,8-dihydroxyanthraquinone*. ***Aloe emodin ω-acetate***
$C_{17}H_{12}O_6$ 312.278
Isol. from roots of *Rumex acetosa* (sorrel). Yellow granules (C_6H_6/petrol). Mp 213-214°.

Tutin, F. *et al., J.C.S.*, 1911, **99**, 946 (*isol*)
Mitter, P.S. *et al., J. Indian Chem. Soc.*, 1932, **9**, 375 (*synth*)
Stone, K.G. *et al., J.A.C.S.*, 1946, **68**, 2742 (*uv*)
Muhtadi, M.J.R. *et al., Tet. Lett.*, 1969, 3751 (*synth, uv, glucoside*)
Okabe, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1254 (*isol, glucoside*)
Fairbairn, J.W. *et al., Pharmacology*, 1976, **14**, 1 (*suppl, rev*)
Sharma, M. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 884 (*isol, synth, acetate*)
Evans, F.G. *et al., Biomed. Mass Spectrom.*, 1979, **6**, 374 (*ms*)
Benfaremo, N. *et al., J.O.C.*, 1985, **50**, 139 (*synth*)
Danielsen, K. *et al., Magn. Reson. Chem.*, 1992, **30**, 359 (*pmr, cmr*)
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, pmr*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1121-1129 (*activity*)
Hofilena, J.G. *et al., ACGC Chem. Res. Commun.*, 2000, **10**, 15-20 (*activity*)
Matsuda, H. *et al., Bioorg. Med. Chem.*, 2001, **9**, 41-50 (*1-glucoside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DMU600

3,4-Dihydroxy-3-hydroxymethylbutanoic acid D-504

$(HOCH_2)_2C(OH)CH_2COOH$

$C_5H_{10}O_5$ 150.131

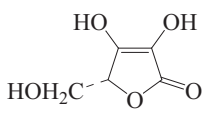
Nitrile, 4-O-β-D-glucopyranoside (3R-): [148965-97-3]

[148966-04-5]
$C_{11}H_{19}NO_8$ 293.273
Constit. of barley (*Hordeum vulgare*).

Pourmohseni, H. *et al., Phytochemistry*, 1993, **33**, 295-297

3,4-Dihydroxy-5-(hydroxymethyl)-2(5*H*)-furanone, 9CI D-505

[13382-28-0]
Pent-2-enono-1,4-lactone. Erythroascorbic acid



$C_5H_6O_5$ 146.099

(*R*)-*form* [138760-70-0]
D-form
Needles (MeCN). Mp 161-162°. $[\alpha]_D^{25}$ +12.5 (c, 1 in MeOH).

1′-O-α-D-Xylopyranoside: [174339-85-6]
$C_{10}H_{14}O_9$ 278.215
Prod. by *Pleurotus ostreatus* (oyster mushroom).

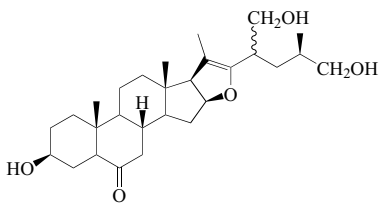
1′-O-α-D-Galactopyranoside: [220448-92-0]
$C_{11}H_{16}O_{10}$ 308.241

1′-O-α-D-Glucopyranoside: [174339-86-7]
$C_{11}H_{16}O_{10}$ 308.241
Prod. by *Hypsizygus mamoreus* (bunashimeji) and *Pleurotus ostreatus* (oyster mushroom).

(*S*)-*form* [26754-35-8]
L-form
Cryst. (Me_2CO/EtOAc). Mp 159-161°. $[\alpha]_D^{25}$ +9.3 (c, 0.268 in 0.01*M* HCl).

Murakawa, S. *et al., Agric. Biol. Chem.*, 1977, **41**, 1799-1800 (*isol*)
Bast, E. *et al., Z. Naturforsch., C*, 1978, **33**, 789-792 (*isol, ms*)
Liang, Y.T.S. *et al., J. Carbohydr. Chem.*, 1990, **9**, 75-84 (*D-form, synth, bibl*)
Gan, L.X. *et al., Carbohydr. Res.*, 1991, **220**, 117-125 (*synth, pmr, cmr*)
Shao, Y.Y. *et al., J. Agric. Food Chem.*, 1993, **41**, 1391-1396 (*synth*)
Okamura, M. *et al., J. Nutr. Sci. Vitaminol.*, 1994, **40**, 81-94 (*isol, glucoside*)
Loewus, F.A. *et al., Biochem. Biophys. Res. Commun.*, 1995, **212**, 196-203 (*isol*)
Wang, X.-Y. *et al., J. Carbohydr. Chem.*, 1995, **14**, 1257-1263 (*cryst struct*)
Pat. Coop. Treaty (WIPO), 1995, 95 29 928; *CA*, **124**, 212049b (*isol, glycosides*)
Keates, S.E. *et al., Phytochemistry*, 1998, **49**, 2397-2401 (*isol, galactoside*)

3,26-Dihydroxy-23-hydroxymethylfurost-20(22)-en-6-one D-506



$C_{28}H_{44}O_5$ 460.653

(3β,5α,23ξ,25*R*)-*form*

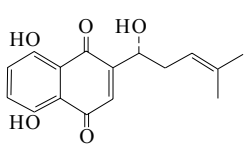
3-O-[β-D-Xylopyranosyl-(1→4)-[α-L-arabinopyranosyl-(1→6)]-β-D-glucopyranoside], 26-O-β-D-glucopyranoside: [187144-80-5] ***Chinenoside IV***
$C_{50}H_{80}O_{23}$ 1049.168
Constit. of *Allium chinense* (rakkyo). Amorph. powder. Mp 172-175°. $[\alpha]_D^{20}$ -35.8 (c, 0.32 in Py).

3-O-[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside], 26-O-β-D-glucopyranoside: [170739-22-7] ***Chinenoside V***
$C_{45}H_{72}O_{19}$ 917.052
Constit. of *Allium chinense* (rakkyo). Amorph. powder. Mp 216-218°. $[\alpha]_D^{20}$ -47.1 (c, 0.57 in Py).

Peng, J. *et al., Planta Med.*, 1996, **62**, 465-468 (*isol, pmr, cmr*)

5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione, 9CI D-507

[54952-43-1]
Shikonin. Alkannin. Arnebin IV. Anchusaic acid. Anchusin. Alkanna red. Alkhanin. Shikalkin



(*R*)-*form*

$C_{16}H_{16}O_5$ 288.299
Historically Shikonin was the (*R*)-form and Alkannin (=Anchusin etc.) the (*S*)-form. Shikalkin was the (±)-form.

(*R*)-*form* [517-89-5]
Red-brown cryst. (C_6H_6). Mp 148° (143°). $[\alpha]_{Hg}^{20}$ +135 (C_6H_6). Log P 1.84 (calc). Component of Tokyo violet λ_{max} 276 (ε 20000); 488 (ε 1200); 525 (ε 8700); 563 (ε 5900) (MeOH) (Derep).
▶ LD_{50} (mus, orl) >1000 mg/kg; LD_{50} (mus, ipr) 20 mg/kg. QL8000200

(*S*)-*form* [517-88-4]
C.I. Natural red 20. C.I. 75530
Red dye component of alkanet root extract used for colouring sausage casings, margarine, confectionery and wine. This extract, formerly FEMA 2016, has been removed from the FEMA GRAS list. Not permitted in Germany. Japan approved. Reddish-bronze needles (Et_2O/EtOH). Mp 116-117° (149°). $[\alpha]_{Hg}^{20}$ -157 (C_6H_6). Log P 1.84 (calc). λ_{max} 276 (ε 20000); 488 (ε 1200); 525 (ε 8700); 563 (ε 5900) (MeOH) (Derep).

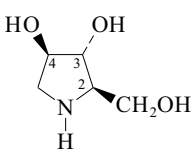
(±)-*form* [11031-58-6]
Mp 148°.

[38222-13-8, 85921-41-1]

Raudnitz, H. *et al., Ber.*, 1934, **67**, 1955-1959; 1935, **68**, 1479-1484 (*isol, struct*)
Brockmann, H. *et al., Annalen*, 1935, **521**, 1-47 (*isol, struct*)
Arakawa, H. *et al., Chem. Ind. (London)*, 1961, 947 (*abs config*)
Shcherbanovskii, L.R. *et al., Khim. Prir. Soedin.*, 1971, **7**, 517-518; **8**, 666; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 491; **8**, 648 (*isol*)
Afzal, M. *et al., J.C.S. Perkin 1*, 1975, 1334-1335 (*Angeloylshikonin, isol*)
Mizukami, H. *et al., Phytochemistry*, 1978, **17**, 95-97 (*isol*)
Papageorgiou, V.P. *et al., Planta Med.*, 1979, **35**, 56-60 (*isol, struct, use*)
Terada, A. *et al., Chem. Comm.*, 1983, 987-988 (*synth*)
Terada, A. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 205-213 (*synth*)
Tanoue, Y. *et al., J.O.C.*, 1987, **52**, 1437-1439 (*synth*)
Braun, M. *et al., Annalen*, 1991, 1157-1164 (*synth, ord*)
Torii, S. *et al., Bull. Chem. Soc. Jpn.*, 1995, **68**, 2917 (*synth*)
Merck Index, 12th edn., 1996, No. 253 (*props, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 74-75
Couladouros, E.A. *et al., Tet. Lett.*, 1997, **38**, 7263-7266 (*synth*)
Papageorgiou, V.P. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 271-300 (***rev***)
Lu, Q. *et al., Chin. Chem. Lett.*, 2002, **13**, 113-114 (*synth*)

3,4-Dihydroxy-2-(hydroxymethyl)pyrrolidine D-508

[98632-49-6]
1,4-Dideoxy-1,4-iminopentitol, 11CI. 2-(Hydroxymethyl)-3,4-pyrrolidinediol, 12CI. DAB-1



(2*R*,3*R*,4*R*)-*form*

$C_5H_{11}NO_3$ 133.147

(2*R*,3*R*,4*R*)-*form* [100937-52-8]
1,4-Dideoxy-1,4-imino-D-arabinitol
Hygroscopic oil. $[\alpha]_D^{20}$ +7.8 (c, 0.46 in H_2O).

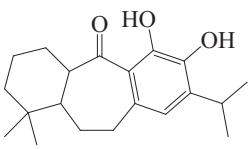
N-*(3-Amino-3-oxopropyl):3,4-Dihydroxy-2-hydroxymethyl-1-pyrrolidinepropanamide*
$C_8H_{16}N_2O_4$ 204.225
Alkaloid from *Morus alba* (white mulberry). $[\alpha]_D$ -53.7 (c, 0.41 in H_2O).

(2*R*,3*R*,4*S*)-*form* [105990-41-8]
1,4-Dideoxy-1,4-imino-D-ribitol
Alkaloid from roots of *Morus alba* (white mulberry). Solid. $[\alpha]_D$ +42 (c, 0.53 in H_2O).

Furukawa, J. *et al., Phytochemistry*, 1985, **24**, 593 (*isol, pmr, cmr, ms, ord, config*)
Nash, R.J. *et al., Phytochemistry*, 1985, **24**, 1620 (*isol, pmr, cmr, ms, struct*)
Fleet, G.W.J. *et al., Tetrahedron*, 1986, **42**, 5685; 1987, **43**, 3083; 1988, **44**, 2637; 2649 (*synth, ir, pmr*)
Setol, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3995 (*synth, ir, pmr*)
Ikota, N. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1087; 3399 (*synth*)
Wehmer, V. *et al., Angew. Chem., Int. Ed.*, 1990, **29**, 1169 (*synth*)
Buchanan, J.G. *et al., J.C.S. Perkin 1*, 1990, 699 (*synth*)
Van der Klein, P.A.M. *et al., Synth. Commun.*, 1992, **22**, 1763 (*synth*)
Asano, N. *et al., Carbohydr. Res.*, 1994, **253**, 235; **259**, 243 (*1,4-Dideoxy-1,4-imino-2-O-β-D-glucopyranosyl-D-arabinitol, 1,4-Dideoxy-1,4-imino-D-ribitol*)
Griffart-Brunet, D. *et al., Tet. Lett.*, 1994, **35**, 2889 (*synth*)
Huang, Y. *et al., J.O.C.*, 1997, **62**, 372-376 (*synth, pmr, ir, cmr*)
Watson, A.A. *et al., Phytochemistry*, 1997, **46**, 255 (*isol, props*)
Huwe, C.M. *et al., Synthesis*, 1997, 61 (*synth, pmr, cmr*)

11,12-Dihydroxy-8,11,13-icetexatrien-20-one D-509

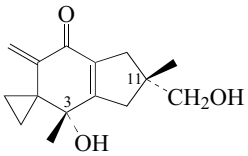
[91729-95-2]
Rosmaridiphenol



$C_{20}H_{28}O_3$ 316.439
Constit. of the leaves of *Rosmarinus officinalis* (rosemary). Cryst. (EtOH). Mp 182-184°.

Houlihan, C.M. *et al., J. Am. Oil Chem. Soc.*, 1984, **61**, 1036-1039 (*isol, pmr, cmr*)
U.S. Pat., 1987, 4 638 095; *CA*, **106**, 99630x (*isol*)

3,12-Dihydroxy-2(9),7(14)-illudadien-8-one D-510



$C_{15}H_{20}O_3$ 248.321

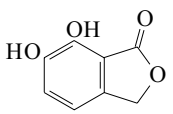
3α-*form* [181294-94-0]
Illudin C₂
Prod. by *Coprinus atramentarius* (common ink cap). Oil. Sol. MeOH, EtOAc. $[\alpha]_D^{20}$ +20 (c, 0.3 in MeOH). λ_{max} 205 (ϵ 9700); 264 (ϵ 5800) (MeOH).

11-Epimer: [181490-81-3] *3,13-Dihydroxy-2(9),7(14)-illudadien-8-one.* ***Illudin C₃***
$C_{15}H_{20}O_3$ 248.321
Prod. by *Coprinus atramentarius* (common ink cap). Oil. Sol. MeOH, EtOAc. $[\alpha]_D^{20}$ -15.4 (c, 0.3 in MeOH). λ_{max} 205 (ϵ 11500); 270 (ϵ 7300) (MeOH).

Lee, I.-K. *et al., J. Antibiot.*, 1996, **49**, 821-822 (*isol, uv, ir, pmr, cmr*)

6,7-Dihydroxy-1(3*H*)-isobenzofuranone, 9CI D-511

[4741-57-5]
6,7-Dihydroxyphthalide, 8CI. Normeconine



$C_8H_6O_4$ 166.133
Cryst. (EtOH). Mp 221-222° dec.

Di-Ac: [61407-18-9]
$C_{12}H_{10}O_6$ 250.207
Cryst. Mp 150.5-153°.

6-Me ether: [29809-16-3] *7-Hydroxy-6-methoxyphthalide*
$C_9H_8O_4$ 180.16
Mp 124-125°.

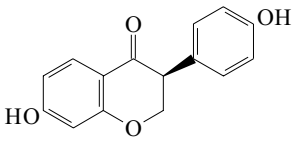
7-Me ether: [78213-30-6] *6-Hydroxy-7-methoxyphthalide*
$C_9H_8O_4$ 180.16
Mp 87-88°.

Di-Me ether: [569-31-3] *6,7-Dimethoxy-1(3H)-isobenzofuranone. 6,7-Dimethoxyphthalide.* ***Meconine****. Opianyl*
$C_{10}H_{10}O_4$ 194.187
Isol. from poppy straw (*Papaver somniferum*). Needles (H_2O). Mp 102.5°. Sublimes.

Wegscheider, R. *et al., Monatsh. Chem.*, 1889, **3**, 351 (*isol, struct*)
Edwards, G.A. *et al., J.C.S.*, 1925, **127**, 195 (*deriv*)
Rodionov, W.M. *et al., Bull. Soc. Chim. Fr.*, 1934, **1**, 653
Schmid, H. *et al., Helv. Chim. Acta*, 1945, **28**, 722 (*isol, deriv*)
Logan, W.R. *et al., J.C.S.*, 1956, 4980
Popoff, T. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 397-402 (*synth, ir, pmr, ms*)
Narasimhan, N.S. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 1257 (*synth*)

4′,7-Dihydroxyisoflavanone D-512

[17238-05-0]
2,3-Dihydro-7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. Dihydrodaidzein



$C_{15}H_{12}O_4$ 256.257

(*R*)-*form* [58865-02-4]
Cryst. Mp 201°.

7-O-β-D-Glucopyranoside: ***Dihydrodaidzin***
$C_{21}H_{22}O_9$ 418.399
Constit. of *Glycine max* (soybeans). Amorph. yellow powder. $[\alpha]_D^{22}$ -12.9 (c, 1 in MeOH). Config. not confirmed λ_{max} 276 (log ϵ 4.27); 310 (log ϵ 4.08) (MeOH).

Di-Ac:
Cryst. (MeOH). Mp 153°. $[\alpha]_D^{24}$ -20.7 ($CHCl_3$).

4′-Me ether: [4626-22-6] *7-Hydroxy-4′-methoxyisoflavanone.* ***Dihydroformononetin***
$C_{16}H_{14}O_4$ 270.284
Constit. of *Myroxylon balsamum* (Tolu balsam) trunkwood. Cryst. (EtOH). Mp 185-188°. No opt. rotn. given.

4′-Me ether, 7-O-β-D-glucopyranoside: [66918-17-0] ***2,3-Dihydroononin***
$C_{22}H_{24}O_9$ 432.426
Mp 269-271°.

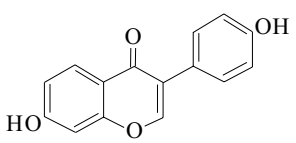
Di-Me ether: [15236-11-0] *4′,7-Dimethoxyisoflavanone*
$C_{17}H_{16}O_4$ 284.311
Cryst. (EtOH). Mp 129-130°.

[71815-35-5]

Donnelly, D.M.X. *et al., J.C.S. Perkin 1*, 1976, 186 (*isol, struct, synth*)
Haźnagy, A. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1978, **311**, 318 (*Dihydroononin*)
de Oliveira, A.B. *et al., Phytochemistry*, 1978, **17**, 593 (*Dihydroformononetin, 7-Hydroxy-4′-methoxyisoflavanone*)
Jain, A.C. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 136 (*synth*)
Hosny, M. *et al., J. Nat. Prod.*, 2002, **65**, 805-813 (*Dihydrodaidzin*)

4′,7-Dihydroxyisoflavone D-513

[486-66-8]
7-Hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Daidzein****. Dimethylbiochanin B. Daizeol. K 251-6. Daidzeol. Tatoin*



$C_{15}H_{10}O_4$ 254.242
Tatoin was impure daidzein. Widespread isoflavone in the Leguminosae, esp.

Phaseolus spp. (broad beans, lima beans); also found in soy and soy products (tofu, miso), chick peas (*Cicer arietinum*) and peanuts (*Arachis hypogaea*) .Nutriceutical with anticancer and bone protective props.. Pale yellow cryst. (EtOH aq.). Mp 330° (323°). λ_{max} 259 (ϵ) (MeOH/NaOH) (Derep). λ_{max} 252 (ϵ 25400) (MeOH) (Derep).

▶ DJ3100040

7-O-β-D-Glucopyranoside: [552-66-9] ***Daidzin***. *Daidzoside*
$C_{21}H_{20}O_9$ 416.384
Isol. from soya bean (*Glycine max*) and soya bean meal, kudzu root (*Pueraria lobata*), alfalfa (*Medicago sativa*) and other Leguminosae. Cryst. + $1H_2O$ (H_2O) becoming anhyd. at 120°. Mp 233-235°. $[\alpha]_D^{20}$ -36.4 (0.02*M* KOH).

▶ DJ3094000

7-O-(6-O-Acetyl-β-D-glucopyranoside): [71385-83-6] ***6″-O-Acetyldaidzin***
$C_{23}H_{22}O_{10}$ 458.421
Isol. from soybean seeds (*Glycine max*); potential nutriceutical. Needles. Mp 186-189°.

7-O-(6-O-Malonyl-β-D-glucopyranoside): [124590-31-4] ***6″-O-Malonyldaidzin***
$C_{24}H_{22}O_{12}$ 502.431
Present in soy foods; potential nutriceutical. Mp 168°. $[\alpha]_D$ -45.2 (c, 0.2 in DMSO).

4′,7-Di-O-β-D-glucopyranoside: [53681-67-7]
$C_{27}H_{30}O_{14}$ 578.526
Stress metab. of cell cultures of azuki bean (*Vigna angularis*). Needles. Mp 241°.

7-Me ether: [486-63-5] *4′-Hydroxy-7-methoxyisoflavone*. ***Isoformononetin***
$C_{16}H_{12}O_4$ 268.268
Isol. from soybean (*Glycine max*) and other plants. Prisms (EtOH). Mp 218-220°.

Farkas, L. *et al., Chem. Ber.*, 1959, **92**, 819 (*synth*)
Markham, K.R. *et al., Phytochemistry*, 1968, **7**, 791 (*isol*)
Gupta, S.R. *et al., Phytochemistry*, 1971, **10**, 877 (*synth*)
Dement, W.A. *et al., Phytochemistry*, 1972, **11**, 1089 (*isol*)
Inone, T. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1422 (*biosynth*)
Jain, A.C. *et al., Indian J. Chem.*, 1975, **13**, 789 (*Isoformononetin*)
Deshpande, V.H. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 201 (*isol*)
Nakayama, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 2398 (*synth*)
Kurosawa, K. *et al., Phytochemistry*, 1978, **17**, 1405 (*Isoformononetin*)
Ohta, N. *et al., Agric. Biol. Chem.*, 1979, **43**, 1415 (*6″-O-Acetyldaidzin*)
Jha, H.C. *et al., Can. J. Chem.*, 1980, **58**, 1211 (*cmr*)
Ayabe, S. *et al., J.C.S. Perkin 1*, 1982, 2725 (*biosynth, ms*)
Kobayashi, M. *et al., Phytochemistry*, 1983, **22**, 1257 (*isol*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Carman, R.M. *et al., Aust. J. Chem.*, 1985, **38**, 485 (*isol*)
Jain, A.C. *et al., J.C.S. Perkin 1*, 1986, 215 (*synth*)
Murthy, M.S.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 225 (*cmr*)
Matsuda, Y. *et al., Agric. Biol. Chem.*, 1988, **52**, 3211 (*isol, props*)
Park, H.H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1978 (*6″-malonyl ester*)
Nishiyama, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 107 (*synth*)
Hirakura, K. *et al., Phytochemistry*, 1997, **46**, 921-928 (*Daidzin, isol, pmr, cmr*)
Lewis, P. *et al., J.C.S. Perkin 1*, 1998, 2481-2484 (*Daidzin, synth, pmr, cmr*)
Balasubramanian, S. *et al., Synth. Commun.*, 2000, **30**, 469-484 (*synth, ethers*)
Hendrich, S. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press,, 2001, 55-75 (*occur, metab*)

5,7-Dihydroxyisoflavone, 8CI D-514

[4044-00-2]
5,7-Dihydroxy-3-phenyl-4H-1-benzopyran-4-one, 9CI

$C_{15}H_{10}O_4$ 254.242
Isol. from hydrolysed flour of *Arachis hypogaea* (peanut). Needles (EtOH aq.). Mp 205° (195-196°).

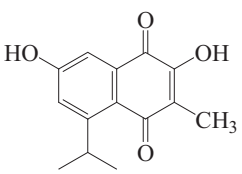
Di-Ac:
Needles (EtOH). Mp 180°.

7-Me ether: [19725-43-0] *5-Hydroxy-7-methoxyisoflavone*
$C_{16}H_{12}O_4$ 268.268
Cryst. (EtOAc). Mp 140-141°.

Di-Me ether: [26964-35-2] *5,7-Dimethoxyisoflavone*
$C_{17}H_{14}O_4$ 282.295
Isol. from peanut (*Arachis hypogaea*) seeds. Plates (EtOH aq.). Mp 122-123° (112°).

Baker, W. *et al., J.C.S.*, 1953, 1852 (*synth*)
Audier, H. *et al., Bull. Soc. Chim. Fr.*, 1966, 2892 (*ms*)
Krishnamurty, H.G. *et al., Tet. Lett.*, 1977, 3071 (*synth*)
Daigle, D.J. *et al., CA*, 1986, **104**, 165440 (*isol*)
Jain, A.C. *et al., J.C.S. Perkin 1*, 1986, 215 (*synth*)
Murthy, M.S.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 225 (*cmr*)

2,7-Dihydroxy-5-isopropyl-3-methyl-1,4-naphthoquinone D-515

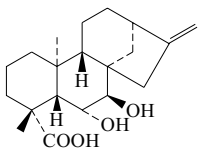


$C_{14}H_{14}O_4$ 246.262

2-Me ether: [253609-43-7] *7-Hydroxy-5-isopropyl-2-methoxy-3-methyl-1,4-naphthoquinone. 15-Nor-2-O-methylisohemigossypolone*
$C_{15}H_{16}O_4$ 260.289
Isol. from infected trunks of *Pachira aquatica* (Malabar chestnut). Yellow syrup.

Shibatani, M. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1777-1780
Sreeramulu, K. *et al., J. Asian Nat. Prod. Res.*, 2001, **3**, 261-265; *CA*, **136**, 352614e (*isol, pmr, cmr*)

6,7-Dihydroxy-16-kauren-19-oic acid D-516



(*ent*-6β,7α)-*form*

$C_{20}H_{30}O_4$ 334.455

(ent-6β,7α)-form [83883-00-5]

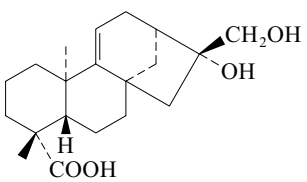
19→6 Lactone: [5691-63-4] ent-*7α-Hydroxy-16-kauren-19,6β-olide*. ***7-Hydroxykaurenolide***
$C_{20}H_{28}O_3$ 316.439
Cryst. (EtOAc/petrol). Mp 187-188°. $[\alpha]_D$ -25 (c, 0.5 in EtOH).

(ent-6α,7α)-form [26109-32-0]
Prod. by *Cucurbita maxima* and in cell-free systems of other plants.

7-Ketone, 6-O-β-D-glucopyranoside: [207240-06-0] ***Australiside A***
$C_{26}H_{38}O_9$ 494.581
Cryst. Mp 143-145°. Stereochem. not clear in ref..

Cross, B. *et al., J.C.S.*, 1963, 2944 (*struct*)
Hanson, J.R. *et al., Chem. Comm.*, 1968, 1689; 1969, 1071 (*biosynth*)
Hanson, J.R. *et al., J.C.S. Perkin 1*, 1974, 2001 (*cmr*)
MacMillan, J. *et al., Phytochemistry*, 1984, **23**, 553; 565 (*isol*)
Turnbull, C.G.N. *et al., Phytochemistry*, 1986, **25**, 97 (*biosynth*)
Li, G. *et al., Zhongguo Zhongyao Zazhi*, 1997, **22**, 548-550; *CA*, **128**, 319311r (*Australiside A*)

16,17-Dihydroxy-9(11)-kauren-19-oic acid D-517

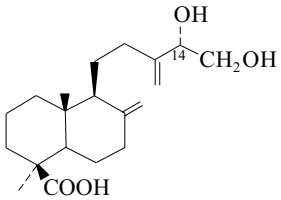


$C_{20}H_{30}O_4$ 334.455

(ent-16βOH)-form [55483-24-4]
Constit. of roasted coffee. Cryst. (Me_2CO). Mp 184-185°. $[\alpha]_D^{20}$ +32.2 (EtOH).

Obermann, H. *et al., Chem. Ber.*, 1975, **108**, 1093
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 2317

14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid D-518



$C_{20}H_{32}O_4$ 336.47

(14*S*)-*form*

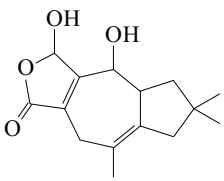
Constit. of *Juniperus communis* (juniper). Oil (as Me ester). $[\alpha]_D$ +43 (c, 1.6 in $CHCl_3$) (Me ester).

de Pascual Teresa, J. *et al., Phytochemistry*, 1980, **19**, 1153

8,14-Dihydroxy-2,6-lactaradien-5,14-olide D-519

[62824-37-7]

Blennin B

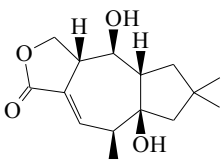


$C_{15}H_{20}O_4$ 264.321

Constit. of *Lactarius blennius* (slimy milk cap). Oil. $[\alpha]_D^{20}$ +70.78 (Me_2CO).

Vidari, G. *et al., Phytochemistry*, 1976, **15**, 1953

2,8-Dihydroxy-4(6)-lactaren-5,14-olide D-520



$C_{15}H_{22}O_4$ 266.336

(2β,3β,7β*H*,8β)-*form* [72601-39-9]

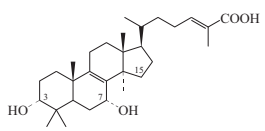
Blennin D

Constit. of *Lactarius blennius* (slimy milk cap). Oil. $[\alpha]_D^{20}$ +51 (Me_2CO).

De Bernardi, N. *et al., Phytochemistry*, 1980, **19**, 99

Garlaschelli, L. *et al., Tetrahedron*, 1994, **50**, 1211 (*struct*)

3,7-Dihydroxylanosta-8,24-dien-26-oic acid D-521



(3α,7α,24*E*)-*form*

$C_{30}H_{48}O_4$ 472.707

(3α,7α,24*E*)-*form* [86377-51-7]

Ganoderic acid T†. *Ganoderic acid U*

Constit. of *Ganoderma lucidum* (reishi). Cryst. Sol. MeOH, CH_2Cl_2; poorly sol. H_2O. Mp 196-199°. $[\alpha]_D$ +35.

3,7-Diketone: [173075-45-1] *3,7-Dioxolanosta-8,24-dien-26-oic acid*. ***Ganoderic acid DM***

$C_{30}H_{44}O_4$ 468.675

Constit. of *Ganoderma lucida* (reishi). $[\alpha]_D^{20}$ +10.9 (c, 0.065 in $CHCl_3$). λ_{max} 214 (log ϵ 3.91); 248 (log ϵ 3.84) (MeOH).

(3β,7α,24*E*)-*form*

7-Ketone, 26-aldehyde: [252351-96-5] *3-Hydroxy-7-oxolanosta-8,24-dien-26-al*. ***Lucidal***

$C_{30}H_{46}O_3$ 454.692

Isol. from *Ganoderma lucidum* (reishi). Cryst. (MeOH/EtOAc). Mp 106-108°. $[\alpha]_D^{25}$ +19 (c, 0.2 in $CHCl_3$). λ_{max} 229 (log ϵ 2); 256 (log ϵ 4.7) (EtOH).

7-Ketone, 26-alcohol: [252351-95-4] *3,26-Dihydroxylanost-8,24-dien-7-one*. ***Lucidadiol***

$C_{30}H_{48}O_3$ 456.707

Isol. from *Ganoderma lucidum* (reishi). Cryst. (MeOH/EtOAc). Mp 163-165°. $[\alpha]_D^{25}$ +80 (c, 0.02 in EtOH). λ_{max} 253 (log ϵ 3.6) (EtOH).

Toth, J.O. *et al., J. Chem. Res., Miniprint*, 1983, 2722 (*isol, pmr*)

Toth, J.O. *et al., Tet. Lett.*, 1983, **24**, 1081

Wang, F.S. *et al., Yaoxue Xuebao*, 1997, **32**, 447-450 (*Ganoderic acid DM*)

González, A.G. *et al., J. Nat. Prod.*, 1999, **62**, 1700-1701 (*Lucidadiol, Lucidal*)

3,15-Dihydroxylanosta-8,24-dien-26-oic acid D-522

$C_{30}H_{48}O_4$ 472.707

(3β,15α,24*E*)-*form*

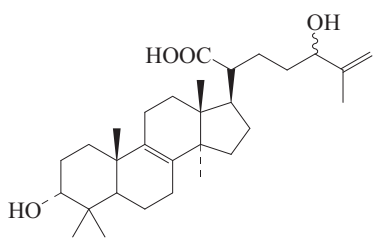
Di-Ac: [117842-20-3] *3β,15α-Diacetoxylanosta-8,24-dien-26-oic acid*

$C_{34}H_{52}O_6$ 556.781

Constit. of *Ganoderma lucidum* (reishi).

Lin, L.-J. *et al., J. Nat. Prod.*, 1988, **51**, 919

3,24-Dihydroxylanosta-8,25-dien-21-oic acid D-523



$C_{30}H_{48}O_4$ 472.707

(3α,24ξ)-*form*

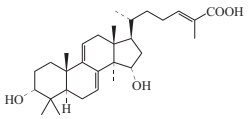
3-Ac: [267649-96-7] ***Tsugaric acid C***

$C_{32}H_{50}O_5$ 514.744

Constit. of *Ganoderma tsugae* (red reishi). Needles (MeOH). Mp 213-215°.

Su, H.-J. *et al., J. Nat. Prod.*, 2000, **63**, 514-516 (*isol, pmr, cmr*)

3,15-Dihydroxylanosta-7,9(11),24-trien-26-oic acid D-524



(3α,5α,15α,24*E*)-*form*

$C_{30}H_{46}O_4$ 470.691

The Ganoderic acid synonyms are confused owing to multiple use by different workers. See also refs. under 3,15,22-Trihydroxylanosta-7,9(11),24-trien-26-oic acid, T-611.

(3α,5α,15α,24*E*)-*form* [112430-67-8]

Ganodermic acid Ja

Metab. of *Ganoderma lucidum* (reishi).

3-Ac: [108026-94-4] ***Ganoderic acid Mf***

$C_{32}H_{48}O_5$ 512.728

Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{24}$ +42 (c, 0.2 in $CHCl_3$).

15-Ac: [86377-53-9] ***Ganoderic acid X***

$C_{32}H_{48}O_5$ 512.728

Metab. of *Ganoderma lucidum* (reishi). λ_{max} 220 ; 233 ; 242 ; 251 (EtOH) (Berdy).

15-Ac, Me ester:

Mp 161-163°. $[\alpha]_D$ +76.

Di-Ac: [108026-93-3] ***Ganoderic acid Me***. *Ganodermic acid R*

$C_{34}H_{50}O_6$ 554.765

Metab. of *Ganoderma lucidum* (reishi). Syrup or amorph. powder ($CHCl_3$/hexane). Mp 126-129°. $[\alpha]_D^{24}$ +53 (c, 0.26 in MeOH).

(3β,5α,15α,24*E*)-*form* [112430-68-9]

Ganodermic acid Jb

Metab. of *Ganoderma lucidum* (reishi). Cryst. Mp 201-202°.

3-Ac: [112430-65-6] ***Ganodermic acid TO***

$C_{32}H_{48}O_5$ 512.728

Metab. of *Ganoderma lucidum* (reishi). Cryst. Mp 160-162°.

15-Ac: [112430-64-5] ***Ganodermic acid TN***

$C_{32}H_{48}O_5$ 512.728

Metab. of *Ganoderma lucidum* (reishi). Cryst. Mp 145-146°. Incorr. called Ganoderic acid TN in CA.

Di-Ac: [112430-63-4] ***Ganodermic acid S***

$C_{34}H_{50}O_6$ 554.765

Metab. of *Ganoderma lucidum* (reishi). Needles ($CHCl_3$/hexane). Mp 123-124°. λ_{max} 235 ; 243 ; 252 (MeOH) (Berdy).

3-Ketone, 15-Ac: [112430-66-7] *15-Acetoxy-3-oxolanosta-7,9(11),24-trien-26-oic acid*. ***Ganodermic acid TQ***

$C_{32}H_{46}O_5$ 510.712

Metab. of *Ganoderma lucidum* (reishi).

3-Ketone, 26-alcohol: [420781-85-7] ***15,26-Dihydroxylanosta-7,9(11),24-trien-3-one***

$C_{30}H_{46}O_3$ 454.692

Cryst. (MeOH). Mp 124-125°. $[\alpha]_D^{20}$ +73 (c, 0.2 in $CHCl_3$). λ_{max} 236 (log ϵ 3.9); 244 (log ϵ 3.9); 252 (log ϵ 3.8) (EtOH).

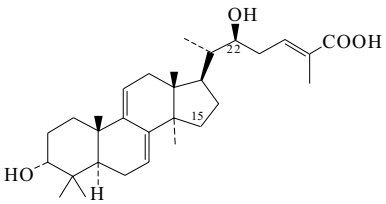
Nishitoba, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 619 (*isol*)

Shiao, M.-S. *et al., J. Nat. Prod.*, 1987, **50**, 886 (*isol*)

Lin, L.-J. *et al., Phytochemistry*, 1988, **27**, 2269

González, A.G. *et al., J. Nat. Prod.*, 2002, **65**, 417-421 (*Dihydroxylanostatrienone*)

3,22-Dihydroxylanosta-7,9(11),24-trien-26-oic acid D-525



$C_{30}H_{46}O_4$ 470.691

Lanostane derivs. have been isol. from *Ganoderma lucidum* by three groups of workers simultaneously, and various Ganoderic acid names have been given to different but closely similar compds. See also under Lanosta-7,9(11),24-triene-3,26-diol, L-40, 3,7,15-Trihydroxy-11,23-dioxolanost-8-en-26-oic acid, T-553 and 3,7,12-Trihydroxy-11,15,23-trioxolanost-8-en-26-oic acid, T-714.

(3α,22*S*,24*E*)-*form*

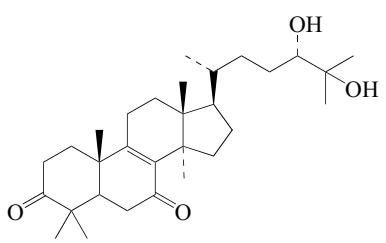
22-Ac: ***Ganoderic acid S***†
$C_{32}H_{48}O_5$ 512.728
Constit. of cultured mycelium of *Ganoderma lucidum* (reishi). Needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 194-196°. $[\alpha]_D$ +19.8 (c, 0.085 in $CHCl_3$). See also under Lanosta-7,9(11),24-triene-3,26-diol, L-40 λ_{max} 231 (ϵ 15800); 240 (ϵ 15600); 248 (ϵ 10000) (MeOH) (Berdy).

Di-Ac: [103963-39-9] ***Ganoderic acid R***†
$C_{34}H_{50}O_6$ 554.765
Constit. of cultured mycelium of *Ganoderma lucidum* (reishi). Needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 201-202°. $[\alpha]_D$ +8.7 (c, 0.092 in $CHCl_3$). λ_{max} 224 (ϵ 10000); 234 (ϵ 10000); 242 (ϵ 10000); 250 (ϵ 6300) (MeOH) (Berdy).

Hirotani, M. *et al., Phytochemistry*, 1987, **26**, 2797

Hirotani, M. *et al., J.C.S. Perkin 1*, 1990, 2751 (*biosynth*)

24,25-Dihydroxylanost-8-ene-3,7-dione D-526

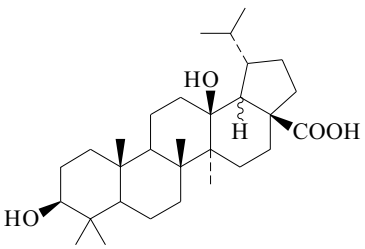


$C_{30}H_{48}O_4$ 472.707

24*S*-*form* [217476-73-8]
Lucidumol A
Constit. of *Ganoderma lucida* (reishi). Needles (C_6H_6/EtOAc). Mp 185-187°. $[\alpha]_D$ +35 (c, 0.1 in EtOH). λ_{max} 251 (log ϵ 4) (no solvent reported).

Min, B.-S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1607-1612 (*isol, pmr, cmr*)

3,13-Dihydroxy-28-lupanoic acid D-527



$C_{30}H_{50}O_4$ 474.723

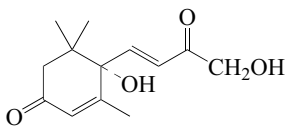
(3β,18ξ,13β)-*form*

28→13 Lactone: [56875-22-0] *3-Hydroxy-28,13-lupanolide*
$C_{30}H_{48}O_3$ 456.707
Constit. of *Dillenia indica* (elephant apple). Cryst. Mp 325° dec. $[\alpha]_D^{27}$ +63.4 ($CHCl_3$).

Banerji, N. *et al., Phytochemistry*, 1975, **14**, 1447 (*isol*)

Suokas, E. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 623 (*struct*)

6,10-Dihydroxy-4,7-megastigmadiene-3,9-dione D-528



$C_{13}H_{18}O_4$ 238.283

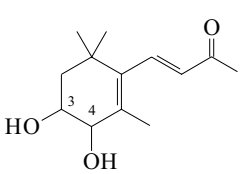
(*S*)-*form*

10-O-β-D-Glucopyranoside: [189344-54-5] ***Corchoionoside B***
$C_{19}H_{28}O_9$ 400.425
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{23}$ +113.7 (c, 0.4 in MeOH).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 464-469 (*isol, pmr, cmr*)

3,4-Dihydroxy-5,7-megastigmadien-9-one D-529

[126585-77-1]
3,4-Dihydroxy-β-ionone



$C_{13}H_{20}O_3$ 224.299
Gum.

3-O-β-D-Glucopyranoside: [126585-76-0] ***Sonchuionoside C***. *Icariside B8*
Constit. of *Vitis vinifera* (Riesling wine). Amorph. powder. $[\alpha]_D^{21}$ -65.2 (c, 0.46 in MeOH).

4-O-β-D-Glucopyranoside: [126585-75-9] ***Sonchuionoside A***
$C_{19}H_{30}O_8$ 386.441
Amorph. powder. $[\alpha]_D^{23}$ -42.7 (c, 0.62 in MeOH).

4-O-[β-D-Apiofuranosyl-(1→?)-β-D-glucopyranoside]: [126527-19-3] ***Sonchuionoside B***
$C_{24}H_{38}O_{12}$ 518.557
Amorph. powder. $[\alpha]_D^{23}$ -77.8 (c, 0.45 in MeOH).

[126176-78-1]

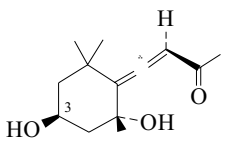
Shimizu, S. *et al., Phytochemistry*, 1989, **28**, 3399 (*isol, pmr, cmr*)

Miyase, T. *et al., Phytochemistry*, 1989, **28**, 3483 (*Icariside B8, pmr, cmr, ms*)

Roscher, R. *et al., J. Agric. Food Chem.*, 1993, **41**, 1452 (*isol, Sonchuionoside C*)

3,5-Dihydroxy-6,7-megastigmadien-9-one D-530

[41703-38-2]
4-(2,4-Dihydroxy-2,6,6-trimethylcyclohexylidene)-3-buten-2-one, 9CI. 2,6,6-Trimethyl-1-(3-oxo-1-butenylidene)-2,4-cyclohexanediol. ***Grasshopper ketone***



$C_{13}H_{20}O_3$ 224.299
Needles (Me_2CO/C_6H_6). Mp 134-136°. $[\alpha]_D^{25}$ -63 (c, 1.15 in MeOH).

3-Ac: [26289-05-4] ***Apo-9′-fucoxanthinone***
$C_{15}H_{22}O_4$ 266.336
Amorph. solid. $[\alpha]_D^{19}$ -284 (c, 0.1 in MeOH). λ_{max} 204 ; 232 (MeOH). λ_{max} 231 (ϵ 2800); 280 (ϵ 700) (MeOH) (Berdy).

3-O-β-D-Glucopyranoside: [109062-00-2] ***Icariside B1***
$C_{19}H_{30}O_8$ 386.441
Amorph. powder. $[\alpha]_D^{25}$ -73.5 (c, 1.00 in MeOH).

5-O-β-D-Glucopyranoside: [120330-44-1] ***Citroside A***
$C_{19}H_{30}O_8$ 386.441
Constit. of *Citrus unshiu* (satsuma mandarin). Amorph. powder + ½H_2O. $[\alpha]_D^{23}$ -95.7 (c, 0.4 in MeOH). λ_{max} 230 (log ϵ 4.12) (MeOH).

3-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [108567-70-0] ***Cinnamoside***
$C_{24}H_{38}O_{12}$ 518.557
Isol. from dried bark of *Cinnamomum cassia* (Chinese cinnamon). Syrup. $[\alpha]_D$ -88.6 (c, 0.5 in MeOH).

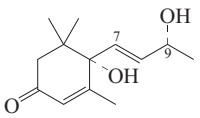
(S)axial Diastereomer, 5-O-β-D-glucopyranoside: [120278-09-3] ***Citroside B***
Constit. of *Citrus unshiu* (satsuma mandarin). Amorph. powder + ½H_2O. $[\alpha]_D^{23}$ -48.2 (c, 0.3 in MeOH). λ_{max} 230 (log ϵ 4.17) (MeOH).

Meinwald, J. *et al., Tet. Lett.*, 1968, 2959 (*isol*)

de Ville, T.E. *et al., Chem. Comm.*, 1970, 1231 (*cryst struct*)

Hlubucek, J.R. *et al., J.C.S. Perkin 1*, 1974, 848 (*synth*)
Mori, K. *et al., Tetrahedron*, 1974, **30**, 1065-1072 (*synth, abs config*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1109 (*Icariside B_1*)
Umehara, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 5004 (*Citrosides*)
Shiraga, Y. *et al., Tetrahedron*, 1988, **44**, 4703-4711 (*Cinnamoside*)
Doi, Y. *et al., J. Nat. Prod.*, 1995, **58**, 1097-1099 (*Apo-9′-fucoxanthinone*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 463-467 (*Apo-9′-fucoxanthinone*)

6,9-Dihydroxy-4,7-megastigmadien-3-one D-531



(6*S*,7*E*,9*R*)-*form*

$C_{13}H_{20}O_3$ 224.299

(6*S*,7*E*,9*R*)-*form* [23526-45-6]
Vomifoliol. *Blumenol A*
Cryst. ($CHCl_3$). Mp 113-114°.

9-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:
$C_{24}H_{38}O_{12}$ 518.557
Isol. from Japanese medlar (*Eriobotrya japonica*) leaves. Powder. $[\alpha]_D^{25}$ +15 (c, 0.14 in MeOH).

9-O-[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]: [126221-59-8]
$C_{24}H_{38}O_{12}$ 518.557
Isol. from apples, *Malus sylvestris* cv Johnathan.

9-O-[β-D-Glucopyranosyl-(1→4)-β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [141947-49-1]
$C_{30}H_{48}O_{17}$ 680.699
Constit. of fruit of apples (*Malus sylvestris*).

9-Ketone: [15764-81-5] *6-Hydroxy-4,7-megastigmadiene-3,9-dione.* ***Dehydrovomifoliol***
$C_{13}H_{18}O_3$ 222.283
Isol. from rice husks (*Oryza sativa* L. cv Koshihikari). Oil. $[\alpha]_D$ +142.7 (c, 0.78 in MeOH).

7,8-Dihydro, 9-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [177261-70-0]
$C_{24}H_{40}O_{12}$ 520.573
Constit. of quince (*Cydonia vulgaris*) leaves.

7,8-Dihydro, 9-O-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [177261-69-7]
$C_{25}H_{42}O_{12}$ 534.6
Constit. of leaves of quince (*Cydonia vulgaris*).

(6*S*,7*E*,9*S*)-*form* [189351-15-3]
Corchoionol C
Powder. $[\alpha]_D^{28}$ +184.3 (c, 0.1 in $CHCl_3$).

9-O-β-D-Glucopyranoside: [185414-25-9]
Corchoionoside C
$C_{19}H_{30}O_8$ 386.441
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{29}$ +25.3 (c, 0.3 in MeOH).

(6ξ,7*E*,9ξ)-*form*

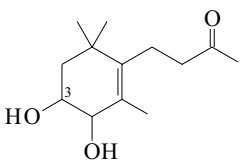
9-O-β-D-Glucopyranoside:
$C_{19}H_{30}O_8$ 386.441
Constit. of *Vitis vinifera* cv. Gewürztraminer. Two epimers isol..

9-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:
$C_{24}H_{38}O_{12}$ 518.557
Constit. of *Vitis vinifera* cv. Gewürztraminer. Two epimers isol..

Takasugi, M. *et al., Chem. Lett.*, 1973, **3**, 245-248 (*Vomifoliol, 9-ketone*)
Mori, K. *et al., Tetrahedron*, 1974, **30**, 1065-1072 (*ketone, synth*)
Kato, T. *et al., Phytochemistry*, 1977, **16**, 45-48 (*Dehydrovomifoliol*)
Higuchi, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 534-535 (*9-apiosylglucoside*)
De Tommasi, N. *et al., J. Nat. Prod.*, 1992, **55**, 1025 (*9-apiosylglucoside*)
Herderich, M. *et al., Phytochemistry*, 1992, **31**, 895-897 (*apple glucoside*)
Sefton, M.A. *et al., Phytochemistry*, 1992, **31**, 1813-1815 (*grape glucoside*)
Baltenweck-Guyot, R. *et al., Phytochemistry*, 1996, **43**, 621-624 (*Vitis vinifera glycosides*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 464-469 (*Corchoionoside C*)
Murai, Y. *et al., Planta Med.*, 2001, **67**, 480-481 (*Corchoionoside C*)
Calis, I. *et al., Phytochemistry*, 2002, **59**, 451-457 (*Corchoionoside C*)

3,4-Dihydroxy-5-megastigmen-9-one D-532

3,4-Dihydroxy-7,8-dihydro-β-ionone

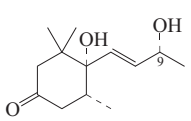


$C_{13}H_{22}O_3$ 226.315

3-O-β-D-Glucopyranoside: [126176-78-1]
Icariside B_8
$C_{19}H_{32}O_8$ 388.457
Constit. of wine grape *Vitis vinifera* leaves (Riesling). $[\alpha]_D^{23}$ -60.9 (c, 0.64 in MeOH).

Miyase, T. *et al., Phytochemistry*, 1989, **28**, 3483 (*isol, pmr, cmr*)
Roscher, R. *et al., J. Agric. Food Chem.*, 1993, **41**, 1452 (*isol*)

6,9-Dihydroxy-7-megastigmen-3-one D-533



(5*R*,6*S*,7*E*,9*R*)-*form*

$C_{13}H_{22}O_3$ 226.315

The various isolates and their glucosides may or may not be stereochemically identical.

(5*R*,6*S*,7*E*,9*R*)-*form*

9-O-β-D-Glucopyranoside: [138665-44-8]
Ampelopsisionoside
$C_{19}H_{32}O_8$ 388.457
Powder. $[\alpha]_D$ -35.1 (c, 0.11 in MeOH).

9-O-[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]: [232601-29-5] ***Platanionoside C***
$C_{24}H_{40}O_{12}$ 520.573
Amorph. powder. $[\alpha]_D^{25}$ -26 (c, 1.23 in MeOH).

(5*R*,6*S*,7*E*,9ξ)-*form*
Oil. $[\alpha]_D^{20}$ +2 (c, 0.25 in $CHCl_3$).

9-O-β-D-Glucopyranoside:
$C_{19}H_{32}O_8$ 388.457

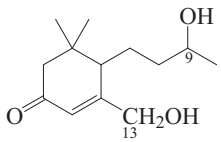
(5ξ,6*S*,7*E*,9*R*)-*form* [142173-08-8] ***4,5-Dihydrovomifoliol***
Constit. of *Vitis vinifera* grapes and Riesling wine.

9-O-β-D-Glucopyranoside: [142235-28-7]

[351343-53-8] ***Dihydroroseoside***
$C_{19}H_{32}O_8$ 388.457
Isol. from a Riesling wine.

Inada, A. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2437 (*isol, pmr, cmr*)
González, A.G. *et al., J. Nat. Prod.*, 1994, **57**, 400 (*isol, pmr, cmr*)
Baltenweck-Guyot, R. *et al., Phytochemistry*, 1996, **43**, 621 (*Vitis vinifera glycosides*)
Tamaki, A. *et al., J. Nat. Prod.*, 1999, **62**, 1074-1076 (*Platanionoside C*)
Otsuka, H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1093-1097 (*Ampelopsisionoside, abs config*)
Shen, Y.B. *et al., J. Wood Sci.*, 2001, **47**, 145-148; *CA*, **135**, 119622a (*Dihydroroseoside*)

9,13-Dihydroxy-4-megastigmen-3-one D-534



$C_{13}H_{22}O_3$ 226.315

9-O-β-D-Glucopyranoside: [188305-07-9]
$C_{19}H_{32}O_8$ 388.457
Constit. of *Hordeum vulgare* (barley).

9-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [224047-74-9]
$C_{25}H_{42}O_{13}$ 550.599

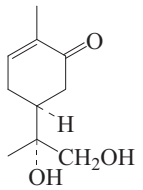
13-Carboxylic acid:9-Hydroxy-3-oxo-4-megastigmen-13-oic acid
$C_{13}H_{20}O_4$ 240.299

13-Carboxylic acid, 9-O-β-D-glucopyranoside: [295343-61-2]
$C_{19}H_{30}O_9$ 402.441

13-Carboxylic acid, 9-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [295343-59-8]
$C_{25}H_{40}O_{14}$ 564.583

Peipp, H. *et al., Phytochemistry*, 1997, **44**, 581-587 (*Hordeum vulgare constit*)
Maier, W. *et al., Planta*, 1999, **207**, 620-623 (*Nicotiana constits*)
Maier, W. *et al., Phytochemistry*, 2000, **54**, 473-479 (*Nicotiana constits*)

8,9-Dihydroxy-*p*-menth-1(6)-en-2-one D-535



(4*S*,8*R*)-*form*

$C_{10}H_{16}O_3$ 184.235

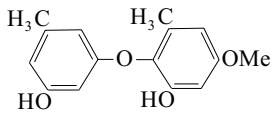
(4*S*,8*R*)-*form* [402593-42-4]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{25}$ -6 (c, 0.1 in MeOH).

(4*S*,8*S*)-*form* [402593-43-5]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{25}$ -7 (c, 0.2 in MeOH).

Matsumura, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 66-72 (*isol, pmr, cmr*)

2,3′-Dihydroxy-4-methoxy-5′,6-dimethyldiphenyl ether D-536

[33716-82-4]
2-(3-Hydroxy-5-methylphenoxy)-5-methoxy-3-methylphenol, 9CI. ***Cyperine***. *LL-V125α. Antibiotic LL-V125α*



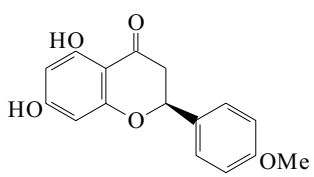
$C_{15}H_{16}O_4$ 260.289
Metab. of a fungal pathogen of *Cyperus rotundus* (nutgrass). Cryst. ($CHCl_3$/petrol). Mp 121.5-122.5°.

Di-Ac:
Mp 75-76°.

McGahren, W.J. *et al., J.O.C.*, 1970, **35**, 2433
Cannon, J.R. *et al., J.C.S. Perkin 1*, 1972, 1200 (*isol, struct, synth*)
Weber, H.A. *et al., J. Nat. Prod.*, 1988, **51**, 879 (*pmr, cmr*)
Stierle, A. *et al., Phytochemistry*, 1991, **30**, 2191 (*isol, pmr*)

5,7-Dihydroxy-4′-methoxyflavanone D-537

[480-43-3]
*2,3-Dihydro-5,7-dihydroxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*. ***Isosakuranetin***. *Kikokunetin. Citrifoliol. Ponciretin*



$C_{16}H_{14}O_5$ 286.284

(*S*)-*form*
Mp 193-194°. $[\alpha]_D^{20}$ -19.7 (EtOH).

7-O-β-D-Xylopyranoside: [83728-89-6]
$C_{21}H_{22}O_9$ 418.399
Isol. from *Prunus cerasoides* (wild Himalayan cherry). Yellow needles (MeOH). Mp 140-142° dec.

7-O-β-D-Glucopyranoside: [491-69-0] ***Isosakuranin***
$C_{22}H_{24}O_{10}$ 448.426
Isol. from *Prunus* spp.. Cryst. (Me_2CO). Mp 214° (184-187°). $[\alpha]_D^{24}$ -73.4 (Py).

7-O-β-D-Galactopyranoside: [28585-70-8] ***Puddumin B***
$C_{22}H_{24}O_{10}$ 448.426
Isol. from *Prunus cerasoides* (wild Himalayan cherry). Needles (MeOH). Mp 178-179°. $[\alpha]_D^{25}$ -51.6 (c, 1.2 in Py). Data given is for synthetic compd..

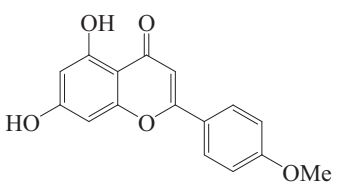
7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [14941-08-3] ***Poncirin***. *Citrifolioside*
$C_{28}H_{34}O_{14}$ 594.568
Isol. from *Citrus* spp.. Cryst. (MeOH). Mp 210-211°. $[\alpha]_D$ -81.7 (c, 1 in DMF).

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [14259-47-3] ***Neoponcirin***. *Didymin*
$C_{28}H_{34}O_{14}$ 594.568
From leaves of *Monarda didyma* (bergamot) and *Citrus* spp.. Fine needles (MeOH). Mp 211-213°. $[\alpha]_D^{26}$ -105.3 (c, 1.44 in MeOH).

Asahina, Y. *et al., CA*, 1929, **23**, 3475 (*isol*)
Hattori, S. *et al., CA*, 1930, **24**, 1862 (*isol*)
Karijone, T. *et al., Yakugaku Zasshi*, 1954, **74**, 363 (*isol*)
Pacheco, H. *et al., Bull. Soc. Chim. Fr.*, 1965, 2937 (*synth*)
Wagner, H. *et al., Tet. Lett.*, 1967, 1837; 1968, 1635; 1976, 1799 (*synth, derivs, nmr*)
Kamiya, A. *et al., Agric. Biol. Chem.*, 1979, **43**, 1529 (*Poncirin*)
Jangwan, J.S. *et al., Int. J. Crude Drug Res.*, 1989, **27**, 223 (*Puddumin B*)
Vasconcelos, J.M.J. *et al., Phytochemistry*, 1998, **49**, 1421-1424 (*isol, pmr, cmr*)
Bae, E.-A. *et al., Planta Med.*, 1999, **65**, 442-443 (*activity*)
Bae, E.-A. *et al., Biol. Pharm. Bull.*, 2000, **23**, 1122-1124 (*activity*)

5,7-Dihydroxy-4′-methoxyflavone, 8CI D-538

[480-44-4]
*5,7-Dihydroxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. Apigenin 4′-methyl ether*. ***Acacetin***. *Linarigenin. Buddleoflavonol*



$C_{16}H_{12}O_5$ 284.268
Pale yellow needles (EtOH). Sol. bases, EtOH; poorly sol. Et_2O. Mp 263°. Log P 1.56 (calc).

▶ LD_{50} (mus, ivn) 993 mg/kg. Exp. reprod. effects. DJ3002000

7-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [239106-94-6]
$C_{27}H_{30}O_{14}$ 578.526
Constit. of the seeds of *Carthamus tinctorius* (safflower). Yellow powder. Mp 240-244°. $[\alpha]_D$ -23 (c, 1 in MeOH). λ_{max} 268 ; 325 (MeOH).

7-O-[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]: [31514-20-2] *Acacetin 7-diglucoside*
$C_{28}H_{32}O_{15}$ 608.552
Isol. from *Tanacetum vulgare* (tansy).

[80443-15-8]

Nakaoki, T. *et al., CA*, 1961, **55**, 10803 (*deriv*)
Nogradi, M. *et al., Chem. Ber.*, 1967, **100**, 2783 (*deriv*)
Wagner, H. *et al., Chem. Ber.*, 1969, **102**, 1445; 2083; 1970, **103**, 851 (*derivs*)
Wanjala, C.C.W. *et al., Phytochemistry*, 1999, **51**, 705-707 (*7-apiosylglucoside*)
Ahmed, K.M. *et al., Pharmazie*, 2000, **55**, 621-622 (*7-apiosylglucoside*)

5,7-Dihydroxy-6-methoxyflavone D-539

[480-11-5]
*5,7-Dihydroxy-6-methoxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI*. ***Oroxylin A***

$C_{16}H_{12}O_5$ 284.268
Yellow cryst. (EtOH). Mp 231-232° (219-220°). λ_{max} 247 (ε 20900); 270 (ε 13490); 317 (ε 13180) (MeOH) (Berdy).

7-O-β-D-Glucopyranoside: [36948-77-3]
$C_{22}H_{22}O_{10}$ 446.41

7-O-β-D-Glucuronopyranoside: [36948-76-2] ***Oroxyloside***
$C_{22}H_{20}O_{11}$ 460.393
Mp 199-201°.

5-O-α-L-Rhamnopyranoside: [163350-29-6]
$C_{22}H_{22}O_9$ 430.41
Constit. of the seeds of *Trichosanthes anguina* (snake gourd). Mp 327°. λ_{max} 248 ; 280 ; 317 (sh) (MeOH).

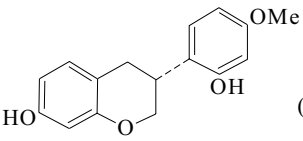
7-O-α-L-Rhamnopyranoside: [254898-91-4]
$C_{22}H_{22}O_9$ 430.41
Yellow needles (MeOH/Et_2O). Mp 221-223°. λ_{max} 248 (sh) ; 270 ; 319 (MeOH).

7-O-[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranoside]: [168771-59-3]
$C_{28}H_{32}O_{14}$ 592.552

Naylor, W.A.H. *et al., J.C.S.*, 1901, **79**, 954 (*isol*)
Sastri, J. *et al., CA*, 1947, **41**, 2417 (*isol*)
Molho, D. *et al., Bull. Soc. Chim. Fr.*, 1963, 607 (*synth*)
Varady, J. *et al., Tet. Lett.*, 1965, 4281 (*synth*)
Popova, T.P. *et al., Farm. Zh. (Kiev)*, 1972, **23**, 84; *CA*, **82**, 28553z (*isol*)
Goudard, M. *et al., Phytochemistry*, 1978, **17**, 145-146 (*ms*)
Nicollier, G.F. *et al., J. Agric. Food Chem.*, 1981, **29**, 1179 (*glucoside*)
Buschi, C.A. *et al., Phytochemistry*, 1981, **20**, 1178-1179 (*isol*)
Yadava, R.N. *et al., Fitoterapia*, 1994, **65**, 554 (*5-rhamnoside*)
Aqil, M. *et al., CA*, 1995, **123**, 251218e (*7-glucosylrhamnoside*)
Yuldashev, M.P. *et al., Khim. Prir. Soedin.*, 1996, **32**, 610-612; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 592-593 (*Oroxyloside*)
Houghton, P.J. *et al., Pharm. Pharmacol. Lett.*, 1997, **7**, 96-98 (*activity*)
Rashad, M.A. *et al., Phytomedicine*, 1998, **5**, 375-381 (*isol, activity*)
Prakash, E.O. *et al., Fitoterapia*, 1999, **70**, 287-289 (*7-rhamnoside*)

2′,7-Dihydroxy-4′-methoxyisoflavan D-540

[56701-24-7]
*3,4-Dihydro-3-(2-hydroxy-4-methoxyphenyl)-2*H*-1-benzopyran-7-ol, 9CI*. ***Vestitol***



(*R*)-*form*

$C_{16}H_{16}O_4$ 272.3
λ_{max} 206 (ϵ 45500); 228 (ϵ 11300); 285 (ϵ 5700) (EtOH) (Berdy).

(*R*)-*form* [35878-41-2]
Needles. Mp 159-160° (154-157°). $[\alpha]_D^{18}$ -35.1 (c, 0.88 in MeOH).

7-O-β-D-Glucopyranoside:
$C_{22}H_{26}O_9$ 434.442
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Needles (MeOH aq.). Mp 143-144°. $[\alpha]_D$ -35.5 (c, 1 in MeOH). λ_{max} 206 (log ϵ 4.68); 223 (log ϵ 4.22); 280 (log ϵ 3.83); 285 (log ϵ 3.8) (MeOH).

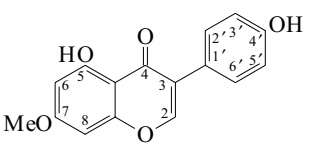
(*S*)-*form* [20879-05-4]
Mp 156°. $[\alpha]_D$ +21.6 (MeOH).

(±)-*form* [52305-03-0]
Cryst. (EtOAc). Mp 173-175°.

Antus, S. *et al., J.C.S. Perkin 1*, 1974, 305 (*synth*)
de Oliveira, A.B. *et al., Phytochemistry*, 1975, **14**, 2495 (*isol, struct, synth*)
Gottlieb, O.R. *et al., Phytochemistry*, 1978, **17**, 1413 (*isol, struct, synth*)
Alves, H.M. *et al., Phytochemistry*, 1978, **17**, 1423 (*abs config*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3267 (*isol*)
Goda, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 5606
Hatano, T. *et al., Phytochemistry*, 1998, **47**, 287-293 (*7-glucoside*)

4′,5-Dihydroxy-7-methoxyisoflavone D-541

[552-59-0]
*5-Hydroxy-3-(4-hydroxyphenyl)-7-methoxy-4*H*-1-benzopyran-4-one, 9CI*. ***Prunetin***. *Padmakastein*. *Prunusetin*



$C_{16}H_{12}O_5$ 284.268
Occurs in several *Prunus* spp. and *Glycyrrhiza glabra* (licorice). Cryst. (EtOH). Mp 246-248°. All isolations of isoflavones from microorganism cultures are considered doubtful.

► DJ3100050

4′-O-β-D-Glucopyranoside: [154-36-9] ***Prunitrin***. *Prunitroside. Trifoside. Prunetrin*
$C_{22}H_{22}O_{10}$ 446.41
Isol. from *Trifolium pratense* (red clover). Mp 181° (sinters from 160°). $[\alpha]_D$ -82.5 (Py). Padmakastin was prob. impure prunitrin.

5-O-β-D-Glucopyranoside: [89595-66-4] ***Prunetinoside***
$C_{22}H_{22}O_{10}$ 446.41
Plates. Mp 237-239°.

4′-O-β-D-Galactopyranoside: [117007-27-9]
$C_{22}H_{22}O_{10}$ 446.41
Mp 182-184°.

4′-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [169181-41-3] ***Coromandelin***
$C_{27}H_{30}O_{14}$ 578.526
Cryst. (MeOH). Mp 192-193°.

[26015-63-4]

Hasegawa, M. *et al., J.A.C.S.*, 1957, **79**, 1738 (*isol*)
Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 594 (*isol, deriv*)
Hudson, A.T. *et al., Chem. Comm.*, 1969, 830 (*isol*)
Farkas, L. *et al., Tetrahedron*, 1969, **25**, 1013 (*struct, synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Sekizaki, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4876 (*synth*)
Narayanan, V. *et al., Phytochemistry*, 1988, **27**, 2364 (*4′-Galactoside*)
Khalid, S.A. *et al., Phytochemistry*, 1989, **28**, 1560 (*Prunetinoside*)
Ramesh, P. *et al., J. Nat. Prod.*, 1995, **58**, 1240 (*cmr, Coromandelin*)

5,7-Dihydroxy-4′-methoxyisoflavone D-542

[491-80-5]
*5,7-Dihydroxy-3-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*. ***Biochanin A***. *Genistein 4′-methyl ether*. *Pratensol*. *Olmelin*

$C_{16}H_{12}O_5$ 284.268
Widespread isoflavone found in alfalfa *(Medicago sativa)*, chick peas *(Cicer arietinum)* and white clover *(Trifolium repens)*. Glycosides also widespread. Potential nutriceutical. Needles (MeOH or EtOH aq.). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 215-216°. λ_{max} 263 (ϵ 30000) (MeOH) (Berdy). λ_{max} 262 (ϵ 40700); 279 (EtOH) (Berdy). λ_{max} 274 (ϵ 30000); 336 (ϵ 9000) (EtOH-NaOH) (Berdy).

7-O-β-D-Glucopyranoside: [5928-26-7] ***Sissotrin***. *Astroside*
$C_{22}H_{22}O_{10}$ 446.41
Constit. of *Cicer arietinum* (chickpea). Mp 220° (212-214°) Mp 223-224.5°. $[\alpha]_D^{30}$ -35.3 (c, 1.644 in DMF). $[\alpha]_D^{20}$ -117.8 (c, 0.98 in DMF).

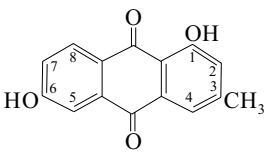
7-O-(6-O-Malonyl-β-D-glucopyranoside):
[34232-17-2]
$C_{25}H_{24}O_{13}$ 532.457
Isol. from leaves of *Trifolium pratense* (red clover). Needles (MeOH). Mp 217°. Revised struct..

7-O-(6-O-Malonyl-β-D-glucopyranoside), Me ester: [34232-19-4]
$C_{26}H_{26}O_{13}$ 546.484
Isol. from leaves of *Trifolium pratense* (red clover). Needles (MeOH). Mp 195°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 95D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 920A (*nmr*)
Baker, W. *et al., J.C.S.*, 1953, 1852 (*synth*)
Wong, E. *et al., Phytochemistry*, 1965, **4**, 89 (*Sissotrin*)
Deryugina, L.I. *et al., Khim. Prir. Soedin.*, 1966, **2**, 315; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 256 (*Astroside*)
Beck, A.B. *et al., Aust. J. Chem.*, 1971, **24**, 1509 (*malonates*)
Pelter, A. *et al., Synthesis*, 1976, 326 (*synth*)
Diedrich, D.F. *et al., J. Chem. Eng. Data*, 1977, **22**, 448 (*pmr*)
Bass, R.J. *et al., J.C.S. Perkin 1*, 1978, 666 (*cmr*)
Ashdown, D.H.J. *et al., Synthesis*, 1978, 843 (*synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Elgamal, M.H.A. *et al., J. Prakt. Chem.*, 1986, **328**, 893 (*ms*)
Murthy, M.S.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 225 (*cmr*)
Sekizaki, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4876 (*synth*)
Aparecida dos Santos, S. *et al., J. Braz. Chem. Soc.*, 1995, **6**, 349 (*pmr, cmr*)
Lewis, P. *et al., J.C.S. Perkin 1*, 1998, 2481-2484 (*Sissotrin, synth, pmr, cmr*)
Balasubramanian, S. *et al., Synth. Commun.*, 2000, **30**, 469-484 (*synth, pmr*)

1,6-Dihydroxy-3-methylanthraquinone, 8CI D-543

[6866-87-1]
1,6-Dihydroxy-3-methyl-9,10-anthracenedione, 9CI. ***Phomarin***. *Digitoemodin*



$C_{15}H_{10}O_4$ 254.242
From roots of *Ruta graveolens* (rue). Orange-red needles (EtOH). Mp 258-260° (200° dec.). λ_{max} 220 (ϵ 28200); 245 (ϵ 10960); 271 (ϵ 28840); 337 (ϵ 1480) (EtOH) (Berdy).

6-Me ether: [34425-59-7] *1-Hydroxy-6-methoxy-3-methylanthraquinone*
$C_{16}H_{12}O_4$ 268.268
Yellow needles (EtOH). Mp 193°.

Bick, I.R.C. *et al., Biochem. J.*, 1966, **98**, 112 (*ir, pmr*)
Brew, E.J.C. *et al., J.C.S.(C)*, 1971, 2007 (*isol*)
Imre, S. *et al., Phytochemistry*, 1976, **15**, 317 (*isol*)
Rozsa, Z. *et al., Planta Med.*, 1977, **32**, 57 (*isol*)
Imre, S. *et al., Z. Naturforsch., C*, 1978, **33**, 592 (*synth*)
Krohn, K. *et al., Tet. Lett.*, 1980, **21**, 3557 (*synth*)
Brisson, C. *et al., J.O.C.*, 1981, **46**, 1810 (*synth*)

1,8-Dihydroxy-3-methylanthraquinone D-544

[481-74-3]
1,8-Dihydroxy-3-methyl-9,10-anthracenedione, 9CI. ***Chrysophanol***. *3-Methylchrysazin*. *Rheic acid*. *Chrysophanic acid*. *Archinin*. *Rumicin*

$C_{15}H_{10}O_4$ 254.242
Constit. of *Rumex, Rheum* spp.. Golden-yellow plates (C_6H_6). Mp 200-201° (196°).

pK_a 8.91 (20°, H_2O). Log P 2.42 (calc). λ_{max} 223 (ϵ 36000); 253 (ϵ 20000); 274 (ϵ 10000); 285 (ϵ 11000); 405 (sh) (ϵ); 427 (ϵ 11000); 450 (sh) (ϵ) (MeOH) (Derep).

▶ CB6725000

1-O-*β*-D-*Glucopyranoside:* [4839-60-5] ***Pulmatin***
$C_{21}H_{20}O_9$ 416.384
Constit. of *Rheum palmatum* (Turkey rhubarb). Mp 232-234°. λ_{max} 223 (ϵ 5300); 258 (ϵ 3640); 430 (MeOH) (Berdy).

8-O-*β*-D-*Glucopyranoside:* [13241-28-6] ***Chrysophanein***. *Chrysophanol 8-glucoside*
$C_{21}H_{20}O_9$ 416.384
Isol. from *Rheum, Rumex* spp.. Fine yellow needles (EtOH). Mp 248-249° (245-246°). Kubo (1992) confirmed Chrysophanein as the 8-glucoside λ_{max} 223 (ϵ 3840); 258 (ϵ 4070); 277 ; 429 (MeOH) (Berdy).

8-O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:Chrysophanol 8-(6-galloylglucoside)*
$C_{28}H_{24}O_{13}$ 568.49
Constit. of the rhizomes of *Rheum undulatum* (rhubarb). Yellow needles (MeOH). Mp 207-210°. $[\alpha]_D^{25}$ +95 (c, 0.1 in MeOH). λ_{max} 220 (log ϵ 4.58); 260 (log ϵ 4.32); 284 (sh) (log ϵ 4.17); 409 (log ϵ 3.79) (MeOH).

8-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [54944-38-6] *Chrysophanol 8-gentiobioside*
$C_{27}H_{30}O_{14}$ 578.526
Constit. of the seeds of *Cassia tora* (charota). Yellow needles + $2H_2O$ (MeOH). Mp 168-170°. $[\alpha]_D$ -55.2 (c, 0.29 in MeOH).

1-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [120181-07-9] *Chrysophanol 1-triglucoside*
$C_{33}H_{40}O_{19}$ 740.668
Constit. of the seeds of *Cassia tora* (charota). Yellow powder. Mp 284-286°.

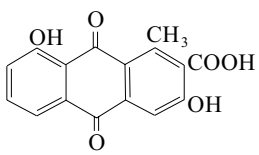
1-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [120181-08-0] *Chrysophanol 1-tetraglucoside*
$C_{39}H_{50}O_{24}$ 902.81
Constit. of the seeds of *Cassia tora* (charota). Yellow needles. Mp 288-290°. λ_{max} 224 ; 260 ; 286 (sh) ; 412 (MeOH).

1-Me ether: [67116-22-7] *8-Hydroxy-1-methoxy-3-methylanthraquinone*
$C_{16}H_{12}O_4$ 268.268
Constit. of *Rumex acetosa* (sorrel). Cryst. Mp 199-200°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 88A (*ir*)
King, F.E. *et al., J.C.S.*, 1952, 4580 (*synth*)
Bloom, H. *et al., J.C.S.*, 1959, 178 (*ir*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1254 (*occur*)
Labadie, R.P. *et al., Pharm. Weekbl.*, 1972, **107**, 535 (*occur*)
Rizk, A.M. *et al., Phytochemistry*, 1972, **11**, 2122 (*deriv*)
Banville, J. *et al., Can. J. Chem.*, 1974, **52**, 80 (*synth, uv, pmr*)
Raghunathan, K. *et al., Indian J. Chem.*, 1974, **12**, 1251 (*8-gentiobioside*)
Harris, T.M. *et al., J.A.C.S.*, 1976, **98**, 6065 (*synth*)
Kraus, G.A. *et al., J.O.C.*, 1983, **48**, 3439 (*synth*)
Kelly, T.R. *et al., J.O.C.*, 1983, **48**, 3573 (*isol*)
Anderson, J.A. *et al., Phytochemistry*, 1986, **25**, 103 (*biosynth*)
Ahmed, S.A. *et al., Chem. Comm.*, 1987, 883 (*synth*)
Thomson, W.H. *et al., Naturally Occurring Quinones, Recent Advances*, Chapman and Hall, 1987, (*occur*)
Wong, S.-M. *et al., Phytochemistry*, 1989, **28**, 211-214 (*1-tetraglucoside*)
Sassa, T. *et al., Agric. Biol. Chem.*, 1991, **55**, 95 (*isol*)
Danielsen, K. *et al., Magn. Reson. Chem.*, 1992, **30**, 359 (*pmr, cmr*)
Kubo, I. *et al., Phytochemistry*, 1992, **31**, 1063 (*Chrysophanein, Pulmatin*)
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, pmr*)
Schripsema, J. *et al., Phytochemistry*, 1996, **42**, 177 (*pmr, struct*)
Guo, H. *et al., Phytochemistry*, 1998, **49**, 1623-1625 (*1-Me ether*)

3,8-Dihydroxy-1-methylanthraquinone-2-carboxylic acid D-545

[69119-31-9]
9,10-Dihydro-3,8-dihydroxy-1-methyl-9,10-dioxo-2-anthracenecarboxylic acid, 9CI



$C_{16}H_{10}O_6$ 298.251
Constit. of *Crocus sativus* (saffron). Orange or yellow needles (AcOH or $CHCl_3$/MeOH/cyclohexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 248-250° (241-244°). λ_{max} 207 (ϵ 13900); 278 (ϵ 13800); 407 (ϵ 3400) (MeOH) (Berdy). λ_{max} 244 (ϵ 8900); 314 (ϵ 10700); 392 (ϵ 2200); 506 (ϵ 3100) (MeOH-NaOH) (Berdy).

Me ester: [53254-89-0] *1,6-Dihydroxy-7-methoxycarbonyl-8-methylanthraquinone.* ***Aloesaponarin I***
$C_{17}H_{12}O_6$ 312.278
Orange needles (MeOH). Mp 199-203° dec. λ_{max} 305 (ϵ); 390 (ϵ); 485 (ϵ) (MeOH/KOH) (Derep). λ_{max} 270 (ϵ 79400); 280 (ϵ 79400); 415 (ϵ 15800); 435 (ϵ 10000) (MeOH) (Derep).

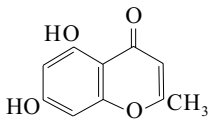
Di-Ac, Me ester: [53254-90-3]
Yellow needles (Me_2CO). Mp 203-206° dec.

3-Me ether: [176327-86-9] *8-Hydroxy-3-methoxy-1-methylanthraquinone-2-carboxylic acid*
$C_{17}H_{12}O_6$ 312.278
Constit. of *Crocus sativus* (saffron).

Yagi, A. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1159 (*isol, deriv*)
Yagi, A. *et al., Phytochemistry*, 1978, **17**, 895 (*biosynth, deriv*)
Roberge, G. *et al., Synthesis*, 1979, 148 (*synth, deriv*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1981, **24**, 2401 (*synth*)
Krupa, J. *et al., Annalen*, 1989, 699 (*isol*)
Gao, W.-Y. *et al., Zhiwu Xuebao*, 1999, **41**, 531-533 (*3-Me ether*)
Uno, H. *et al., Chem. Lett.*, 2000, 1014-1015 (*synth*)

5,7-Dihydroxy-2-methyl-4*H*-1-benzopyran-4-one, 9CI D-546

[1013-69-0]
5,7-Dihydroxy-2-methylchromone. ***Noreugenin***



$C_{10}H_8O_4$ 192.171
Needles (MeOH). Cryst. (EtOH). Mp 279° (275-280°).

5-O-*β*-D-*Glucopyranoside:* [128396-15-6] ***Schumanniofioside A***
$C_{16}H_{18}O_9$ 354.313
Granules (MeOH). Mp 162-163°.

7-O-*β*-D-*Glucopyranoside:* [58108-99-9] ***Undulatoside A***
$C_{16}H_{18}O_9$ 354.313
Needles (MeOH) or hygroscopic solid. Mp 245-248° (235-237°). $[\alpha]_D^{25}$ -50 (Py). $[\alpha]_D^{27}$ -169 (c, 0.71 in MeOH).

7-O-*[β-D-Glucopyranosyl-(1→2)-apiofuranoside]:* [128396-16-7] ***Schumanniofioside B***
$C_{21}H_{26}O_{13}$ 486.429
Cryst. (MeOH). Mp 251-252°.

7-O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [151029-70-8]
$C_{21}H_{26}O_{13}$ 486.429
Solid. $[\alpha]_D^{25}$ -94.2 (c, 1.5 in MeOH).

7-O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [71512-59-9] ***Undulatoside B***
$C_{21}H_{26}O_{13}$ 486.429
Yellow powder + $1H_2O$. Mp 156-157°. $[\alpha]_D^{18}$ -146.5 (c, 0.31 in MeOH).

7-O-*[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:* [31511-96-3] ***Staphylin***
$C_{22}H_{28}O_{14}$ 516.455
Microneedles. Mp 248-250°.

5-Me ether: [3449-40-9] *7-Hydroxy-5-methoxy-2-methyl-4*H*-1-benzopyran-4-one. 7-Hydroxy-5-methoxy-2-methylchromone.* ***Maritimin***†
$C_{11}H_{10}O_4$ 206.198
Prisms (Me_2CO). Mp 215-216° (112-113°).

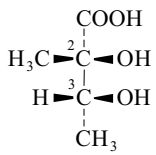
7-Me ether: [480-34-2] *5-Hydroxy-7-methoxy-2-methyl-4*H*-1-benzopyran-4-one. 5-Hydroxy-7-methoxy-2-methylchromone.* ***Eugenin***
$C_{11}H_{10}O_4$ 206.198
Constit. of *Eugenia aromatica* (clove). Cryst. (EtOH). Sol. MeOH, $CHCl_3$, EtOH. Mp 119-120°. λ_{max} 227 (ϵ 16000); 248 (ϵ 33000); 255 (ϵ 35500); 288 (ϵ 7950) (EtOH) (Berdy).

Meijer, T.M. *et al., Helv. Chim. Acta*, 1948, **31**, 1603 (*isol, struct, synth, Eugenin*)

Morita, N. *et al., Yakugaku Zasshi*, 1968, **88**, 1311-1312 (*Staphylin*)
Dorofeenko, G.N. *et al., Khim. Geterotsikl. Soedin.*, 1971, **7**, 1703; *CA*, **76**, 153503k (*synth*)
Chawla, H.M. *et al., Curr. Sci.*, 1975, **44**, 344 (*ir*)
Brown, R.T. *et al., J.C.S. Perkin 1*, 1975, 1776 (*isol, struct*)
Stoessl, A. *et al., Can. J. Bot.*, 1978, **56**, 2589 (*cmr, biosynth*)
Murata, A. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1979, **119**, 1346 (*Eugenin, synth*)
Gujral, V.K. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 40 (*Undulatoside B*)
Gujral, V.K. *et al., Phytochemistry*, 1979, **18**, 181 (*glucoside, Undutaloside A*)
Ito, T. *et al., Anal. Chim. Acta*, 1980, **113**, 343 (*Me ether, detn, Ti*)
Ahluwalia, V.K. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2649-2652 (*Maritimin, synth*)
Ghosal, S. *et al., Phytochemistry*, 1982, **21**, 2943 (*isol*)
Copeland, R.J. *et al., J.C.S. Perkin 1*, 1984, 1013
Tane, P. *et al., Phytochemistry*, 1990, **29**, 1004 (*glycosides*)
Kelly, T.R. *et al., J.O.C.*, 1992, **57**, 1593 (*synth, pmr, ms, ir*)
Abe, F. *et al., Phytochemistry*, 1993, **33**, 1499 (*7-apiosylglucoside*)
Elgamal, M.H.A. *et al., Fitoterapia*, 1998, **69**, 549-550 (*Undulatoside A, cmr*)
Youssef, D.T.A. *et al., Phytochemistry*, 1998, **49**, 2579-2583 (*Maritimin*)

2,3-Dihydroxy-2-methylbutanoic acid, 9CI D-547

[14868-24-7]
2,3-Dimethylglyceric acid

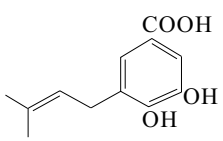


(2*R*,3*R*)-*form*

$C_5H_{10}O_4$ 134.132
Abs. config. assignments are subject to possible revision (1990) (see Mazars *et al*). Occurs in wine.
Christensen, B.W. *et al., Proc. Chem. Soc., London*, 1962, 37 (*abs config*)
Carles, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1966, **262**, 2788 (*synth*)
Robins, D.J. *et al., J.C.S.(C)*, 1970, 1334 (*synth, bibl, pmr*)
Closs, G.L. *et al., J.A.C.S.*, 1978, **100**, 3483 (*synth*)
Nouguier, R. *et al., Tet. Lett.*, 1994, **35**, 8171 (*synth*)

3,4-Dihydroxy-5-(3-methyl-2-butenyl)benzoic acid, 9CI D-548

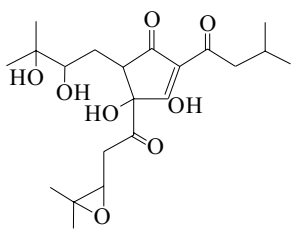
[101330-67-0]
3,4-Dihydroxy-5-prenylbenzoic acid



$C_{12}H_{14}O_4$ 222.24
λ_{max} 265 ; 300 (MeOH).
3-O-β-D-Glucopyranoside, Me ester:
$C_{19}H_{26}O_9$ 398.409
Constit. of apple leaves (*Malus domestica*). $[\alpha]_D$ -37 (c, 0.44 in $CHCl_3$). λ_{max} 208 ; 238 ; 280 (cyclohexane).
3-Me ether: [146367-85-3] *4-Hydroxy-3-methoxy-5-(3-methyl-2-butenyl)benzoic acid. 4-Hydroxy-3-methoxy-5-prenylbenzoic acid.* ***Proglobeflowery acid***
$C_{13}H_{16}O_4$ 236.267
Cryst.(EtOH aq.). Mp 141-142°.
4-Me ether: [101330-66-9] *3-Hydroxy-4-methoxy-5-(3-methyl-2-butenyl)benzoic acid. 3-Hydroxy-5-isopentenyl-4-methoxybenzoic acid. 3-Hydroxy-4-methoxy-5-prenylbenzoic acid*
$C_{13}H_{16}O_4$ 236.267
1′-Oxo: ***Lanceaefolic acid****. 3,4-Dihydroxy-5-(3-methyl-2-butenoyl)benzoic acid*
$C_{12}H_{12}O_5$ 236.224
Orange-yellow needles (Me_2CO). Mp 253-255°. $[\alpha]_D^{24}$ -14.3 (c, 0.1 in MeOH). Opt. rotn. unaccounted for λ_{max} 205 (log ϵ 3.92); 236 (log ϵ 4.29); 338 (log ϵ 3.46) (MeOH).
1′-Oxo, Me ester:
$C_{13}H_{14}O_5$ 250.251
Yellowish needles. Mp 109-110°. $[\alpha]_D^{24}$ -8.6 (c, 0.1 in MeOH). Opt. rotn. unaccounted for λ_{max} 203 (log ϵ 3.67); 240 (log ϵ 4.32); 338 (log ϵ 3.4) (MeOH).
Breuer, M. *et al., Phytochemistry*, 1986, **25**, 495-497 (*isol, pmr, cmr, ms*)
Liu, L.J. *et al., Yaoxue Xuebao*, 1992, **27**, 837-840 (*Proglobeflowery acid*)
Lopez, A. *et al., J. Nat. Prod.*, 2002, **65**, 62-64 (*Lanceaefolic acid*)
Stingl, C. *et al., Nat. Prod. Lett.*, 2002, **16**, 87-93 (*3-glucoside Me ester*)

5-(2,3-Dihydroxy-3-methylbutyl)-4-(3,4-epoxy-4-methylpentanoyl)-3,4-dihydroxy-2-isopentanoyl-2-cyclopenten-1-one D-549

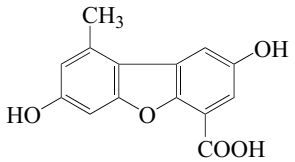
[18964-32-4]



$C_{21}H_{32}O_8$ 412.479
Constit. of hops. Pale-yellow noncryst. solid. Mp 65-68°.
Connett, B.E. *et al., J.C.S.(C)*, 1968, 1193

2,7-Dihydroxy-9-methyl-4-dibenzofurancarboxylic acid, 9CI D-550

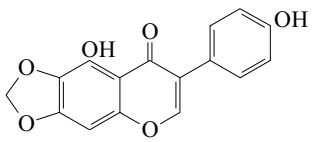
[207285-04-9]
Porric acid C



$C_{14}H_{10}O_5$ 258.23
Constit. of the bulbs of *Allium porrum* (leek). Pale yellow cryst. Mp 230-232°. λ_{max} 238 ; 256 ; 288 ; 298 ; 334 (MeOH).
Carotenuto, A. *et al., Eur. J. Org. Chem.*, 1998, 661-663 (*isol, uv, pmr, cmr*)

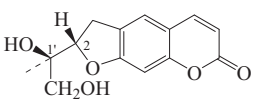
4′,5-Dihydroxy-6,7-methylenedioxyisoflavone D-551

[41653-81-0]
9-Hydroxy-7-(4-hydroxyphenyl)-8H-1,3-dioxolo[4,5-g][1]benzopyran-8-one, 9CI. ***Irilone***



$C_{16}H_{10}O_6$ 298.251
Constit. of *Trifolium pratense* (red clover). Yellow cryst. Mp 231°.
4′-O-β-D-Glucopyranoside: [50868-47-8] *Irilone 4′-glucoside*
$C_{22}H_{20}O_{11}$ 460.393
Isol. from the roots of *Trifolium pratense* (red clover). Amorph. solid. Mp 154°. $[\alpha]_D^{24}$ +47.6 (c, 0.63 in MeOH). λ_{max} 271 (log ϵ 3.56) (MeOH).
Gopinath, K.W. *et al., Tetrahedron*, 1961, **16**, 201 (*isol, struct*)
Dhar, K.L. *et al., Phytochemistry*, 1973, **12**, 734-735 (*Irilone*)
Pegnyemb, D.E. *et al., Fitoterapia*, 1998, **69**, 551 (*Irilone, cmr*)
Atta-ur-Rahman, *et al., Chem. Pharm. Bull.*, 2002, **50**, 1100-1102 (*Germanaism B, Irilone 4′-glucoside*)

2-(1,2-Dihydroxy-1-methylethyl)-2,3-dihydro-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI D-552



(1′*R*,2*S*)-*form*

$C_{14}H_{14}O_5$ 262.262
(1′*R*,2*S*)-*form* [54854-90-9]
Prandiol
Cryst. Mp 131-132° (natural) Mp 157-158° (synthetic).
(1′*S*,2*S*)-*form* [80794-85-0]
Dorsteniol
Constit. of *Apium graveolens*. Prisms. Mp 172-173° (natural) Mp 185-187° (synthetic) Mp 178-180° (as 2′-Ac). $[\alpha]_D$ +45 (c, 1 in $CHCl_3$) (2′-Ac). λ_{max} 231 (log ϵ 3.6); 248 (log ϵ 3.53); 259 (log ϵ 3.48); 300 (log ϵ 3.61); 360 (log ϵ 4.02) (no solvent reported) (2′-Ac).
2′-O-(3-Methyl-2-butenoyl): ***2′-Senecioyl-***

dorsteniol
$C_{19}H_{20}O_6$ 344.363
Cryst. (hexane/CH_2Cl_2). Mp 100-102°. $[\alpha]_D^{20}$ +28 (c, 0.7 in $CHCl_3$). λ_{max} 248 (sh) (log ϵ 3.9); 258 (sh) (log ϵ 3.9); 300 (sh) (log ϵ 3.8); 336 (log ϵ 4.3) (EtOH).

(1′ξ,2*R*)-*form*
2′-O-β-D-Glucopyranoside:
$C_{20}H_{24}O_{10}$ 424.404
Cryst. (H_2O). Mp 152-154.5°. $[\alpha]_D^{20}$ -22 (c, 0.06 in MeOH).

(1′ξ,2*S*)-*form*
2′-O-β-D-Glucopyranoside:
Constit. of *Angelica archangelica* (angelica). Cryst. (H_2O). Mp 184-188°. $[\alpha]_D^{20}$ -25 (c, 0.1 in MeOH).

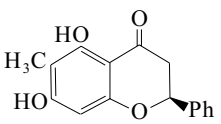
(1′ξ,2ξ)-*form*
1′-O-(3-Methyl-2-butenoyl): [89787-39-3] ***Tortuosinol***. *Prandiol senecioate*
$C_{19}H_{20}O_6$ 344.363
Cryst. Mp 79-81°.

[162555-82-0, 162679-04-1]

Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1974, **10**, 574; 1983, **19**, 704; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 586; 1983, **19**, 668 (*Tortuosinol*)
Garg, S.K. *et al., Planta Med.*, 1981, **43**, 306
Lemmich, J. *et al., Phytochemistry*, 1983, **22**, 553; 1995, **38**, 427 (*glucosides*)
Tovar-Miranda, R. *et al., J. Nat. Prod.*, 1998, **61**, 1216-1220 (*isol, synth, pmr, cmr, abs config*)
Rojas-Lima, S. *et al., Phytochemistry*, 1999, **50**, 863-868 (*isol, uv, cd, ir, pmr, cmr, ms, abs config*)
Jimenez, B. *et al., Phytochemistry*, 2000, **53**, 1025-1031 (*Senecioyldorsteniol*)

5,7-Dihydroxy-6-methylflavanone D-553

[491-66-7]
*2,3-Dihydro-5,7-dihydroxy-6-methyl-2-phenyl-4*H*-1-benzopyran-4-one, 9CI*. ***Strobopinin***. *6-*C*-Methylpinocembrin*



$C_{16}H_{14}O_4$ 270.284

(*S*)-*form* [11023-71-5]
Pale-yellow prisms (AcOH). Mp 225-227°. $[\alpha]_D^{20.5}$ -60.5 (MeOH).

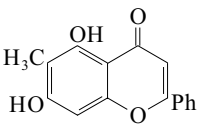
Di-Me ether: [128508-16-7] *5,7-Dimethoxy-6-methylflavanone*
$C_{18}H_{18}O_4$ 298.338
Constit. of *Leptospermum scoparium* (red tea). Needles (Et_2O). Mp 133-135°. $[\alpha]_D^{20}$ +19.2 (c, 0.104 in $CHCl_3$).

[1230-20-2, 80749-76-4, 82571-07-1, 84413-39-8]

Erdtman, H. *et al., Sven. Kem. Tidskr.*, 1944, **56**, 2; *CA*, **40**, 1309 (*isol*)
Linstedt, G. *et al., Acta Chem. Scand.*, 1951, **5**, 1; 121; 129 (*isol, struct*)
Asakawa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 2761 (*isol*)
Gawad, D.H. *et al., Indian J. Chem.*, 1974, **12**, 1033 (*synth*)
Star, A.E. *et al., Phytochemistry*, 1978, **17**, 586 (*isol, deriv*)
Wollenweber, E. *et al., Z. Pflanzenphysiol.*, 1979, **94**, 241; 1981, **104**, 161 (*isol, deriv*)
Byrne, L.T. *et al., Aust. J. Chem.*, 1982, **35**, 1851 (*cmr, struct*)
Markham, K.R. *et al., J. Plant Physiol.*, 1987, **131**, 45 (*derivs, struct*)
Mayer, R. *et al., Phytochemistry*, 1990, **29**, 1340 (*5,7-Dimethoxy-6-methylflavanone*)
Solladie, G. *et al., Eur. J. Org. Chem.*, 1999, 2309-2314 (*synth, pmr, cmr*)

5,7-Dihydroxy-6-methylflavone D-554

[529-52-2]
*5,7-Dihydroxy-6-methyl-2-phenyl-4*H*-1-benzopyran-4-one.* ***Strobochrysin***. *6-Methylchrysin*



$C_{16}H_{12}O_4$ 268.268
Cryst. (EtOH). Mp 312-314° (308-310°).

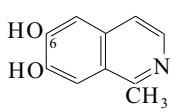
7-Me ether: [55969-57-8] ***5-Hydroxy-7-methoxy-6-methylflavone***
$C_{17}H_{14}O_4$ 282.295
Isol. from *Leptospermum scoparium* (red tea). Yellow needles. Mp 176-179° (170-172°).

Di-Me ether: [109251-29-8] *5,7-Dimethoxy-6-methylflavone.* ***Dimethylstrobochrysin***
$C_{18}H_{16}O_4$ 296.322
Constit. of *Leptospermum scoparium* (red tea). Cryst. (Et_2O). Mp 170-171° (166-168°).

Lindstedt, G. *et al., Acta Chem. Scand.*, 1951, **5**, 1 (*isol*)
Aknin, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 604 (*synth*)
Beirne, J.J. *et al., Tetrahedron*, 1975, **31**, 265 (*synth*)
Seligmann, O. *et al., Tetrahedron*, 1981, **37**, 2601 (*synth, uv*)
Cardona, M.L. *et al., Phytochemistry*, 1982, **21**, 2759 (*7-Me ether*)
Mayer, R. *et al., Phytochemistry*, 1990, **29**, 1340 (*7-Me ether*)
Mayer, R. *et al., Planta Med.*, 1993, **59**, 269 (*Dimethylstrobochrysin*)
Haeberlein, H. *et al., Phytochemistry*, 1994, **35**, 765 (*Di-Me ether*)
Hauteville, M. *et al., Annalen*, 1996, 1217 (*synth, pmr, ms*)

6,7-Dihydroxy-1-methylisoquinoline D-555

1-Methyl-6,7-isoquinolinediol



$C_{10}H_9NO_2$ 175.187
► NW8220000

6-Me ether: [4594-05-2] *6-Methoxy-1-methyl-7-isoquinolinol, 9CI. 7-Hydroxy-6-methoxy-1-methylisoquinoline*
$C_{11}H_{11}NO_2$ 189.213
Needles ($CHCl_3$/MeOH). Mp 121-123°.

Di-Me ether: [4594-02-9] *6,7-Dimethoxy-1-methylisoquinoline, 9CI.* ***Isosalsolidine***.
Nigellimine
$C_{12}H_{13}NO_2$ 203.24
Trace constit. in seeds of *Nigella sativa* (black cumin). Cryst. (Et_2O/EtOAc). Mp 118-119°.

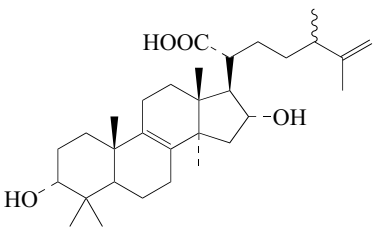
Di-Me ether, N*-oxide:* [96562-85-5] ***Nigellimine* N*-oxide***
$C_{12}H_{13}NO_3$ 219.24
Minor alkaloid from the seeds of *Nigella sativa* (blcak cumin). Amorph.

3,4-Dihydro, di-Me ether:3,4-Dihydro-6,7-dimethoxy-1-methylisoquinoline. ***Dehydrosalsolidine***
$C_{12}H_{15}NO_2$ 205.256
Mp 201-202° (195-197°)(as hydrochloride).

1,2,3,4-Tetrahydro: 1,2,3,4-Tetrahydro-6,7-dihydroxy-1-methylisoquinoline, T-77

Pummangura, S. *et al., J. Nat. Prod.*, 1982, **45**, 277 (*Dehydrosalsolidine*)
Roush, R.A. *et al., Anal. Chem.*, 1985, **57**, 109 (*occur, Isosalsolidine*)
Atta-ur-Rahman, *et al., Heterocycles*, 1985, **23**, 953 (*Nigellimine oxide*)
Atta-ur-Rahman, *et al., J. Nat. Prod.*, 1992, **55**, 676 (*isol, Isosalsolidine*)
Chen, J.J. *et al., Phytochemistry*, 1996, **42**, 1479 (*6-Me ether*)

3,16-Dihydroxy-24-methyllanosta-8,25-dien-21-oic acid D-556



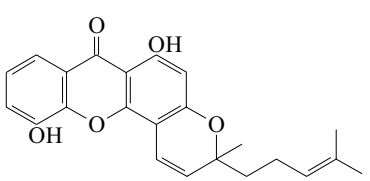
$C_{31}H_{50}O_4$ 486.734

(3α,16α,24ξ)-*form*
3-Ac: [201045-20-7] ***Tsugaric acid B***
$C_{33}H_{52}O_5$ 528.771
Constit. of *Ganoderma tsugae* (red reishi). Powder (MeOH/$CHCl_3$). Mp 240-242°. $[\alpha]_D^{27}$ -15 (c, 0.1 in $CHCl_3$).

Lin, C.-N. *et al., Phytochemistry*, 1997, **46**, 1143-1146 (*isol, pmr, cmr*)

6,11-Dihydroxy-3-methyl-3-(4-methyl-3-pentenyl)-3*H*,7*H*-pyrano[2,3-*c*]xanthen-7-one, 9CI D-557

[35338-77-3]

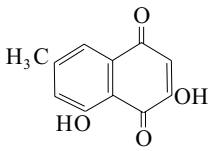


$C_{23}H_{22}O_5$ 378.424
Constit. of the root bark of *Garcinia livingstonei* (imbe). Yellow plates. Mp 140-141°. λ_{max} 250 (ϵ 31500); 266 (ϵ 30000); 308 (ϵ 9900); 329 (ϵ 11000); 370 (ϵ 3000) (MeOH) (Berdy).

Locksley, H.D. *et al., J.C.S.(C)*, 1971, 3804 (*synth*)
Sordat-Diserens, I. *et al., Phytochemistry*, 1992, **31**, 313 (*isol, pmr, cmr*)

2,8-Dihydroxy-6-methyl-1,4-naphthoquinone D-558

[39058-21-4]
3-Hydroxy-7-methyljuglone



$C_{11}H_8O_4$ 204.182
Yellow needles.

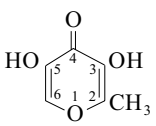
2-Me ether: [1589-92-0] *8-Hydroxy-2-methoxy-6-methyl-1,4-naphthoquinone. 8-Hydroxy-2-methoxy-6-methylnaphthalene-1,4-dione, 9CI. 3-Methoxy-7-methyljuglone*
$C_{12}H_{10}O_4$ 218.209
Root constit. of *Diospyros kaki* (Japanese persimmon). Cryst. (petrol). Mp 210-211° (209-210°).

Di-Me ether: [39058-19-0] *2,8-Dimethoxy-6-methyl-1,4-naphthoquinone*
$C_{13}H_{12}O_4$ 232.235
Yellow needles (C_6H_6). Mp 172°.

Yoshihira, K. *et al., Chem. Pharm. Bull.*, 1971, **19**, 851 (*isol, struct*)
Tezuka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2029 (*synth, pmr*)
Giles, R.G.F. *et al., J.C.S. Perkin 1*, 1976, 2057 (*synth*)
Marston, A. *et al., Planta Med.*, 1984, **50**, 279 (*deriv*)
Savard, J. *et al., Tetrahedron*, 1984, **40**, 3455 (*deriv*)
Budzianowski, J. *et al., Planta Med. (Suppl.)*, 1993, **59**, A654 (*deriv*)

3,5-Dihydroxy-2-methyl-4*H*-pyran-4-one, 9CI D-559

[1073-96-7]
5-Hydroxymaltol



$C_6H_6O_4$ 142.111
Constit. of flavour of roast barley *Hordeum vulgare*. Rhombic plates. Mp 184-184.5°.

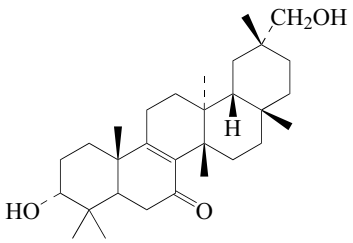
3-O-β-D-Glucopyranoside:
$C_{12}H_{16}O_9$ 304.253
Mp 148°. $[\alpha]_D$ -39.3.

5-O-α-L-Rhamnopyranoside:
$C_{12}H_{16}O_8$ 288.254
Mp 178-179°.

Di-Me ether:3,5-Dimethoxy-2-methyl-4H-pyran-4-one. ***Zanthopyranone***
$C_8H_{10}O_4$ 170.165
Needles(MeOH). Mp 98°. λ_{max} 218 (log ε 4.01); 273 (log ε 4.15) (MeOH).

Matsuto, S. *et al., Agric. Biol. Chem.*, 1970, **34**, 845 (*ms, uv, ir*)
Jureb, G.R. *et al., Carbohydr. Res.*, 1970, **15**, 233
Murakami, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 643 (*glucoside*)
Wada, H. *et al., Yakugaku Zasshi*, 1986, **106**, 989 (*rhamnoside*)
Yang, Y.-P. *et al., Phytochemistry*, 2002, **61**, 567-572 (*Zanthopyranone*)

3,29-Dihydroxy-8-multifloren-7-one D-560



$C_{30}H_{48}O_3$ 456.707
3α-*form*
7-Oxodihydrokarounidiol

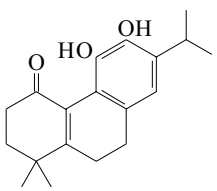
3-Benzoyl: [201685-86-1]
$C_{37}H_{52}O_4$ 560.815
Amorph. solid (Me_2CO/MeOH). Mp 135-140°. λ_{max} 250 (log ε 4.03) (EtOH).

Bis(4-methoxybenzoyl): [361475-68-5]
$C_{46}H_{60}O_7$ 724.976
Constit. of *Momordica cochinchinensis* (Chinese cucumber). Cryst. (EtOH). Mp 212.5-213.5°. $[\alpha]_D^{26}$ -16 (c, 0.5 in $CHCl_3$). λ_{max} 254 (log ε 3.77); 315 (log ε 3.53) ($CHCl_3$).

Akihisa, T. *et al., Phytochemistry*, 1997, **46**, 1261-1266 (*isol, pmr, cmr*)
Shan, M.D. *et al., Nat. Prod. Lett.*, 2001, **15**, 139-145 (*bis-4-methoxybenzoyl, isol, pmr, cmr, cryst struct*)

11,12-Dihydroxy-20-nor-5(10),8,11,13-abietatetraen-1-one D-561

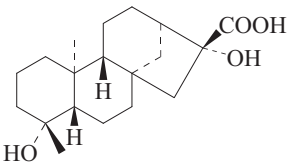
[142546-15-4]
Sageone



$C_{19}H_{24}O_3$ 300.397
Constit. of *Salvia officinalis* (sage). Amorph. yellow solid or oil.

González, A.G. *et al., Phytochemistry*, 1992, **31**, 1297 (*isol, pmr, cmr*)
Tada, M. *et al., Phytochemistry*, 1994, **35**, 539 (*isol, pmr, cmr*)
Majetich, G. *et al., J.O.C.*, 1997, **62**, 6928-6951 (*synth*)

4,16-Dihydroxy-19-nor-17-kauranoic acid D-562

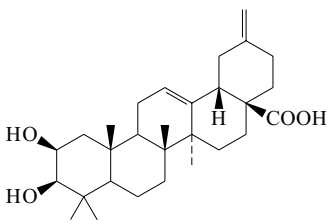


$C_{19}H_{30}O_4$ 322.444
(*ent*-4β*OH*,16β*OH*)-*form*

16-Ac, Me ester: [288627-12-3] ***Annoglabasin F***
$C_{22}H_{34}O_5$ 378.508
Constit. of *Annona glabra* (pond apple). Powder. Mp 164-165°. $[\alpha]_D^{25}$ -64.5 (c, 0.09 in $CHCl_3$).

Chen, C.-Y. *et al., J. Nat. Prod.*, 2000, **63**, 1000-1003 (*isol, pmr, cmr*)

2,3-Dihydroxy-30-nor-12,20(29)-oleanadien-28-oic acid D-563



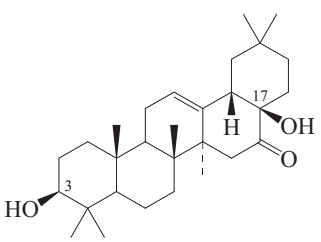
$C_{29}H_{44}O_4$ 456.664
(2β,3β)-*form*

3-O-[α-L-Rhamnopyranosyl-(1→3)-β-D-glucuronopyranoside], β-D-glucopyranosyl ester: [139742-11-3] ***Amaranthussaponin III***
$C_{47}H_{72}O_{19}$ 941.074
Constit. of *Amaranthus hypochondriacus* (prince's feather). Powder. $[\alpha]_D$ +22 (c, 0.4 in Py).

Kohda, H. *et al., Chem. Pharm. Bull.*, 1995, **39**, 2609 (*isol*)

3,17-Dihydroxy-28-nor-12-oleanen-16-one, 9CI D-564

[96861-15-3]



$C_{29}H_{46}O_3$ 442.681
Structs. revised in 2001, formerly assigned as 18-hydroxy.
(3β,17β)-*form* [81426-91-7]
Camellenodiol
Constit. of *Camellia japonica*. Cryst. ($CHCl_3$). Mp 215-216.5°. $[\alpha]_D^{25}$ +30 (c,

0.22 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [380303-64-0]
Camellioside A
$C_{53}H_{84}O_{24}$ 1105.232
Constit. of *Camellia japonica*. Cryst. (MeOH aq.). Mp 226-229°. $[\alpha]_D^{26}$ -32.1 (c, 1.8 in Py).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-[4-O-acetyl-β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [378244-83-8]
Camellioside B
$C_{55}H_{86}O_{25}$ 1147.269
Constit. of *Camellia japonica*. Cryst. (MeOH aq.). Mp 221-224°. $[\alpha]_D^{23}$ -30 (c, 0.8 in Py).

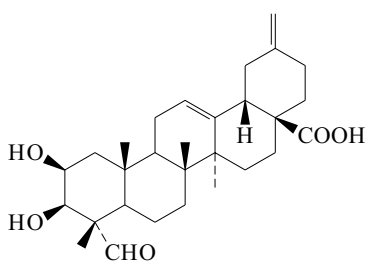
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[α-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [96827-23-5] ***Camellidin II***
$C_{53}H_{84}O_{24}$ 1105.232
From *Camellia japonica*. Cryst. Sol. MeOH, butanol, Py; poorly sol. hexane. Mp 211-212°. $[\alpha]_D^{25}$ -6 (c, 0.5 in MeOH).

17-Ac, 3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→4)-[α-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [96827-22-4] ***Camellidin I***
$C_{55}H_{86}O_{25}$ 1147.269
Constit. of *Camellia japonica*. Cryst. Sol. MeOH, butanol, Py; poorly sol. hexane. Mp 208-209°. $[\alpha]_D^{25}$ +2 (c, 0.5 in MeOH).

3-Ketone: [81426-90-6] *17β-Hydroxy-28-nor-3,16-oleanenedione.* ***Camelledionol***
$C_{29}H_{44}O_3$ 440.665
Constit. of *Camellia japonica*. Cryst. Mp 232-233°. $[\alpha]_D^{26}$ +49 (c, 0.1 in $CHCl_3$).

Itokawa, H. *et al., Phytochemistry*, 1981, **20**, 2539 (*isol*)
Nagata, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 1181 (*isol*)
Nishino, C. *et al., Chem. Comm.*, 1986, 720 (*struct*)
Yoshikawa, M. *et al., Heterocycles*, 2001, 1653-1657 (*Camelliosides, cryst struct*)

2,3-Dihydroxy-30-nor-23-oxo-12,20(29)-oleanadien-28-oic acid D-565



$C_{29}H_{42}O_5$ 470.648
(2β,3β)-*form*

3-O-[α-L-Rhamnopyranosyl-(1→3)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [139742-12-4]
Amaranthussaponin IV
$C_{47}H_{70}O_{20}$ 955.058
Constit. of *Amaranthus hypochondriacus* (prince's feather). Powder. $[\alpha]_D$ +71.9 (c, 0.32 in MeOH).

23-Carboxylic acid:2,3-Dihydroxy-30-nor-12,20(29)-oleanadiene-23,28-dioic acid
$C_{29}H_{42}O_6$ 486.647

23-Carboxylic acid, 3-O-β-D-glucuronopyranoside, 28-O-β-D-glucopyranosyl ester: [214840-34-3]
$C_{41}H_{60}O_{17}$ 824.915
Constit. of *Amaranthus cruentus* (purple amaranth). $[\alpha]_D^{25}$ +43.8.

23-Carboxylic acid, 3-O-[β-D-glucuronopyranosyl-(1→3)-β-D-glucuronopyranoside]: [170894-33-4]
Lindernioside B
$C_{41}H_{58}O_{18}$ 838.898
$[\alpha]_D^{20}$ +51.1 (c, 1.8 in MeOH) (as tetra-Me ester).

Kohda, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2609 (*Amaranthussaponin IV*)
Miyase, T. *et al., Phytochemistry*, 1995, **40**, 1499 (*Lindernioside B*)
Junkuszew, M. *et al., Phytochemistry*, 1998, **49**, 195-198 (*Amaranthus cruentus saponin*)

15,16-Dihydroxyoctadecanoic acid D-566

15,16-Dihydroxystearic acid
$H_3CCH_2CH(OH)CH(OH)(CH_2)_{13}COOH$
$C_{18}H_{36}O_4$ 316.48

(+)-*form*
Prepared from *Camelina sativa* (false flax). Cryst. (petrol). Mp 96-97°. $[\alpha]_D^{20}$ +3.3 (c, 4 in EtOH).

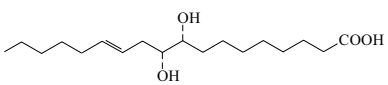
Me ester:
$C_{19}H_{38}O_4$ 330.507
Mp 89.5-90.5°.

Et ester:
$C_{20}H_{40}O_4$ 344.534
Mp 74-74.5°.

Gunstone, F.D. *et al., J.C.S.*, 1959, 2127 (*synth*)

9,10-Dihydroxy-12-octadecenoic acid D-567

[53734-70-6]

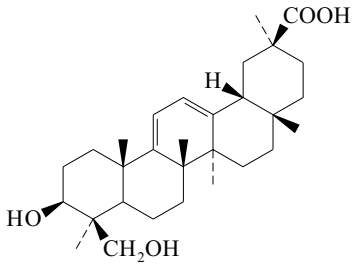


(9*RS*,10*RS*,12*E*)-*form*

$C_{18}H_{34}O_4$ 314.464
(9*RS*,10*RS*,12*E*)-*form* [59959-43-2]
(±)-trans-threo-*form*
Cryst. (Et_2O/petrol). Mp 71-74°.
(9*RS*,10*RS*,12*Z*)-*form* [59959-42-1]
(±)-cis-threo-*form*
Cryst. (Et_2O/petrol). Mp 62-63°.
(9*RS*,10*SR*,12*E*)-*form* [59959-50-1]
(±)-trans-erythro-*form*
Cryst. (Et_2O/petrol). Mp 119-120.5°.
(9*RS*,10*SR*,12*Z*)-*form* [59959-49-8]
(±)-cis-erythro-*form*
Cryst. (Et_2O/petrol). Mp 96-99°.
(9ξ,10ξ,12ξ)-*form*
Isol. from the seeds of *Cucurbita pepo*. Fine needles (hexane/EtOAc). Mp 59-59.5°. $[\alpha]_D^{20}$ +10 (c, 0.2 in MeOH).
[62071-03-8, 125356-85-6, 125356-86-7, 125356-87-8, 125356-88-9]

Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1975, **15**, 174; 198 (*synth, ms*)
Fukui, H. *et al., Agric. Biol. Chem.*, 1977, **41**, 175 (*isol*)
Kato, T. *et al., Tet. Lett.*, 1983, **24**, 4715 (*isol*)
Fukushima, J. *et al., Agric. Biol. Chem.*, 1989, **53**, 3057 (*isol, synth*)
Pang, Z. *et al., Acta Chem. Scand.*, 1994, **48**, 408 (*isol*)

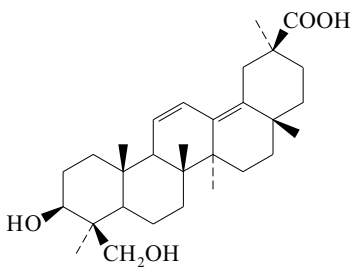
3,24-Dihydroxy-9(11),12-oleanadien-30-oic acid D-568



$C_{30}H_{46}O_4$ 470.691
3β-*form* [56262-33-0]
Isol. from *Glycyrrhiza glabra* (licorice). Mp 265-267° (as Me ester).

Bogatkina, V.F. *et al., Khim. Prir. Soedin.*, 1975, **11**, 101; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 114 (*isol*)

3,24-Dihydroxy-11,13(18)-oleanadien-30-oic acid D-569



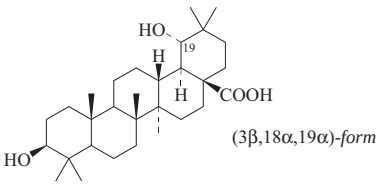
$C_{30}H_{46}O_4$ 470.691
3β-*form*

Me ester: [98063-17-3]
$C_{31}H_{48}O_4$ 484.718
Isol. from *Glycyrrhiza uralensis* (Chinese licorice) and *Glycyrrhiza glabra* (licorice). Mp 247° (as di-Ac).

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Licoricesaponin K2***
$C_{42}H_{62}O_{16}$ 822.942
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Mp 207-209°. $[\alpha]_D^{25}$ +28 (MeOH).

Bogatkina, V.F. *et al., Khim. Prir. Soedin.*, 1975, **11**, 101; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 114 (*isol*)
Shu, Y. *et al., CA*, 1985, **103**, 119932 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1991, **39**, 244 (*Licoricesaponin K2*)

3,19-Dihydroxy-28-oleananoic acid D-570



(3β,18α,19α)-*form*

$C_{30}H_{50}O_4$ 474.723

(3β,18α,19α)-*form* [205439-95-8]
Machaeroceric acid
Amorph. powder. Mp 271-274°. $[\alpha]_D^{20}$ +5.98 (c, 0.35 in $CHCl_3$/MeOH).

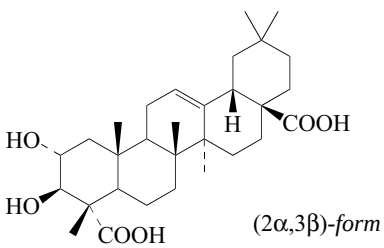
(3β,18α,19β)-*form*

28→19 Lactone: [24035-70-9] ***Oxyallobetulin***
$C_{30}H_{48}O_3$ 456.707
Isol. from *Diospyros lotus* (date plum). Needles (EtOH). Mp 310°.

28→19-Lactone, Ac: [60441-33-0]
Cryst. (Me_2CO). Mp 310°.

Yoshihira, K. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2308 (*isol*)
Nasipuri, D. *et al., J.C.S. Perkin 1*, 1976, 321 (*synth*)
Lillie, T.J. *et al., J.C.S. Perkin 1*, 1976, 2155 (*isol*)
Achari, B. *et al., Tetrahedron*, 1976, **32**, 741 (*struct*)
Ye, Y. *et al., J. Nat. Prod.*, 1998, **61**, 456-460 (*Machaeroceric acid*)

2,3-Dihydroxy-12-oleanene-23,28-dioic acid D-571



(2α,3β)-*form*

$C_{30}H_{46}O_6$ 502.69

(2β,3β)-*form* [599-07-5]
Medicagenic acid. *Catsanogenin. Medicogenic acid*
Aglycone from the roots of *Medicago sativa* (alfalfa) and other *Medicago* spp.. Cryst. (MeOH). Mp 352-353°. $[\alpha]_D^{23}$ +106 (EtOH).

28-O-[β-D-Xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [129570-95-2]
$C_{46}H_{72}O_{18}$ 913.064
Isol. from the roots of *Medicago sativa* (alfalfa).

3-O-β-D-Glucopyranoside: [49792-23-6]
$C_{36}H_{56}O_{11}$ 664.832
Isol. from the roots of *Medicago sativa* (alfalfa). Mp 253-255°. $[\alpha]_D^{23}$ +71.4 (EtOH).

3-O-β-D-Glucopyranoside, 28-O-β-D-glucopyranosyl ester: [106074-96-8]
Medicoside G
$C_{42}H_{66}O_{16}$ 826.974
Isol. from roots of *Medicago sativa* (alfalfa). Sol. H_2O. Mp 255° (242-243°). $[\alpha]_D^{24}$ +35.2 (c, 0.53 in 50% EtOH aq.). Revised struct..

3-O-β-D-Glucopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→2)-β-L-arabinopyranosyl] ester: [125448-43-3]
Medicoside H
$C_{47}H_{74}O_{19}$ 943.09
Isol. from the roots of *Medicago sativa* (alfalfa).

3-O-β-D-Glucopyranoside, 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [120039-30-7]
$C_{52}H_{82}O_{23}$ 1075.206
Isol. from the roots of *Medicago sativa* (alfalfa). Sol. H_2O.

3-O-β-D-Glucopyranoside, 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-L-arabinopyranosyl] ester: [107195-79-9]
Medicoside J
$C_{52}H_{82}O_{23}$ 1075.206
Isol. from the roots of *Medicago sativa* (alfalfa).

3-O-β-D-Glucuronopyranoside: [84161-90-0]
$C_{36}H_{54}O_{12}$ 678.815
Constit. of the roots of *Medicago sativa* (alfalfa). Sol. H_2O.

3-O-β-D-Glucuronopyranoside, 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [128192-15-4]
$C_{52}H_{80}O_{24}$ 1089.19
Isol. from the roots of *Medicago sativa* (alfalfa). Sol. H_2O.

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [120039-31-8]
$C_{58}H_{92}O_{28}$ 1237.348
Isol. from the roots of *Medicago sativa* (alfalfa). Sol. H_2O.

3-O-[α-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]: [49792-25-8] *Medicagenic acid β-maltoside*
$C_{42}H_{66}O_{16}$ 826.974
Constit. of the roots of *Medicago sativa* (alfalfa). Sol. MeOH.

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside]: [37838-43-0]
$C_{48}H_{76}O_{21}$ 989.116
Constit. of the roots of *Medicago sativa* (alfalfa). $[\alpha]_D^{23}$ +10.2 (c, 1 in 80% EtOH).
▶ Highly toxic.

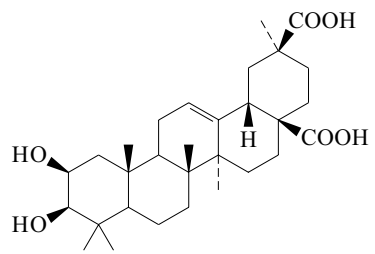
3-O-[α-L-Rhamnopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 28-O-β-D-glucopyranosyl ester: [128784-75-8]
Medicoside L
$C_{60}H_{96}O_{30}$ 1297.4
Constit. of the roots of *Medicago sativa* (alfalfa).

Glycoside: Medicagenic acid triglycoside
$C_{48}H_{74}O_{21}$ 987.1
Isol. from blooms of *Medicago sativa* (alfalfa). Powder. Mp 257-258°. $[\alpha]_D^{23}$ +24 (c, 0.02 in EtOH). Gives Medicagenic acid, L-rhamnose, D-glucose and D-glucuronic acid on hydrol..

[96686-56-5, 107232-01-9]

Morris, R.J. *et al., J.O.C.*, 1961, **26**, 1241-1243; 1963, **28**, 240-242 (*2β,3β-form, glucoside*)
Morris, R.J. *et al., J.O.C.*, 1965, **30**, 166-168 (*2β,3β-form, triglycoside*)
Sastry, C.S.P. *et al., Tetrahedron*, 1967, **23**, 3837-3846 (*2β,3β-form, isol*)
Gestetner, B. *et al., Phytochemistry*, 1971, **10**, 2221-2223 (*2β,3β-form, triglucoside*)
Metzger, J.D. *et al., J.O.C.*, 1972, **37**, 789-793 (*2β,3β-form, synth*)
Anjaneyulu, A.S.R. *et al., J. Indian Chem. Soc.*, 1978, **55**, 1169-1174 (*isol, deriv*)
Timbekova, A.E. *et al., Khim. Prir. Soedin.*, 1984, **20**, 451-458; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 427-433 (*Medicoside G*)
Levy, M. *et al., J. Agric. Food Chem.*, 1986, **34**, 960-963 (*Medicagenic acid glucoside*)
Timbekova, A.E. *et al., Khim. Prir. Soedin.*, 1986, **22**, 610-613; 1989, **25**, 673-677; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 574-577; 1989, **25**, 573-576 (*Medicosides H and J*)
Stoeckli-Evans, H. *et al., Acta Cryst. C*, 1989, **45**, 341-343 (*cryst struct, Medicagenic acid*)
Levy, M. *et al., Carbohydr. Res.*, 1989, **193**, 115-123 (*Medicagenic acid β-maltoside*)
Oleszek, W. *et al., J. Agric. Food Chem.*, 1990, **38**, 1810-1817 (*3-glucuronoside*)
Mil'grom, Y.M. *et al., Khim. Prir. Soedin.*, 1992, **28**, 98-102; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 82-85 (*Medicosides H and J, ms*)

2,3-Dihydroxy-12-oleanene-28,30-dioic acid D-572



$C_{30}H_{46}O_6$ 502.69

(2β,3β)-*form* [57079-94-4]
Acinosolic acid

28-Me ester:
$C_{31}H_{48}O_6$ 516.717
Cryst. Mp 200°.

3-Ac, 28-Me ester: [95260-97-2] ***Acinosolic acid A***
$C_{33}H_{50}O_7$ 558.754
Cryst. Mp 310°.

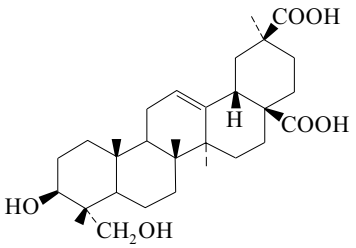
2-Ac, 28-Me ester: [95260-98-3] ***Acinosolic acid B***
$C_{33}H_{50}O_7$ 558.754
Cryst. Mp 345°.

30-Me ester: [75206-90-5] ***Pokeberrygenin***
$C_{31}H_{48}O_6$ 516.717
Isol. from *Phytolacca americana* berries (pokeberry). Amorph. powder (MeOH). Mp 208-209°. $[\alpha]_D^{25}$ +79.2 (c, 0.29 in MeOH).

Glombitza, K.W. *et al., Planta Med.*, 1975, **27**, 367 (*isol*)
Kang, S.S. *et al., J. Nat. Prod.*, 1980, **43**, 510 (*isol*)

Harkar, S. *et al., Phytochemistry*, 1984, **23**, 2893

3,23-Dihydroxy-12-oleanene-28,30-dioic acid D-573



$C_{30}H_{46}O_6$ 502.69

3β-*form* [56283-68-2]
Esculentic acid†
Isol. from *Phytolacca americana* (pokeberry). Mp 360°. $[\alpha]_D^{25}$ +85.6 (c, 0.23 in EtOH).

30-Me ester: [54928-05-1] ***Phytolaccinic acid***. *Phytolaccagenic acid*
$C_{31}H_{48}O_6$ 516.717
Aglycone from the berries of *Phytolacca americana* (pokeberry). Cryst. (EtOAc). Mp 295-299°. $[\alpha]_D^{25}$ -66.5 (c, 1 in MeOH).

3,23-Di-Ac, 28-Me ester: [88202-34-0] ***Isophytolaccinic acid A***
$C_{35}H_{52}O_8$ 600.791
Cryst. (C_6H_6/petrol). Mp 145°.

3-O-*β*-D-*Xylopyranoside:* [139198-58-6] ***Esculentoside O***
$C_{35}H_{54}O_{10}$ 634.806

3-O-*β*-D-*Xylopyranoside, 30-Me ester:* [65608-00-6] ***Phytolaccoside A***
$C_{36}H_{56}O_{10}$ 648.832
Isol. from *Phytolacca americana* (pokeberry). Mp 273-274°. $[\alpha]_D$ +56.5 (c, 0.14 in MeOH).

3-O-*β*-D-*Glucopyranoside, 30-Me ester:* [129715-90-8] ***3-O-β-D-Glucopyranosylphytolaccagenic acid***
$C_{37}H_{58}O_{11}$ 678.859
Pale yellow needles (MeOH/EtOAc). Mp 195-197°. $[\alpha]_D^{22}$ +45.8 (c, 0.12 in MeOH).

3-O-*β*-D-*Glucuronopyranoside, 30-Me ester:* [155556-65-3]
$C_{37}H_{56}O_{12}$ 692.842
Cryst. Mp 238°. $[\alpha]_D^{22}$ +32.5 (MeOH).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*β*-D-*glucopyranosyl ester, 30-Me ester:* [155556-66-4]
$C_{43}H_{66}O_{17}$ 854.984

3-O-*[α*-L-*Arabinopyranosyl-(1→3)-β*-D-*glucuronopyranoside], 28*-O-*β*-D-*glucopyranosyl ester, 30-Me ester:* [329327-64-2]
$C_{48}H_{74}O_{21}$ 987.1
Constit. of *Chenopodium quinoa* (quinoa). Powder. $[\alpha]_D$ +10.8 (c, 0.003 in MeOH).

3-O-*[β*-D-*Xylopyranosyl-(1→3)-β*-D-*glucuronopyranoside], 30-Me ester:* [288303-26-4]
$C_{42}H_{64}O_{16}$ 824.958
Amorph. powder (as Me ester). $[\alpha]_D^{20}$ -34.2 (c, 3 in MeOH) (Me ester). CAS no. refers to Me ester.

3-O-*[β*-D-*Xylopyranosyl-(1→3)-β*-D-*glucuronopyranoside], 28*-O-*β*-D-*glucopyranosyl ester, 30-Me ester:* [288303-27-5]
$C_{48}H_{74}O_{21}$ 987.1
Amorph. powder (as Me ester). $[\alpha]_D^{20}$ -17.6 (c, 2.8 in MeOH) (Me ester). CAS no. refers to Me ester.

3-O-*[β*-D-*Galactopyranosyl-(1→2)-β*-D-*glucuronopyranoside], 28*-O-*[α*-L-*rhamnopyranosyl-(1→2)-[β*-D-*glucopyranosyl-(1→3)]-[2*R-*methylbutanoyl-(→4)]-β*-D-*fucopyranosyl] ester, 30-Me ester:* [325489-37-0]
$C_{66}H_{104}O_{31}$ 1393.529
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*xylopyranoside], 30-Me ester:* [111199-24-7] ***Phytolaccoside D₂***
$C_{42}H_{66}O_{15}$ 810.974
Constit. of *Phytolacca americana* (pokeberry). Amorph. powder. $[\alpha]_D^{22}$ +46.1 (c, 0.74 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*xylopyranoside], 28*-O-*β*-D-*glucopyranosyl ester, 30-Me ester:* [163658-56-8] ***Esculentoside L₁***
$C_{48}H_{76}O_{20}$ 973.116
Cryst. (isopropanol/Et_2O). Mp 215-220°. $[\alpha]_D^{21}$ +20.8 (c, 0.3 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→4)-β*-D-*xylopyranoside], 30-Me ester:* [65931-92-2] ***Phytolaccoside D***
$C_{42}H_{66}O_{15}$ 810.974
Isol. from *Phytolacca americana* (pokeberry). Mp 220-222°. $[\alpha]_D$ +40 (c, 0.3 in MeOH).

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-β*-D-*glucopyranosyl-(1→2)-β*-D-*xylopyranoside]:* [65608-04-0] ***Phytolaccoside I***
$C_{47}H_{74}O_{19}$ 943.09
Constit. of *Phytolacca americana* (pokeberry). Cryst. (MeOH). Mp 250-253°. $[\alpha]_D^{23}$ +26 (c, 0.25 in Py).

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-β*-D-*glucopyranosyl-(1→2)-β*-D-*xylopyranoside], 30-Me ester:* [65497-08-7] ***Phytolaccoside F***
$C_{48}H_{76}O_{19}$ 957.117
Constit. of *Phytolacca americana* (pokeberry). Amorph. solid.

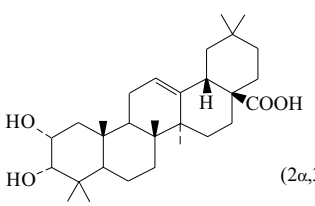
3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-β*-D-*glucopyranosyl-(1→2)-β*-D-*xylopyranoside], 28*-O-*β*-D-*glucopyranosyl ester, 30-Me ester:* [163658-57-9] ***Esculentoside R***
$C_{54}H_{86}O_{24}$ 1119.259
Cryst. (2-propanol/petrol). Mp 212-216°. $[\alpha]_D^{22}$ +4.9 (c, 0.4 in MeOH).

3-O-*[β*-D-*Glucopyranosyl-(1→3)-β*-D-*xylopyranosyl-(1→2)-β*-D-*glucopyranoside], 28*-O-*β*-D-*glucopyranosyl ester, 30-Me ester:* [329327-65-3]
$C_{54}H_{86}O_{25}$ 1135.258
Constit. of *Chenopodium quinoa* (quinoa). Powder. $[\alpha]_D$ +3 (c, 0.004 in MeOH).

23-Ac, 3-O-*[β*-D-*galactopyranosyl-(1→2)-β*-D-*glucuronopyranoside], 28*-O-*[2*S-*methylbutanoyl-(→3)-2*-O-*acetyl-α*-L-*rhamnopyranosyl-(1→2)-[β*-D-*glucopyranosyl-(1→3)]-[2*S-*methylbutanoyl-(→4)]-β*-D-*fucopyranosyl] ester, 30-Me ester:* [325966-86-7] ***Saponin S13***
$C_{75}H_{116}O_{34}$ 1561.721
Constit. of *Quillaja saponaria* (soapbark tree).

Johnson, A. *et al., Tetrahedron*, 1974, **30**, 2033
Woo, W.S. *et al., Phytochemistry*, 1975, **14**, 1885 (*isol, pmr, ms*)
Woo, W.S. *et al., Planta Med.*, 1978, **34**, 87 (*Phytolaccosides*)
Razdan, T.K. *et al., Phytochemistry*, 1983, **22**, 1797 (*Isophytolaccinic acid*)
Harkar, S. *et al., Phytochemistry*, 1984, **23**, 2893 (*isol, cmr*)
Pareda-Miranda, R. *et al., J. Nat. Prod.*, 1986, **46**, 225 (*cmr*)
Kang, S.S. *et al., Planta Med.*, 1987, **53**, 338 (*Phytolaccosides, cmr*)
Bandara, B.M.R. *et al., Planta Med.*, 1990, **56**, 290 (*Phytolaccagenic acid, glucoside*)
Kang, S.S. *et al., Fitoterapia*, 1991, **62**, 532 (*Phytolaccoside I*)
Yi, Y.H. *et al., Yaoxue Xuebao*, 1991, **25**, 745; *CA*, **116**, 158672u (*Esculentoside O*)
Jayasinghe, U.L.B. *et al., Nat. Prod. Lett.*, 1993, **2**, 249 (*Diploclisia glaucescens saponin, glucuronopyranosides*)
Strauss, A. *et al., Phytochemistry*, 1995, **38**, 861 (*Esculentosides*)
Nord, L.I. *et al., Carbohydr. Res.*, 2000, **329**, 817-829 (*Quillaja saponaria saponin*)
Kamel, M.S. *et al., Pharmazie*, 2000, **55**, 460-462 (*Cornulaca monacantha constits*)
Guo, S. *et al., Phytochemistry*, 2000, **55**, 419-428 (*Saponin S13*)
Takahashi, H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 246-248 (*Phytolacca americana constit*)
Dini, I. *et al., J. Agric. Food Chem.*, 2001, **49**, 741-746 (*Chenopodium quinoa constits*)
Soliman, H.S.M. *et al., Magn. Reson. Chem.*, 2001, **39**, 567-576 (*Phytolaccoside F, pmr, cmr*)

2,3-Dihydroxy-12-oleanen-28-oic acid D-574



(2α,3α)-*form*

$C_{30}H_{48}O_4$ 472.707

(2α,3α)-*form* [26563-68-8]
Cryst. Mp 300-302°.

3-Ketone: [73584-62-0] *2-Hydroxy-3-oxo-12-oleanen-28-oic acid*
$C_{30}H_{46}O_4$ 470.691
Constit. of *Salvia officinalis* (sage). Cryst. (MeOH) (as Me ester, Ac). Mp 226-227° (Me ester, Ac). $[\alpha]_D^{20}$ +63 (c, 1.8 in $CHCl_3$) (Me ester, Ac).

(2α,3β)-*form* [4373-41-5]
Crategolic acid. *Maslinic acid*
Cryst. (MeOH aq.). Mp 267-269° (243-245°). $[\alpha]_{Hg}^{20}$ +43 (Py). $[\alpha]_D$ +42.1 (c, 1.02 in Py).

3-O-*β*-D-*Galactopyranoside:* [163634-06-8]

Lucyoside O
$C_{36}H_{58}O_9$ 634.849
Constit. of *Luffa cylindrica* (smooth luffa). Cryst. Mp 181-183°.

3-O-β-D-Glucopyranoside: [157771-37-4]
$C_{36}H_{58}O_9$ 634.849
Constit. of *Luffa cylindrica* (smooth luffa).

3-O-(4-E-Hydroxycinnamoyl): [35482-91-8]
$C_{39}H_{54}O_6$ 618.852
Isol. from *Zizyphus jujuba* (Chinese date). Needles (Me_2CO/C_6H_6). Sol. MeOH, $CHCl_3$; fairly sol. H_2O; poorly sol. hexane. Mp 278-282°. $[\alpha]_D^{20}$ +0.95 (c, 1.05 in Py).

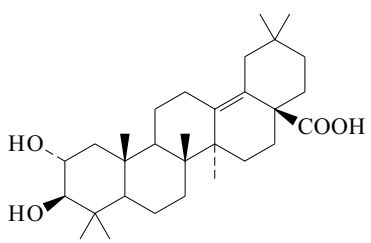
3-O-(4-Z-Hydroxycinnamoyl): [69297-40-1]
$C_{39}H_{54}O_6$ 618.852
Isol. from *Zizyphus jujuba* (Chinese date). Cryst. (Me_2CO/hexane). Mp 190-195°. $[\alpha]_D^{20}$ +9.1 (c, 1.1 in Py).

(2β,3β)-*form* [26707-60-8]
Augustic acid
Cryst. Mp 258-261°.

3-O-[α-L-Rhamnopyranosyl-(1→3)-β-D-glucuronopyranoside], β-D-glucopyranosyl ester: [139742-09-9]
Amaranthussaponin I
$C_{48}H_{76}O_{19}$ 957.117
Constit. of *Amaranthus hypochondriacus* (Prince's feather) and *Amaranthus cruentus* (purple amaranth). Powder. $[\alpha]_D$ +23.3 (c, 0.43 in Py).

Cheung, H.T. *et al., Aust. J. Chem.*, 1972, **25**, 2003-2012 (*isol*)
Yagi, A. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3075-3079 (*Maslinic acid, Zizyphus jujuba constits*)
Brieskorn, C.H. *et al., Planta Med.*, 1980, **38**, 86-90 (*3-ketone*)
Kumar, N.S. *et al., Phytochemistry*, 1985, **24**, 2454-2455 (*isol*)
Kohda, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2609-2612 (*Amaranthussaponin I*)
Pambou Tchivounda, H. *et al., Phytochemistry*, 1991, **30**, 2711-2716 (*Maslinic acid, glycosides*)
Liang, L. *et al., Yaoxue Xuebao*, 1994, **29**, 798; *CA*, **123**, 5581h (*Lucyoside O*)
Junkuszew, M. *et al., Phytochemistry*, 1998, **49**, 195-198 (*Amaranthus cruentus saponin*)

2,3-Dihydroxy-13(18)-oleanen-28-oic acid D-575



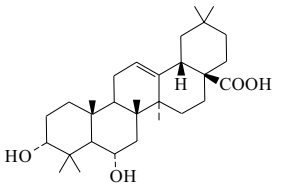
$C_{30}H_{48}O_4$ 472.707

(2α,3β)-*form*
δ-Maslinic acid
Isol. from leaves of *Olea europaea* (olive).

Me ester: [54836-91-8]
Cryst. (hexane). Mp 183-187°. $[\alpha]_D$ -28 (c, 2 in $CHCl_3$).

Caputo, R. *et al., Phytochemistry*, 1974, **13**, 2825 (*isol*)

3,6-Dihydroxy-12-oleanen-28-oic acid D-576



(3α,6α)-*form*

$C_{30}H_{48}O_4$ 472.707

(3α,6α)-*form*
Needles (MeOH). Mp 235-237°. $[\alpha]_D^{20}$ +7 (c, 0.07 in $CHCl_3$).

(3α,6β)-*form*
3-Episumaresinolic acid
Cryst. (as Me ester). Mp 223-224° (Me ester). $[\alpha]_D$ +29.8 (c, 0.7 in $CHCl_3$) (Me ester).

(3β,6α)-*form*
6-Ac: [56119-15-4] ***Karachic acid***
$C_{32}H_{50}O_5$ 514.744
Cryst. (EtOH). Mp 260-261°. $[\alpha]_D$ +79 (Py).

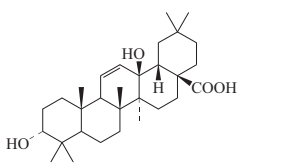
3-Ketone: [32337-18-1] ***6β-Hydroxy-3-oxo-12-oleanen-28-oic acid***
$C_{30}H_{46}O_4$ 470.691
Constit. of *Myroxylon balsamum* (Tolu balsam). Cryst. (hexane/diisopropyl ether) (as Me ester). Mp 190-191° (Me ester). $[\alpha]_D$ +33 (c, 1 in $CHCl_3$) (Me ester).

(3β,6β)-*form* [559-64-8]
Sumaresinolic acid. *Sumaresinol*
Cryst. (EtOH aq.). Mp 298-299°. $[\alpha]_D^{24}$ +102.2 ($CHCl_3$).

3-Ac, Me ester: [32435-06-6]
$C_{33}H_{52}O_5$ 528.771
Needles (EtOH). Mp 220-222°.

Djerassi, C. *et al., Helv. Chim. Acta*, 1955, **38**, 1304 (*Sumaresinolic acid*)
Wahlberg, I. *et al., Acta Chem. Scand.*, 1971, **25**, 70 (*3-ketone, pmr*)
Khan, M.A. *et al., Phytochemistry*, 1975, **14**, 789 (*Karachic acid*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3906 (*isol*)
Chan, W.R. *et al., J. Nat. Prod.*, 1992, **55**, 963 (*3-Episumaresinolic acid*)
Akhtar, N. *et al., Phytochemistry*, 1993, **32**, 1523 (*isol, pmr, cmr*)

3,13-Dihydroxy-11-oleanen-28-oic acid D-577



(3α,13β)-*form*

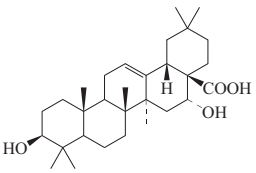
$C_{30}H_{48}O_4$ 472.707

(3β,13β)-*form*

11α,12α-Epoxide, 28→13 lactone, 3-Ac: [35738-25-1]
$C_{32}H_{48}O_5$ 512.728
Constit. of *Rhodomyrtus tomentosa* (hill gooseberry). Cryst. Mp 329-331° (295-296°). $[\alpha]_D$ +45.3 ($CHCl_3$).

Kitagawa, J. *et al., Tetrahedron*, 1972, **28**, 907 (*synth*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3057 (*synth*)
Iwamoto, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1 (*synth*)
Ikuta, A. *et al., Phytochemistry*, 1995, **38**, 1203 (*isol, pmr, cmr*)

3,16-Dihydroxy-12-oleanen-28-oic acid D-578



(3β,16α)-*form*

$C_{30}H_{48}O_4$ 472.707

(3β,16α)-*form* [510-30-5]
Echinocystic acid. *Albizziagenin*
Cryst. (EtOH). Mp 305-312° dec. $[\alpha]_D^{26}$ +27.7 (EtOH). Log P 7.21 (uncertain value) (calc).

28-O-[β-D-Glucopyranosyl-(1→4)-4-hydroxy-E-cinnamoyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-arabinopyranosyl] ester: ***Tragopogonsaponin Q***
$C_{56}H_{82}O_{20}$ 1075.252
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $5H_2O$. $[\alpha]_D^{25}$ +25.4 (c, 0.4 in MeOH). λ_{max} 224 (log ε 3.96); 299 (log ε 4.13); 307 (log ε 4.15) (MeOH).

28-O-[β-D-Glucopyranosyl-(1→3)-[4-hydroxy-E-cinnamoyl-(→2)]-arabinopyranosyl] ester: ***Tragopogonsaponin K***
$C_{50}H_{72}O_{15}$ 913.11
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $3H_2O$. $[\alpha]_D^{25}$ +59.4 (c, 0.9 in MeOH). λ_{max} 213 (log ε 4.09); 229 (log ε 4); 301 (log ε 4.2); 318 (log ε 4.3) (MeOH).

28-O-[β-D-Glucopyranosyl-(1→3)-[3-(4-hydroxyphenyl)propanoyl-(→2)]-arabinopyranosyl] ester: ***Tragopogonsaponin L***
$C_{50}H_{74}O_{15}$ 915.126
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder. Obt. only as a mixt. with Tragopogonsaponin M.

28-O-[β-D-Glucopyranosyl-(1→3)-[3-(4-hydroxy-3-methoxyphenyl)propanoyl-(→2)]-arabinopyranosyl] ester: ***Tragopogonsaponin M***
$C_{51}H_{76}O_{16}$ 945.152
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder.

3-O-β-D-Glucopyranoside, 28-O-[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [168324-02-5]
Asterlingulatoside D
$C_{57}H_{92}O_{25}$ 1177.339

Constit. of *Codonopsis lanceolata* (todok). Amorph. powder. Mp 196-198°. $[\alpha]_D$ -63.2 (c, 1 in Py).

3-O-*β*-D-*Glucopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→3)-[β*-D-*xylopyranosyl-(1→3)-β*-D-*xylopyranosyl-(1→4)-α*-L-*rhamnopyranosyl-(1→2)]-α*-L-*arabinopyranosyl] ester:* [168324-01-4]
$C_{63}H_{102}O_{30}$ 1339.481
Constit. of *Codonopsis lanceolata* (todok).

3-O-*β*-D-*Glucuronopyranoside:* [134361-64-1] ***Tragopogonsaponin A***
$C_{36}H_{56}O_{10}$ 648.832
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $2^1/_4H_2O$ (as Me ester). $[\alpha]_D^{25}$ -8.2 (c, 0.90 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→4)-4-hydroxy-3-methoxy*-E-*cinnamoyl-(→2)-β*-D-*xylopyranosyl] ester:* [134361-67-4] ***Tragopogonsaponin D***
$C_{57}H_{82}O_{22}$ 1119.262
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $3H_2O$ (as Me ester). $[\alpha]_D^{25}$ -4.4 (c, 0.6 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→3)-[3-(4-hydroxyphenyl)propanoyl-(→2)]-arabinopyranosyl] ester:* [134522-28-4] ***Tragopogonsaponin I***
$C_{56}H_{82}O_{21}$ 1091.251
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder (as Me ester). Obt. only as a mixt. with Tragopogonsaponin J Me ester.

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→4)-4-hydroxy-3-methoxy*-E-*cinnamoyl-(→2)-β*-D-*arabinopyranosyl] ester:* [134453-40-0] ***Tragopogonsaponin E***
$C_{57}H_{82}O_{22}$ 1119.262
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $3^1/_2H_2O$ (as Me ester). $[\alpha]_D^{25}$ +7.3 (c, 1.1 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→3)-[3-(4-hydroxyphenyl)propanoyl-(→2)]-β*-D-*xylopyranosyl] ester:* [134361-69-6] ***Tragopogonsaponin G***
$C_{56}H_{82}O_{21}$ 1091.251
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $3H_2O$ (as Me ester). $[\alpha]_D^{25}$ -11.7 (c, 0.95 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→3)-[4-hydroxycinnamoyl-(1→2)]-β*-D-*xylopyranosyl] ester:* [134361-68-5] ***Tragopogonsaponin F***
$C_{56}H_{80}O_{21}$ 1089.235
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $4H_2O$ (as Me ester). $[\alpha]_D^{25}$ +20.9 (c, 1.29 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→3)-[3-(4-hydroxy-3-methoxyphenyl)propanoyl-(→2)]-arabinopyranosyl] ester:* [134361-70-9] ***Tragopogonsaponin J***
$C_{57}H_{84}O_{22}$ 1121.277
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder (as Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→3)-[4-hydroxycinnamoyl-(→2)]-α*-L-*arabinopyranosyl] ester:* [134522-27-3] ***Tragopogonsaponin H***
$C_{56}H_{80}O_{21}$ 1089.235
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $2^1/_2H_2O$ (as Me ester). $[\alpha]_D^{25}$ +7.2 (c, 0.65 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→4)-3-(4-hydroxyphenyl)propanoyl-(→2)-[β*-D-*glucopyranosyl-(1→3)]-β*-D-*xylopyranosyl] ester:* [134361-75-4] ***Tragopogonsaponin O***
$C_{62}H_{92}O_{26}$ 1253.393
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $1^1/_2H_2O$ (as Me ester). $[\alpha]_D^{25}$ 0 (c, 0.40 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→4)-3-(4-hydroxy-3-methoxyphenyl)propanoyl-(→2)-[β*-D-*glucopyranosyl-(1→3)]-arabinopyranosyl] ester:* [134361-77-6] ***Tragopogonsaponin R***
$C_{63}H_{94}O_{27}$ 1283.419
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $4^1/_2H_2O$ (as Me ester). $[\alpha]_D^{25}$ -12.3 (c, 0.5 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→3)-β*-D-*xylopyranosyl-(1→3)-[β*-D-*xylopyranosyl-(1→4)]-α*-L-*rhamnopyranosyl-(1→2)-α*-L-*arabinopyranosyl] ester:* [252979-60-5] ***Foetidissimoside B***
$C_{63}H_{100}O_{31}$ 1353.464
Constit. of *Cucurbita foetidissima* (buffalo gourd). Amorph. powder. $[\alpha]_D^{25}$ -31.8 (c, 0.11 in MeOH). λ_{max} 210 (MeOH).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[4-hydroxy*-E-*cinnamoyl-(→2)-β*-D-*xylopyranosyl] ester:* [134361-65-2] ***Tragopogonsaponin B***
$C_{50}H_{70}O_{16}$ 927.093
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $3H_2O$ (as Me ester). $[\alpha]_D^{25}$ +24.9 (c, 1.27 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→4)-3-(4-hydroxyphenyl)propanoyl-(→2)-[β*-D-*glucopyranosyl-(1→3)]-arabinopyranosyl] ester:* [134453-41-1] ***Tragopogonsaponin P***
$C_{62}H_{92}O_{26}$ 1253.393
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $1^1/_2H_2O$ (as Me ester). $[\alpha]_D^{25}$ -7.2 (c, 0.90 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[4-hydroxy-3-methoxy*-E-*cinnamoyl-(→2)-β*-D-*xylopyranosyl] ester:* [13436-66-3] ***Tragopogonsaponin C***
$C_{51}H_{72}O_{17}$ 957.12
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $2H_2O$ (as Me ester). $[\alpha]_D^{25}$ +24.3 (c, 0.9 in MeOH) (Me ester).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[β*-D-*glucopyranosyl-(1→4)-4-hydroxy*-E-*cinnamoyl-(→2)-[glucopyranosyl-(1→3)]-β*-D-*xylopyranosyl] ester:* [134361-74-3] ***Tragopogonsaponin N***
$C_{62}H_{90}O_{26}$ 1251.377
Isol. from *Tragopogon porrifolius* (salsify). Amorph. powder + $6H_2O$ (as Me ester). $[\alpha]_D^{25}$ -6.7 (c, 0.50 in MeOH) (Me ester).

3-O-*[α*-L-*Arabinopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [78285-89-9] ***Pithecelloside A***
$C_{41}H_{66}O_{13}$ 766.965
Constit. of *Pithecellobium dulce* (manila tamarind). Needles. Mp 216-218°. $[\alpha]_D$ -8.2 (c, 4.6 in MeOH).

3-O-*[*D-*Xylopyranosyl-(1→4)-*L-*rhamnopyranoside], 28*-O-*[*D-*glucopyranosyl-(1→4)-*L-*rhamnopyranosyl-(1→2)-*L-*arabinopyranosyl] ester:* [29108-67-6] ***Helianthoside B***
$C_{58}H_{94}O_{25}$ 1191.366
Isol. from *Helianthus annuus* (sunflower).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-α*-L-*arabinopyranoside], 28*-O-*[β*-D-*xylopyranosyl-(1→6)-β*-D-*glucopyranosyl] ester:* [160955-43-1] ***Dulcin***
$C_{52}H_{84}O_{22}$ 1061.222
Constit. of *Pithecellobium dulce* (manila tamarind). Powder. Mp 260° dec. $[\alpha]_D$ +41.9 (c, 0.3 in Py).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-α*-L-*arabinopyranoside], 28*-O-*[α*-L-*rhamnopyranosyl-(1→4)-β*-D-*glucopyranosyl-(1→4)-β*-D-*glucopyranosyl] ester:* [214219-70-2]
$C_{56}H_{96}O_{27}$ 1201.358
Constit. of *Pithecellobium dulce* (manila tamarind).

3-O-*[β*-D-*Glucopyranosyl-(1→3)-α*-L-*arabinopyranoside], 28*-O-*β*-D-*glucopyranosyl ester:* [289649-54-3] ***Araliasaponin I***
$C_{47}H_{76}O_{18}$ 929.107
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder. $[\alpha]_D$ -28.9 (c, 0.15 in Py).

3-O-*[β*-D-*Glucopyranosyl-(1→3)-β*-D-*glucuronopyranoside]:* [171828-78-7] ***Elatoside H***
$C_{42}H_{66}O_{15}$ 810.974
Constit. of *Aralia elata* (Japanese angelica tree). Needles (MeOH aq.). Mp 214-217.3°. $[\alpha]_D^{29}$ -2.4 (c, 0.1 in MeOH).

3-O-*[α*-L-*Arabinopyranosyl-(1→2)-α*-L-*arabinopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [189161-64-6] ***Pithecelloside D***
$C_{46}H_{74}O_{17}$ 899.08
Constit. of *Pithecellobium dulce* (manila tamarind). Needles. Mp 186-188°. $[\alpha]_D$ -9.8 (c, 6.3 in Py).

3-O-*[β-D-Xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [78285-88-8] ***Prosapogenin***†. *Pitheduloside E*
$C_{46}H_{74}O_{17}$ 899.08
Isol. from *Pithecellobium dulce* (manila tamarind). Needles. Mp 227-229° (219-222°). $[\alpha]_D^{16}$ -11.7 (c, 1.01 in MeOH). $[\alpha]_D$ -8.6 (c, 4.5 in MeOH).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [325489-44-9]
$C_{78}H_{124}O_{42}$ 1733.812
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [289649-66-7] ***Araliasaponin III***
$C_{53}H_{86}O_{23}$ 1091.249
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder. $[\alpha]_D$ -13.3 (c, 0.2 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [340982-21-0] ***Araliasaponin VI***
$C_{54}H_{88}O_{24}$ 1121.275
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder. $[\alpha]_D$ -18.8 (c, 0.2 in Py).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [289649-67-8] ***Araliasaponin IV***
$C_{54}H_{88}O_{24}$ 1121.275
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder. $[\alpha]_D$ -18.8 (c, 0.2 in Py).

3-O-*[α-L-Arabinopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]:* [200127-83-9] ***Pitheduloside K***
$C_{52}H_{84}O_{22}$ 1061.222
Constit. of *Pithecellobium dulce* (manila tamarind). Needles. Mp 200-202°. $[\alpha]_D^{25}$ -4.1 (c, 3.5 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→6)]-β-D-glucopyranoside]:* [139164-70-8]

[24404-55-5] ***Helianthoside A***
$C_{53}H_{86}O_{21}$ 1059.25
Constit. of *Helianthus annuum* (sunflower). No phys. props. reported.

3-O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→3)-[D-xylopyranosyl-(1→6)]-D-glucopyranoside], 28*-O-*[D-glucopyranosyl-(1→4)-L-rhamnopyranosyl-(1→2)-L-arabinopyranosyl] ester:* [25503-42-8] ***Helianthoside C***
$C_{70}H_{114}O_{34}$ 1499.65
Saponin from *Helianthus annuus* (sunflower). Mp 215-217°.

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]:* [374807-02-0] ***Congmunoside XV***
$C_{54}H_{88}O_{24}$ 1121.275
Constit. of *Aralia elata* (Japanese angelica tree).

(3β,16β)-*form* [545-88-0]
Cochalic acid
Plates (MeOH). Mp 303-306°. $[\alpha]_D$ +58 (dioxan). λ_{max} 218 (no solvent reported).

3-O-*[β-D-Galactopyranosyl-(1→3)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [358732-32-8] ***Calendasaponin B***
$C_{48}H_{76}O_{20}$ 973.116
Constit. of flowers of *Calendula officinalis* (pot marigold). Cryst. (MeOH aq.). Mp 245.6-247°. $[\alpha]_D^{27}$ +6.4 (c, 0.1 in MeOH).

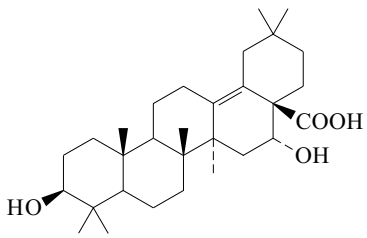
3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [358732-33-9] ***Calendasaponin C***
$C_{54}H_{86}O_{25}$ 1135.258
Constit. of flowers of *Calendula officinalis* (pot marigold).

3-Ketone: [77625-71-9] ***16-Hydroxy-3-oxo-12-oleanen-28-oic acid***
$C_{30}H_{46}O_4$ 470.691
Isol. from *Vitis vinifera* (wine grape). Cryst. Mp 212-214°.

[69280-20-2]

Djerassi, C. *et al., J.A.C.S.*, 1955, **77**, 3579-3582; 1957, **79**, 3525-3528 (*isol, struct*)
Cheban, P.L. *et al., Khim. Prir. Soedin.*, 1968, **4**, 140; 1969, **5**, 59; 129-130; 327; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 121; 1969, **5**, 51-52; 112-113; 277-278 (*Helianthosides*)
Allen, J. *et al., J.C.S. Perkin 1*, 1972, 2994-3001 (*synth*)
Brieskorn, C.H. *et al., CA*, 1981, **94**, 188662k (*3-ketone*)
Warashina, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 388-396 (*Tragopogonsaponins A-R*)
Miyase, T. *et al., Phytochemistry*, 1992, **31**, 2087-2091 (*Tragopogonsides A-I*)
Sahu, N.P. *et al., Phytochemistry*, 1994, **37**, 1425-1427 (*Dulcin*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1878-1882 (*Elatoside H, isol, pmr, cmr*)
Hu, B. *et al., Chin. Chem. Lett.*, 1996, **7**, 1005-1008 (*Asterlingulatosides*)
Shao, Y. *et al., J. Nat. Prod.*, 1997, **60**, 743-746 (*Asterlingulatosides*)
Yoshikawa, K. *et al., J. Nat. Prod.*, 1997, **60**, 1269-1274 (*Pitheduloside K*)
Shao, Y. *et al., Phytochemistry*, 1997, **44**, 337-340 (*Asterlingulatosides*)
Nigam, S.K. *et al., Phytochemistry*, 1997, **44**, 1329-1334 (*Pithedulosides*)
Saxena, V.K. *et al., Proc. Indian Acad. Sci., Chem. Sci.*, 1998, **110**, 409-414 (*Pithecellobium dulce saponin*)
Song, S.-J. *et al., Chem. Pharm. Bull.*, 2000, **48**, 838-842 (*Araliasaponins*)
Gaidi, G. *et al., J. Nat. Prod.*, 2000, **63**, 122-124 (*Foetidissimoside B*)
Guo, S. *et al., Phytochemistry*, 2000, **55**, 419-428 (*Quillaja saponaria saponin*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 863-870 (*Calendasaponins B,C*)
Song, S.J. *et al., Phytochemistry*, 2001, **56**, 491-497 (*Araliasaponin VI*)
Song, S. *et al., Zhongguo Yaowu Huaxue Zazhi*, 2001, **11**, 174-176; *CA*, **136**, 2906a (*Congmunoside XV*)

3,16-Dihydroxy-13(18)-oleanen-28-oic acid D-579



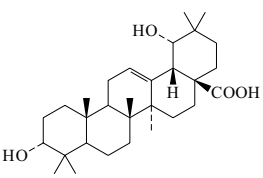
$C_{30}H_{48}O_4$ 472.707

(3β,16α)-*form* [664-40-4]
Albigenic acid
Constit. of *Codonopsis lanceolata* (todok) and from *Helianthus annuus* (sunflower). Cryst. (MeOH). Mp 246-248° dec. $[\alpha]_D^{31}$ -13 (EtOH).

Me ester: [22611-52-5]
Mp 225-230°. $[\alpha]_D$ -12 (EtOH).

Barua, A.K. *et al., Tetrahedron*, 1959, **7**, 19 (*isol*)
Kasprzyk, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1968, **42**, 1463 (*synth*)
Kubota, T. *et al., Tet. Lett.*, 1969, 771 (*synth*)
Han, B.H. *et al., CA*, 1978, **88**, 71431 (*isol*)

3,19-Dihydroxy-12-oleanen-28-oic acid D-580



(3α,19α)-*form*

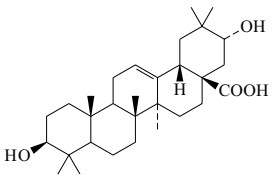
$C_{30}H_{48}O_4$ 472.707

(3β,19α)-*form* [511-77-3]
Siaresinolic acid. *Siaresinol*
Cryst. (MeOH/Et_2O). Mp 274-275°. $[\alpha]_D^{24}$ +98.5 (EtOH).

3-O-*α-L-Arabinopyranoside, 28*-O-*β-D-glucopyranosyl ester:* [356785-71-2]
$C_{41}H_{66}O_{13}$ 766.965
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Amorph. solid. $[\alpha]_D^{25}$ +14 (c, 0.1 in MeOH).

Mimaki, Y. *et al., Phytochemistry*, 2001, **57**, 773-779 (*Sanguisorba officinalis saponin*)

3,21-Dihydroxy-12-oleanen-28-oic acid D-581



(3β,21α)-*form*

$C_{30}H_{48}O_4$ 472.707

(3β,21β)-*form* [25763-71-7]
Machaerinic acid. *Proceric acid*

28-O-β-D-Glucopyranosyl ester: [183294-29-3] ***Lucyoside Q***
$C_{36}H_{58}O_9$ 634.849
Constit. of *Luffa cylindrica* (smooth luffa). Cryst. Mp 238-240°. $[\alpha]_D^{15}$ +23.5 (c, 0.4 in MeOH).

3-O-[α-L-Arabinopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [117804-15-6] ***Cynarasaponin J***
$C_{47}H_{74}O_{19}$ 943.09
Constit. of *Cynara cardunculus* (cardoon). Powder + $2H_2O$ (as Me ester). $[\alpha]_D^{25}$ +15.6 (c, 0.95 in MeOH) (Me ester).

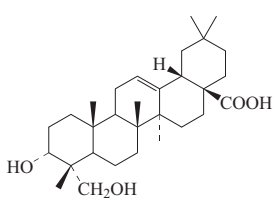
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [135575-15-4] ***Acutoside C***
$C_{58}H_{94}O_{26}$ 1207.365
Constit. of *Luffa acutangula* (Chinese okra). Amorph. powder. Mp 220-225° dec. $[\alpha]_D^{24}$ -15.5 (c, 0.5 in MeOH aq.).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [358732-35-1] ***Calendasaponin D***
$C_{54}H_{86}O_{25}$ 1135.258
Constit. of flowers of *Calendula officinalis* (pot marigold). Cryst. (MeOH aq.). Mp 227-229°. $[\alpha]_D^{24}$ +33 (c, 1.1 in MeOH).

[117804-24-7]

Shimizu, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2466 (*Cynarasaponin J*)
Liang, L. *et al., Yaoxue Xuebao*, 1996, **31**, 122 (*Lucyoside Q*)

3,23-Dihydroxy-12-oleanen-28-oic acid D-582



(3α)-*form*

$C_{30}H_{48}O_4$ 472.707

Many glycosides of Hederagenin are known. See also Hederagenin 3-glycosides, H-12, Hederagenin 28-glycosyl esters and Hederagenin bisdesmosides, H-11.

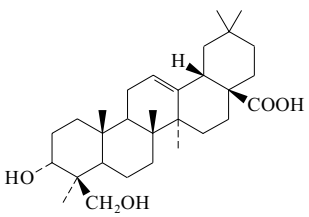
3β-*form* [465-99-6]
Hederagenin. *Caulosapogenin. Hederidin. Kalosapogenin. Melanthigenin. Astrantiagenin E*
Cryst. (EtOH). Mp 334° dec. $[\alpha]_D$ +82 (Py).

3,23-Di-O-β-D-glucopyranoside, 28-O-[β-D-glucopyranosyl-(1→3)-α-L-arabinopyranosyl] ester: [123597-11-5] ***Quinoside A***
$C_{53}H_{86}O_{23}$ 1091.249
Constit. of *Chenopodium quinoa* (quinoa). No phys. props. reported.

[30883-34-2]

Meyer, B.N. *et al., J. Agric. Food Chem.*, 1990, **38**, 205-208 (*Quinoside A*)

3,24-Dihydroxy-12-oleanen-28-oic acid D-583



3α-*form*

$C_{30}H_{48}O_4$ 472.707

3β-*form* [83944-28-9]
Bredemolic acid. *4-Epihederagenin*
Cryst. (Et_2O/petrol). Mp 288-292° Mp 305-307°. $[\alpha]_D^{20}$ +100.5 (Py). $[\alpha]_D$ +74.1 (c, 0.27 in MeOH).

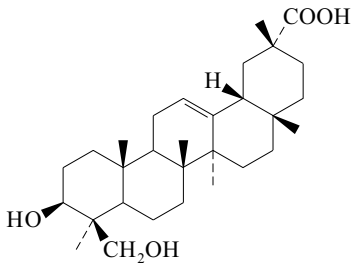
3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[3-hydroxy-3-methylglutaroyl-(→6)-β-D-glucopyranosyl] ester: ***Lablaboside D***
$C_{60}H_{94}O_{28}$ 1263.386
Glycoside from *Dolichos lablab* (hyacinth bean). Cryst. (MeOH aq.). Mp 193.4-195°. $[\alpha]_D^{26}$ -15.1 (c, 2.5 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranosyl] ester: [209802-42-6] ***Lablaboside C***
$C_{60}H_{96}O_{28}$ 1265.402
Constit. of *Dolichos lablab* (hyacinth bean). Cryst. (MeOH aq.). Mp 222-223.5°. $[\alpha]_D^{24}$ -22.9 (c, 0.97 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranosyl] ester: ***Lablaboside E***
$C_{66}H_{106}O_{32}$ 1411.544
Constit. of *Dolichos lablab* (hyacinth bean). Cryst. (MeOH). Mp 202.8-204.5°. $[\alpha]_D^{25}$ -20.3 (c, 2.8 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1960, **93**, 1903
Pereda-Miranda, R. *et al., J. Nat. Prod.*, 1986, **49**, 225
Singh, S.K. *et al., Phytochemistry*, 1990, **29**, 3360 (*isol, pmr, cmr*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 812-816 (*Lablabosides*)
Komatsu, H. *et al., Heterocycles*, 1998, **48**, 703-710 (*Lablabosides*)

3,24-Dihydroxy-12-oleanen-29-oic acid D-584



$C_{30}H_{48}O_4$ 472.707

3β-*form* [86425-21-0]
Azukisapogenol
Isol. from *Vigna angularis* (azuki bean). Needles ($CHCl_3$/MeOH). Mp 286-287°. $[\alpha]_D^{13}$ +38.5 (c, 1.2 in Py).

Me ester: [20476-10-2]
Needles ($CHCl_3$/petrol). Mp 262-263°. $[\alpha]_D^{13}$ +56.4 (c, 1 in $CHCl_3$).

Di-Ac: [5672-32-2]
Fine cryst. (MeOH). Mp 246-247°. $[\alpha]_D^{13}$ +53.5 (c, 1.4 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl(1→2)-β-D-glucuronopyranoside]: [82801-38-5] ***Azukisaponin III***
$C_{42}H_{66}O_{15}$ 810.974
Isol. from seeds of *Vigna angularis* (azuki bean). Cryst. + H_2O (MeOH aq.). Mp 218-221°. $[\alpha]_D^{28}$ +2.5 (c, 1.1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucuronopyranoside], Me ester: [128357-84-6]
$C_{43}H_{68}O_{15}$ 825.001

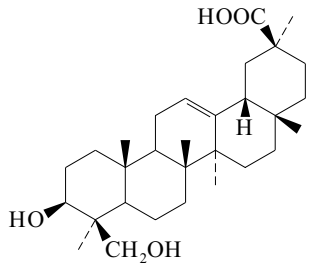
3-O-[β-D-Glucopyranosyl(1→2)-β-D-glucuronopyranoside], [β-D-glucopyranosyl(1→6)-β-D-glucopyranosyl] ester: [82801-39-6] ***Azukisaponin VI***
$C_{54}H_{86}O_{25}$ 1135.258
Isol. from seeds of *Vigna angularis* (azuki bean). Cryst. (MeOH). Mp 223-225°. $[\alpha]_D^{20}$ -5.9 (c, 1.1 in MeOH).

Amide, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucuronopyranoside]: [128309-09-1]
$C_{42}H_{67}NO_{14}$ 809.99

[86500-82-5, 86764-25-2]

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 664; 674; 683 (*isol, struct*)

3,24-Dihydroxy-12-oleanen-30-oic acid D-585

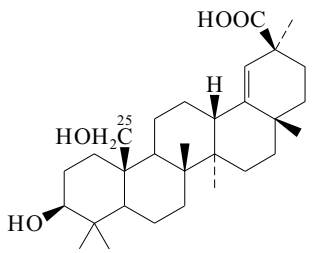


$C_{30}H_{48}O_4$ 472.707

3β-*form*

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: [134250-13-8]
Licoricesaponin J2
$C_{42}H_{64}O_{16}$ 824.958
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Mp 263-265°. $[\alpha]_D^{25}$ +21 (MeOH).
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1991, **39**, 244

3,25-Dihydroxy-18-oleanen-30-oic acid D-586



$C_{30}H_{48}O_4$ 472.707

3β-*form* [85282-03-7]
Periandric acid III
Needles (Me_2CO aq). Mp 265-267°.

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: [74256-70-5]
Periandrin III
$C_{42}H_{64}O_{16}$ 824.958
Constit. of *Periandra dulcis* roots. Natural sweetener. Cryst. with sweet taste. Mp 300°. $[\alpha]_D^{18}$ -24.5 (c, 1.1 in H_2O).

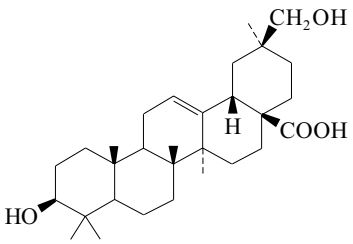
3-Ketone, 25-aldehyde: [84260-73-1] *3,25-Dioxo-18-oleanen-30-oic acid.* ***3-Dehydroperiandric acid I***
$C_{30}H_{44}O_4$ 468.675
Cryst. (Me_2CO aq.). Mp 283-292°. $[\alpha]_D^{23}$ +1.52 (c, 1.275 in $CHCl_3$).

25-Aldehyde: [85317-31-3] *3β-Hydroxy-25-oxo-18-oleanen-30-oic acid.* ***Periandric acid I***
$C_{30}H_{46}O_4$ 470.691
Needles (EtOH aq.). Mp 267-268°.

25-Aldehyde, 3-[O-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: [73565-59-0]
Periandrin I
$C_{42}H_{62}O_{16}$ 822.942
Isol. from *Periandra dulcis* roots. Natural sweetener. Plates + $4H_2O$ (MeOH aq.) with sweet taste. Mp 300°. $[\alpha]_D^{20}$ -23 (c, 1 in H_2O).

25-Aldehyde, 3-O-[β-D-xylopyranosyl-(1→2)-β-D-glucopyranoside]: ***Periandrin V***
$C_{41}H_{64}O_{13}$ 764.949
Constit. of *Periandra dulcis* roots. Natural sweetener. Amorph. powder (MeOH aq.). Mp 300°. $[\alpha]_D^{25}$ -18.5 (c, 0.09 in H_2O).
Hashimoto, Y. *et al., Phytochemistry*, 1982, **21**, 2335; 1984, **23**, 693
Suttiari, R. *et al., Phytochemistry*, 1993, **34**, 405 (*Periandrin V*)

3,30-Dihydroxy-12-oleanen-28-oic acid D-587



$C_{30}H_{48}O_4$ 472.707

3β-*form* [511-82-0]
Queretaroic acid
Constit. of *Chenopodium quinoa* (quinoa), *Stenocereus thurberi* (organ pipe cactus). Cryst. (MeOH). Mp 345-348° (318-323°). $[\alpha]_D$ +81.1 (c, 3 in Py).

Me ester:
Cryst. (C_6H_6/MeOH). Mp 228-228.5°. $[\alpha]_D$ +77.8 ($CHCl_3$).

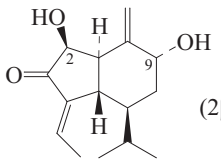
30-O-(3,4-Dihydroxycinnamoyl): [59441-01-9]
$C_{39}H_{54}O_7$ 634.851
Cryst. (EtOH/$CHCl_3$). Mp 230-232°. $[\alpha]_D$ +152.

30-Aldehyde:3-Hydroxy-30-oxo-12-oleanen-28-oic acid. ***Dodecandral***
$C_{30}H_{46}O_4$ 470.691

30-Carboxylic acid: 3-Hydroxy-12-oleanene-28,30-dioic acid, H-662

Djerassi, C. *et al., J.A.C.S.*, 1956, **78**, 3785 (*isol, struct*)
Rangaswami, S. *et al., Tetrahedron*, 1969, **25**, 3701 (*isol*)
Tori, K. *et al., Tet. Lett.*, 1974, 4227 (*cmr*)
Agarwal, J.S. *et al., Phytochemistry*, 1976, **15**, 430 (*deriv, pmr*)
Kircher, H.W. *et al., Phytochemistry*, 1977, **16**, 1078; 1980, **19**, 2707 (*isol*)
Oshima, Y. *et al., Planta Med.*, 1984, **50**, 43 (*deriv, cmr*)
Ikuta, A. *et al., Phytochemistry*, 1986, **25**, 1625 (*cmr*)
Spengel, S.M. *et al., Phytochemistry*, 1996, **43**, 179 (*Dodecandral*)
Ye, Y. *et al., J. Nat. Prod.*, 1998, **61**, 456-460 (*cmr*)

2,9-Dihydroxy-4,10(14)-oplopadien-3-one D-588



(2β,4*E*,9α)-*form*

$C_{15}H_{22}O_3$ 250.337

(2β,4*E*,9α)-*form*

*9-(3-Methyl-2*E*-pentenoyl), 2-(2-methylbutanoyl):* [80489-88-9]
$C_{26}H_{38}O_5$ 430.583
Gum. $[\alpha]_D^{24}$ -95 (c, 0.2 in $CHCl_3$).

(2β,4*Z*,9α)-*form*

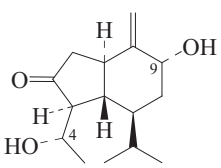
*9-(3-Methyl-2*E*-pentenoyl), 2-(2-methylbutanoyl):* [80514-14-3]
$C_{26}H_{38}O_5$ 430.583
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{24}$ -125 (c, 1 in $CHCl_3$).

*9-(3-Methyl-2*E*-pentenoyl), 2-angeloyl:* [237407-02-2]
$C_{26}H_{36}O_5$ 428.567
Constit. of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D^{28}$ -166.7 (c, 0.04 in $CHCl_3$). λ_{max} 224 (log ϵ 4.5) (MeOH).

*2,9-Bis(3-methyl-2*E*-pentenoyl):* [237407-03-3]
$C_{27}H_{38}O_5$ 442.594
Constit. of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D^{29}$ -173.9 (c, 0.02 in $CHCl_3$). λ_{max} 222 (log ϵ 4.6) (MeOH).

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 2024 (*isol, pmr*)
Kikuchi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2753 (*isol, pmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 705-707 (*isol, pmr, cmr*)

4,9-Dihydroxy-10(14)-oplopen-3-one D-589



$C_{15}H_{24}O_3$ 252.353

(4*S*,9α)-*form*

9-(3-Methylbutanoyl): [348113-04-2]
$C_{20}H_{32}O_4$ 336.47
Constit. of flower buds of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D^{22}$ -39.8 (c, 0.2 in $CHCl_3$).

9-(3-Methylbutanoyl), 4-Ac: [72247-71-3]
Notonipetrone
$C_{22}H_{34}O_5$ 378.508
Oil. $[\alpha]_D^{24}$ -14.3 (c, 2 in $CHCl_3$).

*9-(3-Methyl-2*E*-pentenoyl), 4-Ac:* [104012-37-5]

[126453-63-2] ***Tussilagone***. *Farfaratin*
$C_{23}H_{34}O_5$ 390.519
Constit. of *Tussilago farfara* (coltsfoot). Cryst. Mp 100-101°. $[\alpha]_D^{24}$ -40 (c, 1 in $CHCl_3$).

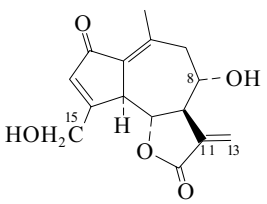
*9-(3-Methyl-2*E*-pentenoyl):* [147742-07-2]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{22}$ -102.4 (c, 0.3 in $CHCl_3$).

9-Angeloyl, 4-Ac: [147742-08-3]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{22}$ -48.8 (c, 0.5 in $CHCl_3$).

*9-(3-Methyl-2*E*-butenoyl), 4-Ac:* [147742-09-4]
$C_{22}H_{32}O_5$ 376.492
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{22}$ -45.8 (c, 0.4 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1063; 1981, **20**, 2024 (*isol, struct, deriv, pmr*)
Bai-Ping, Y. *et al., Huaxue Xuebao*, 1987, **45**, 450 (*cryst struct*)
Wang, C. *et al., Yaoxue Xuebao*, 1989, **24**, 913-915 (*Farfaratin*)
Kikuchi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2753 (*deriv, pmr, cmr*)
Shi, W. *et al., J. Chin. Pharm. Sci.*, 1996, **5**, 63-67; *CA*, **126**, 314812d (*pmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2001, **49**, 645-648 (*9-methylbutanoyl, abs config*)

8,15-Dihydroxy-2-oxo-1(10),3,11(13)-guaiatrien-12,6-olide D-590



$C_{15}H_{16}O_5$ 276.288

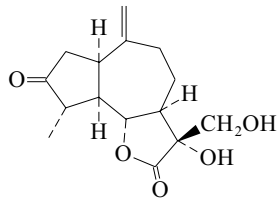
(5α,6α,8α)-*form* [1891-29-8]
Lactucin
Constit. of *Cichorium intybus* (chicory). Cryst. (Me_2CO). Mp 224-228°. $[\alpha]_D$ +49 (c, 0.9 in MeOH). λ_{max} 257 (ε 14000) (EtOH) (Berdy).

8-(4-Hydroxyphenylacetyl): [65725-11-3]
Lactupicrin. *Lactucopicrin. Intybin*
$C_{23}H_{22}O_7$ 410.423
Constit. of *Lactuca sativa* (lettuce), *Cichorium intybus* (chicory) and *Cichorium endivia* (endive). Mp 132-178° dec. $[\alpha]_D$ +73 (Py).

11α,13-Dihydro, 15-aldehyde, 8-(4-hydroxyphenylacetyl): [374536-44-4]
$C_{23}H_{22}O_7$ 410.423
Constit. of *Cichorium intybus* (chicory).

Bachelor, F.W. *et al., Can. J. Chem.*, 1973, **51**, 3626 (*struct*)
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1977, **51**, 2165 (*isol, derivs*)
Ruban, G. *et al., Acta Cryst. B*, 1978, **34**, 1163 (*cryst struct*)
Khalil, A.T. *et al., Planta Med.*, 1991, **57**, 190-191 (*Lactucin, Lactucopicrin, 11,13-Dihydrolactucopicrin*)
Song, Q. *et al., Phytochemistry*, 1995, **40**, 1659-1665 (*biosynth*)
Deng, Y. *et al., Z. Naturforsch., C*, 2001, **56**, 787-796 (*Cichorium intybus constits*)

11,13-Dihydroxy-3-oxo-10(14)-guaien-12,6-olide D-591



$C_{15}H_{20}O_5$ 280.32

(1α,4α,5α,6α,11α)-*form* [255722-99-7]
Cryst. Mp 154-155°.

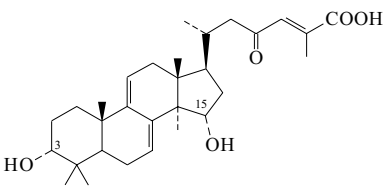
13-Ac: [142449-61-4]
$C_{17}H_{22}O_6$ 322.357
Cryst. (MeOH). Mp 141-143°. Struct. corrected from 11-Ac in 1993.

11,13-Di-Ac:
$C_{19}H_{24}O_7$ 364.394
Gum. $[\alpha]_D^{24}$ +87 (c, 0.1 in $CHCl_3$).

(1α,4α,5α,6α,11ξ)-*form* [83551-03-5] ***8-Deoxy-11,13-dihydroxygrosheimin***
Constit. of *Cynara scolymus* (globe artichoke). Needles (MeOH). Mp 215-218°.

Rustaiyan, A. *et al., Phytochemistry*, 1981, **20**, 2427-2429 (*isol, ir, pmr, ms*)
Oksuz, S. *et al., Phytochemistry*, 1982, **21**, 2747-2749 (*13-Ac*)
Bruno, M. *et al., Phytochemistry*, 1991, **30**, 4165 (*11-Ac, isol, pmr, cmr*)
Barbetti, P. *et al., Nat. Prod. Lett.*, 1993, **3**, 21-30 (*Cynara scolymus constit*)
Öksüz, S. *et al., Phytochemistry*, 1993, **33**, 1267-1268 (*13-Ac, cryst struct*)
González-Platas, J. *et al., Acta Cryst. C*, 1999, **55**, 1837-1839 (*isol, cryst struct*)

3,15-Dihydroxy-23-oxo-7,9(11),24-lanostatrien-26-oic acid D-592



$C_{30}H_{44}O_5$ 484.675

(3α,15α,24*E*)-*form*
3-Ac: [117383-37-6] *3α-Acetoxy-15α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid*
$C_{32}H_{46}O_6$ 526.712
Constit. of *Ganoderma lucidum* (reishi).

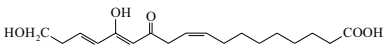
15-Ac: [117383-35-4] *15α-Acetoxy-3α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid*
$C_{32}H_{46}O_6$ 526.712
Constit. of *Ganoderma lucidum* (reishi).

Di-Ac: [117383-36-5] *3α,15α-Diacetoxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid*
$C_{34}H_{48}O_7$ 568.749
Constit. of *Ganoderma lucidum* (reishi).

Shiao, M.-S. *et al., Phytochemistry*, 1988, **27**, 2911

14,18-Dihydroxy-12-oxo-9,13,15-octadecatrienoic acid D-593

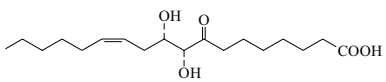
18-Hydroxy-12,14-dioxo-9,15-octadecadienoic acid



$C_{18}H_{28}O_5$ 324.416
Enolised β-diketone. Exists in the enol. form illus..

(9*Z*,13*Z*,15*E*)-*form* [130523-93-2]
Cibaric acid
Isol. from damaged fruit bodies of the edible chanterelle mushroom (*Cantharellus cibarius*). Cryst. (EtOAc). Mp 69.5-70.5°. λ_{max} 237 (ε 6456); 308 (ε 19054) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 100 mg/kg.
Pang, Z. *et al., J.O.C.*, 1991, **56**, 1233 (*struct, ir, uv, ms, pmr, cmr*)

9,10-Dihydroxy-8-oxo-12-octadecenoic acid D-594



$C_{18}H_{32}O_5$ 328.448

(9*R*,10*S*,12*Z*)-*form* [142036-13-3]
Constit. of the edible lions mane mushroom (*Hericium erinaceum*). Fine needles (EtOAc/hexane). Sol. EtOAc, $CHCl_3$, Me_2CO; fairly sol. hexane, MeOH; poorly sol. H_2O. Mp 56-57°. $[\alpha]_D^{22}$ -48.9 (c, 1.49 in $CHCl_3$).

(9*S*,10*S*,12*Z*)-*form* [145308-76-5]
Needles (EtOAc/hexane). Mp 96-97°. $[\alpha]_D^{22}$ +43.5 (c, 1.36 in $CHCl_3$).

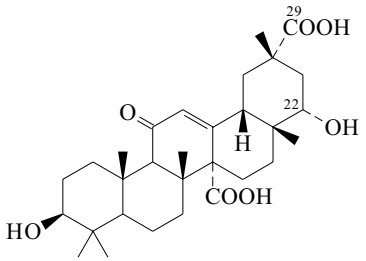
Kawagishi, H. *et al., Agric. Biol. Chem.*, 1990, **54**, 1329 (*isol, pmr, ms*)
Kuwahara, S. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1417 (*synth, abs config*)
Yokota, H. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1562 (*activity*)

9,13-Dihydroxy-10-oxo-11-octadecenoic acid D-595

$H_3C(CH_2)_4CH(OH)CH=CHCOCH(OH)(CH_2)_7COOH$
$C_{18}H_{32}O_5$ 328.448

(9ξ,11*E*,13ξ)-*form*
9-Me ether: [150147-08-3] *13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid*
$C_{19}H_{34}O_5$ 342.475
Isol. from corn. Yellow oil. $[\alpha]_D$ +5.3 (c, 1 in MeOH). λ_{max} 227 (MeOH) (Berdy).
Kuga, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1020 (*isol, deriv*)

3,22-Dihydroxy-11-oxo-12-oleanene-27,29-dioic acid D-596



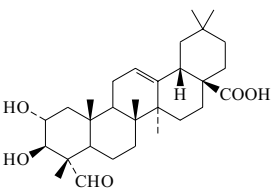
$C_{30}H_{44}O_7$ 516.673

(3β,22α)-*form*

29→22 Lactone, 27-Me ester: [123914-44-3] *Methyl 3-hydroxy-11-oxo-12-oleanen-29,22α-olid-27-oate.* ***Glyuranolide***
$C_{31}H_{44}O_6$ 512.685
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Cryst. Mp 301-303°. $[\alpha]_D^{14}$ +46.

Jia, Q. *et al., Yaoxue Xuebao*, 1989, **24**, 348-351 (*isol, pmr*)

2,3-Dihydroxy-23-oxo-12-oleanen-28-oic acid D-597



(2α,3β)-*form*

$C_{30}H_{46}O_5$ 486.69

(2α,3β)-*form*

2α-Hydroxygypsogenin

3-O-β-D-Glucopyranoside:
$C_{36}H_{56}O_{10}$ 648.832
Constit. of smooth luffa (*Luffa cylindrica*) leaves (the gourd and not the leaves of the plant is a food source).

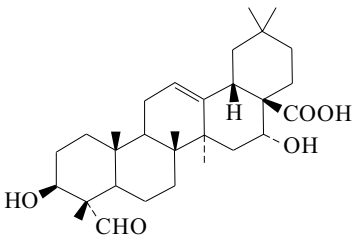
(2β,3β)-*form* [168570-34-1]
Oleragenin. *2β-Hydroxygypsogenin*
Needles (MeOH). Mp 296-298° dec. $[\alpha]_D^{21}$ +67.8 (c, 0.59 in MeOH).

3-O-β-D-Glucuronopyranoside, 28-O-β-D-glucopyranosyl ester: [274677-98-4]
Oleragenoside
$C_{42}H_{64}O_{16}$ 824.958
Constit. of spinach (*Spinacia oleracea*). Amorph. powder. λ_{max} 208 (MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→3)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [139742-10-2]
Amaranthussaponin II
$C_{48}H_{74}O_{20}$ 971.101
Constit. of prince's feather (*Amaranthus hypochondriacus*) and bush greens (*Amaranthus cruentus*) grains. Powder. $[\alpha]_D$ +9.2 (c, 0.87 in MeOH).

Kohda, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2609 (*Amaranthussaponin II*)
Liang, L. *et al., CA*, 1994, **121**, 175208t (*Luffa cylindrica glycoside*)
Maeda, C. *et al., Phytochemistry*, 1994, **37**, 1131 (*isol, pmr, cmr*)
Zhang, D. *et al., Chem. Pharm. Bull.*, 1995, **43**, 966 (*isol, pmr, cmr*)
Junkuszew, M. *et al., Phytochemistry*, 1998, **49**, 195-198 (*Amaranthus cruentus saponin*)
Mithöfer, A. *et al., Nat. Prod. Lett.*, 1999, **14**, 5-10 (*Oleragenoside*)

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid D-598



$C_{30}H_{46}O_5$ 486.69

(3β,16α)-*form* [631-01-6]
Quillaic acid
Cryst. (EtOH). Mp 294°. $[\alpha]_D$ +56.1 (Py).

Me ester: [6151-28-6]
$C_{31}H_{48}O_5$ 500.717
Mp 200-205° dec. $[\alpha]_D$ +50.1 ($CHCl_3$).

28-O-[β-D-Glucopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→6)]-β-D-glucopyranosyl] ester: [158359-81-0]
$C_{48}H_{76}O_{20}$ 973.116
Cryst. Mp 205-207°. $[\alpha]_D^{20}$ +18.1 (MeOH).

3-O-β-D-Glucopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl] ester: [356542-99-9]
$C_{59}H_{94}O_{28}$ 1251.375
Amorph. powder. $[\alpha]_D^{20}$ -2 (c, 0.1 in MeOH).

3-O-β-D-Glucuronopyranoside: [24404-56-6] ***Prosapogenin***†
$C_{36}H_{54}O_{11}$ 662.816
Saponin from peel of *Quillaja saponaria* (soap-bark tree). Cryst. (EtOH). Mp 219-221° dec. $[\alpha]_D^{20}$ +16 (MeOH).

3-O-[β-D-Galactopyranosyl-(1→3)-β-D-glucopyranoside], 28-O-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-[β-D-fucopyranosyl-(1→3)]-α-L-arabinopyranosyl] ester: [202645-16-7]
$C_{70}H_{112}O_{36}$ 1529.633
$[\alpha]_D^{25}$ +17 (c, 1 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside]: [168647-42-5]
$C_{42}H_{64}O_{16}$ 824.958
Constit. of *Quillaja saponaria* (soap-bark tree).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [122587-95-5]
Dubioside A
$C_{53}H_{82}O_{24}$ 1103.216
Amorph. powder (as Me ester). Mp 210-215° dec. (Me ester). $[\alpha]_D^{25}$ -31.9 (c, 2.7 in MeOH) (Me ester).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[α-L-rhamnopyranosyl-(1→2)-[4-methoxy-E-cinnamoyl-(→4)]-β-D-fucopyranosyl] ester: [194040-59-0] ***Jenisseensoside C***
$C_{64}H_{92}O_{26}$ 1277.415

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[α-L-rhamnopyranosyl-(1→2)-[4-methoxy-Z-cinnamoyl-(→4)]-β-D-fucopyranosyl] ester: [194040-60-3] ***Jenisseensoside D***
$C_{64}H_{92}O_{26}$ 1277.415

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [122587-96-6] ***Dubioside B***
$C_{58}H_{90}O_{28}$ 1235.332
Needles (MeOH) (as Me ester). Mp 225-226° (Me ester). $[\alpha]_D^{24}$ -26.1 (c, 1 in MeOH) (Me ester).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[β-D-glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→2)-β-D-[4-methoxy-E-cinnamoyl-(→4)]-fucopyranosyl] ester: [168647-40-3] ***Jenisseensoside A***
$C_{70}H_{102}O_{31}$ 1439.557

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[β-D-glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→2)-β-D-[4-methoxy-Z-cinnamoyl-(→4)]-fucopyranosyl] ester: [168753-25-1] ***Jenisseensoside B***
$C_{70}H_{102}O_{31}$ 1439.557

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [122587-97-7] ***Dubioside C***
$C_{63}H_{98}O_{32}$ 1367.448
Needles (MeOH) (as Me ester). Mp 229-231° (Me ester). $[\alpha]_D^{24}$ -27.6 (c, 0.8 in MeOH aq.).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-arabinofuranosyl-(1→3)]-4-O-acetyl-β-D-fucopyranosyl] ester: [211508-49-5] ***Vaccaroside E***. *Vaccariside E*
$C_{66}H_{102}O_{33}$ 1423.512
Amorph. solid. Mp 230° dec. $[\alpha]_D^{21}$ -22.4 (c, 1 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[5-O-acetyl-α-L-arabinofuranosyl-(1→3)]-4-O-acetyl-β-D-fucopyranosyl] ester: [318959-80-7] ***Segetoside I***
$C_{68}H_{104}O_{34}$ 1465.549

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-[β-D-xylopyranosyl-(1→4)-α-L-

rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4-O-*acetyl-β-D-fucopyranosyl] ester:* [287386-81-6]
$C_{67}H_{104}O_{33}$ 1437.539
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosyl] ester:* [229484-36-0] ***Silenoside B***
$C_{65}H_{102}O_{33}$ 1411.501
Constit. of *Silene vulgaris* (bladder campion). Powder.

3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*[α-L-arabinopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [218167-65-8]
$C_{77}H_{120}O_{42}$ 1717.77
Amorph. powder. $[\alpha]_D^{20}$ -6 (c, 0.132 in H_2O). λ_{max} 210 (MeCN aq.).

3-O-*[β-D-Galactopyranosyl-(1→2)-6*-O-*methyl-β-D-glucuronopyranoside], 28*-O-*[5*-O-*acetyl-α-L-arabinofuranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [223428-32-8] ***Segetoside D***
$C_{69}H_{106}O_{34}$ 1479.576

3-O-*[β-D-Galactopyranosyl-(1→2)-6*-O-*butyl-β-D-glucuronopyranoside], 28*-O-*[5*-O-*acetyl-α-L-arabinofuranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [223428-33-9] ***Segetoside E***
$C_{72}H_{112}O_{34}$ 1521.656

3-O-*[β-D-Galactopyranosyl-(1→3)-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-[β-D-fucopyranosyl-(1→3)]-α-L-arabinopyranosyl] ester:* [202645-08-7]
$C_{70}H_{110}O_{37}$ 1543.617
$[\alpha]_D^{25}$ +23.2 (c, 1 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucuronopyranoside], 28*-O-*[β-D-galactopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-[β-D-fucopyranosyl-(1→3)]-α-L-arabinopyranosyl] ester:* [202645-12-3]
$C_{70}H_{110}O_{37}$ 1543.617
$[\alpha]_D^{25}$ +20.8 (c, 1 in MeOH).

3-O-*[α-L-Arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosyl] ester:* [229484-45-1] ***Silenoside C***
$C_{70}H_{110}O_{37}$ 1543.617
Constit. of *Silene vulgaris* (bladder campion). Powder.

3-O-*[β-D-Xylopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]:* [97892-86-9]
$C_{47}H_{72}O_{20}$ 957.074
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Xylopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*[α-L-rhamnopyranosyl-(1→2)-[4-methoxycinnamoyl-(→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [241485-62-1] ***Silenoside***
$C_{71}H_{102}O_{31}$ 1451.568

3-O-*[α-L-Rhamnopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]:* [210426-59-8]
$C_{48}H_{74}O_{20}$ 971.101
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[α-L-Rhamnopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-3*-O-*[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester:* [263259-79-6]
$C_{94}H_{152}O_{47}$ 2034.207
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[α-L-Rhamnopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*[β-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-4*-O-*[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester:* [263259-76-3]
$C_{94}H_{152}O_{47}$ 2034.207
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[α-L-Rhamnopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-3*-O-*[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester:* [263259-81-0]
$C_{99}H_{160}O_{51}$ 2166.322
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[α-L-Rhamnopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-4*-O-*[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester:* [263259-78-5]
$C_{99}H_{160}O_{51}$ 2166.322
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], Me ester:* [172045-43-1]
$C_{48}H_{74}O_{20}$ 971.101
Amorph. powder.

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-fucopyranosyl-(1→4)-[β-D-galactopyranosyl-(1→3)]-α-L-rhamnopyranosyl] ester:* [172045-45-3]
$C_{65}H_{102}O_{33}$ 1411.501
Amorph. powder.

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [287386-83-8]
$C_{72}H_{112}O_{37}$ 1569.655
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[4*-O-*acetyl-β-D-glucopyranosyl-(1→2)]-β-D-fucopyranosyl] ester:* [180965-44-0] ***Rubicunoside C***
$C_{72}H_{112}O_{38}$ 1585.654
$[\alpha]_D^{16}$ -16 (c, 0.9 in Py).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-64-8]
$C_{72}H_{112}O_{38}$ 1585.654
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[6*-O-*acetyl-β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-68-2]
$C_{74}H_{114}O_{39}$ 1627.691
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-65-9]
$C_{73}H_{114}O_{39}$ 1615.68
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4*-O-*acetyl-*

β-D-fucopyranosyl] ester: [287386-85-0]
$C_{77}H_{120}O_{41}$ 1701.77
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-66-0]
$C_{77}H_{120}O_{42}$ 1717.77
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[4*-O-*acetyl-6-deoxy-β-D-glucopyranosyl-(1→4)]-β-D-fucopyranosyl] ester:* [214552-00-8]
Saponarioside B
$C_{77}H_{120}O_{41}$ 1701.77
Constit. of *Saponaria officinalis*.
Amorph. solid. Mp 236-238° dec. $[\alpha]_D^{20}$ -15 (c, 1.1 in Py).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[2*-O-*acetyl-6-deoxy-β-D-glucopyranosyl-(1→2)]-3*-O-*acetyl-β-D-fucopyranosyl] ester:* [171528-07-7]

[158732-58-2] ***Rubicunoside A***
$C_{79}H_{122}O_{42}$ 1743.808
Cryst. (MeOH). Mp 244-246°. $[\alpha]_D^{16}$ -18.03 (c, 1.1 in Py).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [287386-87-2]
$C_{77}H_{120}O_{41}$ 1701.77
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[α-L-rhamnopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-70-6]
$C_{78}H_{122}O_{42}$ 1731.797
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-3*-O-*[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester:* [263259-80-9]
$C_{93}H_{150}O_{47}$ 2020.18
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-4*-O-*[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester:* [263259-77-4]
$C_{93}H_{150}O_{47}$ 2020.18
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-67-1]
$C_{78}H_{122}O_{43}$ 1747.796
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[6*-O-*acetyl-β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-69-3]
$C_{80}H_{124}O_{44}$ 1789.833
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-3*-O-*[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester:* [154335-25-8]
$C_{98}H_{158}O_{51}$ 2152.296
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [208933-54-4]
$C_{83}H_{130}O_{46}$ 1863.912
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)-4*-O-*acetyl-6-deoxy-β-D-glucopyranosyl-(1→4)]-β-D-fucopyranosyl] ester:* [214551-55-0]
Saponarioside A
$C_{82}H_{128}O_{45}$ 1833.886
Amorph. solid. Mp 243-245° dec. $[\alpha]_D^{20}$ -25.5 (c, 0.9 in Py).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→4)-6-deoxy-β-D-glucopyranosyl-(1→2)]-3*-O-*acetyl-β-D-fucopyranosyl] ester:* [180965-42-8]
Rubicunoside B
$C_{83}H_{130}O_{46}$ 1863.912
$[\alpha]_D^{15}$ -11.3 (c, 1.5 in Py).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-6*-O-*butyl-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[2*-O-*acetyl-6-deoxy-β-D-glucopyranosyl-(1→2)]-3*-O-*acetyl-β-D-fucopyranosyl] ester:* [180965-45-1] ***Rubicunoside D***
$C_{83}H_{130}O_{42}$ 1799.915
$[\alpha]_D^{15}$ -11.6 (c, 1.5 in Py).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [287386-82-7]
$C_{73}H_{114}O_{37}$ 1583.681
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-57-9]
$C_{73}H_{114}O_{38}$ 1599.681
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[6*-O-*acetyl-β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-61-5]
$C_{75}H_{116}O_{39}$ 1641.718
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-58-0]
$C_{74}H_{116}O_{39}$ 1629.707
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-*

*xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester:* [287386-84-9]
$C_{78}H_{122}O_{41}$ 1715.797
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-59-1]
$C_{78}H_{122}O_{42}$ 1731.797
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [287386-86-1]
$C_{78}H_{122}O_{41}$ 1715.797
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosyl] ester:* [96552-96-4] ***Momordicasaponin II***
$C_{76}H_{120}O_{41}$ 1689.759
Isol. from seeds of *Momordica cochinchinensis* (Chinese cucumber). Powder. Mp 241-244° dec. $[\alpha]_D^{19}$ -14.8 (c, 0.7 in 33% MeOH aq.).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[α-L-rhamnopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-63-7]
$C_{79}H_{124}O_{42}$ 1745.823
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-60-4]
$C_{79}H_{124}O_{43}$ 1761.823
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[6*-O-*acetyl-β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [299184-62-6]
$C_{81}H_{126}O_{44}$ 1803.86
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-4*-O-*acetyl-β-D-fucopyranosyl] ester:* [287200-23-1]
$C_{84}H_{132}O_{46}$ 1877.939
Constit. of *Quillaja saponaria* (soapbark tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 28*-O-*[α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [128866-15-9] ***Dubioside D***
$C_{59}H_{94}O_{28}$ 1251.375
Amorph. powder (EtOH). $[\alpha]_D^{24}$ -20 (c, 1 in MeOH).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [128866-16-0] ***Dubioside E***
$C_{64}H_{102}O_{32}$ 1383.491
Amorph. powder. $[\alpha]_D^{24}$ -16.9 (c, 1 in MeOH).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [128887-86-5] ***Dubioside F***
$C_{69}H_{110}O_{36}$ 1515.606
Amorph. powder. $[\alpha]_D^{22}$ -17.3 (c, 1 in MeOH aq.).

3-O-*[6-Deoxy-β-D-glucopyranosyl-(1→4)-β-D-xylopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-3*-O-*acetyl-β-D-fucopyranosyl] ester:* [257880-35-6] ***Vaccariside A***
$C_{78}H_{122}O_{42}$ 1731.797
Powder. Mp 215-217°. $[\alpha]_D^{18}$ -14.9 (c, 0.66 in MeOH). Not the same as Vaccaroside A (cf.).

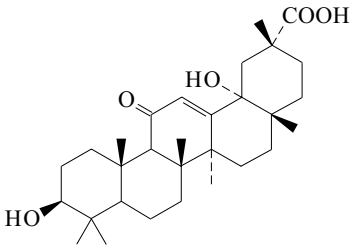
3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→4)-α-L-arabinopyranosyl-(1→4)]-β-D-glucuronopyranoside], 28*-O-*[6-deoxy-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)]-β-D-fucopyranosyl] ester:* [71866-89-2] ***Acanthophylloside D***
$C_{86}H_{136}O_{49}$ 1953.991
Cryst. Mp 235-237°. $[\alpha]_D^{20}$ -13 (c, 1.5 in H_2O).

Glycoside: ***Quillajasaponin***
Constit. of Quillaja bark (*Quillaja saponaria*). Amorph. powder. Mp 292-294° dec. Hydrol. gives quillaic acid, galactose and glucuronic or galacturonic acid.

▶ Produces strong sneezing response.

Bilham, P. *et al., J.C.S.*, 1940, 1469-1477; 1941, 552-554 (*struct*)
Labriola, R.A. *et al., Experientia*, 1969, **25**, 124-125 (*Prosapogenin*)
Kitagawa, I. *et al., Tet. Lett.*, 1974, 469-472 (*struct*)
Tori, K. *et al., Tet. Lett.*, 1974, 4227-4230 (*cmr*)
Putieva, Z.M. *et al., Khim. Prir. Soedin.*, 1979, **15**, 176-180; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 148-151 (*Acanthophylloside D*)
Iwamato, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 464-478 (*isol, pmr, cmr*)
Nagao, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 925-929; 1990, **38**, 378-381 (*Dubiosides*)
Tan, N.-H. *et al., CA*, 1994, **121**, 251219q (*Rubicunoside A*)
Elgamal, E.H.A. *et al., Nat. Prod. Lett.*, 1994, **4**, 217 (*Gypsophila capillaris saponin*)
Tan, N.-H. *et al., Huaxue Xuebao*, 1995, **53**, 1024-1033; *CA*, **124**, 25623x (*Rubicunoside A*)
Liu, Z. *et al., J. Nat. Prod.*, 1995, **58**, 1632-1635 (*Gypsophila oldhamiana glycosides*)
Lacaille-Dubois, M.-A. *et al., Phytochemistry*, 1995, **40**, 509; 1997, **45**, 985-990 (*Jenisseensosides*)
Tan, N.-H. *et al., Huaxue Xuebao*, 1996, **54**, 722-728; *CA*, **125**, 190619d (*Rubicunosides B-D*)
De Tommasi, N. *et al., J. Nat. Prod.*, 1998, **61**, 323-327 (*Spergularia ramosa saponins*)
Jia, Z. *et al., J. Nat. Prod.*, 1998, **61**, 1368-1373 (*Saponariosides*)
Sang, S. *et al., Nat. Prod. Sci.*, 1998, **4**, 268-273; *CA*, **130**, 294009z (*Segetoside D, Segetoside E*)
Guo, S. *et al., Phytochemistry*, 1998, **48**, 175-180 (*Quillaja saponaria saponins*)
Jia, Z. *et al., Phytochemistry*, 1998, **48**, 529-536 (*Vaccaroside E*)
Zou, C. *et al., Chin. Chem. Lett.*, 1999, **10**, 33-36 (*Silenoside A*)
Ma, J. *et al., Chin. Chem. Lett.*, 1999, **10**, 921-924 (*Vaccariside A*)
Lacaille-Dubois, M.-A. *et al., J. Nat. Prod.*, 1999, **62**, 133-136 (*Sitene fortunei saponin*)
Glensk, M. *et al., J. Nat. Prod.*, 1999, **62**, 717-721 (*Silenosides B and C*)
Nybera, N.T. *et al., Carbohydr. Res.*, 2000, **323**, 87-97 (*Quillaja saponaria saponins*)
Sang, S.-M. *et al., J. Asian Nat. Prod. Res.*, 2000, **2**, 187-193; *CA*, **134**, 97862d (*Segetoside I*)
Guo, S. *et al., Phytochemistry*, 2000, **53**, 861-868 (*Quillaja saponaria saponins*)
Guo, S. *et al., Phytochemistry*, 2000, **54**, 615-623 (*Quillaja saponaria saponins*)
Gaidi, G. *et al., J. Nat. Prod.*, 2001, **64**, 920-924 (*Acanthophyllum squarrosum saponin*)

3,18-Dihydroxy-11-oxo-12-oleanen-29-oic acid D-599

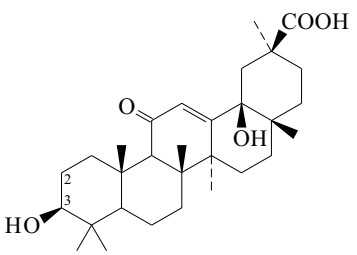


$C_{30}H_{46}O_5$ 486.69

(3β,18α)-*form*

29→18 lactone: [10376-64-4] *3β-Hydroxy-11-oxo-12-oleanen-29,18α-olide.* ***Isoglabrolide***
$C_{30}H_{44}O_4$ 468.675
Constit. of *Glycyrrhiza glabra* (licorice). Cryst. (2-propanol). Mp 318-325° dec. $[\alpha]_D^{20}$ +46 (c, 1.2 in $CHCl_3$).
Canonica, L. *et al., Gazz. Chim. Ital.*, 1966, **96**, 843

3,18-Dihydroxy-11-oxo-12-oleanen-30-oic acid D-600



$C_{30}H_{46}O_5$ 486.69

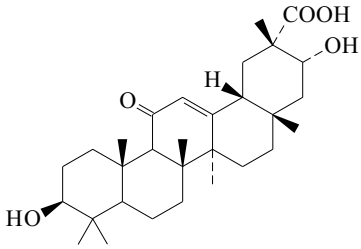
(3β,18β)-*form*

30→18 Lactone, 3-Ac: [67463-79-0] *3β-Acetoxy-11-oxo-12-oleanen-30,18β-olide.* ***Echinolactone A***
$C_{32}H_{46}O_5$ 510.712
Cryst. (MeOH). Mp 245°.

30→18 Lactone, 3-ketone, 2,2-dibromo: [94354-98-0] *2,2-Dibromo-3,11-dioxo-12-oleanen-30,18β-olide.* ***Echinolactone B***
$C_{30}H_{40}Br_2O_4$ 624.452
Cryst. (MeOH). Mp 225°.

(3β,18α)-*form* [17991-67-2] ***18α-Hydroxyglycyrrhetic acid***
Constit. of *Glycyrrhiza uralensis* (Chinese licorice) and *Glycyrrhiza glabra* (licorice). Cryst. ($CHCl_3$/petrol). Mp 252-255° dec. $[\alpha]_D^{20}$ +60 (c, 0.17 in Me_2CO).
Canonica, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 769 (*18α-Hydroxyglycyrrhetic acid*)
Sandiya, R. *et al., Chem. Comm.*, 1984, 1091

3,21-Dihydroxy-11-oxo-12-oleanen-29-oic acid D-601



$C_{30}H_{46}O_5$ 486.69

(3β,21α)-*form* [22327-86-2]
Glabric acid
Isol. from *Glycyrrhiza glabra* (licorice). Cryst. (Me_2CO). Mp 329-333°. $[\alpha]_D$ -26 (c, 1 in Py). $[\alpha]_D$ +23 (EtOH).

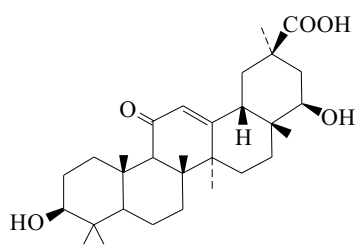
Me ester:
Needles (Me_2CO/petrol). Mp 277-280°. $[\alpha]_D$ +16 (c, 1.3 in $CHCl_3$).

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: [256441-31-3] ***Macedonoside A***
$C_{42}H_{62}O_{17}$ 838.942

Di-Ac, Me ester:
Plates ($CHCl_3$/MeOH). Mp 319-323°. $[\alpha]_D$ +43 (c, 1.7 in $CHCl_3$).

Beaton, J.M. *et al., J.C.S.*, 1956, 2417 (*isol*)
Kir'yalov, N.P. *et al., Khim. Prir. Soedin.*, 1975, **11**, 105; *Chem. Nat. Compd. (Engl. Transl.)*, 123 (*pmr, ms*)
Shibano, M. *et al., Nat. Med. (Tokyo)*, 1999, **53**, 166-172; *CA*, **132**, 119875y (*Macedonoside A*)

3,22-Dihydroxy-11-oxo-12-oleanen-30-oic acid D-602



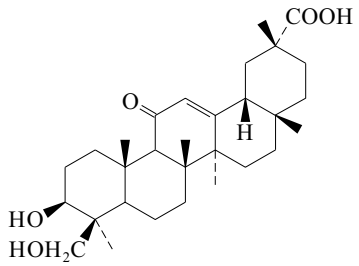
$C_{30}H_{46}O_5$ 486.69

(3β,22β)-*form*

30→22 Lactone: [10401-33-9] *3β-Hydroxy-11-oxo-12-oleanen-30,22β-olide.* ***Glabrolide***
$C_{30}H_{44}O_4$ 468.675
Constit. of *Glycyrrhiza glabra* (licorice) and *Glycyrrhiza uralensis* (Chinese licorice). Cryst. Mp 360-365°. $[\alpha]_D^{20}$ +80.

30→22 Lactone, 3-O-[β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: [119418-01-8] ***Licoricesaponin E2***
$C_{42}H_{60}O_{16}$ 820.926
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice). Dihydrate. Mp 216-219°. $[\alpha]_D^{23}$ +68 (MeOH). MF incorr. given as C_{44}.
Canonica, L. *et al., Gazz. Chim. Ital.*, 1966, **96**, 772 (*isol, uv, ir, pmr, ms, deriv*)
Russo, G. *et al., Corsi. Semin. Chim.*, 1968, **11**, 20 (*isol*)
Ricca, G.S. *et al., Gazz. Chim. Ital.*, 1968, **98**, 602 (*pmr*)
Wahlberg, I. *et al., Acta Chem. Scand.*, 1971, **25**, 3192 (*ms*)
Kir'yalov, N.P. *et al., Khim. Prir. Soedin.*, 1973, **9**, 277; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 268 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3710 (*Licoricesaponin E2*)

3,24-Dihydroxy-11-oxo-12-oleanen-29-oic acid D-603

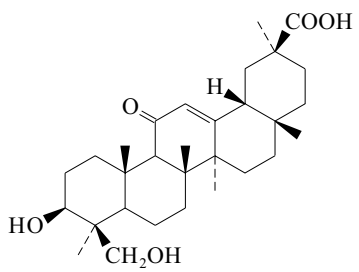


$C_{30}H_{46}O_5$ 486.69

3β-*form*
24-Hydroxyliquiritic acid
Isol. from *Glycyrrhiza glabra* (licorice). Mp 282-286° dec. $[\alpha]_D$ +79 ($CHCl_3$/MeOH).

Di-Ac, Me ester:
Mp 218-220°. $[\alpha]_D$ +53 ($CHCl_3$).
Canonica, L. *et al., Gazz. Chim. Ital.*, 1968, **98**, 712

3,24-Dihydroxy-11-oxo-12-oleanen-30-oic acid D-604



$C_{30}H_{46}O_5$ 486.69

3β-*form* [20528-69-2]
24-Hydroxyglycyrrhetic acid
Isol. from *Glycyrrhiza glabra* (licorice).

Me ester: [18184-26-4]
$C_{31}H_{48}O_5$ 500.717
Cryst. ($CHCl_3$/MeOH). Mp 247-248°. $[\alpha]_D^{20}$ +142.5.

Di-Ac:
Cryst. ($CHCl_3$/MeOH). Mp 255-257°. $[\alpha]_D^{20}$ +123.5.

Di-Ac, Me ester: [18061-38-6]
Cryst. ($CHCl_3$/MeOH). Mp 227°. $[\alpha]_D^{20}$ +123.

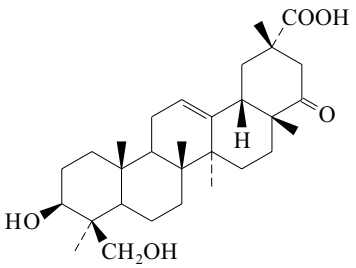
3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Licoricesaponin G2***
$C_{42}H_{62}O_{17}$ 838.942
Constit. of *Glycyrrhiza uralensis* (Chi-

nese licorice). Mp 229-230°. $[\alpha]_D^{20}$ +34 (MeOH).

[52911-55-4]

Russo, G. *et al., Gazz. Chim. Ital.*, 1967, **97**, 1359; 1968, **98**, 602; 712 (*isol, synth*)
Canonica, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 1359
Kir'yalov, N.P. *et al., Khim. Prir. Soedin.*, 1972, **8**, 395; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 393 (*isol*)
Shu, Y. *et al., CA*, 1985, **103**, 119932 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1991, **39**, 244 (*Licoricesaponin G2*)

3,24-Dihydroxy-22-oxo-12-oleanen-29-oic acid D-605



$C_{30}H_{46}O_5$ 486.69

3β-*form* [114702-59-9]
Melilotigenin. *Yunganogenin K*
Constit. of *Melilotus officinalis* (sweet clover). Plates (MeOH). Mp 318-319°. $[\alpha]_D^{18}$ +57.1 (c, 0.04 in MeOH).

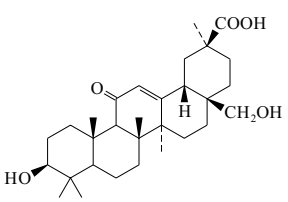
3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Yunganoside K₂***
$C_{42}H_{62}O_{17}$ 838.942
Amorph. powder. $[\alpha]_D^{20}$ -30.4 (c, 0.67 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-xylopyranosyl-(1→2)-β-D-glucuronopyranoside]: [263398-47-6] ***Melilotussaponin O₂***
$C_{47}H_{72}O_{19}$ 941.074
Constit. of *Melilotus officinalis* (sweet clover). Amorph. powder. $[\alpha]_D^{14}$ -45.7 (c, 0.5 in Py).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Yunganoside K₁***
$C_{48}H_{72}O_{21}$ 985.084
Amorph. powder. $[\alpha]_D^{20}$ -10.7 (c, 0.55 in MeOH).

Kang, S.S. *et al., J. Nat. Prod.*, 1988, **51**, 335 (*isol, pmr*)
Ohtani, K. *et al., Phytochemistry*, 1994, **36**, 139 (*Yunganosides*)
Hirakawa, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 286-287 (*Melilotussaponin O₂*)

3,28-Dihydroxy-11-oxo-12-oleanen-30-oic acid D-606



3β-*form*

$C_{30}H_{46}O_5$ 486.69

3β-*form* [56061-86-0]
28-Hydroxyglycyrrhetic acid
Isol. from *Glycyrrhiza glabra* (licorice).

Me ester:
Needles ($CHCl_3$/MeOH). Mp 265°. $[\alpha]_D$ +132.5 ($CHCl_3$).

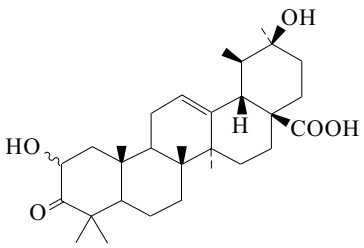
Di-Ac, Me ester:
Mp 303-305°. $[\alpha]_D$ +133 ($CHCl_3$).

(3β,18α)-*form* [75281-84-4] ***Lonchoterpene***

Me ester: [75281-82-2]
Cryst. ($CHCl_3$/MeOH). Mp 300°.

Elgamal, M.H.A. *et al., Planta Med.*, 1975, **27**, 159 (*isol, pmr, ms*)
Iwu, M.M. *et al., Can. J. Pharm. Sci.*, 1980, **15**, 39 (*isol*)
Iwu, M.M. *et al., Fitoterapia*, 1982, **53**, 25 (*isol*)

2,20-Dihydroxy-3-oxo-12-ursen-28-oic acid D-607



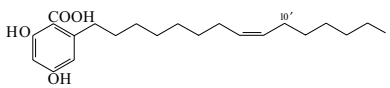
$C_{30}H_{46}O_5$ 486.69

(2ξ,20β)-*form*
Constit. of apple skin.

2-Ac, Me ester:
Cryst. ($CHCl_3$/MeOH). Mp 248-249°. $[\alpha]_D$ +93.2 (c, 1.26 in $CHCl_3$).

Lawrie, W. *et al., J.C.S.(C)*, 1967, 851

2,4-Dihydroxy-6-(8-pentadecenyl)benzoic acid D-608



$C_{22}H_{34}O_4$ 362.508

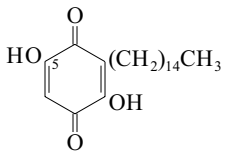
(*Z*)-*form* [62071-06-1]
Constit. of *Ginkgo biloba* (ginkgo).

10′-Acetoxy: [120727-07-3] *6-(10-Acetoxy-8-pentadecenyl)-2,4-dihydroxybenzoic acid*
$C_{24}H_{36}O_6$ 420.545

[120727-09-5]

Gellerman, J.L. *et al., Phytochemistry*, 1976, **15**, 1959 (*isol, uv, pmr*)
Barrero, A.F. *et al., Phytochemistry*, 1989, **28**, 161 (*isol, cmr*)

2,5-Dihydroxy-3-pentadecyl-1,4-benzoquinone D-609



[21551-65-5]
2,5-Dihydroxy-3-pentadecyl-2,5-cyclohexadiene-1,4-dione, 9CI. ***Homorapanone***

$C_{21}H_{34}O_4$ 350.497
λ_{max} 292 (log ε 4.27); 425 (log ε 2.47) (EtOH).

5-Me ether: [21551-64-4] *2-Hydroxy-5-methoxy-3-pentadecyl-1,4-benzoquinone.* ***Dihydromaesanin***
$C_{22}H_{36}O_4$ 364.524
Orange-yellow prisms (Et_2O/hexane). Mp 102-103° (100°). λ_{max} 289 (log ε 4.22); 420 (log ε 2.64) (EtOH).

Di-Me ether: [21551-66-6] *2,5-Dimethoxy-3-pentadecyl-1,4-benzoquinone*
$C_{23}H_{38}O_4$ 378.551
Cryst. (hexane). Mp 72-74°.

8′,9′-Didehydro(Z-): [188414-99-5] *2,5-Dihydroxy-3-(8-pentadecenyl)-1,4-benzoquinone*
$C_{21}H_{32}O_4$ 348.481
Orange cryst. (MeOH aq.). Mp 116-119°. λ_{max} 288 (log ε 4.33); 419 (log ε 2.48) (MeOH/HCl).

10′,11′-Didehydro(Z-): [132362-27-7] *2,5-Dihydroxy-3-(10-pentadecenyl)-1,4-benzoquinone*
$C_{21}H_{32}O_4$ 348.481

10′,11′-Didehydro, 5-Me ether: [82380-21-0] *2-Hydroxy-5-methoxy-3-(10-pentadecenyl)-1,4-benzoquinone.* ***Maesanin***
$C_{22}H_{34}O_4$ 362.508
Yellow needles. Sol. MeOH, hexane; poorly sol. hexane. Mp 77°. λ_{max} 289 (ε 30200); 425 (ε 631) (EtOH) (Derep).

10,11-Didehydro(Z-), di-Me ether: [87746-51-8] *2,5-Dimethoxy-3-(10-pentadecenyl)-1,4-benzoquinone*
$C_{23}H_{36}O_4$ 376.535
Yellow oil.

*8′,9′,11′,12′,14′,15′-Hexadehydro(*all-Z*), 5-Me ether:* [105018-76-6] *2-Hydroxy-5-methoxy-3-(8,11,14-pentadecatrienyl)-1,4-benzoquinone.* ***Sorgoleone 358***
$C_{22}H_{30}O_4$ 358.477
Constit. of the etiolated seedlings of *Sorghum bicolor* (sorghum). Yellow cryst. Mp 50-51° (37-39°). ⁎Sorgoleone⁎ is the name given to the unstable hydroquinone form λ_{max} 283 (ε 7300); 288 (ε 7300); 411 (ε 400) (CH_2Cl_2).

*8′,9′,11′,12′,14′,15′-Hexadehydro(*all-Z*), 5-Et ether:* [210708-13-7] ***5-Ethoxysorgoleone 358***
$C_{23}H_{32}O_4$ 372.503
Constit. of *Sorghum bicolor* (sorghum). Amorph. yellow powder. λ_{max} 285 (log ε 4.33); 289 (log ε 4.19); 413 (log ε 2.89) (CH_2Cl_2).

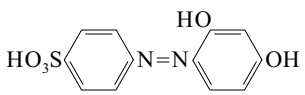
[26915-11-7, 116138-78-4]

Ogawa, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1709-1720 (*synth, uv, ir, pmr*)
Khurana, S.K. *et al., Curr. Sci.*, 1972, **41**, 331; 1975, **44**, 11 (*occur, ms*)
Reinaud, O. *et al., Tet. Lett.*, 1985, **26**, 3993-3996 (*synth, Dihydromaesanin*)
Kubo, I. *et al., Tetrahedron*, 1987, **43**, 2653-2660 (*struct, synth, Maesanin*)

Midiwo, J.O. *et al., Bull. Chem. Soc. Ethiop.*, 1990, **4**, 71-73 (*10′,11′-didehydro, isol*)
Sargent, M.V. *et al., J.C.S. Perkin 1*, 1990, 1429-1434 (*synth, derivs*)
Danheiser, R.L. *et al., Tet. Lett.*, 1990, **31**, 1527-1530 (*synth, Maesanin*)
Marner, F.J. *et al., Helv. Chim. Acta*, 1992, **75**, 1557-1562 (*isol, Dihydromaesanin*)
Yadav, J.S. *et al., J.O.C.*, 1992, **57**, 3242-3245 (*synth, Maesanin*)
Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1993, **41**, 561-565 (*isol, synth, Maesanin*)
Muhammad, I. *et al., Saudi Pharm. J.*, 1993, **1**, 7; *CA*, **121**, 104078 (*isol, Dihydromaesanin*)
Janik, I. *et al., Fitoterapia*, 1994, **65**, 476 (*isol*)
Pfeifer, J. *et al., Annalen*, 1995, 131-137 (*synth, Maesanin, ir, pmr, cmr*)
Lund, A.-K. *et al., Phytochemistry*, 1997, **44**, 679-681 (*8′,9′-didehydro, isol, uv, pmr, cmr, activity*)
Rimando, A.M. *et al., J. Nat. Prod.*, 1998, **61**, 927-930 (*isol*)
Suzuki, Y. *et al., Phytochemistry*, 1998, **47**, 997-1001 (*hexadehydro deriv*)
Podolak, I. *et al., Phytother. Res.*, 1998, **12**, S70-S73 (*activity*)
Poigny, S. *et al., Tetrahedron*, 1998, **54**, 14791-14802 (*synth, Maesanin*)

4-[(2,4-Dihydroxyphenyl)azo]-benzenesulfonic acid, 9CI D-610

[2050-34-2]
2′,4′-Dihydroxyazobenzene-4-sulfonic acid. Resorcinol yellow. C.I. Acid orange 6. C.I. Food yellow 8. Chrysoine S. Tropaeolin O. C.I. 14270. E 103



$C_{12}H_{10}N_2O_5S$ 294.287
The name Resorcinol yellow strictly applies to the sodium salt. Food dye; no longer permitted in the EU.

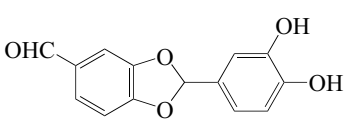
Na salt: [547-57-9]
Sol. H_2O, EtOH, 2-ethoxyethanol; insol. C_6H_6 Me_2CO, $CHCl_3$. λ_{max} 490 (no solvent reported).

[57303-52-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 977B (*ir*)
Perlmutter-Hayman, B. *et al., Inorg. Chem.*, 1976, **15**, 2932 (*use*)
McEwan, C.N. *et al., Anal. Chem.*, 1977, **49**, 922-926 (*ms*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 719

2-(3,4-Dihydroxyphenyl)-1,3-benzodioxole-5-carboxaldehyde D-611

[213903-67-4]
3,4-(3,4-Dihydroxymethylenedioxyphenyl)-benzaldehyde

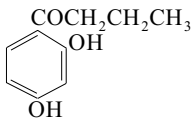


$C_{14}H_{10}O_5$ 258.23
(±)-*form*
Constit. of *Melissa officinalis* (lemon balm). Amorph. pale purple powder. Mp 131-137° dec. λ_{max} 204 (ϵ 2712); 230 (ϵ 2030); 280 (ϵ 1628); 310 (ϵ 1340) (no solvent reported).

Tagashira, M. *et al., Planta Med.*, 1998, **64**, 555-558 (*isol, uv, ir, pmr, cmr*)

1-(2,4-Dihydroxyphenyl)-1-butanone, 9CI D-612

[4390-92-5]
2,4-Dihydroxybutyrophenone. 4-Butyrylresorcinol. Resobutyrophenone



$C_{10}H_{12}O_3$ 180.203
Preservative for food. Needles ($CHCl_3$/C_6H_6). Mp 73°.

Oxime: [22919-59-1]
$C_{10}H_{13}NO_3$ 195.218
Pale-yellow needles. Mp 188-189°.

Brewster, C.M. *et al., J.A.C.S.*, 1930, **52**, 4866 (*synth*)
Price, P. *et al., J.O.C.*, 1964, **29**, 2800 (*synth*)
Desai, M.N. *et al., Microchem. J.*, 1968, **13**, 500 (*use*)
Gandhi, M.H. *et al., Indian J. Appl. Chem.*, 1969, **32**, 360 (*photometric detn*)
Gandhi, M.H. *et al., J. Prakt. Chem.*, 1969, **311**, 171 (*spot test*)
Desai, M.N. *et al., J. Indian Chem. Soc.*, 1973, **50**, 369 (*titrim*)
Gandhi, R.B. *et al., Talanta*, 1979, **26**, 425 (*use*)

4-(3,4-Dihydroxyphenyl)-2-butanone, 9CI D-613

[61152-62-3]

$C_{10}H_{12}O_3$ 180.203
Prisms (Et_2O/petrol). Mp 88-90° (85.5-86°). Bp_8 220-221° Subl.0.05 110.

3-O-β-D-Glucopyranoside: [101705-37-7] ***Myzodendrone***
$C_{16}H_{22}O_8$ 342.345
Isol. from raspberries. Pale yellow cryst. (EtOH/EtOAc). Mp 120-123°.

3-Me ether: [122-48-5] *4-(4-Hydroxy-3-methoxyphenyl)-2-butanone, 9CI, 8CI. Vanillylacetone.* ***Zingerone****. [0]Paradol. FEMA 3124*
$C_{11}H_{14}O_3$ 194.23
Reputed pungent principle of ginger (*Zingiber officinale*). Flavour material used in imitation fruit flavours, ginger beer, ginger ale etc. Also present in cranberry, raspberry and mango. Cryst. (petrol). Mp 41°. Bp 185.5°. Contrary to common assumption, free zingerone is probably not present in ginger and is certainly not its pungent principle. It is however a valuable flavouring agent.
▶ Skin irritant. LD_{50} (rat, orl) 2580 mg/kg. EL8900000

3-Me ether, O-β-D-glucopyranoside: [64703-96-4] ***Zingerone glucoside***
$C_{17}H_{24}O_8$ 356.372
Isol. from Riesling vine leaf. Oil. $[\alpha]_D^{22}$ +31.4 (c, 0.35 in MeOH).

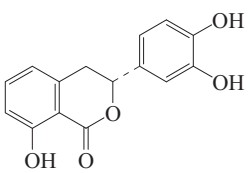
3,4-Methylene ether: [55418-52-5] *4-(3,4-Methylenedioxyphenyl)-2-butanone, 9CI. Piperonylacetone. Heliotropylacetone. FEMA 2701*
$C_{11}H_{12}O_3$ 192.214
Used in food flavouring. Cryst. with intense floral odour. Mp 55° (47-48°). Bp_2 130-131°.

3,4-Didehydro, 3-Me ether: [1080-12-2] *4-(4-Hydroxy-3-methoxyphenyl)-3-buten-2-one.* ***Dehydrozingerone****. Vanillylidene acetone. FEMA 3738*
$C_{11}H_{12}O_3$ 192.214
Flavouring ingredient. Mp 120-124° Mp 129-130°.
▶ EM9960000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 800A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1228A (*ir*)
Lapworth, A. *et al., J.C.S.*, 1917, 777-799 (*Zingerone, isol, struct*)
Chen, Y.-L. *et al., J.A.C.S.*, 1953, **75**, 4287-4289 (*methylene ether, synth*)
Arctander, S. *et al., Perfume and Flavor Chemicals*, Steffen Arctander, 1969, No. 3101 (*Zingerone*)
Banno, K. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1453-1454 (*Zingerone, synth, ir, pmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol., (Suppl.)*, 1976, **14**, 847 (*methylene ether, rev, props*)
De Bernardi, M. *et al., Phytochemistry*, 1976, **15**, 1785-1786 (*Dehydrozingerone*)
Higuchi, R. *et al., Phytochemistry*, 1977, **16**, 1587-1590 (*Zingerone glucoside*)
Reyes, A. *et al., J. Nat. Prod.*, 1986, **49**, 318-320 (*Myzodendrone*)
U.S. Pat., 1987, 4701541; *CA*, **108**, 21874b (*methylene ether, synth*)
Roscher, R. *et al., J. Agric. Food Chem.*, 1993, **41**, 1452-1457 (*Zingerone glucoside*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1117; 1780; 1807 (*Piperonylacetone, Dehydrozingerone, Zingerone*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VFP100

3-(3,4-Dihydroxyphenyl)-3,4-dihydro-8-hydroxyisocoumarin D-614

[480-46-6]
*3-(3,4-Dihydroxyphenyl)-3,4-dihydro-8-hydroxy-1*H*-2-benzopyran-1-one, 9CI.* ***Thunberginol G***



(*R*)-*form*

$C_{15}H_{12}O_5$ 272.257
(R)-form [80394-88-3]
Powder.

4′-Me ether: [21499-23-0] *3,4-Dihydro-8-hydroxy-3-(3-hydroxy-4-methoxyphenyl)-1*H*-2-benzopyran-1-one. 3,4-Dihydro-3-(3-hydroxy-4-methoxyphenyl)-8-hydroxyisocoumarin.* ***Phyllodulcin****. Phyllodulcinol*
Natural sweetener approx. 600-800 times sweeter than sucrose. Cryst. Mp 120°. $[\alpha]_D$ +67.7. Most samples are

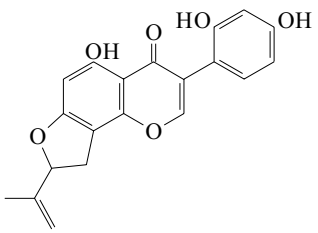
partly racemic.

[37568-82-4]

Asahina, H. *et al., Ber.*, 1931, **64**, 1253 (*Phyllodulcin, isol*)
Arakawa, H. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 2451 (*Phyllodulcin, config*)
Yagi, A. *et al., Phytochemistry*, 1977, **16**, 1098 (*biosynth*)
Takeuchi, N. *et al., Chem. Pharm. Bull.*, 1983, **31**, 4360 (*synth*)
Takeuchi, N. *et al., Heterocycles*, 1993, **35**, 289 (*synth*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1440 (*Phyllodulcin, isol, cmr, activity*)
Ramacciotti, A. *et al., J.O.C.*, 1996, **61**, 5371 (*synth*)

3-(2,4-Dihydroxyphenyl)-8,9-dihydro-5-hydroxy-8-(1-methylethenyl)-4*H*-furo[2,3-*h*]-1-benzopyran-5-one, 9CI D-615

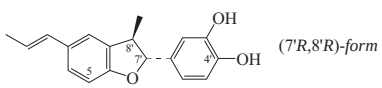
[112147-37-2]
2′,4′,5-Trihydroxy-7,8-[2-(1-methylethenyl)furo]isoflavone



$C_{20}H_{16}O_6$ 352.343
Isol. from seedlings of *Cajanus cajan* (pigeon pea).

Dahiya, J.S. *et al., J. Chromatogr.*, 1987, **409**, 355 (*isol*)

2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3-methyl-5-(1-propenyl)benzofuran D-616



(7′*R*,8′*R*)-*form*

$C_{18}H_{18}O_3$ 282.338
Lignan numbering shown.

(7′*R*,8′*R*)-*form*

3′-Me ether: ***2,3-Dihydro-2-(4-hydroxy-3-methoxyphenyl)-3-methyl-5-(1-propenyl)benzofuran***
$C_{19}H_{20}O_3$ 296.365
Cryst. Mp 105-107°. $[\alpha]_D^{21}$ +94 (c, 1.1 in MeOH).

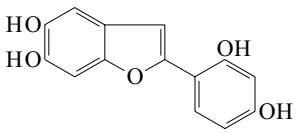
3′,4′-Methylene ether:2,3-Dihydro-2-(3,4-methylenedioxy)-3-methyl-5-(1-propenyl)benzofuran. ***Regnelline***
$C_{19}H_{18}O_3$ 294.349
Amorph. $[\alpha]_D^{21}$ +85.5 (c, 0.06 in MeOH). λ_{max} 232 (ϵ 11250); 265 (ϵ 8750); 290 (ϵ 7500) (MeOH).

(7′*S*,8′*S*)-*form*

3′-Me ether: [119555-99-6]
Constit. of the seed of *Myristica fragrans* (nutmeg).

Achenbach, H. *et al., Phytochemistry*, 1987, **26**, 1159-1166 (*isol*)
Shin, K.H. *et al., Arch. Pharmacal Res.*, 1988, **11**, 240-243 (*isol*)
Benevides, P.J.C. *et al., Phytochemistry*, 1999, **52**, 339-343 (*isol, uv, ir, cd, pmr, cmr, ms*)

2-(2,4-Dihydroxyphenyl)-5,6-dihydroxybenzofuran D-617



$C_{14}H_{10}O_5$ 258.23

6-Me ether:2-(2,4-Dihydroxyphenyl)-5-hydroxy-6-methoxybenzofuran. ***Ebenfuran I***
$C_{15}H_{12}O_5$ 272.257
Yellow solid. λ_{max} 211 (log ϵ 4.55); 231 (sh) (log ϵ 4.27); 243 (sh) (log ϵ 4.03); 274 (log ϵ 4.17); 283 (sh) (log ϵ 4.18); 312 (sh) (log ϵ 4.2); 326 (log ϵ 4.45); 341 (log ϵ 4.45) (EtOH).

4′,6-Di-Me ether: [90664-32-7] *2-(2-Hydroxy-4-methoxyphenyl)-5-hydroxy-6-methoxybenzofuran.* ***Sainfuran***
$C_{16}H_{14}O_5$ 286.284
Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 150-152°. λ_{max} 213 ; 275 ; 284 ; 291 ; 326 ; 342 (EtOH) (Berdy). λ_{max} 213 ; 257 ; 284 ; 346 (EtOH-NaOH) (Berdy).

5,6-Di-Me ether: [67492-33-5] *2-(2,4-Dihydroxyphenyl)-5,6-dimethoxybenzofuran*
$C_{16}H_{14}O_5$ 286.284
Isol. from trunkwood of *Myroxylon balsamum* (Tolu balsam). Mp 178-180°.

2′,4′,6-Tri-Me ether: [94190-37-1] *2-(3,4-Dimethoxyphenyl)-5-hydroxy-6-methoxybenzofuran.* ***Methylsainfuran***
$C_{17}H_{16}O_5$ 300.31
Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 147-148°. λ_{max} 211 ; 275 ; 284 ; 298 ; 326 ; 342 (EtOH) (Berdy). λ_{max} 211 ; 291 ; 317 ; 346 (EtOH-NaOH) (Berdy).

5,6-Methylene ether: See 2-(2,4-Dihydroxyphenyl)-5,6-methylenedioxybenzofuran in *The Combined Chemical Dictionary.*

5,6-Methylene, 4′-Me ether:2-(2-Hydroxy-4-methoxyphenyl)-5,6-methylenedioxybenzofuran
$C_{16}H_{12}O_5$ 284.268
Needles (MeOH). Mp 179-181°.

[67236-31-1]

Komatsu, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1274 (*isol, uv, pmr, struct*)
Braga de Oliviera, A. *et al., Phytochemistry*, 1978, **17**, 593 (*isol, ir, uv, pmr, ms, struct*)
Gottlieb, O.R. *et al., Phytochemistry*, 1978, **17**, 593 (*5,6-di-Me ether*)
Russell, G.B. *et al., Phytochemistry*, 1984, **23**, 1417 (*Sainfuran, Methylsainfuran*)
Burke, J.M. *et al., J. Chem. Res., Synop.*, 1987, 179 (*Sainfuran, synth*)
Halabalaki, M. *et al., J. Nat. Prod.*, 2000, **63**, 1672-1674 (*Ebenfuran I*)

2-(3,5-Dihydroxyphenyl)-5,6-dihydroxybenzofuran D-618

[156098-99-6]
2-(3,5-Dihydroxyphenyl)-5,6-benzofurandiol, 9CI. ***Alfafuran***

$C_{14}H_{10}O_5$ 258.23
Stress metab. of *Medicago sativa* (alfalfa). Pale yellow solid.

5-Me ether, 3′-O-β-D-glucopyranoside: ***Schoenoside***
$C_{21}H_{22}O_{10}$ 434.399
Amorph. powder. $[\alpha]_D^{21}$ -84.2 (c, 0.48 in MeOH).

6-Me ether: [73338-89-3] *2-(3,5-Dihydroxyphenyl)-5-hydroxy-6-methoxybenzofuran.* ***Moracin J***
$C_{15}H_{12}O_5$ 272.257
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. λ_{max} 218 ; 294 ; 325 (MeOH) (Berdy).

5,6-Di-Me ether: [73338-85-9] *2-(3,5-Dihydroxyphenyl)-5,6-dimethoxybenzofuran.* ***Moracin F***
$C_{16}H_{14}O_5$ 286.284
From *Morus alba* (white mulberry) infected by *Fusarium solani*. λ_{max} 217 ; 282 ; 291 ; 321 ; 334 (MeOH) (Berdy).

3′,5-Di-Me ether: ***2-(3-Hydroxy-5-methoxyphenyl)-5-methoxy-6-benzofuranol****. 6-Hydroxy-2-(3-hydroxy-5-methoxyphenyl)-5-methoxybenzofuran*
$C_{16}H_{14}O_5$ 286.284
Brown paste (EtOAc). Mp 82-85°. λ_{max} 216 (log ϵ 3.45); 285 (log ϵ 3.74); 293 (log ϵ 4.04); 324 (log ϵ 4.21) (MeOH).

3′,6-Di-Me ether: [67259-16-9] *2-(3-Hydroxy-5-methoxyphenyl)-6-methoxy-5-benzofuranol.* ***Moracin B***
$C_{16}H_{14}O_5$ 286.284
Phytoalexin from diseased *Morus alba* (mulberry). Mp 184-185°. λ_{max} 218 (ϵ 29300); 285 (ϵ 12400); 294 (ϵ 13900); 325 (ϵ 27300) (EtOH) (Berdy).

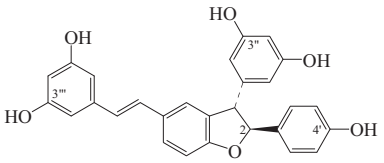
3′,6-Di-Me ether, di-Ac:
Mp 82-84°.

Tetra-Me ether:
Mp 104-105°.

Takasugi, M. *et al., Tet. Lett.*, 1978, 797; 1979, 4675 (*Moracins*)
Binh, V. *et al., Annalen*, 1984, 734 (*synth*)
Burke, J.M. *et al., J. Chem. Res., Synop.*, 1985, 34 (*synth*)
Noguchi, A. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 2312 (*isol*)
Kanchanapoom, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 863-865 (*Schoenoside*)
Wanjala, C.C.W. *et al., Planta Med.*, 2002, **68**, 640-642 (*3′,5-Di-Me ether*)

3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran D-619

Resveratrol dehydrodimer



(2*S*,3*R*)-(*E*)-*form*

$C_{28}H_{22}O_6$ 454.478

(2*S*,3*R*)-(*E*)-*form* [204076-78-8]
Isol. from *Vitis vinifera* (wine grape). Oil. $[\alpha]_D$ -1.7 (c, 0.2 in MeOH). λ_{max} 308 (MeOH).

(2*S*,3*R*)-(*Z*)-*form* [204076-79-9]
λ_{max} 281 (MeOH).

(2*S*,3*S*)-(*E*)-*form*

3″-O-β-D-Glucopyranoside: [328090-92-2]
$C_{34}H_{32}O_{11}$ 616.62
Constit. of the cell cultures of *Vitis vinifera* (wine grape). Powder. $[\alpha]_D^{20}$ -18.9 (c, 0.38 in MeOH). λ_{max} 204 (log ε 4.73); 221 (log ε 4.58); 309 (log ε 4.43); 320 (log ε 4.39) (MeOH).

3‴-O-β-D-Glucopyranoside: [328090-94-4]
$C_{34}H_{32}O_{11}$ 616.62
Constit. of the cell cultures of *Vitis vinifera* (wine grape). Powder. $[\alpha]_D^{20}$ -12 (c, 0.05 in MeOH). λ_{max} 206 (log ε 4.88); 309 (log ε 4.23); 322 (log ε 4.21) (MeOH).

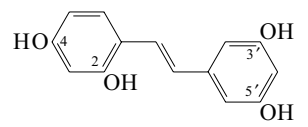
(2*R*,3*R*)-(*Z*)-*form*
Maximol B
Amorph. brown powder. $[\alpha]_D^{25}$ +99.4 (c, 0.34 in MeOH). λ_{max} 205 (log ε 4.9); 298 (log ε 4.5) (MeOH).

(2*R*,3*S*)-(*E*)-*form*
Maximol A
Amorph. brown powder. $[\alpha]_D^{25}$ -16.3 (c, 0.75 in MeOH). λ_{max} 211 (log ε 4.8); 310 (log ε 4.6) (MeOH).

Breuil, A.-C. *et al., Tet. Lett.*, 1998, **39**, 537-540 (*isol, pmr, cmr*)
Cichewicz, R.H. *et al., J. Nat. Prod.*, 2000, **63**, 29-33 (*isol, pmr*)
Waffo-Teguo, P. *et al., J. Nat. Prod.*, 2001, **64**, 136-138 (*glucosides, isol*)
Shikishima, Y. *et al., Phytochemistry*, 2001, **56**, 377-381 (*Maximols*)

1-(2,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene D-620

[4721-07-7]
4-[2-(3,5-Dihydroxyphenyl)ethenyl]-1,3-benzenediol, 9CI. 2,3′,4,5′-Stilbenetetrol, 8CI. 2,3′,4,5′-Tetrahydroxystilbene. ***Oxyresveratrol****. Cudranin*



$C_{14}H_{12}O_4$ 244.246
λ_{max} 218 (ε 25000); 301 (ε 19700); 330 (ε 27100) (EtOH) (Berdy).

(*E*)-*form* [29700-22-9]
Mp 205°.

2-O-β-D-Glucopyranoside:
$C_{20}H_{22}O_9$ 406.388
Amorph. powder. $[\alpha]_D^{21}$ -59.1 (c, 2.1 in MeOH).

3′-O-β-D-Glucopyranoside: [144525-40-6]
$C_{20}H_{22}O_9$ 406.388
Isol. from *Morus alba* (white mulberry). Powder (H_2O). Mp 155-157°. $[\alpha]_D^{22}$ -5.5 (c, 0.3 in MeOH).

3′,4-Di-O-β-D-glucopyranoside: [102841-42-9] ***Mulberroside A***
$C_{26}H_{32}O_{14}$ 568.53
Amorph. powder. $[\alpha]_D^{25}$ -78 (c, 0.88 in MeOH).

Tetra-Ac:
Mp 142°.

Tetra-Me ether:
Mp 84°.

(*Z*)-*form*

3′,4-Di-O-β-D-glucopyranoside: [166734-06-1] **cis-*Mulberroside A***
$C_{26}H_{32}O_{14}$ 568.53
Constit. of *Morus alba* (white mulberry).

Barnes, R.A. *et al., J.A.C.S.*, 1955, **77**, 3259 (*isol*)
Mongolsuk, S. *et al., J.C.S.*, 1957, 2231 (*isol*)
Reimann, E. *et al., Annalen*, 1971, **750**, 109 (*synth*)
Takasugi, M. *et al., Chem. Lett.*, 1978, 1241 (*isol, deriv*)
Hirakura, K. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1088 (*cmr, deriv*)
Hirakura, K. *et al., J. Nat. Prod.*, 1986, **49**, 218 (*deriv*)
Hanawa, F. *et al., Phytochemistry*, 1992, **31**, 3005 (*3-glucoside*)
Qiu, F. *et al., Planta Med.*, 1996, **62**, 559 (*glucosides*)
Kanchanapoom, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 863-865 (*cmr, 2-glucoside*)

1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene D-621

[4339-71-3]
4-[2-(3,5-Dihydroxyphenyl)ethenyl]-1,2-benzenediol, 9CI. 3,3′,4,5′-Stilbenetetrol, 8CI. 3,3′,4,5′-Tetrahydroxystilbene. ***Piceatannol****. Astringenin. NSC 365798*

$C_{14}H_{12}O_4$ 244.246

(*E*)-*form* [10083-24-6]
Needles (EtOAc/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 231-232° (216°). λ_{max} 221 ; 240 (sh) ; 306 ; 326 (ε 27600) (EtOH).
► LD_{50} (mus, ipr) 217 mg/kg.

4′-O-β-D-Glucopyranoside: [116181-54-5]
$C_{20}H_{22}O_9$ 406.388
Isol. from Chinese rhubarb (*Rheum* sp.). Amorph. powder + $1^1/_2H_2O$. $[\alpha]_D^{22}$ -35.8 (c, 0.84 in Me_2CO).

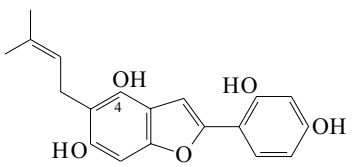
4′-O-[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]: [116107-19-8]
$C_{27}H_{26}O_{13}$ 558.495
Isol. from Chinese rhubarb (*Rheum* sp.). Off-white powder + $1^1/_2H_2O$. $[\alpha]_D^{22}$ -73.2 (c, 0.7 in Me_2CO).

3″,4′-Di-O-β-D-glucopyranoside: [282736-93-0] *Piceatannol 3,4′-diglucoside*
$C_{26}H_{32}O_{14}$ 568.53
Constit. of *Rheum undulatum* (rhubarb).

4′-Me ether: [500-65-2] *1-(3,5-Dihydroxyphenyl)-2-(3-hydroxy-4-methoxyphenyl)ethylene. 3,3′,5-Trihydroxy-4′-methoxystilbene.* ***Rhapontigenin****. Pontigenin*
$C_{15}H_{14}O_4$ 258.273
Isol. from rhizomes of *Rheum undulatum* (rhubarb). Mp 186-187°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1161A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 405A (*nmr*)
Grassman, W. *et al., J.C.S.*, 1965, 4579 (*isol, struct*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1545-1549 (*4′-glucosides*)
Ko, S.K. *et al., Arch. Pharmacal Res.*, 2000, **23**, 159-162 (*3″,4′-diglucoside*)

2-(3,4-Dihydroxyphenyl)-4,6-dihydroxy-5-prenylbenzofuran D-622



$C_{19}H_{18}O_5$ 326.348

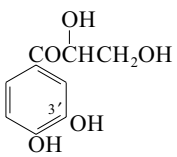
4-Me ether: [118524-14-4] *2-(3,4-Dihydroxyphenyl)-6-hydroxy-4-methoxy-5-prenylbenzofuran. 4-[6-Hydroxy-4-methoxy-5-(3-methyl-2-butenyl)-2-benzofuranyl]-1,3-benzenediol, 9CI.* ***Licocoumarone***
$C_{20}H_{20}O_5$ 340.375
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice). Needles (EtOH aq.). Mp 183-185°.

4,6-Di-Me ether: [126716-36-7] *2-(3,4-Dihydroxyphenyl)-4,6-dimethoxy-5-prenylbenzofuran. 4-[4,6-Dimethoxy-5-(3-methyl-2-butenyl)-2-benzofuranyl]-1,3-benzenediol, 9CI.* ***Gancaonin I***
$C_{21}H_{22}O_5$ 354.402
Isol. from *Glycyrrhiza uralensis* (Chinese licorice) and other *Glycyrrhiza* spp.. Prisms + $1H_2O$ ($CHCl_3$/petrol). Mp 67-70° Mp 125-127° (Double Mp).

Demizu, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3474 (*Licocoumarone*)
Fukai, T. *et al., Heterocycles*, 1989, **29**, 1761 (*Gancaonin I*)
Hwang, J.O. *et al., Nat. Prod. Sci.*, 1998, **4**, 130-135; *CA*, **130**, 63528b (*activity*)

1-(3,4-Dihydroxyphenyl)-2,3-dihydroxy-1-propanone D-623

2,3,3′,4′-Tetrahydroxypropiophenone



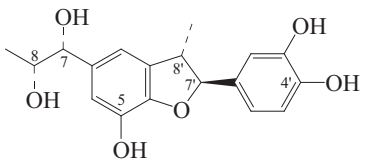
$C_9H_{10}O_5$ 198.175

3′-Me ether: [168293-10-5] *2,3-Dihydroxy-*

1-(4-hydroxy-3-methoxyphenyl)-1-propanone. 2,3,4′-Trihydroxy-3′-methoxypropiophenone. C-Veratroylglycol
$C_{10}H_{12}O_5$ 212.202
Constit. of Riesling wine. Gum. λ_{max} 207 ; 231 ; 279 ; 306 (MeOH).

Kijjoa, A. *et al., Phytochemistry*, 1995, **40**, 191-193 (*isol, pmr*)
Jones, L. *et al., Fitoterapia*, 2000, **71**, 580-583 (*isol, pmr, cmr*)
Baderschneider, B. *et al., J. Agric. Food Chem.*, 2001, **49**, 2788-2798 (*isol, pmr, cmr*)

2-(3,4-Dihydroxyphenyl)-5-(1,2-dihydroxypropyl)-2,3-dihydro-6-hydroxy-3-methylbenzofuran D-624



(7*R*,7'*S*,8*R*,8'*S*)-*form*

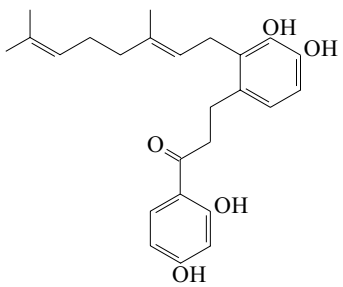
$C_{18}H_{20}O_6$ 332.352
Lignan numbering shown.

(7ξ,7′*R*,8ξ,8′*R*)-*form*
3′,5,7-Tri-Me ether: [114394-19-3] ***Fragransol A***
$C_{21}H_{26}O_6$ 374.433
Constit. of *Myristica fragrans* (nutmeg). Oil.

Hada, S. *et al., Phytochemistry*, 1988, **27**, 563-568 (*Fragransols*)
Juhasz, L. *et al., J. Nat. Prod.*, 2000, **63**, 866-870 (*Fragransol A, synth, pmr, cmr*)

1-(2,4-Dihydroxyphenyl)-3-[2-(3,7-dimethyl-2,6-octadienyl)-3,4-dihydroxyphenyl]-1-propanone, 9CI D-625

[118026-33-8]



$C_{25}H_{30}O_5$ 410.509

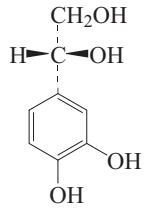
(*E*)-*form* [113866-89-0]
2-Geranyl-2′,3,4,4′-tetrahydroxydihydrochalcone. AC-5-1
Constit. of *Artocarpus communis* (breadfruit). Powder. Mp 132-136°.

Nakano, J. *et al., Heterocycles*, 1989, **29**, 427-430 (*synth*)
McLean, S. *et al., Magn. Reson. Chem.*, 1996, **34**, 719-722 (*isol, pmr, cmr*)

1-(3,4-Dihydroxyphenyl)-1,2-ethanediol, 8CI D-626

[3343-19-9]

4-(1,2-Dihydroxyethyl)-1,2-benzenediol, 9CI. 3,4-Dihydroxyphenylglycol



(*R*)-*form*

$C_8H_{10}O_4$ 170.165

(*R*)-*form* [109835-90-7]
4′-Me ether: [213466-88-7] *1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol*
$C_9H_{12}O_4$ 184.191
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder (nat.); cryst. (synthetic). Mp 97-98° (synthetic). $[\alpha]_D^{23}$ -22.5 (c, 0.2 in MeOH) (natural). $[\alpha]_D$ -34.2 (c, 0.54 in MeOH) (synthetic).
*4′-Me ether, 3′-*O*-β-D-glucopyranoside:* [217972-13-9]
$C_{15}H_{22}O_9$ 346.333
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder. $[\alpha]_D^{23}$ -52 (c, 0.3 in MeOH).
*3′,4′-Di-Me ether, 1-*O*-β-D-glucopyranoside:* [251905-98-3]
$C_{16}H_{24}O_9$ 360.36
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder. $[\alpha]_D^{24}$ -87 (c, 0.1 in MeOH).
*3′,4′-Di-Me ether, 2-*O*-β-D-glucopyranoside:* [251913-30-1]
$C_{16}H_{24}O_9$ 360.36
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder. $[\alpha]_D^{24}$ -45 (c, 0.1 in MeOH).

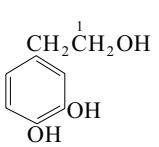
(ξ)-*form*
Constit. of the fruit of *Olea europeae* (olives).

[55254-51-8, 64998-12-5, 64998-13-6]

Benigni, J.D. *et al., J. Med. Chem.*, 1963, **6**, 607 (*synth*)
Bianchi, G. *et al., Phytochemistry*, 1994, **35**, 1335 (*isol*)
De Tommasi, N. *et al., Phytochemistry*, 1996, **42**, 163 (*β-Hydroxy-3′,4′-dimethoxyphenylethyl glucoside*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1587-1590; 1999, **47**, 1448-1450 (*isol, 4′-Me derivs, 3′,4′-di-Me glucosides*)
Fisher, A.J. *et al., Synth. Commun.*, 1998, **28**, 2959-2968 (*4′-Me ether*)

2-(3,4-Dihydroxyphenyl)ethanol D-627

[10597-60-1]
4-(2-Hydroxyethyl)-1,2-benzenediol, 9CI. 3,4-Dihydroxyphenethyl alcohol, 8CI. 3,4-Dihydroxybenzeneethanol. Hydroxytyrosol



$C_8H_{10}O_3$ 154.165

Indicator of maturity in olives which increases as the fruit ripens. Oil. $Bp_{0.02}$ 170-175° part. dec.. Previously incorrectly descr. as cryst., Mp 81-83°.

*1-*O*-β-D-Glucopyranoside:* [76873-99-9]

[123078-38-6, 147731-98-4] *3,4-Dihydroxyphenethyl glucoside*
$C_{14}H_{20}O_8$ 316.307
Constit. of *Prunus* sp.. Pale yellow powder. Mp 40.5-42° (as hexa-Ac). $[\alpha]_D^{15}$ -23.8 (c, 1 in MeOH). $[\alpha]_D^{20}$ -12.3 (c, 7.1 in $CHCl_3$) (hexa-Ac).

*1-*O*-[α-L-Rhamnopyranosyl-(1→3)-β-D-glucopyranoside]:* [61548-34-3] ***Verbasoside***. *Dicaffeoylacteoside*
$C_{20}H_{30}O_{12}$ 462.45
Isol. from *Stachys sieboldii* (Chinese artichoke). Powder. $[\alpha]_D^{24}$ -49.3 (c, 0.34 in MeOH).

*1-*O*-[α-L-Rhamnopyranosyl-(1→3)-[3,4-dihydroxy-*E*-cinnamoyl-(→4)]-β-D-glucopyranoside]:* [61276-17-3] ***Acteoside***. *Verbascoside. Kusaginin*
$C_{29}H_{36}O_{15}$ 624.594
The main hydroxycinnamic deriv. in olives. Yellow powder. $[\alpha]_D^{20}$ -84.9 (c, 1.15 in MeOH).

*1-*O*-[α-L-Arabinopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→3)-[4-hydroxy-3-methoxy-*E*-cinnamoyl-(→4)]-β-D-glucopyranoside]:* [140147-66-6] ***Leonoside A***. *Stachyoside C. Stachyoside B*
$C_{35}H_{46}O_{19}$ 770.737
Constit. of *Stachys sieboldii* (Chinese artichoke). Amorph. $[\alpha]_D^{26}$ -49.3 (c, 1.05 in MeOH). Application of names Stachyoside C and Stachyoside B is confused. See 1991 paper for clarification.

*1-*O*-[α-L-Arabinopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→3)-[3,4-dihydroxy-*E*-cinnamoyl-(→4)]-β-D-glucopyranoside]:* [117895-00-8] ***Lavandulifolioside***. *Stachyoside A*
$C_{34}H_{44}O_{19}$ 756.71
Constit. of *Stachys sieboldii* (Chinese artichoke). Amorph. $[\alpha]_D^{20}$ -40.3 (c, 0.6 in H_2O).

*4′-Me ether, 1-*O*-[α-L-arabinopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→3)-[4-hydroxy-3-methoxy-*E*-cinnamoyl-(→4)]-β-D-glucopyranoside]:* [140147-67-7]

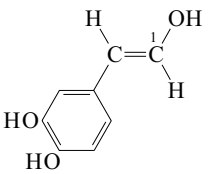
[135010-56-9] ***Leonoside B***. *Stachyoside D*†. *Stachyoside C*†
$C_{36}H_{48}O_{19}$ 784.764
Isol. from tubers of *Stachys sieboldii* (Chinese artichoke). Amorph. $[\alpha]_D^{26}$ -42 (c, 0.52 in MeOH). In some lit. erroneously referred to as Stachyoside C.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1169C; 1169D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 412A; 412B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1087B; 1087C (*ir*)
Kudo, K. *et al., Planta Med.*, 1980, **40**, 250 (*1-glucoside*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2732 (*Acteoside*)
Andary, C. *et al., Phytochemistry*, 1982, **21**, 1123; 1985, **24**, 362 (*Acteoside, Poliumoside*)

Baraldi, P.G. *et al., Annalen*, 1983, 684 (*synth, ir, pmr, bibl*)
Karasawa, H. *et al., Yakugaku Zasshi*, 1986, **106**, 562; 721 (*Verbasoside, Cistanoside H*)
Basaran, A.A. *et al., Helv. Chim. Acta*, 1988, **71**, 1483; 1989, **72**, 631 (*Lavandulifolioside*)
Bianco, A. *et al., Synth. Commun.*, 1988, **15**, 1765 (*synth*)
Calis, I. *et al., Phytochemistry*, 1990, **29**, 1253-1257; 1992, **31**, 357-359 (*Phlinosides, Leonosides*)
Nishimura, H. *et al., Phytochemistry*, 1990, **29**, 3303; 1991, **30**, 965 (*Verbasoside*)
Miyase, T. *et al., Yakugaku Zasshi*, 1990, **110**, 652; 932 (*Stachyosides*)
Nishimura, H. *et al., Phytochemistry*, 1991, **30**, 965 (*Stachyosides*)
Esti, M. *et al., J. Agric. Food Chem.*, 1998, **46**, 32-35 (*occur*)
Benkrief, R. *et al., Phytochemistry*, 1998, **47**, 825-832 (*Acteoside 6-cinnamate, Acteoside*)
Park, H.-J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1029-1031 (*1-glucoside*)
Duynstee, H.I. *et al., Eur. J. Org. Chem.*, 1999, 2623-2632 (*synth, pmr, cmr*)
Hara, R. *et al., J.A.C.S.*, 1999, **121**, 3072-3082 (*synth, derivs*)

2-(3,4-Dihydroxyphenyl)ethenol D-628

2-(3,4-Dihydroxyphenyl)vinyl alcohol. 3,4-Dihydroxystyryl alcohol



(*E*)-*form*

$C_8H_8O_3$ 152.149

Enol-form of 3,4-Dihydroxyphenylacetaldehyde.

(*E*)-*form*

1-O-*3,4-Dihydroxycinnamoyl(*E-*):* [99816-39-4]
$C_{17}H_{14}O_6$ 314.294
Isol. from the callus cultures of *Lavandula angustifolia* (lavender). Oil.

(*Z*)-*form*

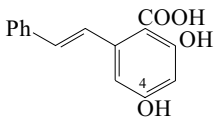
1-O-*3,4-Dihydroxycinnamoyl(*E-*):* [55486-06-1]
Isol. from *Perilla frutescens* (perilla) and the callus cultures of *Lavandula angustifolia* (lavender). Yellow cryst. Mp 183-185° (dec.). λ_{max} 213 (ϵ 20900); 250 (ϵ 15900); 340 (ϵ 19100) (EtOH) (Berdy).

[157961-35-8, 157961-40-5, 158080-70-7]

Banthorpe, D.V. *et al., Phytochemistry*, 1985, **24**, 2677-2680 (*caffeoyl derivs*)
Nakanishi, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1772-1774 (*caffeoyl derivs*)

2,4-Dihydroxy-6-(2-phenylethenyl)benzoic acid, 9CI D-629

2,4-Dihydroxy-6-styrylbenzoic acid. 3,5-Dihydroxy-2-stilbenecarboxylic acid. ***Pinosylvic acid***



$C_{15}H_{12}O_4$ 256.257

(*E*)-*form* [38232-09-6]
Mp 162-165°.

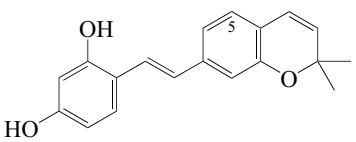
4-O-*β*-D-*Glucopyranoside:* [38232-08-5] ***Gaylussacin***
$C_{21}H_{22}O_9$ 418.399
Constit. of the leaves of *Gaylussacia baccata* (black huckleberry) and *Gaylussacia frondosa* (dangleberry). Mp 235-236°. $[\alpha]_D^{22}$ -95.8 (MeOH/Py).

4-Me ether: [149697-30-3] *2-Hydroxy-4-methoxy-6-styrylbenzoic acid.* ***4-O-Methylpinosylvic acid***
$C_{16}H_{14}O_4$ 270.284
Constit. of the leaves of *Cajanus cajan* (pigeon pea).

Askari, A. *et al., J. Nat. Prod.*, 1972, **35**, 49 (*synth, Gaylussacin*)
Miyaichi, Y. *et al., CA*, 1989, **110**, 141364y (*isol*)
Ohwaki, Y. *et al., CA*, 1993, **119**, 135604 (*deriv*)

7-[2-(2,4-Dihydroxyphenyl)ethenyl]-2,2-dimethyl-2*H*-1-benzopyran D-630

*7-(2,4-Dihydroxystyryl)-2,2-dimethyl-2*H*-1-benzopyran*



$C_{19}H_{18}O_3$ 294.349

(*E*)-*form*

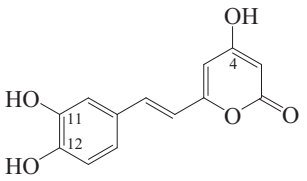
Di-Me ether: [106009-66-9] *7-[2-(2,4-Dimethoxyphenyl)ethenyl]-2,2-dimethyl-2*H*-1-benzopyran*
$C_{21}H_{22}O_3$ 322.403
Needles (EtOH). Mp 108°.

5-Hydroxy: [194144-02-0] *7-(2,4-Dihydroxystyryl)-5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran.* ***Artocarbene***
$C_{19}H_{18}O_4$ 310.349
Constit. of *Artocarpus incisus* (breadfruit). Yellow powder.

Garcia, M. *et al., Phytochemistry*, 1986, **25**, 2425 (*isol*)
Shimizu, K. *et al., Phytochemistry*, 1997, **45**, 1297-1298 (*Artocarbene*)

6-[2-(3,4-Dihydroxyphenyl)ethenyl]-4-hydroxy-2*H*-pyran-2-one, 9CI D-631

[555-55-5]
6-(3,4-Dihydroxystyryl)-4-hydroxy-α-pyrone. Hispidin†



$C_{13}H_{10}O_5$ 246.219

(*E*)-*form*

Yellow needles (EtOH aq.). Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. acids, H_2O, hexane. Mp 259°. λ_{max} 223 ; 248 ; 367 (MeOH) (Berdy). λ_{max} 206 (ϵ 30200); 223 (ϵ 31620); 253 (ϵ 13800); 366 (ϵ 17380) (EtOH) (Berdy). λ_{max} 257 (ϵ 19050); 373 (ϵ 11750) (EtOH/NaOH) (Berdy).

4,11-Di-Me ether: [77900-31-3] *6-[2-(4-Hydroxy-3-methoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one. 6-(4-Hydroxy-3-methoxystyryl)-4-methoxy-2-pyrone.* ***11-Methoxynoryangonin***
$C_{15}H_{14}O_5$ 274.273
Isol. from a *Piper* sp. from New Guinea. Yellow cryst. (EtOH aq.). Mp 218-219°.

4,12-Di-Me ether: [77900-30-2] ***11-Hydroxyyangonin***
$C_{15}H_{14}O_5$ 274.273
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002).

Tri-Me ether: [2743-14-8]

[56070-89-4] *6-[2-(3,4-Dimethoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one. 6-(3,4-Dimethoxystyryl)-4-methoxy-2-pyrone.* ***11-Methoxyyangonin***
$C_{16}H_{16}O_5$ 288.299
Isol. from *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Yellow needles (EtOH). Mp 166-167° (162-164°).

5,6-Dihydro, tri-Me ether: ***5,6-Dihydro-11-methoxyyangonin***
$C_{16}H_{18}O_5$ 290.315
Isol. from *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Yellow semisolid. $[\alpha]_D^{25}$ +70 (c, 0.02 in $CHCl_3$). λ_{max} 228 (log ϵ 4.04); 266 (log ϵ 3.87) (MeOH).

*5,6*S*,7,8-Tetrahydro, 4,12-di-Me ether:* [38146-59-7] *4-Methoxy-6-[2-(3-hydroxy-4-methoxyphenyl)ethyl]-5,6-dihydro-2*H*-pyran-2-one.* ***11-Hydroxy-12-methoxydihydrokawain***
$C_{15}H_{18}O_5$ 278.304
Constit. of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Cryst. (MeOH). Mp 165-167°. $[\alpha]_D^{20}$ +35 (c, 0.2 in $CHCl_3$).

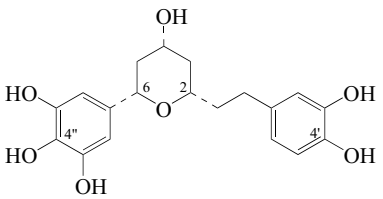
*5,6*S*,7,8-Tetrahydro, tri-Me ether:* [38146-60-0] *6-[(3,4-Dimethoxyphenyl)ethyl]-5,6-dihydro-4-methoxy-2*H*-pyran-2-one.* ***11,12-Dimethoxydihydrokawain****. 5,6,7,8-Tetrahydro-11-methoxyyangonin. 7,8-Dihydro-11,12-dimethoxykawain*
$C_{16}H_{20}O_5$ 292.331
Constit. of *Piper methysticum* (kava).

FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Needles (Et_2O); plates (C_6H_6). Mp 124-125° (121-123°). $[\alpha]_D^{20}$ +32 (c, 0.32 in $CHCl_3$) (+27.7).

Edwards, R.L. *et al., J.C.S.*, 1961, 4995; 5003 (*Hispidin, isol, struct, synth*)
Bu'Lock, J.D. *et al., J.A.C.S.*, 1962, 2085 (*Hispidin, isol*)
Ueno, A. *et al., Chem. Pharm. Bull.*, 1964, **112**, 376 (*Hispidin, isol*)
Haensel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1966, **299**, 503; 507 (*11-Hydroxyyangonin, 11-Methoxynoryangonin, 11-Methoxyyangonin*)
Adam, W. *et al., Synthesis*, 1994, 1133 (*Hispidin, synth*)

2-[2-(3,4-Dihydroxypheny- D-632 l)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol

7-(3,4-Dihydroxyphenyl)-1,5-epoxy-3-hydroxy-1-(3,4,5-trihydroxyphenyl)heptane



(2*S*,4*R*,6*S*)-*form*

$C_{19}H_{22}O_7$ 362.379

(2*S*,4*R*,6*S*)-*form*

3′,3″-Di-Me ether: [182227-93-6]
$C_{21}H_{26}O_7$ 390.432
Constit. of *Zingiber officinale* (ginger). Amorph. $[\alpha]_D^{25}$ -61.6 (c, 1 in EtOH). λ_{max} 226 (sh) (log ϵ 4.2); 280 (log ϵ 3.65) (EtOH).

3′,3″-Di-Me ether, 4-Ac: [182227-92-5]
$C_{23}H_{28}O_8$ 432.469
Constit. of *Zingiber officinale* (ginger). Oil. $[\alpha]_D^{25}$ -31.2 (c, 1.3 in EtOH). λ_{max} 226 (sh) (log ϵ 4.32); 280 (log ϵ 3.75) (EtOH).

3′,3″,5″-Tri-Me ether: [182227-94-7]
$C_{22}H_{28}O_7$ 404.459
Constit. of *Zingiber officinale* (ginger). $[\alpha]_D^{25}$ -48.6 (c, 0.6 in EtOH). λ_{max} 226 (sh) (log ϵ 4.09); 280 (log ϵ 3.59) (EtOH).

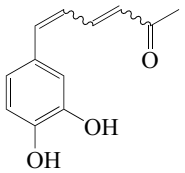
(2*S*,4*S*,6*S*)-*form*

3′,3″-Di-Me ether: [182369-54-6]
$C_{21}H_{26}O_7$ 390.432
Constit. of *Zingiber officinale* (ginger). Oil. $[\alpha]_D^{25}$ -41.6 (c, 0.9 in EtOH). λ_{max} 225 (sh) (log ϵ 4.03); 280 (log ϵ 3.51) (EtOH).

3′,3″-Di-Me ether, 4-Ac: [182369-53-5]
$C_{23}H_{28}O_8$ 432.469
Constit. of *Zingiber officinale* (ginger). Oil. $[\alpha]_D^{25}$ -23.3 (c, 0.5 in EtOH). λ_{max} 226 (sh) (log ϵ 4.33); 280 (log ϵ 3.76) (EtOH).

Kikuzaki, H. *et al., Phytochemistry*, 1996, **43**, 273-277 (*isol, uv, ir, pmr, cmr, ms*)

6-(3,4-Dihydroxyphenyl)-3,5- D-633 hexadien-2-one



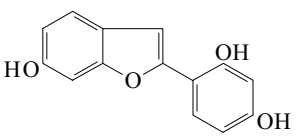
$C_{12}H_{12}O_3$ 204.225

Methylene ether: [17172-93-9] *6-(3,4-Methylenedioxyphenyl)-3,5-hexadien-2-one, 8CI. 3,4-Methylenedioxycinnamylideneacetone*
$C_{13}H_{12}O_3$ 216.236
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Mp 89°.

Jossang, P. *et al., J. Chromatogr.*, 1967, **31**, 375-383 (*isol*)

2-(2,4-Dihydroxyphenyl)-6-hy- D-634 droxybenzofuran

[67736-22-5]
4-(6-Hydroxy-2-benzofuranyl)-1,3-benzenediol, 9CI



$C_{14}H_{10}O_4$ 242.231
Brownish needles. Mp 207-208°.

Tri-Ac:
Mp 154-156°.

2′-Me ether: [74048-90-1] *6-Hydroxy-2-(4-hydroxy-2-methoxyphenyl)benzofuran.* ***6-O-Demethylvignafuran***
$C_{15}H_{12}O_4$ 256.257
λ_{max} 212 ; 282 ; 321 ; 337 (EtOH) (Berdy). λ_{max} 217 ; 299 ; 343 ; 359 (EtOH/NaOH) (Berdy).

4′-Me ether: [67685-33-0] *6-Hydroxy-2-(2-hydroxy-4-methoxyphenyl)benzofuran.* ***Centrolobofuran***
$C_{15}H_{12}O_4$ 256.257
Glistening needles (C_6H_6). Mp 165-166°.

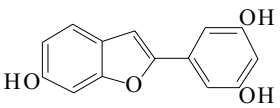
2′,6-Di-Me ether: [57800-41-6] *2-(4-Hydroxy-2-methoxyphenyl)-6-methoxybenzofuran.* ***Vignafuran***
$C_{16}H_{14}O_4$ 270.284
Constit. of *Lablab niger* (hyacinth bean). Glass. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 210 (ϵ 30200); 282 (ϵ 14800); 320 (ϵ 39000); 335 (ϵ 33200) (EtOH) (Berdy). λ_{max} 336 ; 347 (EtOH/NaOH) (Berdy).

2′,6-Di-Me ether, Ac: [57800-42-7]
Needles (MeOH). Mp 94-94.5°.

Preston, N.W. *et al., Phytochemistry*, 1975, **14**, 1843 (*isol, struct, uv, ms, pmr, synth, Vignafuran*)
Duffley, R.P. *et al., J.C.S. Perkin 1*, 1977, 802 (*synth, pmr, uv*)
Ingham, J.L. *et al., Phytochemistry*, 1978, **17**, 535; 1980, **19**, 289 (*Demethylvignafuran*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2205; 1984, **32**, 3267 (*isol, uv, ms*)
Jurd, L. *et al., Aust. J. Chem.*, 1984, **37**, 1127 (*Centrolobofuran*)
Watanabe, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 579 (*synth*)
Miyase, T. *et al., Phytochemistry*, 1999, **52**, 303-310 (*isol, cmr*)
Hiroya, K. *et al., J.C.S. Perkin 1*, 2000, 4339-4346 (*synth, Vignafuran*)

2-(3,5-Dihydroxyphenyl)-6-hy- D-635 droxybenzofuran

[56317-21-6]
*5-(6-Hydroxy-2-benzofuranyl)-1,3-benzenediol, 9CI. **Moracin M**. Veraphenol*



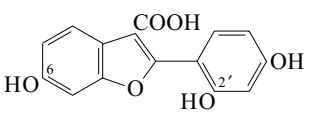
$C_{14}H_{10}O_4$ 242.231
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. Light pink cryst. Mp 275° (238-240°). λ_{max} 217 (ϵ 30200); 316 (ϵ 33400); 330 (ϵ 27900) (MeOH) (Berdy).

3′-O-β-D-Glucopyranoside: [152041-26-4]
$C_{20}H_{20}O_9$ 404.373
Pale yellow cryst. Mp 284°.

3′,6-Di-O-β-D-glucopyranoside: ***Mulberroside F***
$C_{26}H_{30}O_{14}$ 566.515
Constit. of the leaves of *Morus alba* (white mulberry). Yellowish powder. Mp 231-234°. $[\alpha]_D^{22}$ +75. λ_{max} 210 ; 271 (sh) ; 313 (MeOH).

Takasugi, M. *et al., CA*, 1980, **92**, 160540 (*isol, struct*)
Watanabe, M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 579 (*synth*)
Mann, I.S. *et al., Tetrahedron*, 1991, **47**, 7981; 7991 (*synth*)
Basnet, P. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1238-1243 (*isol*)
Zhou, C.X. *et al., Planta Med.*, 1999, **65**, 480-482 (*Veraphenol, pmr, cmr*)
Lee, S.H. *et al., Biol. Pharm. Bull.*, 2002, **25**, 1045-1048 (*Mulberroside F*)

2-(2,4-Dihydroxyphenyl)-6-hy- D-636 droxy-3-benzofurancarboxylic acid



$C_{15}H_{10}O_6$ 286.24

2′,6-Di-Me ether, Me ester: [151228-01-2]
$C_{18}H_{16}O_6$ 328.321
Isol. from the root exudates of iron-deficient *Medicago sativa* (alfalfa).

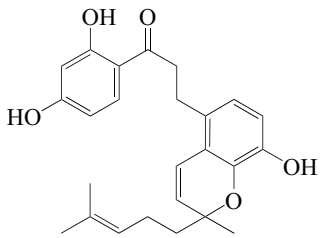
Aldehyde, 4′,6-di-Me ether:2-(2-Hydroxy-4-methoxyphenyl)-6-methoxy-3-benzofurancarboxaldehyde. ***Melimessanol C***
$C_{17}H_{14}O_5$ 298.295
Amorph. solid. λ_{max} 241 ; 344 (MeOH).

Koshino, H. *et al., Phytochemistry*, 1993, **33**, 1075 (*isol, deriv*)

Macias, F.A. *et al., Phytochemistry*, 1999, **50**, 35-46 (*Melimessanol C*)
Hiroya, K. *et al., J.C.S. Perkin 1*, 2000, 4339-4346 (*synth*)

1-(2,4-Dihydroxyphenyl)-3-[8-hydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-5-yl]-1-propanone, 9CI D-637

[116207-29-5]

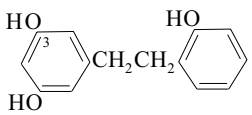


$C_{25}H_{28}O_5$ 408.493
Constit. of *Artocarpus communis* (breadfruit).

Koshihara, Y. *et al., Biochem. Pharmacol.*, 1988, **37**, 2161-2165 (*isol, props*)
McLean, S. *et al., Magn. Reson. Chem.*, 1996, **34**, 719-722 (*isol, pmr, cmr*)

1-(3,5-Dihydroxyphenyl)-2-(2-hydroxyphenyl)ethane D-638

[113276-63-4]
5-[2-(2-Hydroxyphenyl)ethyl]-1,3-benzenediol. 2′,3,5-Trihydroxybibenzyl. ***Demethylbatatasin IV***



$C_{14}H_{14}O_3$ 230.263
Isol. from *Dioscorea alata* (greater yam), *Dioscorea bulbifera* (air potato) and *Dioscorea rotundata* (white guinea yam) infected with *Botryodiplodia theobromae*. λ_{max} 267 ; 272 (sh) ; 275 ; 282 (sh) (MeOH).

2′-Me ether:5-[2-(2-Methoxyphenyl)ethyl]-1,3-benzenediol. 1-(3,5-Dihydroxyphenyl)-2-(2-methoxyphenyl)ethane. 3,5-Dihydroxy-2′-methoxybibenzyl. ***Stilbostemin A***
$C_{15}H_{16}O_3$ 244.29
λ_{max} 214 (log ϵ 4.17); 224 (sh) (log ϵ 4.04); 274 (log ϵ 3.48); 278 (log ϵ 3.47) (MeOH).

3-Me ether: [60347-67-3] *1-(2-Hydroxyphenyl)-2-(3-hydroxy-5-methoxyphenyl)ethane. 3-[2-(2-Hydroxyphenyl)ethyl]-5-methoxyphenol, 9CI. 2,3′-Dihydroxy-5′-methoxybibenzyl.* ***Batatasin IV***
$C_{15}H_{16}O_3$ 244.29
Constit. of the bulbs of *Dioscorea batatus* (Chinese yam). Needles ($CHCl_3$/CCl_4). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 99.5-100.5°. λ_{max} 209 (ϵ 4000); 274 (ϵ 600) (EtOH) (Berdy).

Hashimoto, T. *et al., Phytochemistry*, 1978, **17**, 1179-1184 (*Batatasin IV, isol, synth*)
Fagboun, D.E. *et al., Phytochemistry*, 1987, **26**, 3187-3189 (*Batatasin IV, isol, cmr*)
Adensanya, S.A. *et al., Phytochemistry*, 1989, **28**, 773-774 (*isol*)
Pacher, T. *et al., J. Nat. Prod.*, 2002, **65**, 820-827 (*Stilbostemin A*)

1-(3,5-Dihydroxyphenyl)-2-(3-hydroxyphenyl)ethane D-639

3,3′,5-Trihydroxybibenzyl. 5-[2-(3-Hydroxyphenyl)ethyl]-1,3-benzenediol
$C_{14}H_{14}O_3$ 230.263

3-Me ether: [56684-87-8] *3-[2-(3-Hydroxyphenyl)ethyl]-5-methoxyphenol, 9CI. 3,3′-Dihydroxy-5-methoxybibenzyl.* ***Batatasin III***
$C_{15}H_{16}O_3$ 244.29
Constit. of *Dioscorea batatas* (Chinese yam). Rods ($CHCl_3$/CCl_4). Mp 93.5-94.5°.

3-Me ether, 5-O-β-D-glucopyranoside:
$C_{21}H_{26}O_8$ 406.432
Powder. λ_{max} 238 (log ϵ 4.07); 269 (log ϵ 4.04); 286 (log ϵ 3.88) (MeOH).

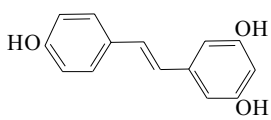
3,3′-Di-Me ether:3-Hydroxy-5-[2-(3-methoxyphenyl)ethyl]phenol. 1-(3-Hydroxy-5-methoxyphenyl)-2-(3-methoxyphenyl)ethane. ***3′-O-Methylbatatasin III***
$C_{16}H_{18}O_3$ 258.316
Viscous solid.

3,3′-Di-Me ether, 5-O-β-D-glucopyranoside:
$C_{22}H_{28}O_8$ 420.458
Needles (MeOH). Mp 154-155°. λ_{max} 225 (log ϵ 3.2); 272 (log ϵ 2.53); 280 (log ϵ 2.5) (MeOH).

Hasegawa, K. *et al., Planta*, 1972, **108**, 369 (*isol*)
Hasegawa, K. *et al., Phytochemistry*, 1974, **13**, 2849 (*synth*)
Sachdev, K. *et al., Phytochemistry*, 1986, **25**, 499 (*isol, activity*)
Bai, L. *et al., Phytochemistry*, 1997, **44**, 1565 (*5-glucosides, isol, uv, ir, pmr, cmr*)

1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene D-640

[36469-58-6]
5-[2-(4-Hydroxyphenyl)ethenyl]-1,3-benzenediol, 9CI. 3,4′,5-Stilbenetriol, 8CI. 3,4′,5-Trihydroxystilbene. ***Resveratrol***



(E)-form

$C_{14}H_{12}O_3$ 228.247

(E)-form [501-36-0]
Phytoalexin from the wine grape (*Vitis vinifera*) and peanut (*Arachis hypogaea*). Resveratrol in red wines has been postulated to be associated with beneficial health effects. Nutriceutical with a positive influence on blood lipid profile. Cryst. (MeOH aq.). Sol. EtOH, Me_2CO; poorly sol. H_2O. Mp 265-267°. λ_{max} 218 (ϵ 21400); 227 (sh) (ϵ 14800); 307 (ϵ 27500); 320 (ϵ 26900) (EtOH).

3-O-β-D-Glucopyranoside: [27208-80-6]
Piceid. *Polydatin*
$C_{20}H_{22}O_8$ 390.389
Present in grapeskins and red wine. Isol. from *Polygonum cuspidatum* (Japanese knotweed). Pale yellow needles. Mp 130-140° (resolidifies at 170°, remelts at 228-230°). $[\alpha]_D^{19}$ -65.26 (c, 0.19 in MeOH). λ_{max} 211 (ϵ 17000); 304 (ϵ 17800); 315 (ϵ 14800) (isomeric form recorded) (Derep). λ_{max} 217 (ϵ 2000); 306 (ϵ 16200); 314 (ϵ 13200); 320 (ϵ 13800) (EtOH) (Derep).

3-O-β-D-Glucopyranoside, 4′-O-sulfate:
$C_{20}H_{22}O_{11}S$ 470.453
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + 1 H_2O (as K salt). $[\alpha]_D^{24}$ -70.6 (c, 0.08 in MeOH) (K salt). λ_{max} 211 ; 229 (sh) ; 301 ; 312 (MeOH) (K salt).

3-O-β-D-Glucopyranoside, 5-O-sulfate:
$C_{20}H_{22}O_{11}S$ 470.453
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + 2H_2O (as K salt). $[\alpha]_D^{24}$ -67 (c, 0.07 in MeOH) (K salt). λ_{max} 207 ; 232 (sh) ; 305 ; 320 (MeOH) (K salt).

3-O-(2-O-Sulfo-β-D-glucopyranoside):
$C_{20}H_{22}O_{11}S$ 470.453
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + 3½ H_2O (as K salt). $[\alpha]_D^{24}$ -60 (c, 0.19 in MeOH) (K salt). λ_{max} 215 ; 233 (sh) ; 306 ; 319 (MeOH) (K salt).

3-O-(4-O-Sulfo-β-D-glucopyranoside):
$C_{20}H_{22}O_{11}S$ 470.453
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + 1 H_2O (as K salt). $[\alpha]_D^{24}$ -59.5 (c, 0.08 in MeOH) (K salt). λ_{max} 212 ; 236 (sh) ; 306 ; 322 (MeOH) (K salt).

3-O-(6-O-Sulfo-β-D-glucopyranoside):
$C_{20}H_{22}O_{11}S$ 470.453
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder (as K salt). $[\alpha]_D^{24}$ -105 (c, 0.13 in MeOH) (K salt). λ_{max} 215 ; 236 (sh) ; 306 ; 322 (MeOH) (K salt).

4′-O-β-D-Glucopyranoside: [38963-95-0]
Resveratroloside
$C_{20}H_{22}O_8$ 390.389
Constit. of Rhizoma rhei. Mp 235-238°. $[\alpha]_D^{20}$ -72 (c, 0.125 in EtOH).

4′-O-[3,4,5-Trihydroxybenzoyl-(→2)-β-D-glucopyranoside]: [105304-51-6] *Resveratrol 4′-(2-galloylglucoside)*
$C_{27}H_{26}O_{12}$ 542.495
Isol. from commercial rhubarbs (*Rheum* spp.). Amorph. powder + 1H_2O. $[\alpha]_D^{27}$ +25.2 (c, 0.69 in Me_2CO).

4′-O-[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]: [64898-03-9] *Resveratrol 4′-(6-galloylglucoside)*
$C_{27}H_{26}O_{12}$ 542.495
Isol from coml. Japanese rhubarbs (*Rheum* spp.). Pale brown needles + ½H_2O ($CHCl_3$/MeOH). Mp 258°. $[\alpha]_D^{20}$ -86 (c, 1.0 in MeOH).

3-Me ether, 4′-O-β-D-glucopyranoside: [58762-96-2] ***Pinostilbenoside***
$C_{21}H_{24}O_8$ 404.416
Isol. from the bark of *Picea koraiensis* (Korean pine). Needles (MeOH/

$CHCl_3$). $[\alpha]_D^{22}$ -52.5 (c, 2.0 in MeOH).

4′-Me ether, 3-O-β-D-glucopyranoside:
$C_{21}H_{24}O_8$ 404.416
Constit. of rhubarb (*Rheum rhaponticum*) root. Cryst. (EtOH aq.). Mp 226-228°. λ_{max} 307 (ε 31000); 320 (ε 30700) (MeOH).

(*Z*)-*form* [61434-67-1]
Phytoalexin from hypocotyls of germinating peanuts (*Arachis hypogaea*). Powder (MeOH aq.). Mp 170-174°. λ_{max} 210 ; 220 (sh) ; 286 (EtOH).

3-O-β-D-Glucopyranoside: [148766-36-3]
cis-*Piceid*
$C_{20}H_{22}O_8$ 390.389
Constit. of the wine grape (*Vitis vinifera*). Cryst. (MeOH aq.). Mp 126-129°.

3-O-β-D-Glucopyranoside, 5-O-sulfate:
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + 3 H_2O (as K salt). $[\alpha]_D^{24}$ -31 (c, 0.4 in MeOH) (K salt). λ_{max} 216 ; 232 (sh) ; 290 ; 322 (sh) (MeOH) (K salt).

3-O-(2-O-Sulfo-β-D-glucopyranoside):
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + 2 H_2O (as Na salt). $[\alpha]_D^{24}$ -44 (c, 0.3 in MeOH) (Na salt). λ_{max} 217 ; 234 (sh) ; 290 ; 321 (sh) (MeOH) (Na salt).

3-O-(3-O-Sulfo-β-D-glucopyranoside):
$C_{20}H_{22}O_{11}S$ 470.453
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + $2H_2O$ (as K salt). $[\alpha]_D^{24}$ -40 (c, 0.2 in MeOH) (K salt). λ_{max} 217 ; 235 (sh) ; 286 ; 322 (sh) (MeOH) (K salt).

3-O-(4-O-Sulfo-β-D-glucopyranoside):
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + 1 H_2O (as K salt). $[\alpha]_D^{24}$ -32.3 (c, 0.18 in MeOH) (K salt). λ_{max} 216 ; 232 (sh) ; 288 ; 322 (sh) (MeOH) (K salt).

3-O-(6-O-Sulfo-β-D-glucopyranoside):
Constit. of *Polygonum cuspidatum* (Japanese knotweed). Amorph. powder + $1\frac{1}{2}$ H_2O (as Na salt). $[\alpha]_D^{24}$ -33.6 (c, 0.25 in MeOH) (Na salt). λ_{max} 215 ; 233 (sh) ; 284 (MeOH) (Na salt).

4′-O-β-D-Glucopyranoside: [151716-27-7]
$C_{20}H_{22}O_8$ 390.389
Constit. of the wine grape (*Vitis vinifera*). Cryst. (MeOH aq.). Mp 140-143°.

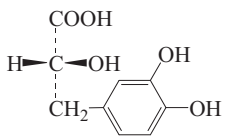
3,4′-Di-O-β-D-glucopyranoside:
$C_{26}H_{32}O_{13}$ 552.531
Isol. from cell suspension cultures of *Vitis vinifera* (wine grape). Amorph. powder. $[\alpha]_D^{25}$ -42 (c, 1 in MeOH). λ_{max} 282 (log ε 4.14) (MeOH).

[33626-08-3, 54443-64-0]

Späth, E. *et al., Ber.*, 1941, **74**, 189 (*synth*)
Banks, H.J. *et al., Aust. J. Chem.*, 1971, **24**, 2427 (*isol, derivs*)
Murakami, T. *et al., Tet. Lett.*, 1972, 2965 (*isol, uv*)
Kumar, N. *et al., Phytochemistry*, 1974, **13**, 633 (*isol*)
Gromova, A.S. *et al., Khim. Prir. Soedin.*, 1975, **11**, 677; 1977, **13**, 275; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 715; 1977, **13**, 236 (*Pinostilbenoside, Resveratroloside*)
Ingham, J.L. *et al., Phytochemistry*, 1976, **15**, 1791 (*isol, uv, ms*)
Aritomi, M. *et al., Phytochemistry*, 1976, **15**, 2006 (*isol, uv*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2300 (*isol, uv, ir, pmr, derivs*)
Langcake, P. *et al., Phytochemistry*, 1977, **16**, 1193 (*biosynth*)
Nakajima, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3050 (*isol, ir, uv, pmr*)
Moreno-Mañas, M. *et al., An. Quim.*, 1985, **81**, 157 (*synth*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3237 (*2-galloylglucoside*)
Etoh, H. *et al., Agric. Biol. Chem.*, 1990, **54**, 2443 (*6-Coumarylpiceid, Polydatin, Rhaponticin*)
Jayatilake, G.S. *et al., J. Nat. Prod.*, 1993, **56**, 1805 (*pmr, props, synth, cis-isomers*)
Sotheeswaran, S. *et al., Phytochemistry*, 1993, **32**, 1083 (*rev, bibl*)
Powell, R.G. *et al., Phytochemistry*, 1994, **35**, 335 (*occur*)
Lamuela-Raventós, R.M. *et al., J. Agric. Food Chem.*, 1995, **43**, 281-283 (*Piceid, occur*)
Mattivi, F. *et al., J. Agric. Food Chem.*, 1995, **43**, 1820 (*cis-4′-glucoside*)
Waffo Teguo, P. *et al., J. Nat. Prod.*, 1996, **59**, 1189 (*cis-Piceid*)
Waffo Teguo, P. *et al., Phytochemistry*, 1996, **42**, 1591 (*Piceid, uv, ir, pmr, cmr*)
Orsini, F. *et al., J. Nat. Prod.*, 1997, **60**, 1082-1087 (*Piceid, synth, isol, pmr, cmr*)
Xiao, K. *et al., J. Nat. Prod.*, 2000, **63**, 1373-1376 (*Polygonum sulfoglucosides*)
Likhitwitayawuid, K. *et al., Planta Med.*, 2000, **66**, 275-277 (*activity*)
Decendit, A. *et al., Phytochemistry*, 2002, **60**, 795-798 (*cis-3,4′-diglucoside*)
Guiso, M. *et al., Tet. Lett.*, 2002, **43**, 597-598 (*synth*)

3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid D-641

[23028-17-3]
α,3,4-Trihydroxybenzenepropanoic acid, 9CI. 3-(3,4-Dihydroxyphenyl)lactic acid



(R)-form

$C_9H_{10}O_5$ 198.175

(*R*)-*form* [76822-21-4]
Prisms ($EtOAc/C_6H_6$). Mp 84-87°. $[\alpha]_D^{18}$ +10.8 (c, 3.7 in MeOH).

Amide:2-Hydroxy-3-(3,4-dihydroxyphenyl)propanamide. 3-(3,4-Dihydroxyphenyl)lactamide
$C_9H_{11}NO_4$ 197.19
Isol. from rhizomes of sage plant. Amorph. yellow powder. $[\alpha]_D^{20}$ +15.8 (c, 0.1 in MeOH). λ_{max} 208 (log ε 4.04); 280 (log ε 3.54) (MeOH).

2-O-(3,4-Dihydroxy-E-cinnamoyl): [537-15-5]

[20283-92-5] ***Rosmarinic acid***. *Labiatenic acid. Rosemarinic acid*
$C_{18}H_{16}O_8$ 360.32
Isol. from rosemary, mint, sage, thyme, lemon balm and other plants. Cryst. + $2H_2O$. Mp 204° dec. $[\alpha]_D^{20}$ +145. Log P 1.01 (calc). λ_{max} 230 ; 329 (MeOH) (Berdy).

► LD_{50} (mus, ivn) 561 mg/kg. GD8990000

2-O-(3,4-Dihydroxy-E-cinnamoyl), Me ester: [99353-00-1]

[179462-75-0] *Methyl rosmarinate*
$C_{19}H_{18}O_8$ 374.346
Isol. from *Salvia* (sage) spp.. Amorph. $[\alpha]_D^{18}$ +138 (c, 0.6 in MeOH). λ_{max} 287 ; 326 (MeOH).

2-O-[β-D-Glucopyranosyl-(→3)-3,4-dihydroxy-E-cinnamoyl]: [178895-25-5]
Salviaflaside
$C_{24}H_{26}O_{13}$ 522.462
Isol. from *Salvia* (sage) spp.. Amorph. yellow powder. $[\alpha]_D$ +18.5 (c, 0.065 in MeOH).

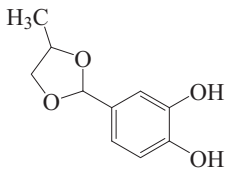
2-O-[β-D-Glucopyranosyl-(→3)-3,4-dihydroxy-E-cinnamoyl], Me ester: [178860-70-3] *Salviaflaside methyl ester*
$C_{25}H_{28}O_{13}$ 536.488
Constit. of sage (*Salvia flava*). Amorph. yellow powder. $[\alpha]_D$ -9.1 (c, 0.12 in MeOH). λ_{max} 205 (log ε 4.55); 287 (log ε 4.07); 320 (log ε 4.11) (no solvent reported).

[42085-50-7, 67810-33-7, 67920-52-9, 69339-96-4, 81075-52-7]

Kelley, C.J. *et al., J.O.C.*, 1975, **40**, 1804; 1976, **41**, 449-455 (*pmr, cmr, Rosmarinic acid*)
Razzaque, A. *et al., Planta*, 1977, **137**, 287 (*biosynth, Rosmarinic acid*)
Ellis, B.E. *et al., Planta*, 1979, **147**, 163 (*biosynth, Rosmarinic acid*)
Parnham, M.J. *et al., Drugs of the Future*, 1985, **10**, 756 (*rev, Rosmarinic acid*)
Englberger, W. *et al., Int. J. Immunopharmacol.*, 1988, **10**, 729 (*pharmacol, Rosmarinic acid*)
Peake, P.W. *et al., Int. J. Immunopharmacol.*, 1991, **13**, 853 (*pharmacol, Rosmarinic acid*)
Pabsch, K. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1991, **110**, 199 (*synth, Rosmarinic acid*)
Mahmood, N. *et al., Antiviral Chem. Chemother.*, 1993, **4**, 235 (*anti-HIV activity, nmr, ms, Rosmarinic acid*)
Zou, Z.W. *et al., Yaoxue Xuebao*, 1993, **28**, 241 (*pharmacol, Rosmarinic acid*)
Zhao, L.M. *et al., Chin. Chem. Lett.*, 1996, **7**, 449-452 (*Salviaflaside*)
Abraham, S.K. *et al., Food Chem. Toxicol.*, 1996, **34**, 15-20 (*activity, Rosmarinic acid*)
Binutu, O.A. *et al., Planta Med.*, 1996, **62**, 352-353 (*activity, Rosmarinic acid*)
Robinson, W.E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 6326-6331 (*activity, Rosmarinic acid*)
Eicher, T. *et al., Synthesis*, 1996, 755 (*synth, Rosmarinic acid*)
Bogucki, D.E. *et al., Can. J. Chem.*, 1997, **75**, 1783-1794 (*synth, Rosmarinic acid*)
Reimann, E. *et al., Monatsh. Chem.*, 1997, **128**, 995-1008; 1998, **129**, 187-193 (*synth, Rosmarinic acid*)
Kusano, G. *et al., Biol. Pharm. Bull.*, 1998, **21**, 997-999 (*activity, Rosmarinic acid*)
Kuo, Y.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 2000, **47**, 241-246 (*Methyl rosmarinate*)
Choi, J.S. *et al., Fitoterapia*, 2001, **72**, 30-34 (*amide*)
Hou, Z.-F. *et al., J. Chin. Chem. Soc. (Taipei)*, 2002, **49**, 255-258 (*Ethyl rosmarinate*)

2-(3,4-Dihydroxyphenyl)-4-methyl-1,3-dioxolane D-642

4-(4-Methyl-1,3-dioxolan-2-yl)-1,2-benzenediol, 9CI



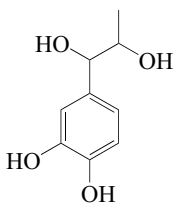
$C_{10}H_{12}O_4$ 196.202

3′-Me ether: [68527-74-2] *2-Methoxy-4-(4-methyl-1,3-dioxolan-2-yl)phenol, 9CI. Vanillin propylene glycol acetate*
$C_{11}H_{14}O_4$ 210.229
Present in food as an artifact arising from reaction of Vanillin (see D-382) flavouring and 1,2-Propanediol, P-471 solvent.

3′-Et ether: [68527-76-4] *2-Ethoxy-4-(4-methyl-1,3-dioxolan-2-yl)phenol, 9CI. Ethyl vanillin propylene glycol acetal*
$C_{12}H_{16}O_4$ 224.256
Present in food as an artifact arising from reaction of Ethylvanillin (see D-382) flavouring and 1,2-Propanediol, P-471 solvent.

Shu, C.K. *et al., CA*, 1997, **126**, 6734j (*occur*)
Woefel, K. *et al., ACS Symp. Ser.*, 1998, **705**, 193-210 (*ms*)

1-(3,4-Dihydroxyphenyl)-1,2-propanediol D-643



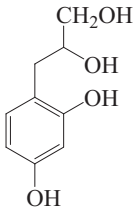
$C_9H_{12}O_4$ 184.191

3′,4′-Methylene ether: [189067-47-8] *1-(1,3-Benzodioxol-5-yl)-1,2-propanediol, 9CI. 1-(3,4-Methylenedioxyphenyl)-1,2-propanediol*
$C_{10}H_{12}O_4$ 196.202
Oil. $[\alpha]_D$ +12.9 (c, 0.6 in $CHCl_3$).

3-Chloro, 3′-Me ether:3-Chloro-1-(4-hydroxy-3-methoxyphenyl)-1,2-propanediol
$C_{10}H_{13}ClO_4$ 232.663
Constit. of the fruit of *Pimenta dioica* (allspice). Needles ($CHCl_3$). Mp 121°. $[\alpha]_D^{25}$ -2 (c, 0.52 in EtOH). Possesses *threo*-config..

Sy, L.-K. *et al., Phytochemistry*, 1997, **44**, 1099-1108 (*isol, pmr, cmr, ms*)
Kikuzaki, H. *et al., Phytochemistry*, 1999, **52**, 1307-1312 (*chloro deriv*)

3-(2,4-Dihydroxyphenyl)-1,2-propanediol D-644



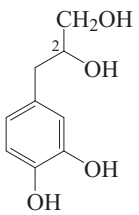
$C_9H_{12}O_4$ 184.191

2′-Me ether, 4′-O-β-D-glucopyranoside: [455947-72-5]
$C_{16}H_{24}O_9$ 360.36
Constit. of the fruit of *Anethum graveolens* (dill). Amorph. powder. $[\alpha]_D^{24}$ -29 (c, 1.1 in MeOH). Isol. as a mixt. of stereoisomers.

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 501-507 (*isol, pmr, cmr*)

3-(3,4-Dihydroxyphenyl)-1,2-propanediol D-645

4-(2,3-Dihydroxypropyl)-1,2-benzenediol



$C_9H_{12}O_4$ 184.191

(ξ)-*form*

3′-Me ether: [220006-74-6]

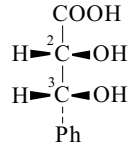
[27391-18-0] *3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol*
$C_{10}H_{14}O_4$ 198.218
Constit. of allspice (*Pimenta dioica*). $[\alpha]_D$ -6. $[\alpha]_D$ -12 (c, 1 in EtOH). Both isolates were a mixt. of stereoisomers.

3′-Me ether, 2-O-[(3,4,5-trihydroxybenzoyl)(→6)-β-D-glucopyranoside]:
$C_{23}H_{28}O_{13}$ 512.466
Constit. of the fruit of allspice (*Pimenta dioica*). Viscous liq. $[\alpha]_D^{20}$ -27.7 (c, 0.15 in MeOH).

Kikuzaki, H. *et al., Phytochemistry*, 1999, **52**, 1307-1312 (*isol, config*)
Kikuzaki, H. *et al., J. Nat. Prod.*, 2000, **63**, 749-752 (*3′-Me, 2-6-galloylglucoside*)

2,3-Dihydroxy-3-phenylpropanoic acid, 9CI D-646

[5695-95-4]
α,β-Dihydroxybenzenepropanoic acid, 9CI. 3-Phenylglyceric acid, 8CI. α,β-Dihydroxyhydrocinnamic acid



(2*R*,3*R*)-*form*

$C_9H_{10}O_4$ 182.176

(2*R*,3*R*)-*form* [70094-91-6]
(-)-erythro-*form*
Cryst. Mp 97-98°. $[\alpha]_D^{20}$ -25.6 (H_2O).

2-Phenylethylamide: [140848-74-4]

[151670-52-9, 151670-53-0, 157366-45-5] ***Secodemethylclausenamide***
$C_{17}H_{19}NO_3$ 285.342
Alkaloid from *Clausena lansium* (wampee). Mp 151-152°. $[\alpha]_D^{28}$ +38 (c, 0.3 in MeOH). Abs. config. revised in 1994 λ_{max} 255 (log ϵ 2.6) (MeOH).

2-Phenylethylamide, N-*Me:* [140848-73-3]

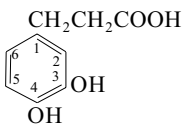
[157332-69-9] ***Secoclausenamide***
$C_{18}H_{21}NO_3$ 299.369
Alkaloid from *Clausena lansium* (wampee). Mp 145-147°. $[\alpha]_D^{22}$ -65.8 (c, 0.2 in $CHCl_3$). Abs. config. revised in 1994 λ_{max} 256 (log ϵ 2.8) (MeOH).

[60209-23-6, 65870-46-4, 65870-48-6, 65870-49-7, 73610-80-7]

Yang, M.H. *et al., Chin. Chem. Lett.*, 1991, **2**, 775-776 (*Secoclausenamides*)
Du, J.F. *et al., Chin. Chem. Lett.*, 1994, **5**, 179-180; 269-270 (*Secoclausenamides*)

3-(3,4-Dihydroxyphenyl)propanoic acid D-647

[1078-61-1]
3,4-Dihydroxybenzenepropanoic acid, 9CI. 3,4-Dihydroxyhydrocinnamic acid, 8CI. Hydrocaffeic acid



$C_9H_{10}O_4$ 182.176
Leaflets (H_2O). Mp 139°. pK_{a1} 4.56; pK_{a2} 9.36; pK_{a3} 11.6 (30°, 0.1*M* $NaClO_4$).

▶ MW5143500

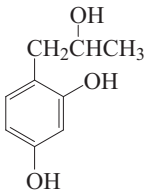
4-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside], Me ester: [134860-04-1] ***Citrusin F***
$C_{22}H_{32}O_{14}$ 520.486
Isol. from lemon peel oil (*Citrus limon*). Oil. $[\alpha]_D^{22}$ -4.68 (c, 0.1 in MeOH).

3-Me ether, 4-O-β-D-glucopyranoside, Me ester: [134860-03-0] ***Citrusin E***
Isol. from oil of lemon peel (*Citrus limon*). Mp 108°. $[\alpha]_D^{17}$ -35.68 (c, 0.1 in MeOH).

Matsubara, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 647 (*Citrusins*)

1-(2,4-Dihydroxyphenyl)-2-propanol D-648

4-(2-Hydroxypropyl)-1,3-benzenediol



$C_9H_{12}O_3$ 168.192

(ξ)-*form*

4′-Me ether: [212516-43-3] *1-(2-Hydroxy-4-methoxyphenyl)-2-propanol.* ***Verimol J***
$C_{10}H_{14}O_3$ 182.219
Constit. of *Illicium verum* (Chinese star anise). Oil.

Sy, L.K. *et al., J. Nat. Prod.*, 1998, **61**, 987-992 (*Verimol J*)

3-(3,4-Dihydroxyphenyl)-1-propanol D-649

[46118-02-9]
4-(3-Hydroxypropyl)-1,2-benzenediol, 9CI. 4-(3-Hydroxypropyl)catechol

$C_9H_{12}O_3$ 168.192

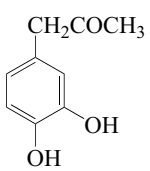
3′-O-β-D-Glucopyranoside:
$C_{15}H_{22}O_8$ 330.334
Constit. of the fruit of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{23}$ -41 (c, 0.2 in MeOH).

3′-Me ether, 4′-O-β-D-glucopyranoside: [17609-06-2] ***Dihydroconiferin***
$C_{16}H_{24}O_8$ 344.361
Constit. of *Pinus sylvestris* (Scotch pine). Needles (MeOH/Me_2CO). Mp 143° (130-132°). $[\alpha]_D^{18}$ -52.2 (c, 0.5 in MeOH).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 413A (*nmr*)
Higuchi, R. *et al., Phytochemistry*, 1977, **16**, 1007 (*Dihydroconiferin*)
Cram, D.J. *et al., J.O.C.*, 1978, **43**, 2758 (*synth*)
Fang, J.M. *et al., J. Chin. Chem. Soc. (Taipei)*, 1985, **32**, 75; 477 (*isol*)
Cordona, M.L. *et al., Phytochemistry*, 1990, **29**, 629 (*isol, pmr, cmr*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*3′-glucoside*)

1-(3,4-Dihydroxyphenyl)-2-propanone D-650

[2503-44-8]
3,4-Dihydroxyphenylacetone



$C_9H_{10}O_3$ 166.176
Component of wood smokes, present in smoked meats. Metabolite of 2-Amino-3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid and *N*,α-Dimethyl-3,4-(methylenedioxy)phenethylamine.

3′-Me ether: [2503-46-0] *1-(4-Hydroxy-3-methoxyphenyl)-2-propanone, 9CI. Guaiacylacetone. Methyl vanillyl ketone*
$C_{10}H_{12}O_3$ 180.203
Oil. Bp_4 155° $Bp_{0.2}$ 115°.

3′-Me ether, 2,4-dinitrophenylhydrazone:
Orange needles (EtOH). Mp 125°.

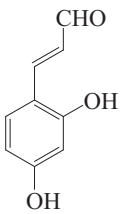
Di-Me ether: [776-99-8] *1-(3,4-Dimethoxyphenyl)-2-propanone*
$C_{11}H_{14}O_3$ 194.23
Yellow oil. $Bp_{0.15}$ 93°. n_D^{20} 1.5358.

5′-Methoxy, 3′-Me ether: [19037-58-2] *1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-propanone.* ***Syringylacetone***
$C_{11}H_{14}O_4$ 210.229
Not to be confused with syringalacetones A and B.

Freudenberg, K. *et al., Ber.*, 1943, **76**, 997 (*synth, 3′-Me ether*)
Skurikhin, I.M. *et al., Khim. Prir. Soedin.*, 1967, **3**, 339; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 286 (*uv, 3′-Me ether*)
Chang, C.-F. *et al., Agric. Biol. Chem.*, 1975, **39**, 573 (*isol*)
Morgan, P.H. *et al., Tetrahedron*, 1975, **31**, 2595 (*di-Me ether*)
Lim, H.K. *et al., Cryst. Res. Technol.*, 1988, **1**, 370 (*synth, pmr, 3′-Me ether*)
An, Z.W. *et al., Synthesis*, 1992, 1229 (*di-Me ether*)
Brozla, D. *et al., Pharmazie*, 1994, **49**, 573 (*synth, ir, pmr, ms*)

3-(2,4-Dihydroxyphenyl)-2-propenal D-651

2,4-Dihydroxycinnamaldehyde



$C_9H_8O_3$ 164.16

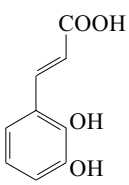
(ξ)-*form*

2′-Me ether: [127321-19-1] *3-(4-Hydroxy-2-methoxyphenyl)-2-propenal. 4-Hydroxy-2-methoxycinnamaldehyde*
$C_{10}H_{10}O_3$ 178.187
Constit. of sunflower and vanilla. Yellowish powder.

Sun, R. *et al., J. Agric. Food Chem.*, 2001, **49**, 5161-5164 (*isol, pmr, ms*)

3-(2,3-Dihydroxyphenyl)-2-propenoic acid, 9CI D-652

[31082-90-3]
2,3-Dihydroxycinnamic acid. Anthenobilic acid



$C_9H_8O_4$ 180.16

(*E*)-*form* [38481-04-8]
Identified in *Anthemis nobilis* (Roman chamomile). Mp 218° dec.

3-Me ether: [3626-94-6] *3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid, 9CI. 2-Hydroxy-3-methoxycinnamic acid. o-Ferulic acid. Orthoferulic acid*
$C_{10}H_{10}O_4$ 194.187
Present in wheat shoots. Mp 183-184°.

Di-Me ether: [7345-82-6]

[7461-60-1] *3-(2,3-Dimethoxyphenyl)-2-propenoic acid, 9CI. 2,3-Dimethoxycinnamic acid, 8CI*
$C_{11}H_{12}O_4$ 208.213
Cryst. (EtOH aq.). Mp 182-184°.

Di-Me ether, Me ester: [15854-60-1]
$C_{12}H_{14}O_4$ 222.24
Cryst. Mp 53-54°.

Methylene ether: [38489-70-2] *3-(2,3-Methylenedioxyphenyl)propenoic acid. 3-(1,3-Benzodioxol-4-yl)-2-propenoic acid, 9CI. 2,3-Methylenedioxycinnamic acid, 8CI*
$C_{10}H_8O_4$ 192.171
Prisms (MeOH aq. or EtOAc). Mp 194°.

Perkin, W.H. *et al., J.C.S.*, 1926, 2925 (*methylene ether*)
El-Basyouni, S. *et al., Can. J. Biochem.*, 1964, **42**, 493 (*deriv*)
Hevisset, A. *et al., CA*, 1971, **74**, 50555 (*occur*)
Santavy, *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1825 (*methylene ether*)
Mathison, I.W. *et al., J.O.C.*, 1974, **39**, 2852 (*synth*)
Dupin, J.F.E. *et al., Synth. Commun.*, 1985, **15**, 581-586 (*synth, pmr*)
Peterson, J.R. *et al., J. Chem. Eng. Data*, 1988, **33**, 534-537 (*di-Me ether, synth, pmr*)

3-(3,4-Dihydroxyphenyl)-2-propenoic acid, 9CI D-653

[331-39-5]

[2316-26-9]
3,4-Dihydroxycinnamic acid, 8CI. ***Caffeic acid***

$C_9H_8O_4$ 180.16
Sol. MeOH, EtOAc; fairly sol. H_2O; poorly sol. $CHCl_3$, hexane. Log P 0.82 (calc). λ_{max} 217 (ε 20100); 300 (ε 20700); 332 (ε 24500) (as Me ester) (Derep). λ_{max} 219 (ε 14700); 235 (ε 10100); 244 (ε 10500); 300 (ε 13500); 329 (ε 17100) (EtOH) (Derep). λ_{max} 235 ; 290 ; 320 (MeOH) (Berdy).

▶ GD8950000

(*E*)-*form* [501-16-6]
Widespread in plants, free and as glycosides. Present in fruits, cereals, wine and coffee in free and conjugated forms. Yellow cryst. Mp 223-225° dec. pK_{a1} 4.62; pK_{a2} 9.07 (25°). Log P 0.82 (calc). Forms a monohydrate. Pharmacol. active isomer.

▶ Mod. allergen.

Vinyl ester: ***Vinyl caffeate***
$C_{11}H_{10}O_4$ 206.198
Constit. of *Perilla frutescens* var. *crispa*. Cryst. Mp 133-140°. λ_{max} 221 (ε 17000); 247 (ε 13000); 339 (ε 22000) (EtOH).

[β-D-Apiofuranosyl-(1→6)-β-D-

glucopyranosyl] ester:
$C_{20}H_{26}O_{13}$ 474.418
Constit. of *Salvia officinalis* (sage). Cryst. (MeOH). Mp 69-71°. $[\alpha]_D^{23}$ -21.8 (c, 0.15 in MeOH).

4′-O-β-D-Glucopyranoside: [17093-82-2] ***Glucocaffeic acid***. *Linocaffein*
$C_{15}H_{18}O_9$ 342.302
Isol. from flax (*Linum usitatissimum*). Needles (MeOH). Mp 208° Mp 133-135°. $[\alpha]_D^{25}$ -87.3 (MeOH). Some doubt about the identity of Linocaffein and Glucocaffeic acid in view of the widely differing Mp's reported.

4′-Me ether: [537-73-5]

[24276-84-4] *3-(3-Hydroxy-4-methoxyphenyl)-2-propenoic acid, 9CI. 3-Hydroxy-4-methoxycinnamic acid.* ***Isoferulic acid***. *Hesperetic acid. Hesperetinic acid*
$C_{10}H_{10}O_4$ 194.187
Used as a food additive; listed in the EAFUS Food Additive Database (Jan 2001). Plates. λ_{max} 241 (sh) (ε 25100); 291 (ε 26900); 322 (ε 27500) (MeOH) (Derep).

▶ UD3365400

4′-Me ether, octacosyl ester: [102607-46-5] *Octacosyl (*E*)-isoferulate.* ***Erythrinasinate A***. *Erythrinassinate A*
$C_{38}H_{66}O_4$ 586.937
Isol. from the stem bark of *Erythrina glauca* (gallito). Cryst. (CH_2Cl_2/hexane). Mp 75-76°.

Di-Me ether: [14737-89-4] *3-(3,4-Dimethoxyphenyl)-2-propenoic acid, 9CI. 3,4-Dimethoxycinnamic acid, 8CI. Dimethylcaffeic acid*
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Cryst. (EtOH aq.). Mp 180-181.5°.

(*Z*)-*form* [4361-87-9]
Isocaffeic acid
Found in olive oil, peanuts and other plant sources.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 184B; 184D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1057C; 1058B (*nmr*)
Hermann, F.X. *et al., Pharmazie*, 1956, **11**, 433 (*rev*)
Bate-Smith, E.C. *et al., Sci. Proc. R. Dublin Soc.*, 1956, **27**, 165 (*occur*)
Klosterman, H.J. *et al., J.A.C.S.*, 1959, **81**, 2188 (*Linocaffein*)
Jizba, J. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 2867 (*Glucocaffeic acid*)
Dewick, P.M. *et al., Chem. Comm.*, 1968, 673 (*biosynth*)
Swain, T. *et al., Phytochemistry*, 1970, **9**, 2115 (*biosynth*)
Achenbach, H. *et al., Chem. Ber.*, 1971, **104**, 1468 (*isol, deriv*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 957
Bowden, B.F. *et al., Aust. J. Chem.*, 1975, **28**, 91 (*derivs*)
Kelley, C.J. *et al., J.O.C.*, 1976, **41**, 449 (*cmr*)
de Silva, S.O. *et al., Can. J. Chem.*, 1979, **57**, 1598 (*synth, deriv*)
Fomum, Z.T. *et al., Phytochemistry*, 1986, **25**, 757 (*Erythrinasinate A*)
Garcá-Granda, S. *et al., Acta Cryst. C*, 1987, **43**, 683 (*cryst struct*)
Stuart, J.G. *et al., J. Het. Chem.*, 1987, **24**, 1589 (*synth, ir, pmr, deriv*)
Bankova, V. *et al., J. Nat. Prod.*, 1990, **53**, 821 (*caffeates*)
Saha, M.M. *et al., Phytochemistry*, 1991, **30**, 3834 (*isol, esters*)
IARC Monog., 1993, **56**, 115 (*Caffeic acid, rev, tox*)
Mellidis, A.S. *et al., J. Nat. Prod.*, 1993, **56**, 949 (*isol, esters*)
Wang, M. *et al., J. Nat. Prod.*, 1999, **62**, 454-456 (*apiosylglucosyl ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAK375

3-(3,5-Dihydroxyphenyl)-2-propenoic acid, 9CI D-654

[28374-93-8]
3,5-Dihydroxycinnamic acid, 8CI

$C_9H_8O_4$ 180.16
Isol. from peach buds. Needles (H_2O). Mp 245-246°.

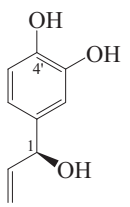
3-Me ether, 5-O-β-D-glucopyranoside, Me ester: ***Linusitamarin***
$C_{17}H_{22}O_9$ 370.355
Constit. of *Linum usitatissimum* (flax). Amorph. powder.

Di-Me ether: [16909-11-8] *3,5-Dimethoxycinnamic acid*
$C_{11}H_{12}O_4$ 208.213
Needles (H_2O). Mp 175-176°. pK_{a1} 4.36 (25°).

Di-Me ether, pyrrolidide: [102934-29-2] **N-*(3,5-Dimethoxycinnamoyl)pyrrolidine***. *3,5-Dimethoxycinnamic acid pyrrolidide*
$C_{15}H_{19}NO_3$ 261.32

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 184A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1057B (*nmr*)
Mauthner, F. *et al., J. Prakt. Chem.*, 1925, **110**, 126 (*synth*)
Altree-Williams, S. *et al., Aust. J. Plant Physiol.*, 1975, **2**, 105; *CA*, **83**, 40204 (*isol*)
Mukherjee, J. *et al., Indian J. Chem.*, 1975, **13**, 859 (*deriv*)
Achenbach, H. *et al., Planta Med.*, 1986, **52**, 12-18 (*pyrrolidide*)
Luyengi, L. *et al., J. Nat. Prod.*, 1993, **56**, 2012 (*Linusitamarin*)

1-(3,4-Dihydroxyphenyl)-2-propen-1-ol D-655



S-form

$C_9H_{10}O_3$ 166.176

(*S*)-*form*

3′-Me ether, 1,4′-di-Ac: [52946-23-3]

[53890-24-7, 108093-85-2] *1′-Acetoxyeugenol acetate*
$C_{14}H_{16}O_5$ 264.277
Constit. of *Alpinia galanga* (greater galangal). Oil. $[\alpha]_D^{20}$ -17.8 (c, 0.44 in EtOH).

(ξ)-*form*

3′-Me ether, 4′-(2-methylpropanoyl), 1-Ac: [142824-99-5] *1′-Acetoxy-4-*O*-isobutyryleugenol*
$C_{16}H_{20}O_5$ 292.331
Dark yellow oil. $Bp_{0.005}$ 130°. $[\alpha]_D^{25}$ -81 (c, 0.7 in $CHCl_3$). λ_{max} 219 (ε 7080); 273 (ε 2344) (MeOH) (Berdy).

3′-Me ether, 1,4′-bis(2-methylpropanoyl): [55249-41-7]
$C_{18}H_{24}O_5$ 320.385
Oil. $Bp_{0.005}$ 130°.

3′-Me ether, 4′-(2-methylpropanoyl), 1-(2-methylbutanoyl): [120692-49-1]
$C_{19}H_{26}O_5$ 334.411

3′-Me ether, 4′-(2-methylpropanoyl), 1-(3-methylbutanoyl): [120692-50-4]
$C_{19}H_{26}O_5$ 334.411
Oil. $[\alpha]_D^{25}$ -150 (c, 1 in $CHCl_3$). λ_{max} 218 (log ε 3.9); 273 (log ε 3.4) (MeOH).

3′,4′-Di-Me ether:1-(3,4-Dimethoxyphenyl)-2-propen-1-ol
$C_{11}H_{14}O_3$ 194.23
Pale yellow oil. $[\alpha]_D^{25}$ +1.46 (c, 1 in MeOH).

Tri-Me ether: [84744-55-8] *1,2-Dimethoxy-4-(1-methoxy-2-propenyl)benzene. 1,2-Dimethoxy-4-(1-methoxyallyl)benzene. 3-(3,4-Dimethoxyphenyl)-3-methoxy-1-propene.* ***Morinin G***
$C_{12}H_{16}O_3$ 208.257
Yellowish oil. $[\alpha]_D^{25}$ +6.5. $[\alpha]_D^{25}$ -1.2 (c, 1.38 in $CHCl_3$). λ_{max} 243 (log ε 3.59); 280 (log ε 3.35) ($CHCl_3$).

[20665-84-3]

Bohlmann, F. *et al., Chem. Ber.*, 1968, **101**, 3243 (*isol, synth*)
Noro, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 244-248 (*1′-Acetoxyeugenol acetate*)
Thron, U. *et al., Z. Naturforsch., C*, 1989, **44**, 7; 573 (*isol, pmr, cmr, ms*)
Pistelli, L. *et al., J. Nat. Prod.*, 1995, **58**, 112 (*tri-Me ether, isol*)
Fuzzati, N. *et al., Phytochemistry*, 1995, **39**, 409 (*isol, uv, pmr, cmr, ms*)
Ikeda, R. *et al., Chem. Pharm. Bull.*, 1998, **46**, 875-878 (*3′,4′-di-Me ether*)
Su, B.N. *et al., J. Nat. Prod.*, 1999, **47**, 1363-1366 (*Morinin G*)
Mata, R. *et al., J. Nat. Prod.*, 2002, **65**, 1030-1032 (*Cosmos pringlei esters*)

3-(3,4-Dihydroxyphenyl)-2-propen-1-ol D-656

[3598-26-3]
4-(3-Hydroxy-1-propenyl)-1,2-benzenediol, 9CI. Caffeyl alcohol. 3,4-Dihydroxycinnamyl alcohol

$C_9H_{10}O_3$ 166.176
(*E*)-config. assumed for derivs. except where (*Z*)-config. is certain.

(*E*)-*form*
Mp 144-145°.

3′-Me ether, 1-O-β-D-glucopyranoside: [65995-51-9] ***Citrusin D***. *Isoconiferin*
$C_{16}H_{22}O_8$ 342.345
Isol. from *Citrus limon* (lemon), *Citrus unshiu* (satsuma mandarin), *Fortunella japonica* (round kumquat) and *Pinus sylvestris* (Scotch pine). $[\alpha]_D^{20}$ -16.9 (c, 4.1 in MeOH). λ_{max} 275 (ε 5000) (MeOH).

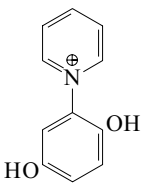
*3′-Me ether, 4′-*O*-β-D-glucopyranoside:* [531-29-3] *Abietin*†. ***Coniferin***. *Coniferoside. Laricin*†
$C_{16}H_{22}O_8$ 342.345
Isol. from *Scorzonera hispanica* (scorzonera). Needles + $2H_2O$. Mp 185°. $[\alpha]_D^{20}$ -66.9 (Py aq.).

[18604-50-7, 77355-78-3, 81532-11-8, 113349-27-2, 115330-92-2, 125164-73-0]

Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 1835 (*isol, Coniferin*)
Sawabe, A. *et al., Nippon Kagaku Kaishi*, 1988, **62**, 1067 (*Citrusin D*)
Daubresse, N. *et al., Synthesis*, 1998, 157-161 (*Coniferin, synth*)

N-(2,5-Dihydroxyphenyl)pyridinium(1+) D-657

[33354-74-4]

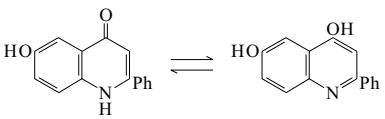


$C_{11}H_{10}NO_2^{\oplus}$ 188.205
Isol. from the leaves of *Punica granatum* (pomegranate). Needles (as chloride). CAS no. refers to chloride.

Nawwar, M.A.M. *et al., Phytochemistry*, 1994, **37**, 1175 (*isol, uv, pmr, cmr, struct*)

4,6-Dihydroxy-2-phenylquinoline D-658

[147197-84-0]
*6-Hydroxy-2-phenyl-4(1*H*)-quinolinone. 2-Phenyl-4,6-quinolinediol*



$C_{15}H_{11}NO_2$ 237.257
Red powder + 0.9 AcOH (AcOH). Mp 243-245°.

NH-form

O,N-*Di-Me:* [6878-08-6] *6-Methoxy-1-methyl-2-phenyl-4(1*H*)-quinolinone, 9CI*. ***Eduline***
$C_{17}H_{15}NO_2$ 265.311
Alkaloid from seeds of *Casimiroa edulis* (Mexican apple). Plates (Me_2CO/Et_2O). Mp 187-188°.

O,N-*Di-Me, perchlorate:*
Needles (Me_2CO/Et_2O). Mp 250-252°.

O,N-*Di-Me, picrate:*
Golden-yellow plates (MeOH). Mp 225-227° dec.

OH-form

Di-Me ether: [22680-65-5] *4,6-Dimethoxy-2-phenylquinoline*
$C_{17}H_{15}NO_2$ 265.311
Mp 118°.

Dziewoński, K. *et al., CA*, 1935, **29**, 1092 (*synth*)
Kincl, F.A. *et al., J.C.S.*, 1956, 4163 (*isol, uv, Eduline*)
Beyerman, H.C. *et al., CA*, 1961, **55**, 10488b (*struct, synth, Eduline*)
Dreyer, D.L. *et al., J.O.C.*, 1968, **33**, 3577 (*isol, pmr, Eduline*)
Boyd, D.R. *et al., J.C.S.(C)*, 1970, 556 (*isol, pmr, ms, Eduline*)
Sato, S. *et al., J. Het. Chem.*, 1999, **36**, 1189-1193 (*synth, ir, pmr*)

4,7-Dihydroxy-2-phenylquinoline D-659

*7-Hydroxy-2-phenyl-4(1*H*)-quinolinone. 2-Phenyl-4,7-quinolinediol*
$C_{15}H_{11}NO_2$ 237.257
Mp 200-201°.

NH-form

7-Me ether, N-*Me:* [483-51-2] *7-Methoxy-1-methyl-2-phenyl-4(1*H*)-quinolinone.* ***Eduleine***
$C_{17}H_{15}NO_2$ 265.311
Alkaloid from *Casimiroa edulis* (Mexican apple). Needles (EtOH). Mp 200-201°.

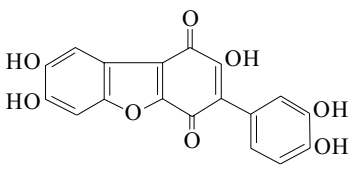
7-Me ether, N-*Me, hydrochloride:*
Needles (5% HCl). Mp 248.5° dec.

7-Me ether, N-*Me, picrate:*
Yellow needles (EtOH). Mp 220-220.5° (191-192°).

Johnstone, R. *et al., Aust. J. Chem.*, 1958, **11**, 562 (*isol, uv, ir, struct, synth*)
Sondheimer, F. *et al., J.O.C.*, 1958, **23**, 762 (*isol, ir, struct*)

3-(3,4-Dihydroxyphenyl)-2,7,8-trihydroxydibenzofuran-1,4-dione, 9CI D-660

[55692-59-6]
Cyclovariegatin

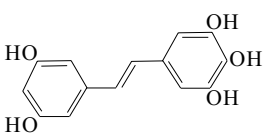


$C_{18}H_{10}O_8$ 354.272
The name Cyclovariegatin not used by the original authors. Isol. from sporophores of *Suillus grevillei* (larch bolete). Dark-red needles. Mp 300°.

Edwards, R.L. *et al., J.C.S. Perkin 1*, 1975, 351-354 (*isol, uv, ir, ms*)

1-(3,5-Dihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethylene D-661

5-[2-(3,5-Dihydroxyphenyl)ethenyl]-1,2,3-benzenetriol, 9CI. 3,3′,4,5,5′-Pentahydroxystilbene



(*E*)-*form*

$C_{14}H_{12}O_5$ 260.246
(***E***)-***form*** [35154-48-4]
Prisms (MeOH aq.). Mp 243-245°.

Penta-Ac: [52961-90-7]
$C_{24}H_{22}O_{10}$ 470.432
Plates. Mp 174°.

4″-Me ether: [89946-11-2] *5-[2-(3,5-Dihydroxyphenyl)ethenyl]-2-methoxy-1,3-benzenediol. 3,3′,5,5′-Tetrahydroxy-4-methoxystilbene*
$C_{15}H_{14}O_5$ 274.273
Isol. from *Phoenix dactylifera* (date). Cryst. ($MeOH/CHCl_3$). Mp 165-168°.

Penta-Me ether: [52961-88-3]
$C_{19}H_{22}O_5$ 330.38
Pale-yellow needles. Mp 134-135°.

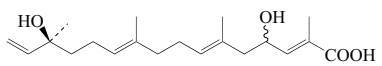
(***Z***)-***form*** [52961-87-2]
Pale-brown needles (EtOH aq.). Mp 128-130°.

4″-Me ether: [89946-10-1]
Isol. from *Phoenix dactylifera* (date). Oil.

King, F.E. *et al., J.C.S.*, 1956, 4477 (*isol, derivs*)
Hathaway, D.E. *et al., Biochem. J.*, 1962, **83**, 80 (*occur*)
Drewes, S.E. *et al., J.C.S. Perkin 1*, 1974, 961 (*isol, ms, pmr, synth*)
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2819 (*isol*)

3,13-Dihydroxy-1,6,10,14-phytatetraen-16-oic acid D-662

4,14-Dihydroxy-2,6,10,14-tetramethyl-2,6,10,15-hexadecatetraenoic acid

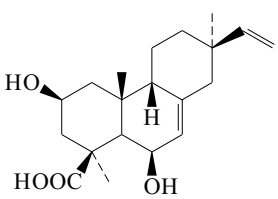


$C_{20}H_{32}O_4$ 336.47
(3*S*,6*E*,10*E*,13ξ,14*E*)-*form*

*3-*O*-[β-D-Glucopyranosyl(1→2)-D-glucopyranoside]:* [121924-04-7] ***Capsianoside I***. *Capsianside I*
$C_{32}H_{52}O_{14}$ 660.754
Constit. of *Capsicum annuum* var. *fascuilatum*. Powder. $[\alpha]_D^{23}$ -7.6 (c, 0.5 in MeOH).

Izumitani, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1299-1307 (*isol, ir, pmr, cmr, ms*)

2,6-Dihydroxy-7,15-pimaradien-19-oic acid D-663

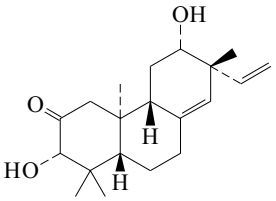


$C_{20}H_{30}O_4$ 334.455
(2β,6β,9β*H*)-*form*

19→6 Lactone: [62394-07-4] *2-Hydroxy-7,15-pimaradien-19,6-olide.* ***Momilactone C***
$C_{20}H_{28}O_3$ 316.439
Constit. of *Oryza sativa* (rice). Cryst. ($CHCl_3$/hexane). Mp 227-228°.

Kato, T. *et al., Phytochemistry*, 1977, **16**, 45

3,12-Dihydroxy-8(14),15-pimaradien-2-one D-664

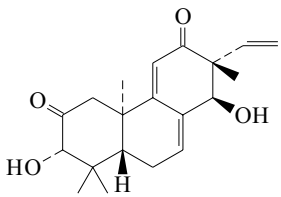


$C_{20}H_{30}O_3$ 318.455

(*ent*-3β,12β)-*form* [119642-82-9]
Yucalexin P17
Constit. of cassava roots (*Manihot esculenta*).

Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769

3,14-Dihydroxy-7,9(11),15-pimaratriene-2,12-dione D-665

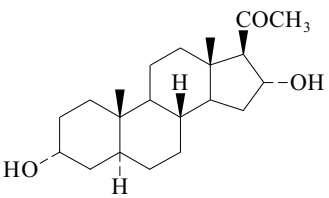


$C_{20}H_{26}O_4$ 330.423

(*ent*-3β,14α)-*form* [119626-52-7]
Yucalexin P15
Constit. of cassava roots (*Manihot esculenta*).

Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769

3,16-Dihydroxypregnan-20-one, 9CI D-666

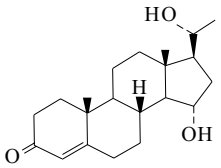


$C_{21}H_{34}O_3$ 334.498

(3β,5α,16β)-*form* [20745-29-3]
Lycopersiconol
Isol. from *Lycopersicon esculentum* (tomato). Cryst. (Me_2CO). Mp 255-258° (dec.)(202-204°). $[\alpha]_D^{27}$ +51.3 (c, 0.95 in MeOH/$CHCl_3$). $[\alpha]_D^{18}$ +58.3 (c, 0.309 in $CHCl_3$).

Yoshihara, T. *et al., Phytochemistry*, 1988, **27**, 3982 (*Lycopersiconol*)

15,20-Dihydroxypregn-4-en-3-one D-667



(15α,20*R*)-*form*

$C_{21}H_{32}O_3$ 332.482

(15α,20*R*)-*form*
Constit. of the aglycone from *Carthamus tinctorius* (safflower). Cryst. (MeOH). Mp 132-134°.

20-O-*[β-D-Glucopyranosyl-(1→4)-6*-O-*acetyl-β-D-glucopyranoside]:*
$C_{35}H_{54}O_{14}$ 698.803
Constit. of *Carthamus tinctorius* (safflower). Cryst. Mp 145-146°. $[\alpha]_D^{18}$ +57.9 (c, 0.6 in MeOH). λ_{max} 241 (ε 15700) (MeOH).

(15α,20*S*)-*form*

20-O-*[α-L-Rhamnopyranosyl-(1→4)-4-hydroxy-3-methoxybenzoyl-(→6)-β-D-glucopyranoside]:* [212624-67-4]
Moschatine
$C_{41}H_{58}O_{15}$ 790.9
Gum. λ_{max} 218 (log ε 4.3); 246 (log ε 4.1); 255 (log ε 4.02); 290 (log ε 3.97) (MeOH).

(15β,20*R*)-*form* [55487-66-6]
Cryst. Mp 188-190°. $[\alpha]_D^{24}$ +44 (c, 0.8 in $CHCl_3$).

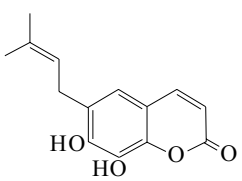
(15β,20*S*)-*form* [34783-65-8]
Cryst. (EtOAc/petrol). Mp 210-212°. $[\alpha]_D^{18}$ +60 (c, 0.4 in $CHCl_3$).

[34783-64-7]

Schildknecht, H. *et al., Naturwissenschaften*, 1969, **56**, 37 (*isol*)
Palter, R. *et al., Phytochemistry*, 1972, **11**, 819 (*isol, struct*)
Holland, H.L. *et al., Can. J. Chem.*, 1975, **53**, 845 (*synth*)
Smith, K.E. *et al., J. Steroid Biochem.*, 1989, **33**, 927 (*synth, pmr, 15α,20*R*-form*)
Nagatsu, A. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1044-1047 (*6′-acetylcellobioside, cryst struct*)
Sarker, S.D. *et al., Phytochemistry*, 1998, **48**, 1039-1043 (*Moschatine*)

7,8-Dihydroxy-6-prenylcoumarin D-668

*7,8-Dihydroxy-6-(3-methyl-2-butenyl)-2*H-*1-benzopyran-2-one, 9CI*



$C_{14}H_{14}O_4$ 246.262

7-Me ether: [34211-17-1] *8-Hydroxy-7-methoxy-6-(3-methyl-2-butenyl)-2*H-*1-benzopyran-2-one, 9CI. 8-Hydroxy-7-methoxy-6-prenylcoumarin.* ***Brosiparin****. Arnottianol*
$C_{15}H_{16}O_4$ 260.289
Yellow cryst. (Me_2CO/hexane). Mp 121-122°.

8-Me ether: [72963-64-5] *7-Hydroxy-8-methoxy-6-(3-methyl-2-butenyl)-2*H-*1-benzopyran-2-one. 7-Hydroxy-8-methoxy-6-prenylcoumarin.* ***Apigravin***
$C_{15}H_{16}O_4$ 260.289
Isol. from *Apium graveolens*. Granules. Mp 167-169°.

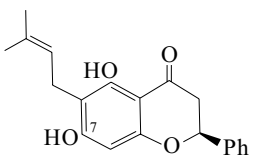
Di-Me ether: [72963-65-6] *7,8-Dimethoxy-6-(3-methyl-2-butenyl)-2*H-*1-benzopyran-2-one. 7,8-Dimethoxy-6-prenylcoumarin*
$C_{16}H_{18}O_4$ 274.316
Mp 93-94°.

7-Me ether, 8-O-*(3-methyl-2-butenyl):* [40046-39-7] **O-*Prenylbrosiparin***
$C_{20}H_{24}O_4$ 328.407
Oil.

Braz Filho, R. *et al., Phytochemistry*, 1972, **11**, 3307
Gottlieb, O.R. *et al., Phytochemistry*, 1972, **11**, 3479
Garg, S.K. *et al., Phytochemistry*, 1979, **18**, 1580 (*Apigravin*)
Raizada, M.B. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 918 (*synth*)
Mali, R.S. *et al., Chem. Comm.*, 1994, 251 (*synth*)

5,7-Dihydroxy-6-prenylflavanone D-669

[72018-32-7]
*2,3-Dihydro-5,7-dihydroxy-6-(3-methyl-2-butenyl)-2-phenyl-4*H-*1-benzopyran-4-one, 9CI. 6-Prenylpinocembrin*



$C_{20}H_{20}O_4$ 324.376

(*S*)-*form* [55051-77-9]
Constit. of *Glycyrrhiza glabra* (licorice). Cryst. (C_6H_6). Mp 212-214°.

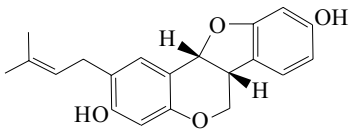
7-Me ether: [55051-79-1] ***5-Hydroxy-7-methoxy-6-prenylflavanone***
$C_{21}H_{22}O_4$ 338.402
Cryst. (petrol). Mp 90-92°.

[57943-33-6, 59718-54-6]

Gottlieb, O.R. *et al., Phytochemistry*, 1975, **14**, 1454; 1674 (*isol*)
Braz Filho, R. *et al., Phytochemistry*, 1975, **14**, 261 (*isol*)
Manchanda, V.P. *et al., Curr. Sci.*, 1976, **45**, 322 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1851; 1980, **19**, 873; 1983, **22**, 2877 (*isol*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 271 (*isol*)
Batirov, E.K. *et al., Khim. Prir. Soedin.*, 1986, **22**, 111; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 107 (*isol*)

3,9-Dihydroxy-2-prenylpterocarpan D-670

[53802-77-0]
*6a,11a-Dihydro-2-(3-methyl-2-butenyl)-6*H-*benzofuro[3,2-c][1]benzopyran-3,9-diol, 9CI.* ***Calopocarpin***



$C_{20}H_{20}O_4$ 324.376

This struct. was prev. given to Homoedudiol. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 180°. λ_{max} 211 ; 288 (MeOH) (Berdy). λ_{max} 211 ; 241 ; 300 (MeOH-NaOH) (Berdy).

*3-Me ether:9-Hydroxy-3-methoxy-2-prenylpterocarpan. 3-*O*-Methylcalopocarpin.* ***Orientanol B***
$C_{21}H_{22}O_4$ 338.402
Constit. of *Erythrina glauca* (gallito). Amorph. solid. $[\alpha]_D$ -235 (c, 0.3 in $CHCl_3$). λ_{max} 214 (log ϵ 4.59); 230 (sh) (log ϵ 4.15); 287 (log ϵ 3.88) (MeOH).

Ingham, J.L. *et al., Z. Naturforsch., C*, 1985, **40**, 482
McKee, T.C. *et al., J. Nat. Prod.*, 1997, **60**, 431 (*3-O-Methylcalopocarpin*)
Nkengfack, A.E. *et al., Phytochemistry*, 1997, **46**, 573-578 (*isol, cmr*)
Tanaka, H. *et al., Phytochemistry*, 1998, **47**, 475-477 (*Orientanol B*)
Yenesew, A. *et al., Phytochemistry*, 1998, **48**, 1439-1443 (*isol, uv, ir, cd, cmr*)

3,9-Dihydroxy-4-prenylpterocarpan D-671

$C_{20}H_{20}O_4$ 324.376

9-Me ether: [202815-29-0] *3-Hydroxy-9-methoxy-4-prenylpterocarpan.* ***Licoagrocarpin***
$C_{21}H_{22}O_4$ 338.402
Isol. from the hairy root cultures of *Glycyrrhiza glabra* (licorice). Powder. $[\alpha]_D^{24}$ -78.6 (c, 0.5 in MeOH). λ_{max} 284 (log ϵ 3.87); 290 (sh) (log ϵ 3.71) (MeOH).

Asada, Y. *et al., Phytochemistry*, 1998, **47**, 389-392 (*isol, uv, ir, cd, pmr, cmr, ms*)

3,9-Dihydroxy-10-prenylpterocarpan D-672

[37831-70-2]
6a,11a-Dihydro-10-(3-methyl-2-butenyl)-6H-benzofuro[3,2-c][1]benzopyran-3,9-diol, 9CI. ***Phaseollidin***

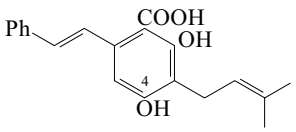
$C_{20}H_{20}O_4$ 324.376
Isol. from kidney bean *Phaseolus vulgaris*, mung bean *Phaseolus aureus*, rice bean *Phaseolus calcaratus*, papadi *Dolichos biflorus*, and hyacinth bean *Lablab niger*. Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. Mp 67-69°. λ_{max} 208 (ϵ 39800); 237 (sh) (ϵ 19100); 281 (ϵ 7940); 286 (ϵ 8910) (EtOH) (Derep). λ_{max} 230 ; 248 ; 289 ; 291 (EtOH-NaOH) (Berdy).

9-Me ether: [74515-46-1] *3-Hydroxy-9-methoxy-10-prenylpterocarpan.* ***Sandwicensin***
$C_{21}H_{22}O_4$ 338.402
$[\alpha]_D$ -190 (c, ca. 0.02 in MeOH). λ_{max} 214 (ϵ 37100); 281 (ϵ 5890); 287 (ϵ 630) (MeOH) (Berdy). λ_{max} 212 ; 252 ; 290 (EtOH-NaOH) (Berdy).

Scheffer, T.C. *et al., Annu. Rev. Phytopathol.*, 1966, **4**, 147 (*rev*)
Perrin, D.R. *et al., Tet. Lett.*, 1972, 1673 (*struct, nmr, uv, ms*)
Burden, R.S. *et al., Tet. Lett.*, 1972, 4175 (*isol, struct*)
Perrin, D.R. *et al., Aust. J. Chem.*, 1974, **27**, 1607 (*struct*)
Ingham, J.L. *et al., Phytochemistry*, 1980, **19**, 1203-1205 (*Sandwicensin, activity*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1980, **35**, 384 (*Sandwicensin*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
McKee, T.C. *et al., J. Nat. Prod.*, 1997, **60**, 431 (*isol, cmr, Sandwicensin*)

2,4-Dihydroxy-3-prenyl-6-styrylbenzoic acid D-673

2,4-Dihydroxy-3-(3-methyl-2-butenyl)-6-(2-phenylethenyl)benzoic acid. 1-Carboxy-2,4-dihydroxy-3-prenylstilbene



$C_{20}H_{20}O_4$ 324.376

(*E*)-*form*

4-Me ether: [87402-84-4] *2-Hydroxy-4-methoxy-3-(3-methyl-2-butenyl)-6-(2-phenylethenyl)benzoic acid. 2-Hydroxy-4-methoxy-3-prenyl-6-styrylbenzoic acid*
$C_{21}H_{22}O_4$ 338.402
Constit. of *Cajanus cajan* (pigeon pea). Pale yellow needles (MeOH aq.). Mp 150-165°.

[86660-10-8]

Cooksey, C.J. *et al., Phytochemistry*, 1982, **21**, 2935

4,6-Dihydroxy-3-prenyl-2-styrylbenzoic acid D-674

4,6-Dihydroxy-3-(3-methyl-2-butenyl)-2-(2-phenylethenyl)benzoic acid. 1-Carboxy-2,4-dihydroxy-5-prenylstilbene

$C_{20}H_{20}O_4$ 324.376

(*E*)-*form*

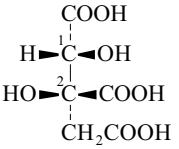
4-Me ether: [87402-83-3] *6-Hydroxy-4-methoxy-3-(3-methyl-2-butenyl)-2-(2-phenylethenyl)benzoic acid. 6-Hydroxy-4-methoxy-3-prenyl-2-styrylbenzoic acid*
$C_{21}H_{22}O_4$ 338.402
Constit. of *Cajanus cajan* (pigeon pea). Pale yellow needles (MeOH aq.). Mp 144-146°.

[86660-09-5]

Cooksey, C.J. *et al., Phytochemistry*, 1982, **21**, 2935

1,2-Dihydroxy-1,2,3-propanetricarboxylic acid, 8CI D-675

[6205-14-7]
3-C-Carboxy-2-deoxypentaric acid, 9CI. Hydroxycitric acid



(1*R*,2*S*)-*form*

$C_6H_8O_8$ 208.124
9CI numbering starts from the other end of the chain.

(1*R*,2*S*)-*form* [6205-15-8]
L-threo-*form*

γ-Lactone:
$C_6H_6O_7$ 190.109
Mp 179-180.5°. $[\alpha]_D^{25}$ +106.4 (H_2O).

(1*S*,2*R*)-*form* [27750-11-4] *D*-threo-*form. (+)*-allo-*form.* ***Hibiscus acid***
$[\alpha]_D$ +44 (c, 0.16 in H_2O).

γ-Lactone:
$[\alpha]_D^{25}$ +110 (c, 1.37 in H_2O).

(1*S*,2*S*)-*form* [27750-10-3] *D*-erythro-*form.* ***Garcinia acid***
Isol. from *Garcinia atroviridis* (gelugor), *Garcinia indica* (kokam) and *Garcinia cambogia*. $[\alpha]_D^{25}$ -20 (H_2O).

α,ω-Dibutyl, γ-Me ester:1,5-Dibutyl methyl hydroxycitrate
$C_{15}H_{26}O_8$ 334.366
Constit. of the fruit of *Garcinia atroviridis* (gelugor). Cryst. (hexane). $[\alpha]_D$ +150 (c, 0.01 in MeOH). Poss. artifact. Abs. config. not certain λ_{max} 217 (log ϵ 2.5) (MeOH).

*1-*O*-(4-Hydroxy-*E*-cinnamoyl):* [62345-85-1] *2-*O*-p-Coumaroylhydroxycitric acid*
$C_{15}H_{14}O_{10}$ 354.27
Constit. of *Zea mays* (sweet corn). Cryst. + ½H_2O (EtOAc/C_6H_6). Mp 155° dec. $[\alpha]_D^{22}$ +27 (c, 0.73 in H_2O).

*1-*O*-(3,4-Dihydroxy-*E*-cinnamoyl):* [62345-87-3] *2-*O*-Caffeoylhydroxycitric acid*
$C_{15}H_{14}O_{11}$ 370.269
Constit. of *Spondias mombin* (yellow mombin) and *Zea mays* (sweet corn). Cryst. (EtOAc aq.). Mp 158° dec. $[\alpha]_D$ +40 (H_2O).

*1-*O*-(4-Hydroxy-3-methoxy-E-cinnamoyl):* [62345-86-2] *2-*O*-Feruloylhydroxycitric acid*
$C_{16}H_{16}O_{11}$ 384.296
Constit. of *Zea mays* (sweet corn). Cryst. (H_2O). Mp 154° dec. $[\alpha]_D^{22}$ +25 (c, 1.06 in H_2O).

γ-Lactone: [27750-13-6]
Mp 178°. $[\alpha]_D^{25}$ +100 (H_2O).

γ-Lactone, di-Me ester:
$C_8H_{10}O_7$ 218.163
$[\alpha]_D^{25}$ +92.1 (c, 0.3 in MeOH).

γ-Lactone, dibutyl ester:
$C_{14}H_{22}O_7$ 302.324
Constit. of the fruit of *Garcinia atroviridis* (gelugor). Yellow oil. $[\alpha]_D$ -60 (c, 0.02 in MeOH). Abs. config. not certain λ_{max} 220 (log ϵ 2.5) (MeOH).

(1*RS*,2*RS*)-*form* *(±)*-erythro-*form*

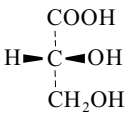
γ-Lactone:
Cryst. (Et_2O). Mp 175°.

Lewis, Y.S. *et al., Phytochemistry*, 1965, **4**, 619 (*isol*)
Boll, P.M. *et al., Acta Chem. Scand.*, 1969, **23**, 286 (*synth*)

Glusker, J.P. *et al., Arch. Biochem. Biophys.*, 1969, **13**, 573 (*cryst struct, abs config*)
Brandange, S. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 307 (*synth*)
Ozawa, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 359 (*isol esters*)
Perry, C.W. *et al., Synthesis*, 1977, 492 (*resoln*)
Corthout, J. *et al., Phytochemistry*, 1992, **31**, 1979 (*caffeoyl ester*)
Jena, B.S. *et al., J. Agric. Food Chem.*, 2002, **50**, 10-22 (*rev, chem, biochem*)
Mackeen, M.M. *et al., Z. Naturforsch., C*, 2002, **57**, 291-295 (*dibutyl Me ester*)

2,3-Dihydroxypropanoic acid, 9CI D-676

[473-81-4]
Glyceric acid. Glyceronic acid



(*R*)-form

$C_3H_6O_4$ 106.078

(*R*)-*form* [6000-40-4]
D-form
Isol. from various plants, e.g. *Vicia faba* and cress. Thick gum. Dec. on dist. Laevorotatory.

(ξ)-*form*

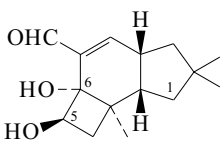
2-O-(E-p-Hydroxycinnamoyl): [154639-28-8]
$C_{12}H_{12}O_6$ 252.223
Constit. of *Eleusine coracana* (finger millet). $[\alpha]_D^{24}$ -55 (c, 1.5 in MeOH).

2-O-(Z-p-Hydroxycinnamoyl): [154639-27-7]
$C_{12}H_{12}O_6$ 252.223
Constit. of *Eleusine coracana* (finger millet). $[\alpha]_D^{24}$ +70 (c, 1.5 in MeOH). Config. not confirmed.

[115136-20-4]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 855C (*nmr*)
Karrer, P. *et al., Helv. Chim. Acta*, 1924, **7**, 931 (*synth*)
Sallach, *et al., J.A.C.S.*, 1952, **74**, 2415 (*synth, bibl*)
Isherwood, F.A. *et al., Biochem. J.*, 1954, **56**, 15 (*isol*)
Ballou, C.E. *et al., J.A.C.S.*, 1954, **76**, 3188-3193 (*R-form, 3-phosphate*)
Ashworth, J.M. *et al., J.C.S.*, 1963, 2563
Biochem. Prep., 1966, **11**, 50 (*synth*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1967, 128 (*synth*)
Kim, C.-S. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 380 (*2-hydroxycinnamates*)
Popek, T. *et al., Acta Cryst. C*, 1996, **52**, 2716 (*cryst struct, salts*)

5,6-Dihydroxy-7-protoilluden-14-al D-677



$C_{15}H_{22}O_3$ 250.337

(5β,6α)-*form*

5-(2,4-Dihydroxy-6-methylbenzoyl): [82869-08-7] ***Melleolide***
$C_{23}H_{28}O_6$ 400.471
Isol. from *Armillaria mellea* (honey mushroom). Cryst. (MeOH aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 198-200°. $[\alpha]_D$ +183.3 (c, 0.93 in $CHCl_3$). λ_{max} 218 (ε 37000); 240 (ε 22000); 313 (ε 24000) (MeOH/NaOH) (Derep). λ_{max} 218 (ε 31000); 267 (ε 16500); 305 (ε 6700) (MeOH) (Derep). λ_{max} 218 (ε 31000); 267 (ε 16500); 305 (ε 6700) (MeOH) (Berdy). λ_{max} 218 (ε 37000); 240 (ε 27000); 313 (ε 24000) (MeOH-NaOH) (Berdy).

5-(2-Hydroxy-4-methoxy-6-methylbenzoyl): [83329-14-0] ***Armillarin***
$C_{24}H_{30}O_6$ 414.497
Isol. from *Armillaria mellea* (honey mushroom). Cryst. Mp 122°. $[\alpha]_D^{30}$ +228 (c, 0.49 in $CHCl_3$).

5-(3-Chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [96684-80-9] ***Armillaridin***
$C_{24}H_{29}ClO_6$ 448.942
From *Armillaria mellea* (honey mushroom). Needles (Et_2O/petrol). Mp 132-134°. $[\alpha]_D^{18}$ +151 (c, 0.23 in $CHCl_3$).

5-(3-Chloro-4,6-dihydroxy-2-methylbenzoyl): ***Melleolide K***
$C_{23}H_{27}ClO_6$ 434.915
Isol. from *Armillariella mellea* (honey mushroom). Powder. Mp 71-74°. $[\alpha]_D$ +121.9 (c, 1 in MeOH). λ_{max} 219 (log ε 4.39); 262 (log ε 3.93); 310 (log ε 3.66) (MeOH).

6-Me ether, 5-(2,4-dihydroxy-6-methylbenzoyl): [96627-13-3] ***4-O-Methylmelleolide***
$C_{24}H_{30}O_6$ 414.497
From *Armillaria mellea* (honey mushroom). Prisms (EtOAc/hexane). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 189-191°. $[\alpha]_D^{21}$ +71 (c, 0.31 in $CHCl_3$). λ_{max} 215 (ε 32000); 262 (ε 16800); 299 (ε 6405) (MeOH) (Berdy).

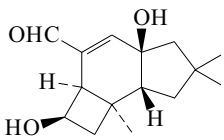
6-Me ether, 5-(3-chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [126006-70-0] ***6-O-Methylarmillaridin***. *4-O-Methylarmillaridin*
$C_{25}H_{31}ClO_6$ 462.969
Metab. of *Armillaria mellea* (honey mushroom). Cryst. (EtOAc/hexane). Sol. MeOH, hexane; poorly sol. H_2O. Mp 132-136°. $[\alpha]_D^{21}$ +74 (c, 0.2 in MeOH). λ_{max} 261 (ε 29030); 310 (ε 20179) (MeOH) (Berdy).

5-Ketone, 14-alcohol: [181644-53-1] *6,14-Dihydroxy-7-protoilluden-5-one.* ***Lentinellone***
$C_{15}H_{22}O_3$ 250.337
Oil. $[\alpha]_D^{23}$ +286 (c, 0.36 in $CHCl_3$). λ_{max} 208 (ε 3600); 310 (ε 195) (MeOH) (Berdy).

14-Carboxylic acid, 5-(2,4-dihydroxy-6-methylbenzoyl): [129251-06-5] ***Armillaric acid***
$C_{23}H_{28}O_7$ 416.47
Isol. from *Armillaria mellea* (honey mushroom). Brown powder. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 222 (ε 25200); 266 (ε 15198); 302 (ε 3930) (MeOH) (Berdy).

Midland, S.L. *et al., Tet. Lett.*, 1982, 2515 (*isol, cryst struct*)
Junshan, Y. *et al., Planta Med.*, 1984, **50**, 288 (*isol*)
Yang, J. *et al., Planta Med.*, 1984, **50**, 288 (*Melleolide*)
Donnelly, D.M.X. *et al., J. Nat. Prod.*, 1985, **48**, 10; 1986, **49**, 111 (*4-O-Methylmelleolide*)
Arnone, A. *et al., Gazz. Chim. Ital.*, 1988, **118**, 517 (*bibl*)
Hayek, E.W.H. *et al., Phytochemistry*, 1989, **28**, 2229 (*rev*)
Donnelly, D.M.X. *et al., Phytochemistry*, 1990, **29**, 179 (*derivs*)
Obuchi, T. *et al., Planta Med.*, 1990, **56**, 198 (*Armillaric acid*)
Wunder, A. *et al., Z. Naturforsch., C*, 1996, **51**, 493 (*Lentinellone*)
Momose, I. *et al., J. Antibiot.*, 2000, **53**, 137-143 (*Melleolide K*)
Cremin, P. *et al., J.C.S. Perkin 1*, 2325-2329 (*iso, activity*)

5,9-Dihydroxy-7-protoilluden-14-al D-678



$C_{15}H_{22}O_3$ 250.337

(5β,9β)-*form*

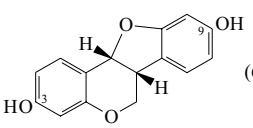
5-(2,4-Dihydroxy-6-methylbenzoyl): [135247-96-0] ***Armillaritin***
$C_{23}H_{28}O_6$ 400.471
Metab. of *Armillaria mellea* (honey mushroom). Gum. $[\alpha]_D$ +136.5 (c, 0.52 in $CHCl_3$).

5-(2-Hydroxy-4-methoxy-6-methylbenzoyl): [129741-56-6] ***Armillaripin***
$C_{24}H_{30}O_6$ 414.497
Constit. of *Armillaria mellea* (honey mushroom). Mp 202-204°. $[\alpha]_D^{15}$ +130 (c, 0.05 in $CHCl_3$).

Yang, J.S. *et al., Yaoxue Xuebao*, 1990, **25**, 353
Yang, J.S. *et al., Yaoxue Xuebao*, 1991, **26**, 117; *CA*, **115**, 89082s

3,9-Dihydroxypterocarpan D-679

6a,11a-Dihydro-6H-benzofuro[3,2-c][1]benzopyran-3,9-diol, 9CI. Demethylmedicarpin



(6a*R*,11a*R*)-*form*

$C_{15}H_{12}O_4$ 256.257
λ_{max} 211 ; 284 (EtOH) (Berdy). λ_{max} 215 ; 248 ; 297 (EtOH/NaOH) (Berdy).

(6a*R*,11a*R*)-*form* [61135-91-9]
Pale yellow amorph. powder. λ_{max} 282 (sh) ; 286 (MeOH).

3-Me ether: [74560-05-7] *9-Hydroxy-3-methoxypterocarpan*. ***Isomedicarpin***
$C_{16}H_{14}O_4$ 270.284
Constit. of *Psophocarpus tetragonolobus* (winged bean). Cryst. Mp 106°. $[\alpha]_D^{18}$ -

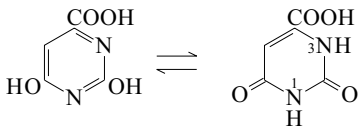
201 ($CHCl_3$). λ_{max} 283 (sh) (log ϵ 3.78); 286 (log ϵ 3.82); 292 (sh) (log ϵ 3.63) (EtOH) (Berdy).

[70144-19-3, 129262-45-9]

Preston, N.W. *et al., Phytochemistry*, 1977, **16**, 2044-2045 (*Isomedicarpin*)
Ingham, J.L. *et al., Phytochemistry*, 1980, **19**, 1203-1207 (*Isomedicarpin*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1-266 (*rev, occur*)

2,6-Dihydroxy-4-pyrimidinecarboxylic acid D-680

[65-86-1]
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid, 9CI. ***Orotic acid, BAN, INN****. Uracil-6-carboxylic acid. Vitamin B_{13}. Whey factor. Many other names*



$C_5H_4N_2O_4$ 156.098

Intermediate tautomers also possible. Exists as the dioxo tautomer in the cryst. state. Occurs in milk and other biol. systems. Salts used as dietary and mineral supplements. Cryst. + $1H_2O$ (H_2O). Mp 322-325° Mp 345-346°. pK_{a1} 1.8; pK_{a2} 9.55 (25°). Log P -0.75 (calc).

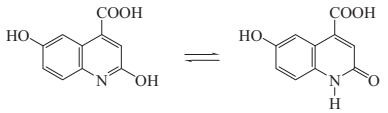
► LD_{50} (mus, orl) 2000 mg/kg. RM3180000

[154-85-8, 5266-20-6, 22454-86-0, 24598-73-0, 50887-69-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 834A (*ir*)
Sadtler Standard C-13 NMR Spectra, 16598 (*cmr*)
Nyc, J.F. *et al., J.A.C.S.*, 1947, **69**, 1382 (*synth*)
Deghenghi, R. *et al., Can. J. Chem.*, 1960, **38**, 1255 (*synth*)
Kokko, J.P. *et al., J.A.C.S.*, 1962, **84**, 1042 (*pmr*)
Rambacher, P. *et al., Angew. Chem., Int. Ed.*, 1968, **7**, 383 (*synth*)
Takusagawa, F. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2011 (*cryst struct*)
Ivin, B.A. *et al., Zh. Org. Khim.*, 1976, **12**, 1836; *J. Org. Chem. USSR (Engl. Transl.)*, 1976, **12**, 1802 (*synth*)
Walther, H. *et al., Pharmazie*, 1979, **34**, 309 (*pharmacol*)
Cihak, A. *et al., Orotic Acid*, MTP: Lancaster, U.K., 1980, (*book*)
Falk, M. *et al., Pharmazie*, 1985, **40**, 377 (*rev, props*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A12**, 156 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 261
Mirzoyan, V.S. *et al., Khim. Geterotsikl. Soedin.*, 1990, 520; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1990, 446 (*ms*)
Párkányi, C. *et al., Struct. Chem.*, 1992, **3**, 277 (*uv*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1396
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OJV500

2,6-Dihydroxy-4-quinolinecarboxylic acid D-681

[4363-99-9]
1,2-Dihydro-6-hydroxy-2-oxo-4-quinolinecarboxylic acid. 2,6-Dihydroxycinchoninic acid. β-Acid



$C_{10}H_7NO_4$ 205.17
Mp 326° (browns at 300°).

Me ester: [66416-75-9]
$C_{11}H_9NO_4$ 219.196
Alkaloid from the aleurone layer of rice *Oryza sativa* cv. *heugjinmi*. Pale yellow needles. Mp >320° λ_{max} 242 (log ϵ 4.8); 280 (log ϵ 4.4); 382 (log ϵ 4.2) (MeOH).

Sahashi, Y. *et al., Biochem. Z.*, 1927, **189**, 208
Makino, K. *et al., Bull. Chem. Soc. Jpn.*, 1944, **19**, 95
Chung, H.S. *et al., J. Nat. Prod.*, 2001, **64**, 1579-1580 (*Me ester, isol*)

2,8-Dihydroxy-4-quinolinecarboxylic acid D-682

[30536-55-1]
1,2-Dihydro-8-hydroxy-2-oxo-4-quinolinecarboxylic acid. 2,8-Dihydroxycinchoninic acid. 8-Hydroxy-2(1H)-quinolinone-4-carboxylic acid. ***Zeanic acid***

$C_{10}H_7NO_4$ 205.17
Isol. from corn steep liquor. Needles ($CHCl_3$/MeOH). Mp 340° dec.

O-*β-D-Glucopyranoside:* [113202-67-8]
Zeanoside B
$C_{16}H_{17}NO_9$ 367.312
Isol. from immature corn kernels (*Zea mays*) (Gramineae). Sl. yellow needles. Mp 297-302°. $[\alpha]_D^{23}$ -69.4 (c, 0.1 in NH_4OH).

Me ether: [37749-17-0] *1,2-Dihydro-8-methoxy-2-oxo-4-quinolinecarboxylic acid. 2-Hydroxy-8-methoxy-4-quinolinecarboxylic acid*
$C_{11}H_9NO_4$ 219.196
Mp 310° dec.

Matsushima, M. *et al., Agric. Biol. Chem.*, 1970, **34**, 1430
Fukumi, H. *et al., Yakugaku Zasshi*, 1974, **94**, 768
Tateishi, K. *et al., Agric. Biol. Chem.*, 1987, **51**, 3445 (*Zeanoside B*)
Shibata, H. *et al., Agric. Biol. Chem.*, 1989, **53**, 849; 2545 (*Zeanoside B*)

4,6-Dihydroxy-2-quinolinecarboxylic acid D-683

1,4-Dihydro-6-hydroxy-4-oxo-2-quinolinecarboxylic acid, 9CI. 6-Hydroxykynurenic acid

$C_{10}H_7NO_4$ 205.17
Alkaloid from *Ginkgo biloba* (ginkgo). Mp 287° dec.

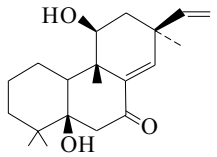
6-Me ether: [52980-06-0] *1,4-Dihydro-6-methoxy-4-oxo-2-quinolinecarboxylic acid. 4-Hydroxy-6-methoxy-2-quinolinecarboxylic acid.* ***6-Methoxykynurenic acid***

$C_{11}H_9NO_4$ 219.196
Cryst. (MeOH). Mp 298-300° dec. (294-295° dec.).

[3778-29-8, 52980-07-1]

Macnicol, P.K. *et al., Biochem. J.*, 1968, **107**, 473 (*isol, struct, synth, ir, pmr, uv, occur*)
Hall, C.M. *et al., J. Med. Chem.*, 1974, **17**, 685 (*synth, 6-Methoxykynurenic acid*)
Mendez, J. *et al., Phytochemistry*, 1975, **14**, 1136 (*isol*)
Schennen, A. *et al., Planta Med.*, 1986, 235 (*isol, cmr*)
Starratt, A.N. *et al., Phytochemistry*, 1996, **42**, 1477 (*isol, 6-Methoxykynurenic acid*)

5,11-Dihydroxy-8(14),15-rosadien-7-one D-684

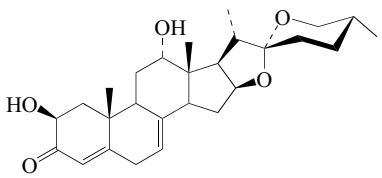


$C_{20}H_{30}O_3$ 318.455

(5β,11β)-*form* [62574-18-9]
Ineketone
Isol. from *Oryza sativa* (rice). Cryst. (EtOH/hexane). Mp 206-209°.

Kato, T. *et al., Phytochemistry*, 1977, **16**, 45

2,12-Dihydroxyspirosta-4,7-dien-3-one D-685

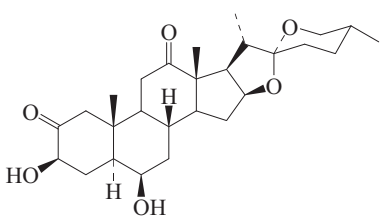


$C_{27}H_{38}O_5$ 442.594

(2β,12α,25*R*)-*form* [197080-19-6]
Muzanzagenin
Constit. of the wild asparagus (*Asparagus africanus*). Pale yellow needles (MeOH aq.). Mp 230°. $[\alpha]_D^{21}$ -99.9 (c, 0.8 in MeOH). λ_{max} 237 (log ϵ 4.18) (MeOH).

Oketch-Rabah, H.A. *et al., J. Nat. Prod.*, 1997, **60**, 1017-1022 (*isol, pmr, cmr, cryst struct*)

3,6-Dihydroxyspirostane-2,12-dione D-686



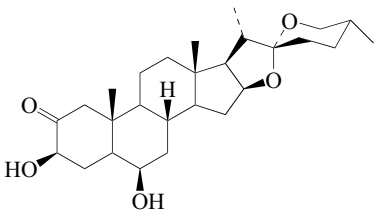
$C_{27}H_{40}O_6$ 460.609

(3β,5α,6β,25*R*)-*form*
3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-

xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [289690-77-3]
$C_{50}H_{78}O_{25}$ 1079.151
Constit. of *Allium porrum* (leeks). $[\alpha]_D^{25}$ -13 (c, 0.003 in MeOH).

Fattorusso, E. *et al., J. Agric. Food Chem.*, 2000, **48**, 3455-3462 (*isol, pmr, cmr*)

3,6-Dihydroxyspirostan-2-one D-687



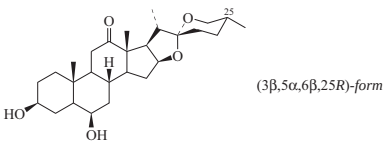
$C_{27}H_{42}O_5$ 446.626

(3β,5α,6β,25*R*)-*form* [196607-73-5]
Porrigenin B
Constit. of *Allium porrum* (leeks). Powder. $[\alpha]_D^{25}$ -28 (c, 0.03 in $CHCl_3$/MeOH).

(3β,5α,6β,25*S*)-*form* [196607-74-6]
Neoporrigenin B
Constit. of *Allium porrum* (leeks). Powder. $[\alpha]_D^{25}$ -42 (c, 0.003 in $CHCl_3$/MeOH).

Carotenuto, A. *et al., J. Nat. Prod.*, 1997, **60**, 1003-1007 (*isol, pmr, cmr*)

3,6-Dihydroxyspirostan-12-one D-688



$C_{27}H_{42}O_5$ 446.626

(3β,5α,6β,25*R*)-*form* [189014-45-7]
12-Ketoporrigenin
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -13 (c, 0.03 in $CHCl_3$).

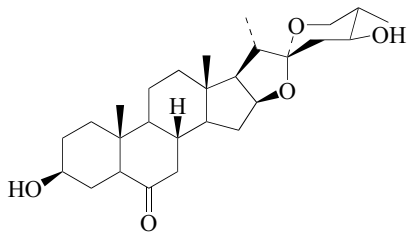
3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [289690-76-2]
$C_{50}H_{80}O_{24}$ 1065.168
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -13 (c, 0.003 in MeOH).

Diketone: [214681-60-4] ***Spirostane-3,6,12-trione***
$C_{27}H_{38}O_5$ 442.594
Cryst. (MeOH). Mp 267-269°.

(3β,5α,6β,25*S*)-*form* [189007-91-8]
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -31 (c, 0.003 in $CHCl_3$).

Carotenuto, A. *et al., Tetrahedron*, 1997, **53**, 3401-3406 (*isol, pmr, cmr*)
Xu, Y.X. *et al., Phytochemistry*, 1998, **49**, 199-201 (*trione*)
Fattorusso, E. *et al., J. Agric. Food Chem.*, 2000, **48**, 3455-3462 (*Allium porrum constit*)

3,24-Dihydroxyspirostan-6-one D-689



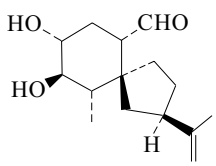
$C_{27}H_{42}O_5$ 446.626

(3β,24*S*,25*R*)-*form*
3-O-[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside], 24-O-β-D-glucopyranoside: [200483-13-2] ***Chinenoside VI***
$C_{44}H_{70}O_{19}$ 903.026
Constit. of *Allium chinense* (rakkyo). Amorph. powder. Mp 219-221°.

Jiang, Y. *et al., Chin. Chem. Lett.*, 1997, **8**, 965-966 (*isol, pmr, cmr*)
Jiang, Y. *et al., Stud. Plant Sci.*, 1999, **6**, 212-219 (*isol, pmr, cmr*)

2,3-Dihydroxy-11-spirovetiven-14-al D-690

[55784-90-2]
Oxylubimin. *4-Hydroxylubimin*



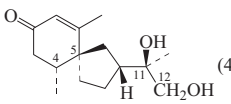
$C_{15}H_{24}O_3$ 252.353
Isol. from potato tubers infected with *Phytophthora infestans*. Cryst. Mp 96-98° (85-86°). $[\alpha]_D^{32}$ +55 (c, 0.5 in EtOH).

10-Epimer: [69350-60-3] ***Epioxylubimin***
$C_{15}H_{24}O_3$ 252.353
Isol. from potato tubers infected with *Phytophthora infestans*. Cryst. (diisopropyl ether). Sol. H_2O; poorly sol. MeOH, hexane. Mp 123-124°. $[\alpha]_D$ -12.1 ($CHCl_3$).

Birnbaum, G.I. *et al., Chem. Comm.*, 1976, 330 (*biosynth*)
Matsunaga, A. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 1217 (*struct*)
Birnbaum, G.I. *et al., Can. J. Chem.*, 1977, **55**, 1619 (*cryst struct*)
Stoessl, A. *et al., Can. J. Chem.*, 1978, **56**, 645 (*biosynth*)
Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2424 (*Epilubimin*)
Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 2286; 2291 (*synth*)
Iwata, C. *et al., Chem. Pharm. Bull.*, 1990, **38**, 361 (*synth*)

11,12-Dihydroxy-1(10)-spirovetiven-2-one D-691

[62574-30-5]
2-(1,2-Dihydroxy-1-methylethyl)-6,10-dimethylspiro[4.5]dec-6-en-8-one, 9CI



$C_{15}H_{24}O_3$ 252.353

(4*R***,5***S***,7***R***,11***R***)-*form***
Constit. of potato tubers infected with *Phoma foveata* and *Fusarium* spp.. $[\alpha]_D$ -72 (c, 0.4 in MeOH). λ_{max} 242 (MeOH).

(4*R***,5***S***,7***R***,11***S***)-*form***
Constit. of potato tubers infected with *Phoma foveata* and *Fusarium* spp.. $[\alpha]_D$ -120 (c, 0.9 in MeOH). λ_{max} 242 (MeOH).

11-O-β-D-Glucopyranoside:
$C_{21}H_{34}O_8$ 414.495
Constit. of potato tubers infected with *Phoma foveata* and *Fusarium* spp.. $[\alpha]_D$ -84 (c, 0.5 in MeOH). λ_{max} 242 (MeOH).

(4*R***,5***S***,7***R***,11ξ)-*form***
Constit. of potatoes infected with *Phoma exigua*. Amorph. $[\alpha]_D^{23}$ -55 (c, 0.1 in EtOH). λ_{max} 242 (EtOH).

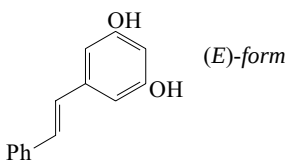
12-O-β-D-Glucopyranoside: [62574-29-2]
$C_{21}H_{34}O_8$ 414.495
Isol. from potatoes infected with *Phoma exigua*. Amorph. $[\alpha]_D^{23}$ -75.7 (c, 0.1 in EtOH). Obt. as a mixture of diastereoisomers.

[62623-86-3, 62623-87-4, 65634-25-5, 76648-57-2]

Anderson, R.C. *et al., Chem. Comm.*, 1977, 27-28 (*isol, abs config, cmr*)
Malmberg, A.G. *et al., Phytochemistry*, 1980, **19**, 1739-1742 (*isol*)
Afzal, M. *et al., Heterocycles*, 1986, **24**, 2943-2961 (*pmr, cmr*)
Engström, K. *et al., Phytochemistry*, 1998, **47**, 985-990 (*isol, pmr, cmr*)

3,5-Dihydroxystilbene D-692

[102-61-4]
5-(2-Phenylethenyl)-1,3-benzenediol, 9CI. 1-(3,5-Dihydroxyphenyl)-2-phenylethylene. 5-Styrylresorcinol. 3,5-Stilbenediol. ***Pinosylvin***



$C_{14}H_{12}O_2$ 212.248

(E)*-*form [22139-77-1]
Needles (AcOH). Sol. EtOH, Me_2CO, Et_2O; fairly sol. H_2O. Mp 160° (155.5-156°). Log P 3.1 (calc). λ_{max} 305 (ε 30900) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 20 mg/kg ; LD_{50} (mus, ipr) 20 mg/kg. WJ5580000

Di-Ac:
$C_{18}H_{16}O_4$ 296.322
Mp 100-101°.

Mono-O-β-D-glucopyranoside: [119600-62-3]
$C_{20}H_{22}O_7$ 374.39

Di-O-β-D-glucopyranoside: [156302-22-6] ***Pinosylvin diglucoside***

$C_{26}H_{32}O_{12}$ 536.532
Cryst. (MeOH). Mp 178-180° (synthetic). $[\alpha]_D$ -82.7 (c, 0.1 in Me_2CO aq.) (synthetic).

Mono-Me ether: [5150-38-9] *3-Methoxy-5-(2-phenylethenyl)phenol, 9CI. 3-Hydroxy-5-methoxystilbene. 5-Methoxy-3-stilbenol*
$C_{15}H_{14}O_2$ 226.274
Cryst. Mp 122-123°.

Di-Me ether: [21956-56-9]
$C_{16}H_{16}O_2$ 240.301
Isol. from wood of *Pinus palustris* (pitch pine). Prisms (MeOH). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 56-57°. λ_{max} 305 (ϵ 24550) (MeOH) (Berdy).

(*Z*)-*form* [106325-78-4]

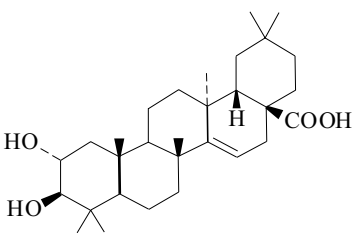
Mono-Me ether:
Gum.

Di-Me ether: [21956-55-8]
$Bp_{0.02}$ 123°.

Erdtman, H. *et al., Annalen*, 1939, **539**, 116 (*isol, struct*)
Cox, R.F.B. *et al., J.A.C.S.*, 1940, **62**, 3512 (*isol, struct*)
Liebherr, E. *et al., Ber.*, 1941, **74**, 869 (*synth*)
Erdtman, H. *et al., Phytochemistry*, 1966, **5**, 927 (*isol*)
Rowe, J.W. *et al., Phytochemistry*, 1969, **8**, 235 (*isol, derivs*)
Bachelor, F.W. *et al., Can. J. Chem.*, 1970, **48**, 1554 (*synth*)
Cardona, L. *et al., Tetrahedron*, 1986, **42**, 2725 (*synth, pmr, cmr*)
Miyaichi, Y. *et al., CA*, 1989, **110**, 141364y (*monoglucoside*)
Zhang, J.-Z. *et al., Planta Med.*, 1994, **60**, 190 (*diglucoside*)

2,3-Dihydroxy-14-taraxeren-28-oic acid D-693

2,3-Dihydroxy-D-friedoolean-14-en-28-oic acid, 9CI



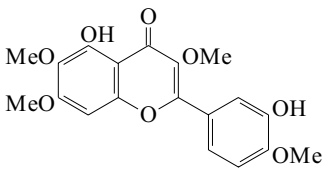
$C_{30}H_{48}O_4$ 472.707

(2α,3β)-*form* [94390-09-7]
Sebiferenic acid. *2α-Hydroxymaprounic acid. 2α-Hydroxyaleuritolic acid*
Constit. of *Sapium sebiferum* (Chinese tallowtree). Cryst. Mp 297-299° Mp 325° dec. $[\alpha]_D$ +25 (c, 0.18 in Py). $[\alpha]_D$ +32 ($CHCl_3$).

Wani, M.C. *et al., J. Nat. Prod.*, 1983, **46**, 537 (*isol*)
Pradhan, B.P. *et al., Phytochemistry*, 1984, **23**, 2593
McPhail, A.T. *et al., J. Nat. Prod.*, 1989, **52**, 212 (*struct*)
Pengsuparp, T. *et al., J. Nat. Prod.*, 1994, **57**, 415 (*isol*)
Chaudhuri, S.K. *et al., J. Nat. Prod.*, 1995, **58**, 1 (*isol, pmr, cmr*)

3′,5-Dihydroxy-3,4′,6,7-tetramethoxyflavone D-694

[479-91-4]
*5-Hydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6,7-trimethoxy-4*H*-benzopyran-4-one, 9CI*. ***Casticin***. *Vitexicarpin*



$C_{19}H_{18}O_8$ 374.346

Originally thought to be 3,5-Dihydroxy-3′,4′,7,8-tetramethoxyflavone. Struct. revised in 1989. Constit. of *Vitex agnus-castus* (agnus castus) seeds. Prisms (C_6H_6/petrol). Mp 186-187°. λ_{max} 233 (sh) (ϵ 11500); 268 (ϵ 14800); 335 (ϵ 6760); 375 (ϵ 5750) (MeOH/NaOH) (Derep). λ_{max} 257 (ϵ 10200); 267 (sh) (ϵ 8710); 347 (ϵ 11000) (MeOH) (Derep).

3′-O-β-D-Glucopyranoside: [71827-14-0]
$C_{25}H_{28}O_{13}$ 536.488
Pale yellow needles (MeOH aq.). Mp 179-183°.

Belič, I. *et al., J.C.S.*, 1961, 2523
Hörhammer, L. *et al., Tet. Lett.*, 1964, 323 (*struct*)
Hansel, R. *et al., Phytochemistry*, 1965, **4**, 19 (*isol*)
Djermanović, M. *et al., Phytochemistry*, 1975, **14**, 1873 (*isol, uv, ms, pmr*)
Rodriguez, E. *et al., Biochem. Syst. Ecol.*, 1977, **5**, 207 (*isol*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 708 (*cmr*)
Collins, F.W. *et al., Z. Naturforsch., C*, 1981, **36**, 730 (*uv, pmr, ms, glycoside*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Esteban, M.D. *et al., Phytochemistry*, 1986, **25**, 1502 (*isol*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Horie, T. *et al., Phytochemistry*, 1989, **28**, 2869 (*isol, struct*)
You, K.M. *et al., Planta Med.*, 1998, **64**, 546-550 (*activity*)
Ragasa, C. *et al., Philipp. J. Sci.*, 1999, **128**, 21-29 (*isol, activity*)
Ko, W.G. *et al., Food Chem. Toxicol.*, 2000, **38**, 861-865 (*activity*)

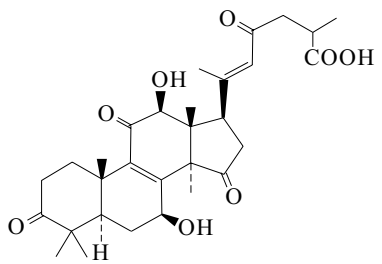
5,7-Dihydroxy-3′,4′,6,8-tetramethoxyflavone D-695

[56003-01-1]
*2-(3,4-Dimethoxyphenyl)-5,7-dihydroxy-6,8-dimethoxy-4*H*-1-benzopyran-4-one, 9CI*. ***Hymenoxin***

$C_{19}H_{18}O_8$ 374.346
Isol. from *Mentha piperita* (peppermint). Yellow cryst. (MeOH). Mp 215-216°. λ_{max} 281 (ϵ 17400); 340 (ϵ 20300) (MeOH) (Berdy). λ_{max} 253 ; 378 (MeOH/NaOH) (Berdy).

Thomas, M.B. *et al., J.O.C.*, 1967, **32**, 3254 (*isol, synth, uv, ir, pmr*)
Waddell, T.G. *et al., Phytochemistry*, 1973, **12**, 2061 (*isol, pmr, ms*)
Ohno, N. *et al., Phytochemistry*, 1981, **20**, 2393 (*isol*)
Zakharova, O.I. *et al., Khim. Prir. Soedin.*, 1982, **18**, 652; 1983, **19**, 645; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 619; 1983, **19**, 611 (*isol*)
Herz, W. *et al., Phytochemistry*, 1983, **22**, 2021 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Schilling, E. *et al., Biochem. Syst. Ecol.*, 1985, **13**, 403 (*isol*)
Chen, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 1235-1238 (*isol, uv, pmr, cmr, ms*)

7,12-Dihydroxy-3,11,15,23-tetraoxolanosta-8,20(22)-dien-26-oic acid D-696

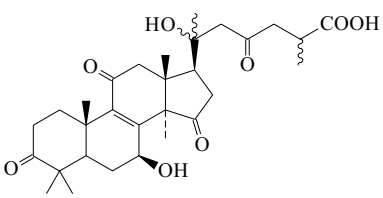


$C_{30}H_{40}O_8$ 528.641

(7β,12β,20(22)*E*)-*form* [110241-23-1]
Ganoderenic acid E
Constit. of *Ganoderma lucidum* (reishi). Cryst. (EtOAc/MeOH) (as Me ester). Mp 227-229° (Me ester).

Nishitoba, T. *et al., Phytochemistry*, 1987, **26**, 1777

7,20-Dihydroxy-3,11,15,23-tetraoxolanost-8-en-26-oic acid D-697



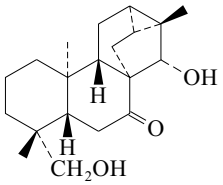
$C_{30}H_{42}O_8$ 530.657

(7β,20ξ)-*form* [110241-19-5]
Ganoderic acid N
Constit. of *Ganoderma lucidum* (reishi). Cryst. (EtOAc/cyclohexane) (as Me ester). Mp 164-167° (Me ester). $[\alpha]_D^{24}$ +153 (c, 0.2 in MeOH) (Me ester).

7-Ketone: [110241-21-9] ***Ganoderic acid O***†. *20ξ-Hydroxy-3,7,11,15,23-pentaoxolanost-8-en-26-oic acid*
$C_{30}H_{40}O_8$ 528.641
Constit. of *Ganoderma lucidum* (reishi). Pale yellow needles (Et_2O/hexane) (as Me ester). Mp 168-171° (Me ester). Not the same as Ganoderic acid O in 3,7,15,22-Tetrahydroxylanosta-8,24-dien-26-oic acid, T-228.

Nishitoba, T. *et al., Phytochemistry*, 1987, **26**, 1777

15,19-Dihydroxy-7-trachylobanone D-698



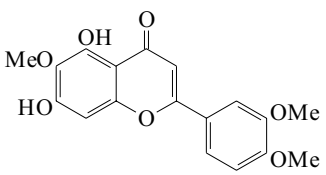
$C_{20}H_{30}O_3$ 318.455

(*ent*-15β)-*form* [137648-01-2]
Constit. of *Helianthus annuus* (sunflower).

Alfatafta, A.A. *et al., Phytochemistry*, 1992, **31**, 4109 (*isol, pmr, cmr*)

5,7-Dihydroxy-3′,4′,6-trimethoxyflavone D-699

[22368-21-4]
*2-(3,4-Dimethoxyphenyl)-5,7-dihydroxy-6-methoxy-4*H*-1-benzopyran-4-one, 9CI.* ***Eupatilin***



$C_{18}H_{16}O_7$ 344.32

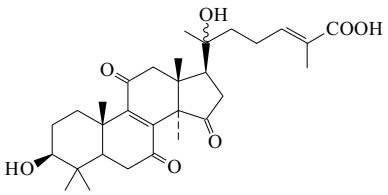
Not to be confused with Eupalitin. Isol. from *Tanacetum vulgare* (tansy). Cryst. (EtOAc). Mp 241-242° (234-236°). λ_{max} 243 (ϵ 20500); 277 (ϵ 17000); 340 (ϵ 26300) (EtOH) (Berdy).

► Cytotoxic.

Di-Ac:
Cryst. (C_6H_6/petrol); needles (MeOH). Mp 154-155° Mp 165-167° Mp 220-221°.

Kupchan, S.M. *et al., Tetrahedron*, 1969, **25**, 1603 (*isol, struct*)
Horie, T. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 3198 (*synth*)
Wagner, H. *et al., Chem. Ber.*, 1974, **107**, 1049 (*synth*)
Midge, M.D. *et al., Indian J. Chem.*, 1975, **13**, 541 (*synth*)
Goudard, M. *et al., Phytochemistry*, 1978, **17**, 145 (*ms*)
Gupta, S.R. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 37 (*synth*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Horie, T. *et al., Yakugaku Zasshi*, 1985, **105**, 232 (*synth*)
Nakasugi, T. *et al., J. Agric. Food Chem.*, 2000, **48**, 3256-3266 (*activity*)

3,20-Dihydroxy-7,11,15-trioxolanosta-8,24-dien-26-oic acid D-700

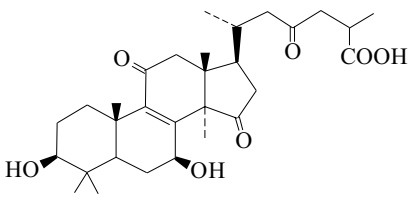


$C_{30}H_{42}O_7$ 514.658

(3β,20ξ,24*E*)-*form* [150033-91-3]
Ganoderic acid V₁
Metab. of *Ganoderma lucidum* (reishi). Cryst. Mp 234-234.5°. $[\alpha]_D^{21}$ +100 (c, 0.12 in $CHCl_3$).

Hirotani, M. *et al., Phytochemistry*, 1993, **33**, 379 (*isol, pmr, cmr*)

3,7-Dihydroxy-11,15,23-trioxolanost-8-en-26-oic acid D-701



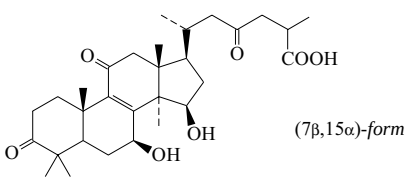
$C_{30}H_{44}O_7$ 516.673

(3β,7β)-*form* [81907-61-1]
Ganoderic acid B
Constit. of *Ganoderma lucidum* (reishi). Amorph. powder. Sol. MeOH, bases, $CHCl_3$; poorly sol. H_2O, hexane.

Me ester:
Cryst. (EtOAc). Mp 202.5-203°.

Kubota, T. *et al., Helv. Chim. Acta*, 1982, **65**, 611
Kohda, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1367-1374 (*isol*)
Koyama, I.K. *et al., Planta Med.*, 1997, **63**, 224-227 (*activity*)

7,15-Dihydroxy-3,11,23-trioxolanost-8-en-26-oic acid D-702



(7β,15α)-*form*

$C_{30}H_{44}O_7$ 516.673

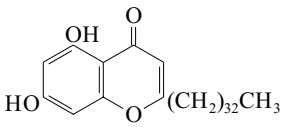
(7β,15α)-*form* [81907-62-2]
Ganoderic acid A
Constit. of *Ganoderma lucidum* (reishi). Amorph. powder. Sol. MeOH, bases, $CHCl_3$; poorly sol. H_2O, hexane, acids. $[\alpha]_D^{27}$ +153.8 (c, 0.156 in $CHCl_3$).

Me ester:
Cryst. (EtOH). Mp 196-197°.

Kubota, T. *et al., Helv. Chim. Acta*, 1982, **65**, 611
Hirotani, U. *et al., Phytochemistry*, 1985, **24**, 2055-2061 (*isol*)
Koyama, K. *et al., Planta Med.*, 1997, **63**, 224-227 (*activity*)
Lee, S. *et al., Planta Med.*, 1998, **64**, 303-308 (*activity*)

5,7-Dihydroxy-2-tritriacontyl-4*H*-1-benzopyran-4-one D-703

5,7-Dihydroxy-2-tritriacontylchromone



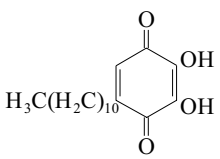
$C_{42}H_{72}O_4$ 641.028

7-Me ether: [144049-68-3] *5-Hydroxy-7-methoxy-2-tritriacontyl-4*H*-1-benzopyran-4-one, 9CI. 5-Hydroxy-7-methoxy-2-tritriacontylchromone*
$C_{43}H_{74}O_4$ 655.055
Constit. of the famine food *Agave americana*. Needles ($CHCl_3$/petrol). Mp 83°. λ_{max} 251 (MeOH) (Berdy).

Parmer, V.S. *et al., Tetrahedron*, 1992, **48**, 1281

2,3-Dihydroxy-5-undecyl-1,4-benzoquinone D-704

[145040-57-9]
2,3-Dihydroxy-5-undecyl-2,5-cyclohexadiene-1,4-dione, 9CI. ***Myrsinone***

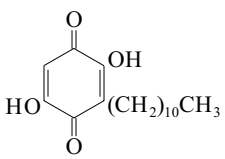


$C_{17}H_{26}O_4$ 294.39
Constit. of *Myrsine africana* (cape myrtle). Orange-red cryst. (CH_2Cl_2/hexane). Mp 120-122°.

Midiwo, J.O. *et al., Bull. Chem. Soc. Ethiop.*, 1992, **6**, 15 (*isol, pmr, cmr*)

2,5-Dihydroxy-3-undecyl-1,4-benzoquinone D-705

[550-24-3]
2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione, 9CI. ***Embelin****. Embelic acid. Embeliaquinone*



$C_{17}H_{26}O_4$ 294.39
Orange cryst. (MeOH or hexane/EtOH). Insol. H_2O. Mp 145-146°. Log P 5.14 (calc). λ_{max} 292 (ϵ 16200); 424 (ϵ 280) (95% EtOH) (Derep). λ_{max} 292 (ϵ 17400); 426 (ϵ 340) (MeOH) (Berdy).

► Exp. reprod. effects (male and female). DK4230000

Di-Ac:
$C_{21}H_{30}O_6$ 378.464

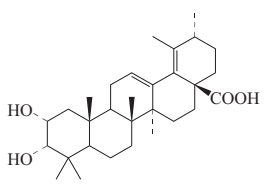
Yellow cryst. (MeOH aq.). Mp 54° Mp 59°.

5-Me ether: [56005-10-8] *2-Hydroxy-5-methoxy-3-undecyl-1,4-benzoquinone.* ***5-O-Methylembelin***
$C_{18}H_{28}O_4$ 308.417
Constit. of *Myrsine africana* (cape myrtle). Orange cryst. Mp 95-96°. λ_{max} 285 (ϵ 398) (95% EtOH) (Derep).

Di-Me ether:
$C_{19}H_{30}O_4$ 322.444
Cryst. (MeOH aq.). Mp 58°.

Merian, M. *et al., Helv. Chim. Acta*, 1948, **31**, 2237 (*isol*)
Fieser, L.F. *et al., J.A.C.S.*, 1948, **70**, 71 (*synth*)
Rao, C.B. *et al., Fresenius' Z. Anal. Chem.*, 1960, **175**, 114; 1961, **178**, 277; 1963, **198**, 183 (*detn, Th, U, Al, Be, Ba, Ca, Mg, Sr*)
Natori, S. *et al., Chem. Pharm. Bull.*, 1964, **12**, 236 (*ir, uv*)
Dallacker, F. *et al., Chem. Ber.*, 1972, **105**, 614 (*synth*)
Desai, H.K. *et al., Indian J. Chem., Sect. B*, 1975, **13**, 97; 1977, **15**, 291 (*isol*)
Joshi, B.S. *et al., J.C.S. Perkin 1*, 1975, 327 (*isol, ms, pmr*)
Thappa, R.K. *et al., Indian J. Pharm.*, 1976, **38**, 17 (*synth, pharmacol*)
Gupta, O.P. *et al., Indian J. Physiol. Pharmacol.*, 1977, **21**, 31 (*pharmacol*)
Gomez, E. *et al., J. Nat. Prod.*, 1989, **52**, 649 (*5-O-Methylembelin*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 42
Pfeifer, J. *et al., Annalen*, 1995, 131 (*synth, deriv, ir, pmr, cmr*)
Poigny, S. *et al., Tetrahedron*, 1998, **54**, 14791-14802 (*synth*)
Miles, D.H. *et al., Tetrahedron*, 2001, **57**, 5769-5772 (*5-O-Methylembelin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAJ600

2,3-Dihydroxy-12,18-ursadien-28-oic acid D-706



(2α,3α)-*form*

$C_{30}H_{46}O_4$ 470.691

(2α,3α)-*form* [138771-34-3]
Powder ($CHCl_3$). Mp 178°. $[\alpha]_D^{28}$ +89 (c, 0.5 in $CHCl_3$).

(2α,3β)-*form* [129058-59-9]

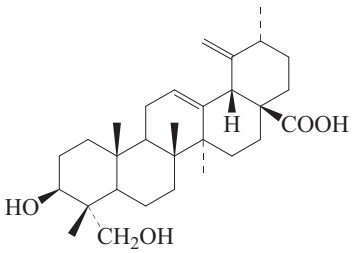
[138771-35-4]
Goreishic acid I
Cryst. (MeOH). Mp 189-199°. $[\alpha]_D^{26}$ +161 (c, 0.6 in MeOH).

(2ξ,3ξ)-*form*

Di-Ac: [273379-39-8]
$C_{34}H_{50}O_6$ 554.765
Constit. of *Pyrus communis* (pear).

Numata, A. *et al., Chem. Pharm. Bull.*, 1990, **38**, 942 (*isol, pmr, cmr*)
Ruecker, G. *et al., Planta Med.*, 1991, **57**, 468-470 (*isol, pmr, cmr, ms*)
Yang, S.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 1995, **42**, 573 (*isol, pmr, cmr*)
Younes, M.E. *et al., Egypt. J. Chem.*, 1999, **42**, 573-586; *CA*, **133**, 28459v (*di-Ac*)

3,23-Dihydroxy-12,19(29)-ursadien-28-oic acid D-707



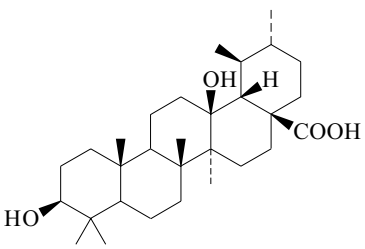
$C_{30}H_{46}O_4$ 470.691

3β-*form*

3-O-α-L-Arabinopyranoside, 28-O-β-D-glucopyranosyl ester: [356785-73-4]
$C_{41}H_{64}O_{13}$ 764.949
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Amorph. solid. $[\alpha]_D^{25}$ +24 (c, 0.1 in MeOH).

Mimaki, Y. *et al., Phytochemistry*, 2001, **57**, 773-779 (*isol, pmr, cmr*)

3,13-Dihydroxy-28-ursanoic acid D-708



$C_{30}H_{50}O_4$ 474.723

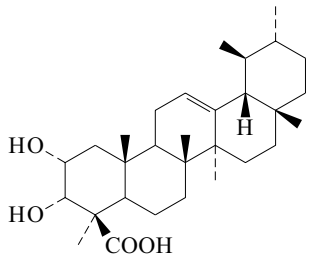
3β-*form*

28→13 Lactone: [29428-70-4] ***3β-Hydroxy-28,13-ursanolide.*** *Ursolic acid lactone*
$C_{30}H_{48}O_3$ 456.707
Isol. from *Helichrysum italicum* (curry plant). Cryst. Mp 253°. $[\alpha]_D^{20}$ +13 ($CHCl_3$).

28→13 Lactone, 3-Ac: [28290-51-9] *3β-Acetoxy-28,13-ursanolide.* ***Ursololactone***
$C_{32}H_{50}O_4$ 498.745
Isol. from *Helichrysum italicum* (curry plant). Mp 252-253°. $[\alpha]_D^{25}$ +12 ($CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1952, 78 (*synth*)
Mezzetti, T. *et al., Boll. Chim. Farm.*, 1969, **108**, 540; *CA*, **72**, 121740m (*isol*)
Schiaffella, F. *et al., Phytochemistry*, 1975, **14**, 584 (*isol*)
Katai, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1567 (*pmr, cmr*)
Begum, S. *et al., J. Nat. Prod.*, 2000, **63**, 1265-1268 (*isol, activity*)

2,3-Dihydroxy-12-ursen-24-oic acid D-709

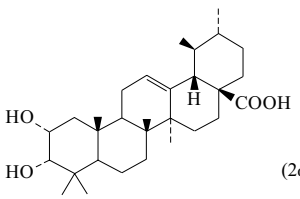


$C_{30}H_{48}O_4$ 472.707

(2α,3α)-*form* [164920-64-3]
Constit. of *Boswellia serrata* (Indian olibanum). Cryst. (EtOAc/petrol). Mp 174°.

Mahajan, B. *et al., Phytochemistry*, 1995, **39**, 453 (*isol, pmr, cmr*)

2,3-Dihydroxy-12-ursen-28-oic acid D-710



(2α,3α)-*form*

$C_{30}H_{48}O_4$ 472.707

(2α,3α)-*form* [52213-27-1]

*3-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* [351333-71-6]
$C_{40}H_{56}O_7$ 648.878
Constit. of *Eriobotrya japonica* (loquat). Amorph. powder. $[\alpha]_D^{22}$ +7.2 (c, 0.12 in MeOH). λ_{max} 217 (log ϵ 4.14); 237 (log ϵ 4.04); 297 (sh) (log ϵ 4.04); 324 (log ϵ 4.18) (MeOH).

(2α,3β)-*form* [4547-24-4]
Corosolic acid. *2α-Hydroxyursolic acid*
Cryst. (EtOH). Mp 243-245° dec. $[\alpha]_D$ +42.1 (c, 1 in Py).

3-(4-Hydroxy-Z-cinnamoyl):
$C_{39}H_{54}O_6$ 618.852
Constit. of *Leptospermum scoparium* (red tea). Amorph. powder (MeOH). Mp 200-203°.

*2-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):*
$C_{40}H_{56}O_7$ 648.878
Constit. of *Leptospermum scoparium* (red tea).

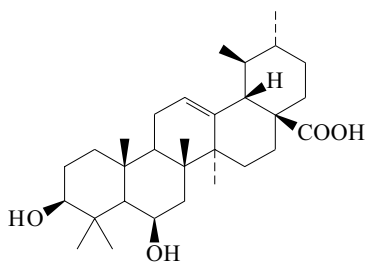
*3-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):*
$C_{40}H_{56}O_7$ 648.878
Constit. of *Leptospermum scoparium* (red tea). Cryst. (MeOH). Mp 186-188°.

*3-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):*
$C_{40}H_{56}O_7$ 648.878
Constit. of *Leptospermum scoparium* (red tea). Amorph. powder.

Glen, A.T. *et al., J. Solution Chem.*, 1967, 510 (*isol*)
Biessels, H.W.A. *et al., Phytochemistry*, 1974, **13**, 203 (*isol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1975, **28**, 91 (*isol*)

Seo, S. *et al., Chem. Comm.*, 1975, 270; 954 (*biosynth, pmr*)
Seo, S. *et al., Tet. Lett.*, 1975, 7 (*cmr*)
Ogura, M. *et al., Phytochemistry*, 1977, **16**, 286 (*deriv*)
Manzoor-i-Khuda, M. *et al., Z. Naturforsch., B*, 1979, **34**, 1320 (*deriv*)
Kojima, H. *et al., Phytochemistry*, 1986, **25**, 729; 1989, **28**, 1703 (*cmr*)
Siddiqui, S. *et al., Planta Med.*, 1987, **53**, 424 (*deriv*)
Kojimo, H. *et al., Phytochemistry*, 1989, **28**, 1703 (*pmr, cmr*)
Yang, M.-H. *et al., Planta Med.*, 1992, **38**, 227 (*cmr*)
Begum, S. *et al., Aust. J. Chem.*, 1993, **46**, 1067 (*synth*)
Häberlein, H. *et al., Phytochemistry*, 1994, **35**, 765 (*derivs*)
Monte, F.J.Q. *et al., Magn. Reson. Chem.*, 1997, **35**, 802-805 (*pmr, cmr*)
Ahn, K.-S. *et al., Planta Med.*, 1998, **641**, 468-470 (*activity*)
Ito, H. *et al., J. Nat. Prod.*, 2001, **64**, 737-740 (*Eriobotrya japonica ester*)

3,6-Dihydroxy-12-ursen-28-oic acid D-711



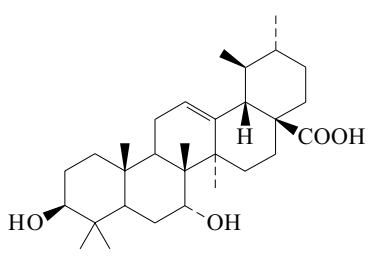
$C_{30}H_{48}O_4$ 472.707

(3β,6β)-*form* [89786-85-6]
6-Hydroxyursolic acid
Cryst. (MeOH). Mp 230-235°. $[\alpha]_D$ +36.7 (c, 1.25 in MeOH).

6-Ketone, 3-benzoyl: [205699-24-7] ***3-Benzoyloxy-6-oxo-12-ursen-28-oic acid***
$C_{37}H_{50}O_5$ 574.799
Constit. of the famine food *Momordica dioica*. Cryst. ($CHCl_3$/MeOH). Mp 256-259°.

Sakakibara, J. *et al., Phytochemistry*, 1983, **22**, 2553
Luo, L. *et al., Yunnan Zhiwu Yanjiu*, 1997, **19**, 316-320; *CA*, **128**, 268191s (*6-ketone-3-benzoyl*)

3,7-Dihydroxy-12-ursen-28-oic acid D-712



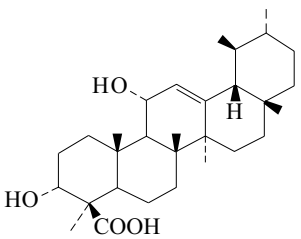
$C_{30}H_{48}O_4$ 472.707

(3β,7α)-*form* [28348-90-5]
Rubitic acid
Constit. of *Rubus fruticosus* (blackberry). Amorph. solid. Mp 252-254°. $[\alpha]_D$ +65 (MeOH).

3-Ketone: [94662-96-1] *7α-Hydroxy-3-oxo-12-ursen-28-oic acid.* ***Rubinic acid***
Constit. of *Rubus fruticosus* (blackberry). Cryst. (MeOH/$CHCl_3$). Mp 259-261°. $[\alpha]_D^{25}$ +72 (MeOH).

Sarkar, A. *et al., Phytochemistry*, 1978, **17**, 1983
Mukherjee, M. *et al., Phytochemistry*, 1984, **23**, 2581

3,11-Dihydroxy-12-ursen-24-oic acid D-713



$C_{30}H_{48}O_4$ 472.707

(3α,11α)-*form*

3-Ac:
$C_{32}H_{50}O_5$ 514.744
Cryst. (as Me ester). Mp 210-214° (Me ester). $[\alpha]_D$ +24 (c, 1 in $CHCl_3$) (Me ester).

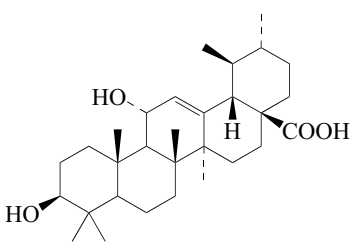
11-Ketone: [17019-92-0] *3-Hydroxy-11-oxo-12-ursen-24-oic acid.* ***11-Keto-β-boswellic acid***
$C_{30}H_{46}O_4$ 470.691
Constit. of *Boswellia serrata* (Indian olibanum). Cryst. (MeOH). Mp 190-191°. $[\alpha]_D$ +77.8.

11-Ketone, 3-Ac: [67416-61-9]
$C_{32}H_{48}O_5$ 512.728
Isol. from *Boswellia serrata* (Indian olibanum). Cryst. (C_6H_6/hexane). Mp 271°. $[\alpha]_D$ +87.3 (c, 4.2 in $CHCl_3$).

11-Ketone, 3-Ac, Me ester: [17019-95-3]
$C_{33}H_{50}O_5$ 526.755
Isol. from Olibanum. Mp 188-190°.

Corsano, S. *et al., Gazz. Chim. Ital.*, 1964, **94**, 328
Savoir, R. *et al., Bull. Soc. Chim. Belg.*, 1967, **76**, 368
Snatzke, G. *et al., Monatsh. Chem.*, 1967, **98**, 121
Pardhy, R.S. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 176

3,11-Dihydroxy-12-ursen-28-oic acid D-714



$C_{30}H_{48}O_4$ 472.707

(3β,11α)-*form*

11-Me ether, 3-Ac, Me ester: [189139-96-6]
$C_{34}H_{54}O_5$ 542.798
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. Mp 140.5-141°. $[\alpha]_D$ -82 (c, 0.25 in $CHCl_3$).

3-Ketone: [240473-11-4] ***11-Hydroxy-3-oxo-12-ursen-28-oic acid***
$C_{30}H_{46}O_4$ 470.691
Amorph. solid. $[\alpha]_D^{28}$ +10 (c, 0.32 in $CHCl_3$).

11-Ketone: [105870-59-5] *3-Hydroxy-11-oxo-12-ursen-28-oic acid.* ***Obtusilin***
$C_{30}H_{46}O_4$ 470.691
Needles (MeOH) (as Me ester). Mp 159-161° (Me ester).

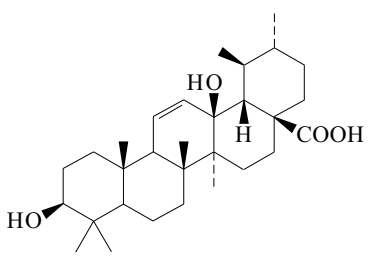
11-Ketone, 3-Ac:
$C_{32}H_{48}O_5$ 512.728
Cryst. (MeOH) (as Me ester). Mp 235-237° (Me ester).

11-Ketone, 3-benzoyl: [205699-23-6] *3-Benzoyloxy-11-oxo-12-ursen-28-oic acid*
$C_{37}H_{50}O_5$ 574.799
Constit. of the famine food *Momordica dioica*. Cryst. ($CHCl_3$/MeOH). Mp 248-249°. λ_{max} 250 (MeOH).

3,11-Diketone, 28-alcohol: [184092-59-9] *28-Hydroxy-12-ursene-3,11-dione.* ***Krukovine B***
$C_{30}H_{46}O_3$ 454.692
Amorph. solid. Mp 239-241°. $[\alpha]_D^{25}$ +85.7 (c, 0.65 in $CHCl_3$). λ_{max} 250 (log ϵ 3.78) (MeOH).

Siddiqui, S. *et al., Phytochemistry*, 1990, **29**, 3615 (*isol, pmr, cmr, Obtusilin*)
Syamasundar, K.V. *et al., Phytochemistry*, 1991, **30**, 362 (*isol, pmr, cmr, Obtusilin*)
Shirota, O. *et al., J. Nat. Prod.*, 1996, **59**, 1072-1075 (*Krukovine B*)
Honda, T. *et al., J. Nat. Prod.*, 1997, **60**, 1174-1177 (*synth*)
Santos, G.G. *et al., Phytochemistry*, 1997, **44**, 1309-1312 (*isol, pmr, cmr, deriv*)
Luo, L. *et al., Yunnan Zhiwu Yanjiu*, 1997, **19**, 316-320; *CA*, **128**, 268191s (*11-ketone 3-benzoyl*)
Luis, J.G. *et al., Nat. Prod. Lett.*, 1999, **13**, 187-194 (*3-ketone*)

3,13-Dihydroxy-11-ursen-28-oic acid D-715



$C_{30}H_{48}O_4$ 472.707

(3β,13β)-*form* [180005-32-7]
Needles. Mp 238°.

28→13 Lactone: [35959-05-8] *3β-Hydroxy-11-ursen-28,13-olide.* ***11,12-Dehydroursolic acid lactone***
$C_{30}H_{46}O_3$ 454.692
Cryst. Mp 278° (262-265°) dec. $[\alpha]_D^{10}$ +44.

28→13 Lactone, 3-Ac: [35959-08-1]
$C_{32}H_{48}O_4$ 496.729
Cryst. (EtOAc). Mp 252°. $[\alpha]_D^{20}$ +46 ($CHCl_3$).

28→13 Lactone, 3-formyl: [208997-68-6] ***Camaldulin***
$C_{31}H_{46}O_4$ 482.702
Needles ($CHCl_3$/MeOH). Mp 280-281°.

28→13-Lactone, 3-O-(p-hydroxycinnamoyl): [149725-21-3] ***Tereticornate B***
$C_{39}H_{52}O_5$ 600.837
Cryst. (MeOH). Mp 270-274°. $[\alpha]_D$ +37.3 (c, 1 in $CHCl_3$).

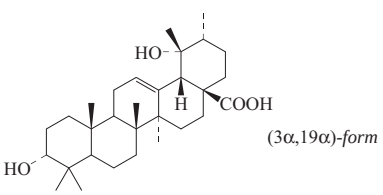
28→13 Lactone, 3-O-(4-hydroxy-3-methoxycinnamoyl): [149751-81-5] ***Tereticornate A***
$C_{40}H_{54}O_6$ 630.863
Cryst. (MeOH). Mp 267-270°. $[\alpha]_D$ +27 (c, 1 in $CHCl_3$).

28→13 Lactone, 3-ketone: [105870-60-8] *3-Oxo-11-ursen-28,13-olide.* ***Camarolide***
$C_{30}H_{44}O_3$ 452.676
Needles (MeOH). Mp 204-205°. λ_{max} 210 (MeOH).

28-Alcohol, 3-ketone, 28-Me ether: ***Momoridcin***
$C_{31}H_{50}O_3$ 470.734
Constit. of *Momordica charantia* (bitter melon). Needles. Mp 121-122°. $[\alpha]_D^{27}$ +62 (c, 0.12 in $CHCl_3$).

Horn, D.H.S. *et al., Aust. J. Chem.*, 1964, **17**, 477 (*isol*)
Mezzetti, T. *et al., Planta Med.*, 1970, **18**, 326; 1971, **20**, 244 (*isol, synth*)
Schiaffella, F. *et al., Phytochemistry*, 1975, **14**, 584 (*isol*)
Katai, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1567 (*isol*)
Wang, H. *et al., Phytochemistry*, 1993, **33**, 151 (*Tereticornates*)
Hao, H. *et al., Phytochemistry*, 1996, **42**, 1665 (*isol, pmr, cmr*)
Begum, S. *et al., Phytochemistry*, 1997, **44**, 1313 (*Momordicin*)
Siddiqui, B.S. *et al., Heterocycles*, 2000, **53**, 681-687 (*Camarolide*)
Begum, S. *et al., J. Nat. Prod.*, 2000, **63**, 1265-1268 (*Camaldulin*)

3,19-Dihydroxy-12-ursen-28-oic acid D-716



$C_{30}H_{48}O_4$ 472.707

(3β,19α)-*form* [13849-91-7]
Pomolic acid. *Benthamic acid. Randialic acid A*
Constit. of apple peel. Cryst. Mp 301-303°. $[\alpha]_D^{20}$ +37 (c, 2.0 in THF).

28-O-β-D-Glucopyranosyl ester: [83725-24-0]
$C_{36}H_{58}O_9$ 634.849
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Cryst. (MeOH). Mp 279-280°.

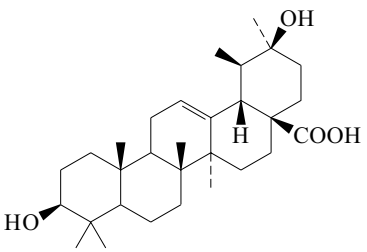
3-O-α-L-Arabinopyranoside, 28-O-[3,4,5-trihydroxybenzoyl-(→6)-β-D-glucopyranosyl] ester: [356785-75-6]
$C_{48}H_{70}O_{17}$ 919.071
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Amorph. solid. $[\alpha]_D^{25}$ +10 (c, 0.1 in MeOH).

3-O-β-D-Arabinopyranoside, Me ester: [243470-00-0]
$C_{36}H_{58}O_8$ 618.849
Constit. of *Dendrocalamus strictus* (male bamboo). Cryst. ($CHCl_3$). Mp 278°.

3-Ketone: [13849-90-6] *19-Hydroxy-3-oxo-12-ursen-28-oic acid.* ***Pomonic acid***
$C_{30}H_{46}O_4$ 470.691
Isol. as the Me ester from apple (*Pyrus malus*). Mp 204° (Me ester). $[\alpha]_D^{20}$ +50 (c, 2.0 in $CHCl_3$) (Me ester).

Tandon, A.S. *et al., Indian J. Chem.*, 1966, **4**, 483 (*isol*)
Brieskorn, C.H. *et al., Chem. Ber.*, 1967, **100**, 1252 (*isol*)
Takahashi, K. *et al., Chem. Pharm. Bull.*, 1974, **72**, 650 (*isol*)
Nakanishi, T. *et al., Phytochemistry*, 1982, **21**, 1373 (*isol*)
Cheng, D.-L. *et al., Phytochemistry*, 1992, **31**, 1317 (*28-glycosyl ester*)
Kakuno, T. *et al., Phytochemistry*, 1992, **31**, 3553 (*cmr*)
Rai, R. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 518-520 (*3-arabinoside Me ester*)
Mimaki, Y. *et al., Phytochemistry*, 2001, **57**, 773-779 (*Sanguisorba officinalis saponin*)

3,20-Dihydroxy-12-ursen-28-oic acid D-717



$C_{30}H_{48}O_4$ 472.707

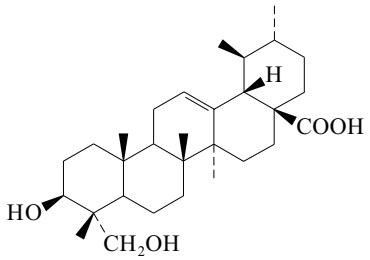
3β-*form* [58213-73-3]
20β-Hydroxyursolic acid
Constit. of apple skin and elder blossoms. Cryst. Mp 210-212°.

Me ester: [15371-66-1]
Cryst. (MeOH). Mp 220-225°. $[\alpha]_D$ +56.7 (c, 0.3 in $CHCl_3$).

20-Ac: ***Camaldulic acid***. *20β-Acetoxyursolic caid*
$C_{32}H_{50}O_5$ 514.744
Needles ($CHCl_3$/MeOH). Mp 218-219°. $[\alpha]_D$ +71 (c, 0.1 in $CHCl_3$). λ_{max} 205 (MeOH).

Lawrie, W. *et al., J.C.S.(C)*, 1967, 851 (*isol*)
Haensel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1975, **308**, 790 (*isol*)
Begum, S. *et al., J. Nat. Prod.*, 1997, **60**, 20 (*Camaldulic acid*)

3,23-Dihydroxy-12-ursen-28-oic acid D-718



$C_{30}H_{48}O_4$ 472.707

3β-*form*
Mp 180-181.5° Mp 266-268°.

Di-Ac, Me ester: [94492-28-1]
Needles (EtOH). Mp 180-181.5°. $[\alpha]_D^{21}$ +64.1 (c, 0.22 in $CHCl_3$).

3-O-α-L-Arabinopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [160669-29-4] ***Scheffursoside C***
$C_{53}H_{86}O_{22}$ 1075.249
Amorph. powder. $[\alpha]_D^{18}$ +2.3 (c, 0.47 in Py).

28-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester, 23-O-sulfate: [120190-30-9] ***Sulfapatrinoside I***
$C_{42}H_{68}O_{17}S$ 877.055
Cryst. (EtOH). Mp 239-242°. $[\alpha]_D^{20}$ +19.2 (c, 0.33 in Py).

3-O-β-D-Glucuronopyranoside, 28-O-β-D-glucopyranosyl ester: [117804-11-2] ***Cynarasaponin E***
$C_{42}H_{66}O_{15}$ 810.974
Constit. of *Cynara cardunculus* (cardoon). Powder + $2H_2O$ (as Me ester). $[\alpha]_D^{25}$ +3.7 (c, 0.95 in MeOH) (Me ester).

3-O-[α-L-Arabinopyranosyl-(1→2)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [117804-10-1] ***Cynarasaponin D***
$C_{47}H_{74}O_{19}$ 943.09
Constit. of *Cynara cardunculus* (cardoon). Powder + $2H_2O$ (as Me ester). $[\alpha]_D^{25}$ +7.6 (c, 1.16 in MeOH) (Me ester).

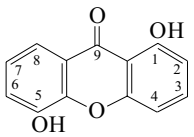
3-Ketone: ***23-Hydroxy-3-oxo-12-ursen-28-oic acid***
$C_{30}H_{46}O_4$ 470.691
Cryst. (EtOAc). Mp 170°.

[117827-84-6, 117849-92-0]

Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3906 (*isol*)
Sousa, M.P. *et al., Phytochemistry*, 1984, **23**, 2589 (*isol*)
Furuya, T. *et al., Phytochemistry*, 1987, **26**, 715 (*isol, pmr, cmr*)
Shimizu, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2466 (*Cynarasaponins*)
Inada, A. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4269 (*Sulfapatrinoside I*)
Mata, R. *et al., Phytochemistry*, 1988, **27**, 1887
Srivastava, S.K. *et al., Phytochemistry*, 1989, **28**, 644 (*cmr*)
Fourie, G. *et al., Phytochemistry*, 1989, **28**, 2851 (*isol, pmr, cmr*)
Maeda, C. *et al., Phytochemistry*, 1994, **37**, 1131 (*Scheffursoside C*)

1,5-Dihydroxyxanthone D-719

[14686-65-8]
*1,5-Dihydroxy-9*H*-xanthen-9-one, 9CI*



$C_{13}H_8O_4$ 228.204
Constit. of *Garcinia* spp., *Mammea americana* (mamey). Yellow needles (C_6H_6 or EtOAc/petrol). Mp 286° (265-266°). λ_{max} 203 ; 248 ; 309 ; 355 (MeOH) (Berdy).

1-Me ether: [27770-13-4] *5-Hydroxy-1-methoxyxanthone*
$C_{14}H_{10}O_4$ 242.231
Needles (MeOH). Mp 250-252°. λ_{max} 246 ; 304 ; 352 (MeOH) (Berdy).

5-Me ether: [15069-45-1] *1-Hydroxy-5-methoxyxanthone*
$C_{14}H_{10}O_4$ 242.231
Yellow needles (Me_2CO aq.). Mp 215°.

Di-Me ether: [14869-88-6] *1,5-Dimethoxyxanthone*
$C_{15}H_{12}O_4$ 256.257
Plates (petrol). Mp 206-208° (194-196°).

Jackson, B. *et al., J.C.S.(C)*, 1967, 785; 1968, 2579 (*isol, synth*)
Locksley, H.D. *et al., J.C.S.(C)*, 1971, 1332 (*isol, struct*)
Quillinan, A.J. *et al., J.C.S. Perkin 1*, 1972, 1382 (*isol, synth*)
Finnegan, R.A. *et al., J.C.S. Perkin 1*, 1972, 1896 (*isol, synth*)
Gunasekera, S.P. *et al., J.C.S. Perkin 1*, 1975, 2447; 1977, 1505 (*isol*)
Westermann, P.W. *et al., Org. Magn. Reson.*, 1977, **9**, 631 (*cmr*)
Patel, G.N. *et al., Synth. Commun.*, 1989, **19**, 1641 (*synth*)

1,7-Dihydroxyxanthone D-720

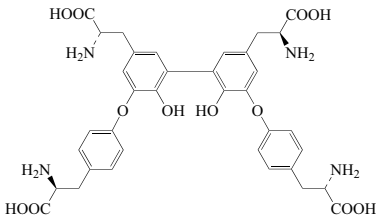
[529-61-3]
*1,7-Dihydroxy-9*H*-xanthen-9-one, 9CI.* ***Euxanthone****. Eyxanthone. Purrenone*

$C_{13}H_8O_4$ 228.204
Occurs in *Mammea americana* (mamey), *Platonia insignis* (bakuri) and *Mangifera indica* (mango). Yellow needles (toluene). Mp 240°.

Antonaccio, L.D. *et al., Ann. Acad. Bras. Ci&eenc.*, 1965, **37**, 229; *CA*, **65**, 2622 (*isol, deriv*)
Locksley, H.D. *et al., J.C.S.(C)*, 1966, 430; 1969, 1567; 1971, 1332 (*isol, synth*)
Finnegan, R.A. *et al., J.C.S. Perkin 1*, 1972, 1896 (*isol, synth*)
Bandaranayake, W.M. *et al., Phytochemistry*, 1975, **14**, 265; 1878 (*isol*)
Westermann, P.W. *et al., Org. Magn. Reson.*, 1977, **9**, 631 (*cmr*)
Daroust, D. *et al., Org. Magn. Reson.*, 1978, **11**, 547 (*pmr*)
Gunatilake, A.A.L. *et al., Phytochemistry*, 1982, **21**, 1751 (*isol*)
Patel, G.N. *et al., Synth. Commun.*, 1989, **19**, 1641 (*synth*)

Diisodityrosine D-721

[175889-19-7]



$C_{36}H_{38}N_4O_{12}$ 718.716
Isol. from hydrolysate of cell walls of tomato cell cultures.

Brady, J.D. *et al., Biochem. J.*, 1996, **315**, 323-327 (*isol, struct*)

Diisopropyl disulfide D-722

[4253-89-8]
Bis(1-methylethyl) disulfide, 9CI. Isopropyl disulfide. FEMA 3827
$(H_3C)_2CH\text{-}S\text{-}S\text{-}CH(CH_3)_2$
$C_6H_{14}S_2$ 150.309
Flavour ingredient. Constit. of fruit and seeds of *Nigella sativa* (black cumin). Poss. isol. from *Brassica oleracea* var. *capitata*, durian *Durio zibethinus*, guava and fried foods. Bp 177° Bp_{56} 95°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 268A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 430C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 351D (*ir*)
Cumper, C.W.N. *et al., J.C.S.*, 1965, 5323; *J.C.S.(A)*, 1966, 239 (*props*)
Aida, T. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1441 (*synth*)
Cohen, V.I. *et al., Helv. Chim. Acta*, 1976, **59**, 840 (*synth, bibl*)
Uemura, S. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 220 (*synth*)
Masaki, M. *et al., Chem. Lett.*, 1977, 151 (*synth*)
Jonczyk, A. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 217 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **4**, 430
Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*occur*)

Diisopropyl sulfide D-723

[625-80-9]
2,2′-Thiobispropane, 9CI. Isopropyl sulfide, 8CI
$(H_3C)_2CHSCH(CH_3)_2$
$C_6H_{14}S$ 118.243
Present in simulated meat flavours derived from autolysed baker's yeast. d_4^{20} 0.81. Bp 120-121°. n_D^{20} 1.4381.

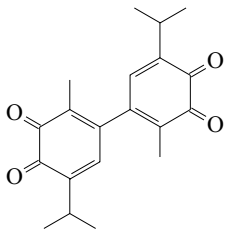
S-*Oxide:* [2211-89-4] *2,2′-Sulfinylbispropane, 9CI. Diisopropyl sulfoxide*
$C_6H_{14}OS$ 134.242
$Bp_{0.9}$ 59°.
► NW3325000

S,S-*Dioxide:* [595-50-6] *2,2′-Sulfonylbispropane, 9CI. Diisopropyl sulfone*
$C_6H_{14}O_2S$ 150.241
Cryst. (Et_2O). Sol. H_2O. Mp 36°. $Bp_{0.5}$ 78°.
► WR6210000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 267D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 430B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 351C (*ir*)
Claus, A. *et al., Ber.*, 1875, **8**, 532 (*synth*)
Cumper, C.W.N. *et al., J.C.S.(A)*, 1966, 239; 323 (*synth, uv*)
Golovnya, R.V. *et al., Nahrung*, 1983, **27**, 237-249 (*occur*)

5,5-Diisopropyl-2,2′-dimethylbiphenyl-3,3′,4,4′-tetrone D-724

[122548-31-6]

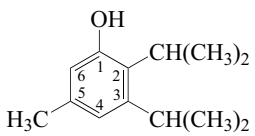


$C_{20}H_{22}O_4$ 326.391
Constit. of the leaves of thyme *Thymus vulgaris*. Shows antioxidant activity. Brown oil.

Nakatani, N. *et al., Agric. Biol. Chem.*, 1989, **53**, 1375 (*isol, pmr, cmr*)

2,3-Diisopropyl-5-methylphenol D-725

[76138-68-6]
5-Methyl-2,3-bis(1-methylethyl)phenol, 9CI. 5,6-Diisopropyl-m-*cresol*



$C_{13}H_{20}O$ 192.3
Constit. of the essential oil of *Coridothymus capitatus* (Spanish oregano).

Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 1513 (*isol*)

2,4-Diisopropyl-3-methylphenol D-726

[76138-69-7]
3-Methyl-2,4-bis(1-methylethyl)phenol, 9CI. 2,4-Diisopropyl-m-*cresol*

$C_{13}H_{20}O$ 192.3
Constit. of the essential oil of *Coridothymus capitatus* (Spanish oregano).

Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 1513 (*isol*)

2,4-Diisopropyl-5-methylphenol D-727

[40625-96-5]
5-Methyl-2,4-bis(1-methylethyl)phenol, 9CI. 4,6-Diisopropyl-m-*cresol*

$C_{13}H_{20}O$ 192.3

Constit. of the essential oil of *Coridothymus capitatus* (Spanish oregano). Oil.

Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 1513 (*isol*)
Ramanamma, C.V. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 517 (*synth*)

2,5-Diisopropyl-3-methylphenol D-728

[76138-70-0]
3-Methyl-2,5-bis(1-methylethyl)phenol, 9CI. 2,5-Diisopropyl-m-*cresol*

$C_{13}H_{20}O$ 192.3
Constit. of the essential oil of *Coridothymus capitatus* (Spanish oregano). Mp 59-60°.

Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 1513 (*isol*)
Baeckstroem, P. *et al., J.O.C.*, 1985, **50**, 3728 (*synth, pmr*)

2,5-Diisopropyl-4-methylphenol D-729

[15269-16-6]
4-Methyl-2,5-bis(1-methylethyl)phenol, 9CI. 2,5-Diisopropyl-p-*cresol, 8CI*

$C_{13}H_{20}O$ 192.3
Constit. of the essential oil of *Coridothymus capitatus* (Spanish oregano). Mp 52.7° (51-52°).

Bassus, J. *et al., Bull. Soc. Chim. Fr.*, 1974, 3031
Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 1513 (*isol*)
Baeckstroem, P. *et al., J.O.C.*, 1985, **50**, 3728 (*synth, pmr*)
Ramanamma, C.V. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 517 (*synth*)

2,6-Diisopropyl-3-methylphenol D-730

[28434-93-7]
3-Methyl-2,6-bis(1-methylethyl)phenol, 9CI. 2,6-Diisopropyl-m-*cresol, 8CI*

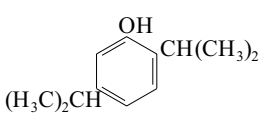
$C_{13}H_{20}O$ 192.3
Constit. of essential oils of Spanish oregano (*Coridothymus capitatus*) and *Origanum* spp.. Oil. Bp_{50} 161° Bp 70-72°.

Phenylurethane:
Mp 157°.

Stroh, R. *et al., Angew. Chem.*, 1957, **69**, 699 (*synth*)
James, R. *et al., J. Med. Chem.*, 1980, **23**, 1350 (*synth*)
Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 89 (*isol, pmr*)
Benjilali, B. *et al., Lebensm.-Wiss. Technol.*, 1986, **19**, 22 (*isol*)
Ramanamma, C.V. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 517 (*synth*)

2,5-Diisopropylphenol, 8CI D-731

[35946-91-9]
2,5-Bis(1-methylethyl)phenol, 9CI

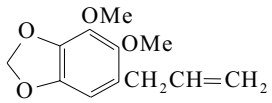


$C_{12}H_{18}O$ 178.274
Occurs in Spanish origanum oil. Cryst. (EtOH aq.). Mp 95.5°.

Dewar, M.J.S. *et al., J.C.S.*, 1960, 959 (*synth*)
Shrewsbury, D.D. *et al., Spectrochim. Acta*, 1960, **16**, 1294 (*ir*)
Sendra, J. *et al., Phytochemistry*, 1980, **19**, 1513 (*isol*)

Dillapiol D-732

[484-31-1]
4,5-Dimethoxy-6-(2-propenyl)-1,3-benzodioxole, 9CI. 1-Allyl-2,3-dimethoxy-4,5-methylenedioxybenzene. Dill apiole



$C_{12}H_{14}O_4$ 222.24
Constit. of Japanese, Indian (*Anethum sowa*) and European (*Anethum graveolens*) dill oils and *Piper* spp. Also from seeds of *Bunium persicum* (black caraway). Mp 29.5°. Bp 285° Bp_{11} 162° $Bp_{0.8}$ 100°. n_D^{25} 1.5278. Log P 1.95 (calc).

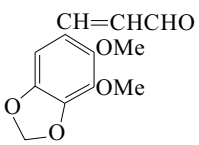
▶ CY2490000

Picrate:
Mp 81.5°.

Baker, W. *et al., J.C.S.*, 1934, 1682 (*synth*)
Dallacker, F. *et al., Chem. Ber.*, 1969, **102**, 2663 (*synth*)
Fujita, H. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3553 (*synth*)
Bernhard, H.O. *et al., Helv. Chim. Acta*, 1978, **61**, 2273 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 112 (*rev*)
Martins, A.P. *et al., Phytochemistry*, 1998, **49**, 2019-2033 (*isol*)
Benevides, P.J.C. *et al., Phytochemistry*, 1999, **52**, 339-343 (*isol, pmr, cmr*)
Farediah, A. *et al., ACGC Chem. Res. Commun.*, 2000, **10**, 63-66; *CA*, **133**, 293544v (*activity*)

Dillapional D-733

[38971-74-3]
2,3-Dimethoxy-4,5-methylenedioxycinnamaldehyde. 3-(2,3-Dimethoxy-4,5-methylenedioxyphenyl)-2-propen-1-al



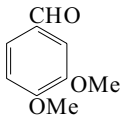
$C_{12}H_{12}O_5$ 236.224
Minor constit. of *Anethum sowa* (Indian dill) oil. Needles (C_6H_6). Mp 101-102°.

2,4-Dinitrophenylhydrazone:
Orange cryst. Mp 213-215°.

Tomar, S.S. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 723

3,4-Dimethoxybenzaldehyde, 9CI D-734

[120-14-9]
Veratric aldehyde. Protocatechuic aldehyde dimethyl ether. Vanillin methyl ether. Veratraldehyde. Veratrumaldehyde. Methylvanillin. FEMA 3109



$C_9H_{10}O_3$ 166.176
Isol. from peppermint, raspberry, ginger and Bourbon vanilla. Used in vanilla flavours. Needles (Et_2O, petrol, CCl_4 or toluene) with woody vanilla odour. Mp 44° Mp 58°. Bp_{18} 172-175°.

▶ Skin irritant. LD_{50} (rat, orl) 2000 mg/kg. YX5088000

Oxime: [39627-82-2]
$C_9H_{11}NO_3$ 181.191
Cryst. (petrol). Mp 94-95°.

2,4-Dinitrophenylhydrazone:
Orange prisms (EtOAc). Mp 264-265°.

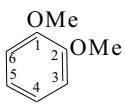
Semicarbazone:
Mp 177°.

Di-Me acetal: [59276-33-4] *4-(Dimethoxymethyl)-1,2-dimethoxybenzene*
$C_{11}H_{16}O_4$ 212.245
$Bp_{0.05}$ 94°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 118B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 955B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1299B (*ir*)
Barger, G. *et al., J.C.S.*, 1928, **133**, 2924 (*synth*)
Org. Synth., 1936, **14**, 91 (*synth*)
Weijlard, J. *et al., J.A.C.S.*, 1947, **69**, 2070 (*synth*)
de Kowalewski, D.G. *et al., J. Mol. Struct.*, 1973, **16**, 395 (*nmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 923 (*rev, tox*)
Napolitano, E. *et al., J.O.C.*, 1983, **48**, 3653 (*deriv, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 795
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2906-2907
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VHK000

1,2-Dimethoxybenzene, 9CI D-735

[91-16-7]
Veratrol. Veratrole. Catechol dimethyl ether. FEMA 3799



$C_8H_{10}O_2$ 138.166
Food additive listed in the EAFUS Food Additive Database (Jan 2001). Found in raw and cooked foods, e.g. cheeses, grapes and asparagus. Cryst. (petrol). Mp 22.5°. Bp_{759} 206° Bp_{10} 88-90°.

▶ Fl. p. 87°. LD_{50} (rat, orl) 890 mg/kg. CZ6475000

Picrate:
Red plates. Mp 56-57°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1037C (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 180B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 965B (*ir*)
Perkin, W.H. *et al., J.C.S.*, 1906, **89**, 1649
King, H. *et al., J.C.S.*, 1939, 1168 (*synth*)
Antoniades, H.N. *et al., Chemist-Analyst*, 1955, **44**, 34 (*detn, Ce*)
Wright, G.E. *et al., Tetrahedron*, 1973, **29**, 3775 (*nmr*)
Starkov, S. *et al., CA*, 1974, **82**, 43030 (*synth*)
Lille, V. *et al., CA*, 1976, **85**, 46138 (*glc*)
Marczenko, Z. *et al., Separation and Spectrophotometric Determination of Elements*, Horwood, Chichester, 1986,
Emsley, J.W. *et al., J.C.S. Perkin 2*, 1991, 583 (*conformn*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 436
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOA200

1,3-Dimethoxybenzene, 9CI D-736

[151-10-0]

$C_8H_{10}O_2$ 138.166

Present in fungi. Mushroom odorant substance. d_{25}^{25} 1.05. Mp -52° approx. Bp 216.5-217.7°. pK_a -6.4.

► Fl. p. 88°. LD_{50} (mus, ipr) 900 mg/kg. CZ6474000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1040D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 183C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 968D (*ir*)
Wright, G.E. *et al., Tetrahedron*, 1973, **29**, 3775 (*nmr*)
Kuznetsov, V.A. *et al., Dokl. Akad. Nauk SSSR*, 1974, **216**, 812 (*ir*)
Messer, C. *et al., CA*, 1999, **131**, 71415y (*isol*)

1,4-Dimethoxybenzene, 9CI D-737

[150-78-7]

Hydroquinone dimethyl ether. FEMA 2386

$C_8H_{10}O_2$ 138.166

Flavouring ingredient. Plates. Mp 55-56°. Bp 212-216° Bp_{20} 109°.

► Fl. p. >66°. Skin irritant. LD_{50} (rat, orl) 3600 mg/kg. CZ6650000

1,3,5-Trinitrobenzene complex: Bright red prisms. Mp 86.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1042D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 184C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 971A (*ir*)
Dyson, G.M. *et al., J.C.S.*, 1927, 440 (*synth*)
Santavy, F. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1825 (*uv*)
Ger. Pat., 1973, 2 148 589; *CA*, **78**, 159200 (*synth*)
Wright, G.E. *et al., Tetrahedron*, 1973, **29**, 3775 (*nmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **16**, 715 (*rev*)
Konz, E. *et al., Synthesis*, 1979, 603 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 170
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 840-841
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOA400

6,7-Dimethoxy-1(3*H*)-benzoxazolone D-738

2-Hydroxy-6,7-dimethoxybenzoxazole



$C_9H_9NO_4$ 195.174

Constit. of the dried tissues of *Zea mays* (sweet corn). Amber cryst. (H_2O). Mp 180°.

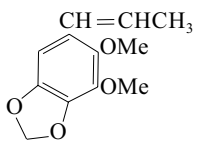
4-Chloro:4-Chloro-6,7-dimethoxy-2-benzoxazolinone
$C_9H_8ClNO_4$ 229.619
Isol. from light-grown sweet corn shoots (*Zea mays*).

Klun, J.A. *et al., J. Agric. Food Chem.*, 1970, **18**, 663 (*isol, struct, synth*)
Anai, T. *et al., Phytochemistry*, 1996, **42**, 273-275 (*deriv*)

2,3-Dimethoxy-4,5-methylenedioxy-1-propenylbenzene D-739

[23731-63-7]

4,5-Dimethoxy-6-(1-propenyl)-1,3-benzodioxole, 9CI. ***Isodillapiole***



$C_{12}H_{14}O_4$ 222.24

Present in *Crithmum maritimum* (rock samphire). Leaflets or needles (EtOH). Mp 55-56°.

Sahdev, R. *et al., J. Inst. Chem. (India)*, 1975, **47**, 234 (*synth*)

Dimethyl carbonate D-740

[616-38-6]

Carbonic acid dimethyl ester, 9CI. Methyl carbonate. E242

$O{=}C(OMe)_2$

$C_3H_6O_3$ 90.079

Used for cold sterilisation of beverages. Effective against typical beverage-spoiling microorganisms, like yeasts and fermentative bacteria. Liq. Sol. EtOH, Et_2O, insol. H_2O. d_4^{20} 1.07. Mp 0.5°. Bp 90-91°. n_D^{20} 1.3687.

► Highly flammable, fl. p. 19°. Reacts violently with potassium *tert*-butoxide. FG0450000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 928A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 610D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 633C (*ir*)
Hood, H.P. *et al., J. Phys. Chem.*, 1919, **23**, 508 (*synth*)
Kling, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1920, **170**, 111 (*synth*)
Kondo, K. *et al., Tet. Lett.*, 1971, 4885 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 234
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 361 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIF000
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1158
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 504

Dimethyl diselenide, 9CI D-741

[7101-31-7]

Methyl diselenide, 8CI. Diselenobismethane

Me–Se–Se–Me

$C_2H_6Se_2$ 187.989

Constit. of *Allium* sp.. Orange oil. Bp 156-158° Bp_{15} 63-65°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 425C (*nmr*)
Bird, M.L. *et al., J.C.S.*, 1942, 570 (*synth*)
Lardon, M. *et al., J.A.C.S.*, 1970, **92**, 5063 (*nmr*)
D'Antonio, P. *et al., J. Chem. Phys.*, 1971, **55**, 1071 (*struct*)
McFarlane, W. *et al., J.C.S. Dalton*, 1972, 1397 (*nmr*)
Gladysz, J.A. *et al., J.O.C.*, 1978, **43**, 1204 (*synth*)
Syper, L. *et al., Synthesis*, 1984, 439 (*synth*)
Clarembeau, M. *et al., Tetrahedron*, 1985, **41**, 4793 (*synth*)
Barton, D.H.R. *et al., Tetrahedron*, 1986, **42**, 4983 (*synth, pmr*)
Luthra, N.P. *et al., J. Organomet. Chem.*, 1988, **354**, 51 (*Se-77 nmr*)
Anderson, J.A. *et al., Organometallics*, 1988, **7**, 267 (*cmr*)
Krief, A. *et al., Synthesis*, 1988, 131 (*synth*)
McKillop, A. *et al., Tet. Lett.*, 1990, **31**, 5007 (*synth*)
Cai, X.J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081 (*occur*)

Dimethyl disulfide, 9CI D-742

[624-92-0]

Methyl disulfide. 2,3-Dithiabutane. FEMA 3536

Me–S–S–Me

$C_2H_6S_2$ 94.201

Isol. from garlic oil (*Allium sativum*), also in onion (*Allium cepa*), ramsons (*Allium ursinum*), morello cherry, melon, pineapple, strawberry, wheat bread, cocoa, roasted barley, roasted filberts, roasted peanuts, crispbread, American potato chips, soybean and other foodstuffs. Flavouring ingredient.. Liq. d_4^{16} 1.06. Mp -98°. Bp 110° (116-118°) Bp_{12} 40°. n_D^{16} 1.5219.

► LC_{50} (rat, ihl) *ca.* 16 mg m^{-3} (2h exposure). Highly flammable, fl. p. < 21°. JO1927500

S-*Oxide:* [13882-12-7]

[85085-08-1, 111769-09-6, 133773-40-7] S-*Methyl methanesulfinothioate. Methyl methanethiosulfinate*

$C_2H_6OS_2$ 110.201

Constit. of *Allium* spp.. $Bp_{1.1}$ 65°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 264C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 425B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 347C (*ir*)

McAllan, D.T. *et al., J.A.C.S.*, 1951, **73**, 3627 (*synth*)
Cumper, C.W.N. *et al., J.C.S.*, 1965, 5323; 5860 (*synth, props*)
Schultz, O.E. *et al., Pharmazie*, 1965, **20**, 441 (*isol*)
Cumper, C.W.N. *et al., J.C.S.(A)*, 1966, 239 (*synth*)
Moore, T.L. *et al., J.O.C.*, 1966, **31**, 3587-3592 (*oxide, synth*)
Beagley, B. *et al., Trans. Faraday Soc.*, 1971, **67**, 3216 (*struct*)
Block, E. *et al., J.A.C.S.*, 1974, **96**, 3921-3929 (*oxide, synth*)
Zack, N.R. *et al., J. Fluorine Chem.*, 1975, **5**, 153 (*ms*)
Dauphin, G. *et al., Org. Magn. Reson.*, 1979, **12**, 557 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 189; *Fieser and Fieser's Reagents for Organic Synthesis, Wiley*, 1980, **9**, 91; 281; 473 (*use*)
Connell, R.J. *et al., Anal. Chem. Symp. Ser.*, (Chem. Sens.), 1990, **6**, 725
Casida, J.E. *et al., J. Agric. Food Chem.*, 1992, **40**, 1425 (*pmr, cmr*)
Meyer, M. *et al., J. Mol. Struct.*, 1992, **273**, 99 (*ir, Raman, microwave*)
Block, E. *et al., Pure Appl. Chem.*, 1993, **65**, 625-632 (*oxide, occur*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 2067-2070 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1755-1756 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DRQ400

Dimethyl peroxide D-743

[690-02-8]

Me–O–O–Me

$C_2H_6O_2$ 62.068

Constit. of *Basella rubra* (Malabar spinach). Gas or liq. Bp 10°.

▶ Heat and shock sensitive explosive.

Rieche, A. *et al., Ber.*, 1928, **61**, 951 (*synth*)
Hanst, P.L. *et al., J. Phys. Chem.*, 1959, **63**, 104 (*synth*)
Baker, G. *et al., Chem. Ind. (London)*, 1964, 1988
Shanley, E.S. *et al., Organic Peroxides*, (ed. Swern, D.), 1972, 341 (*haz, rev*)
Kameoka, H. *et al., J. Food Compos. Anal.*, 1991, **4**, 315-321 (*isol*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0869
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 516
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTJ000

Dimethyl selenide D-744

[593-79-3]

Selenobismethane, 9CI. Methyl selenide, 8CI

$SeMe_2$

C_2H_6Se 109.029

Constit. of *Allium* spp.. d^{25} 1.43. Mp -87.2°. Bp 57.7°.

▶ LD_{50} (rat, ipr) 2200 mg/kg. VS6880000

Se-*Oxide:* [4371-90-8] ***Seleninylbismethane, 9CI***. *Dimethyl selenoxide*
C_2H_6OSe 125.029
Needles. Mp 92-94° (in sealed capillary).

Se,Se-*Dioxide:* [22089-69-6] *Selenonylbismethane. Dimethyl selenone*
$C_2H_6O_2Se$ 141.028
Cryst. (MeOH). Mp 147-148°.

Bird, M.L. *et al., J.C.S.*, 1942, 570-574 (*synth*)
Dransfield, P.B. *et al., J.C.S.*, 1955, 1153-1160 (*synth*)
Tideswell, N.W. *et al., J.A.C.S.*, 1957, **79**, 1031-1033 (*uv*)
Paetzold, R. *et al., Z. Anorg. Allg. Chem.*, 1968, **360**, 293-299 (*oxide, dioxide, synth*)
McFarlane, W. *et al., J.C.S. Dalton*, 1972, 1397-1402 (*pmr*)
Rebane, E. *et al., Chem. Scr.*, 1973, **4**, 219-230 (*oxide, ms*)
Price, C.C. *et al., J.O.C.*, 1973, **38**, 615-616 (*pmr*)
v. Loon, J.C. *et al., Chem. Can.*, 1976, **28**, 15; *CA*, **85**, 41651 (*anal*)
McFarlane, W. *et al., Bull. Soc. Chim. Belg.*, 1977, **86**, 457-463 (*cmr, Se-77 nmr, oxide*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 224; **8**, 197 (*oxide, use*)
Micolajczyk, M. *et al., J.O.C.*, 1978, **43**, 2132-2138 (*oxide, use*)
Odom, J.D. *et al., J.A.C.S.*, 1979, **101**, 5815-5822 (*use*)
Syper, L. *et al., Synthesis*, 1984, 439-442 (*oxide, synth, props*)
Krief, A. *et al., Chem. Comm.*, 1985, 569-570 (*dioxide, synth*)
Ip, C. *et al., Cancer Res.*, 1991, **51**, 595-600 (*oxide, synth, activity*)
Block, E. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081-2084 (*isol*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 2130-2131 (*Se-oxide, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DUB200

Dimethyl sulfoxide, BAN, INN, USAN D-745

[67-68-5]

Sulfinylbismethane, 9CI. Methyl sulfoxide. Methylsulfinylmethane. DMSO. Dermavet. Iduridine. NSC 763. FEMA 3875. Many other names

MeSOMe

C_2H_6OS 78.135

Found in broad bean *Phaseolus vulgaris*, alfalfa *Medicago sativa* and many other plants. Flavouring agent. Liq. Misc. H_2O, org. solvs. d_4^{20} 1.1. Mp 18.5°. Bp 189° $Bp_{0.37}$ 20°. n_D^{25} 1.4790 ((1.4775)). Log P -1.38 (calc). Dielectric constant ϵ 46.45. Dipole moment 4.3d. Viscosity 1.991 cP. Virtually odourless when pure, most coml. samples contain traces of odorous Bis(-methylthio)methane, B-150. Stable to 150°, sl. dec. above this temp. requiring addn. of an acid scavenger, e.g $NaHCO_3$. Forms a Na deriv., Dimsyl sodium.

▶ Fl. p. 95° (oc), autoignition temp. 215°. Can decompose exothermically at 150°. May dec. explosively in presence of high concs. of halide ions. Can cause redness, itching and scaling of skin and damage to eyes. Low oral toxicity, but readily absorbed by skin with adverse systemic effects reported. Can act as a carrier for skin absorption of other chemicals. PV6210000

[2206-27-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 879A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1417A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 831A (*ir*)
U.S. Pat., 1952, 2 581 050; *CA*, **46**, 8669 (*synth*)
Martin, D. *et al., Angew. Chem., Int. Ed.*, 1967, **6**, 318 (*rev*)
Jacob, S.W. *et al., Arzneim.-Forsch.*, 1967, **17**, 1553 (*pharmacol, tox*)
Allan, G.G. *et al., Chem. Ind. (London)*, 1967, 1706 (*haz*)
Dimethyl Sulfoxide, (eds. Jacob, S.W. *et al*) M. Dekker, New York, 1971, (*tox, pharmacol*)
Jacob, S.W. *et al., Ann. N.Y. Acad. Sci.*, Eds., 1975, **243**, (*book*)
Large, R. *et al., Org. Mass Spectrom.*, 1976, **11**, 582 (*ms*)
Frolov, Y.L. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1978, 1042; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 901 (*uv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 198; 1981, **9**, 189; 1982, **10**, 166; 1984, **11**, 214; 1986, **12**, 212; 1988, **13**, 124; 1992, **16**, 149 (*use*)
Pearson, T.W. *et al., J. Agric. Food Chem.*, 1981, **29**, 1089 (*occur*)
Mancuso, J. *et al., Synthesis*, 1981, 165 (*rev, bibl*)
Kharasch, N. *et al., Ann. N.Y. Acad. Sci.*, 1983, **411**, 391 (*rev, struct, props*)
Swanson, B.N. *et al., Rev. Clin. Basic Pharmacol.*, 1985, **5**, 1 (*rev, pharmacol*)
Cataliotti, R.S. *et al., Spectrochim. Acta A*, 1986, **42**, 855 (*ir, Raman*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 64
Martin, G.F. *et al., Synth. Commun.*, 1987, **17**, 1667 (*purifn*)
Itoh, S. *et al., Z. Naturforsch., A*, 1987, **42**, 858 (*struct*)
Casida, J.E. *et al., J. Agric. Food Chem.*, 1992, **40**, 1425 (*cmr, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1223
www.gaylordchem.com, (*bibl*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0867
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 524
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DUD800
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 2087

Dimethyl tetrasulfide, 9CI D-746

[5756-24-1]

Methyl tetrasulfide, 8CI. 2,3,4,5-Tetrathiahexane

MeS-S-S-SMe

$C_2H_6S_4$ 158.333

Constit. of various *Allium* spp. and *Lentinus* sp.. $Bp_{0.07}$ 70°.

Milligan, B. *et al., J.C.S.*, 1963, 3608 (*synth*)
Morel, G. *et al., Synthesis*, 1980, 918 (***synth***)
Barany, G. *et al., J.O.C.*, 1983, **48**, 4750 (*pmr*)
Mott, A.W. *et al., Sulfur Lett.*, 1984, **2**, 137 (*synth*)

Dimethyl trisulfide, 9CI D-747

[3658-80-8]

Methyl trisulfide, 8CI. 2,3,4-Trithiapen-

tane. FEMA 3275

Me-S-S-S-Me

$C_2H_6S_3$ 126.267

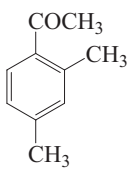
Found in essential oil of hop (*Humulus lupulus*), garlic (*Allium sativum*), shallot (*Allium cepa*) and ramsons (*Allium ursinum*). Also found in pineapple, raw cabbage, kohlrabi, roasted filberts, roasted peanuts, edible mushrooms, brussel sprouts, fermented radish, Chinese cabbage, parsnips, scallop and squid. The major off-flavour principle of overcooked brassicas. Flavouring ingredient. Liq. with powerful onion-like odour. Bp 165-170° Bp_{30} 70-71°. n_D^{20} 1.6010.

Milligan, B. *et al., J.C.S.*, 1963, 3608-3614 (*synth*)
Armitage, D.A. *et al., J.C.S.(C)*, 1971, 2840-2842 (*synth, pmr, glc*)
Schreyen, N. *et al., J. Agric. Food Chem.*, 1976, **24**, 336-341
Peppard, T.L. *et al., Phytochemistry*, 1977, **16**, 2020-2021 (*isol, ms, glc*)
Snyder, J.P. *et al., Tet. Lett.*, 1978, 197-200 (*conformn*)
Dauphin, G. *et al., Org. Magn. Reson.*, 1979, **12**, 557-560 (*cmr*)
Whitfield, F.B. *et al., Chem. Ind. (London)*, 1981, 692-693 (*isol*)
Capozzi, G. *et al., Tet. Lett.*, 1989, **30**, 2991-2994 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 881-882 (*use, occur*)
Kubec, R. *et al., J. Agric. Food Chem.*, 1998, **46**, 4334-4340 (*formn*)

2′,4′-Dimethylacetophenone, 8CI D-748

[89-74-7]

1-(2,4-Dimethylphenyl)ethanone, 9CI. 4-Acetyl-m-*xylene. FEMA 2387*



$C_{10}H_{12}O$ 148.204

Flavouring ingredient. Liq. d^{20} 1.01. Bp 228° Bp_{27} 122-123°. Bp also given as 234-235°.

Oxime:

$C_{10}H_{13}NO$ 163.219

Needles (petrol). Mp 63-64°. Bp_{15} 153-154°.

2,4-Dinitrophenylhydrazone:

Mp 174-175° (169-170°).

Semicarbazone:

Mp 185-187° Mp 192-193°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 820C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1238B (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 859A (*ir*)
v. Auwers, K. *et al., Ber.*, 1925, **58**, 36 (*synth*)
Perkin, W.H. *et al., J.C.S.*, 1925, 2275 (*synth*)
Mecke, R. *et al., Chem. Ber.*, 1960, **93**, 210 (*uv, ir*)
Dhami, D.S. *et al., Can. J. Chem.*, 1965, **43**, 479 (*cmr*)
Uzarewicz, A. *et al., CA*, 1969, **70**, 3468q (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 172
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 844-845

Dimethylamine D-749

[124-40-3]

N-*Methylmethanamine, 9CI*

Me_2NH

C_2H_7N 45.084

Aminating agent in the manuf. of ion-exchange resins for food processing. Gas at r.t. V. sol. H_2O, sol. EtOH, Et_2O. d_4^0 0.68. Mp -96°. Bp 7°. pK_a 3.28 (25°).

▶ Extremely flammable, fl. p. -6°, autoignition temp. 400°. Eye, skin and respiratory tract irritant (gas or aq. solns.) Prolonged exposure can cause dermatitis and conjunctivitis. IP8750000

Hydrochloride: [506-59-2] *Dimethylammonium chloride*

C_2H_8ClN 81.545

Volatile cryst. Sol. H_2O, EtOH, $CHCl_3$; insol. Et_2O. Mp 171°.

▶ IQ0220000

DMSO complex (1:1):Dimsulf

$C_4H_{13}NOS$ 123.219

Distillable liq.

N-*Benzoyl:* See *N,N*-Dimethylbenzamide in *The Combined Chemical Dictionary.*

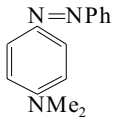
[17000-01-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 294B; 294C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 470A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 378C (*ir*)
Werner, E.A. *et al., J.C.S.*, 1917, **111**, 850 (*synth*)
Ger. Pat., 1929, 468 895; *CA*, **23**, 846 (*synth*)
U.S. Pat., 1948, 2 456 599; *CA*, **43**, 3440g (*manuf*)
Gohlke, R.S. *et al., Acta Chim. Hung.*, 1962, **34**, 1281 (*ms*)
Suhr, H. *et al., Chem. Ber.*, 1963, **96**, 1720 (*pmr*)
Serban, S. *et al., Rev. Chim. (Bucharest)*, 1963, **14**, 451; *CA*, **60**, 5097b (*synth*)
Audier, H. *et al., Bull. Soc. Chim. Fr.*, 1964, 3034 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 119
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 846-847
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 207
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 73 (*tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0887
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 492
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOQ800; DOR000; DOR600

4-(Dimethylamino)azobenzene D-750

[60-11-7]

N,N-*Dimethyl-4-(phenylazo)benzenamine, 9CI.* N,N-*Dimethyl*-p-*(phenylazo)aniline, 8CI. Butter yellow. Dimethyl yellow. Methyl yellow. C.I. Solvent yellow 2. C.I. 11020. Many other names*



$C_{14}H_{15}N_3$ 225.293

Formerly used as a food dye, use discontinued. Yellow leaflets (EtOH). Sol. EtOH, Me_2CO, C_6H_6; insol. H_2O. Mp 115° Mp 117°. pK_{a1} 3.34 (20°). pK_{a1} 3.25.

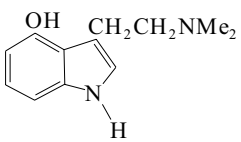
▶ Possible human carcinogen. Can cause contact dermatitis. LD_{50} (rat, orl) 200 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects. BX7350000

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1452G (*ir*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 472
Möhlau, G. *et al., Ber.*, 1884, **17**, 1491 (*synth*)
Cray, I.M. *et al., Trans. Faraday Soc.*, 1925, **21**, 326
Rosenhauer, E. *et al., Ber.*, 1928, **61**, 396 (*synth*)
Kotthoff, I.M. *et al., J.A.C.S.*, 1938, **60**, 2516
Guss, L.S. *et al., J.A.C.S.*, 1940, **62**, 249
IARC Monog., 1975, **8**, 125; *Suppl.* 7, 62 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOT300
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 245
Lewis, R.J. *et al., Reproductively Active Chemicals*, Van Nostrand Reinhold, 1991, DOT300

3-(2-Dimethylaminoethyl)-4-hydroxyindole D-751

[520-53-6]

*3-(2-Dimethylaminoethyl)-1*H-*indol-4-ol, 9CI.* N,N-*Dimethyl-4-hydroxytryptamine.* ***Psilocine****. CX 59*



$C_{12}H_{16}N_2O$ 204.271

Sol. MeOH, butanol; fairly sol. H_2O. Mp 173-176° dec. Log P 1.16 (calc). λ_{max} 222 (ϵ 39800); 260 (ϵ 5000); 267 (ϵ 6300); 283 (ϵ 5000); 293 (ϵ 4000) (MeOH) (Berdy).

▶ LD_{50} (rat, ivn) 75 mg/kg. NM2625000

O-*Phosphate:* [520-52-5] ***Psilocybine, BAN, INN****. Indocybin. CY 39*

$C_{12}H_{17}N_2O_4P$ 284.251

Cryst. (MeOH or H_2O). Sol. MeOH, H_2O, butanol. Mp 220-228° (185-195°). λ_{max} 221 (ϵ 18620); 268 (ϵ 6920); 280 (ϵ 5500); 290 (ϵ 4360) (MeOH) (Berdy). λ_{max} 220 (ϵ 39800); 267 (ϵ 6300); 290 (ϵ 4000) (EtOH) (Berdy).

▶ Human adverse systemic effects by ingestion and intraperitoneal routes incl. toxic psychosis. LD_{50} (rat, ivn) 280 mg/kg ; LD_{50} (mus, ivn) 275 mg/kg , LD_{50} (mus,

ipr) 420 mg/kg. NM3150000

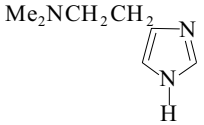
N-*De-Me,* O-*phosphate:* [21420-58-6]
Baeocystine
$C_{11}H_{15}N_2O_4P$ 270.224
Mp 254-258° dec.

Di-N-*de-Me,* O-*phosphate:* [21420-59-7]
Norbaeocystine
$C_{10}H_{13}N_2O_4P$ 256.197
Mp 188-192° dec.

Hofmann, A. *et al., Experientia*, 1958, **14**, 107; 397; 1959, **15**, 101 (*isol, synth, ir, uv*)
Julia, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1959, **269**, 51 (*synth*)
Leung, A.Y. *et al., J. Pharm. Sci.*, 1967, **56**, 146; 1968, **57**, 1667 (*derivs*)
Agurell, S. *et al., Acta Chem. Scand.*, 1968, **22**, 1210 (*biosynth*)
Hofmann, A. *et al., Bull. Narc.*, 1971, **23**, 3 (*rev*)
Aboul-Enein, H.Y. *et al., Am. J. Pharm.*, 1974, **146**, 91 (*rev, Psilocybine*)
Weber, H.P. *et al., J.C.S. Perkin 2*, 1974, 942; 946 (*cryst struct*)
Repke, D.B. *et al., J. Pharm. Sci.*, 1977, **66**, 113; 743 (*isol, glc, ms, derivs*)
Unger, S.E. *et al., Anal. Lett.*, 1979, **12**, 1157 (*ms*)
White, P.C. *et al., J. Chromatogr.*, 1979, **169**, 453 (*deriv*)
Weeks, R.A. *et al., J. Nat. Prod.*, 1979, **49**, 469 (*isol, uv, ms*)
Chilton, W.S. *et al., J. Psychedelic Drugs*, 1979, **11**, 61 (*rev*)
Repke, D.B. *et al., J. Het. Chem.*, 1981, **18**, 175 (*synth, bibl*)
Seeger, R. *et al., Dtsch. Apoth. -Ztg.*, 1985, **125**, 65 (*rev, Psilocybine*)
Brenneisen, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 487 (*synth, uv, ir, pmr, cmr, P-31 nmr, ms, bibl, Baeocystine*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1407
Sakagami, H. *et al., Heterocycles*, 1999, **51**, 1131-1135 (*synth*)
Nichols, D.E. *et al., Synthesis*, 1999, 935-938 (*Psilocine, Psilocybine*)
Gathergood, N. *et al., Org. Lett.*, 2003, **5**, 921-923 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HKE000; PHU500

4-[2-(Dimethylamino)ethyl]imidazole, 8CI D-752

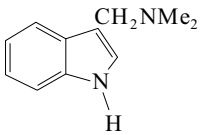
[673-46-1]
N,N-*Dimethyl-1*H-*imidazole-4-ethanamine, 9CI.* ***N$^{\pi}$,N$^{\pi}$-Dimethylhistamine.*** *Hippospongine*†



$C_7H_{13}N_3$ 139.2
The application of the name Hippospongine to this compound is tentative. Alkaloid from *Coprinus comatus* (shaggy ink cap) and *Casimiroa edulis* seeds (Mexican apple).
▶ NI4840000
Hydrochloride (1:2):
Mp 182-184°.
Dipicrate:
Mp 229-230°.
Ackermann, D. *et al., Z. Biol. (Munich)*, 1924, **82**, 278 (*isol*)
Garforth, B. *et al., J.C.S.*, 1935, 489 (*synth*)
Huebner, C.F. *et al., J.A.C.S.*, 1949, **71**, 3942 (*synth*)
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1958, **291**, 502 (*isol*)
Major, R.T. *et al., J.O.C.*, 1958, **23**, 1564 (*isol*)
Ling, J.S.L. *et al., J. Pharmacol. Exp. Ther.*, 1958, **122**, 44A (*pharmacol*)
Erspamer, V. *et al., Experientia*, 1963, **19**, 346 (*occur*)
Ingle, P.H.B. *et al., J. Pharm. Pharmacol.*, 1963, **15**, 620 (*synth*)
Erspamer, V. *et al., Arch. Biochem. Biophys.*, 1964, **105**, 620 (*occur*)
German, V.F. *et al., J. Pharm. Sci.*, 1971, **60**, 495 (*isol, pmr, ms*)
Roseghini, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1976, **54**, 31 (*occur*)
Roseghini, M. *et al., Z. Naturforsch., C*, 1976, **31**, 118 (*occur*)
Ferrigni, N.R. *et al., J. Ethnopharmacol.*, 1982, **5**, 359 (*isol*)
Wagner, H. *et al., Planta Med.*, 1982, **45**, 95 (*isol*)
Romero, M.L. *et al., J. Chromatogr.*, 1983, **281**, 245 (*hplc*)
Ferrigni, N.R. *et al., Rev. Latinoam. Quim.*, 1984, **14**, 131; *CA*, **101**, 23790a (*pmr, cmr*)

3-(Dimethylaminomethyl)indole D-753

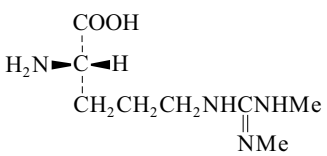
[87-52-5]
N,N-*Dimethyl-1*H-*indole-3-methanamine, 9CI.* ***Gramine.*** *Donaxine. Doranine*



$C_{11}H_{14}N_2$ 174.245
Isol. from cabbage and barley shoots. Mp 138-139°. pK_a 16 (25°,NH, aq. KOH).
▶ LD_{50} (mus, ipr) 122 mg/kg ; LD_{50} (mus, ipr) 122 mg/kg. NL7525000
[6170-37-2]
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 131B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 660B (*ir*)
Kühn, H. *et al., Ber.*, 1937, **70**, 567 (*synth*)
Marion, L. *et al., J.A.C.S.*, 1951, **73**, 305 (*ir*)
Jamieson, W.D. *et al., Phytochemistry*, 1970, **9**, 2029 (*ms*)
Leete, E. *et al., Phytochemistry*, 1975, **14**, 471 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DYC000

N^{G},N$'^{G}$-Dimethylarginine D-754

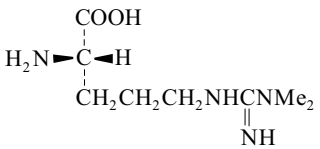
N^5-*[(Methylamino)(methylimino)methyl]ornithine, 9CI.* N^5-*(N,N′-Dimethylamidino)ornithine, 8CI*



$C_8H_{18}N_4O_2$ 202.256
(S)-form [30344-00-4]
L-form
Isol. from broad bean (*Vicia faba*) seed proteins. Cryst. (H_2O) (as diflavianate). Mp 237-239° (diflavianate).
Kakimoto, Y. *et al., J. Biol. Chem.*, 1970, **245**, 5751 (*isol, struct, synth, pmr*)
Baldwin, G.S. *et al., Biochem. J.*, 1971, **123**, 69 (*isol*)
Nakajima, T. *et al., Biochim. Biophys. Acta*, 1971, **230**, 212 (*isol, struct*)
Deibler, G.E. *et al., J. Biol. Chem.*, 1973, **248**, 2387 (*anal*)
Paik, W.K. *et al., Amino Acids*, 1993, **4**, 267 (*rev, biosynth, metab*)

N^{G},N^{G}-Dimethylarginine D-755

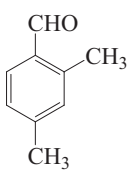
N^5-*[(Dimethylamino)iminomethyl]ornithine, 9CI.* N^5-*(N,N-Dimethylamidino)ornithine, 8CI*



$C_8H_{18}N_4O_2$ 202.256
(S)-form [30315-93-6]
[65005-57-4]
L-form
Isol. from broad bean seeds (*Vicia faba*). Cryst. (EtOH aq.) (as hydrochloride). Mp 198-201° (hydrochloride).
Hempel, K. *et al., Naturwissenschaften*, 1968, **55**, 37 (*isol*)
Kakimoto, Y. *et al., J. Biol. Chem.*, 1970, **245**, 5751 (*isol, synth*)
Nakajima, T. *et al., Biochim. Biophys. Acta*, 1971, **230**, 212; **243**, 31 (*isol*)
Deibler, G.E. *et al., J. Biol. Chem.*, 1973, **248**, 2387 (*anal*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 2449 (*isol, synth, pmr, ir*)
Paik, W.K. *et al., Amino Acids*, 1993, **4**, 267 (*rev, biosynth, metab*)

2,4-Dimethylbenzaldehyde D-756

[15764-16-6]
m-*Xylylaldehyde. FEMA 3427*



$C_9H_{10}O$ 134.177
Flavouring ingredient. Liq. Mp -9°. Bp 215-216° Bp_{10} 99°. n_D^{20} 1.5490.
(E)-Oxime:
$C_9H_{11}NO$ 149.192
Prisms (petrol). Mp 84-85° Mp 88°.
(Z)-Oxime:
$C_9H_{11}NO$ 149.192
Small needles (EtOH). Mp 126°.
Dimethylhydrazone: [134172-79-5]
$C_{11}H_{16}N_2$ 176.261
Liq. Bp_5 85-87°.
Phenylhydrazone: [86726-05-8]
Leaflets (AcOH aq.). Mp 88°.

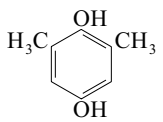
2,4-Dinitrophenylhydrazone:
Cryst. (C_6H_6/xylene). Mp 228-229°.

Semicarbazone:
Mp 225-227°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 115D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 950B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1295D (*ir*)
Aldrich Library of NMR Spectra, **6**, 87D (*pmr*)
Sadtler Standard C-13 NMR Spectra, 3634 (*cmr*)
Gattermann, L. *et al., Annalen*, 1906, **347**, 347 (*synth*)
Hinkel, L.E. *et al., J.C.S.*, 1932, 2793 (*synth*)
Weygand, F. *et al., Chem. Ber.*, 1955, **88**, 301 (*synth*)
Ryang, M. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 341 (*synth*)
Smith, W.E. *et al., J.O.C.*, 1972, **37**, 3972 (*synth*)
Venkoji, P. *et al., Proc. Indian Acad. Sci., Chem. Sci.*, 1984, **93**, 105 (*ir, Raman*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 173
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 847-848

2,6-Dimethyl-1,4-benzenediol, 9CI D-757

[654-42-2]
2,6-Dimethylhydroquinone, 8CI. 2,5-Dihydroxy-m-*xylene. 2,6-Dimethylquinol.* m-*Xylohydroquinone. 2,6-Xylohydroquinone*



$C_8H_{10}O_2$ 138.166
Claimed isoln. from *Pisum sativum* (pea). Cryst. (xylene). Mp 149-151°. Steam-volatile. Isoln. as nat. prod. unconfirmed.
▶ Human and exp. reprod. effects (reduced fertility). Exp. teratogenic effects. LD_{50} (mus, orl) 186 mg/kg. MX5900000

1-Me ether:4-Methoxy-3,5-dimethylphenol
$C_9H_{12}O_2$ 152.193
Plates. Mp 84-85°. Incorrectly named as "2,6-dimethyl-4-methoxyphenol" and incorrect formula of $C_9H_{14}O_3$ given.

4-Me ether: [2431-91-6] *4-Methoxy-2,6-dimethylphenol*
$C_9H_{12}O_2$ 152.193
Needles (petrol). Mp 77°. pK_{a1} 10.84 (25°).

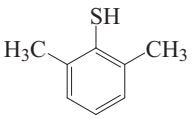
Di-Me ether:1,4-Dimethoxy-2,6-dimethylbenzene
$C_{10}H_{14}O_2$ 166.219
Oil.

[21111-81-9]

Bamberger, E. *et al., Annalen*, 1901, **316**, 302 (*synth*)
Bruice, T.C. *et al., J.O.C.*, 1953, **18**, 83 (*1-Me ether*)
Nilsson, J.L.G. *et al., Acta Pharm. Suec.*, 1968, **5**, 215; *CA*, **69**, 106132 (*synth*)
Carpino, L.A. *et al., J.O.C.*, 1989, **54**, 3303 (*synth, pmr*)
Elix, J.A. *et al., Aust. J. Chem.*, 1993, **46**, 95 (*di-Me ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DSG700
Lewis, R.J. *et al., Reproductively Active Chemicals*, Van Nostrand Reinhold, 1991, DSG700

2,6-Dimethylbenzenethiol, 9CI D-758

[118-72-9]
2,6-Xylenethiol, 8CI. m-*Xylene-2-thiol. 2,6-Dimethylthiophenol. 2,6-Thioxylenol. 2-Mercapto*-m-*xylene. FEMA 3666*



$C_8H_{10}S$ 138.233
Present in boiled beef. Flavouring ingredient. Liq. with a strong odour. d_4^{25} 1.04. Bp_{50} 122° Bp_{25} 110°. n_D^{20} 1.5753. Bp also given as 91°/50 mm.

S-*Me:* [4163-79-5] *1,3-Dimethyl-2-(methylthio)benzene, 9CI. Methyl 2,6-xylyl sulfide*
$C_9H_{12}S$ 152.26
Bp 217-218°.

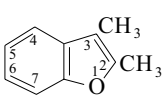
S-*Ph:* [54088-93-6] *1,3-Dimethyl-2-(phenylthio)benzene, 9CI. Phenyl 2,6-xylyl sulfide*
$C_{14}H_{14}S$ 214.331
Bp_3 137-138°.

[25550-52-1]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 425B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1097A (*ir*)
Al-Kazimi, H.R. *et al., J.A.C.S.*, 1955, **77**, 2479-2482 (*synth*)
Campaigne, E.E. *et al., J.O.C.*, 1957, **22**, 561-562 (*synth*)
Bartkus, E.A. *et al., J.O.C.*, 1957, **22**, 1185-1186 (*synth*)
Baliah, V. *et al., Tetrahedron*, 1963, **19**, 455-464 (*S-Me, synth*)
van der Laan, R. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1985, **104**, 220 (*pmr*)
Dupont, J. *et al., J.C.S. Dalton*, 1989, 1715-1720 (*S-Me, synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 195
Perumal, S. *et al., Magn. Reson. Chem.*, 1995, **33**, 779-790 (*S-Ph, synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 880-881
Sridhar, M. *et al., Synth. Commun.*, 1997, **27**, 1347-1350 (*synth*)

2,3-Dimethylbenzofuran D-759

[3782-00-1]
FEMA 3535



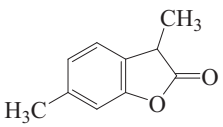
$C_{10}H_{10}O$ 146.188
Present in coffee and roasted onion. Flavorant. Oil. d_{20} 1.55. Bp_{19} 101-102° Bp_8 86-86.5°.

Picrate:
Yellow needles (EtOH). Mp 90-91°.

Gaertner, R. *et al., J.A.C.S.*, 1952, **74**, 5319 (*synth*)
Bisagni, M. *et al., J.C.S.*, 1955, 3688
Wilhalm, B. *et al., Tetrahedron*, 1964, **20**, 1185 (*ms*)
Veselovskaya, T.K. *et al., Zh. Obshch. Khim.*, 1964, **34**, 560 (*synth*)
Binon, F. *et al., Bull. Soc. Chim. Belg.*, 1965, **74**, 306 (*ir*)
Platzer, N. *et al., Bull. Soc. Chim. Fr.*, 1974, 906 (*synth, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 174 (*props, use*)

3,6-Dimethyl-2(3*H*)-benzofuranone, 9CI D-760

[65817-24-5]
Furaminton. FEMA 3863

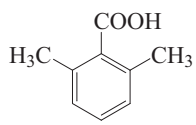


$C_{10}H_{10}O_2$ 162.188
(±)-*form*
Flavouring agent for candies etc.. Mp 39°. $Bp_{0.3}$ 76°.

Piccolo, O. *et al., J. Chem. Res., Synop.*, 1985, 258-259 (*synth, pmr*)
Eur. Pat., 1999, 953 294; *CA*, **131**, 310543x (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1142 (*use*)

2,6-Dimethylbenzoic acid, 9CI, 8CI D-761

[632-46-2]
vic-m-*Xylylic acid*



$C_9H_{10}O_2$ 150.177
Cryst. (H_2O). Mp 115-116°. pK_{a1} 3.35 (25°).
▶ DG8734010

Me ester: [14920-81-1]
$C_{10}H_{12}O_2$ 164.204
Oil. Bp_{19} 109°.

β-D-Glucopyranosyl ester: [97400-73-2] *β-D-Glucopyranosyl 2,6-dimethylbenzoate.* ***Moringyne***
$C_{15}H_{20}O_7$ 312.319
Constit. of the seeds of *Moringa oleifera* (horseradish tree).

Chloride: [21900-37-8]
C_9H_9ClO 168.622
Liq. Bp 217° $Bp_{0.3}$ 40-41°.

Amide: [55321-98-7]
$C_9H_{11}NO$ 149.192
Cryst. (EtOH). Mp 139°.

Nitrile: [6575-13-9] *2,6-Dimethylbenzonitrile. 2-Cyano-1,3-dimethylbenzene*

C_9H_9N 131.177
Needles (MeOH). Mp 90-91°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 203A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1091A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1329A (*ir*)
Hufferd, R.W. *et al., J.A.C.S.*, 1921, **43**, 929 (*synth*)
Anca, R. *et al., Acta Cryst.*, 1967, **23**, 110 (*cryst struct*)
Hojo, M. *et al., Tetrahedron*, 1971, **27**, 2713 (*synth*)
Smeyers, Y.G. *et al., Theor. Chim. Acta*, 1973, **28**, 355 (*uv*)
Guilleme, J. *et al., An. Quim.*, 1976, **72**, 35 (*pmr*)
Morcillo, J. *et al., An. Quim.*, 1977, **73**, 334 (*ir, Raman*)
Memon, G.M. *et al., Pak. J. Sci. Ind. Res.*, 1985, **28**, 7-9; *CA*, **103**, 51180m (*Moringyne*)
Drew, M.G.B. *et al., Acta Cryst. C*, 1991, **47**, 221 (*nitrile, cryst struct*)
Behringer, C. *et al., J. Prakt. Chem.*, 1997, **339**, 184 (*nitrile*)

3,4-Dimethylbenzoic acid, 9CI, 8CI D-762

[619-04-5]
unsym-o-*Xylylic acid*

$C_9H_{10}O_2$ 150.177
Isol. from *Eryngium foetidum* (culantro). Prisms. Mp 166°. pK_a 4.5 (25°). Sublimes.
▶ DG8734020

Me ester: [38404-42-1]
$C_{10}H_{12}O_2$ 164.204
Liq. Bp_{38} 132°.

Chloride: [21900-23-2]
C_9H_9ClO 168.622
Liq. Bp_{10} 122°.

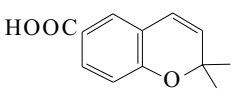
Amide: [5580-33-6]
$C_9H_{11}NO$ 149.192
Cryst. (EtOH). Mp 131° (113-114°).

Nitrile: [22884-95-3] *3,4-Dimethylbenzonitrile. 4-Cyano-1,2-dimethylbenzene*
C_9H_9N 131.177
Cryst. Mp 66°. Bp 231-232°.
▶ DI4357500

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 208D (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 205A (*nmr*)
Laham, S. *et al., Mikrochim. Acta*, 1969, 654 (*uv, ir*)
Yeh, P.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1974, **21**, 139; *CA*, **82**, 34950t (*isol*)
Guilleme, J. *et al., An. Quim.*, 1976, **72**, 35; 1977, **73**, 93 (*pmr, cmr*)
Morcillo, J. *et al., An. Quim.*, 1977, **73**, 334 (*ir, Raman*)
Mukherjee-Müller, G. *et al., Helv. Chim. Acta*, 1977, **60**, 1758 (*synth*)

2,2-Dimethyl-2*H*-1-benzopyran-6-carboxylic acid D-763

[34818-56-9]
2,2-Dimethyl-6-chromenecarboxylic acid. ***Anofinic acid***



$C_{12}H_{12}O_3$ 204.225
Metab. of *Lactarius deliciosus*. Cryst. (hexane/C_6H_6). Mp 160°.

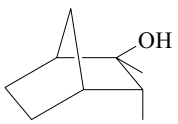
Me ester: [34818-57-0]
$C_{13}H_{14}O_3$ 218.252
Cryst. Mp 43-45° (synthetic).

Nitrile: [33143-29-2] *6-Cyano-2,2-dimethyl-2*H*-1-benzopyran*
$C_{12}H_{11}NO$ 185.225
Cryst. (hexane). Mp 48-49.5° (36-37°).

Shima, K. *et al., Yakugaku Zasshi*, 1971, **91**, 1124 (*isol, synth*)
Ahluwalia, V.K. *et al., Tetrahedron*, 1982, **38**, 3673 (*synth*)
Yamaguchi, S. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 442 (*synth, uv, pmr*)
Dáz, D.P.P. *et al., Phytochemistry*, 1987, **26**, 809 (*isol*)
Alberola, A. *et al., Heterocycles*, 1994, **38**, 819 (*synth, pmr, ms*)
Ayer, W.A. *et al., J. Nat. Prod.*, 1994, **57**, 839 (*isol, cmr*)
Bell, D. *et al., Synthesis*, 1995, 707 (*nitrile*)
Cristina, D. *et al., Phytochemistry*, 1999, **51**, 899-902 (*isol, uv, ir, pmr, cmr*)

2,3-Dimethylbicyclo[2.2.1]heptan-2-ol D-764

[59432-92-7]
Santene hydrate

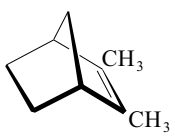


$C_9H_{16}O$ 140.225
Constit. of the famine food *Santalum album* (sandalwood). Flavouring ingredient. Cryst. Mp 102-103°. Mp refers to synthetic racemate. No indication of opt. rotn. of nat. prod. All 4 racemates are known synthetically.

Beckman, S. *et al., Chem. Ber.*, 1961, **94**, 1905 (*synth*)
Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*isol*)

2,3-Dimethylbicyclo[2.2.1]-hept-2-ene D-765

[529-16-8]
2,3-Dimethyl-2-norbornene. ***Santene***

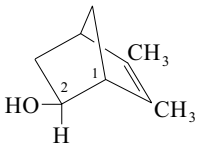


C_9H_{14} 122.21
Flavouring ingredient. Constit. of sandalwood oil. Oil. Bp 140-141°. n_D^{17} 1.4688.

Ryhage, R. *et al., Acta Chem. Scand.*, 1963, **17**, 2025 (*ms*)
Degny, E. *et al., Bull. Soc. Chim. Fr.*, 1972, 4770 (*synth*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)

5,6-Dimethylbicyclo[2.2.1]-hept-5-en-2-ol, 9CI D-766

[59300-41-3]
5,6-Dimethyl-5-norbornen-2-ol, 8CI



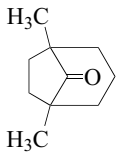
$C_9H_{14}O$ 138.209

(1R*,2S*)-form
exo-*form*
Constit. of the oil of East Indian sandalwood (*Santalum album*). Food flavouring. Liq. Bp_{10} 87°.

Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*isol, synth*)
Swiss Pat., 1978, 600 799; *CA*, **89**, 414992m (*synth*)

1,5-Dimethylbicyclo[3.2.1]octan-8-one, 9CI D-767

[21922-58-7]



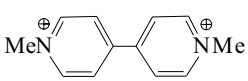
$C_{10}H_{16}O$ 152.236
Bp_{10} 72-74°.

Oxime: [75147-23-8] *Buccoxime*
$C_{10}H_{17}NO$ 167.25
Fragrance ingredient with a blackcurrant-like aroma.

Ger. Pat., 1980, 2 945 812; *CA*, **93**, 167745d (*synth*)
Ger. Pat., 1983, 3 129 934; *CA*, **98**, 197671x (*oxime*)
Haufe, G. *et al., Tetrahedron*, 1986, **42**, 4719-4728 (*synth, ir, pmr, cmr, ms*)

1,1′-Dimethyl-4,4′-bipyridinium(2+), 9CI, 8CI D-768

[4685-14-7]
N,N′-*Dimethyl-4,4′-bipyridyl(2+). Paraquat, ANSI, BSI, ISO, JMAF, WSSA. MV(2+)*



$C_{12}H_{14}N_2^{\oplus}$ 186.256
Herbicide.
▶ DW1960000

Dichloride: [1910-42-5] *Paraquat dichloride.* N,N′-*Dimethylviologen. Methyl viologen. Dextrone X. Gramoxone. Esgram*
$C_{12}H_{14}Cl_2N_2$ 257.161
Constit. of numerous proprietary herbicides. V. air-sensitive needles (MeOH/Me_2CO). V. sol. H_2O; sl. sol. MeOH, EtOH; insol. nonpolar solvs. Mp 300° approx. dec.
▶ OES: long-term 0.1 mg m^{-3} (respirable dust). Conc. commercial formulations irritate skin, eyes and mucous membranes, and can injure eyes by direct contact.

Many fatalities are associated with ingestion of 20% w/v solns., with death delayed for up to 2-3 weeks. Effects of ingestion incl. oesophageal ulceration, severe gastrointestinal effects, and damage to kidneys, liver, lungs and pancreas. The lung is a particular target organ for paraquat. LD_{50} (rat, orl) 57 mg/kg. LD_{50} (rat, skn) 80 mg/kg. Exp. reprod. and teratogenic effects. DW2275000

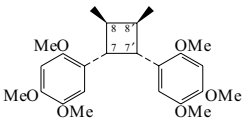
Bis(methylsulfate): [2074-50-2]
$C_{14}H_{20}N_2O_8S_2$ 408.453
Mp 300° approx. dec.

▶ DW2010000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 238A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 731A (*ir*)
Michaelis, L. *et al., J.A.C.S.*, 1933, **55**, 1481 (*synth*)
Brian, R.C. *et al., Nature (London)*, 1958, **181**, 446 (*rev*)
Haque, R. *et al., J.A.C.S.*, 1969, **91**, 3822 (*pmr*)
Russell, J.H. *et al., Acta Cryst. B*, 1972, **28**, 1527 (*cryst struct*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, 520 (*use*)
Verhoeven, J.W. *et al., Helv. Chim. Acta*, 1974, **57**, 2503 (*uv*)
Petersen, J.D. *et al., J.A.C.S.*, 1977, **99**, 8417 (*cmr*)
Carey, J.G. *et al., J.C.S. Perkin 1*, 1977, 2429; 2431 (*synth*)
Lott, P.F. *et al., J. Chromatogr. Sci.*, 1978, **16**, 390 (*rev, detn*)
Ross, J.H. *et al., J. Agric. Food Chem.*, 1980, **28**, 1026 (*synth, pmr*)
Summers, L.A. *et al., The Bipyridinium Herbicides*, Academic Press, London, 1980, (*book*)
Hester, R.E. *et al., J. Raman Spectrosc.*, 1982, **12**, 36 (*ir, Raman*)
Barofsky, D.F. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1983, **46**, 359 (*ms*)
Poizat, O. *et al., J. Chem. Soc., Faraday Trans.*, 1984, **80**, 3257 (*ir, Raman*)
Smith, L.L. *et al., Rev. Biochem. Toxicol.*, (ed., Hodgson, E., *et al*), Elsevier, New York, 1987, **8**, 37 (*tox*)
Dangerous Prop. Ind. Mater. Rep., 1988, **8**, 67 (*rev*)
Bockman, T.M. *et al., J.O.C.*, 1990, **55**, 4127 (*reactions*)
Kochi, J.K. *et al., J.O.C.*, 1990, **55**, 4127 (*props*)
Pesticide Manual, 9th edn., 1991, No. 9320
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A310
Cousson, A. *et al., Acta Cryst. C*, 1993, **49**, 942 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1129
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAI990; PAI995; PAJ000; PAJ250
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1356 (*tox, rev*)
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 452

1,2-Dimethyl-3,4-bis(2,4,5-trimethoxyphenyl)cyclobutane D-769

1,1′-(3,4-Dimethyl-1,2-cyclobutanediyl)-bis[2,4,5-trimethoxybenzene], 9CI. 2,2′,4,4′,5,5′-Hexamethoxy-7,7′-cyclolignan



(7α,7′α,8β,8′β)-*form*

$C_{24}H_{32}O_6$ 416.513
Lignan numbering shown.

(7α,7′α,8β,8′β)-*form* [70280-35-2]
Heterotropan
Constit. of *Piper cubeba* (cubeb pepper). Viscous liq. Opt. inactive (*meso*-).

(7α,7′β,8α,8′β)-*form* [81861-74-7]
Magnosalin
Cryst. (Et_2O/hexane). Mp 98-99°. $[\alpha]_D^{23}$ -4.6 (c, 0.25 in $CHCl_3$). Chiral molecule, may be racemic. Config. revised in 1993 λ_{max} 208 (ϵ 40738); 231 (ϵ 16980); 298 (ϵ 10715) (MeOH) (Berdy).

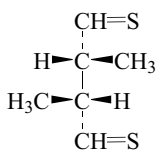
(7α,7′β,8β,8′α)-*form* [130323-08-9]
Andamanicin
Powder. Mp 110-112°. $[\alpha]_D^{20}$ +2.8 (c, 0.5 in $CHCl_3$). Chiral molecule, may be racemic. Config. revised in 1993.

(7ξ,7′ξ,8ξ,8′ξ)-*form* [73036-51-8]
Acoradin. *Bisasaricin*
Constit. of *Acorus calamus* (sweet flag). Prisms (Et_2O/petrol). Mp 101°. $[\alpha]_D$ 0 ($CHCl_3$).

[84172-46-3, 113349-60-3]

Niwa, M. *et al., Tet. Lett.*, 1978, 4891 (*isol, struct, synth*)
Patra, A. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 412 (*Acoradin*)
Yamamura, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 3573 (*isol, Heterotropan*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1112 (*Magnosalin*)
Badheka, L.P. *et al., Phytochemistry*, 1987, **26**, 2033-2036 (*isol*)
Kadota, S. *et al., Tet. Lett.*, 1987, **28**, 2857 (*synth*)
Kimura, M. *et al., Int. Arch. Allergy Appl. Immunol.*, 1990, **93**, 365-370 (*activity*)
Malhotra, S. *et al., Phytochemistry*, 1990, **29**, 2733-2734 (*Andamanicin*)
Mahindru, R.N. *et al., Phytochemistry*, 1993, **32**, 1073-1075 (*cryst struct*)
Ryu, J.-H. *et al., Bioorg. Med. Chem. Lett.*, 2002, **12**, 649-651 (*isol, pmr, cmr*)

2,3-Dimethyl-1,4-butanedithial D-770

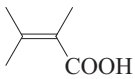


$C_6H_{10}S_2$ 146.277

(2*RS*,3*RS*)-*form*
(±)-form
S,S′-*Dioxide(Z,Z-):* [127793-93-5] ***Bissulfine***
$C_6H_{10}O_2S_2$ 178.276
Constit. of onion (*Allium cepa*). Solid. Mp 48° dec.
Block, E. *et al., J.A.C.S.*, 1990, **112**, 4584-4585; 1996, **118**, 2799-2810 (*isol, synth, pmr, cmr, ms*)

2,3-Dimethyl-2-butenoic acid, 9CI D-771

[4411-97-6]
Trimethylacrylic acid. 2,3-Dimethylcrotonic acid



$C_6H_{10}O_2$ 114.144
Long needles (H_2O). Mod. sol. H_2O. Mp 70-71°. pK_a 4.4 (25°).

Et ester: [13979-28-7]
$C_8H_{14}O_2$ 142.197
Liq. Bp_{59} 93-94°.

tert-*Butyl ester:*
$C_{10}H_{18}O_2$ 170.251
Liq. Bp_{20} 81-82°.

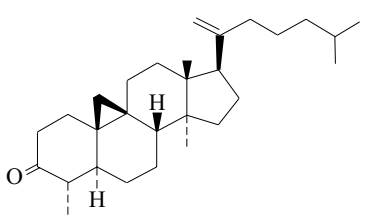
Benzyl ester: [7492-69-5] *FEMA 2143*
$C_{13}H_{16}O_2$ 204.268
Flavouring agent.

Chloride:
C_6H_9ClO 132.589
Liq. Bp_{50} 81°. Contd. *ca.* 5% benzene.

Nitrile:2-Cyano-3-methyl-2-butene
C_6H_9N 95.144
Yellow oil.

Perkin, W.H. *et al., J.C.S.*, 1896, **69**, 1479 (*synth*)
Huston, R.C. *et al., J.A.C.S.*, 1946, **68**, 2504 (*deriv*)
Braude, E.A. *et al., J.C.S.*, 1955, 3331 (*synth*)
McCollough, J.J. *et al., J.A.C.S.*, 1982, **104**, 4644 (*deriv*)
Freeman, F. *et al., J.O.C.*, 1986, **51**, 1654 (*synth, pmr, cmr, ms*)
Ceccherelli, P. *et al., Synth. Commun.*, 1991, **21**, 17 (*synth*)
Hansen, J.F. *et al., J. Het. Chem.*, 1994, **31**, 105 (*tert-butyl ester, chloride*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 59 (*benzyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 266-267 (*benzyl ester*)
Verdegem, P.J.E. *et al., J.O.C.*, 2001, **66**, 1269-1282 (*nitrile, pmr, cmr*)

4,14-Dimethyl-9,19-cyclocholest-20-en-3-one D-772



$C_{29}H_{46}O$ 410.682

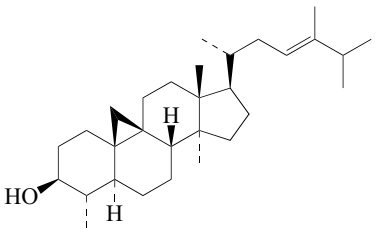
(4α,5α)-*form* [83118-62-1]
Constit. of *Musa paradisiaca* (banana). Cryst. (Me_2CO). Mp 138-139°. $[\alpha]_D^{30}$

+51.2.

Banerji, N. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 387 (*isol*)

4,14-Dimethyl-9,19-cycloergost-23-en-3-ol D-773

4,14,24-Trimethyl-9,19-cyclocholest-23-en-3-ol



$C_{30}H_{50}O$ 426.724

(3β,4α,5α,23*E*)-*form* [77704-67-7]

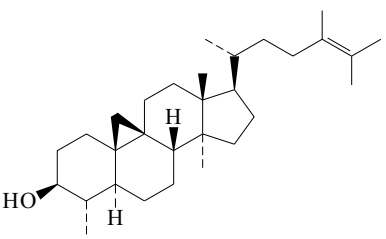
Isol. from olive oil and sweet corn (*Zea mays*).

Itoh, T. *et al., J. Am. Oil Chem. Soc.*, 1981, **58**, 545 (*isol*)

Scheid, F. *et al., Phytochemistry*, 1982, **21**, 1959 (*isol*)

4,14-Dimethyl-9,19-cycloergost-24-en-3-ol D-774

4,14,24-Trimethyl-9,19-cyclocholest-24-en-3-ol



$C_{30}H_{50}O$ 426.724

(3β,4α,5α,9β)-*form* [64543-35-7]

Constit. of rapeseed (*Brassica napus*).

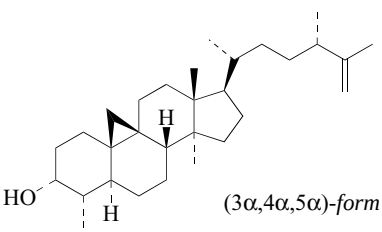
Ac:

Cryst. Mp 159-160°.

Itoh, T. *et al., Phytochemistry*, 1977, **16**, 1448

4,14-Dimethyl-9,19-cycloergost-25-en-3-ol, 9CI D-775

4,14,24-Trimethyl-9,19-cyclocholest-25-en-3-ol



(3α,4α,5α)-*form*

$C_{30}H_{50}O$ 426.724

(3α,4α,5α)-*form* [207850-20-2]

3-Epicyclomusalenol

Constit. of *Musa sapientum* (banana).

Cryst. Mp 121-122°.

(3α,4β,5α)-*form* [92694-03-6]

24-Methyl-28-norcycloart-25-en-3-ol

Constit. of *Musa sapientum* (banana).

3-Ketone: [2315-18-6] *4,14-Dimethyl-9,19-cycloergost-25-en-3-one. 24-Methyl-28-norcycloart-25-en-3-one.* ***4-Epicyclomusalenone***

$C_{30}H_{48}O$ 424.709

Constit. of *Musa sapientum* (banana).

Cryst. Mp 125-127°.

(3β,4α,5α)-*form* [2464-44-0]

[107439-26-9]

31-Norcyclolaudenol. *24-Methyl-29-norcycloart-25-en-3-ol. Cyclomusalenol*

Constit. of *Musa sapientum* (banana). Also from the mushrooms *Clitocybe nebularis* (clouded agaric) and *Hydnum repandum* (hedgehog fungus). Mp 137-139°.

Ac: [10376-46-2]

$C_{32}H_{52}O_2$ 468.762

3-Ketone: [30452-60-9]

[107439-27-0] *24-Methyl-29-norcycloart-25-en-3-one.* ***31-Norcyclolaudenone***. *Cyclomusalenone*

$C_{30}H_{48}O$ 424.709

Constit. of *Musa sapientum* (banana).

Knapp, F.F. *et al., Steroids*, 1970, **16**, 329-351 (*ketone, isol*)

Itoh, T. *et al., Steroids*, 1976, **27**, 275-285 (*pmr*)

Morelli, I. *et al., Fitoterapia*, 1981, **52**, 45-47 (*isol*)

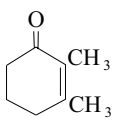
Akihisa, T. *et al., Lipids*, 1986, **21**, 494-497 (*Cyclomusalenone*)

Ageta, H. *et al., J. Nat. Prod.*, 1990, **53**, 325-332 (*isol*)

Akihisa, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 744-746 (*4-Epicyclomusalenone*)

2,3-Dimethyl-2-cyclohexen-1-one, 9CI D-776

[1122-20-9]



$C_8H_{12}O$ 124.182

Has been used in food flavouring. Liq. Bp_{12} 118-119°.

Semicarbazone:

Mp 225° dec.

2,4-Dinitrophenylhydrazone:

Mp 199-200° (170°).

Bergmann, E. *et al., J.O.C.*, 1939, **4**, 266 (*synth*)

Smith, L.I. *et al., J.A.C.S.*, 1943, **65**, 631 (*synth*)

Fenselau, C. *et al., J.A.C.S.*, 1969, **91**, 112 (*ms*)

Ramage, R. *et al., Tet. Lett.*, 1971, 649 (*synth*)

Pletcher, D. *et al., J.C.S. Perkin 1*, 1975, 948 (*synth*)

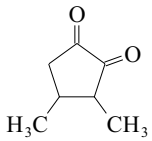
Corey, E.J. *et al., Chem. Ber.*, 1978, **111**, 1337 (*synth*)

Harding, C.E. *et al., J.O.C.*, 1992, **57**, 883 (*synth, pmr, ir, ms*)

3,4-Dimethyl-1,2-cyclopentanedione, 9CI D-777

[13494-06-9]

2-Hydroxy-3,4-dimethyl-2-cyclopenten-1-one. FEMA 3268



$C_7H_{10}O_2$ 126.155

Constit. of coffee. Flavouring additive with sugary/maple/caramel taste. Mp 71-72°. Config. not known (1994).

Gianturco, M.A. *et al., Tetrahedron*, 1963, **19**, 2039; 2051 (*isol, synth, struct*)

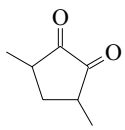
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*detn, ms, coffee*)

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 446

3,5-Dimethyl-1,2-cyclopentanedione, 9CI D-778

[13494-07-0]

2-Hydroxy-3,5-dimethyl-2-cyclopenten-1-one, 9CI. FEMA 3269



$C_7H_{10}O_2$ 126.155

Constit. of coffee and cooked cured pork. Flavouring agent. Mp 91-92°.

Gianturco, M.A. *et al., Tetrahedron*, 1963, **19**, 2039; 2051 (*isol, synth, struct*)

Sato, K. *et al., J.O.C.*, 1973, **38**, 551 (*synth*)

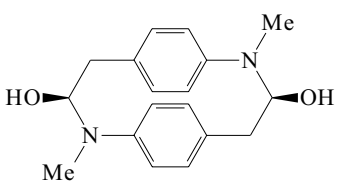
Cookson, R.C. *et al., Chem. Comm.*, 1976, 804 (*synth*)

Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*detn, ms, coffee*)

2,9-Dimethyl-2,9-diazatricyclo[10.2.2.2^{5,8}]octadeca-5,7,12,14,15,17-hexaene-3,10-diol, 9CI D-779

[124190-18-7]

N,α′,N′,α-Cyclodi(4-methylaminobenzeneethanol)

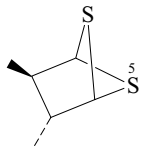


$C_{18}H_{22}N_2O_2$ 298.384

Alkaloid from peelings of *Citrus unshiu* (satsuma mandarin).

Matsubara, Y. *et al., CA*, 1990, **112**, 73757; **113**, 17474 (*isol, pmr, cmr, ms, struct*)

2,3-Dimethyl-5,6-dithiabicyclo[2.1.1]hexane D-780



(2*R**,3*R**)-*form*

$C_6H_{10}S_2$ 146.277

(2*R,3*R**)-*form***
trans-*form*

5α-Oxide: [120709-22-0] ***Zwiebelane B***
$C_6H_{10}OS_2$ 162.276
Constit. of onion (*Allium cepa*). There are two possible isomeric mono-*S*-oxides of the *trans*-form but only this isomer was detected.

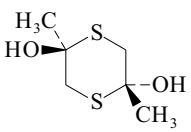
(2*RS*,3*SR*)-*form*
cis-*form*

5α-Oxide: [120637-81-2] ***Zwiebelane A***
$C_6H_{10}OS_2$ 162.276
Constit. of onion (*Allium cepa*). Oil. There are four possible isomeric mono-*S*-oxides of the *cis*-form but only this one was detected.

Bayer, T. *et al., J.A.C.S.*, 1989, **111**, 3085; 1990, **112**, 4584 (*isol, struct, synth*)
Block, E. *et al., J. Agric. Food Chem.*, 1992, **40**, 2431 (*glc, ms*)
Block, E. *et al., J.A.C.S.*, 1996, **118**, 2791; 2799 (*synth, pmr, cmr, ms*)

2,5-Dimethyl-1,4-dithiane-2,5-diol, 9CI D-781

[55704-78-4]
2,5-Dihydroxy-2,5-dimethyl-1,4-dithiane. FEMA 3450



$C_6H_{12}O_2S_2$ 180.292
Flavouring ingredient.

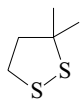
(2*RS*,5*SR*)-*form* [146511-93-5]
trans-*form*
Cryst. (C_6H_6). Mp 117-118° Mp 136-138° (dimorph.). Cryst. form depends on method of prepn. *meso*-.

[90200-29-6]

Haberl, R. *et al., Monatsh. Chem.*, 1955, **86**, 551 (*synth, ir, cryst struct*)
Brown, M.D. *et al., J.C.S. Perkin 1*, 1985, 1623 (*synth, ir, pmr, ms, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 176
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 853-854

3,3-Dimethyl-1,2-dithiolane, 9CI D-782

[58384-57-9]



$C_5H_{10}S_2$ 134.266
Detected in aroma of coffee. Yellow oil. Bp_{14} 68°. Rapidly polymerizes.

Schoeberl, A. *et al., Annalen*, 1958, **614**, 66 (*synth*)
Crump, D.R. *et al., J. Chem. Ecol.*, 1980, **6**, 837
Tressl, R. *et al., J. Agric. Food Chem.*, 1981, **29**, 1078 (*occur*)
Schildknecht, H. *et al., Chem.-Ztg.*, 1983, **107**, 267 (*occur*)
Buglass, A.J. *et al., Z. Naturforsch., C*, 1991, **46**, 166

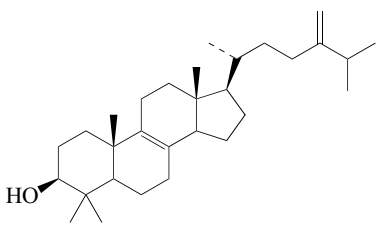
2,4-Dimethyldodecane D-783

[6117-99-3]
$(H_3C)_2CHCH_2CH(CH_3)CH_2(CH_2)_6CH_3$
$C_{14}H_{30}$ 198.391
Constit. of the flowers of *Viola odorata* (sweet violet). d_{20} 0.76. Bp_{13} 115°.

Petrov, A.A. *et al., CA*, 1960, **54**, 1257g (*synth*)
Zil'berg, G.A. *et al., CA*, 1966, **64**, 11046d (*synth*)
Cu, J.Q. *et al., Phytochemistry*, 1992, **31**, 571 (*occur*)

4,4-Dimethylergosta-8,24(28)-dien-3-ol D-784

4,4-Dimethyl-24-methylenecholest-8-en-3-ol

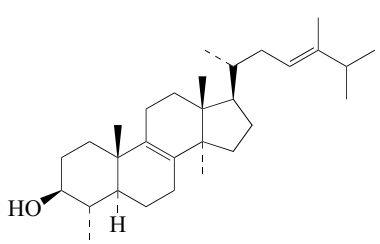


$C_{30}H_{50}O$ 426.724

(3β,5α)-*form* [14250-23-8]
Metab. of *Marasmius oreades* (fairy ring mushroom). Cryst. Mp 163-164°. $[\alpha]_D$ +14 (c, 0.03 in $CHCl_3$).

Fattorusso, E. *et al., Steroids*, 1992, **57**, 119 (*isol, pmr, cmr*)

4,14-Dimethylergosta-8,23-dien-3-ol D-785



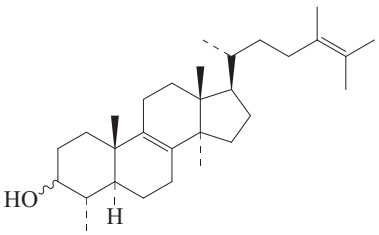
$C_{30}H_{50}O$ 426.724

(3β,4α,5α,23*E*)-*form* [84886-39-5]
Isol. from etiolated corn coleoptiles (*Zea mays*).

Scheid, F. *et al., Phytochemistry*, 1982, **21**, 1959 (*isol, ms*)

4,14-Dimethylergosta-8,24-dien-3-ol D-786

4,14,24-Trimethylcholesta-8,24-dien-3-ol



$C_{30}H_{50}O$ 426.724

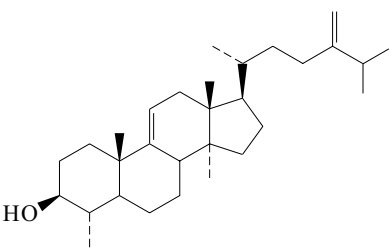
(3ξ,4α,5α,14α)-*form* [64543-34-6]
Constit. of rapeseed (*Brassica napus*).

Ac:
Cryst. Mp 139-140°.

Itoh, T. *et al., Phytochemistry*, 1977, **16**, 1448

4,14-Dimethylergosta-9(11),24(28)-dien-3-ol D-787

4,14-Dimethyl-24-methylenecholest-9(11)-en-3-ol



$C_{30}H_{50}O$ 426.724

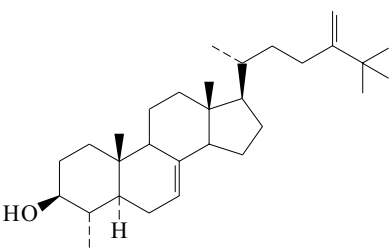
(3β,4α,5α)-*form* [77704-66-6]
Isol. from seeds of *Phaseolus vulgaris* (kidney bean). Mp 105-107° (as acetate).

[105097-80-1, 108944-19-0]

Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219 (*isol*)

4,25-Dimethylergosta-7,24(28)-dien-3-ol, 9CI D-788

4,25-Dimethyl-24-methylenecholest-7-en-3-ol



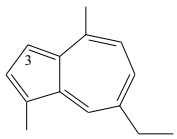
$C_{30}H_{50}O$ 426.724

(3β,4α,5α)-*form* [123086-79-3]
25-Methylgramisterol
Constit. of bean (*Phaseolus vulgaris*) seeds.

Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219

1,4-Dimethyl-7-ethylazulene D-789

[529-05-5]
Chamazulene. Camazulene. Lindazulene. Dimethulene

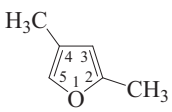


$C_{14}H_{16}$ 184.28
Isol. as artifact from various sesquiterpene oils, e.g. from *Achillea* and *Artemisia* spp.. Blue oil. Bp_{12} 161°. Log P 5.34 (calc).
▶ LD_{50} (rat, orl) 10000 mg/kg. CO4780000
Picrate:
Cryst. (MeOH). Mp 116°.
3,6-Dihydro: [18454-88-1] *7-Ethyl-3,6-dihydro-1,4-dimethylazulene*
$C_{14}H_{18}$ 186.296
Minor constit. of *Artemisia absinthium* (wormwood). Pale-yellow unstable oil.
5,6-Dihydro: [18454-89-2] *7-Ethyl-5,6-dihydro-1,4-dimethylazulene*
$C_{14}H_{18}$ 186.296
Minor constit. of *Artemisia absinthium* (wormwood). Orange-black unstable oil.

Takeda, K. *et al., Chem. Pharm. Bull.*, 1953, **75**, 3865 (*struct*)
Bertelli, D.J. *et al., Tetrahedron*, 1968, **24**, 2079 (*isol, struct*)
Mukherjee, D. *et al., J.A.C.S.*, 1979, **101**, 251 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 755
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995, (*bibl*)
Adam, K.-P. *et al., Phytochemistry*, 1998, **48**, 953-959 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DRV000

2,4-Dimethylfuran, 9CI D-790

[3710-43-8]



C_6H_8O 96.129
Found in garlic and leek oil. Flavouring ingredient. Bp 94-98°.

Gilman, H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1932, **51**, 672
Morel, T.H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1951, **70**, 35
Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)
Scharf, H.-D. *et al., Chem. Ber.*, 1978, **111**, 639 (*synth*)
Yu, T.H. *et al., J. Agric. Food Chem.*, 1989, **37**, 725-730 (*isol*)
Ancerewicz, J. *et al., Helv. Chim. Acta*, 1996, **79**, 1393 (*synth, pmr*)

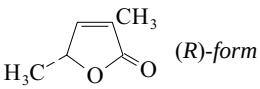
2,5-Dimethylfuran, 9CI D-791

[625-86-5]

C_6H_8O 96.129
Maillard product. Mp -63°. Bp 93-94°. n_D^{20} 1.4363.
▶ Highly flammable, fl. p. 16°. LU0875000
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 15C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 580B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1450C (*ir*)
Reddy, G.S. *et al., J. Phys. Chem.*, 1961, **65**, 1539 (*nmr*)
Reddy, G.S. *et al., J.A.C.S.*, 1961, **83**, 5020 (*nmr*)
Hillers, S. *et al., Khim. Geterotsikl. Soedin.*, 1966, 487 (*ir, Raman*)
Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)
Scott, L.T. *et al., Synthesis*, 1973, **4**, 209 (*synth*)
Kiewiet, A. *et al., Org. Magn. Reson.*, 1974, **6**, 461 (*nmr*)
Scharf, H.-D. *et al., Chem. Ber.*, 1978, **111**, 639 (*synth*)
Hashimi, A.S.K. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 1581 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DSC000

3,5-Dimethyl-2(5*H*)-furanone, 9CI D-792

[5584-69-0]
2,4-Dimethyl-2-buten-4-olide. 4-Hydroxy-2-methyl-2-pentenoic acid γ-lactone



$C_6H_8O_2$ 112.128
(*R*)-*form* [59417-65-1]
Liq. Bp_{16} 120°.
(*S*)-*form* [127418-12-6]
Liq. $[\alpha]_D^{25}$ +91.5 (c, 1.24 in $CHCl_3$).
(±)-*form*
Liq. Bp_{45} 100-103° $Bp_{0.05}$ 30°. n_D^{22} 1.4532.
(ξ)-*form*
Flavour component of the edible miller mushroom (*Coprinus comatus*), cooked bacon and smoke condensates.

Volger, H.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 1203 (*synth, pmr, ms, glc*)
Gorewit, B. *et al., J.O.C.*, 1973, **38**, 2257 (*synth, pmr*)
Hussain, S.A.M.T. *et al., J.C.S. Perkin 1*, 1975, 1480 (*synth, pmr*)
Kawamata, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 277 (*synth, pmr, ir*)
Guntrum, E. *et al., Synthesis*, 1986, 921 (*synth, pmr, cmr, ir*)
Corbera, J. *et al., J.O.C.*, 1988, **53**, 4393 (*synth, pmr, cmr, R-form*)
Chiarello, J. *et al., Synth. Commun.*, 1989, **19**, 3379 (*synth, pmr, ir, S-form*)

5,5-Dimethyl-2(5*H*)-furanone, 9CI D-793

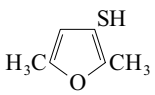
[20019-64-1]
4,4-Dimethyl-2-butenolide

$C_6H_8O_2$ 112.128
Aroma component of hop extract, and of lavender, sagebrush, narcissus and salmon oils. Liq. with burnt camphor-menthol odour. Bp 210° Bp_{14} 94° Bp_{10} 80°. n_D^{18} 1.4470.

Haynes, L.J. *et al., J.C.S.*, 1946, 954 (*synth*)
Nobuhara, A. *et al., Agric. Biol. Chem.*, 1970, **11**, 1745 (*synth, props*)
King, G.S. *et al., J.C.S. Perkin 1*, 1974, 1499 (*synth, pmr, ms, gc*)
Torii, S. *et al., J.O.C.*, 1974, **39**, 2486 (*synth*)
Barluenga, J. *et al., Chem. Comm.*, 1986, 183 (*synth, cmr*)
Tanikaga, R. *et al., Synthesis*, 1986, 416 (*synth*)
Alper, H. *et al., J.O.C.*, 1991, **56**, 5357 (*synth*)

2,5-Dimethyl-3-furanthiol D-794

[55764-23-3]
3-Mercapto-2,5-dimethylfuran. FEMA 3451

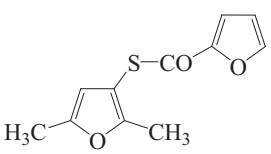


C_6H_8OS 128.195
Component of chicken volatiles. Flavouring agent. Red liq. Bp_{10} 80-150° (bulb).
▶ LU6230000
S-*Me:* [63359-63-7] *2,5-Dimethyl-3-(methylthio)furan*
$C_7H_{10}OS$ 142.221
Occurs in coffee aroma. Faintly yellow liq. Bp_1 71°.

Huber, U.A. *et al., Helv. Chim. Acta*, 1993, **76**, 2528 (*synth, pmr, bibl*)

S-(2,5-Dimethyl-3-furanyl) 2-furancarbothioate, 9CI D-795

[55764-31-3]
2,5-Dimethyl-3-(2-thiofuroyl)furan

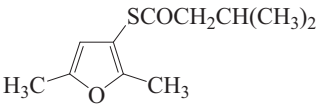


$C_{11}H_{10}O_3S$ 222.264
Flavouring agent with hydrolysed vegetable-type aroma and flavour.

U.S. Pat., 1975, 3 922 288; *CA*, **84**, 721636e (*synth, ms, pmr, use*)

S-2,5-Dimethyl-3-furanyl 3-methylbutanethioate, 9CI D-796

[55764-28-8]
2,5-Dimethyl-3-(thioisovaleryl)furan. FEMA 3482



$C_{11}H_{16}O_2S$ 212.312
Flavouring agent. Liq. with creamy, cocoa-like sweet aroma. d_4^{20} 1.03. Bp_6 124-125°.

U.S. Pat., 1973, 3 910 966; *CA*, **84**, 30860g (*use, ms, pmr*)
U.S. Pat., 1976, 3 958 029; *CA*, **85**, 159857m (*synth, use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 195 (*props, use*)

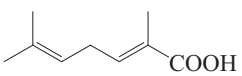
2,6-Dimethyl-2,4-heptadiene D-797

[4634-87-1]
$(H_3C)_2CHCH{=}CHCH{=}C(CH_3)_2$
C_9H_{16} 124.225
Constit. of *Osmanthus fragrans* (sweet osmanthus). Bp 139-143°.

(*E*)-*form* [62716-22-7]
Liq.

Kizhner, N. *et al., CA*, 1912, **7**, 3965
Nakada, Y. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 1724 (*synth*)
Otieno, D.A. *et al., J.C.S. Perkin 1*, 1977, 196 (*synth*)
Ding, D. *et al., J. Essent. Oil Res.*, 1989, **1**, 295 (*occur*)

2,6-Dimethyl-2,5-heptadienoic acid D-798



$C_9H_{14}O_2$ 154.208

(*E*)-*form* [261949-42-2]
Constit. of *Passiflora quadrangularis* (giant grandilla). Oil.

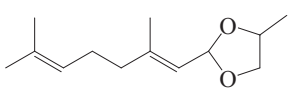
β-D-Glucopyranosyl ester: [261949-43-3]
$C_{15}H_{24}O_7$ 316.35
Constit. of *Passiflora quadrangularis* (giant grandilla). Oil. $[\alpha]_D^{25}$ +12.6 (c, 0.78 in MeOH).

Osorio, C. *et al., Phytochemistry*, 2000, **53**, 97-101 (*isol, pmr, cmr*)

2-(2,6-Dimethyl-1,5-heptadienyl)-4-methyl-1,3-dioxolane, 9CI, 8CI D-799

[10444-50-5]

[170556-22-6, 170556-23-7, 170556-24-8, 170556-25-9, 197718-75-5, 197719-38-3]
Citral propylene glycol acetal



$C_{13}H_{22}O_2$
Flavouring ingredient. Oily liq. with citrus orange-lemon odour and lemon flavour in aq. media. $Bp_{0.5}$ 82°.

Welch, R.C. *et al., J. Agric. Food Chem.*, 1980, **28**, 870-872 (*ms*)
Kula, J. *et al., Parfuem. Kosmet.*, 1995, **76**, 368 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 613 (*use, props*)
U.S. Pat., 1997, 5 626 852 (*use*)
Sharma, A. *et al., J. Agric. Food Chem.*, 1998, **46**, 654-656 (*synth, props*)

3,4-Dimethylheptane, 9CI D-800

[922-28-1]
$H_3CCH_2CH_2CH(CH_3)CH(CH_3)CH_2CH_3$
C_9H_{20} 128.257
Constit. of the flowers of *Osmanthus fragrans* (sweet osmanthus) and *Viola odorata* (sweet violet). Bp 140.1°. Mixt. of diastereoisomers.

[52896-82-9, 57031-63-7, 57031-64-8, 75110-09-7, 75110-10-0]

Henne, A.L. *et al., J.A.C.S.*, 1944, **66**, 392 (*synth*)
Dvoretsky, I. *et al., Anal. Chem.*, 1963, **35**, 545 (*synth*)
Beierbeck, H. *et al., Can. J. Chem.*, 1977, **55**, 771; 1980, **58**, 1258 (*conformn, cmr*)
Yaws, C.L. *et al., Hydrocarbon Process. Int. Ed.*, 1989, **68**, 61 (*props*)

2,6-Dimethyl-4-heptanol, 9CI D-801

[108-82-7]
Diisobutylcarbinol. FEMA 3140
$(H_3C)_2CHCH_2CH(OH)CH_2CH(CH_3)_2$
$C_9H_{20}O$ 144.256
Flavouring ingredient. Insol. H_2O, sol. EtOH, Et_2O. d^{20} 0.81. Bp 179° Bp_{14} 72°. n_D^{20} 1.4238.

▶ Eye, skin and respiratory tract irritant. Adverse hepatic and CNS effects reported by ingestion. LD_{50} (rat, orl) 3160 mg/kg. LD_{50} (rbt, skn) 4600 mg/kg. MJ3325000

1-Naphthylurethane:
Mp 71-74°.

Ac:
$C_{11}H_{22}O_2$ 186.294
Bp_{60} 125-126°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 188A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 180A (*ir*)
Ipatieff, V.N. *et al., J.O.C.*, 1942, **7**, 189-198 (*synth*)
Sarel, S. *et al., J.A.C.S.*, 1956, **78**, 5416-5420 (*Ac*)
Sokolova, E.B. *et al., CA*, 1962, **56**, 8652 (*synth*)
Brown, H.C. *et al., Synthesis*, 1978, 676-677 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 178
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 856-857
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DNH800

2,6-Dimethyl-4-heptanone, 9CI D-802

[108-83-8]
Diisopropylacetone. Isovalerone. Diisobutyl ketone. Isobutyl ketone. FEMA 3537
$(H_3C)_2CHCH_2COCH_2CH(CH_3)_2$
$C_9H_{18}O$ 142.241
Flavouring ingredient. Oil. Sl. sol. H_2O, sol. EtOH. Bp 165-166° Bp_{11} 56°. n_D^{20} 1.4128.

▶ Flammable, fl. p. 49/51°, autoignition temp. 388°. Eye, skin and respiratory tract irritant. High vapour conc. narcotic. Lower conc. may cause headache, nausea. LD_{50} (rat, orl) 5750 mg/kg. OES: long-term 25 ppm. MJ5775000

Oxime: [52435-41-3]
$C_9H_{19}NO$ 157.255
Bp 205-210° Bp_{20} 114-116°.

2,4-Dinitrophenylhydrazone:
Mp 92°.

Semicarbazone:
Mp 126° (110°).

Registry of Mass Spectral Data, Wiley, 1974, 321-6 (*ms*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 409D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 638B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 493D (*ir*)
Aldrich Library of IR Spectra, 2nd Ed., 218C (*ir*)
Aldrich Library of NMR Spectra, **2**, 109B (*pmr*)
Sadtler Standard C-13 NMR Spectra, 806 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 10135 (*uv*)
Hammell, M. *et al., J.O.C.*, 1950, **15**, 1628 (*synth*)
Davis, R. *et al., J.O.C.*, 1962, **27**, 854 (*synth*)
Carlson, B.A. *et al., J.A.C.S.*, 1973, **95**, 6876 (*synth*)
Karimov, M. *et al., CA*, 1976, **85**, 77589 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 179
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 857-858
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4770 (*tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 476
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DNI800

2,6-Dimethyl-5-heptenal, 9CI D-803

[106-72-9]
Melonal. FEMA 2389
$(H_3C)_2C{=}CHCH_2CH_2CH(CH_3)CHO$
$C_9H_{16}O$ 140.225
Oil.

▶ Skin and eye irritant. MJ8797000

(±)-*form*
Perfumery and flavouring ingredient. Liq. with melon-like odour and taste. Bp_{100} 116-124°.

Oxime: [22457-24-5]
$C_9H_{17}NO$ 155.239
$Bp_{0.9}$ 80-81°.

Semicarbazone:
Mp 135°.

2,4-Dinitrophenylhydrazone:
Mp 87°.

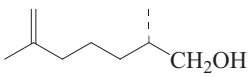
1-Carboxylic acid:2,6-Dimethyl-5-heptenoic acid
$C_9H_{16}O_2$ 156.224
Oil.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 737C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 561A (*ir*)

Dominguez, X.A. *et al., CA*, 1956, **50**, 8445 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 793 (*rev, tox*)
Ayer, S.W. *et al., Experientia*, 1983, **39**, 255-256 (*isol*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DSD775
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

2,6-Dimethyl-6-hepten-1-ol, 9CI D-804

[40326-01-0]
α-Melonol. FEMA 3663



(S)-form

$C_9H_{18}O$ 142.241

(*S*)-*form* [138381-56-3]
Liq. $[\alpha]_D^{20}$ -11.8 (c, 1.0 in $CHCl_3$).

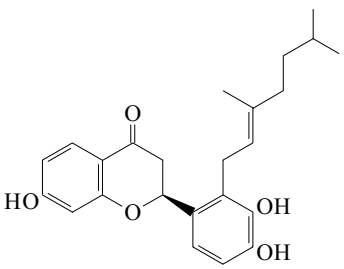
(±)-*form* [36806-46-9]
Flavouring ingredient. Liq. with pleasant melon odour. d^{20} 0.86. Bp_1 62°. n_D^{20} 1.4515.

(ξ)-*form*
Oil.

[138381-57-4]

Wu, J. *et al., Agric. Biol. Chem.*, 1991, **55**, 2667-2668 (*synth*)
Shanghnessy, K.H. *et al., J.A.C.S.*, 1995, **117**, 5873-5874 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 859
Schinzer, D. *et al., Chem. Eur. J.*, 1999, **5**, 2492-2500 (*synth, ir, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 452

2′-(3,6-Dimethyl-2-heptenyl)-3′,4′,7-trihydroxyflavanone D-805



$C_{24}H_{28}O_5$ 396.482

(*S*)-(*E*)-*form* [116207-28-4]
Constit. of *Artocarpus communis* (breadfruit).

Koshihara, Y. *et al., Biochem. Pharmacol.*, 1988, **37**, 2161 (*isol, props*)

8-(3,6-Dimethyl-2-heptenyl)-4′,5,7-trihydroxyflavanone D-806

$C_{24}H_{28}O_5$ 396.482

(*S*)-(*E*)-*form* [116207-30-8]
Constit. of *Artocarpus communis* (breadfruit). Cryst. Mp 146-148°.

Koshihara, Y. *et al., Biochem. Pharmacol.*, 1988, **37**, 2161-2165 (*isol, props*)
McLean, S. *et al., Magn. Reson. Chem.*, 1996, **34**, 719-722 (*isol, pmr, cmr*)

2,3-Dimethylhexane D-807

[584-94-1]
Isopropylmethylpropylmethane
$(H_3C)_2CHCH(CH_3)CH_2CH_2CH_3$
C_8H_{18} 114.23

(-)-*form*
Liq. Bp 113-114°. $[\alpha]_D^{25}$ -0.92.

(±)-*form*
Liq. d^{20} 0.71. Bp 115.8°.
► Highly flammable, fl. p. 7° (oc), autoignition temp. 438°. High vapour conc. prob. narcotic.

(ξ)-*form*
Volatile component of starfruit.

Clark, L. *et al., J.A.C.S.*, 1911, **33**, 529 (*synth*)
Levene, P.A. *et al., J. Biol. Chem.*, 1933, **100**, 769 (*synth*)
Beierbeck, H. *et al., Can. J. Chem.*, 1977, **55**, 771 (*cmr*)
Dimov, N. *et al., Anal. Chim. Acta*, 1987, **201**, 217 (*detn*)
Daub, R.J. *et al., HRC & CC, J. High Resolut. Chromatogr. Chromatogr. Commun.*, 1988, **11**, 649 (*gc, rev*)
MacLeod, G. *et al., Phytochemistry*, 1990, **29**, 165 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DSE509

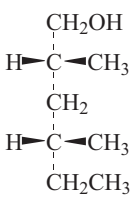
3,3-Dimethylhexane, 9CI D-808

[563-16-6]
$H_3CCH_2CH_2C(CH_3)_2CH_2CH_3$
C_8H_{18} 114.23
Constit. of the oil of *Osmanthus fragrans* (sweet osmanthus) and ginseng. d_4^{20} 0.71. Bp 111-112°. n_D^{20} 1.4008.

Noller, C.R. *et al., J.A.C.S.*, 1929, **51**, 598 (*synth*)
Marker, R.E. *et al., J.A.C.S.*, 1938, **60**, 2598 (*synth*)
Khromov, S.I. *et al., CA*, 1959, **53**, 2149 (*synth*)
Pines, H. *et al., J.O.C.*, 1965, **30**, 3540 (*synth*)
Beierbeck, H. *et al., Can. J. Chem.*, 1977, **55**, 771 (*conformn, cmr*)

2,4-Dimethyl-1-hexanol, 9CI D-809

[3965-59-1]



(2R,4R)-form

$C_8H_{18}O$ 130.23

(2*R*,4*R*)-*form* [130322-50-8]
Oil. $[\alpha]_D^{22}$ +3.7 (c, 1.67 in $CHCl_3$).

(2*S*,4*S*)-*form* [139684-72-3]
Oil. $[\alpha]_D^{27}$ -456 (c, 1.64 in $CHCl_3$). $[\alpha]_D$ -3.9 (c, 1.63 in $CHCl_3$).

Hexadecanoyl:
$C_{24}H_{48}O_2$ 368.642

Octadecanoyl:
$C_{26}H_{52}O_2$ 396.696

9Z-Octadecenoyl:
$C_{26}H_{50}O_2$ 394.68

9Z,12Z-Octadecadienoyl:
$C_{26}H_{48}O_2$ 392.664

Eicosanoyl:
$C_{28}H_{56}O_2$ 424.749

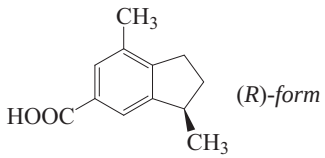
(2ξ,4ξ)-*form*
Aroma and taste producing constit. of wine.

[111675-63-9, 139684-73-4, 159346-50-6]

Lardicci, L. *et al., Tetrahedron*, 1966, **22**, 1991-2001 (*synth*)
Chenyaga, B.S. *et al., Prikl. Khromatogr.*, 1984, 157-167; *CA*, **102**, 130376n (*glc*)
White, J.D. *et al., J.O.C.*, 1994, **59**, 3347-3358 (*synth, ir, pmr, cmr, ms*)
Stoermer, D. *et al., J.O.C.*, 1996, **61**, 9115-9125 (*S,S-form, synth, ir, pmr, cmr*)
Nakamura, S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1330-1333 (*synth, ir, pmr, cmr*)
Sakata, T. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 919-927 (*esters, isol, synth*)

3,7-Dimethyl-5-indanecarboxylic acid D-810

*2,3-Dihydro-3,7-dimethyl-1*H*-indene-5-carboxylic acid, 9CI*



(R)-form

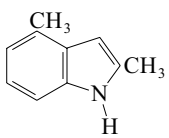
$C_{12}H_{14}O_2$ 190.241

(*R*)-*form* [217802-61-4]
Constit. of *Curcuma zedoaria* (zedoary). Needles (hexane). Mp 153-155°. $[\alpha]_D^{25}$ +18 (c, 1 in C_6H_6).

Syu, W.-J. *et al., J. Nat. Prod.*, 1998, **61**, 1531-1534 (*isol, ir, pmr, cmr, ms*)

2,4-Dimethyl-1*H*-indole, 9CI D-811

[10299-61-3]



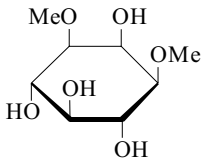
$C_{10}H_{11}N$ 145.204
Alkaloid from fruit bodies of the unpalatable mushrooms *Tricholoma sciodes* and *Tricholoma virgatum*. Liq. $Bp_{0.5}$ 94-96°.

Picrate:
Cryst. Mp 164.5°.

Marion, L. *et al., Can. J. Res., Sect. B*, 1947, **25**, 1 (*synth*)
Gassman, P.G. *et al., J.A.C.S.*, 1974, **96**, 5495 (*synth*)
McDonald, B.G. *et al., J.C.S. Perkin 1*, 1975, 1446 (*synth*)
Bard, R.R. *et al., J.O.C.*, 1980, **45**, 1546 (*synth*)
Garlaschelli, L. *et al., Tetrahedron*, 1994, **50**, 3571 (*isol, uv, ir, pmr, cmr, ms*)
Söderberg, B.C. *et al., J.O.C.*, 1999, **64**, 9731-9734 (*synth*)

1,3-Di-*O*-methyl-*myo*-inositol, 9CI, 8CI D-812

[523-94-4]
Dambonitol. *Dambonite*



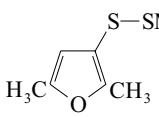
$C_8H_{16}O_6$ 208.211
Latex used for manuf. of chewing gum. Cryst. (EtOH) with sweet taste. Mp 210°. Exhibits polymorphism. Opt. inactive (*meso*-).

Tetra-Ac: [109338-68-3] *2,4,5,6-Tetra*-O-*acetyldambonitol*
$C_{16}H_{24}O_{10}$ 376.36
Cryst. (MeOH). Mp 195°.

Comollo, A.J. *et al., J.C.S.*, 1953, 3319 (*isol, constit*)
Kiang, A.K. *et al., J.C.S.*, 1956, 480-483 (*struct*)
Angyal, S.J. *et al., J.C.S.*, 1957, 1417-1422 (*isol, struct*)
Kindl, H. *et al., Monatsh. Chem.*, 1966, **97**, 1778 (*biosynth*)
Dorman, E.D. *et al., J.A.C.S.*, 1970, **92**, 1351 (*cmr*)
Anderson, L. *et al., The Carbohydrates*, Academic Press, 1972, **1A**, 519 (*rev*)
Paart, E. *et al., J. Chromatogr.*, 1973, **85**, 93 (*chromatog*)
Sakurai, K. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 975 (*isol, pmr, cmr, props*)

2,5-Dimethyl-3-(methyldithio)furan, 9CI D-813

[61197-06-6]
2,5-Dimethyl-3-furanyl methyl disulfide

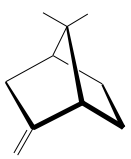


$C_7H_{10}OS_2$ 174.287
Component of coffee aroma. Red liq. $Bp_{0.75}$ 54°.

Huber, U.A. *et al., Helv. Chim. Acta*, 1993, **76**, 2528-2536 (*synth, bibl*)

7,7-Dimethyl-2-methylenebicyclo[2.2.1]heptane D-814

[471-84-1]
α-Fenchene



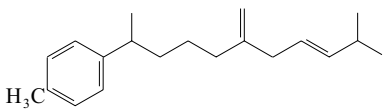
Relative configuration

$C_{10}H_{16}$ 136.236
(-)-*form* [7378-37-2]
Constit. of *Valeriana officinalis* (valerian). Oil. Bp 155-160°. $[\alpha]_D$ -42.62 (EtOAc). n_D^{20} 1.4742.

Hückel, W. *et al., Annalen*, 1963, **664**, 31
Kokke, W.C.M.C. *et al., J.O.C.*, 1973, **38**, 2989

1-(1,9-Dimethyl-5-methylene-8-decenyl)-4-methylbenzene D-815

[6089-98-1]
ar-*Artemisene*



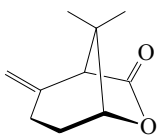
$C_{20}H_{30}$ 270.457
Constit. of Wormwood oil (*Artemisia absinthium*). Oil. $[\alpha]_D$ -19.2.

[19907-39-2]

Sorm, F. *et al., Coll. Czech. Chem. Comm.*, 1951, **16**, 268 (*isol*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1965, **42**, 773 (*synth*)
Crawford, R.J. *et al., J.O.C.*, 1972, **37**, 3543 (*synth, pmr*)

8,8-Dimethyl-2-methylene-6-oxabicyclo[3.2.1]octan-7-one D-816

[28449-87-8]
Karahana lactone



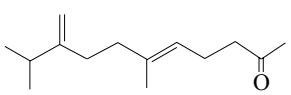
(−)-*form*

$C_{10}H_{14}O_2$ 166.219
Constit. of hops.
(-)-*form*
Cryst. (hexane). Mp 57.5-58.5°. $[\alpha]_D^{25}$ -295 (c, 1 in $CHCl_3$). The nat. prod. is nearly racemic (1.3% ee).

Naya, Y. *et al., CA*, 1970, **73**, 43892
Mori, K. *et al., Tetrahedron*, 1985, **41**, 5487 (*synth*)
Galano, J.-M. *et al., Tetrahedron*, 2000, **56**, 7477-7481 (*synth, cryst struct*)

6,10-Dimethyl-9-methylene-5-undecen-2-one D-817

9-Isopropyl-6-methyl-5,9-decadien-2-one



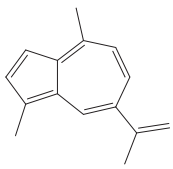
$C_{14}H_{24}O$ 208.343
(E)-form [64854-44-0]
Constit. of *Costus* root oil (*Saussurea lappa*). Oil.

[64854-46-2]

Maurer, B. *et al., Chem. Comm.*, 1977, 353 (*isol, synth*)
Maurer, B. *et al., Helv. Chim. Acta*, 1977, **60**, 6191
Dubs, P. *et al., Helv. Chim. Acta*, 1978, **61**, 984 (*isol, synth*)
Morizur, J.-P. *et al., Tet. Lett.*, 1982, **23**, 5275 (*synth*)

1,4-Dimethyl-7-(1-methylethenyl)azulene, 9CI D-818

[489-85-0]
7-Isopropenyl-1,4-dimethylazulene. ***Lactarazulene***

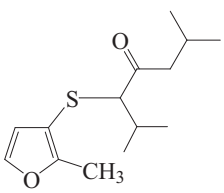


$C_{15}H_{16}$ 196.291
Constit. of *Lactarius deliciosus*. Blue liq. $Bp_{0.01}$ 85-90°.

Šorm, F. *et al., Coll. Czech. Chem. Comm.*, 1954, **19**, 357

2,6-Dimethyl-3-[(2-methyl-3-furanyl)thio]-4-heptanone, 9CI D-819

[61295-51-0]
FEMA 3538

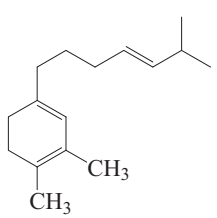


$C_{14}H_{22}O_2S$ 254.393
Flavouring ingredient. Liq. with meat-like odour. d_4^{25} 1.02. $Bp_{0.2}$ 90-92°. n_D^{20} 1.4925.

Ger. Pat., 1976, 2 600 707; *CA*, **86**, 29610k (*synth, use*)
Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-62; 64-66; 68-70 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 182 (*props, use*)

1,2-Dimethyl-4-(6-methyl-4-heptenyl)-1,3-cyclohexadiene D-820

7-(3,4-Dimethyl-1,3-cyclohexadienyl)-2-methyl-3-heptene

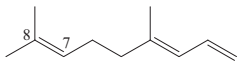


$C_{16}H_{26}$ 218.381
Constit. of the oil of turmeric, *Curcuma longa*.

Jayaprakasha, G.K. *et al., Z. Naturforsch., C*, 2001, **56**, 40-44

4,8-Dimethyl-1,3,7-nonatriene D-821

1,2,3,15-Tetranor-4,6,10-farnesatriene



$C_{11}H_{18}$ 150.263

(*E*)-*form*

Constit. of essential oil of *Elettaria cardamomum* (cardamom). Oil.

*7*R,*8-Epoxide:* [406214-57-1] *7,8-Epoxy-4,8-dimethyl-1,3-nonadiene*
$C_{11}H_{18}O$ 166.263

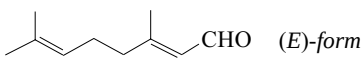
*7*S,*8-Epoxide:* [162460-30-2]
$[\alpha]_D^{22}$ +17.8 (c, 0.045 in Et_2O).

[21214-62-0]

Pattenden, G. *et al., J.C.S.(C)*, 1968, 1984 (*synth*)
Maurer, B. *et al., Tet. Lett.*, 1986, **27**, 2111 (*struct, synth*)
Boland, W. *et al., Helv. Chim. Acta*, 1989, **72**, 247 (*biosynth, bibl*)
Boland, W. *et al., Tetrahedron*, 1998, **54**, 14725-14736 (*biosynth*)
Wegener, R. *et al., Tetrahedron*, 2002, **58**, 315-319 (*epoxide*)

3,7-Dimethyl-2,6-octadienal D-822

[5392-40-5]
Citral. FEMA 2303



$C_{10}H_{16}O$ 152.236

►Fl. p. 91°. Human and exp. skin irritant. LD_{50} (rat, orl) 4960 mg/kg. Exp. reprod. effects (large dose). RG5075000

(*E*)-*form* [141-27-5]
Geranial. *Citral a*
Occurs in lemon grass oil (*Cymbopogon citratus*), lemon, orange and many other essential oils; flavouring ingredient. Bp 229° Bp_{20} 119°. n_D^{20} 1.4898.

►RG5075100

Semicarbazone:
Cryst. Mp 164°.

Di-Me acetal: [7549-37-3] *1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene, 9CI. FEMA 2305*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. with a fresh lemon-like odour. Coml. product is a mixt. of (*E*)- and (*Z*)-isomers.

Di-Et acetal: [7492-66-2] *1,1-Diethoxy-3,7-dimethyl-2,6-octadiene. FEMA 2304*
$C_{14}H_{26}O_2$ 226.358
Flavouring ingredient. Liq. with woody-citrus odour and a green, oily, citrus-peel flavour. Bp_{15} 140-142°. n_D^{20} 1.4503. Props. prob. refer to a mixt. with the *Z*-isomer.

►RG5080000

(*Z*)-*form* [106-26-3]
Neral. *Citral b*
Sol. Me_2CO, hexane; poorly sol. H_2O. Bp_{12} 103°. n_D^{20} 1.4809.

Semicarbazone:
Cryst. Mp 171°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 475D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 743A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 565B (*ir*)
Org. Synth., 1943, **23**, 78 (*synth*)
Simonsen, J.L. *et al., The Terpenes*, 2nd Ed., Cambridge Univ. Press, 1947, **1**, 83 (*rev*)
Org. Synth., Coll. Vol., 3, 1955, 747
Ohtsura, M. *et al., J.C.S.(B)*, 1967, 1033 (*pmr*)
Kogami, K. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 2508 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 371 (*occur*)
Vortkevich, S.A. *et al., Parfums, Cosmet. Savons Fr.*, 1972, **2**, 407 (*rev*)
Robacker, D.C. *et al., J. Chem. Ecol.*, 1977, **3**, 563
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 259 (*rev, tox*)
Akhila, A. *et al., Phytochemistry*, 1985, **24**, 2585 (*biosynth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTC800
Bauer, K. *et al., Common Fragrance and Flavor Materials, Preparation, Properties and Uses*, 2nd Ed., VCH Weinheim, 1990, 29 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1386
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 121-122
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 610-613
Picquet, M. *et al., Eur. J. Org. Chem.*, 2000, 2361-2366 (*synth, ir, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOE000; DTC800

3,7-Dimethyl-3,6-octadienal D-823

[1754-00-3]
Isocitral. *β-Isogeranial*

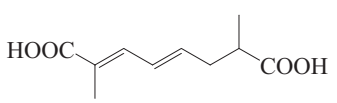
$C_{10}H_{16}O$ 152.236
Constit. of *Melissa officinalis* (lemon balm) and *Origanum* spp.. Bp_4 70°. n_D^{20} 1.4685.

[55722-59-3, 72203-97-5, 72203-98-6]

Bedoukian, P.Z. *et al., CA*, 1960, **54**, 46536 (*synth*)
Cant, P.A.E. *et al., Aust. J. Chem.*, 1975, **28**, 621-630 (*synth, ir, pmr*)
Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 89-92 (*isol*)

2,7-Dimethyl-2,4-octadiene-dioic acid D-824

[112250-63-2]



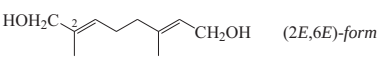
$C_{10}H_{14}O_4$ 198.218

(2*E*,4*E*)-*form* [110107-15-8]
Prod. by a mutant tomato variety 'flacca' deficient in abscisic acid. Cryst. (hexane/Et_2O). Mp 124-126°.

Di-Me ester: [110107-18-1]
$Bp_{0.1}$ 180-190°.

Linforth, R.S.T. *et al., Phytochemistry*, 1987, **26**, 1631-1634 (*isol, synth, pmr, cmr, ms*)
Milburrow, B.V. *et al., Plant Sci. (Limerick, Irel.)*, 1988, **56**, 49-53 (*isol*)
Wenkert, E. *et al., Helv. Chim. Acta*, 1999, **82**, 511-514 (*synth, bibl*)

2,6-Dimethyl-2,6-octadiene-1,8-diol D-825



$C_{10}H_{18}O_2$ 170.251

(2*E*,6*E*)-*form*
8-Hydroxygeraniol

8-O-*β*-D-*Glucopyranoside:*
$C_{16}H_{28}O_7$ 332.393
Constit. of fresh ginger (*Zingiber officinale*).

(2*E*,6*Z*)-*form*
8-O-*β*-D-*Glucopyranoside:*
Constit. of fresh ginger (*Zingiber officinale*).

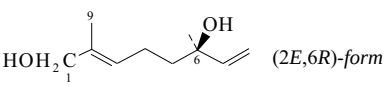
(2*Z*,6*E*)-*form* [32663-40-4]
9-Hydroxygeraniol
Constit. of tarragon (*Artemisia dracunculus*).

Bis(3-methylbutanoyl):
$C_{20}H_{34}O_4$ 338.486
Oil.

Jakupovic, J. *et al., Planta Med.*, 1991, **57**, 450 (*isol, pmr*)
Abdel-Kader, M.S. *et al., Phytochemistry*, 1993, **34**, 1367 (*isol, pmr, cmr*)
Jaensch, M. *et al., Phytochemistry*, 1993, **34**, 1367 (*isol, pmr*)
Otsuka, H. *et al., Phytochemistry*, 1994, **37**, 461 (*isol, pmr, cmr*)
Sekiwa, Y. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 384-389 (*8-glucosides*)

2,6-Dimethyl-2,7-octadiene-1,6-diol D-826

[64142-78-5]
9-Hydroxylinalool



$C_{10}H_{18}O_2$ 170.251

Numbering systems vary.

(2*E*,6*R*)-*form* [61434-50-2]
Oil. $[\alpha]_D^{25}$ -12.8 (c, 1.08 in MeOH).

1-O-*β*-D-*Glucopyranoside:* [64776-96-1]
Betulalbuside A
$C_{16}H_{28}O_7$ 332.393
Constit. of *Chaenomeles japonica* (dwarf quince). Oil.

(2*Z*,6*R*)-*form*

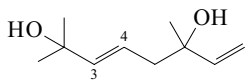
1-O-*β*-D-*Glucopyranoside:* [64813-08-7]
Betulalbuside B
$C_{16}H_{28}O_7$ 332.393
Constit. of *Chaenomeles japonica* (dwarf quince). Oil.

[74984-70-6, 75991-61-6, 103619-06-3, 162302-46-7]

Tschesche, R. *et al., Chem. Ber.*, 1977, **110**, 3111-3117 (*Betulalbusides*)
Caliş, İ. *et al., Phytochemistry*, 1995, **38**, 163-165 (*Betulalbuside A*)

2,6-Dimethyl-3,7-octadiene-2,6-diol, 9CI D-827

[13741-21-4]



$C_{10}H_{18}O_2$ 170.251
Detected in many fruits and aromatic oils and in wines. Oil. $[\alpha]_D^{24}$ +3.6 (c, 0.38 in $CHCl_3$).

2-O-β-D-Glucopyranoside:
$C_{16}H_{28}O_7$ 332.393

3,4-Dihydro: ***2,6-Dimethyl-7-octene-2,6-diol***. *3,7-Dimethyl-1-octene-3,7-diol*
$C_{10}H_{20}O_2$ 172.267
Constit. of the wine grape (*Vitis vinifera*). Cryst. Mp 51-52°.

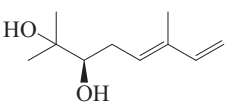
2-Hydroperoxide, 6-O-[3,4-di-O-angeloyl-β-D-glucopyranoside]: [358721-99-0]
$C_{26}H_{40}O_{10}$ 512.596
Oil. $[\alpha]_D^{20}$ -13.1 (c, 0.48 in $CHCl_3$). λ_{max} 216 (log ϵ 4.29) (MeOH).

[51276-34-7, 76540-50-6, 112420-84-5]

Takaoka, D. *et al., Phytochemistry*, 1976, **15**, 330 (*isol, pmr*)
Williams, P.J. *et al., Phytochemistry*, 1980, **19**, 1137 (*dihydro*)
Bruno, M. *et al., Phytochemistry*, 1988, **27**, 1871 (*isol*)
Manns, D. *et al., Phytochemistry*, 1995, **39**, 1115 (*glycoside*)
Jung, C.M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 912-914 (*Aster scaber constit*)

2,6-Dimethyl-5,7-octadiene-2,3-diol D-828

[87563-25-5]
6,7-Dihydro-6,7-ocimenediol



(*S,E*)-form

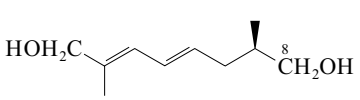
$C_{10}H_{18}O_2$ 170.251

(S,E)-form [261917-31-1]
Isol. from *Passiflora quadrangularis* (giant grandilla). Oil. $[\alpha]_D^{23}$ -19.7 (c, 0.62 in CH_2Cl_2) (80% o.p.). Obt. as a partial racemate.

(Z)-form
Oil.

Tsankova, E. *et al., Phytochemistry*, 1983, **22**, 1285 (*Z-form*)
Osorio, C. *et al., Phytochemistry*, 2000, **53**, 97-101 (*S,E-form*)

2,7-Dimethyl-2,4-octadiene-1,8-diol D-829



$C_{10}H_{18}O_2$ 170.251

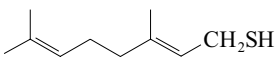
(2E,4E,7R)-form

8-O-β-D-Glucopyranoside:
$C_{16}H_{28}O_7$ 332.393
Constit. of quince fruit (*Cydonia oblonga*). Viscous yellow oil. $[\alpha]_D^{21}$ -15.5 (c, 0.31 in MeOH).

Lutz, A. *et al., Tet. Lett.*, 1991, **32**, 5943 (*isol, pmr, cmr*)
Kitahara, T. *et al., J. Nat. Prod.*, 1998, **61**, 551-554 (*synth*)

3,7-Dimethyl-2,6-octadiene-1-thiol, 9CI D-830

[38237-00-2]



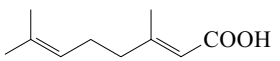
$C_{10}H_{18}S$ 170.318

(E)-form [39067-80-6]
Thiogeraniol
Flavouring and perfumery ingredient.

Mantegani, A. *et al., Eur. J. Med. Chem. (Chim. Ther.)*, 1972, **7**, 411 (*synth*)
Ger. Pat., 1972, 2 221 626; *CA*, **78**, 71402 (*synth, use*)
U.S. Pat., 1976, 3 975 311; *CA*, **86**, 55594c (*synth, use*)

3,7-Dimethyl-2,6-octadienoic acid D-831

[459-80-3]
Geranic acid. *Geranoic acid*



(*E*)-form

$C_{10}H_{16}O_2$ 168.235
Present in petitgrain, lemongrass and other essential oils.

(E)-form [4698-08-2]
Geranic acid a
Oil. $Bp_{0.02}$ 85-87°.

Me ester: [1189-09-9]
Oil. $Bp_{0.35}$ 63°.

Nitrile: [5146-66-7] *Geranonitrile*
$C_{10}H_{15}N$ 149.235
Bp_{10} 110°. Bp refers to a mixt. of (*E*)- and (*Z*)-forms.

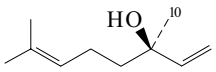
(Z)-form [4613-38-1]
Geranic acid b. Nerolic acid
Oil. $Bp_{0.08}$ 90°.

Me ester:
Oil. $Bp_{0.4}$ 58°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 844C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1360A (*nmr*)
Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*synth, pmr*)
Albright, J.A. *et al., Org. Prep. Proced. Int.*, 1972, **4**, 215 (*synth, derivs*)
Kabayashi, S. *et al., Chem. Lett.*, 1974, 705 (*synth*)
Campbell, R.V.M. *et al., J.C.S. Perkin 1*, 1975, 897 (*synth*)
Fujita, Y. *et al., Chem. Lett.*, 1978, 533 (*nitrile*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 785 (*rev, tox*)
Free, J.B. *et al., Bee World*, 1984, **65**, 175
Kadas, I. *et al., Org. Prep. Proced. Int.*, 1998, **30**, 79-85 (*synth*)

3,7-Dimethyl-1,6-octadien-3-ol D-832

[78-70-6]
Linalool. *Linalol. Linalyl alcohol. Licareol. Coriandrol. β-Linalool. FEMA 2635*



(*R*)-form

$C_{10}H_{18}O$ 154.252
Flavouring agent. Widespread natural occurrence as the optically active and racemic forms in over 200 essential oils. Also present in numerous fruits.. Log P 2.55 (calc). Natural enantiomeric composition of the various esters of Linalool is mostly not well documented. The phys. props. are given here under the racemates but some props. may refer to opt. active samples.

▶ Fl. p. 71/76°. Skin irritant. LD_{50} (rat, orl) 2790 mg/kg. RG5775000

(R)-form [126-91-0]
Constit. of many essential oils including *Melissa officinalis* (lemon balm), rose, neroli and lavender. Major component of oil of field mint (*Mentha arvensis*). Oil. Bp_{756} 197-200°. $[\alpha]_D^{20}$ -17. Log P 2.55 (calc).

▶ LD_{50} (mus, ivn) 180 mg/kg. RG5800000

O-*β-D-Glucopyranoside:* [99096-59-0]
$C_{16}H_{28}O_6$ 316.394
Constit. of wine grape (*Vitis vinifera*).

3-O-[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]: [134553-54-1] ***Neohancoside A***
$C_{21}H_{36}O_{10}$ 448.509
Aroma precursor from tea (*Camellia sinensis* var. *sinensis*). Cryst. (EtOAc). Mp 92-94°. $[\alpha]_D^{25}$ -26 (c, 0.47 in MeOH).

(S)-form [126-90-9]
Constit. of coriander and other essential oils. Oil. Bp 198-200° Bp_{20} 85-90°.

3-O-β-D-Glucopyranoside: [104154-37-2]
$C_{16}H_{28}O_6$ 316.394
Aroma precursor of Linalool from the flower buds of Arabian jasmine (*Jasminum sambac*). Oil. $[\alpha]_D^{22}$ -160 (c, 4 in MeOH).

O-*(6-O-Malonyl-β-D-glucopyranoside):*
$C_{19}H_{30}O_9$ 402.441
Constit. of Arabian jasmine (*Jasminum sambac*) buds.

(ξ)-form

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [84543-11-3]
$C_{21}H_{36}O_{10}$ 448.509
Constit. of wine grapes (*Vitis vinifera*).

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [84534-33-8]
$C_{22}H_{38}O_{10}$ 462.536
Constit. of wine grapes (*Vitis vinifera*).

(±)-form [22564-99-4]
Bp 198°. n_D^{20} 1.4616.

Formyl: [115-99-1] *Linalyl formate. FEMA 2642*
$C_{11}H_{18}O_2$ 182.262
Found in oils of lavender, peach, apricot, lime, clary and petitgrain. Present in *Prunus* spp.. Used in perfumery and food flavouring. d 0.91. Bp 202° $Bp_{0.07}$

45-47°.

Ac: [115-95-7] *Linalool acetate. Linalyl acetate. FEMA 2636*
$C_{12}H_{20}O_2$ 196.289
Isol. from numerous plants and essential oils, e.g. clary sage, lavender, lemon etc. Flavouring ingredient. Persistent sweet acrid taste. d 0.9. Bp 220° $Bp_{0.2}$ 44°.

▶ RG5910000

Propanoyl: [144-39-8] *Linalyl propionate. FEMA 2645*
$C_{13}H_{22}O_2$ 210.316
Found in lavender and sage oils in an enantiomeric form. Used in perfumery and food flavouring. d 0.89. Bp 226° $Bp_{0.1}$ 52-54°.

Butanoyl: [78-36-4] *Linalyl butyrate. FEMA 2639*
$C_{14}H_{24}O_2$ 224.342
Used in perfumery and food flavouring. Present in oils of kumquat peel, lavender and *Artemesia porrecta* var. *coerulea*. d 0.9. Bp 238° $Bp_{0.2}$ 80-82°. n_D^{25} 1.4483.

2-Methylpropanoyl: [78-35-3] *Linalyl isobutyrate. FEMA 2640*
$C_{14}H_{24}O_2$ 224.342
Used in perfumery and food flavouring. Found in lavender and Ceylon cinnamon oils. d 0.88. Bp 230° $Bp_{0.1}$ 63-65°.

3-Methylbutanoyl: [1118-27-0]

[50649-12-2] *Linalyl isovalerate. FEMA 2646*
$C_{15}H_{26}O_2$ 238.369
Used in perfumery and food flavouring. Present in *Salvia* spp. e.g. sage (*Salvia officinalis*).

Hexanoyl: [7779-23-9] *Linalyl hexanoate. Linalyl caproate. FEMA 2643*
$C_{16}H_{28}O_2$ 252.396
Food flavorant. d 0.9. Bp 252°. Poorly documented.

Octanoyl: [10024-64-3] *Linalyl octanoate. Linalyl caprylate. FEMA 2644*
$C_{18}H_{32}O_2$ 280.45
Used in perfumery and food flavouring. Present in lemongrass. Oil with sweet apricot/plum taste. d 0.88. Bp 264°. Poorly documented.

Benzoyl: [126-64-7] *Linalyl benzoate. FEMA 2638*
$C_{17}H_{22}O_2$ 258.36
Found in ylang-ylang and tuberose essential oils and mushrooms. Used in perfumery and food flavouring. d 0.98. Bp 263° $Bp_{0.05}$ 98°.

2-Aminobenzoyl: [7149-26-0] *Linalyl anthranilate. FEMA 2637*
$C_{17}H_{23}NO_2$ 273.374
Used in food flavouring. Liq. with sweet orange-like flavour. d 1.06. Bp >320°.

Cinnamoyl: [78-37-5] *Linalyl cinnamate. FEMA 2641*
$C_{19}H_{24}O_2$ 284.397
Used in perfumery and food flavouring. d 0.99. Bp 353°. n_D^{20} 1.5330.

Phenylacetyl: [7143-69-3] *Linalyl phenylacetate. FEMA 3501*
$C_{18}H_{24}O_2$ 272.386
Flavouring ingredient. Viscous liq. with sweet Neroli-rose type odour. Bp 371°.

[82928-12-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 148C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 225B; 967C (*nmr*)
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U.K. Pat., 1957, 774 621; *CA*, **51**, 16517f (*esters*)
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Nair, G.V. *et al., Tet. Lett.*, 1966, 5097 (*synth*)
Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1480 (*biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 120 (*occur*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1975, **13**, 827; 833; 835; 839; 1976, **14**, 459; 461; 463; 465; 1978, **16**, 811 (*rev, bibl, esters*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Takabe, K. *et al., Tet. Lett.*, 1975, 3005 (*synth*)
Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1976, 513 (*synth*)
Scarborough, R.M. *et al., J.O.C.*, 1979, **44**, 1742 (*synth*)
Japan. Pat., 1980, 80 36 417; *CA*, **93**, 94821p (*esters*)
Tange, K. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 2763 (*biosynth*)
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Zdero, C. *et al., Phytochemistry*, 1989, **28**, 1949
Uchiyama, T. *et al., Phytochemistry*, 1989, **28**, 3369 (*isol*)
Howell, A.R. *et al., J.C.S. Perkin 1*, 1990, 2715 (*synth*)
Konda, Y. *et al., J. Nat. Prod.*, 1992, **55**, 1447; 1993, **56**, 1437 (*Neohancoside A*)
Guo, W. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1532 (*primeveroside*)
Moon, J.-H. *et al., Phytochemistry*, 1994, **36**, 1435 (*glucopyranoside*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 431-439 (*acyl derivs*)
Manns, D. *et al., Phytochemistry*, 1995, **39**, 1115 (*glucoside, isol*)
Fujii, N. *et al., J.C.S. Perkin 1*, 1996, 865 (*synth*)
Konda, Y. *et al., Tet. Lett.*, 1996, **37**, 4015 (*Neohancoside A, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1585-1587; 1588-1590; 1590-1591; 1591-1592; 1592-1593; 1593-1594; 1594-1595; 1595-1596; 1596-1597; 1597-1598; 1598-1599; 1599-1600; 1600-1601 (*use, occur, props, acyl derivs, esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LFX000; LFY000; LFY100

3,7-Dimethyl-2,6-octadien-1-ol D-833

[624-15-7]

$C_{10}H_{18}O$ 154.252

(E)-form [106-24-1]
Geraniol. *Geranyl alcohol. Lemonol. β-Geraniol. FEMA 2507*
Found in free state and as esters in many essential oils including geranium oil. Most prolific natural source is palmarosa oil. Flavouring agent. Oil with sweet rose odour. Bp 230°. n_D^{30} 1.4777. λ_{max} 195 (ϵ 19000) (MeOH) (Berdy).

▶ Skin irritant. LD_{50} (rat, orl) 3600 mg/kg. RG5830000

O-*β-D-Glucopyranoside:* [22850-13-1]
$C_{16}H_{28}O_6$ 316.394
Isol. from *Rosa* spp., rose geranium (*Pelargonium graveolens*) and wine grapes (*Vitis vinifera*).

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [84534-32-7]
$C_{21}H_{36}O_{10}$ 448.509
Constit. of wine grapes (*Vitis vinifera*).

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [152520-94-0] ***Kenposide A***
$C_{21}H_{36}O_{10}$ 448.509
Constit. of Chinese raisin tree leaves and damask rose (*Rosa damascena var. bulgaria*).. Oil. $[\alpha]_D^{22}$ -50 (c, 4 in MeOH).

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [150995-11-2]
$C_{21}H_{36}O_{10}$ 448.509
Constit. of tea (*Camellia sinensis*) leaves. $[\alpha]_D^{20}$ -51 (c, 0.69 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [84534-31-6]
$C_{22}H_{38}O_{10}$ 462.536
Constit. of wine grapes (*Vitis vinifera*).

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [120163-17-9] ***Acuminoside***
$C_{21}H_{36}O_{10}$ 448.509
Constit. of damask rose (*Rosa damascena*) and wine grapes (*Vitis vinifera*). Amorph. Mp 39-41°. $[\alpha]_D^{19}$ -94.6 (c, 0.9 in MeOH).

Formyl: [105-86-2] *FEMA 2514*
$C_{11}H_{18}O_2$ 182.262
Constit. of geranium oil, orange peel oil, lemon peel oil, hop oil, white wine and black tea. Flavouring agent. Oil with rose odour. Bp_{15} 113-114°.

▶ Skin and eye irritant. LD_{50} (rat, orl) >6000 mg/kg. RG5925700

Ac: [105-87-3] *Geranyl acetate. FEMA 2509*
$C_{12}H_{20}O_2$ 196.289
Constit. of citronella, orange and other oils. Flavouring agent. Oil with fragrant odour. Bp_{22} 130-132°.

▶ Skin irritant. LD_{50} (rat, orl) 6330 mg/kg. RG5920000

Propanoyl: [105-90-8]

[105-89-5] *Geranyl propionate. FEMA 2517*
$C_{13}H_{22}O_2$ 210.316
Found in citrus peel oils, kumquat peel oil, muscadine grape (*Vitis rotundifolia*), hop oil and cardamon (*Ellettaria cardamomum*). Flavouring agent. d_{30}^{30} 0.92. Bp_8 118-120°. n_D^{30} 1.4583.

▶ RG5927906

Butanoyl: [106-29-6] *Geranyl butyrate. FEMA 2512*
$C_{14}H_{24}O_2$ 224.342
Found in citrus peel oils, kumquat peel oil, celery leaves/stalks, tomato, yellow passion fruit, lavender oil and other essential oils. Flavouring agent. Liq. with fresh, fruity, rose-like odour and apricot-like taste. Bp_{18} 151-153°.

▶ ES9990000

2-Methylpropanoyl: [2345-26-8] *Geranyl 2-methylpropanoate. Geranyl isobutyrate. FEMA 2513*
$C_{14}H_{24}O_2$ 224.342
Flavouring ingredient. Liq. with sweet, apricot-like taste. d^{15} 0.9. Bp 245°. n_D^{20} 1.4576.

3-Oxobutanoyl: [10032-00-5] *Geranyl acetoacetate. FEMA 2510*
$C_{14}H_{22}O_3$ 238.326
Flavouring ingredient. Liq. d^{25} 0.96. n_D^{25} 1.4670.

Pentanoyl: [10402-47-8] *Geranyl pentanoate. Geranyl valerate*
$C_{15}H_{26}O_2$ 238.369
Isol. from sassafras oil. Mp 291°.

3-Methylbutanoyl: [109-20-6] ***Geranyl 3-methylbutanoate****. Geranyl isovalerate. FEMA 2518*
$C_{15}H_{26}O_2$ 238.369
Constit. of various plant spp. including kumquat peel oil and lovage leaf and root. Flavouring ingredient. Liq. with rose odour and sweet apple-like taste. Bp_7 135-138°. n_D^{20} 1.4538.

Hexanoyl: [10032-02-7] ***Geranyl hexanoate****. Geranyl caproate. FEMA 2515*
$C_{16}H_{28}O_2$ 252.396
Found in kumquat peel and palmarosa oils, also in purple passion fruit and pawpaw. Flavouring agent. $d_4^{15.5}$ 0.89. Bp 290°. n_D^{20} 1.4500.

2-Ethylbutanoyl: [73019-14-4] *Geranyl 2-ethylbutyrate. FEMA 3339*
$C_{16}H_{28}O_2$ 252.396
Flavouring ingredient.

Benzoyl: [94-48-4] *Geranyl benzoate. FEMA 2511*
$C_{17}H_{22}O_2$ 258.36
Flavouring ingredient. d_{25}^{25} 0.98. Bp_{15} 198-200° Bp 305°.

Phenylacetyl: [102-22-7] *Geranyl phenylacetate. Phenylacetyl geranate. FEMA 2516*
$C_{18}H_{24}O_2$ 272.386
Flavouring ingredient.

(*Z*)-*form* [106-25-2]
Nerol*. Neryl alcohol. β-Nerol. FEMA 2770*
Constit. of many essential oils including neroli and bergamot oils. In essential oils it is a minor component always accompanied by geraniol. Flavouring agent. Oil with flowery odour. Bp 225-226°. n_D^{20} 1.4744.
▶ Skin irritant. LD_{50} (rat, orl) 4500 mg/kg. RG5840000

O-*β-D-Glucopyranoside:* [22850-14-2]
$C_{16}H_{28}O_6$ 316.394
Isol. from *Rosa* spp., rose geranium (*Pelargonium graveolens*) and grapes. Plates (EtOH aq.) (as tetra-Ac). Mp 68-70° (tetra-Ac).

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [84582-22-9]
$C_{21}H_{36}O_{10}$ 448.509
Isol. from wine grapes (*Vitis vinifera*).

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [84582-21-8]
$C_{22}H_{38}O_{10}$ 462.536
Isol. from wine grapes (*Vitis vinifera*).

Formyl: [2142-94-1] *Neryl formate. FEMA 2776*
$C_{11}H_{18}O_2$ 182.262
Food flavouring. d 0.92. Bp 225°.

Ac: [141-12-8] *Neryl acetate. FEMA 2773*
$C_{12}H_{20}O_2$ 196.289
Found in citrus, kumquat and pummelo peel oils, ginger, cardamon, clary sage, myrtle leaf and myrtle berries. Flavouring agent. Liq. with honey-like flavour and raspberry undertones. d_4^{25} 0.91. Bp 231° Bp_{25} 134°.
▶ RG5921000

Propanoyl: [105-91-9] *Neryl propionate. FEMA 2777*
$C_{13}H_{22}O_2$ 210.316
Flavouring ingredient. Liq. with sweet plumlike taste. d_{15}^{15} 0.9. Bp 233°. n_D^{20} 1.4550.

Butanoyl: [999-40-6] *Neryl butyrate. FEMA 2774*
$C_{14}H_{24}O_2$ 224.342
Flavouring ingredient. Liq. with sweet cocoa-like taste. $d_{15}^{15.5}$ 0.9. Bp 239-240°. n_D^{20} 1.4539.

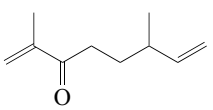
2-Methylpropanoyl: [2345-24-6] *Neryl isobutyrate. FEMA 2775*
$C_{14}H_{24}O_2$ 224.342
Flavouring ingredient. Liq. with a sweet, strawberry taste. d^{15} 0.89. Bp_3 232°. n_D^{20} 1.4508.

3-Methylbutanoyl: [3915-83-1] ***Neryl isovalerate****. FEMA 2778*
$C_{15}H_{26}O_2$ 238.369
Constit. of numerous plant spp. Flavouring agent. Liq. with fruity odour and berry-like flavour. d_4^{15} 0.89. Bp 252°. n_D^{20} 1.4531.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 148D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 224C; 225A; 968A; 968B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 219A; 219B; 668D (*ir*)
Erdmann, E. *et al., J. Prakt. Chem.*, 1852, **56**, 14 (*benzoyl*)
Erdmann, E. *et al., Ber.*, 1898, **31**, 356 (*esters*)
Morel, *et al., Soap, Perfum. Cosmet.*, 1952, **26**, 174 (*esters*)
Bates, R.B. *et al., J.O.C.*, 1963, **28**, 1086 (*struct*)
Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*synth*)
Francis, M.J.O. *et al., Phytochemistry*, 1969, **8**, 1339 (*isol, glucoside*)
Kogami, K. *et al., Kogyo Kagaku Zasshi*, 1971, **74**, 2304 (*synth, pmr, ms, deriv*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 118; 119 (*occur*)
Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 2904 (*isol*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Casey, C.P. *et al., Synth. Commun.*, 1973, **3**, 321 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 881 (*rev, tox, Geraniol*)
Tengo, J. *et al., J. Chem. Ecol.*, 1975, **1**, 253
Pitzele, B.S. *et al., J.O.C.*, 1975, **40**, 269 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1976, **14**, 783; 785 (*revs, esters*)
Banthorpe, D.V. *et al., Phytochemistry*, 1976, **15**, 91; 1983, **22**, 2459 (*biosynth*)
Derguini-Boumechal, F. *et al., Tet. Lett.*, 1977, 1181 (*synth*)
Pickett, J.A. *et al., J. Chem. Ecol.*, 1980, **6**, 425
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 149 (*isol*)
Mathew, K.K. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 340 (*synth*)
Williams, P.J. *et al., Phytochemistry*, 1982, **21**, 2013 (*6-arabinosylglucosides, rutinosides*)
Free, J.B. *et al., Bee World*, 1984, **65**, 175 (*β-nerol*)
Bredenkamp, M.W. *et al., Phytochemistry*, 1988, **28**, 263 (*Acuminoside*)
Ackermann, I.E. *et al., Annalen*, 1989, 79 (*synth, glucosides*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTD000; DTD200; DTD800
Voirin, S.G. *et al., Carbohydr. Res.*, 1990, **207**, 39 (*synth, glycosides, pmr, cmr*)
Voirin, S.G. *et al., J. Agric. Food Chem.*, 1990, **38**, 1373 (*Acuminoside*)
Howell, A.R. *et al., J.C.S. Perkin 1*, 1990, 2715 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1355; 1372
Guo, W. *et al., Phytochemistry*, 1993, **33**, 1373 (*xylopyranosylglucopyranoside*)
Yoshikawa, K. *et al., Phytochemistry*, 1993, **34**, 1431 (*Kenposide A*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 184; 294-299; 590-594 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1186-1197; 864; 1181-1182; 1941-1942; 1945-1951 (*geranyl esters, neryl esters, use, props*)
Oka, N. *et al., Nat. Prod. Lett.*, 1997, **10**, 187-192 (*Rosa damascena glycosides*)
Eisenreich, W. *et al., Tet. Lett.*, 1997, **38**, 3889-3892 (*biosynth*)
Sy, L.-K. *et al., J. Nat. Prod.*, 1998, **61**, 907-912 (*Geranyl benzoate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTD000; GCY000; DTD200; DTD800

2,6-Dimethyl-1,7-octadien-3-one D-834

[211303-27-4]

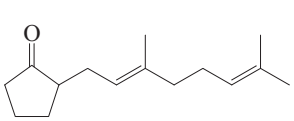


$C_{10}H_{16}O$ 152.236
Constit. of *Tagetes minuta* (Mexican marigold). $[\alpha]_D^{18}$ -17.5 (c, 0.75 in $CHCl_3$).

Garg, S.N. *et al., Phytochemistry*, 1998, **48**, 395-396 (*isol, pmr, cmr*)

2-(3,7-Dimethyl-2,6-octadienyl)cyclopentanone, 9CI D-835

[68133-79-9]
Decenylcyclopentanone



$C_{15}H_{24}O$ 220.354

(±)-(*E*)-*form* [74016-19-6]
Geranylcyclopentanone*. Apritone. FEMA 3829*
Flavouring agent for baked goods and candies. Liq. with apricot odour. Bp_3

130°. n_D^{21} 1.4871.

Dreux, J. *et al., Bull. Soc. Chim. Fr.*, 1955, 1312-1315 (*synth*)

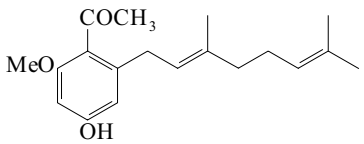
Kurth, M.J. *et al., J.O.C.*, 1985, **50**, 3846-3848 (*synth, ir, pmr*)

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 458 (*use*)

2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone D-836

[121379-44-0]

1-[2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyphenyl]ethanone, 9CI



$C_{19}H_{26}O_3$ 302.413

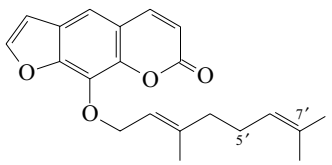
Constit. of *Dioscorea bulbifera* (air potato). Cryst. Mp 225°.

Gupta, D. *et al., Phytochemistry*, 1989, **28**, 947

9-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI D-837

[7437-55-0]

8-Geranyloxypsoralen. 9-Geranyloxypsoralen



$C_{21}H_{22}O_4$ 338.402

Constit. of lemon oil. Needles (petrol). Mp 53-54°. The 8-numbering derives from an obsolete system.

$\Delta^{5'}$-Isomer, 7′-hydroxy: [144398-34-5] *8-(7-Hydroxy-3,7-dimethyl-2,5-octadienyloxy)psoralen*
$C_{21}H_{22}O_5$ 354.402
Gum.

$\Delta^{5'}$-Isomer, 7′-hydroperoxy: [205115-74-8] ***Lansiumarin B***
$C_{21}H_{22}O_6$ 370.401
Constit. of *Clausena lansium* (wampee). Pale yellow oil. λ_{max} 207 ; 217 (sh) ; 243 ; 248 (sh) ; 263 (sh) ; 296 (MeOH).

$\Delta^{7'}$-Isomer, 6′-oxo: [205115-73-7] ***Lansiumarin A***
$C_{21}H_{20}O_5$ 352.386
Constit. of *Clausena lansium* (wampee). Pale yellow oil. λ_{max} 206 (sh) ; 218 ; 243 (sh) ; 248 ; 264 (sh) ; 300 (MeOH).

$\Delta^{7'}$-Isomer, 6′ξ-hydroxy: [205115-75-9] ***Lansiumarin C***
$C_{21}H_{22}O_5$ 354.402
Constit. of *Clausena lansium* (wampee). Pale yellow oil. $[\alpha]_D$ +8 (c, 0.06 in $CHCl_3$). λ_{max} 207 ; 218 ; 242 (sh) ; 249 ; 265 (sh) ; 299 (MeOH).

$\Delta^{7'}$-Isomer, 6′S-hydroperoxy: [144398-35-6] *8-(6-Hydroperoxy-3,7-dimethyl-2,7-octadienyloxy)psoralen*
$C_{21}H_{22}O_6$ 370.401
Gum. $[\alpha]_D$ -13 (c, 0.3 in $CHCl_3$).

6′,7′-Dihydro, 6′-oxo: [220391-49-1] *8-(3,7-Dimethyl-6-oxo-2-octenyloxy)psoralen*
$C_{21}H_{22}O_5$ 354.402
Gum. $[\alpha]_D^{22}$ -23 (c, 0.5 in $CHCl_3$). Possesses unexplained opt. rotation.

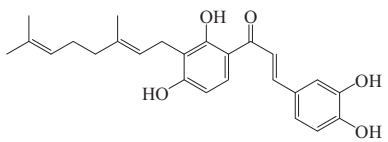
Sharma, Y.N. *et al., Tetrahedron*, 1966, **22**, 3221-3225 (*Geranyloxypsoralen*)

Rashid, M.A. *et al., J. Nat. Prod.*, 1992, **55**, 851-858 (*$\Delta^{5'}$-Isomer-7′-hydroxy, Lansiumarin B*)

Ito, C. *et al., Chem. Pharm. Bull.*, 1998, **46**, 341-343 (*Lansiumarins*)

Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1939-1940 (*Dimethyloxooctenyloxypsoralen*)

3′-(3,7-Dimethyl-2,6-octadienyl)-2′,3,4,4′-tetrahydroxychalcone D-838



$C_{25}H_{28}O_5$ 408.493

(E,E)-form

3′-Geranyl-2′,3,4,4′-tetrahydroxychalcone

Constit. of *Artocarpus incisus* (breadfruit). Yellow powder.

Shimizu, K. *et al., Phytochemistry*, 2000, **54**, 737-739

3′-(3,7-Dimethyl-2,6-octadienyl)-2′,4,4′,6′-tetrahydroxychalcone D-839

$C_{25}H_{28}O_5$ 408.493

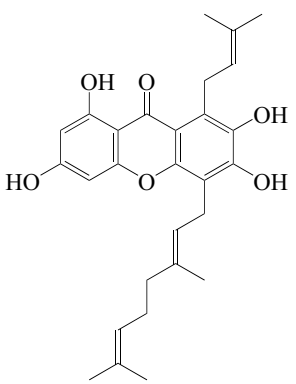
(E,E)-form [189299-03-4]

3′-Geranyl-2′,4,4′,6′-tetrahydroxychalcone

Constit. of hops (*Humulus lupulus*). Yellow powder. λ_{max} 310 (sh) ; 367 (MeOH).

Stevens, J.F. *et al., Phytochemistry*, 1997, **44**, 1575 (*isol, pmr, cmr, ms*)

4-(3,7-Dimethyl-2,6-octadienyl)-2,3,6,8-tetrahydroxy-1-prenylxanthone D-840



$C_{28}H_{32}O_6$ 464.557

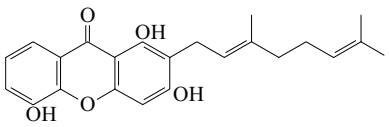
(E)-form [175617-23-9]

4-Geranyl-2,3,6,8-tetrahydroxy-1-prenylxanthone. ***Dulciol A***

Constit. of *Garcinia dulcis* (mundu). Amorph. yellow solid. λ_{max} 209 ; 240 (sh) ; 253 ; 280 ; 328 (MeOH).

Iinuma, M. *et al., J. Nat. Prod.*, 1996, **59**, 472 (*isol, uv, ir, pmr, cmr, ms*)

2-(3,7-Dimethyl-2,6-octadienyl)-1,3,5-trihydroxyxanthone D-841



$C_{23}H_{24}O_5$ 380.44

(E)-form [166197-40-6]

2-Geranyl-1,3,5-trihydroxyxanthone. ***Mangostinone***

Constit. of the pericarps of *Garcinia mangostana* (mangosteen). Amorph. yellow powder.

Asai, F. *et al., Phytochemistry*, 1995, **39**, 943 (*isol, uv, pmr, cmr, ms*)

4-(3,7-Dimethyl-2,6-octadienyl)-1,3,5-trihydroxyxanthone D-842

4-Geranyl-1,3,5-trihydroxyxanthone

$C_{23}H_{24}O_5$ 380.44

(E)-form [136364-54-0]

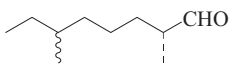
Isol. from the root bark of *Garcinia livingstonei* (imbe). Yellow plates. Mp 129-130°. λ_{max} 244 (ϵ 32300); 259 (ϵ 26300); 320 (ϵ 15500); 365 (ϵ 3800) (MeOH) (Berdy).

Sordat-Diserens, I. *et al., Phytochemistry*, 1992, **31**, 313 (*isol, pmr, cmr*)

2,6-Dimethyloctanal D-843

[7779-07-9]

Dihydrocitronellal. FEMA 2390



(2*R*)-*form*

$C_{10}H_{20}O$ 156.267

Both the 2*R*-form and the racemate are doubtless mixtures of diastereomers. Flavouring ingredient. Liq. with powerful, sweet odour of fruit and somewhat green flavour. Enantiomeric form not designated by FEMA.

(2R)-form

d_4^{18} 0.83. $Bp_{4.5}$ 67°. $[\alpha]_D^{20}$ +9 (neat). n_D^{21} 1.4253.

Semicarbazone:
Mp 78°.

Di-Me acetal:1,1-Dimethoxy-2,6-dimethyloctane
$C_{12}H_{26}O_2$ 202.336
d_4^{20} 0.83. $[\alpha]_D^{20}$ +3.48 (neat). n_D^{20} 1.4270.

(±)-form

Bp_{11} 78-79°.

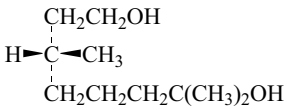
Semicarbazone:
Mp 97°.

Rupe, H. *et al., Helv. Chim. Acta*, 1928, **11**, 656-669 (*synth*)

Suzuki, K. *et al., Chem. News*, 1929, **139**, 153 (*R-form, synth*)
Mueller, A. *et al., Ber., B*, 1941, **74**, 1745-1750 (*R-form, synth, di-Me acetal*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 460 (*use, props*)

3,7-Dimethyl-1,7-octanediol, 9CI, 8CI D-844

[107-74-4]
Hydroxycitronellol. FEMA 2586



(*R*)-*form*

$C_{10}H_{22}O_2$ 174.283

(*R*)-*form* [122612-23-1]
d_4^{20} 0.94. Bp_{15} 156°. $[\alpha]_D^{10}$ +1.4. n_D^{20} 1.4610. (*S*)-form also known.

(±)-*form*
Flavouring ingredient. Oil with rose-hyacinth odour. d_4^{20} 0.93. Bp_2 80-82°. n_D^{25} 1.4354.

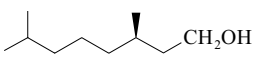
1-Ac: [33730-41-5]
$C_{12}H_{24}O_3$ 216.32
$Bp_{0.02}$ 82-84°. n_D^{25} 1.4436.

[98206-63-4]

Meerwein, H. *et al., J. Prakt. Chem.*, 1937, **141**, 225 (*synth*)
Désalbres, L. *et al., Bull. Soc. Chim. Fr.*, 1956, 761 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, 923 (*rev, tox*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Beckwith, A.L.J. *et al., Aust. J. Chem.*, 1977, **30**, 2177 (*synth, pmr, 1-Ac*)
Beckwith, A.L.J. *et al., Chem. Comm.*, 1979, 690 (*synth*)
Borbaruah, M. *et al., Tet. Lett.*, 1987, **28**, 5741 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 360
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1365-1366

3,7-Dimethyl-1-octanol, 9CI D-845

[106-21-8]
Dihydrocitronellol. Tetrahydrogeraniol. Perhydrogeraniol. FEMA 2391



(*R*)-*form*

$C_{10}H_{22}O$ 158.283
►Skin irritant. RH0900000

(*R*)-*form* [1117-60-8]
Flavouring ingredient. Oil with rose odour and bitter taste. Bp 212-213° Bp_{10} 105-106°.

Ac:
$C_{12}H_{24}O_2$ 200.32
Found in essential oil of *Mentha* spp.. $Bp_{0.3}$ 60-62°.

4-Methylbenzenesulfonyl:
$C_{17}H_{28}O_3S$ 312.472
Oil. $Bp_{0.05}$ 58°. $[\alpha]_D$ +2 (c, 4.00 in C_6H_6).

(*S*)-*form*
Sol. Et_2O. Bp 212-213° Bp_{15} 109°.

(±)-*form* [59204-02-3]
Oil with rose odour and bitter taste. Bp 212-213°.

Ac: [20780-49-8]
Bp_{12} 109-110°.
►Skin irritant. RH0920000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 175A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 165D (*ir*)
Jarolin, V. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 596 (*use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 535 (*rev, tox*)
Nagai, K. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 265 (*synth*)
Chan, K.-E. *et al., J.O.C.*, 1976, **41**, 3497 (*synth, use*)
Cohen, N. *et al., J.O.C.*, 1976, **41**, 3505 (*synth, use*)
Fuganti, C. *et al., Chem. Comm.*, 1979, 995 (*synth, use*)
Schmidt, M. *et al., Helv. Chim. Acta*, 1979, **62**, 464 (*synth, use*)
Zell, R. *et al., Helv. Chim. Acta*, 1979, **62**, 474 (*synth, use*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTE600
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ; DTE800

3,7-Dimethyl-3-octanol, 9CI D-846

[78-69-3]
Tetrahydrolinalool. 2,6-Dimethyl-6-octanol. FEMA 3060

$C_{10}H_{22}O$ 158.283
►RH0905000

(*R*)-*form* [56577-25-4]
$Bp_{2.2}$ 57°. $[\alpha]_D$ +0.96 (c, 15.5 in hexane).

4-Nitrobenzoyl: [39998-98-6]
$[\alpha]_D$ +1.67 (C_6H_6).

(*S*)-*form*
Bp_5 54-59.5°. $[\alpha]_D$ -0.63 (pentane).

4-Nitrobenzoyl: [39999-20-7]
Mp 39.5-40°. $[\alpha]_D^{16.5}$ -0.93 (c, 26.5 in C_6H_6).

Me ether:
$C_{11}H_{24}O$ 172.31
Liq. Bp_{10} 70°. $[\alpha]_D^{20}$ -2.7 (c, 56.6 in $CHCl_3$) (78% ee).

Et ether:
$C_{12}H_{26}O$ 186.337
Liq. $[\alpha]_D^{20}$ -1.6 (c, 25 in $CHCl_3$) (80.0% ee).

Ph ether:
$C_{16}H_{26}O$ 234.381
Bp_4 140-145°. $[\alpha]_D^{24.2}$ -5.53.

(±)-*form* [57706-88-4]
Flavouring ingredient. Liq. with a sweet, oily, floral odour. Bp_{715} 185-186°.

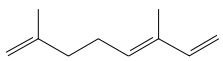
Ac: [20780-48-7] *Tetrahydrolinalyl acetate*
$C_{12}H_{24}O_2$ 200.32
Liq.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 192A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 187A (*ir*)
Stevens, P.G. *et al., J.A.C.S.*, 1939, **61**, 1295 (*config*)
Cornforth, R.H. *et al., Annalen*, 1960, **634**, 197 (*abs config*)
Corman, R.H. *et al., Aust. J. Chem.*, 1960, **29**, 133 (*synth, pmr*)
Verkade, P.E. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1964, **83**, 367 (*config*)
Mehta, G. *et al., Tetrahedron*, 1973, **29**, 1119 (*synth*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 909 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 746
Schulz, S. *et al., Annalen*, 1996, 941 (*pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2763
Müller, P. *et al., J.C.S. Perkin 2*, 2000, 2232-2237 (*S-form, synth, Me ether, Et ether, ir, pmr, cmr*)

3,7-Dimethyl-1,3,7-octatriene D-847

[502-99-8]

[29714-87-2]
***α*-Ocimene**



$C_{10}H_{16}$ 136.236

(*E*)-*form* [6874-10-8]

[27400-72-2]
Oil.

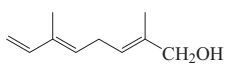
(*Z*)-*form* [6874-44-8]

[27400-71-1]
Odour contributor to green odour of unripe mango and of mango ginger rhizome *Curcuma amada* used in oriental pickles. Oil.

Thieme, H. *et al., Pharmazie*, 1972, **27**, 255
Gholap, A.S. *et al., J. Sci. Food Agric.*, 1977, **28**, 885 (*isol*)

2,6-Dimethyl-2,5,7-octatrien-1-ol D-848

[113378-77-1, 113378-78-2, 304443-48-9, 304443-49-0]
8-Ocimenyl alcohol



(*E,E*)-*form*

$C_{10}H_{16}O$ 152.236Synth. as (2*E*,6*E*)-form.

Ac:

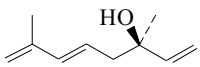
[223705-75-7, 223705-76-8, 223705-77-9, 223705-78-0] *8-Ocimenyl acetate. FEMA 3886. Piperitanate*
$C_{12}H_{18}O_2$ 194.273
Flavouring ingredient for alcoholic or nonalcoholic beverages, chewing gum and candy with fruity aroma. Oil with penetrating, fruity, pineapple-like odour. Geometrical form not specified by FEMA. Props. refer to a mixt. of all four geometrical isomers. Characterised spectroscopically.

Strauss, C.R. *et al., J. Agric. Food Chem.*, 1988, **36**, 569-573 (*ms*)

Desai, S.R. *et al., Synth. Commun.*, 1990, **20**, 523-533 (*E,E-form, synth, pmr*)
Ger. Pat., 1999, 19 748 774; *CA*, **130**, 325271k (*Ac, synth, use, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1329-1330 (*Ac, use*)

3,7-Dimethyl-1,5,7-octatrien-3-ol D-849

[29957-43-5]
Dehydrolinalool



$C_{10}H_{16}O$ 152.236
Flavouring ingredient.

(*R*,*E*)-*form* [20053-88-7]
Hotrienol. FEMA 3830
Present in wine and kiwifruit. Flavouring ingredient for beverages, confectionery etc.. Oil. Bp_2 62°. $[\alpha]_D^{20}$ -15.2. $[\alpha]_D^{20}$ -23 (c, 10 in EtOH). n_D^{20} 1.4913.

(*S*,*E*)-*form* [24278-80-6]
Constit. of black tea flavour. Oil. $[\alpha]_D$ +11.9.

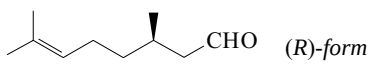
(±)-(*E*)-*form*
Liq. Bp_2 62°.

[38818-60-9, 53834-70-1, 83541-43-9]

Yoshida, T. *et al., Agric. Biol. Chem.*, 1969, **33**, 343-352 (*Hotrienol, isol*)
Nakatani, Y. *et al., Agric. Biol. Chem.*, 1969, **33**, 967-968 (*S,E-form, isol, abs config*)
Moiseenkov, A.M. *et al., Chem. Comm.*, 1982, 109-110 (*S,E-form, R,S-form, (±)-form Hotrienol, synth*)
Böhmer, J. *et al., Synthesis*, 1997, 661-667 (*(±)-form, synth, ir, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 462

3,7-Dimethyl-6-octenal D-850

[106-23-0]
Citronellal. *Rhodinal. FEMA 2307*



(*R*)-*form*

$C_{10}H_{18}O$ 154.252
Isol. from essential oils, esp. citronella oils. Also present in citrus peel oil, kumquat peel oil, parsley seed oil, ginger, pepper, cocoa, lovage root and other foods. Prod. synthetically by hydrogenation of 3,7-Dimethyl-2,6-octadienal, D-822 or hydrogenation of 3,7-Dimethyl-6-octen-1-ol, D-857. Flavouring ingredient. Oil with powerful fresh herbaceous-citrus odour. Enantiomer composition of natural citronellal varies widely, e.g. from 89% (*S*-) in lemon peel oil to 86.5% (*R*-) in citronella oil. Enantiomers have similar odour props..

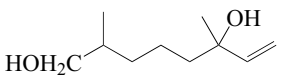
(*R*)-*form* [2385-77-5]
Constit. of citronella oil. Also in citrus, lavender, eucalyptus oils and others. Flavouring agent. Bp 204-205° Bp_{14} 90°. $[\alpha]_D^{18}$ +13.1. n_D^{20} 1.4477.

(*S*)-*form* [5949-05-3]
Reported from oils of *Backhousia citriodora* and Mauritius papeda (*Citrus hystrix*). $[\alpha]_D^{20}$ -13.1.

(±)-*form* [26489-02-1]
Major component (85%) of oil of the lemon-scent gum (*Eucalyptus citriodora*).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 738B; 738C (*nmr*)
Arigoni, D. *et al., Helv. Chim. Acta*, 1954, **37**, 881 (*abs config*)
O'Donnell, G.W. *et al., Aust. J. Chem.*, 1966, **19**, 525
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 366; 367 (*occur*)
Sokol'skii, D.V. *et al., Dokl. Akad. Nauk SSSR*, 1978, **242**, 1126 (*synth*)
Akhila, A. *et al., Phytochemistry*, 1986, **25**, 421 (*biosynth*)
Chimirri, A. *et al., Heterocycles*, 1987, **26**, 2469
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CMS845
Bauer, K. *et al., Common Fragrance and Flavor Materials, Preparation, Properties and Uses*, 2nd Ed., VCH, Weinheim, 1990, 31 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1355
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 124 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 619-621 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMS845

2,6-Dimethyl-7-octene-1,6-diol D-851

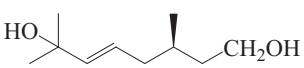


$C_{10}H_{20}O_2$ 172.267

8-O-*β*-D-*Glucopyranoside:* [219814-33-2]
$C_{16}H_{30}O_7$ 334.409
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder.

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1748-1751 (*isol, pmr, cmr*)

3,7-Dimethyl-5-octene-1,7-diol D-852



$C_{10}H_{20}O_2$ 172.267

(3*R*,5*E*)-*form*

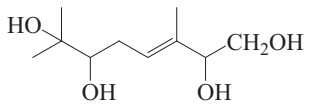
1-O-*β*-D-*Glucopyranoside:*
$C_{16}H_{30}O_7$ 334.409
Constit. of *Rosa damascena* (damask rose). $[\alpha]_D^{22}$ -12.2 (c, 0.1 in H_2O).

Watanabe, N. *et al., Nat. Prod. Lett.*, 1998, **12**, 5-10 (*isol, pmr, cmr, synth*)

3,7-Dimethyl-3-octene-1,2,6,7-tetrol D-853

[261949-44-4]

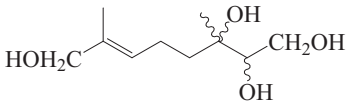
[260355-82-6, 260355-87-1]



$C_{10}H_{20}O_4$ 204.266
Constit. of *Passiflora quadrangularis* (giant grandilla). Oil. $[\alpha]_D^{25}$ -11.9 (c, 0.67 in MeOH). Mixture of stereoisomers.

Osorio, C. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 4313-4319 (*stereochem*)
Osorio, C. *et al., Phytochemistry*, 2000, **53**, 97-101 (*isol, pmr, cmr*)

3,7-Dimethyl-6-octene-1,2,3,8-tetrol D-854



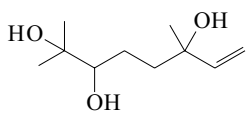
$C_{10}H_{20}O_4$ 204.266

(2ξ,3ξ,6*E*)-*form* [240495-79-8]
Constit. of *Foeniculum vulgare* (fennel). Syrup. $[\alpha]_D^{23}$ -41.8 (c, 0.2 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 805-808 (*isol, pmr, cmr*)

2,6-Dimethyl-7-octene-2,3,6-triol D-855

[73815-21-1]

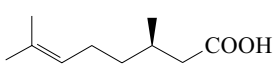


$C_{10}H_{20}O_3$ 188.266
Constit. of *Vitis vinifera* (wine grape). Oil. Bp_1 126-128°.

Williams, P.J. *et al., Phytochemistry*, 1980, **19**, 1137
Manns, D. *et al., Phytochemistry*, 1995, **39**, 1115 (*isol, pmr, cmr*)

3,7-Dimethyl-6-octenoic acid D-856

[502-47-6]
Citronellic acid. *Rhodinic acid. Callitrol. FEMA 3142*



(*R*)-*form*

$C_{10}H_{18}O_2$ 170.251
Flavouring ingredient.
► Skin irritant. LD_{50} (rat, orl) 2610 mg/kg. LD_{50} (rbt, skn) 450 mg/kg. RH3230000

(*R*)-*form* [18951-85-4]
Oil. Bp 257° Bp_{10} 143°. $[\alpha]_D$ +10.3 (c, 5.0 in $CHCl_3$) (98% ee). n_D^{25} 1.4520.

Nitrile: [35931-93-2] *Citronellonitrile*
$C_{10}H_{17}N$ 151.251

(*S*)-*form* [2111-53-7]
$Bp_{0.6}$ 118°. $[\alpha]_D^{24}$ -6.6.

(±)-*form* [57030-77-0]
Bp_4 126°.

(ξ)-*form*

Me ester: [2270-60-2]

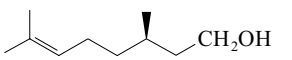
$C_{11}H_{20}O_2$ 184.278
Present in pepper (*Piper nigrum*) and lemon balm (*Melissa officinalis*). Flavouring ingredient.

[51566-62-2]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 780C; 781A; 781B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 587A (*ir*)
Lukeš, R. *et al., Croat. Chem. Acta*, 1957, **29**, 201; *CA*, **53**, 17898e (*synth, abs config*)
Overberger, C.G. *et al., J.A.C.S.*, 1967, **89**, 5640 (*synth*)
Valentine, D.V. *et al., J.O.C.*, 1976, **41**, 62 (*bibl*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1983, **20**, 653 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 125
He, W. *et al., Helv. Chim. Acta*, 1995, **78**, 391 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 866-867; 1755
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMT125; CMU000

3,7-Dimethyl-6-octen-1-ol D-857

[106-22-9]
Citronellol. *β-Rhodinol. β-Citronellol. Yacarol. Rhodinol*†



(R)-form

$C_{10}H_{20}O$ 156.267
Occurs in many essential oils, usually as a partial racemate. Obt. mainly from geranium oil or synthetically. Flavour for use in citrus compositions. Esters used in foods etc. are mostly of unreported enantiomeric composition. They are given here under the racemate and the props. reported presumably refer to the racemic forms.

► Fl. p. >100°. Skin irritant. LD_{50} (rat, orl) 3450 mg/kg. LD_{50} (rbt, skn) 2650 mg/kg. RH3400000

(*R*)-*form* [1117-61-9]
Constit. of black cumin (*Nigella sativa*) seeds. A common constit. of plant oils, esp. in the Rutaceae. Oil with sweet rose odour and bitter taste. d^{20} 0.86. Bp 108° $Bp_{0.5}$ 68°. $[\alpha]_D$ +5.45 (neat). n_D^{20} 1.4558.

O-*β-D-Glucopyranoside:* [117895-55-3]
$C_{16}H_{30}O_6$ 318.409
Constit. of wine grapes (*Vitis vinifera*).

Ac:Citronellyl acetate
$C_{12}H_{22}O_2$ 198.305

Propanoyl:
$C_{13}H_{24}O_2$ 212.331

Butanoyl:
$C_{14}H_{26}O_2$ 226.358

Pentanoyl:
$C_{15}H_{28}O_2$ 240.385

(*S*)-*form* [7540-51-4]
Constit. of geranium and citronella oils. Oil with sweet odour, more delicate than *R*-enantiomer, and sweet peach-like taste. $Bp_{0.5}$ 68-70°. $[\alpha]_D$ -4.76.

O-*β-D-Glucopyranoside:* [99096-57-8]
$C_{16}H_{30}O_6$ 318.409
Constit. of wine grapes (*Vitis vinifera*).

(±)-*form* [26489-01-0]
FEMA 2309
Bp 213-215° Bp_{12} 107-108°.

Ac: [67650-82-2]

[150-84-5] *FEMA 2311*
Flavouring ingredient. Constit. of citronella oil, orange juice, lemon juice and peel, grapefruit peel, swangi (*Citrus hystrix*), ginger, tarragon, myrtle leaf, West Indian lemongrass oil and beer. Bp 229° Bp_{15} 119-121°.

Propanoyl: [141-14-0]

[76444-23-0] *Citronellyl propionate. FEMA 2316. E410*
Flavouring ingredient. Constit. of tomato. Liq. with rose-like odour and bittersweet plum-like taste. Bp 242° Bp_{14} 122-124°.

Butanoyl: [141-16-2]

[76444-24-1] *Citronellyl butyrate. FEMA 2312. E275*
Constit. of Ceylon citronella oil, tomato, orange juice and passion fruit juice. Flavouring ingredient. Liq. with rose-like odour and sweet plum-like taste. d_4^4 0.9. Bp 243° Bp_{12} 134-135°.

2-Methylpropanoyl: [97-89-2]

[76444-25-2] *Citronellyl isobutyrate. FEMA 2313*
$C_{14}H_{26}O_2$ 226.358
Constit. of Ceylon citronella oil. Flavouring ingredient. Liq. with sweet, fruity, rose-like odour and apricot-like taste. Bp 249°.

Pentanoyl: [7540-53-6]

[76444-26-3] *Citronellyl pentanoate. Citronellyl valerate. E469. FEMA 2317*
Flavouring ingredient. Constit. of *Boronia citriodora* essence. Liq. with rose, herb, honey-like odour. $d^{15.5}$ 0.89. Bp 237°. n_D^{20} 1.4435.

3-Methylbutanoyl: [68922-10-1] *Citronellyl isovalerate*
$C_{15}H_{28}O_2$ 240.385
Used in food flavouring. Liq. d 0.88. Bp 253°.

Hexanoyl: [10580-25-3] *Citronellyl hexanoate. Citronellyl caproate*
$C_{16}H_{30}O_2$ 254.412
Used in food flavouring. Liq. Bp 240°.

Phenylacetyl: [139-70-8] *Citronellyl phenylacetate. Citronellyl α-toluate. E 2157. FEMA 2315*
$C_{18}H_{26}O_2$ 274.402
Flavouring ingredient and flavour enhancer for fruit flavours. Not reported in nature. Liq. with sweet, faintly honey, rose-like odour with a definite waxy undertone. $d_4^{15.5}$ 0.99 d^{20} 1.51. Bp 342°. n_D^{20} 1.5100.

Cinnamoyl: [10482-79-8] *Citronellyl cinnamate*
$C_{19}H_{26}O_2$ 286.413
Used in food flavouring. Liq. d 0.99. Bp 380°.

(ξ)-*form*

1-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [209681-41-4] ***Citronellyl β-sophoroside***
$C_{22}H_{40}O_{11}$ 480.551
Constit. of flowers of damask rose (*Rosa damascena* var. *bulgaria*). $[\alpha]_D^{22}$ -16 (c, 0.1 in H_2O).

Formyl: [105-85-1] *Citronellyl formate. FEMA 2314*
$C_{11}H_{20}O_2$ 184.278
Occurs in essential oils of geranium, mandarin, satsuma, kumquat and other spp. Also present in lovage root and honey. Flavouring ingredient. Liq. with rose-like odour and sweet fruity taste. Bp 235° Bp_{11} 97-98°.

[22850-15-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 145C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 216B; 216C; 217A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 213A; 213C; 213D (*ir*)
Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 111 (*occur*)
Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3545-3548 (*biosynth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1011-1081 (*formyl*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037-1064 (*ir*)
Wollmann, H. *et al., Pharmazie*, 1973, **28**, 56 (*isol*)
Shono, T. *et al., Tet. Lett.*, 1974, 1295-1298 (*synth*)
Hidai, M. *et al., Chem. Comm.*, 1975, 170-171 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 757-758 (*rev, tox*)
Corey, E.J. *et al., J.O.C.*, 1976, **41**, 380-381 (*synth*)
Chan, K.-K. *et al., J.O.C.*, 1976, **41**, 3497-3505 (*synth*)
Lanza, E. *et al., Phytochemistry*, 1977, **16**, 1555-1560 (*biosynth*)
Grundschuber, F. *et al., Toxicology*, 1977, **8**, 387-390 (*phenylacetyl, tox*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 693 (*2-methylpropanoyl, rev*)
Hiroma, M. *et al., J.O.C.*, 1985, **50**, 127-129 (*synth*)
Soai, K. *et al., J.C.S. Perkin 1*, 1987, 1909-1904; 1988, 415 (*synth*)
Ackermann, I.E. *et al., Annalen*, 1989, 79-81 (*synth, glucosides*)
Bauer, K. *et al., Common Fragrance and Flavor Materials, Preparation, Properties and Uses*, VCH, Weinheim, 2nd. edn., 1990, 25 (*rev*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 113S-114S (*rev, tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1409
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 126-130
Org. Synth., 1995, **72**, 74-85 (*S-form, synth, pmr*)
Sharma, A. *et al., Annalen*, 1996, 529-531 (*resoln, pmr, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 622-630
Oka, N. *et al., Phytochemistry*, 1998, **47**, 1527-1529 (*Citronellyl β-sophoroside*)
McDaniel, C.J. *et al., Z. Naturforsch., C*, 1998, **53**, 932-934 (*Caiman latirostris esters*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 317; 319; 320; 321; 322; 323; 324; 325 (*esters, use, props, occur*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMT250

3,7-Dimethyl-7-octen-1-ol, 9CI D-858

[141-25-3]
Rhodinol. α-Citronellol. FEMA 2980

$C_{10}H_{20}O$ 156.267
Flavouring ingredient. d_4^{20} 0.85. $Bp_{1.8}$ 68-70°. n_D^{20} 1.4517.

(±)-*form*

Formyl: [141-09-3] *Rhodinyl formate. FEMA 2984*
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient. Liq.

Ac: [141-11-7]

[20777-37-1, 130980-16-4] *Rhodinyl acetate. FEMA 2981*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Bp 237°.

Propanoyl: [105-89-5] *Rhodinyl propionate. FEMA 2986*
$C_{13}H_{24}O_2$ 212.331
Flavouring ingredient. Oil. Bp_{14} 122°.

Butanoyl: [141-15-1] *Rhodinyl butyrate. FEMA 2982*
$C_{14}H_{26}O_2$ 226.358
Flavouring ingredient. Liq.with sweet blackberry-like taste. Bp_{13} 137°.

2-Methylpropanoyl: [138-23-8] *Rhodinyl isobutyrate. FEMA 2983*
$C_{14}H_{26}O_2$ 226.358
Flavouring ingredient. Oil. Bp 260°.

3-Methylbutanoyl: [7778-96-3] *Rhodinyl isovalerate. FEMA 2987*
$C_{15}H_{28}O_2$ 240.385
Flavouring ingredient. d^{15} 0.88. Bp_{14} 147°. n_D^{20} 1.4465.

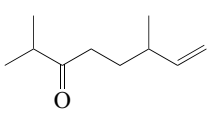
Phenylacetyl: [10486-14-3] *Rhodinyl phenylacetate. FEMA 2985*
$C_{18}H_{26}O_2$ 274.402
Flavouring ingredient. Liq. Bp 340°.

[5713-07-5]

Eschinazi, H.E. *et al., J.O.C.*, 1961, **26**, 3072-3076 (*synth*)
Rienaecker, R. *et al., Chimia*, 1973, **27**, 97-99 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 849-853; 1979, **17**, 901 (*esters, rev*)
Ford, R.A. *et al., Food Cosmet. Toxicol.*, 1988, **26**, 405 (*phenylacetate, rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 716-720
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2422-2428

2,6-Dimethyl-7-octen-3-one D-859

[19776-07-9]



$C_{10}H_{18}O$ 154.252
Constit. of *Tagetes minuta* (Mexican marigold). $[\alpha]_D^{18}$ +2.7 (c, 0.27 in $CHCl_3$).

Garg, S.N. *et al., Phytochemistry*, 1998, **48**, 395-396 (*isol, pmr, cmr*)

[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde, 9CI D-860

[7492-67-3]
6,10-Dimethyl-3-oxa-9-undecanal. Citronellyloxyacetaldehyde. Muguet aldehyde. FEMA 2310

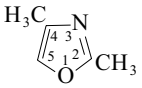
$(H_3C)_2C{=}CHCH_2CH_2CH(CH_3)CH_2CH_2OCH_2CHO$
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. with powerful green muguet-lily odour. Bp 239° Bp_{12} 128-130°.

[124932-08-7]

Sabetay, S. *et al., Bull. Soc. Chim. Fr.*, 1929, **45**, 1161 (*synth*)
Opdyka, D.L.J. *et al., CA*, 1977, **86**, 145725a (*rev, synth, props, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 127
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 623

2,4-Dimethyloxazole D-861

[7208-05-1]



C_5H_7NO 97.116
Constit. of Arabica coffee aroma. Liq. Sol. H_2O. Bp 108°. pK_a 2.86 (20°).

Oesterreich, M. *et al., Ber.*, 1897, **30**, 2255 (*synth*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, pmr*)
Prager, R.H. *et al., J.C.S. Perkin 1*, 1997, 2665-2672 (*synth, pmr, cmr*)

2,5-Dimethyloxazole D-862

[23012-11-5]

C_5H_7NO 97.116
Constit. of Arabica coffee aroma. Liq. Misc. H_2O. Bp 117-118°.

Picrate:
Mp 124°.

Wredl, F. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1933, **218**, 128 (*synth*)
Bowie, J.H. *et al., Org. Mass Spectrom.*, 1968, **1**, 13 (*ms*)
Brown, D.J. *et al., J.C.S.(B)*, 1969, 270 (*pmr, uv*)
Wiegand, E.E. *et al., Synthesis*, 1970, 648 (*synth, pmr*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, pmr*)

4,5-Dimethyloxazole D-863

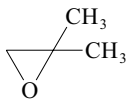
[20662-83-3]

C_5H_7NO 97.116
Constit. of Arabica coffee aroma, roasted peanut and roast beef volatiles. Liq. Bp 129-135°. pK_a 2.05 (20°, HCl aq.).

Bredereck, H. *et al., Chem. Ber.*, 1953, **86**, 88 (*synth*)
Bowie, J.H. *et al., Org. Mass Spectrom.*, 1968, **1**, 13 (*ms*)
Brown, D.J. *et al., J.C.S.(B)*, 1969, 270 (*uv, pmr*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, pmr, coffee*)
Hartman, G.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1030-1033 (*detn, roast beef*)

2,2-Dimethyloxirane, 9CI D-864

[558-30-5]
1,2-Epoxy-2-methylpropane, 8CI. Isobutylene oxide

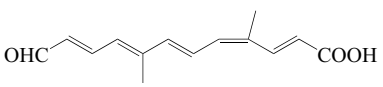


C_4H_8O 72.107
Isol. from essential oil of *Angelica glauca*. Liq. Bp 52°.

▶ TZ3580000

Fourneau, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1907, **145**, 438 (*synth*)
Evseeva, L.A. *et al., Zh. Fiz. Khim.*, 1969, **43**, 845; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1969, **43**, 468 (*ir, Raman*)
Whitham, G.H. *et al., J.C.S. Perkin 2*, 1975, 861 (*cmr*)
Collins, D.J. *et al., Aust. J. Chem.*, 1989, **42**, 1235 (*synth, pmr*)
Bouchoux, G. *et al., Rapid Commun. Mass Spectrom.*, 1992, **6**, 37 (*ms*)
Zhang, H. *et al., CA*, 1993, **118**, 219586j (*isol*)
Liu, J. *et al., J.O.C.*, 1998, **63**, 8565-8569 (*synth, pmr, cmr, ms, ir*)

4,8-Dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoic acid D-865



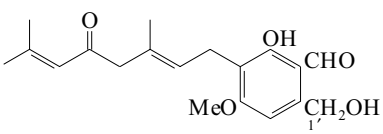
$C_{14}H_{16}O_3$ 232.279

(2*E*,4*Z*,6*E*,8*E*,10*E*)-*form*

Me ester: [201996-40-9]
$C_{15}H_{18}O_3$ 246.305
Constit. of the seeds of *Bixa orellana* (annatto). λ_{max} 350 ; 367 ; 387 (no solvent reported).

Mercadante, A.Z. *et al., Phytochemistry*, 1997, **46**, 1379-1383 (*isol, ester, pmr, cmr, ms*)

3-(3,7-Dimethyl-5-oxo-2,6-octadienyl)-2-hydroxy-6-(hydroxymethyl)-4-methoxybenzaldehyde D-866



$C_{19}H_{24}O_5$ 332.396

1′-O-Hexadecanoyl: [137592-03-1] ***Hericenone C***
$C_{35}H_{54}O_6$ 570.808
Isol. from the edible lion's mane mushroom (*Hericium erinaceum*). Cryst. Mp 38-40°. λ_{max} 225 (ε 22800); 231 (sh) (ε 21500); 236 (ε 21900); 267 (sh) (ε 5100); 294 (ε 14500) (MeOH) (Derep).

1′-O-Octadecanoyl: [137592-04-2] ***Herice-***

none D
$C_{37}H_{58}O_6$ 598.862
From the edible lion's mane mushroom (*Hericium erinaceum*). Cryst. Mp 41-43°. λ_{max} 225 (ϵ 22800); 231 (sh) (ϵ 21500); 236 (ϵ 21900); 267 (sh) (ϵ 5100); 294 (ϵ 14500) (MeOH) (Derep).

1′-O-(9Z,12Z-Octadecadienoyl): [137592-05-3] ***Hericenone E***
$C_{37}H_{54}O_6$ 594.83
From the edible lion's mane mushroom (*Hericium erinaceum*). Oil. λ_{max} 225 (ϵ 22800); 231 (sh) (ϵ 21500); 236 (ϵ 21900); 267 (sh) (ϵ 5100); 294 (ϵ 14500) (MeOH) (Derep).

5′-Deoxo: [158314-36-4] *3-(3,7-Dimethyl-2,6-octadienyl)-2-hydroxy-6-(hydroxymethyl)-4-methoxybenzaldehyde*
Oil.

5′-Deoxo, 1′-O-hexadecanoyl: [157207-54-0] ***Hericene A***
$C_{35}H_{56}O_5$ 556.824
From the edible lion's mane mushroom (*Hericium erinaceum*). Oil.

5′-Deoxo, 1′-O-octadecanoyl: [157207-56-2] ***Hericene C***
$C_{37}H_{60}O_5$ 584.878
From the edible lion's mane mushroom (*Hericium erinaceum*). Oil.

5′-Deoxo, 1′-O-(9Z-octadecenoyl): [157207-55-1] ***Hericene B***
$C_{37}H_{58}O_5$ 582.862
From the edible lion's mane mushroom (*Hericium erinaceum*). Oil.

[34593-50-5]

Kawagishi, H. *et al., Tet. Lett.*, 1991, **32**, 4561 (*Hericenones*)
Arnone, A. *et al., J. Nat. Prod.*, 1994, **57**, 602 (*Hericenes*)

2,4-Dimethyl-3-pentanone, 9CI D-867

[565-80-0]
Diisopropyl ketone. Isopropyl ketone. Isobutyrone
$(H_3C)_2CHCOCH(CH_3)_2$
$C_7H_{14}O$ 114.187
Isol. from lavender oil (*Lavendula officinalis* hybrid). Liq. d_4^{20} 0.81. Bp 124-125°. n_D^{20} 1.4001.
▶ Highly flammable, fl. p. 15°. LD_{50} (rat, orl) 3536 mg/kg. SA8575500

Oxime: [1113-74-2]
$C_7H_{15}NO$ 129.202
Needles (EtOH). Sol. alcohols. Mp 34°. Bp 181-185° Bp_{12} 82-85°.

2,4-Dinitrophenylhydrazone: [7153-35-7]
Mp 94-98°.

Semicarbazone: [5338-14-7]
Cryst. (EtOH aq.). Mp 160°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 634C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 407C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 489C (*ir*)
Aldrich Library of NMR Spectra, **2**, 106D (*pmr*)
Pfeiffer, G.J. *et al., J.A.C.S.*, 1931, **53**, 1043 (*props*)
Hauser, C.R. *et al., J.A.C.S.*, 1937, **59**, 1823 (*synth*)
Stadler, P.A. *et al., Helv. Chim. Acta*, 1960, **43**, 1601 (*isol*)
Dunn, P.J. *et al., Mikrochim. Acta*, 1975, **2**, 129 (*oxime, detn, Pd*)
Cooks, R.G. *et al., J.A.C.S.*, 1976, **98**, 2011 (*ms*)
Andrieu, C.G. *et al., Org. Magn. Reson.*, 1978, **11**, 528 (*cmr*)
Boulton, A.J. *et al., J.C.S. Perkin 1*, 1987, 2073 (*oxime*)
Konaka, S. *et al., J. Phys. Chem.*, 1990, **94**, 1793 (*ir, Raman, ed, conformn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTI600

2,4-Dimethyl-2-pentenoic acid, 9CI D-868

[66634-97-7]
FEMA 3143
$(H_3C)_2CHCH{=}C(CH_3)COOH$
$C_7H_{12}O_2$ 128.171
Flavouring ingredient. Liq. Bp_{15} 115-117°. (*E,Z*)-mixt..

Me ester: [87117-10-0]
$C_8H_{14}O_2$ 142.197
Liq. Bp_6 46-49°.

Et ester: [13979-26-5]
$C_9H_{16}O_2$ 156.224
Liq.

Chloride: [134124-24-6]

[89609-13-2, 125427-95-4]
$C_7H_{11}ClO$ 146.616
Liq. Bp 160-163° Bp_2 37°.

Amide:
$C_7H_{13}NO$ 127.186
Cryst. Mp 82-84°.

(E)-form [3876-52-6]
$Bp_{1.5}$ 88-92°.

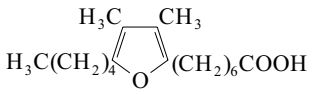
(S)-1-Methylbutyl ester: [80510-16-3] ***Dominicalure 2***
$C_{12}H_{22}O_2$ 198.305
Liq. $[\alpha]_D$ +10.9 (c, 1.26 in Et_2O) (ca. 98% op).

[3876-51-5, 20515-17-7, 20515-18-8, 21016-46-6, 21016-47-7, 89301-91-7, 134680-45-8]

McGreer, D.E. *et al., Can. J. Chem.*, 1968, **46**, 2225 (*synth, ir, pmr*)
Williams, H.J. *et al., J. Chem. Ecol.*, 1981, **7**, 759 (*Dominicalure 2*)
Larson, G.L. *et al., J.O.C.*, 1984, **49**, 3385 (*synth, pmr*)
Etemad-Moghadam, G. *et al., Tetrahedron*, 1984, **40**, 5153 (*synth*)
Coutrot, P. *et al., Synthesis*, 1986, 790 (*synth, pmr*)
Vyehara, T. *et al., Chem. Comm.*, 1987, 410 (*synth*)
Henin, F. *et al., Tetrahedron*, 1989, **45**, 6171 (*chloride, esters*)
Lin-Yu, L. *et al., J. Chem. Ecol.*, 1990, **16**, 1921 (*Dominicalure 2*)
Rossi, R. *et al., Synth. Commun.*, 1992, **22**, 603 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 186
Razkin, J. *et al., J. Chem. Ecol.*, 1996, **22**, 673 (*synth, Dominicalure 2*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 867

3,4-Dimethyl-5-pentyl-2-furanheptanoic acid, 9CI D-869

[92745-17-0]
8,11-Epoxy-9,10-dimethyl-8,10-hexadienoic acid. F_0 acid

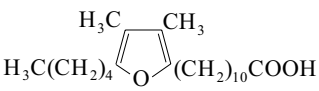


$C_{18}H_{30}O_3$ 294.433
Component of F acid fraction present in beef blood serum.

Okajima, H. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3281 (*isol*)
Puchta, V. *et al., Annalen*, 1988, 25 (*occur*)
Hannemann, K. *et al., Lipids*, 1989, **24**, 296 (*occur*)

3,4-Dimethyl-5-pentyl-2-furanundecanoic acid, 9CI D-870

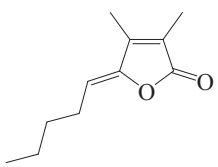
[57818-36-7]
12,15-Epoxy-13,14-dimethyleicosa-12,14-dienoic acid. F_6 Acid



$C_{22}H_{38}O_3$ 350.54
The most common member of a series of furanoid acids varying in chain length and in the number of methyl groups; see also 3-Methyl-5-pentyl-2-furannonanoic acid, M-568. Present in fish lipids. Component of F acid fraction present in beef blood serum.

Glass, R.L. *et al., Lipids*, 1977, **12**, 828
Gunstone, F.D. *et al., J. Sci. Food Agric.*, 1978, **29**, 539
Puchta, V. *et al., Annalen*, 1988, 25 (*occur*)
Batna, A. *et al., Annalen*, 1991, 861 (*biosynth*)

3,4-Dimethyl-5-pentylidene-2(5*H*)-furanone, 9CI D-871



$C_{11}H_{16}O_2$ 180.246

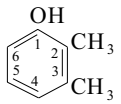
(Z)-form [774-64-1]
Bovolide
Constit. of peppermint oil.
▶ Exp. neoplastigenic data. LU4025000

Demole, E. *et al., Helv. Chim. Acta*, 1972, **55**, 1866 (*isol*)
Katsuhiro, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 1535 (*isol*)
Wulff, W.D. *et al., J.A.C.S.*, 1986, **108**, 520 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMK500

2,3-Dimethylphenol D-872

[526-75-0]

[1300-71-6, 25155-23-1]
o-*3-Xylenol. 3-Hydroxy*-o-*xylene. 1,2,3-Xylenol. 2,3-Xylenol.* vic-o-*Xylenol*



$C_8H_{10}O$ 122.166
Constit. of *Valerianella locusta* (corn salad). Cryst. (EtOH aq.). Mp 75°. Bp 218° Bp_{20} 120°. n_D^{20} 1.5420. pK_a 10.54 (25°).

▶ ZE5500000

Ac: [22618-22-0]
$C_{10}H_{12}O_2$ 164.204
Oil. Bp 226-228° Bp_{14} 107° Bp_8 104°.

Benzoyl: [5554-27-8]
$C_{15}H_{14}O_2$ 226.274
Mp 55-57°.

Me ether: [2944-49-2] *1-Methoxy-2,3-dimethylbenzene, 9CI. 2,3-Dimethylanisole*
$C_9H_{12}O$ 136.193
Cryst. Mp 29°. Bp 199° Bp_{15} 110°.

Et ether: [61808-02-4] *1-Ethoxy-2,3-dimethylbenzene, 9CI. 2,3-Dimethylphenetole*
$C_{10}H_{14}O$ 150.22
Low-melting cryst. Mp 10°. Bp 212.5°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 191A; 256C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1045D; 1080D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 974C; 1013B (*ir*)
Aldrich Library of NMR Spectra, **4**, 117A (*pmr*)
Smith, L.I. *et al., J.O.C.*, 1941, **6**, 427 (*synth*)
McLamoe, W.M. *et al., J.A.C.S.*, 1951, **73**, 2221 (*synth*)
Adv. Chem. Ser., 1955, **15**, 277 (***props***)
Green, J.H.S. *et al., Spectrochim. Acta A*, 1972, **28**, 33 (*ir, Raman*)
Neuman, A. *et al., Acta Cryst. B*, 1973, **29**, 1017 (*cryst struct*)
Eisner, T. *et al., J. Chem. Ecol.*, 1977, **3**, 321
Netzel, D.A. *et al., Org. Magn. Reson.*, 1978, **11**, 58 (*cmr*)
Ganguly, T. *et al., Spectrochim. Acta A*, 1978, **34**, 617 (*uv*)
Box, V.G.S. *et al., Heterocycles*, 1990, **31**, 1261 (*Me ether, synth*)
Knölker, H. *et al., Helv. Chim. Acta*, 1993, **76**, 2500 (*Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, XKJ000

2,4-Dimethylphenol D-873

[105-67-9]

[1300-71-6, 25155-23-1]
2,4-Xylenol, 8CI. m-*4-Xylenol. 4-Hydroxy*-m-*xylene*

$C_8H_{10}O$ 122.166
Needles (EtOH aq. or C_6H_6). Sol. Me_2CO, EtOH; mod. sol. H_2O. Mp 27-28°. Bp 210° Bp_{14} 97-98°. pK_a 10.6 (25°).

▶ LD_{50} (rat, orl) 3200 mg/kg; LD_{50} (rat, skn) 1040 mg/kg. ZE5600000

Ac: [877-53-2]
$C_{10}H_{12}O_2$ 164.204
Oil. Bp_{13} 107.5-108.5°.

Benzoyl: [76048-43-6]
$C_{15}H_{14}O_2$ 226.274
Cryst. (AcOH). Mp 37-38°. Bp_{15} 110.5-111°.

Me ether: [6738-23-4] *1-Methoxy-2,4-dimethylbenzene, 9CI. 2,4-Dimethylanisole. FEMA 3828*
$C_9H_{12}O$ 136.193
Food addiitive listed in the EAFUS Food Additive Database (Jan 2001). Found in camembert cheese. Food flavour. Oil. Bp 191° Bp_{13} 73-75°.

Et ether: [35338-30-8] *1-Ethoxy-2,4-dimethylbenzene, 9CI. 2,4-Dimethylphenetole*
$C_{10}H_{14}O$ 150.22
Oil. Bp 202-203°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 193C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1047C; 1082B; 1087B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 976A; 1020B (*ir*)
Aldrich Library of NMR Spectra, **4**, 122A (*pmr*)
Lambooy, J.P. *et al., J.A.C.S.*, 1950, **72**, 5327 (*synth*)
Adv. Chem. Ser., 1955, **15**, 278 (***props***)
Wessely, F. *et al., Monatsh. Chem.*, 1963, **94**, 227 (*synth*)
Green, J.H.S. *et al., Spectrochim. Acta A*, 1972, **28**, 33 (*ir, Raman*)
Norwitz, G. *et al., Anal. Chim. Acta*, 1977, **89**, 177; 1978, **98**, 323; 1979, **105**, 335; **109**, 373 (*use*)
Netzel, D.A. *et al., Org. Magn. Reson.*, 1978, **11**, 58 (*cmr*)
Yus, M. *et al., Tetrahedron*, 1992, **48**, 2709 (*synth, ms, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, XKJ500

2,5-Dimethylphenol, 9CI D-874

[95-87-4]

[1300-71-6, 25155-23-1]
2,5-Xylenol, 8CI. p-*2-Xylenol. Hydroxy*-p-*xylene. FEMA 3595*

$C_8H_{10}O$ 122.166
Present in coffee and whisky. Flavouring ingredient. Cryst. (EtOH). Mp 71-73°. Bp 210° Bp_{10} 89.3°. pK_a 10.41 (25°).

▶ LD_{50} (rat, orl) 444 mg/kg. ZE5775000

Ac: [877-48-5]
$C_{10}H_{12}O_2$ 164.204
Oil. Bp 237°.

4-Nitrobenzoyl: [135838-96-9]
Cryst. Mp 88°.

Me ether: [1706-11-2] *2-Methoxy-1,4-dimethylbenzene, 9CI. 2,5-Dimethylanisole*
$C_9H_{12}O$ 136.193
Liq. Bp 194°.

Et ether: [61808-03-5] *2-Ethoxy-1,4-dimethylbenzene, 9CI. 2,5-Dimethylphenetole*
$C_{10}H_{14}O$ 150.22
Liq. Bp 199°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1047D; 1087C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 194A; 265C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 976B; 1020C (*ir*)
Adv. Chem. Ser., 1955, **15**, 279 (***props***)
Green, J.H.S. *et al., Spectrochim. Acta A*, 1972, **28**, 33 (*ir, Raman*)
Neuman, A. *et al., Acta Cryst. B*, 1973, **29**, 1017 (*cryst struct*)
Rao, G.C. *et al., Chem. Comm.*, 1974, 584 (*synth*)
Gornostaeva, L.I. *et al., CA*, 1978, **88**, 117789 (*isol*)
Netzel, D.A. *et al., Org. Magn. Reson.*, 1978, **11**, 58 (*cmr*)
Szczecinski, P. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1978, **52**, 1225 (*pmr*)
Ganguly, T. *et al., Spectrochim. Acta A*, 1978, **34**, 617 (*uv*)
Minami, N. *et al., Chem. Pharm. Bull.*, 1979, **27**, 816 (*synth*)
Lau, C.K. *et al., Can. J. Chem.*, 1989, **67**, 1384 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 797
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2965-2966
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, XKS000

2,6-Dimethylphenol, 9CI D-875

[576-26-1]

[1300-71-6, 25155-23-1]
2,6-Xylenol, 8CI. m-*2-Xylenol. 2-Hydroxy*-m-*xylene. 1,3,2-Xylenol. FEMA 3249*

$C_8H_{10}O$ 122.166
Present in whisky and coffee. Flavouring ingredient. Leaflets or flat needles. Sol. EtOH, AcOH; mod. sol. H_2O. Mp 49°. Bp 203°. pK_a 10.62 (25°).

▶ Eye irritant. LD_{50} (rat, orl) 296 mg/kg. ZE6125000

Ac: [876-98-2]
$C_{10}H_{12}O_2$ 164.204
Oil. Bp 215-216° $Bp_{0.3}$ 60°.

4-Nitrobenzoyl:
Cryst. Mp 99°.

Me ether: [1004-66-6] *2-Methoxy-1,3-dimethylbenzene. 2,6-Dimethylanisole*
$C_9H_{12}O$ 136.193
Liq. Bp 182-183° Bp_{20} 79°.

Et ether: [26620-08-6] *2-Ethoxy-1,3-dimethylbenzene. 2,6-Dimethylphenetole*
$C_{10}H_{14}O$ 150.22
Liq. Bp 195.5-196.5°.

Ph ether: [22040-02-4] *1,3-Dimethyl-2-phenoxybenzene, 9CI*
$C_{14}H_{14}O$ 198.264
Mp 55-56.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1045B; 1081D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 190C; 258B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 974A; 1014B (*ir*)
Cox, R. *et al., J.O.C.*, 1960, **25**, 1083 (*synth*)
Hartley, A.M. *et al., Anal. Chem.*, 1963, **35**, 1207 (*use*)
Andrews, D.W. *et al., Analyst (London)*, 1964, **89**, 730 (*use*)
Green, J.H.S. *et al., Spectrochim. Acta A*, 1972, **28**, 33 (*ir, Raman*)
Kuts, V.S. *et al., Zh. Org. Khim.*, 1972, **8**, 142; *J. Org. Chem. USSR (Engl. Transl.)*, 1972, **8**, 145 (*pmr*)
Odinokov, V.N. *et al., Zh. Org. Khim.*, 1972, **8**, 2162; *J. Org. Chem. USSR (Engl. Transl.)*, 1972, **8**, 2206 (*synth, Ac*)
Antona, D. *et al., Acta Cryst. B*, 1973, **29**, 1372 (*cryst struct*)
Krokhin, A.V. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1975, 2334; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1975, 2219 (*ms*)

Gornostaeva, L.I. *et al., CA*, 1978, **88**, 117789 (*isol*)
Gerrard, D.L. *et al., Spectrochim. Acta A*, 1978, **34**, 1225 (*uv*)
Minami, N. *et al., Chem. Pharm. Bull.*, 1979, **27**, 816 (*synth*)
Kitching, W. *et al., Org. Magn. Reson.*, 1980, **14**, 502 (*cmr*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1988, **13**, 1 (*rev, polymers*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 798
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2966
Reichardt, C. *et al., Liebigs Ann./Recl.*, 1997, 707-720 (*Me ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, XLA000

3,4-Dimethylphenol, 9CI D-876

[95-65-8]

[1300-71-6, 25155-23-1]
3,4-Xylenol, 8CI. 4-Hydroxy-o-*xylene. 1,2,4-Xylenol.* asym-o-*Xylenol. FEMA 3596*

$C_8H_{10}O$ 122.166
Present in coffee. Flavouring ingredient. Cryst. (H_2O). Sol. EtOH; mod. sol. H_2O. Mp 62-64°. Bp 227°. pK_{a1} 10.36 (25°).
▶ LD_{50} (rbt, orl) 800 mg/kg. ZE6300000

Ac: [22618-23-1]
$C_{10}H_{12}O_2$ 164.204
Oil. Bp 220° Bp_{80} 140°.

Benzoyl: [3845-63-4]
$C_{15}H_{14}O_2$ 226.274
Mp 55-57°.

4-Nitrobenzoyl:
Cryst. Mp 128°.

Me ether: [4685-47-6] *4-Methoxy-1,2-dimethylbenzene, 9CI. 3,4-Dimethylanisole*
$C_9H_{12}O$ 136.193
Oil. Bp 204-205° Bp_{17} 96-97°.

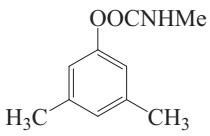
Et ether: [61808-04-6] *4-Ethoxy-1,2-dimethylbenzene, 9CI. 3,4-Dimethylphenetole*
$C_{10}H_{14}O$ 150.22
Oil. Bp 218°.

[22618-23-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1047A; 1086A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 193B; 264C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 975D; 1019B (*ir*)
Adv. Chem. Ser., 1955, **15**, 281 (***props***)
Vitullo, V.P. *et al., J.O.C.*, 1970, **35**, 3976 (*synth*)
Green, J.H.S. *et al., Spectrochim. Acta A*, 1972, **28**, 33 (*ir, Raman*)
Vandenborre, M.T. *et al., Acta Cryst. B*, 1973, **29**, 2488 (*cryst struct*)
Marx, J.N. *et al., J.A.C.S.*, 1974, **96**, 2121 (*synth, pmr*)
Elton-Bott, R.R. *et al., Anal. Chim. Acta*, 1977, **90**, 215 (*use*)
Netzel, D.A. *et al., Org. Magn. Reson.*, 1978, **11**, 58 (*cmr*)
Osibanjo, O. *et al., Analyst (London)*, 1980, **105**, 908 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 798
Stanger, A. *et al., J.O.C.*, 1996, **61**, 2549 (*Ac, synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2967
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, XLJ000

3,5-Dimethylphenyl methylcarbamate, 9CI D-877

[2655-14-3]
3,5-Xylyl methylcarbamate. XMC, JMAF. Cosban. Macbal

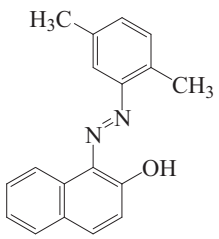


$C_{10}H_{13}NO_2$ 179.218
Agricultural insecticide, particularly for rice and tea. Cryst. Sol. most org. solvs.; v. spar. sol. H_2O. Mp 99°.
▶ LD_{50} (rat, orl) 542 mg/kg. FC8925000

Metcalf, R.L. *et al., J. Econ. Entomol.*, 1963, **56**, 862
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A922
Pesticide Manual, 11th edn., 1997, No. 755
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTN200

1-[(2,5-Dimethylphenyl)azo]-2-naphthalenol, 9CI D-878

[85-82-5]
1-(2,5-Xylylazo)-2-naphthol, 8CI

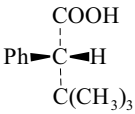


$C_{18}H_{16}N_2O$ 276.337
Food dye; delisted for foods by FDA. Needles with green highlights (EtOH). Mp 150-151°.
▶ QL5950000

Bamberger, E. *et al., Ber.*, 1902, **35**, 1874 (*synth*)
Gasparic, J. *et al., Coll. Czech. Chem. Comm.*, 1960, **26**, 2757 (*synth*)
Smyth, R.H. *et al., Chromatographia*, 1961, **5**, 395 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG080

3,3-Dimethyl-2-phenylbutanoic acid D-879

[83357-74-8]
α-(1,1-Dimethylethyl)benzeneacetic acid, 9CI. tert-*Butylphenylacetic acid*



(*R*)-*form*

$C_{12}H_{16}O_2$ 192.257

(*R*)-*form*
Mp 141-142°. $[\alpha]_D^{21}$ -61.45 (c, 0.31 in $CHCl_3$).

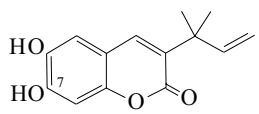
Me ester: [82372-89-2]
$C_{13}H_{18}O_2$ 206.284
Cryst. (hexane). Mp 33-34°. Bp_{15} 122°. $[\alpha]_D$ -58.32 (neat).

(±)-*form*
Cryst. (petrol). Mp 105-108°.

Aaron, C. *et al., J.O.C.*, 1967, **32**, 2797 (*synth*)
Craig, J.C. *et al., Tetrahedron*, 1971, **27**, 1173 (*abs config*)
Lardicci, L. *et al., J.O.C.*, 1972, **37**, 1060 (*synth*)
Imajo, S. *et al., J.O.C.*, 1979, **44**, 3587 (*resoln*)
Bright, D.A. *et al., J.O.C.*, 1982, **47**, 3521 (*synth, bibl*)

3-(1,1-Dimethyl-2-propenyl)-6,7-dihydroxy-2*H*-1-benzopyran-2-one D-880

3-(1,1-Dimethylallyl)-6,7-dihydroxycoumarin



$C_{14}H_{14}O_4$ 246.262

6-Me ether: [19723-23-0] *3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-6-methoxy-2*H*-1-benzopyran-2-one.* ***3-(1,1-Dimethylallyl)scopoletin***
$C_{15}H_{16}O_4$ 260.289
Constit. of *Ruta graveolens* (rue). Yellow needles (petrol). Mp 132-135°.

*6-Me ether, 7-*O*-β-D-glucopyranoside:* [208333-72-6]
$C_{21}H_{26}O_9$ 422.431
Constit. of *Ruta graveolens* (rue). Cryst. Mp 112-114°.

7-Me ether: [110209-94-4] *3-(1,1-Dimethyl-2-propenyl)-6-hydroxy-7-methoxy-2*H*-1-benzopyran-2-one.* ***3-(1,1-Dimethylallyl)isoscopoletin****. 6-De-*O*-methylrutacultin*
$C_{15}H_{16}O_4$ 260.289

Di-Me ether: [31526-60-0] *3-(1,1-Dimethyl-2-propenyl)-6,7-dimethoxy-2*H*-1-benzopyran-2-one, 9CI. 3-(1,1-Dimethylallyl)-6,7-dimethoxycoumarin.* ***Rutacultin***
$C_{16}H_{18}O_4$ 274.316
Constit. of *Ruta graveolens* (rue). Pale yellow needles (petrol). Mp 103-104°.

Steck, W. *et al., Phytochemistry*, 1971, **10**, 191 (*isol*)
Ballantyne, M.M. *et al., Tetrahedron*, 1971, **27**, 871 (*synth*)
von Brocke, W. *et al., Z. Naturforsch., B*, 1971, **26**, 1252 (*isol*)
Bergenthal, D. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1978, **311**, 1026 (*cmr*)
Borges del Castillo, J. *et al., An. Quim., Ser. C*, 1987, **83**, 15 (*Dimethylallylisoscopoletin*)

Srivastava, S.D. *et al., Fitoterapia*, 1998, **69**, 80-81 (*3-(1,1-Dimethylallyl)scopolatin 7-glucoside*)

3-(1,1-Dimethyl-2-propenyl)-7,8-dihydroxy-2*H*-1-benzopyran-2-one D-881

3-(1,1-Dimethylallyl)-7,8-dihydroxycoumarin

$C_{14}H_{14}O_4$ 246.262

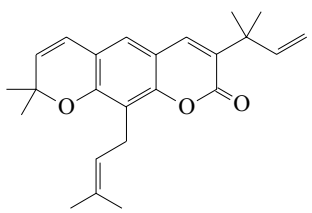
7-Me ether: [61899-42-1] ***3-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2H-1-benzopyran-2-one***. *3-(1,1-Dimethylallyl)-8-hydroxy-7-methoxycoumarin*
$C_{15}H_{16}O_4$ 260.289
Mp 98-100°.

Di-Me ether: [30310-54-4] ***3-(1,1-Dimethyl-2-propenyl)-7,8-dimethoxy-2H-1-benzopyran-2-one, 9CI***. *3-(1,1-Dimethylallyl)-7,8-dimethoxycoumarin*
$C_{16}H_{18}O_4$ 274.316
Isol. from roots of *Ruta graveolens* (rue). Cryst. (hexane). Mp 85-86°.

Reisch, J. *et al., Tet. Lett.*, 1970, 4305 (*isol*)
González, A.G. *et al., An. Quim.*, 1976, **72**, 191 (*isol, synth, deriv*)

3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin D-882

[30310-55-5]
3-(1,1-Dimethylallyl)-8-(3,3-dimethylallyl)xanthyletin



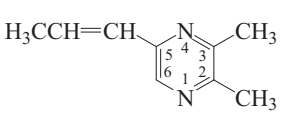
$C_{24}H_{28}O_3$ 364.483
Isol. from roots of *Ruta graveolens* (rue). λ_{max} 226 (sh) (log ϵ 4.39); 265 (log ϵ 4.24); 335 (log ϵ 4.11) (MeOH).

Reisch, J. *et al., Tet. Lett.*, 1970, 4305 (*isol*)
Sharma, R.B. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 538 (*synth*)

2,3-Dimethyl-5-(1-propenyl)-pyrazine, 9CI D-883

[80033-12-1]

[55138-72-2, 55138-76-6]



$C_9H_{12}N_2$ 148.207
Maillard product. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Flamont, I. *et al., Bull. Soc. Chim. Belg.*, 1979, **88**, 941-950 (*E-form, synth, ms, pmr*)
Ger. Pat., 1981, 3 048 031; *CA*, **96**, 6757f (*E-form, synth, ms, pmr*)
Farouk, A. *et al., Nahrung*, 2000, **44**, 188-192 (*occur*)

2,3-Dimethyl-5-(2-propenyl)-pyrazine, 9CI D-884

[55138-68-6]
5-Allyl-2,3-dimethylpyrazine

$C_9H_{12}N_2$ 148.207
Constit. of roasted peanut volatiles. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Ku, K.-L. *et al., J. Agric. Food Chem.*, 1998, **46**, 3220-3224 (*occur*)

2,5-Dimethyl-3-(1-propenyl)-pyrazine, 9CI D-885

[55138-73-3, 55138-77-7]

$C_9H_{12}N_2$ 148.207
Maillard product. Constit. of roasted green tea. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Wu, C.-M. *et al., J. Agric. Food Chem.*, 2000, **48**, 2438-2442 (*occur*)

2,5-Dimethyl-3-(2-propenyl)-pyrazine, 9CI D-886

[55138-69-7]
3-Allyl-2,5-dimethylpyrazine

$C_9H_{12}N_2$ 148.207
Maillard product. Constit. of baked potato. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Oruna-Concha, M.J. *et al., J. Agric. Food Chem.*, 2001, **49**, 2414-2421 (*occur*)

3,5-Dimethyl-2-(1-propenyl)-pyrazine D-887

[55138-74-4, 55138-78-8]

$C_9H_{12}N_2$ 148.207
Maillard product. Constit. of roasted green tea. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Hofmann, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1998, **207**, 229-236 (*occur*)

3,5-Dimethyl-2-(2-propenyl)-pyrazine, 9CI D-888

[55138-70-0]
2-Allyl-3,5-dimethylpyrazine

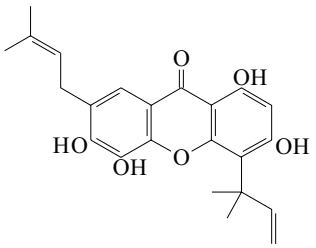
$C_9H_{12}N_2$ 148.207
Claimed food uses are not well documented. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)

4-(1,1-Dimethyl-2-propenyl)-1,3,5,6-tetrahydroxy-7-prenylxanthone D-889

[92609-73-9]

4-(1,1-Dimethyl-2-propenyl)-1,3,5,6-tetrahydroxy-7-(3-methyl-2-butenyl)-9H-xanthen-9-one, 9CI

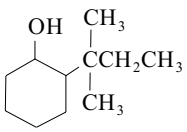


$C_{23}H_{24}O_6$ 396.439
Constit. of the root bark of *Rheedia brasiliensis* (bakupari). Cryst. (Et_2O/hexane). Mp 173-174°.

Delle Monache, G. *et al., J. Nat. Prod.*, 1984, **47**, 620 (*isol, uv, pmr, ms*)

2-(1,1-Dimethylpropyl)cyclohexanol D-890

2-tert-Pentylcyclohexanol. 2-tert-Amylcyclohexanol



$C_{11}H_{22}O$ 170.294
Bp_2 76-79°. Mixt. of stereoisomers.

Ac: [67874-72-0] *Coniferan*
$C_{13}H_{24}O_2$ 212.331
Listed in the EAFUS Food Additive Database (Jan. 2001) but with no current reported use. Bp_2 76°.

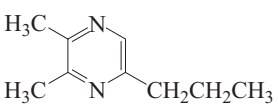
3,5-Dinitrobenzoyl:
Mp 92-92.5°.

Kheifits, L.A. *et al., Zh. Obshch. Khim.*, 1962, **32**, 1467; *CA*, **58**, 8921h (*synth, deriv*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, (Suppl.), 1976, **14**, 679; *CA*, **91**, 198642f (*rev*)

2,3-Dimethyl-5-propylpyrazine, 9CI D-891

[32262-98-9]

[97485-48-8]



$C_9H_{14}N_2$ 150.223
Maillard product. Volatile constit. of cooked shrimp and roasted wheat germ. Flavouring ingredient. Bp_{10} 79-82°. Characterised spectroscopically.

Riezebo, G. *et al., J.C.S.(C)*, 1971, 1627-1632 (*synth, pmr*)
U.S. Pat., 1975, 3 881 025; *CA*, **78**, 109541p (*synth, ms, use*)
Flament, I. *et al., Bull. Soc. Chim. Belg.*, 1979, **88**, 941-950 (*synth, ms*)
Ger. Pat., 1981, 3 048 031; *CA*, **96**, 6757f (*synth, ms*)

Kubota, K. *et al., Agric. Biol. Chem.*, 1986, **50**, 2867-2873 (*occur, shrimp*)
El-Saharty, Y.S. *et al., Adv. Food Sci.*, 1998, **20**, 53-58 (*occur, wheatgerm*)

2,5-Dimethyl-3-propylpyrazine, 9CI D-892

[18433-97-1]

$C_9H_{14}N_2$ 150.223
Maillard product.

Cavill, G.W.K. *et al., Aust. J. Chem.*, 1974, **27**, 879-889 (*occur*)

3,5-Dimethyl-2-propylpyrazine, 9CI D-893

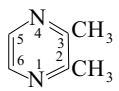
[32350-16-6]

$C_9H_{14}N_2$ 150.223
Volatile constit. of roasted coconut, cooked shrimp, roast beef and cocoa. Characterised spectroscopically.

Flament, I. *et al., Helv. Chim. Acta*, 1971, **54**, 1911-1913 (*synth, ms, occur, beef*)
U.S. Pat., 1975, 3 881 025; *CA*, **78**, 109541p (*synth, ms*)
Jinap, S. *et al., J. Sci. Food Agric.*, 1998, **77**, 441-448 (*occur, cocoa*)

2,3-Dimethylpyrazine, 9CI D-894

[5910-89-4]
FEMA 3271



$C_6H_8N_2$ 108.143
Flavour additive and odorant in foods, Present in papaya, crispbread, Swiss cheeses, black or green tea, asparagus, kohlrabi, baked potato, French fries, bell pepper, roasted filberts or pecans, roasted barley and other foodstuffs.. Sol. H_2O, org. solvs. d_4^0 1.02. Bp 156-158°. pK_{a1} 2.24; pK_{a2} -4.17 (25°, H_2O). Steam-volatile. Odour threshold 2500 ppb in H_2O.

▶ LD_{50} (rat, orl) 613 mg/kg. UQ2625000

Picrate:
Mp 150°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 841A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 399A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1556D (*ir*)
Das, B.K. *et al., J. Indian Chem. Soc.*, 1968, **45**, 1075 (*uv*)
Rizzi, G.P. *et al., J.O.C.*, 1968, **33**, 1333 (*synth*)
Oertel, R.P. *et al., Anal. Chem.*, 1972, **44**, 1589 (*Raman*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTU400
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 873 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

2,5-Dimethylpyrazine, 9CI D-895

[123-32-0]
FEMA 3272

$C_6H_8N_2$ 108.143
Used as flavour additive and odorant in foods. Present in asparagus, wheat bread, crispbread, Swiss cheeses, black or green tea, soya, malt, raw shrimp and squid. Liq. or solid with potato chip flavour. Sol. H_2O, EtOH, Et_2O. Mp 15°. Bp 155°. pK_{a1} 1.85; pK_{a2} -4.6 (27°, H_2SO_4 aq.). pK_{a1} 1.99; pK_{a2} -4.42 (25°, H_2O). Steam-volatile. Odour threshold 1800 ppb in H_2O.

▶ Fl. p. 64° (oc). LD_{50} (rat, orl) 1020 mg/kg. UQ2800000

Picrate:
Mp 157°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 840D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 398C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1556C (*ir*)
Langdon, W.K. *et al., Ind. Eng. Chem. Prod. Res. Dev.*, 1964, **3**, 8 (*synth*)
Wilen, S.H. *et al., Chem. Ind. (London)*, 1969, **8**, 237 (*synth*)
Paudler, W.W. *et al., Org. Mass Spectrom.*, 1970, **4**, 513 (*ms*)
Paudler, W.W. *et al., Org. Magn. Reson.*, 1971, **3**, 217 (*nmr*)
Oertel, R.P. *et al., Anal. Chem.*, 1972, **44**, 1589 (*Raman*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
von Stralendorff, F. *et al., J. Chem. Ecol.*, 1987, **13**, 655
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTU600
Boyer, M.L. *et al., J. Chem. Ecol.*, 1989, **15**, 649
Eiermann, U. *et al., Chem. Ber.*, 1990, **123**, 523 (*uv*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 874 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTU600

2,6-Dimethylpyrazine, 9CI D-896

[108-50-9]
FEMA 3273

$C_6H_8N_2$ 108.143
Flavour additive and odorant in foods. Present in raw asparagus, baked potato, French fries, wheat bread, crispbread, black or green tea, roasted barley, roasted filberts or pecans, malt, peated malt, wort, wild rice (*Zizania aquatica*) and squid. Prisms with sweet fried odour. Sol. H_2O, EtOH, Et_2O. Mp 47-48°. Bp 155.6° Bp_{35} 78-90°. pK_{a1} 1.9; pK_{a2} -4.57 (27°, H_2SO_4 aq.).

▶ LD_{50} (mus, ipr) 1080 mg/kg. UQ2975000

Picrate:
Mp 175-176°.

1-Oxide: [31396-37-9]
$C_6H_8N_2O$ 124.142
Prisms (hexane). Mp 108-110° (105-106°).

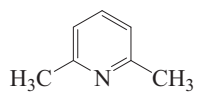
4-Oxide: [31396-38-0]
$C_6H_8N_2O$ 124.142
Prisms (hexane). Mp 57-58° (55°).

1,4-Dioxide: [74428-43-6]
$C_6H_8N_2O_2$ 140.141
Prisms (hexane). Mp 227° (224-225°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 840C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 398B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1556B (*ir*)
Kamal, M. *et al., J.O.C.*, 1962, **27**, 1355 (*synth*)
Paudler, W.W. *et al., Org. Mass Spectrom.*, 1970, **4**, 513 (*ms*)
Paudler, W.W. *et al., Org. Magn. Reson.*, 1971, **3**, 217 (*nmr*)
Oertel, R.P. *et al., Anal. Chem.*, 1972, **44**, 1589 (*Raman*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Ohta, A. *et al., J. Het. Chem.*, 1983, **20**, 311 (*synth, bibl, oxides*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTU800
Eiermann, U. *et al., Chem. Ber.*, 1990, **123**, 523 (*uv*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 875 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTU800

2,6-Dimethylpyridine, 9CI D-897

[108-48-5]
2,6-Lutidine, 8CI. FEMA 3540



C_7H_9N 107.155
Present in bread, tea and whisky. Flavouring agent. Liq. Sol. EtOH, Et_2O, cold H_2O; less sol. hot H_2O. d^{20} 0.92. Mp -6°. Bp 139-141° (145.6-145.8°). n_D^{20} 1.4977. pK_a 6.6 (25°).

▶ Flammable, fl. p. 33°. Toxic. OK9700000

Hydrochloride: [15439-85-7]
Cryst. (EtOH). Mp 230-231° dec.

Picrate: [2798-38-1]
Yellow needles (EtOH). Mp 163-164°.

N-*Oxide:* [1073-23-0]
C_7H_9NO 123.154
Liq. Bp_{18} 115-119°.

N-*Oxide; hydrochloride:* [6890-58-0]
Mp 219.5°.

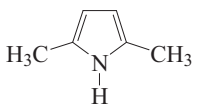
[27175-64-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 740B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 252C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1520B (*ir*)
Biddiscombe, D.P. *et al., J.C.S.*, 1954, 1957 (*synth, props*)
Červinka, O. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 567 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 626
Green, J.H.S. *et al., Spectrochim. Acta A*, 1970, **26**, 2139 (*ir, Raman*)
Hejda, Z. *et al., Coll. Czech. Chem. Comm.*, 1978, **43**, 3035 (*ms*)

Schuster, I.I. *et al., J.O.C.*, 1979, **44**, 2658 (*cmr*)
Bedford, G.R. *et al., Org. Magn. Reson.*, 1983, **21**, 637 (*pmr*)
Yajima, H. *et al., J. Phys. Chem.*, 1986, **90**, 2589 (*uv, fluor*)
Org. Synth., Coll. Vol., 6, 1988, 611
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 192
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 876-877
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTV089

2,5-Dimethyl-1*H*-pyrrole, 9CI D-898

[625-84-3]



C_6H_9N 95.144
Listed in the EAFUS Food Additive Database (Jan 2001) but with no reported use. Oil. Prac. insol. H_2O. d_4^{20} 0.94. Bp_{760} 165° Bp_8 50-53°. n_D^{20} 1.5036. Steam-volatile.

► LD_{50} (rat, orl) 59 mg/kg. UX9465930

N-*Ac:* [5044-31-5]
$C_8H_{11}NO$ 137.181
Bp_{27} 122-125°.

N-*Me:* [930-87-0] *1,2,5-Trimethyl-1*H*-pyrrole*
$C_7H_{11}N$ 109.171
Maillard product. Liq. Bp_{746} 169° Bp_9 55-56°. pK_a -0.24.

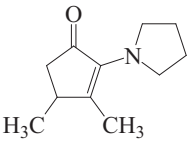
N-*Et:* [5044-19-9] *1-Ethyl-2,5-dimethylpyrrole*
$C_8H_{13}N$ 123.197
Liq. Bp_{739} 174° Bp_{45} 103.5-104.5°. n_D^{20} 1.4884.

N-*Benzyl:* [5044-20-2]
$C_{13}H_{15}N$ 185.268
Pale yellow cryst. solid. Mp 40-41°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 566A; 566B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 2A; 2C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1445C; 1446A (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 219 (*synth*)
Leonard, N.J. *et al., J.A.C.S.*, 1953, **75**, 6249 (*N-Et*)
Abraham, R.J. *et al., Can. J. Chem.*, 1959, **37**, 1056 (*pmr*)
Budzikiewicz, H. *et al., J.C.S.*, 1964, 1949 (*ms*)
Page, T.F. *et al., J.A.C.S.*, 1965, **87**, 5333 (*cmr*)
Jones, R.A. *et al., Aust. J. Chem.*, 1966, **19**, 107; 289 (*synth, ir, deriv*)
Jones, R.A. *et al., Tetrahedron*, 1967, **23**, 4469 (*pmr*)
Heaney, H. *et al., J.C.S. Perkin 1*, 1973, 499 (*N-Me*)
Cushley, R.J. *et al., Can. J. Chem.*, 1975, **53**, 148 (*N-Me*)
Baldwin, J.E. *et al., Chem. Comm.*, 1982, 624 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DTV300
Gangjee, A. *et al., J. Med. Chem.*, 1992, **35**, 3678 (*N-benzyl*)
Rousseau, B. *et al., Synthesis*, 1996, 1336 (*synth*)
Trofimov, B.A. *et al., Synthesis*, 2000, 1585-1590 (*synth, ir, pmr*)

3,4-Dimethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one D-899

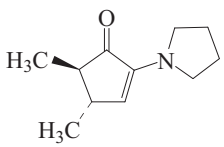
[97826-62-5]



$C_{11}H_{17}NO$ 179.261
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*synth, ms, pmr, ir*)

4,5-Dimethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one D-900



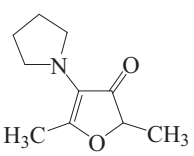
$C_{11}H_{17}NO$ 179.261

(4*R*,5*R*)-*form* [97826-63-6]
trans-*form*
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*synth, ms, pmr, ir*)

2,5-Dimethyl-4-(1-pyrrolidinyl)-3(2*H*)-furanone D-901

[80873-59-2]
DMPF

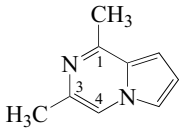


$C_{10}H_{15}NO_2$ 181.234
Proline-derived Maillard product. Flavouring agent. Constit. of dark malt. Pale yellow oil with intense oral cooling action and nutty odour.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*occur, isol, ms*)
Debrauwer, L. *et al., Bull. Soc. Chim. Fr.*, 1991, **128**, 244-254 (*occur*)
Japan. Pat., 1995, 07 242 661; *CA*, **124**, 254123q (*synth, use*)
Ottinger, H. *et al., J. Agric. Food Chem.*, 2001, **49**, 1336-1344 (*synth, ms, pmr, cmr*)

1,3-Dimethylpyrrolo[1,2-*a*]pyrazine, 9CI D-902

[64608-62-4]



$C_9H_{10}N_2$ 146.191
Component of roast beef aroma. Yellow oil. Bp_{10} 125°. Obt. as mixt. with 1,4-Dimethylpyrrolo[1,2-*a*]pyrazine, D-903.

Flament, I. *et al., Helv. Chim. Acta*, 1977, **60**, 1872 (*occur, synth, ir, pmr, ms*)
Houminer, Y. *et al., J. Het. Chem.*, 1981, **18**, 445 (*synth*)

1,4-Dimethylpyrrolo[1,2-*a*]pyrazine, 9CI D-903

[64608-63-5]

$C_9H_{10}N_2$ 146.191
Component of roast beef aroma. Yellow oil. Bp_{10} 125°. Obt. as a mixt. with 1,3-Dimethylpyrrolo[1,2-*a*]pyrazine, D-902.

Flament, I. *et al., Helv. Chim. Acta*, 1977, **60**, 1872 (*occur, synth, uv, pmr, ms*)
Houminer, Y. *et al., J. Het. Chem.*, 1981, **18**, 445 (*synth*)

3,4-Dimethylpyrrolo[1,2-*a*]pyrazine, 9CI D-904

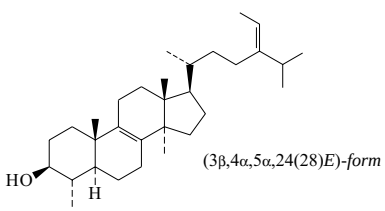
[64608-64-6]

$C_9H_{10}N_2$ 146.191
Component of roast beef aroma. Mp 50°.

Flament, I. *et al., Helv. Chim. Acta*, 1977, **60**, 1872 (*occur, synth, ir, pmr, ms*)

4,14-Dimethylstigmasta-8,24(28)-dien-3-ol D-905

24-Ethylidene-4,14-dimethylcholest-8-en-3-ol



(3β,4α,5α,24(28)*E*)-*form*

$C_{31}H_{52}O$ 440.751

(3β,4α,5α,24(28)*E*)-*form* [123164-57-8]
Constit. of *Phaseolus vulgaris* (kidney bean).

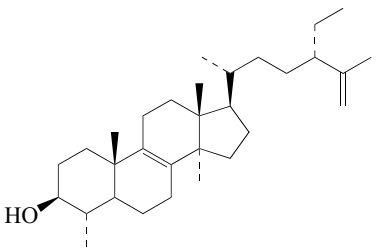
(3β,4α,5α,24(28)*Z*)-*form* [73148-03-5]
Constit. of *Phaseolus vulgaris* (kidney bean).

[123086-82-8, 123116-16-5]

Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219

4,14-Dimethylstigmasta-8,25-dien-3-ol, 9CI D-906

24-Ethyl-4,14-dimethylcholesta-8,25-dien-3-ol



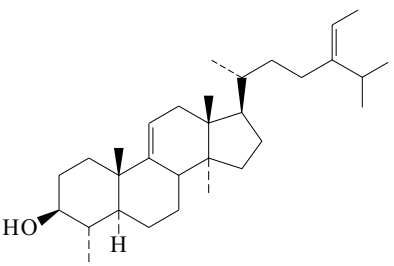
$C_{31}H_{52}O$ 440.751

(3β,4α,5α,24*S*)-*form* [80735-22-4]
Constit. of *Lagenaria leucantha* (bottle gourd). Mp 129-130° (as Ac).

Itoh, T. *et al., Phytochemistry*, 1981, **20**, 1929-1933 (*isol, pmr, cmr, ms*)

4,14-Dimethylstigmasta-9(11),24(28)-dien-3-ol, 9CI D-907

24-Ethylidene-4,14-dimethylcholest-9(11)-en-3-ol. 24-Ethylidene-29-norlanost-9(11)-en-3-ol



$C_{31}H_{52}O$ 440.751

(3β,4α,5α,24(28)*Z*)-*form* [123086-83-9]
Constit. of *Phaseolus vulgaris* (kidney bean).

(3β,4α,5α,24(28)*E*)-*form* [178275-58-6]

Ac: [178275-63-3]
Cryst. Mp 126-128°.

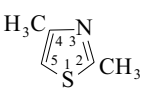
[123086-84-0]

Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219

Akikisa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1202 (*isol, pmr, ms*)

2,4-Dimethylthiazole, 9CI D-908

[541-58-2]



C_5H_7NS 113.183
Constit. of beef aroma. Sol. EtOH, Et_2O, cold H_2O, less sol. hot H_2O. d_4^{15} 1.51. Bp_{50} 70-73°. pK_a 3.92 (25°).

► LD_{50} (mus, ipr) 250 mg/kg. XJ4375000

Hydrochloride:
Mp 189°.

Picrate:
Yellow plates. Mp 140-141°.

N-*Me:2,3,4-Trimethylthiazolium(1+)*
$C_6H_{10}NS^{\oplus}$ 128.218
Mp 260° dec. (as iodide).

Hantzsch, A. *et al., Annalen*, 1889, **250**, 265
Steude, M. *et al., Annalen*, 1891, **261**, 41
Fisher, N.I. *et al., J.C.S.*, 1930, 2509
Org. Synth., 1945, **25**, 35
Kurkjy, R.P. *et al., J.A.C.S.*, 1952, **74**, 5778
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 202
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511 (*ms*)
Hojo, M. *et al., J.O.C.*, 1988, **53**, 2209 (*synth, deriv, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DUG200

2,5-Dimethylthiazole D-909

[4175-66-0]

C_5H_7NS 113.183
Organoleptic agent. Food flavour/aroma component. Reported in roasted peanuts and roasted sesame seeds together with isomers. Liq. with meaty odour. Sol. EtOH, Et_2O. Bp_{80} 86°. pK_a 3.91 (25°). Steam-volatile.

Picrate:
Mp 172° (166-167°).

Gabriel, S. *et al., Ber.*, 1910, **43**, 1283-1287 (*synth*)
Kurkjy, R.P. *et al., J.A.C.S.*, 1952, **74**, 5778 (*synth*)
Nishimura, O. *et al., Koryo*, 1990, **165**, 91-101; *CA*, **113**, 210350s (*isol*)

4,5-Dimethylthiazole D-910

[3581-91-7]
FEMA 3274

C_5H_7NS 113.183
Flavouring agent. Sol. Et_2O, EtOH. Mp 83-84°. Bp 158° Bp_{47} 75°. pK_a 3.73 (25°).

► XJ4380000

Picrate:
Cryst. (EtOH). Mp 186-187°.

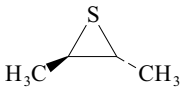
N-*Oxide:*
C_5H_7NOS 129.182
Cryst. (EtOAc/hexane). Mp 116-117°.

N-*Me:3,4,5-Trimethylthiazolium*
$C_6H_{10}NS^{\oplus}$ 128.218
Cryst. (EtOH) (as iodide). Mp 223-223.5° dec. (iodide).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 109C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1492D (*ir*)
Buchman, E.R. *et al., J.O.C.*, 1941, **6**, 764
Kurkjy, R.P. *et al., J.A.C.S.*, 1952, **74**, 5778 (*synth*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511 (*ms*)
Begtrup, M. *et al., Acta Chem. Scand.*, 1992, **46**, 372 (*oxide*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 194
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 879

2,3-Dimethylthiirane, 9CI D-911

[4426-36-2]
2-Butene episulfide. 2,3-Epithiobutane



(2*R*,3*R*)-*form*

C_4H_8S 88.173

(2*R*,3*R*)-*form* [70095-46-4]
(+)-trans-*form*
n_D^{25} 1.4390.

(2*S*,3*S*)-*form* [64474-58-4]
(-)-trans-*form*
Liq. d_4^{25} 0.89. Bp_{735} 88-89° Bp_{180} 54-55°. $[\alpha]_D^{25}$ -96.73 (neat). n_D^{20} 1.4648.

(2*RS*,3*RS*)-*form* [5955-98-6]
(±)-trans-*form*
Bp 88-89° Bp_{155} 45-45.5°. n_D^{20} 1.4640.

(2*RS*,3*SR*)-*form* [5954-71-2]
cis-*form*
Component of food flavours. Bp_{735} 98.5° Bp_{130} 51°. n_D^{20} 1.4775. n_D^{25} 1.4684.

S-*Oxide:* [10306-90-8]
C_4H_8OS 104.173
Oil.

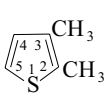
S,S-*Dioxide:* [54697-52-8]
$C_4H_8O_2S$ 120.172
Long needles (EtOH). Mp 57° dec. Dec. to 2-Butene.

[6668-16-2, 10306-89-5, 24302-63-4, 29027-23-4, 70492-83-0, 125125-34-0]

Price, C.C. *et al., J.A.C.S.*, 1953, **75**, 2396 (*config*)
Helmkamp, G.K. *et al., Tetrahedron*, 1957, **2**, 304 (*synth*)
Neureiter, N.P. *et al., J.A.C.S.*, 1959, **81**, 578 (*synth*)
Helmkamp, G.K. *et al., J.O.C.*, 1960, **25**, 1754 (*synth*)
Sidhu, K.S. *et al., J.A.C.S.*, 1966, **88**, 254 (*ms*)
Hartzell, G.E. *et al., J.O.C.*, 1967, **32**, 459 (*synth, oxide*)
Lautenschlaeger, F. *et al., J.O.C.*, 1969, **34**, 3991 (*synth*)
Kondo, K. *et al., Tet. Lett.*, 1969, 2461 (*oxide, dioxide*)
Fisher, N.H. *et al., Synthesis*, 1970, 393 (*dioxide*)
Bucciarelli, M. *et al., Tetrahedron*, 1977, **33**, 999 (*synth, abs config*)
Cohen, D. *et al., J. Phys. Chem.*, 1983, **87**, 4585 (*uv*)
Arad-Yellin, R. *et al., J.A.C.S.*, 1983, **105**, 4561 (*synth, config*)
Paradisi, C. *et al., J. Het. Chem.*, 1989, **26**, 465 (*ms*)
Opitz, G. *et al., Tet. Lett.*, 1989, **30**, 3131 (*dioxide*)
Opitz, G. *et al., Chem. Ber.*, 1990, **123**, 1989 (*dioxide*)
Dishington, A.P. *et al., J.C.S. Perkin 1*, 1997, 323-337 (*dioxide, synth, ir, pmr, cmr, ms*)

2,3-Dimethylthiophene, 9CI D-912

[632-16-6]



C_6H_8S 112.195
Odorant used in food flavouring. Insol. H_2O, v. sol. Et_2O, EtOH, C_6H_6. d_4^{20} 1. Fp -49. Bp 140-141°. n_D^{20} 1.5192.

Grünewald, W. *et al., Ber.*, 1887, **20**, 2586
Shepard, A.F. *et al., J.A.C.S.*, 1932, **54**, 2951
Adv. Chem. Ser., 1955, **15**, 188 (***props***)

Nishimura, H. *et al., J.O.C.*, 1975, **40**, 1567 (*synth, ir, ms, pmr*)

2,4-Dimethylthiophene D-913

[638-00-6]

C_6H_8S 112.195

Constit. of *Allium* spp.. Also found in various cooked foods. Odorant used in food flavouring. Insol. H_2O; sol. Et_2O, EtOH, C_6H_6. d^{20} 1. Bp 140.7°. n_D^{20} 1.5104.

Zelinsky, N. *et al., Ber.*, 1887, **20**, 2018
Adv. Chem. Ser., 1955, **15**, 189 (***props***)
Nishimura, H. *et al., J.O.C.*, 1975, **40**, 1567 (*synth, ir, ms, pmr*)
Mubarak, A.M. *et al., Phytochemistry*, 1990, **29**, 3351 (*isol*)
Takeshita, M. *et al., J.O.C.*, 1991, **56**, 2837 (*synth*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 1030

2,5-Dimethylthiophene, 9CI D-914

[638-02-8]

C_6H_8S 112.195

Odorant used in food flavouring. Insol. H_2O; sol. Et_2O, EtOH, C_6H_6. d^{20} 0.99. Fp -62.6. Bp 136.8°. n_D^{20} 1.5129.

S,S-*Dioxide:* [50590-79-9]
$C_6H_8O_2S$ 144.194
Cryst. Mp 88°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 44C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 592C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1467D (*ir*)
Adv. Chem. Ser., 1955, **15**, 190 (***props***)
Jean, G.N. *et al., J.O.C.*, 1955, **20**, 1363 (*synth*)
Jeffery, G.H. *et al., J.C.S.*, 1961, 570
Lanum, W.J. *et al., J. Chem. Eng. Data*, 1969, **14**, 93 (*ms, ir, uv, Raman*)
Nishimura, H. *et al., J.O.C.*, 1975, **40**, 1567 (*synth, ms, ir, pmr*)
Rozen, S. *et al., Chem. Comm.*, 1994, 1959 (*dioxide*)

3,4-Dimethylthiophene D-915

[632-15-5]

C_6H_8S 112.195

Odorant used in food flavouring. d^{20} 1.01. Bp 144°. n_D^{20} 1.5212.

S,S-*Dioxide:*
$C_6H_8O_2S$ 144.194
Cryst.

Shepard, A.F. *et al., J.A.C.S.*, 1934, **56**, 1355
Adv. Chem. Ser., 1955, **15**, 191 (***props***)
Koenig, B. *et al., Chem. Ber.*, 1974, **107**, 2931 (*synth, spectra*)
Nishimura, H. *et al., J.O.C.*, 1975, **40**, 1567 (*synth, ir, ms, pmr*)
Houge-Frydrych, C.S.V. *et al., Chem. Comm.*, 1987, 1819 (*dioxide*)

2,5-Dimethyltridecane D-916

[56292-66-1]

$H_3C(CH_2)_7CH(CH_3)CH_2CH_2CH(CH_3)_2$

$C_{15}H_{32}$ 212.418

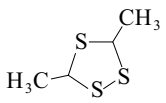
(±)-*form*
Mp -27.2°. Bp 250.4°. n_D^{20} 1.4310.

(ξ)-*form*
Constit. of pickled mustard tuber (*Brassica juncea*).

Pichler, H. *et al., Brennst.-Chem.*, 1962, **43**, 199 (*synth*)
Costa Neto, A. *et al., Ann. Acad. Bras. Ci&eenc.*, 1979, **51**, 255 (*pmr*)
Zhang, H. *et al., CA*, 1985, **103**, 51202v (*occur*)
Lin, Z. *et al., CA*, 1986, **105**, 189690a (*occur*)
Chen, Y. *et al., Chromatographia*, 1987, **23**, 502 (*occur*)

3,5-Dimethyl-1,2,4-trithiolane D-917

[23654-92-4]
FEMA 3541



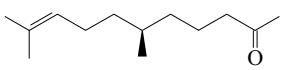
$C_4H_8S_3$ 152.305

Occurs in roast or boiled pork, beef, mutton and chicken. Also in roasted filberts and cooked potato, beans, shrimp and clam. Flavouring ingredient.. Bp_{17} 77-78°. Mixt. of *cis*- and *trans*- forms.

Chang, S.S. *et al., Chem. Ind. (London)*, 1968, 1659 (*isol*)
Brinkman, H.W. *et al., J. Agric. Food Chem.*, 1972, **20**, 177 (*isol*)
Dubs, P. *et al., Helv. Chim. Acta*, 1978, **61**, 1404 (*synth, bibl*)
Ritzau, M. *et al., Annalen*, 1993, 871 (*isol*)

6,10-Dimethyl-9-undecen-2-one D-918

[4433-36-7]
Dihydrogeranylacetone. Tetrahydropseudoionone. FEMA 3059



(*R*)-*form*

$C_{13}H_{24}O$ 196.332

Used in perfumery and food flavouring.

(R)-form [114976-95-3]
Liq. $Bp_{0.16}$ 84-93°. $[\alpha]_D^{23}$ +0.5 (c, 1.02 in $CHCl_3$). n_D^{23} 1.4431.

(S)-form [50718-54-2]
Liq. $Bp_{0.4}$ 89-90°. $[\alpha]_D^{23}$ -0.6 (c, 1.02 in $CHCl_3$). $n_D^{22.5}$ 1.4425.

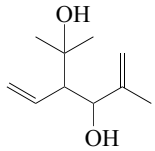
(±)-*form* [93303-24-3]
Liq. Bp 234° Bp_5 110-113°.

Semicarbazone:
Cryst. (EtOH aq.). Mp 83.5-84°.

Bhalerao, H.T. *et al., J.A.C.S.*, 1971, **93**, 105 (*ms*)
Szykula, J. *et al., Annalen*, 1987, 709 (*synth, pmr*)
Mori, K. *et al., Annalen*, 1988, 717 (*synth, R-form, S-form*)
Cane, D.E. *et al., Biochemistry*, 1990, **29**, 5476 (*synth, pmr, cmr*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 123S (*rev, bibl*)

2,5-Dimethyl-3-vinyl-5-hexene-2,4-diol D-919

3-Ethenyl-2,5-dimethyl-5-hexene-2,4-diol



$C_{10}H_{18}O_2$ 170.251

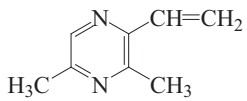
2-Ac: [79507-90-7]
$C_{12}H_{20}O_3$ 212.288
Constit. of *Artemisia vulgaris* (mugwort). Mixt. of diastereoisomers.

4-Ketone, 2-Ac: [79507-89-4]
$C_{12}H_{18}O_3$ 210.272
Constit. of *Artemisia vulgaris* (mugwort).

Näf-Müller, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1424-1430 (*isol, pmr*)

3,5-Dimethyl-2-vinylpyrazine D-920

[157615-33-3]
2-Ethenyl-3,5-dimethylpyrazine, 9CI



$C_8H_{10}N_2$ 134.18

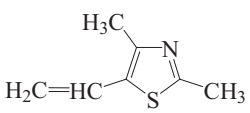
Formed by thermal interaction of ribose and cysteine. Odour constit. of roasted coffee. Also present in fried beef volatiles. Odour threshold 0.012 µg/L in air.

[81352-79-6]

Specht, K. *et al., J. Agric. Food Chem.*, 1994, **42**, 2246-2253 (*occur*)
Czerny, M. *et al., J. Agric. Food Chem.*, 1996, **44**, 3268-3272; 1999, **47**, 695-699 (*occur, synth, pmr, ms*)
Hoffman, T. *et al., Z. Lebensm.-Unters. - Forsch.*, 1998, **207**, 229-236 (*occur*)

2,4-Dimethyl-5-vinylthiazole D-921

[65505-18-2]
5-Ethenyl-2,4-dimethylthiazole, 9CI. FEMA 3145



C_7H_9NS 139.221

Present in cooked beef volatiles. Flavouring ingredient. No phys. props. reported.

Wilson, R.A. *et al., J. Agric. Food Chem.*, 1973, **21**, 873-876 (*glc, occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 198 (*use*)

Dimeticone, INN, JAN D-922

[9006-65-9]
Dimethicone, BAN. *Poly(dimethyl siloxane). Dimethylpolysiloxane*
Used in foods as a defoaming agent.

Component of Altacaps, Cobadex, Diovol, Siloxyl and Vasogen.

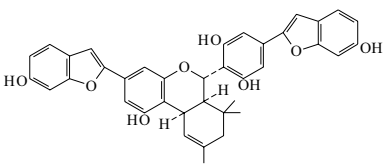
Mixt. with silicon dioxide: [8050-81-5]
Simethicone, USAN. *Simeticone, BAN, INN. Mylicon. Silain*
Viscous oil. Component of Gelusil, Mylanta and Tricone.

► LD_{50} (dog, ivn) 900 mg/kg. VW6200000

Ger. Pat., 1971, 2 057 239, (*Richardson-Merrell*); *CA*, **75**, 91 323v (*synth, pharmacol*)
Cox, H.L.M. *et al., Pharm. Weekbl.*, 1976, **111**, 973 (*activity*)
Grape, W. *et al., Parfuem. Kosmet.*, 1986, **67**, 326 (*manuf, props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1109
Brečević, L. *et al., J. Appl. Toxicol.*, 1994, **14**, 207 (*Simethicone, pharmacol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 871-873

Dimoracin D-923

[84323-11-5]

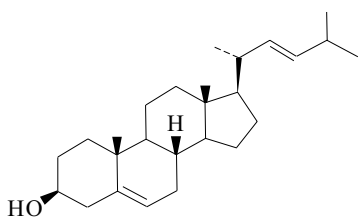


$C_{38}H_{32}O_8$ 616.666
Phytoalexin from *Morus alba* (white mulberry) infected with *Fusarium solani*. Cryst. Poorly sol. hexane. Mp 238-240°. $[\alpha]_D$ -5 (EtOH). λ_{max} 220 (ϵ 64200); 254 (ϵ 21200); 261 (ϵ 17600); 320 (ϵ 76000); 334 (ϵ 67200) (EtOH) (Berdy).

Takasugi, M. *et al., Chem. Lett.*, 1982, 1217

26,27-Dinorergosta-5,22-dien-3-ol, 9CI D-924

24-Norcholesta-5,22-dien-3-ol



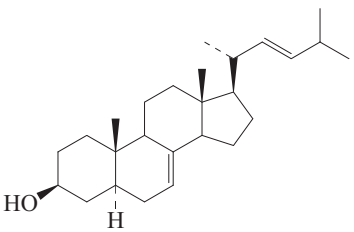
$C_{26}H_{42}O$ 370.617
(3β,22*E*)-*form* [38788-81-7]
Constit. of *Mytilus edulis* (blue mussel) and other crustaceans, molluscs and sponges. Cryst. Mp 138-140° (122-124°). $[\alpha]_D$ -31 ($CHCl_3$).
(3β,22*Z*)-*form* [52745-87-6]
Needles (MeOH). Mp 163-166°. $[\alpha]_D$ -63 ($CHCl_3$).

[34428-92-7, 76250-41-4, 77880-46-7]

Idler, D.R. *et al., Steroids*, 1970, **16**, 451 (*isol, struct*)
Fryberg, M. *et al., Chem. Comm.*, 1971, 1194 (*synth*)
Viala, J. *et al., Bull. Soc. Chim. Fr.*, 1972, 3626 (*pmr, ms*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095 (*isol*)
Metayer, A. *et al., Tet. Lett.*, 1974, 598 (*synth*)
Sheikh, Y.M. *et al., Steroids*, 1975, **26**, 129 (*synth*)

26,27-Dinorergosta-7,22-dien-3-ol D-925

24-Norcholesta-7,22-dien-3-ol

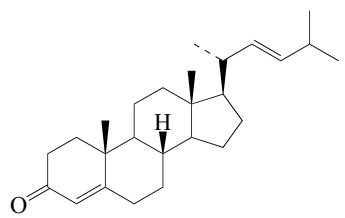


$C_{26}H_{42}O$ 370.617
(3β,5α,22*E*)-*form* [30674-32-9]
Asterosterol
Found in clams and oysters. Cryst. (MeOH). Mp 130-131°. $[\alpha]_D$ -6.4 (c, 1 in $CHCl_3$).

Kobayashi, M. *et al., Tetrahedron*, 1973, **29**, 1193 (*isol, struct*)
Boll, P.M. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 270 (*synth*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 236 (*synth*)

26,27-Dinorergosta-4,22-dien-3-one D-926

[182257-20-1]
24-Norcholesta-4,22-dien-3-one

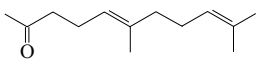


$C_{26}H_{40}O$ 368.601
(*E*)-*form*
Constit. of dried prawns (*Nematopalaemon tenuipes*).

Indap, M.M. *et al., Indian J. Exp. Biol.*, 1996, **34**, 588-589; *CA*, **125**, 270867y (*isol, pmr*)

1,2-Dinor-6,10-farnesadien-3-one D-927

[689-67-8]
6,10-Dimethyl-5,9-undecadien-2-one, 9CI



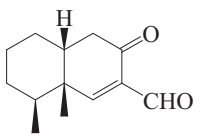
(*E*)-*form*

$C_{13}H_{22}O$ 194.316
► Skin irritant. YQ1190000
(*E*)-*form* [3796-70-1]
Geranylacetone. *FEMA 3542*
Constit. of many essential oils including peppermint (*Mentha piperita*) and Carolina vanilla (*Carphephorus odoratissimus*). Used in food flavouring. Bp_{10} 124°.

Semicarbazone:
Mp 96-97°.
2,4-Dinitrophenylhydrazone:
Mp 54-55°.
(*Z*)-*form* [3879-26-3] ***Nerylacetone***
Semicarbazone:
Mp 90-91°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 416B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 647B; 647C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 502B (*ir*)
Isler, O. *et al., Helv. Chim. Acta*, 1956, **39**, 897-904; 1958, **41**, 786-807 (*E-form, synth, use*)
Trost, B.M. *et al., J.A.C.S.*, 1977, **99**, 6124-6126 (*E-form, synth*)
Fujita, Y. *et al., Chem. Lett.*, 1978, 533-534 (*synth, E,Z-isom*)
Jorgenson, J.W. *et al., Science (Washington, D.C.)*, 1978, **199**, 796-798 (*E-form, occur*)
Shimizu, I. *et al., Tet. Lett.*, 1980, **21**, 3199-3202 (*synth*)
Tsuji, J. *et al., Pure Appl. Chem.*, 1982, **54**, 197-206 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GDE400

12,13-Dinor-8-oxo-6-eremophilen-11-al D-928



$C_{13}H_{18}O_2$
10β-*form* [348119-86-8]
Constit. of *Petasites japonicus* ssp. *giganteus* (Japanese butterbur). Oil. $[\alpha]_D$ +5.05 (c, 0.21 in $CHCl_3$). λ_{max} 235 (EtOH).

Goto, Y. *et al., Phytochemistry*, 2001, **57**, 109-113 (*isol, pmr, cmr*)

Dioctyl phosphate, 9CI D-929

[3115-39-7]
Dioctyl hydrogen phosphate. Dioctyl phosphoric acid
$[H_3C(CH_2)_7O]_2P(O)OH$
$C_{16}H_{35}O_4P$ 322.424
Oil or cryst. Mp 29-30°. n_D^{20} 1.4464 (supercooled). pK_a 3.32 (75% v/v EtOH aq.).

Me_4N salt:
Solid. Mp 173°.

Chloride: Dioctyl phosphorochloridate. Dioctyl phosphoryl chloride. Dioctyl chlorophosphate
$C_{16}H_{34}ClO_3P$ 340.869
Liq. n_D^{25} 1.4452.

Chabrier, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1957, **244**, 2730 (*synth*)
Petrov, K.A. *et al., Zh. Obshch. Khim.*, 1961, **31**, 1709; *J. Gen. Chem. USSR (Engl. Transl.)*, 1961, **31**, 1596 (*synth*)
Grosse-Ruyken, H. *et al., J. Prakt. Chem.*, 1962, **18**, 287 (*synth, chloride*)
Navratil, O. *et al., Hydrometallurgy*, 1981, **7**, 289 (*use*)

Dioctyltin isooctylthioglycolate D-930

[15571-58-1]

2-Ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate, 14CI. Dioctyltin bis(isooctylmercaptoacetate). Dioctyltin S,S′-bis(2-ethylhexylthioglycolate)

$[H_3C(CH_2)_7]_2Sn[SCH_2COOCH_2CH(CH_2CH_3)(CH_2)_3CH_3]_2$

$C_{36}H_{72}O_4S_2Sn$ 751.804

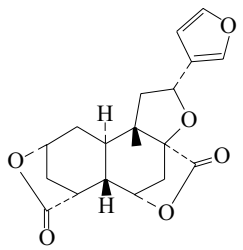
Used as a heat stabiliser for rigid PVC used in food and drink applications. Colourless viscous oil. Sol. common org. solvs. n_D^{20} 1.4992.

Schumann, H. *et al., Organotin Compd.*, (Ed. Sawyer, A.K.), Marcel Dekker, 1971, **2**, 297-508 (*synth, props*)
Figge, K. *et al., J. Chromatogr.*, 1977, **131**, 317-327 (*anal*)
Lequan, M. *et al., Eur. Polym. J.*, 1980, **16**, 1109-1113 (*synth, ir, use*)
Allen, D.W. *et al., J. Organomet. Chem.*, 1980, **199**, 299-310 (*Mössbauer*)
Michel, A. *et al., Polym. Degrad. Stab.*, 1980, **2**, 277-293 (*pmr*)
Senich, G.A. *et al., Polymer*, 1982, **23**, 1385-1387 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 46, 1983, **10**, 111-113 (*rev, props*)
Cooray, B.B. *et al., Polym. Degrad. Stab.*, 1984, **7**, 1-12 (*use*)
Blunden, S.J. *et al., J. Organomet. Chem.*, 1985, **282**, 9-16 (*synth, pmr, ir*)
Mueller, H.A. *et al., Makromol. Chem., Macromol. Symp.*, 1989, **29**, 197-207; *CA*, **112**, 57374k (*Sn-119 nmr*)

Diosbulbin B D-931

[20086-06-0]

8β,12α:15,16-Diepoxy-19-nor-13(16),14-clerodadiene-17,6β:18,2α-diolide



Absolute configuration

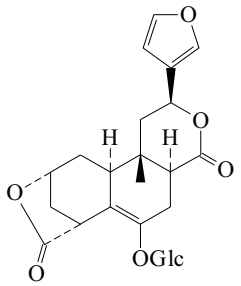
$C_{19}H_{20}O_6$ 344.363

Constit. of *Dioscorea bulbifera* (air potato). Cryst. (Me_2CO). Mp 285° dec. $[\alpha]_D^{20}$ +92 (c, 0.75 in Py).

Kawasaki, T. *et al., Chem. Pharm. Bull.*, 1968, **16**, 2430 (*isol*)
Komori, T. *et al., Annalen*, 1973, 978 (*struct*)
Komori, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1701 (*abs config*)
Yonemitsu, M. *et al., Planta Med.*, 1993, **59**, 577 (*isol, pmr, cmr*)
Singh, A. *et al., Acta Cryst. C*, 1999, **55**, 559-561 (*cryst struct*)

Diosbulbinoside D D-932

[66756-59-0]



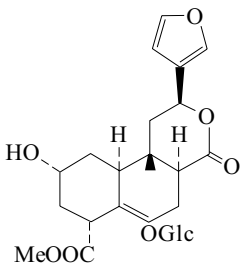
$C_{25}H_{30}O_{11}$ 506.505

Isol. from *Dioscorea bulbifera* (air potato). Cryst. ($CHCl_3$/MeOH). Mp 169-173° dec. $[\alpha]_D$ -31 (c, 0.8 in MeOH).

Ida, Y. *et al., Chem. Pharm. Bull.*, 1978, **26**, 435

Diosbulbinoside F D-933

[66756-58-9]



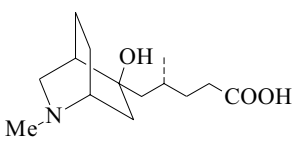
$C_{26}H_{34}O_{12}$ 538.547

Isol. from *Dioscorea bulbifera* (air potato). Cryst. (MeOH). Mp 193-195° dec. $[\alpha]_{350}$ -25 (c, 0.3 in MeOH).

Ida, Y. *et al., Chem. Pharm. Bull.*, 1978, **26**, 435-439 (*isol, pmr*)

Dioscoretine D-934

[128637-87-6]



$C_{13}H_{23}NO_3$ 241.33

Alkaloid from the tubers of the famine food *Dioscorea dumetorum*.

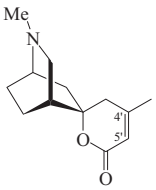
▶ CL5602600

Iwu, M.M. *et al., Planta Med.*, 1990, **56**, 119 (*isol, cmr, struct*)

Dioscorine D-935

[3329-91-7]

2,4′-Dimethylspiro[2-azabicyclo[2.2.2]octane-5,2′-[2H]pyran]-6′(3′H)-one, 9CI



Absolute Configuration

$C_{13}H_{19}NO_2$ 221.299

Alkaloid from the tubers of wild yam *Dioscorea hispida*. Mp 43.5° (34-35°). $[\alpha]_D^{18}$ -35 (c, 3.4 in $CHCl_3$). Log P 0.76 (calc).

▶ LD_{50} (mus, ipr) 60 mg/kg. Exp. convulsant effects. JG5787500

Hydrochloride:
Mp 210-211° dec.

Picrate:
Mp 187° dec.

N-*Oxide:*

[171432-58-9, 171595-79-2] ***Dioscorine* N-oxide**

$C_{13}H_{19}NO_3$ 237.298

4′S,5′-Dihydro: [96552-66-8] ***Dihydrodioscorine***

$C_{13}H_{21}NO_2$ 223.314

Alkaloid from the tubers of the famine food *Dioscorea dumetorum*. Oil. Sol. H_2O. $[\alpha]_D^{18}$ -42.2 (c, 3.4 in $CHCl_3$). Dihydrodioscorine cannot be obt. by hydrogenation of Dioscorine λ_{max} 208 (MeOH) (Berdy).

▶ Convulsive poison ; LD_{50} (mus, ipr) 0.65 mg/kg.

4′S,5′-Dihydro, hydrochloride:
Mp 209°.

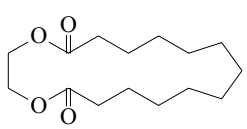
4′S,5′-Dihydro, picrate:
Mp 189°.

Pinder, A.R. *et al., J.C.S.*, 1952, 2236 (*isol, uv, ir*)
Broadbent, J.L. *et al., Br. J. Pharmacol.*, 1958, **13**, 213 (*pharmacol*)
Bevan, C.W.L. *et al., Chem. Ind. (London)*, 1958, 103 (*Dihydrodioscorine, isol*)
Davies, W.A.M. *et al., Chem. Ind. (London)*, 1961, 1410 (*struct*)
Correia Alves, A. *et al., CA*, 1963, **59**, 6452d (*Dihydrodioscorine, isol*)
Beecham, A.F. *et al., Tet. Lett.*, 1969, 3745 (*config*)
Leete, E. *et al., Phytochemistry*, 1977, **16**, 1704 (*biosynth, cmr*)
Corley, D.G. *et al., Tet. Lett.*, 1985, **26**, 1615 (*Dihydrodioscorine, isol, struct, abs config*)
Goh, S.-H. *et al., Malays. J. Sci.*, 1994, **15**, 23; *CA*, **124**, 25562b (*Dioscorine N-oxide*)

1,4-Dioxacycloheptadecane-5,17-dione, 9CI D-936

[105-95-3]

Ethylene brassylate. Astratone. Musk T



$C_{15}H_{26}O_4$ 270.368

Component of fragrances for soaps, detergents, food etc.. Oil with sweetish musky odour. Mp 0-7°. Bp 332° $Bp_{2.5}$ 160-170° (lit. gives a pressure range). n_D^{20}

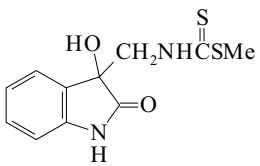
1.4702.

▶ YQ1927500

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 91 (*synth*)
U.S. Pat., 1982, 4 331 603; *CA*, **97**, 72395h (*synth*)
U.S.S.R. Pat., 1984, 1 077 893; *CA*, **104**, 68894r (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EJQ500

Dioxibrassinin D-937

[(2,3-Dihydro-3-hydroxy-2-oxo-1H-indol-3-yl)methyl]carbamodithioic acid methyl ester, 9CI. Dioxybrassinin



$C_{11}H_{12}N_2O_2S_2$ 268.36

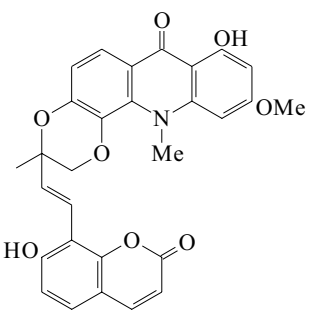
(-)-*form* [133761-64-5]
Alkaloid from cabbage inoculated with *Pseudomonas cichorii*. $[\alpha]_D$ -7.6 (c, 0.6 in MeOH).

(±)-*form* [137821-31-9]
Mp 164-166°.

Powell, R.G. *et al., Experientia*, 1991, **47**, 304 (*isol, pmr, cmr, ms, cryst struct*)
Monde, K. *et al., Phytochemistry*, 1991, **30**, 2915 (*isol, uv, ir, pmr, ms, struct, synth*)

Dioxinoacrimarine A D-938

[158182-14-0]

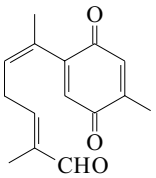


$C_{29}H_{23}NO_8$ 513.503
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisi*) and Dancy tangerine (*Citrus tangerina*)] (Rutaceae). Yellow cubes (Me_2CO). Mp 179-181°. $[\alpha]_D$ +18 (c, 0.1 in $CHCl_3$).

Takemura, Y. *et al., Heterocycles*, 1994, **38**, 1937 (*isol, uv, ir, pmr, cmr, ms, struct*)

1,4-Dioxo-2,5,7,10-bisabolatetraen-12-al D-939

Glandulone B

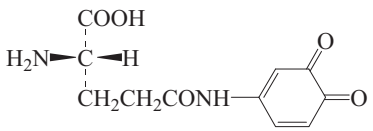


$C_{15}H_{16}O_3$ 244.29
Constit. of *Helianthus annuus* (sunflower). Brown oil. $[\alpha]_D^{25}$ -3.3 (c, 0.12 in MeOH). λ_{max} 235 ; 263 (MeOH) (Berdy).

Spring, O. *et al., Phytochemistry*, 1992, **31**, 1541 (*isol, pmr*)

N^5-(3,4-Dioxo-1,5-cyclohexadien-1-yl)glutamine D-940

γ-Glutaminyl-3,4-benzoquinone



$C_{11}H_{12}N_2O_5$ 252.226

(*S*)-*form* [30382-25-3]
L-form
Isol. from the mushroom *Agaricus bisporus* (button mushroom). Red solid. λ_{max} 440 (no solvent reported).

Weaver, R.F. *et al., J. Biol. Chem.*, 1971, **246**, 2013-2018 (*isol, synth*)
Boekelheide, K. *et al., J. Biol. Chem.*, 1980, **255**, 4766-4771 (*biosynth*)
Mize, P.D. *et al., J.O.C.*, 1980, **45**, 3540-3543 (*synth*)
Tavantzis, S.M. *et al., Phytopathology*, 1982, **72**, 619-621 (*activity*)

2,4-Dioxohexanoic acid, 9CI D-941

[4383-93-1]
Propionylpyruvic acid
$H_3CCH_2COCH_2COCOOH$
$C_6H_8O_4$ 144.127
Cryst. Mp 83°.

Me ester: [20577-62-2]
$C_7H_{10}O_4$ 158.154
Bp_4 90-95°.

Et ester: [13246-52-1] *FEMA 3278*
$C_8H_{12}O_4$ 172.18
Flavouring ingredient. Bp_{11} 108-111°.

Breusch, F.L. *et al., Enzymologia*, 1945, **11**, 356-360; *CA*, **40**, 5702 (*synth*)
Earl, E. *et al., J.A.C.S.*, 1945, **67**, 1508-1509 (*Me ester*)
Schinz, H. *et al., Helv. Chim. Acta*, 1947, **30**, 1349-1373 (*Et ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 229 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 969 (*Et ester*)
Brecker, L. *et al., New J. Chem.*, 1999, **23**, 437-446 (*synth, uv, pmr, cmr*)

2,5-Dioxo-3-hexenal D-942

5-Hydroxy-2-oxo-3,5-hexadienal. ***Tamarindienal***
$H_3CCOCH{=}CHCOCHO \Leftrightarrow H_2C{=}C(OH)CH{=}CHCOCHO$
$C_6H_6O_3$ 126.112

(*Z*)-*form* [149575-43-9]
Constit. of *Tamarindus indica* (tamarind). Brown bitter liq. Sol. H_2O, EtOH, C_6H_6, $CHCl_3$; insol. petrol, CCl_4, Et_2O. λ_{max} 295 (EtOH).

Imbabi, E.S. *et al., Fitoterapia*, 1992, **63**, 537-538 (*isol, struct*)

Diphenyl disulfide, 9CI D-943

[882-33-7]
Phenyl disulfide, 8CI. Dithiobisbenzene. FEMA 3225
Ph-S-S-Ph
$C_{12}H_{10}S_2$ 218.343
Flavouring ingredient. Needles (EtOH). Mp 62-63°. Bp 295° Bp 310° Bp_{15} 192°. Dec. on prolonged heating to Ph_2S.

▶ LD_{50} (mus, ipr) 100 mg/kg. SS6825000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1183C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 440C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1102D (*ir*)
Sadtler Standard C-13 NMR Spectra, 73 (*cmr*)
Sadtler Standard Infrared Spectra, 107 (*ir*)
Sadtler Standard NMR Spectra, 286 (*pmr*)
Sadtler Standard Ultraviolet Spectra, 2094 (*uv*)
Mukaiyama, T. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 2388-2391 (*synth*)
Kresze, G. *et al., Annalen*, 1974, 847-852 (*synth*)
Sacerdoti, M. *et al., Acta Cryst. B*, 1975, **B31**, 327-329 (*cryst struct*)
Spyroudis, S. *et al., Synthesis*, 1975, 445-447 (*synth*)
Kuwajima, I. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 2183-2184 (*use*)
Asaoka, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 3008-3010 (*use*)
Jones, I.W. *et al., Phosphorus Sulfur Relat. Elem.*, 1978, **5**, 57-60 (*ms*)
Hiroi, K. *et al., Chem. Pharm. Bull.*, 1979, **27**, 2338-2344 (*use*)
Boykin, D.W. *et al., J.O.C.*, 1979, **44**, 424-428 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 210; 1989, **14**, 155; 1982, **10**, 171; 1984, **11**, 220; 1981, **9**, 386; 1980, **8**, 416; 1981, **9**, 429 (*use*)
Kagabu, S. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 388-390 (*synth*)
Meshram, H.M. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 232-233 (*synth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2214-2218 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 198
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2190-2191
Noureldin, N.A. *et al., Synthesis*, 1998, 1587-1589 (*synth, ir, pmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PEW250

Diphenyl ether D-944

[101-84-8]
1,1'-Oxybisbenzene, 9CI. Phenyl ether, 8CI. Phenoxybenzene. Diphenyl oxide.

FEMA 3667

PhOPh

$C_{12}H_{10}O$ 170.21

Present in muscat grapes, green tea, vanilla, lemon balm, buckwheat, potato chips and grilled beef. Flavouring ingredient. Low-melting cryst. with a harsh geranium-type odour. Mp 37-39° (28°). Bp 259°.

► Fl. p. 96/112°, autoignition temp. 610/618°. Eye and mild skin irritant. LD_{50} (rat, orl) 3370 mg/kg. Prolonged or repeated exposure causes liver, spleen, kidney and thyroid injury in chronic studies. OES: long-term 1 ppm (vapour). KN8970000

[8004-13-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1056C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 211A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 987C (*ir*)
Adv. Chem. Ser., 1955, **15**, 521 (***props***)
Netherlands Pat., 1965, 6 411 079; *CA*, **63**, 9872a (*synth*)
Milyakh, S.V. *et al., CA*, 1973, **79**, 104842y (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 707 (*rev, tox*)
Epshtein, L.M. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1977, 1981 (*uv*)
Bradamante, S. *et al., J.O.C.*, 1980, **45**, 114 (*cmr*)
Bates, R.B. *et al., J.O.C.*, 1982, **47**, 4374 (*synth, pmr*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 199
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 888
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 471
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 3252
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 550
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PFA850
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 498 (*tox*)

Diphenylamine, 8CI D-945

[122-39-4]

N-*Phenylbenzenamine, 9CI*

PhNHPh

$C_{12}H_{11}N$ 169.226

Used for control of superficial scald in stored apples. Cryst. Sol. EtOH, Et_2O, C_6H_6; insol. H_2O. Mp 52-54°. Bp 302°. pK_a 0.78 (24°, HCl aq.). pK_a 22.73 (25°, DMSO aq.).

► Eye, skin and mucous membrane irritant. Exp. teratogenic effects. Hepatotoxic and nephrotoxic in chronic studies. JJ7800000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1190B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 453B; 1361A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1109B; 1109D (*ir*)
Brownlee, R.C. *et al., J.A.C.S.*, 1968, **90**, 1757
Mellier, A. *et al., Acta Cryst. B*, 1973, **276**, 177 (*cryst struct*)
Mornon, J.-P. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 779 (*cryst struct*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 723 (*rev, tox*)
Bradamante, S. *et al., J.O.C.*, 1980, **45**, 114 (*cmr*)
Schiemenz, G.P. *et al., Phosphorus Sulfur Relat. Elem.*, 1985, **21**, 259 (*uv*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DVX800; DWI000; PDX500

2,4-Diphenyl-1-butene, 8CI D-946

[16606-47-6]

1,1′-(1-Methylene-1,3-propanediyl)bisbenzene, 9CI. SD-2

$H_2C{=}CHPhCH_2CH_2Ph$

$C_{16}H_{16}$ 208.302

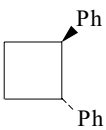
Styrene dimer. Present as an impurity in polystyrene food containers and other products - liberated on heating. Oil. $Bp_{2.5}$ 140° (lit. gives a pressure range).

Marion, L. *et al., Can. J. Res., Sect. B*, 1938, **16**, 213
Parkhurst, R.M. *et al., J.O.C.*, 1963, **28**, 120 (*synth, ir, pmr*)
Mayo, F.R. *et al., J.A.C.S.*, 1968, **90**, 1289 (*synth, ir*)
Kurze, J. *et al., Angew. Makromol. Chem.*, 1970, **12**, 25
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol, pmr, cmr*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; *CA*, **129**, 42008w; **130**, 251409n (*detn*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox*)

1,2-Diphenylcyclobutane, 8CI D-947

[3018-21-1]

1,1′-(1,2-Cyclobutanediyl)bisbenzene, 9CI



(1*RS*,2*RS*)-*form*

$C_{16}H_{16}$ 208.302

Styrene dimer. Present as an impurity in polystyrene food containers and other products - liberated on heating.

(1*RS*,2*RS*)-*form* [20071-09-4]
(±)-trans-*form. SD-4*
Oil.

(1*RS*,2*SR*)-*form* [7694-30-6]
cis-*form. SD-3*
Mp 38-39°.

Dodson, R.M. *et al., J.O.C.*, 1967, **32**, 28 (*synth, nmr*)
Gross, M.L. *et al., Tet. Lett.*, 1969, 3875 (*ms*)
Harpp, D.N. *et al., J.O.C.*, 1970, **35**, 3256 (*synth, pmr*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; 390-398; *CA*, **129**, 42008w; **130**, 251409n (*detn*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox*)

1,7-Diphenyl-4,6-heptadien-3-ol D-948

$PhCH_2CH_2CH(OH)CH{=}CHCH{=}CHPh$

$C_{19}H_{20}O$ 264.366

(*E*,*E*)-*form* [152323-34-7]
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Powder (hexane/Me_2CO). Mp 78-80°.

Claeson, P. *et al., Planta Med.*, 1993, **59**, 451-454

1,7-Diphenyl-4,6-heptadien-3-one, 9CI D-949

[38940-11-3]

$PhCH_2CH_2COCH{=}CHCH{=}CHPh$

$C_{19}H_{18}O$ 262.351

(*E*,*E*)-*form* [33457-62-4]
Alnustone
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Pale yellow needles (EtOH). Mp 63-63.5° (61-62.5°).

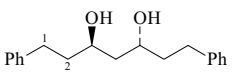
2,4-Dinitrophenylhydrazone: [38940-16-8] Red cryst. (EtOAc). Mp 188-189°.

4,5-Dihydro: [87030-31-7] *1,7-Diphenyl-6-hepten-3-one*
$C_{19}H_{20}O$ 264.366
Oil.

[58506-34-6]

Sakakibaba, M. *et al., Agric. Biol. Chem.*, 1972, **36**, 1825 (*synth*)
Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2058 (*isol*)
Vig, O.P. *et al., Indian J. Chem.*, 1975, **13**, 1129 (*synth*)
Jurgens, T.M. *et al., J. Nat. Prod.*, 1994, **57**, 230-235 (*1,7-Diphenyl-6-hepten-3-one*)

1,7-Diphenyl-3,5-heptanediol D-950



(3*R*,5*R*)-*form*

$C_{19}H_{24}O_2$ 284.397

(5ξ)-*form*
3-Ketone, Me ether: [100667-54-7] ***5-Methoxy-1,7-diphenyl-3-heptanone***
$C_{20}H_{24}O_2$ 296.408
Constit. of rhizomes of *Alpinia officinarum* (lesser galangal). Oil.

[52393-54-1, 55836-43-6, 87095-80-5, 93603-99-7, 99781-95-0, 100761-20-4]

Asakawa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 2223; 1975, **45**, 1794
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1544-1550 (*derivs*)
Hashimoto, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1846
Rychnovsky, S.D. *et al., J.O.C.*, 1991, **56**, 5161 (*synth, ir, pmr, cmr, ms*)
Ngo, K.S. *et al., Phytochemistry*, 1998, **47**, 1117-1123 (*isol, 5-ketone, 4′-hydroxy-5-ketone*)

1,7-Diphenyl-6-hepten-3-ol, 9CI D-951

α-(4-Phenyl-3-butenyl)benzenepropanol, 9CI

$PhCH_2CH_2CH(OH)CH_2CH_2CH{=}CHPh$

$C_{19}H_{22}O$ 266.382

(3ξ,6*E*)-*form* [87095-76-9]
Constit. of seeds of *Curcuma xanthorrhiza* (Java turmeric). Plates (Me_2CO/hexane). Mp 47-49° (44-46°). $[\alpha]_D^{23}$ +7 (c, 1.2 in $CHCl_3$). Described as racemic.

Ac: [155167-05-8]
$C_{21}H_{24}O_2$ 308.419
Oil.

Claeson, P. *et al., Planta Med.*, 1993, **59**, 451-454
Jurgens, T.M. *et al., J. Nat. Prod.*, 1994, **57**, 230-235
Ngo, K.S. *et al., Phytochemistry*, 1998, **47**, 1117-1123

1,7-Diphenyl-4-hepten-3-one D-952

[79559-59-4]
$PhCH_2CH_2CH{=}CHCOCH_2CH_2Ph$
$C_{19}H_{20}O$ 264.366
Isol. from rhizomes of *Alpinia officinarum* (lesser galangal). Oil.

Itokawa, H. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2383-2385 (*isol, spectra*)
Kato, N. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3323-3326 (*synth*)
Tori, M. *et al., Phytochemistry*, 1995, **40**, 1263-1264 (*isol*)

1,3-Diphenylpropane, 8CI D-953

[1081-75-0]
1,1′-(1,3-Propanediyl)bisbenzene, 9CI. Dibenzylmethane. SD1
$PhCH_2CH_2CH_2Ph$
$C_{15}H_{16}$ 196.291
Styrene dimer. Present as an impurity in polystyrene food containers and other products - liberated on heating. Mp -20.78° Mp 6°. $Bp_{1.7}$ 123-124°.

Tuot, M. *et al., Bull. Soc. Chim. Fr.*, 1947, 1087 (*synth*)
Sarijan, K.T. *et al., J.A.C.S.*, 1951, **73**, 4766 (*synth*)
Gilman, H. *et al., J.O.C.*, 1959, **24**, 821 (*synth*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; 390-398; *CA*, **129**, 42008w; **130**, 251409n (*anal*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox*)

1,3-Diphenyl-1-propanone, 9CI D-954

[1083-30-3]
ω-Benzylacetophenone. Phenethyl phenyl ketone. Dihydrochalcone. Hydrocinnamophenone. Hydrochalcone
$PhCOCH_2CH_2Ph$
$C_{15}H_{14}O$ 210.275
Isol. from *Phallus impudicus* (common stinkhorn). Leaflets (EtOH). Mp 72-73°. Bp 360°.

Oxime: [5371-55-1]
$C_{15}H_{15}NO$ 225.29
Needles (EtOH aq.). Mp 87°.

2,4-Dinitrophenylhydrazone: [5371-54-0]
Mp 143-145°.

Semicarbazone: [33745-39-0]
Cryst. (EtOH). Mp 148-148.5°.

Di-Et acetal:1,1-Diethoxy-1,3-diphenylpropane
$C_{19}H_{24}O_2$ 284.397
Liq. d_4^{22} 1.04. Bp_{18} 189°.

Org. Synth., Coll. Vol., 4, 1963, 101 (*synth*)
Freunel, B. *et al., Planta Med.*, 1968, 123; *CA*, **70**, 54869 (*isol*)
Shemyakin, M.M. *et al., Tetrahedron*, 1971, **27**, 2811 (*synth*)
Weber, F.G. *et al., Tetrahedron*, 1973, **29**, 2479 (*synth, pmr*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556 (*isol*)
Judaš, N. *et al., Acta Cryst. C*, 1995, **51**, 2656 (*cryst struct*)
Pande, P.P. *et al., Synth. Commun.*, 1998, **28**, 4193-4200 (*synth, ir, pmr*)
Wang, H. *et al., Synth. Commun.*, 1999, **29**, 129-134 (*synth, ir, pmr*)

1,3-Diphenyl-2-propanone, 9CI D-955

[102-04-5]
1,3-Diphenylacetone. Dibenzyl ketone. Benzyl ketone. FEMA 2397
$PhCH_2COCH_2Ph$
$C_{15}H_{14}O$ 210.275
Flavouring agent. Cryst. (EtOH aq., Et_2O or petrol) with a fruity odour. Mp 35-36°. Bp 331° $Bp_{0.1}$ 112-125°.

Oxime: [1788-31-4]
$C_{15}H_{15}NO$ 225.29
Mp 125°.

Phenylhydrazone:
Needles or leaflets. Mp 128-129°.

2,4-Dinitrophenylhydrazone: [1555-81-3]
Orange cryst. (EtOH). Mp 110°.

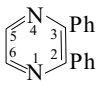
Semicarbazone:
Mp 123-124° Mp 146°.

4-Methylbenzenesulfonylhydrazone:
[19816-88-7] *Diphenylacetone tosylhydrazone*
$C_{22}H_{22}N_2O_2S$ 378.494
Mp 185-186° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1D; 983D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 790B; **3**, 545C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1222C (*ir*)
Hurd, C.D. *et al., J.A.C.S.*, 1933, **55**, 2589; 1936, **58**, 1240
Ashley, J.N. *et al., J.C.S.*, 1942, 103
Rabjohn, N. *et al., J.A.C.S.*, 1953, **75**, 2259
Shapiro, E.L. *et al., J.A.C.S.*, 1953, **75**, 4769
MacKenzie, S. *et al., J.O.C.*, 1963, **28**, 717 (*uv*)
Mislow, K. *et al., J.A.C.S.*, 1964, **86**, 1710 (*pmr*)
Tagaki, W. *et al., Bull. Chem. Soc. Jpn.*, 1965, **38**, 414
Keana, J.F.W. *et al., J.O.C.*, 1973, **38**, 3815 (*synth, tosylhydrazone*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 123 (*use*)
Casanova, J. *et al., Tet. Lett.*, 1977, 1773 (*cmr, config, tosylhydrazone*)
Lipton, M.F. *et al., J. Organomet. Chem.*, 1980, **186**, 155 (*synth, pmr, ms, use, tosylhydrazone*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 200
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 888-889

2,3-Diphenylpyrazine, 9CI D-956

[1588-89-2]



$C_{16}H_{12}N_2$ 232.284
Food flavorant. Monoclinic cryst. (EtOH aq.). Sol. EtOH, Et_2O, C_6H_6, spar. sol. petrol, insol. H_2O.

Monoxide:
$C_{16}H_{12}N_2O$ 248.284
Needles (EtOH or petrol). Mp 179.5-180° (171-172°).

Dioxide:
$C_{16}H_{12}N_2O_2$ 264.283
Platelets (EtOH). Mp 262° dec.

Mason, A.T. *et al., J.C.S.*, 1893, **63**, 1297
Landquist, J.K. *et al., J.C.S.*, 1956, 1885 (*oxides*)
Shibamoto, T. *et al., CA*, 1976, **84**, 149375t (*use*)
Kitano, Y. *et al., Acta Cryst. B*, 1983, **39**, 136 (*cryst struct*)
Sato, N. *et al., J.C.S. Perkin 1*, 1994, 885 (*monoxide*)

N,N′-Diphenylurea, 9CI D-957

[102-07-8]

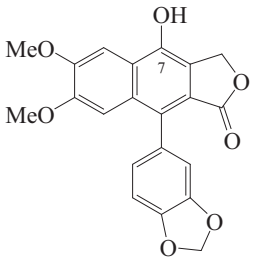
[26763-63-3]
Carbanilide
PhNHCONHPh
$C_{13}H_{12}N_2O$ 212.251
Isol. from coconut milk. Prisms. Mp 239-240°. Bp 260°.

▶ FD9800000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 387A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1418C; 1420C; 1421A (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 453 (*synth*)
Shantz, E.M. *et al., J.A.C.S.*, 1952, **74**, 6133; 1955, **77**, 6351 (*isol*)
Baker, J.W. *et al., J.C.S.*, 1957, 4652 (*synth*)
Novacek, A. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 1712 (*synth*)
Deshapande, S.V. *et al., Acta Cryst. B*, 1968, **24**, 1396 (*cryst struct*)
Knobler, Y. *et al., Isr. J. Chem.*, 1971, **9**, 165 (*synth*)
Norikov, E.G. *et al., Zh. Prikl. Spektrosk.*, 1971, **14**, 833 (*uv*)
Siti, M.P. *et al., J.O.C.*, 1979, **44**, 3017 (*cmr, N-15 nmr*)
Ayyangar, N.R. *et al., Chem. Ind. (London)*, 1988, 599 (*synth, bibl, derivs*)
Laufer, D.A. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 771 (*synth*)
Cooper, C.F. *et al., Synth. Commun.*, 1995, **25**, 2467 (*synth*)
Jimenez Blanco, J.L. *et al., Synthesis*, 1999, 1907-1914 (*synth*)

Diphyllin D-958

[22055-22-7]
9-(1,3-Benzodioxol-5-yl)-4-hydroxy-6,7-dimethoxynaphtho[2,3-c]-furan-1(3H)-one, 9CI. 7-Hydroxy-4,5-dimethoxy-3′,4′-methylenedioxy-2,7′-cycloligna-7,7′-dien-9′,9-olide

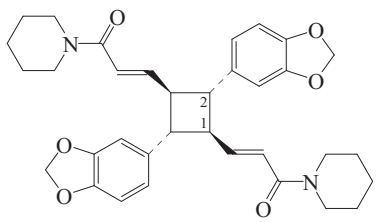


$C_{21}H_{16}O_7$ 380.353
Needles (EtOH). Mp 291°. λ_{max} 230 ; 267 ; 358 (EtOH) (Berdy).

O-*[β-D-Glucopyranosyl-(1→4)-2,3-di-O-methyl-β-D-xylopyranoside]:* [133882-75-4] ***Ramontoside***
$C_{34}H_{38}O_{16}$ 702.665
Isol. from *Flacourtia ramontchii* (governor's plum). Cryst. Mp 140-142°. λ_{max} 265 (ε 126000); 320 (ε 26400); 355 (ε 11220) (MeOH) (Berdy).

Satyanarayana, V. *et al., Phytochemistry*, 1991, **30**, 1026 (*Ramontoside*)

Dipiperamide A D-959

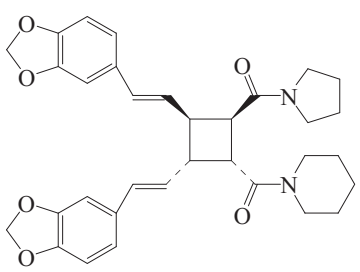


$C_{34}H_{38}N_2O_6$ 570.684
Alkaloid from white pepper, *Piper nigrum*. Racemic λ_{max} 203 (log ε 4.9); 238 (sh) (log ε 4.4); 287 (log ε 4) (EtOH).

1,2-Diepimer: ***Dipiperamide B***
$C_{34}H_{38}N_2O_6$ 570.684
Alkaloid from white pepper, *Piper nigrum*. Racemic λ_{max} 204 (log ε 4.8); 237 (sh) (log ε 4.4); 273 (sh) (log ε 4.3); 289 (sh) (log ε 4.2) (EtOH).

Tsukamoto, S. *et al., Tetrahedron*, 2002, **58**, 1667-1671 (*isol, pmr, cmr, ms*)

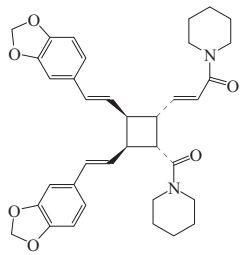
Dipiperamide C D-960



$C_{33}H_{36}N_2O_6$ 556.657
Alkaloid from white pepper, *Piper nigrum*. Racemic λ_{max} 207 (log ε 4.6); 268 (log ε 4.3); 278 (sh) (log ε 4.2); 308 (log ε 4.1); 325 (sh) (log ε 3.8) (EtOH).

Tsukamoto, S. *et al., Tetrahedron*, 2002, **58**, 1667-1671 (*isol, pmr, cmr, ms*)

Dipiperamide D D-961

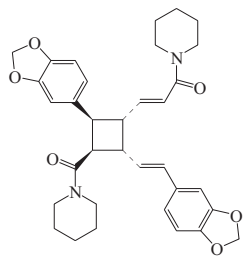


Relative Configuration

$C_{36}H_{40}N_2O_6$ 596.722
Alkaloid from white pepper, *Piper nigrum*. λ_{max} 209 (log ε 4.6); 266 (log ε 4.3) (EtOH).

Tsukamoto, S. *et al., Bioorg. Med. Chem.*, 2002, **10**, 2981-2985 (*isol, pmr, cmr*)

Dipiperamide E D-962



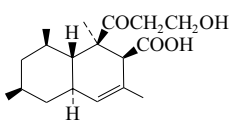
Relative Configuration

$C_{34}H_{38}N_2O_6$ 570.684
Alkaloid from white pepper, *Piper nigrum*. λ_{max} 206 (log ε 3.8); 242 (sh) (log ε 4.1); 266 (sh) (log ε 4); 289 (log ε 4.2) (EtOH).

Tsukamoto, S. *et al., Bioorg. Med. Chem.*, 2002, **10**, 2981-2985 (*isol, pmr, cmr*)

Diplodiatoxin D-963

[41060-01-9]
1,2,4a,5,6,7,8,8a-Octahydro-1-(3-hydroxy-1-oxopropyl)-1,3,6,8-tetramethyl-2-naphthalenecarboxylic acid, 9CI



Absolute configuration

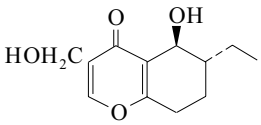
$C_{18}H_{28}O_4$ 308.417
Metab. of *Diplodia maydis* (parasite of sweet corn). Toxin causing diplodiosis disease of cattle and sheep. Cryst. ($CHCl_3$). Sol. MeOH, C_6H_6, $CHCl_3$; poorly sol. H_2O, hexane. Mp 187°. $[\alpha]_D^{28}$ +101 (c, 4 in $CHCl_3$). λ_{max} 293 (ε 50) (EtOH) (Berdy).

▶ Toxic ; LD_{50} (mus, ipr) .05 mg/kg.

Steyn, P.S. *et al., Tetrahedron*, 1972, **28**, 4775 (*isol, pmr, cmr, ms, ir, uv*)
Kruger, G.J. *et al., Cryst. Struct. Commun.*, 1977, **6**, 193 (*cryst struct*)
Ichihara, A. *et al., Tet. Lett.*, 1986, **27**, 1347 (*synth, abs config, bibl*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 916

Diplosporin D-964

[69199-05-9]
*6-Ethyl-5,6,7,8-tetrahydro-5-hydroxy-3-(hydroxymethyl)-4*H*-1-benzopyran-4-one, 9CI. Diplodiol*



$C_{12}H_{16}O_4$ 224.256
Mycotoxin prod. by *Diplodia macrospora* isol. from infected maize. Cryst. (C_6H_6/petrol). Mp 82.5-84°. λ_{max} 219 (ε 5370); 258 (ε 5250) (MeOH) (Derep). λ_{max} 217 (ε 7940); 251 (ε 7940) (EtOH) (Berdy).

▶ LD_{50} (mus, orl) 88.4 mg/kg. DJ3100650

5-Deoxy: ***5-Deoxydiplosporin***
$C_{12}H_{16}O_3$ 208.257
Mycotoxin prod. by *Diplodia macrospora* isol. from infected maize. Oil. Poorly sol. H_2O. $[\alpha]_D^{20}$ +55 (c, 1.1 in MeOH). λ_{max} 219 (ε 5370); 258 (ε 5250) (MeOH) (Derep).

5-Epimer: [109361-64-0] **epi-*Diplosporin***
$C_{12}H_{16}O_4$ 224.256
Metab. of *Diplodia macrospora* isol. from infected maize.

Chalmers, A.A. *et al., J.C.S. Perkin 1*, 1979, 1481 (*isol, struct*)
Probst, A. *et al., Helv. Chim. Acta*, 1982, **65**, 1543 (*isol, pmr*)
Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1983, 1357 (*biosynth, struct*)
Gorst-Allman, C.P. *et al., S. Afr. J. Chem.*, 1987, **40**, 116 (*biosynth, epimer*)

Dipotassium phosphate, 9CI, 8CI D-965

[7758-11-4]

[16068-46-5]
Dipotassium monohydrogenphosphate. Potassium phosphate (K_2HPO_4). Potassium phosphate dibasic, JAN, USAN

K_2HPO_4
HK_2O_4P 174.176
Used in foods as a sequestrant, a pH control agent, and a nutrient in fermentation processes. Deliquescent white powder. V. sol. H_2O (167 g per 100 cm^3 at 20°); v. sol. EtOH. Undergoes a phase change at 315-320° (311°), dec. → Potassium diphosphate ($K_4(P_2O_7)$), P-431 at 400-450°.

Trihydrate: [16788-57-1]
Colourless cryst. Mp 53° (48°) (incongr.). Loses H_2O at *ca*. 110° (1 H_2O), 132° (1H_2O), and 158° (1H_2O). A hexahydrate has also been reported.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1267D (*ir*)
Peterson, S.W. *et al., Acta Cryst.*, 1953, **6**, 273 (*nd*)
Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Steger, E. *et al., Z. Anorg. Allg. Chem.*, 1964, **331**, 169 (*ir, Raman*)
McDonald, J.L. *et al., J. Dent. Res.*, 1970, **49**, 1042 (*metab*)
Pelavin, M. *et al., J. Phys. Chem.*, 1970, **74**, 1116 (*pe*)

Marshall, W.L. *et al., J. Inorg. Nucl. Chem.*, 1981, **43**, 449
Radzhnabov, R. *et al., CA*, 1982, **96**, 45312 (*dta, ir, trihydrate*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **42**, 335 (*P-31 nmr*)
Baran, J. *et al., J. Mol. Struct.*, 1989, **195**, 159 (*ir, cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 858
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2311-2313

Di-1-propenyl disulfide D-966

[53925-82-9]
1,1′-Dithiobis-1-propene

$H_3CCH{=}CH{-}S{-}S{-}CH{=}CHCH_3$

$C_6H_{10}S_2$ 146.277
Bp_{10} 78-84°.

(*E*,*E*)-*form* [23838-23-5]
Constit. of the essential oil of *Allium* spp.. Liq.

(*E*,*Z*)-*form* [121609-82-3]
Pale yellow liq.

(*Z*,*Z*)-*form* [23838-22-4]
Constit. of *Allium* spp.. Yellow oil.

Wijers, H.E. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 519 (*synth*)
Block, E. *et al., J.O.C.*, 1992, **57**, 5815 (*synth, pmr, cmr*)
Block, E. *et al., J.A.C.S.*, 1996, **118**, 2799 (*synth, pmr, cmr, ms*)

Di-2-propenyl disulfide, 9CI D-967

[2179-57-9]
Diallyl disulfide. Allyl disulfide. 4,5-Dithia-1,7-octadiene. ***Garlicin***†. *FEMA 2028*

$H_2C{=}CHCH_2{-}S{-}S{-}CH_2CH{=}CH_2$

$C_6H_{10}S_2$ 146.277
Principal constituent of oil of garlic (*Allium sativum*). Present in onion (*Allium cepa*), ramsons (*Allium ursinum*), chive (*Allium schoenoprasum*) and Chinese chives (*Allium tuberosum*). Also present in raw cabbage and seeds of herb-Sophia (*Descurainia sophia*). Flavouring ingredient. Potential nutriceutical. d_4^{15} 1.01. Bp 138-139° Bp_{16} 78-80°. n_D^{20} 1.5410.

▶ BB1000000

S-*Oxide:* See Allicin, A-176

S,S-*Dioxide:* S-*2-Propenyl 2-propene-1-sulfonothioate*
$C_6H_{10}O_2S_2$ 178.276
Constit. of garlic (*Allium sativum*). Oil.

[72869-75-1]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 354A (*ir*)
Banerjee, M.N. *et al., Z. Anorg. Allg. Chem.*, 1913, **83**, 113 (*synth*)
Twiss, D.F. *et al., J.C.S.*, 1914, **105**, 36 (*synth*)
Milligan, B. *et al., J.C.S.*, 1963, 3608 (*glc*)
Schultz, O.E. *et al., Pharmazie*, 1965, **20**, 441 (*isol*)
Martin, D.J. *et al., Anal. Chem.*, 1966, **38**, 1604 (*pmr*)
Amonkar, S.V. *et al., Science (Washington, D.C.)*, 1971, **174**, 1343
Nishimura, H. *et al., J.O.C.*, 1975, **40**, 1567 (*synth, ir, ms*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 297
Bartkowska, B. *et al., Acta Cryst. C*, 1997, **53**, 1064-1066 (*cryst struct*)
Hu, Q. *et al., J. Agric. Food Chem.*, 2002, **50**, 1059-1062 (*S,S-dioxide, isol*)

Di-2-propenyl heptasulfide D-968

[139693-24-6]
Allyl heptasulfide. Diallyl heptasulfide. 4,5,6,7,8,9,10-Heptathia-1,12-tridecadiene

$H_2C{=}CHCH_2S{-}S{-}S{-}S{-}S{-}SCH_2CH{=}CH_2$

$C_6H_{10}S_7$ 306.607
Constit. of garlic *Allium sativum*. Antioxidant.

Horie, T. *et al., Planta Med.*, 1992, **58**, 468-469 (*isol*)

Di-2-propenyl hexasulfide D-969

[137443-18-6]
Allyl hexasulfide. Diallyl hexasulfide. 4,5,6,7,8,9-Hexathia-1,11-dodecadiene

$H_2C{=}CHCH_2{-}S{-}S{-}S{-}S{-}S{-}CH_2CH{=}CH_2$

$C_6H_{10}S_6$ 274.541
Constit. of garlic (*Allium sativum*). Antioxidant.

Horie, T. *et al., Planta Med.*, 1992, **58**, 468-469

Di-2-propenyl pentasulfide D-970

[118686-45-6]
Allyl pentasulfide. Diallyl pentasulfide. 4,5,6,7,8-Pentathia-1,10-undecadiene

$H_2C{=}CHCH_2{-}S{-}S{-}S{-}S{-}CH_2CH{=}CH_2$

$C_6H_{10}S_5$ 242.475
Constit. of garlic (*Allium sativum*). Antioxidant.

Horie, T. *et al., Planta Med.*, 1992, **58**, 468-469 (*isol*)
Hu, Q. *et al., J. Agric. Food Chem.*, 2002, **50**, 1059-1062 (*isol*)

Di-1-propenyl sulfide D-971

[33922-80-4]

[37981-36-5, 37981-37-6]
1,1′-Thiobis-1-propene, 9CI. 4-Thia-2,5-heptadiene

$(H_3CCH{=}CH)_2S$

$C_6H_{10}S$ 114.211
Volatile constit. of garlic, onion and other *Allium* spp.. d_4^{20} 0.9. Bp_{28} 60-61°. n_D^{20} 1.5112. Props. refer to a mixt. of geom. isomers.

Price, C.C. *et al., J.O.C.*, 1962, **27**, 4639-4641 (*synth, ir*)
Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1962, **81**, 33-38 (*synth*)
Kuo, M.C. *et al., J. Agric. Food Chem.*, 1992, **40**, 1906-1910 (*occur*)
Yu, T.H. *et al., J. Agric. Food Chem.*, 1993, **41**, 800-805 (*occur*)

Di-2-propenyl sulfide D-972

[592-88-1]
3,3′-Thiobis-1-propene, 9CI. Thiobis-2-propene. Diallyl sulfide. Allyl sulfide. 4-Thia-1,6-heptadiene. FEMA 2042

$H_2C{=}CHCH_2SCH_2CH{=}CH_2$

$C_6H_{10}S$ 114.211
Present in *Allium* spp., Japanese horseradish (*Wasabia japonica*) and black mustard (*Brassica nigra*) powder and cooked beef. Formed by hydrol. dec. of cabbage. Flavouring ingredient. Neutriceutical with anti-cancer props.. Oil with garlic odour. d_4^{27} 0.89. Bp 139° Bp_4 27-28°. n_D^{20} 1.4880. Log P 1.99 (calc).

▶ Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 2980 mg/kg. BC4900000

S-*Oxide:* [14180-63-3] *3,3′-Sulfinylbis[1-propene], 9CI. Diallyl sulfoxide*
$C_6H_{10}OS$ 130.21
Brownish-red liq. d_4^{20} 1.03. Bp_7 107-109° Bp_3 98-102°. n_D^{20} 1.5115.

S,S-*Dioxide:* [16841-48-8] *3,3′-Sulfonylbis[1-propene], 9CI. Diallyl sulfone*
$C_6H_{10}O_2S$ 146.21
Liq. d_4^{20} 1.12. Bp_5 114°. n_D^{20} 1.4891.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 269C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 432C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 353D (*ir*)
Cahours, A. *et al., Annalen*, 1857, **102**, 291
Levin, L.N. *et al., J. Prakt. Chem.*, 1930, **127**, 77 (*oxide, dioxide*)
Backer, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1948, **67**, 451 (*dioxide*)
Gabel', Y.O. *et al., Zh. Obshch. Khim.*, 1951, **2**, 1649; *CA*, **46**, 4471 (*synth*)
Edwards, D. *et al., J.C.S.*, 1954, 3272 (*oxide*)
Bateman, L. *et al., J.C.S.*, 1955, 1596 (*oxide*)
Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1963, **82**, 68 (*synth*)
Bernhard, R.A. *et al., Arch. Biochem. Biophys.*, 1964, **107**, 137 (*isol*)
Prochazka, M. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 3149 (*uv*)
Foa, M. *et al., Gazz. Chim. Ital.*, 1975, **105**, 1199 (*dioxide*)
Nishimura, H. *et al., J.O.C.*, 1975, **40**, 1567 (*synth, ir, ms*)
Schmidt, H. *et al., J. Prakt. Chem.*, 1977, **319**, 979 (*synth*)
Liv, K.-T. *et al., J.O.C.*, 1978, **43**, 2717 (*oxide*)
Bock, H. *et al., J.A.C.S.*, 1982, **104**, 312 (*use*)
Fujisaki, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 2429 (*synth*)
Trifomov, B.A. *et al., Sulfur Lett.*, 1985, **3**, 145 (*synth*)
Mishelanie, E.A. *et al., Anal. Chem.*, 1986, **58**, 918 (*hplc*)
Yu, H.T. *et al., J. Agric. Food Chem.*, 1989, **37**, 725 (*chromatog, ms*)
da Silva Correa, C.M.M. *et al., Tetrahedron*, 1990, **46**, 3061 (*synth, ir, pmr*)
Bartkouska, B. *et al., Acta Cryst. C*, 1997, **53**, 1064-1066 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGS250

Di-2-propenyl tetrasulfide, 9CI D-973

[2444-49-7]
Allyl tetrasulfide, 8CI. Diallyl tetrasulfide. 4,5,6,7-Tetrathia-1,9-decadiene

$H_2C{=}CHCH_2{-}S{-}S{-}S{-}S{-}CH_2CH{=}CH_2$

$C_6H_{10}S_4$ 210.409
Isol. from garlic oil (*Allium sativum*). Oil with penetrating odour. Bp_{16} 122°.

[72869-75-1]

Milligan, B. *et al., J.C.S.*, 1963, 3608 (*synth*)
Martin, D.J. *et al., Anal. Chem.*, 1966, **38**, 1604 (*pmr*)
Apparao, M. *et al., Phytochemistry*, 1978, **17**, 1660 (*isol*)

Block, E. *et al., J.A.C.S.*, 1988, **110**, 7813 (*ms, cmr*)

Di-2-propenyl trisulfide, 9CI D-974

[2050-87-5]

Allyl trisulfide, 8CI. Diallyl trisulfide. 4,5,6-Trithia-1,8-nonadiene. ***Allitridin****. FEMA 3265*

$H_2C{=}CHCH_2\text{-}S\text{-}S\text{-}S\text{-}CH_2CH{=}CH_2$

$C_6H_{10}S_3$ 178.343

Volatile component from onion (*Allium sativum*), garlic (*Allium sativum*) and other commercial garlics. Potential nutriceutical. d^{15} 1.09. Bp 140° $Bp_{0.07}$ 66-67°.

▶ LD_{50} (mus, orl) 100 mg/kg. BC6168000

[72869-75-1]

Milligan, B. *et al., J.C.S.*, 1961, 4850; 1963, 3608 (*synth*)
Morel, G. *et al., Synthesis*, 1980, 918 (*synth*)
Banerji, A. *et al., Tet. Lett.*, 1980, 3003 (*synth*)
Nishimura, H. *et al., J. Agric. Food Chem.*, 1988, **36**, 563 (*isol*)
Yu, T.H. *et al., J. Agric. Food Chem.*, 1989, **37**, 725 (*isol*)
Devlin, M.T. *et al., J. Mol. Struct.*, 1990, **238**, 119 (*Raman, conformn*)
Lawson, L.D. *et al., Planta Med.*, 1991, **57**, 363 (*isol, hplc*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 352

Dipropyl disulfide, 9CI D-975

[629-19-6]

Propyl disulfide, 8CI. 4,5-Dithiaoctane. FEMA 3228

$H_3CCH_2CH_2\text{–}S\text{–}S\text{–}CH_2CH_2CH_3$

$C_6H_{14}S_2$ 150.309

Constit. of garlic, onion and other *Allium* spp. Also present in raw cabbage, roast beef and roasted peanuts. Flavouring agent. Liq. d_4^{20} 0.96. Bp_{754} 194° Bp_{60} 105-107°.

S-*Oxide:* [1948-52-3] *S-Propyl 1-propanesulfinothioate, 9CI*
$C_6H_{14}OS_2$ 166.308
Isol. from onions, garlic and other alliums. Liq. λ_{max} 240 (no solvent reported).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 266B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 428B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 349D (*ir*)
Carson, J.F. *et al., J.O.C.*, 1961, **26**, 1467-1470 (*synth, oxide*)
Allum, K.G. *et al., Spectrochim. Acta A*, 1968, **24**, 927
Ho, T.-L. *et al., Synthesis*, 1974, 872 (*synth*)
Aida, T. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1441 (*synth*)
Christensen, L.W. *et al., Synthesis*, 1978, 50 (*synth, pmr*)
Olah, G.A. *et al., Synthesis*, 1979, 721 (*synth*)
Gladysz, J.A. *et al., Tetrahedron*, 1979, **35**, 2329 (*synth, pmr*)
Gupta, D. *et al., Can. J. Chem.*, 1981, **59**, 543 (*ms*)
Tada, M. *et al., Agric. Biol. Chem.*, 1988, **52**, 2383-2385 (*isol, oxide*)
Bayer, T. *et al., Phytochemistry*, 1989, **28**, 2373-2377 (*isol, oxide*)
Barton, D.H.R. *et al., Tetrahedron*, 1991, **47**, 6127 (*synth, ir, pmr, cmr*)

Dipropyl trisulfide, 9CI D-976

[6028-61-1]

4,5,6-Trithianonane. FEMA 3276

$H_3CCH_2CH_2\text{–}S\text{–}S\text{–}S\text{–}CH_2CH_2CH_3$

$C_6H_{14}S_3$ 182.375

Component of onion oil. Flavouring ingredient. Liq. with a powerful garlic-like odour. Bp_8 86-90°. n_D^{25} 1.5382.

Decker, Q.W. *et al., J.O.C.*, 1957, **22**, 145-146 (*synth, uv*)
Oaks, D.M. *et al., Anal. Chem.*, 1964, **36**, 1560-1565 (*synth, glc*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 200
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 889-890

Diptocarpilidine D-977

[75272-86-5]

[139450-85-4]

7-(Methylsulfinyl)heptanenitrile, 9CI. Dipthocarpilidine

$NC(CH_2)_6SOMe$

$C_8H_{15}NOS$ 173.279

Oil. Bp_4 193-194°. $[\alpha]_D$ -49 ($CHCl_3$). λ_{max} 206 (log ϵ 3.15) (no solvent reported).

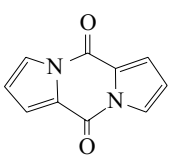
S-*Deoxo:* [75272-78-5] *7-(Methylthio)heptanenitrile*
$C_8H_{15}NS$ 157.279
Constit. of *Wasabia japonica* (Japanese horseradish).

Aripova, S.F. *et al., Khim. Prir. Soedin.*, 1984, **20**, 84-86; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 79-81 (*isol, pmr, ms*)
Tolstikov, A.G. *et al., Khim. Prir. Soedin.*, 1991, **27**, 261-263; *Chem. Nat. Compd. (Engl. Transl.)*, 1991, **27**, 225-226 (*synth, cmr*)
Kumagai, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 2131-2135 (*deriv, isol*)
Pedras, M.S.C. *et al., Phytochemistry*, 1998, **49**, 1959-1965 (*isol, ir, pmr, cmr, ms*)

5*H*,10*H*-Dipyrrolo[1,2-*a*:1′,2′-*d*]pyrazine-5,10-dione, 9CI D-978

[484-73-1]

Pyrocoll



$C_{10}H_6N_2O_2$ 186.17

Obt. from gelatine. Plates (AcOH), cryst. (C_6H_6). Mp 272-273° (sealed tube). Gives 1*H*-Pyrrole-2-carboxylic acid with KOH.

Ciamician, G. *et al., Monatsh. Chem.*, 1880, **1**, 279; *Ber.*, 1884, **17**, 105
Hale, W.J. *et al., J.A.C.S.*, 1916, **38**, 1065
Mold, J.D. *et al., Tob. Int.*, 1960, **4**, 130; *CA*, **54**, 25597
Johnson, A.W. *et al., J.C.S. Perkin 1*, 1972, 2681
Boatman, R.J. *et al., J.O.C.*, 1976, **41**, 3050

Disodium ethylenediaminetetraacetate D-979

[139-33-3]

[6381-92-6]

Ethylenediaminetetraacetic acid disodium salt. N,N′-1,2-Ethanediylbis(N-carboxymethyl)glycine disodium salt, 9CI. (Ethylenedinitrilo)tetraacetic acid, disodium salt, 8CI

$NaOOCCH_2N(CH_2\text{-}COOH)CH_2CH_2N(CH_2COOH)CH_2\text{-}COONa$

$C_{10}H_{14}N_2Na_2O_8$ 336.209

Sequestrant, preservative and discolouration inhibitor for foods.

▶ AH4375000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 567B (*ir*)
Novak, A. *et al., Bull. Soc. Chim. Fr.*, 1965, 1440 (*ir*)
Stolyarov, K.P. *et al., CA*, 1967, **66**, 60467 (*uv-vis*)
Nuttall, R.H. *et al., J.C.S. Dalton*, 1977, 1884 (*Raman*)
Djordjevic, C. *et al., J. Less-Common Met.*, 1983, **94**, 355 (*cmr, pmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1606D (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 916-920
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EIX500

Disodium phosphate, 9CI, 8CI D-980

[7558-79-4]

Disodium monohydrogenphosphate. Sodium phosphate (Na_2HPO_4). Sodium phosphate dibasic, USAN

Na_2HPO_4

HNa_2O_4P 141.959

^{32}P labelled compd. is used as an antineoplastic and antipolycythermic agent and as a neoplasm diagnostic aid (Phosphote). Used in foods as a sequestrant, emulsifier, buffering agent, absorbent, pH control agent, protein modifier, source of alkalinity, stabiliser and nutrient supplement. Hygroscopic powder. Sol. H_2O (6.4 g per 100 cm^3 at 18°; 12.1 g per 100 cm^3 at 25°). Dehydrates to Sodium diphosphate ($Na_4(P_2O_7)$), S-126 at 290-380°. ΔH_f° -1746 kJ mol^{-1}.

▶ Eye and skin irritant. WC4500000

Dihydrate: [10028-24-7] *Sorenson's sodium phosphate. Sorenson's salt*
$H_5Na_2O_6P$ 177.989
V. sol. H_2O (100 g per 100 cm^3 at 50°; 117 g per 100 cm^3 at 80°). Orthorhombic. Two independent distorted Na polyhedra (coordination numbers 5(or 6) and 6(or 7)) share corners, edges or faces. $PO_3(OH)$ tetrahedra are H-bonded and lie between the Na chains. ΔH_f -2344 kJ mol^{-1}. Loss $2H_2O$ at 95°.

Heptahydrate: [7782-85-6]
$H_{15}Na_2O_{11}P$ 268.065
Colourless monoclinic prisms (H_2O at 40°). V. sol. H_2O. ΔH_f -3821 kJ mol^{-1}. The prominent structural feature is a column of face- and edge-sharing $[Na_2(OH_2)_7]^{2\oplus}$ octahedra H-bonded to tetrahedral $PO_3(OH)$ groups. Mean Na –O 241.8, P–O 155.1 pm, OPO 102.7-114.2°. Loses $7H_2O$ at 60-140°.

▶ WC4600000

Dodecahydrate: [10039-32-4]
$H_{25}Na_2O_{16}P$ 358.141
Colourless efflorescent cryst. (H_2O) or white powder; β-form cryst. < 30°, α-form at 30-35°. Sol. H_2O (87 g per 100 cm^3 at 34°); insol. EtOH. ΔH_f -5299 kJ mol^{-1}. β-Form consists of close-packed layers of $[Na(OH_2)_6]^{\oplus}$ octahedra, 1/3 of which are replaced by PO_4 tetrahedra, with no interstitial H_2O molecules; the PO_4 tetrahedra each lie at the centre of a pseudo-hexagonal mesh of Na octahedra. Mean P–O 153.6 pm. Loses $12H_2O$ at ≤ 120°.

▶ TC5725000

H_2O_2 complex (1:1): [25215-15-0] *Disodium phosphate peroxohydrate. Phosphoric acid disodium salt compd. with H_2O_2 (1:1), 11CI*
Colourless, hygroscopic solid.

Telluric acid (H_6TeO_6) complex (1:1), monohydrate: [70929-99-6]
Colourless, hexagonal-bipyramidal cryst. Hexagonal. P–O 154, Te–$O_{av.}$ 192 pm and OPO 109.3-109.7°.

[7632-05-5, 118830-14-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1267A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1480B (*ir*)
Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301 (*hydrates, Raman*)
Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir, dodecahydrate*)
Zsoldos, E. *et al., Acta Cryst.*, 1962, **15**, 614 (*dihydrate, cryst struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 348; 1967, **4**, 1582 (*rev, bibl*)
Chapman, A.C. *et al., Spectrochim. Acta*, 1964, **20**, 937 (*dihydrate, ir*)
Steger, E. *et al., Z. Anorg. Allg. Chem.*, 1964, **331**, 169 (*ir, Raman*)
Rommel, M.A. *et al., Talanta*, 1967, **14**, 1205 (*chromatog*)
Nakatani, H. *et al., CA*, 1969, **71**, 119082 (*ir, xrd, tga*)
Baur, W.H. *et al., Acta Cryst. B*, 1970, **26**, 1584 (*cryst struct*)
Berezkhina, L.G. *et al., Zh. Fiz. Khim.*, 1974, **48**, 2935; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1974, **48**, 1723 (*props*)
Fluck, E. *et al., Pure Appl. Chem.*, 1975, **44**, 373 (*pe*)
Catti, M. *et al., Acta Cryst. B*, 1977, **33**, 3449; 1978, **34**, 369 (*cryst struct*)
Durif, A. *et al., Acta Cryst. B*, 1979, **35**, 1444 (*adduct, cryst struct*)
Gerothanassis, I.P. *et al., J. Magn. Reson.*, 1982, **46**, 423 (*O-17 nmr*)
Wiench, D.M. *et al., Z. Anorg. Allg. Chem.*, 1983, **501**, 95 (*cryst struct*)
Ramakrishnan, V. *et al., Infrared Phys.*, 1986, **26**, 293 (*adduct, ir, Raman*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Griffiths, L. *et al., J.C.S. Dalton*, 1986, 2247 (*P-31 nmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 454-456
Baldus, M. *et al., J.A.C.S.*, 1995, **117**, 5141 (*Na-23 nmr, powder struct*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1181
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2586-2589
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJH090

Disodium pyrophosphate, 8CI D-981

[7758-16-9]
Disodium diphosphate, 9CI. Disodium dihydrogen diphosphate. Sodium phosphate ($Na_2H_2P_2O_7$). Sodium acid pyrophosphate. E450a

$Na_2H_2P_2O_7$

$H_2Na_2O_7P_2$ 221.938
Employed in food processing as a preservative, emulsifying agent and leavening agent. Monoclinic lattice.

▶ UX6475000

Hexahydrate: [13510-98-0]
$H_{14}Na_2O_{13}P_2$ 330.03

Collin, R.L. *et al., Acta Cryst. B*, 1971, **27**, 291 (*cryst struct*)
De Sallier-Dupin, A. *et al., Bull. Soc. Chim. Fr.*, 1975, 1105; 1976, 417; 1977, 629 (*synth, props*)
Griffiths, L. *et al., J.C.S. Dalton*, 1986, 2247 (*P-31 nmr*)
Marshall, W.L. *et al., J.C.S. Faraday 2*, 1989, **85**, 1963 (*Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2519
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXF800

Disodium tetraborate, 11CI, 10CI, 9CI, 8CI D-982

[1330-43-4]
Borax ($B_4Na_2O_7$), 10CI. Boron sodium oxide ($B_4Na_2O_7$), 10CI. Boric acid, disodium salt, 8CI. Anhydrous borax. Borax, fused

$Na_2O.2B_2O_3$

$B_4Na_2O_7$ 201.219
Known in three forms, α- and metastable β- and γ-forms. Contains $[B_8O_{14}]^{4\ominus}$ anions consisting of linked B_3O_3 and B_5O_6 groups. Listed in the EAFUS Food Additive Database (Jan. 2001) but with no reported use. Colourless solid. Sol. H_2O (1.1 g per 100 cm^3 at 0°, 8.8 g per 100 cm^3 at 40°), MeOH, ethylene glycol. Mp 743° (α-form) Mp 720° (β-form) Mp 663° (γ-form). Bp 1575°. ΔH_f° -3259 kJ mol^{-1}; ΔG_f° -3082 kJ mol^{-1}; S° 189.5 J K^{-1} mol^{-1}.

▶ Irritant. ED4588000

Monohydrate: [12447-36-8]
$B_4H_2Na_2O_8$ 219.234
Colourless cryst. Sol. H_2O → $Na_2B_4O_7.5H_2O$. Correctly formulated as $Na_2B_4O_6(OH)_2$.

Dihydrate: ***Metakernite***
$B_4H_4Na_2O_9$ 237.25
Amorph. powder. Correctly formulated as $Na_2B_4O_5(OH)_4$.

Tetrahydrate: See Disodium tetraborate tetrahydrate in *The Combined Chemical Dictionary.*

Pentahydrate: See Disodium tetraborate pentahydrate in *The Combined Chemical Dictionary.*

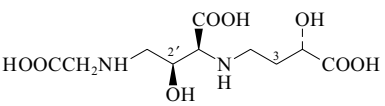
Decahydrate: See Borax, B-167

[14312-40-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1271A (*ir*)
Onak, T.P. *et al., J. Phys. Chem.*, 1959, **63**, 1533 (*B-11 nmr*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 266; 1966, **3**, 1271 (*rev, bibl*)
Thomas, G. *et al., Bull. Soc. Chim. Fr.*, 1970, 4202 (*synth, dihydrate*)
Krogh-Moe, J. *et al., Acta Cryst. B*, 1974, **30**, 578 (*cryst struct*)
Bertoluzza, A. *et al., CA*, 1974, **81**, 81583 (*ir, Raman*)
Epperlein, B.W. *et al., Z. Naturforsch., A*, 1975, **30**, 955 (*B-10 nmr, B-11 nmr, D nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **4**, 90 (*manuf, uses*)
Nies, N.P. *et al., Mellor Compr. Treat. Inorg. Theor. Chem.*, 1980, 383 (*rev, bibl*)
Fedulov, S.A. *et al., Inorg. Mater. (Engl. Transl.)*, 1983, **19**, 445 (*thermal anal*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 296 (*thermodyn*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3155B (*haz*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 295 (*use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4631-4632 (*use*)

Distichonic acid A D-983

[84495-20-5]
N-*(3-Carboxy-3-hydroxypropyl)-4-[(carboxymethyl)amino]-L-allothreonine*



$C_{10}H_{18}N_2O_8$ 294.261
Prod. by *Hordeum vulgare* (barley). Mp 220-221°.

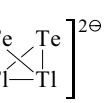
2′-Epimer: [117858-19-2] *2′-Epidistichonic acid*
$C_{10}H_{18}N_2O_8$ 294.261
Powder. Mp 215-217° dec. $[\alpha]_D$ -13.3 (c, 0.09 in $CHCl_3$).

2′-Deoxy, 3-hydroxy: [84495-21-6] ***Distichonic acid B***
$C_{10}H_{18}N_2O_8$ 294.261
From *Hordeum vulgare* (barley). Mp 124-128°. Undetermined 3-config..

Japan. Pat., 1982, 82 144 248; *CA*, **98**, 69034 (*isol, pmr, cmr, ms*)
Tashiro, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 893 (*2′-Epidistichonic acid*)

Dithallateditellurate(2-) D-984

[77321-81-4]



$Te_2Tl_2^{\ominus}$ 663.966
Butterfly shape (arises from square planar geometry with dihedral angle of 49.9°) (C_{2v} symm.).

▶ Toxic.

Bis[(2.2.2)crypt potassium(1+)] salt:
Dark brown cryst.

Burns, R.C. *et al., J.A.C.S.*, 1981, **103**, 2627 (*synth*)

Cave, R.J. *et al., J.A.C.S.*, 1989, **111**, 8105 (*theory*)

2,2′-Dithenyl sulfide D-985

[15832-01-6]
2,2′-[Thiobis(methylene)]bisthiophene, 9CI. 2,2′-(Thiodimethylene)dithiophene, 8CI. Bis(2-thienylmethyl) sulfide



$C_{10}H_{10}S_3$ 226.387
Flavouring agent. Liq. d_4^{25} 1.63. $Bp_{1.5}$ 129-131° $Bp_{0.05}$ 113°.

S,S-*Dioxide:* [15832-04-9] *2,2′-Dithenyl sulfone. 2,2′-[Sulfonylbis(methylene)]-bisthiophene, 9CI. 2,2′-(Sulfonyldimethylene)dithiophene, 8CI. Bis(2-thienylmethyl) sulfone*
$C_{10}H_{10}O_2S_3$ 258.386
Cryst. (EtOH). Mp 147-148°.

Kipnis, F. *et al., J.A.C.S.*, 1949, **71**, 3571 (*synth*)
Jones, E. *et al., J.C.S.(C)*, 1967, 1443 (*synth, ir, uv, dioxide*)

1,3-Dithiane, 9CI D-986

[505-23-7]
m-*Dithiane, 8CI. 1,3-Dithiacyclohexane*



$C_4H_8S_2$ 120.239
Constit. of garlic and other *Allium* spp.. Cryst. (MeOH). Mp 54°. Sublimes.

▶ JO5070000

[63865-78-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 271C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 435A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 356D (*ir*)
Adams, W.J. *et al., J. Mol. Struct.*, 1977, **37**, 261-274 (*cryst struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 217; 246; 1981, **9**, 48; 235; 1982, **10**, 231; 1984, **11**, 285; 1986, **12**, 573; 1992, **16**, 161 (*use*)
Org. Synth., Coll. Vol., 6, 1988, 556-558 (*synth*)
Labiad, B. *et al., Synth. Commun.*, 1989, **19**, 31-38 (*synth, ir, pmr*)
Patney, H.K. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 377-378 (***synth***)
Juaristi, E. *et al., J.A.C.S.*, 1995, **116**, 5796-5804 (*pmr*)

1,4-Dithiane, 9CI D-987

[505-29-3]
p-*Dithiane, 8CI. Tetrahydro-1,4-dithiin. Diethylene disulfide. 1,4-Dithiacyclohexane. FEMA 3831*

$C_4H_8S_2$ 120.239
Food additive listed in the EAFUS food additive database (Jan. 2001). Flavouring used in seasonings. Monoclinic prisms with a seafood-like odour and onion taste. Sol. EtOH, Et_2O, Me_2CO, AcOH; spar. sol. H_2O. Mp 112-113°. Bp 199-200°. Subl. at r.t., volatile in steam and EtOH.

▶ JO5069000

S-*Oxide:*
$C_4H_8OS_2$ 136.239
Mp 125.5-127°.

S^1,S^1-*Dioxide:*
$C_4H_8O_2S_2$ 152.238
Mp 200°.

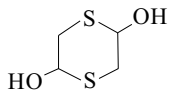
S^1,S^4-*Dioxide* (trans-)*:* [10348-98-8]
Cryst. (EtOH aq.). Mp 261-262° dec.

[10348-97-7, 57983-04-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 271D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 435C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 357A (*ir*)
Org. Synth., Coll. Vol., 4, 1963, 396 (*synth*)
Hunter, G. *et al., J.C.S. Perkin 2*, 1978, 712 (*pmr*)
Sandell, E.A. *et al., Photometric Determination of Traces of Metals*, Wiley, New York, 1978, (*use*)
Juaristi, E. *et al., Tetrahedron*, 1984, **40**, 1477 (*S-oxide, synth, cmr*)
Fujihara, H. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 4451 (*S-oxide, synth, ir, pmr*)
Fujihara, H. *et al., J.O.C.*, 1987, **52**, 4254 (*sulfoxide, synth, ir*)
Clennan, E.J. *et al., J.A.C.S.*, 1992, **114**, 3021 (*dioxide, synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 487

1,4-Dithiane-2,5-diol, 9CI D-988

[40018-26-6]
Mercaptoacetaldehyde dimer. 2,5-Dihydroxy-1,4-dithiane. FEMA 3826



$C_4H_8O_2S_2$ 152.238
Two forms known, probably *cis* and *trans*. Food flavour component with meaty/toasted/sulfurous odour.

α-form
Stout prisms. Mp 138-143°.

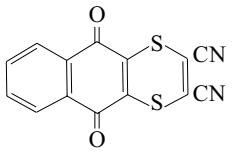
β-form
Clusters. Mp 138-143°.

[28631-86-9, 87602-21-9, 87602-27-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 272B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 447B (*nmr*)
Hesse, G. *et al., Chem. Ber.*, 1952, **85**, 924 (*synth*)
Hromatka, O. *et al., Monatsh. Chem.*, 1954, **85**, 1088; *CA*, **49**, 15878f (*synth*)
McIntosh, J.M. *et al., Can. J. Chem.*, 1983, **61**, 1872 (*synth*)
Inamori, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 243 (*pmr, biochem*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 429

Dithianon, BSI D-989

[3347-22-6]
5,10-Dihydro-5,10-dioxonaphtho[2,3-b]-1,4-dithiin-2,3-dicarbonitrile, 9CI. Delan



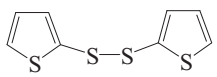
$C_{14}H_4N_2O_2S_2$ 296.33
Agricultural and horticultural fungicide. Brown cryst. Mp 225°.

▶ LD_{50} (rat, orl) 638 mg/kg. QL0700000

U.S. Pat., 1957, 2 976 296; *CA*, **56**, 3486c
Flemming, H. *et al., Z. Pflanzenkrankh. Pflanzenschutz.*, 1963, **70**, 4 (*props, activity, use*)
Suzuki, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 1433 (*glc*)
Pesticide Manual, 11th edn., 1997, No. 258
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DLK200

Di-2-thienyl disulfide D-990

[6911-51-9]
2,2′-Dithiobisthiophene, 9CI. 2-Thienyl disulfide. FEMA 3323

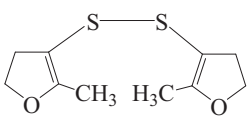


$C_8H_6S_4$ 230.399
Meat-like flavouring agent. Pale yellow needles (EtOH aq.). Mp 56-57°.

U.S. Pat., 1972, 3 706 577; *CA*, **78**, 83062f (*use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Bock, H. *et al., Phosphorus Sulfur Relat. Elem.*, 1983, **14**, 211-223 (*synth, pmr, epr*)
Christensen, T.B. *et al., Sulfur Lett.*, 1989, **9**, 289-290 (*pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 752 (*use*)
Vyas, R. *et al., Chem. Lett.*, 1998, 43-44 (*synth*)

3,3′-Dithiobis[4,5-dihydro-2-methylfuran], 9CI D-991

[85196-66-3]
Bis(2-methyl-4,5-dihydro-3-furyl) disulfide

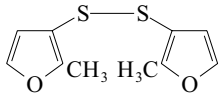


$C_{10}H_{14}O_2S_2$ 230.351
Component of meat aroma model systems. Cysteine-derived Maillard product. Characterised spectroscopically.

Hartman, G.J. *et al., J. Agric. Food Chem.*, 1984, **32**, 1015-1018 (*occur*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*synth, ms, pmr*)

3,3′-Dithiobis[2-methylfuran], 9CI, 8CI D-992

[28588-75-2]
Bis(2-methyl-3-furanyl) disulfide. FEMA 3259



$C_{10}H_{10}O_2S_2$ 226.32
Cysteine derived maillard product. Occurs in yeast autolysate, cooked beef and black and green tea. Flavouring agent for meat prods.. Yellow liq. with sulfurous roasted-meat odour. $Bp_{0.5}$ 90-92° $Bp_{0.15}$ 90°. Odour threshold 0.0006 - 0.0024 ng/l in air.

Blank, I. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 239-245 (*detn, coffee*)
Huber, U.A. *et al., Helv. Chim. Acta*, 1993, **76**, 2528-2536 (*synth, uv, ir, pmr, bibl*)
Mottram, D.S. *et al., Dev. Food Sci.*, 1998, **40**, 483-492 (*formn*)
Demir, A.S. *et al., Tetrahedron*, 1999, **55**, 12399-12404 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1125 (*use, occur*)

3,3′-Dithiobispropanoic acid, 9CI D-993

[1119-62-6]
3,3′-Dithiodipropionic acid. Diethyl disulfide β,β′-dicarboxylic acid
$HOOCCH_2CH_2SSCH_2CH_2COOH$
$C_6H_{10}O_4S_2$ 210.275
Cryst. (H_2O) with strong unpleasant odour. Mp 157-159°. pK_{a1} 3.88; pK_{a2} 4.47 (20°, 0.15*M* $NaClO_4$).

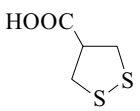
Di-Me ester: [15441-06-2]
$C_8H_{14}O_4S_2$ 238.328
Cryst. (H_2O). Mp 87.5-88°.

Didodecyl ester: [5926-55-6] *Dilauryl 3,3′-thiodipropionate*
$C_{30}H_{58}O_4S_2$ 546.918
Food and polymer antioxidant.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 820B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 529D (*ir*)
Japan. Pat., 1965, 12 171; *CA*, **64**, 5262 (*didodecyl ester*)
Gibson, H.W. *et al., J.O.C.*, 1970, **35**, 2994 (*synth*)
Stout, E.I. *et al., J.O.C.*, 1974, **39**, 562 (*synth*)

1,2-Dithiolane-4-carboxylic acid, 9CI D-994

[2224-02-4]
Asparagusic acid



$C_4H_6O_2S_2$ 150.222
Isol. from asparagus (*Asparagus officinalis*). Yellow prisms (C_6H_6/cyclohexane). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 75.7-76.5°.

▶ JP0705000

*1-Oxide(*cis-*):* [42258-87-7]

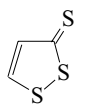
[3083-96-3]
$C_4H_6O_3S_2$ 166.222
Isol. from asparagus (*Asparagus officinalis*). Mp 118-120°.

*1-Oxide(*trans-*):* [42258-86-6]
$C_4H_6O_3S_2$ 166.222
Mp 127-128.5°.

Field, L. *et al., J.O.C.*, 1972, **37**, 2710 (*synth, pmr*)
Yanagawa, H. *et al., Tet. Lett.*, 1972, 2549 (*isol*)
Yanagawa, H. *et al., Synthesis*, 1973, 607; 1073 (*synth*)
Parry, R.J. *et al., J.A.C.S.*, 1985, **107**, 2512 (*biosynth*)
Teuber, L. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 629 (*synth, ir, uv, pmr, cmr*)

3*H*-1,2-Dithiole-3-thione, 9CI, 8CI D-995

[534-25-8]
1,2-Dithia-4-cyclopentene-3-thione



$C_3H_2S_3$ 134.247
Isol. from *Brassica oleracea* var. *capitata* and other crucifers. Potential nutriceutical. Cryst. (C_6H_6 or MeOH). Sol. EtOH, $CHCl_3$; insol. H_2O. Mp 81-82°.

Methiodide:
Mp 175°.

Jirousek, L. *et al., Naturwissenschaften*, 1958, **45**, 386
Busev, A.I. *et al., Zh. Anal. Khim.*, 1970, **25**, 953 (*detn, Pd*)
Meinetsberger, E. *et al., Synthesis*, 1977, 802 (*synth, pmr, ir*)
Pedersen, C.T. *et al., Adv. Heterocycl. Chem.*, 1982, **31**, 63 (*rev*)
Wei, C.H. *et al., Acta Cryst. C*, 1985, **41**, 1768 (*cryst struct*)
Poleschner, H. *et al., Phosphorus Sulfur Relat. Elem.*, 1985, **25**, 193; 1987, **29**, 187 (*synth, cmr*)
Jeffery, E.H. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 169-191

Divinyl sulfide D-996

[627-51-0]
1,1′-Thiobisethene, 9CI. Vinyl sulfide, 8CI. Divinyl thioether. Diethenyl sulfide. 3-Thia-1,4-pentadiene
$H_2C{=}CHSCH{=}CH_2$
C_4H_6S 86.157
Present in oil of *Allium* spp.. Liq. with odour of garlic. Sl. sol. H_2O; misc. EtOH, Et_2O. Mp 20°. Bp 85-86°. Undergoes radical cyclopolym. and cationic polym..

▶ KM7350000

S-*Oxide:* [1115-15-7] *Divinyl sulfoxide. 1,1′-Sulfinylbisethene, 9CI. Vinyl sulfoxide, 8CI*
C_4H_6OS 102.157
Liq. Bp_{18} 86-87°.

▶ YZ9800000

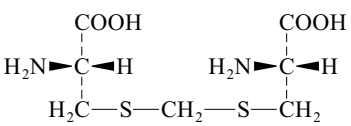
S,S-*Dioxide:* [77-77-0] *Divinyl sulfone. 1,1′-Sulfonylbisethene, 9CI. Vinyl sulfone*
$C_4H_6O_2S$ 118.156
d^{25} 1.18. Mp -26°. Bp 234.5° Bp_8 90-92°. n_D^{20} 1.4765.

▶ Vesicant, mild lachrymator. KM7175000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 882A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1420C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 832A (*ir*)
Alexander, J.R. *et al., J.C.S.*, 1931, **134**, 1913 (*synth*)
Ford-Moore, A.H. *et al., J.C.S.*, 1949, 2126 (*oxide, synth*)
Overberger, C.G. *et al., J.O.C.*, 1954, **19**, 1486 (*dioxide, synth*)
Stackman, R.W. *et al., J. Macromol. Sci., Part A: Chem.*, 1971, **5**, 2101 (*copolym, dioxide*)
Guaita, M. *et al., Makromol. Chem.*, 1971, **143**, 1 (*cyclopolym*)
Nunn, E.E. *et al., Tet. Lett.*, 1976, 4199 (*dioxide, use*)
Annenkova, V.Z. *et al., Vysokomol. Soedin., Ser. B*, 1976, **18**, 144; *CA*, **85**, 6439b (*cationic polym*)
Trofimov, B.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1977, 340 (*ir*)
Hargittai, I. *et al., J.C.S. Dalton*, 1978, 861 (*struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 23 (*use*)
Bzhezovskii, V.M. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1981, 2507 (*cmr, pmr*)
Rooney, R.P. *et al., Org. Magn. Reson.*, 1981, **16**, 266 (*synth, cmr, oxide*)
Trofimov, B.A. *et al., Sulfur Rep.*, 1984, **3**, 323 (*rev*)
Wils, E.R.J. *et al., Fresenius' Z. Anal. Chem.*, 1985, 321 (*ms*)
Sinegovskaya, L.M. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 115 (*uv*)
Trofimov, B.A. *et al., Zh. Org. Khim.*, 1985, **21**, 2324 (*synth*)
Krivdin, L.B. *et al., Zh. Org. Khim.*, 1987, **23**, 2070 (*cmr*)
Gusarova, N.K. *et al., Sulfur Rep.*, 1989, **9**, 95 (*rev, oxide*)
Amosova, S.V. *et al., Zh. Org. Khim.*, 1989, **25**, 302; 743 (*synth, use*)
Afonin, A.V. *et al., Izv. Akad. Nauk Kaz. SSR, Ser. Khim.*, 1990, 1978 (*conformn, cmr, pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2314-2315 (*S,S-dioxide, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXR200

Djenkolic acid D-997

S,S′-*Methylenebiscysteine, 9CI*



$C_7H_{14}N_2O_4S_2$ 254.331

(*R*,*R*)-*form* [498-59-9]
L-*form*
Needles (H_2O or HCl). Mp 300-350° dec. $[\alpha]_D^{20.5}$ -65 (c, 1 in HCl). Forms THF solvate, Mp 72-73.5°.

Hydrochloride: [4508-48-9]
Mp 250-300° dec.

S-*Oxide:* [21631-29-8] *3-[[[(2-Amino-2-carboxyethyl)thio]methyl]sulfinyl]alanine, 8CI.* ***Djenkolic acid sulfoxide***
$C_7H_{14}N_2O_5S_2$ 270.33

S,S′-*Dioxide:* [20584-40-1] *3,3′-(Methylenedisulfinyl)dialanine, 8CI.* ***Djenkolic acid disulfoxide***
$C_7H_{14}N_2O_6S_2$ 286.329

Di-Et ester:
$C_{11}H_{22}N_2O_4S_2$ 310.438
Cryst. (EtOH) (as dihydrochloride). Mp 171-173° (dihydrochloride). $[\alpha]_D^{25}$ -40 (c, 1 in DMF). Forms THF solvate, Mp 72-73.5°.

N-*Ac:*
$C_9H_{16}N_2O_5S_2$ 296.368
Isol. from *Acacia farnesiana* (sweet acacia). Mp 170° dec. $[\alpha]_D^{23}$ -22 (c, 1 in H_2O).

N-*Ac,* S-*oxide:***N-*Acetyldjenkolic acid sulfoxide***
$C_9H_{16}N_2O_6S_2$ 312.367

Dibenzoyl:
$C_{21}H_{22}N_2O_6S_2$ 462.547
Mp 85°.

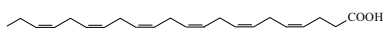
N-*Glutamyl:* [21631-28-7] **N-*γ*-*Glutamyldjenkolic acid***
$C_{12}H_{21}N_3O_7S_2$ 383.446

du Vigneaud, V. *et al., J. Biol. Chem.*, 1947, **168**, 373 (*synth*)
Gmelin, R. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1959, **316**, 164 (*isol*)
Gmelin, R. *et al., Phytochemistry*, 1961, **1**, 233 (*deriv*)
Warren, R.J. *et al., J. Assoc. Off. Anal. Chem.*, 1966, **49**, 1083 (*ir*)
Bartle, K.D. *et al., Biochim. Biophys. Acta*, 1968, **160**, 106 (*nmr*)
Seneviratne, A.S. *et al., Phytochemistry*, 1968, **17**, 1039 (*sulfoxides*)
Bigoli, F. *et al., Acta Cryst. B*, 1982, **38**, 498 (*cryst struct*)

4,7,10,13,16,19-Docosahexaenoic acid D-998

[2091-24-9]

[25167-62-8]



$C_{22}H_{32}O_2$ 328.494
►JR1230200
(all-Z)-form [6217-54-5]

[32839-18-2]
Clupanodonic acid. ***Doconexent, INN.***
Cervonic acid
Extensively marketed as a dietary supplement in Japan. Log P 7.44 (uncertain value) (calc). Component of Omega-3 Marine Triglycerides, O-156.

Me ester: [2566-90-7]

[301-01-9]
$C_{23}H_{34}O_2$ 342.52
Oil.

Et ester: [81926-94-5]

[84494-72-4]
$C_{24}H_{36}O_2$ 356.547
Oil.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 786B (*nmr*)
Hands, A.R. *et al., Biochem. J.*, 1963, **87**, 263
Beach, D.H. *et al., Biochim. Biophys. Acta*, 1974, **369**, 16 (*biosynth*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Sanders, T.A.B. *et al., Am. J. Clin. Nutr.*, 1978, **31**, 805
Moreno, V.J. *et al., Lipids*, 1979, **14**, 15 (*biosynth*)
Selivonchick, D.P. *et al., Lipids*, 1979, **14**, 66 (*isol*)
Dyerberg, J. *et al., Nutr. Rev.*, 1986, **44**, 125 (*rev*)
Bazan, N.G. *et al., Prog. Clin. Biol. Res.*, 1989, **312**, 95 (*rev*)
Kim, H.Y. *et al., Prostaglandins*, 1990, **40**, 539 (*metab*)
Anderson, R.E. *et al., Adv. Exp. Med. Biol.*, 1992, **318**, 285 (*rev*)
Aursand, M. *et al., Chem. Phys. Lipids*, 1992, **62**, 239 (*cmr*)
Taber, D.F. *et al., J.O.C.*, 1995, **60**, 139-142 (*Et ester, synth, pmr, cmr, ir, ms*)
Sandri, J. *et al., J.O.C.*, 1995, **60**, 6627 (*synth, ir, pmr, cmr*)

4,6-Docosanedione D-999

$H_3C(CH_2)_{15}COCH_2COCH_2CH_2CH_3$
$C_{22}H_{42}O_2$ 338.573
Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-docosanone
$C_{22}H_{44}O_2$ 340.588
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

5,7-Docosanedione D-1000

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_3CH_3$
$C_{22}H_{42}O_2$ 338.573
Constit. of the pollen of *Helianthus annuus* (sunflower).

5-Alcohol:5-Hydroxy-7-docosanone
$C_{22}H_{44}O_2$ 340.588
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

6,8-Docosanedione D-1001

$H_3C(CH_2)_{13}COCH_2CO(CH_2)_4CH_3$
$C_{22}H_{42}O_2$ 338.573
Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-8-docosanone
$C_{22}H_{44}O_2$ 340.588
Constit. of the pollen of *Helianthus annuus* (sunflower).

8-Alcohol:8-Hydroxy-6-docosanone
$C_{22}H_{44}O_2$ 340.588
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

7,9-Docosanedione D-1002

$H_3C(CH_2)_{12}COCH_2CO(CH_2)_5CH_3$
$C_{22}H_{42}O_2$ 338.573
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

4,8,12,15,19-Docosapentaenoic acid D-1003

[2548-85-8]

[25448-00-4, 32839-34-2]

$H_3CCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2COOH$
$C_{22}H_{34}O_2$ 330.509

The name Clupanodonic acid was prev. applied to a mixt. with, 4,7,10,13,16,19-Docosahexaenoic acid, D-998. It is now applied to the hexaenoic acid alone. Constit. of many fish oils e.g. sardine, mackerel and herring.

Me ester:
d_{15} 0.94. $Bp_{0.07}$ 169-170°. n_D^{15} 1.4933.

Tsujimoto, M. *et al., Chem. Zentralbl.*, 1923, **1**, 38
Toyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1935, **10**, 433; 441 (*isol, struct*)
Baudent, P. *et al., C. R. Trav. Fac. Sci. Univ. Aix-Marseille*, 1941, **1**, 79; 1942, 86; 1943, 127 (*isol, struct*)
Varanasi, U. *et al., Biochim. Biophys. Acta*, 1975, **409**, 304 (*isol*)

7,10,13-Docosatrienoic acid D-1004

$H_3C(CH_2)_7CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_5COOH$
$C_{22}H_{38}O_2$ 334.541

(all-Z)-form [28874-30-8]
Metab. of Oleic acid prod. particularly under conditions of essential fatty acid deficiency.

Kunau, W.H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1971, **352**, 1297

13,16,19-Docosatrienoic acid D-1005

[59708-86-0]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_{11}COOH$
$C_{22}H_{38}O_2$ 334.541

(all-Z)-form [28845-86-5]
Isol. from rape seed oil. Found in lipids of egg yolk.

[108698-01-7]

Haeffner, E. *et al., Lipids*, 1970, **5**, 430 (*isol, struct*)
Moreno, V.J. *et al., Lipids*, 1979, **14**, 15; 313 (*biosynth*)
Diaz, G.B. *et al., Lipids*, 1988, **23**, 1125; 1990, **25**, 724 (*occur*)
Berger, A. *et al., Lipids*, 1990, **25**, 473 (*biosynth*)

2,4,10-Docosatrienoic isobutylamide D-1006

$H_3C(CH_2)_{10}CH{=}CH(CH_2)_4CH{=}CHCH{=}CHCONHCH_2CH(CH_3)_2$
$C_{26}H_{47}NO$ 389.663

(E,E,Z)-form [62726-18-5]
Filfiline
Constit. of the fruits of *Piper officinarum* (Javanese long pepper). Cryst. (petrol). Mp 66-66.5°.

Gupta, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 912 (*isol*)
Gupta, O.P. *et al., Indian J. Pharm. Sci.*, 1978, **40**, 113 (*use*)

11-Docosenoic acid D-1007

[506-36-5]

[25378-26-1]

$H_3C(CH_2)_9CH{=}CH(CH_2)_9COOH$
$C_{22}H_{42}O_2$ 338.573

(E)-form [62600-37-7]
Catelaidic acid

Constit. of partially hydrogenated fish oil.

(Z)-form [1002-96-6]

[28929-01-3]

Cetoleic acid

Esters occur commonly in oil from marine mammals and fish and rapeseed. Mp 33-33.7°.

Toyama, Y. *et al., CA*, 1928, **22**, 575 (*isol*)
Ackman, R.G. *et al., Fette, Seifen, Anstrichm.*, 1977, **79**, 15
Gudbjarnason, S. *et al., Biochim. Biophys. Acta*, 1977, **487**, 10
Kirk, R.S. *et al., J. Sci. Food Agric.*, 1978, **29**, 880 (*glc*)
Loew, F.M. *et al., Nutr. Metab.*, 1978, **22**, 207
Thomas, D.C. *et al., Arch. Microbiol.*, 1978, **117**, 239

2,4-Dodecadienal, 9CI D-1008

[13162-47-5]

[96348-49-1]

$H_3C(CH_2)_6CH{=}CHCH{=}CHCHO$

$C_{12}H_{20}O$ 180.289

$Bp_{0.01}$ 72-83°. Bp data is for a 17:83 mixt. of *E*,*Z*- and *E*,*E*-isomers.

(2E,4E)-form [21662-16-8]

FEMA 3670

Flavouring ingredient esp. for fats and oils. Reported in angelica root, oxidised soybean oil, oxidised milk, potato chips and cured ham. Oily liq. with oily fried meat aroma.

(2E,4Z)-form [21662-15-7]

Present in roasted chicken, roasted guinea hen and citrus fruit peels. Characterised spectroscopically.

U.S. Pat., 1972, 3 664 851; *CA*, **73**, 75860w (*E-E-form, use*)
Naef, F. *et al., Helv. Chim. Acta*, 1974, **57**, 1309-1317 (*synth*)
Noleau, I. *et al., Lebensm.-Wiss. Technol.*, 1987, **20**, 37-41 (*occur*)
Kann, N. *et al., J.O.C.*, 1990, **55**, 5312-5323 (*synth, pmr, cmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 491-492 (*E,E-form, use, occur*)
Naef, R. *et al., J. Essent. Oil Res.*, 2001, **13**, 154-157 (*occur*)

2,6-Dodecadienal, 9CI D-1009

$H_3C(CH_2)_4CH{=}CHCH_2CH_2CH{=}CHCHO$

$C_{12}H_{20}O$ 180.289

Component of cooked chicken flavour.

[21662-13-5, 21662-14-6]

Meijboom, P.W. *et al., Fette, Seifen, Anstrichm.*, 1968, **70**, 477
Harkes, P.D. *et al., J. Am. Oil Chem. Soc.*, 1974, **51**, 356 (*occur*)

2,4-Dodecadienoic acid D-1010

$H_3C(CH_2)_6CH{=}CHCH{=}CHCOOH$

$C_{12}H_{20}O_2$ 196.289

(2E,4E)-form [24738-48-5]

Cryst. (petrol). Mp 49-51°.

Me ester: [24738-46-3]
$C_{13}H_{22}O_2$ 210.316
$Bp_{0.3}$ 106-108°.

2-Methylpropylamide: [24738-51-0] ***2,4-Dodecadienoic acid isobutylamide***
$C_{16}H_{29}NO$ 251.411
Mp 89-90°.

Pyrrolidide: [117137-69-6] *2,4-Dodecadienoic acid pyrrolidide. 1-(2,4-Dodecadienoyl)pyrrolidine*
$C_{16}H_{27}NO$ 249.395
Constit. of pepper (*Piper nigrum*) (Piperaceae). Not obt. completely pure.

Holman, R.T. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 356 (*isol*)
Burden, R.S. *et al., J.C.S.(C)*, 1969, 2477 (*isol, synth*)
Greger, H. *et al., Phytochemistry*, 1981, **20**, 2579 (*isol, ms, struct*)
Kiuichi, F. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2452 (*pyrrolidide*)
Abarbri, M. *et al., Synthesis*, 1996, 82 (*synth, ir, pmr, cmr, ms*)

2,6-Dodecadienoic acid D-1011

$H_3C(CH_2)_4CH{=}CHCH_2CH_2CH{=}CHCOOH$

$C_{12}H_{20}O_2$ 196.289

(2E,6Z)-form

Me ester: [28369-22-4]
$C_{13}H_{22}O_2$ 210.316
Constit. of Bartlett pears.

Et ester: [28380-08-7]
$C_{14}H_{24}O_2$ 224.342
Constit. of Bartlett pears.

Creveling, R.K. *et al., J. Agric. Food Chem.*, 1970, **18**, 19
Naf, F. *et al., Helv. Chim. Acta*, 1972, **55**, 82 (*synth*)

2,8-Dodecadienoic acid D-1012

$H_3C(CH_2)_2CH{=}CH(CH_2)_4CH{=}CHCOOH$

$C_{12}H_{20}O_2$ 196.289

(2E,8E)-form

Large plates. Mp 34-35°. $Bp_{0.8}$ 140°.

S-*Benzylthiouronium salt:*
Plates (EtOAc). Mp 159°.

2-Methylpropylamide:
Needles (petrol). Mp 53°.

(2Z,8E)-form

Bp_1 127-129°.

S-*Benzylthiouronium salt:*
Plates (EtOAc). Mp 148°.

2-Methylpropylamide:
$Bp_{0.6}$ 154° $Bp_{0.03}$ 142°.

(2ξ,8ξ)-form

*2-Methylpropylamide:*N-*Isobutyl-2,8-dodecadienamide.* ***Herculin***
$C_{16}H_{29}NO$ 251.411
Isol. from *Zanthoxylum clava-herculis* (Hercules' club). Pungent needles (hexane). Mp 59-60°. Struct. doubtful.

Jacobson, M. *et al., J.A.C.S.*, 1948, **70**, 4234 (*isol, struct*)
Raphael, R.A. *et al., J.C.S.*, 1950, 115; 1951, 2693 (*synth*)
Crombie, L. *et al., J.C.S.*, 1952, 2997 (*synth, struct*)

3,6-Dodecadien-1-ol D-1013

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH_2OH$

$C_{12}H_{22}O$ 182.305

(E,E)-form [116264-82-5]

Oil.

(Z,Z)-form [29125-78-8]

Isol. from *Jasminum sambac* (Arabian jasmine). Yellowish liq.

[116264-83-6]

Carvalho, J.F. *et al., J.O.C.*, 1984, **49**, 1251 (*synth, ir, pmr, cmr, bibl*)
Wilson, S.R. *et al., J.O.C.*, 1988, **53**, 4682 (*synth, pmr, cmr*)
Morisaki, N. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2945 (*synth, pmr*)
Carpita, A. *et al., Synth. Commun.*, 1994, **24**, 2281 (*synth, pmr, cmr, ms*)
Hutzinger, M.W. *et al., J.O.C.*, 1995, **60**, 4595 (*synth, ir, pmr, cmr, ms*)
Vasilev, A.A. *et al., J. Chem. Res., Synop.*, 1998, 706-707 (*synth*)
Khanapure, S. *et al., J.O.C.*, 1998, **63**, 337-342 (*synth, pmr, cmr*)

Dodecanal D-1014

[112-54-9]

Lauric aldehyde. Laurylaldehyde. FEMA 2615

$H_3C(CH_2)_{10}CHO$

$C_{12}H_{24}O$ 184.321

Occurs in peel oil from *Citrus* spp. and kumquat. Also present in ginger, coriander, chervil and scallop. Flavouring agent. Cryst. with fatty, woody taste. Poorly sol. H_2O. d_{25}^{25} 0.83. Mp 44.5°. Bp_{100} 184-185° Bp_{22} 142-143°.

▶ Skin and eye irritant. LD_{50} (rat, orl) 23000 mg/kg. JR1910000

Oxime: [13372-76-4]

[106915-67-7, 106915-68-8]
$C_{12}H_{25}NO$ 199.336
Mp 73°.

2,4-Dinitrophenylhydrazone: [1726-78-9]
Mp 106°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 361B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 469D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 556B (*ir*)
Kraft, F. *et al., Ber.*, 1880, **13**, 1413-1418 (*synth*)
Davies, R.R. *et al., J.C.S.*, 1943, 84-86 (*synth*)
Ikeda, R.M. *et al., J. Agric. Food Chem.*, 1962, **10**, 98-102 (*isol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 483 (*rev, tox*)
Boss, B.D. *et al., Anal. Chem.*, 1976, **48**, 417-420 (*glc, ms*)
Tengoe, J. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **55**, 179-188 (*occur*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DXT000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1542-1543 (*occur, props*)
Aurell, M.J. *et al., Tetrahedron*, 1997, **53**, 10883-10898 (*synth, pmr*)
Sharma, A. *et al., J.O.C.*, 1999, **22**, 8059-8062 (*synth, ir, pmr*)
Singh, R.S. *et al., Chem. Eur. J.*, 2002, **8**, 900-909 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

1,12-Dodecanediol D-1015

[5675-51-4]

Dodecamethylenediol

$HOCH_2(CH_2)_{10}CH_2OH$

$C_{12}H_{26}O_2$ 202.336
Cryst. (EtOH aq. or C_6H_6). Mp 80-81°. Bp_{12} 189°.

Di-Ac:
$C_{16}H_{30}O_4$ 286.411
Mp 36.5-37.5°.

Di-Me ether: [73120-52-2] *1,2-Dimethoxydodecane*
$C_{14}H_{30}O_2$ 230.39
Mp 11.5°. Bp_{15} 155-156°.

Di-Ph ether: [61575-03-9] *1,1′-[1,12-Dodecanediylbis(oxy)]bisbenzene, 9CI. 1,12-Diphenoxydodecane*
$C_{24}H_{34}O_2$ 354.531
Isol. from the leaves of *Arachis hypogaea* (peanuts) infected with *Puccinia arachidis*.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 137A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 206B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 199A (*ir*)
Chuit, P. *et al., Helv. Chim. Acta*, 1926, **9**, 264 (*synth*)
Guyer, A. *et al., Helv. Chim. Acta*, 1955, **38**, 976-982 (*synth*)
Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 1248 (*synth*)
White, R.W. *et al., Tet. Lett.*, 1971, 3587 (*synth*)
Rosen, M.J. *et al., J. Am. Oil Chem. Soc.*, 1976, **53**, 742 (*di-Ph ether*)
Rao, P.V.S. *et al., Oleagineux*, 1991, **46**, 501; *CA*, **116**, 252152 (*di-Ph ether*)
Nakamura, N. *et al., Acta Cryst. C*, 1997, **53**, 1883-1885 (*cryst struct*)

Dodecanoic acid, 9CI D-1016

[143-07-7]
Lauric acid. Laurostearic acid. FEMA 2614
$H_3C(CH_2)_{10}COOH$
$C_{12}H_{24}O_2$ 200.32
For salts see Dodecanoic acid salts, D-1017. Defoamer, lubricant. Used in fruit coatings. Occurs as glyceride in coconut oil and palm kernel oil. Simple esters are flavour ingredients. Cryst. (EtOH). d^{20} 0.88. Mp 44°. Bp_{100} 225° $Bp_{0.65}$ 141-142° (lit. gives a pressure range). pK_a 5.3 (20°).
▶ LD_{50} (rat, orl) 12000 mg/kg. OE9800000

Me ester: [111-82-0] *Methyl dodecanoate. Methyl laurate. FEMA 2715*
$C_{13}H_{26}O_2$ 214.347
Found in concord grape (*Vitis labrusca*), melon, pineapple, heated blackberry, red chilli (*Capsicum frutescens*) and other fruits. Also present in cheeses, hop oil, white wine, spirits and other foodstuffs. Flavouring agent. d_4^{20} 0.87. Mp 5°. Bp 261-262° Bp_{15} 141°. n_D^{20} 1.4320.
▶ OF0670000

Et ester: [106-33-2] *Ethyl dodecanoate. Ethyl laurate. FEMA 2441*
$C_{14}H_{28}O_2$ 228.374
Present in various fruits, eg. apple, apricot, guava, melon, etc.. Also present in wheatbread, crispbread, ginger, whisky, fruit brandies and wine. flavouring agent. Liq. with floral, fruity odour. d_4^{25} 0.86. Bp_{25} 272-273° Bp_{25} 163°.

Butyl ester: [106-18-3] *Butyl dodecanoate. Butyl laurate. FEMA 2206*
$C_{16}H_{32}O_2$ 256.428
Present in apple, papaya, cape gooseberry, spineless monkey orange and malt whisky. Used in fruit flavouring. d_4^{20} 0.86. Mp -7°. Bp_{30} 194° $Bp_{4.5}$ 153.5°. n_D^{20} 1.4362.

3-Methylbutyl ester: [6309-51-9] *3-Methylbutyl dodecanoate. Isoamyl laurate. FEMA 2077*
$C_{17}H_{34}O_2$ 270.454
Flavouring ingredient. Oil.

[2224-49-9, 37811-72-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 484A; 608C; 731A; 761B; 840A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 755A; 924C; 1168C; 1196C; 1245A; 1355B (*nmr*)
Vogel, A.I. *et al., J.C.S.*, 1948, 624-644 (*butyl ester*)
Org. Synth., 1950, **30**, 106
Warren, C.H. *et al., Can. J. Chem.*, 1973, **51**, 3901 (*Raman*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 93 (*rev, tox, Et ester*)
Kameoka, H. *et al., Yukagaku*, 1976, **25**, 490 (*isol*)
Goto, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 70 (*cryst struct*)
Barton, F.E. *et al., J. Am. Oil Chem. Soc.*, 1978, **55**, 574 (*cmr*)
Shostenko, A.G. *et al., CA*, 1979, **90**, 103343b (*synth*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ELY700; LBL000
Yokoyama, I. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 400 (*ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 381 (*3-methylbutyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 348-349; 1003-1004; 1428-1429; 1540-1541; 1790-1791 (*occur, props, esters*)
Kiessling, A.J. *et al., Synth. Commun.*, 1997, **27**, 923-935 (*esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXT400; LBL000; ELY700

Dodecanoic acid salts D-1017

Dodecanoates. Laurates
For parent acid see Dodecanoic acid, D-1016.

Na salt: [629-25-4] *Sodium dodecanoate. Sodium laurate*
$C_{12}H_{23}NaO_2$ 222.302
Used in foods as a binder, emulsifier and anticaking agent.

K salt: [10124-65-9] *Potassium dodecanoate. Potassium laurate*
$C_{12}H_{23}KO_2$ 238.411
Used in foods as a binder, emulsifier and anticaking agent.

Mg salt: [4040-48-6] *Magnesium dodecanoate. Magnesium laurate*
$C_{24}H_{46}MgO_4$ 422.93
Used in foods as a binder, emulsifier and anticaking agent. Mp 75° Mp 150.4°.

Ca salt: [4696-56-4] *Calcium dodecanoate. Calcium laurate*
$C_{24}H_{46}CaO_4$ 438.703
Used in foods as a binder, emulsifier and anticaking agent. Needles. Mp 182-183°.

Al salt: [7230-93-5] *Aluminium dodecanoate. Aluminium laurate*
$C_{36}H_{69}AlO_6$ 624.919
Used in foods as a binder, emulsifier and anticaking agent.

[629-25-4, 2437-23-2, 10124-65-9]

Lomer, T.R. *et al., Acta Cryst.*, 1952, **5**, 11-17 (*K salt, cryst struct*)
Gilmour, A. *et al., J.C.S.*, 1956, 1972-1976 (*Al salt*)
Wood, D.E. *et al., J. Appl. Chem.*, 1958, **8**, 237-246 (*Al salt*)
Muller, B.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1977, **310**, 693-704 (*Mg salt*)
Amesubi, M. *et al., J. Mol. Struct.*, 1982, **81**, 61-67 (*ir, salts*)
Reichmuth, G. *et al., Thermochim. Acta*, 1985, **85**, 485-488 (*synth*)
Seddon, A.B. *et al., Thermochim. Acta*, 1986, **106**, 341-344 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 111-112; 396-397; 1625-1626; 2304-2305; 2566-2567 (*salts*)

1-Dodecanol D-1018

[112-53-8]
Dodecyl alcohol. Lauryl alcohol. FEMA 2617
$H_3C(CH_2)_{10}CH_2OH$
$C_{12}H_{26}O$ 186.337
Present in apple, banana, morello cherry, melon, pawpaw, white wine, roasted peanut, coriander leaf, Bourbon vanilla, rice, licorice and crab. Flavouring agent. Cryst. (EtOH aq.) with fatty, waxy flavour. Mp 24° Mp 26°. Bp 260-262° Bp_{18} 145-148°.
▶ Severe skin irritant. LD_{50} (rat, orl) *ca.* 13000 mg/kg. JR5775000

Ac: [112-66-3] *Dodecyl acetate. Acetate C12. FEMA 2616*
$C_{14}H_{28}O_2$ 228.374
Present in morello cherry, citrus peel oils and cardamom. Flavouring agent. Liq. with citrus-rose odour and flavour on dilution. Bp_{15} 150.5-151.5°.
▶ AH3525000

[27342-88-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 112A; 603C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 166C; 903C (*nmr*)
Adkins, H. *et al., J.A.C.S.*, 1931, **53**, 1095 (*synth*)
Salgues, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1956, **242**, 2392 (*isol*)
Hoshino, H. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3043 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 109 (*rev, tox*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Nagai, T. *et al., Yukagaku*, 1974, **23**, 43 (*nmr*)
Precht, D. *et al., Fette, Seifen, Anstrichm.*, 1976, **78**, 145; 189 (*cryst struct*)
Ohashi, M. *et al., Org. Mass Spectrom.*, 1978, **13**, 642 (*ms*)
Rossi, R. *et al., Tetrahedron*, 1982, **38**, 639 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DXV600

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 428
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1543-1544; 1544-1545 (*occur, props, Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXV400; DXV600

2-Dodecanone D-1019

[6175-49-1]

$H_3C(CH_2)_9COCH_3$

$C_{12}H_{24}O$ 184.321

Constit. of essential oil of rue (*Ruta graveolens*). Also in hop oil (*Humulus lupulus*) and tomato leaf oil. Mp 21°. Bp_{100} 177-178° $Bp_{3.5}$ 101°. n_D^{20} 1.4340.

2,4-Dinitrophenylhydrazone: [81874-90-0] Mp 81°.

Semicarbazone:
Needles (EtOH). Mp 122-123°.

Pickard, R.H. *et al., J.C.S.*, 1911, **99**, 57 (*synth*)
Asinger, F. *et al., Ber.*, 1944, **77**, 73 (*synth*)
U.S. Pat., 1968, 3 365 499; *CA*, **69**, 35440 (*manuf*)
Yeo, A.N.H. *et al., Chem. Comm.*, 1970, 987 (*ms*)
Cooke, M.P. *et al., J.O.C.*, 1973, **38**, 4082 (*synth*)
Bente, P.F. *et al., J. Phys. Chem.*, 1975, **79**, 713 (*ms*)
Kabalka, G.W. *et al., J. Chem. Educ.*, 1976, **53**, 549 (*synth*)
Hokanson, E.C. *et al., J.O.C.*, 1985, **50**, 462 (*synth, pmr*)
McDowell, P.G. *et al., Phytochemistry*, 1988, **27**, 2519 (*isol*)

2,4,8,10-Dodecatetraenoic acid D-1020

$H_3CCH{=}CHCH{=}CHCH_2CH_2CH{=}CHCH{=}CHCOOH$

$C_{12}H_{16}O_2$ 192.257

N-*Isobutylamide:*
$C_{16}H_{25}NO$ 247.38The (2*E*,4*E*,8*Z*,10*E*)- and (2*E*,4*E*,8*Z*,10*Z*)-isomers were isol..

N-*2-Hydroxy-2-methylpropylamide:* ***Sanshoamide***
$C_{16}H_{25}NO_2$ 263.379
Alkaloid from fresh unripe fruits of *Zanthoxylum piperitum* (Japanese pepper tree). Needles (C_6H_6). Mp 110-111°.

Aihara, T. *et al., Yakugaku Zasshi*, 1951, **71**, 1112
Yasuda, I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 564 (*isobutylamide*)
Herz, W. *et al., Phytochemistry*, 1985, **24**, 173-174 (*isobutylamide*)

2,6,8,10-Dodecatetraenoic acid D-1021

$H_3CCH{=}CHCH{=}CHCH{=}CHCH_2CH_2CH{=}CHCOOH$

$C_{12}H_{16}O_2$ 192.257

(all-E)-form

N-*(2-Methylpropyl)amide:* *β-Sanshool*
Cryst. (hexane). Mp 100-101°.

2-Hydroxy-2-methylpropylamide: [97465-69-5] ***Hydroxy-β-sanshool***
$C_{16}H_{25}NO_2$ 263.379
Powder.

(2E,6Z,8E,10E)-form [18744-21-3]
Cryst. (hexane). Mp 93.5-95°. Material contaminated with some *all-E*-isomer.

2-Methylpropylamide: [504-97-2] ***Neoherculin***. N-*Isobutyl-2,6,8,10-dodecatetraenamide. Echinacein*. *α-Sanshool*
$C_{16}H_{25}NO$ 247.38
Constit. of *Zanthoxylum* spp.. Cryst. (petrol). Mp 69° (61-63°). Unstable in air.

2-Hydroxy-2-methylpropylamide: [83883-10-7] ***Hydroxy-α-sanshool***
$C_{16}H_{25}NO_2$ 263.379
Constit. of *Zanthoxylum piperitum* (Japanese pepper tree). Unstable oil. λ_{max} 260 (ε 22400); 269 (ε 29200); 280 (ε 23200) (EtOH).

[119719-30-1]

Crombie, L. *et al., J.C.S.*, 1952, 2997; 1955, 995; 1957, 2760 (*isol, uv, ir, struct*)
Crombie, L. *et al., Nature (London)*, 1954, **174**, 833
Sonnet, P.E. *et al., J.O.C.*, 1969, **34**, 1147 (*synth, uv*)
Yasuda, I. *et al., Phytochemistry*, 1982, **21**, 1295 (*isol, pmr, cmr, ms, occur*)
Mizutani, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2362 (*isol, ir, pmr, cmr*)
Nakamura, N. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2647 (*ir*)

2-Dodecenal D-1022

[4826-62-4]
FEMA 2402

$H_3C(CH_2)_8CH{=}CHCHO$

$C_{12}H_{22}O$ 182.305

► JR5150000

(E)-form [20407-84-5]
Present in many foods including citrus peel, ginger, carrots, milk, roast peanuts, roast beef and cured pork. Flavouring agent. Oil with citrus-like odour and a mandarin taste. Bp_{10} 125-128° $Bp_{0.5}$ 73.4°.

► Skin irritant. LD_{50} (rat, orl) >5000 mg/kg.

Semicarbazone: [16742-26-0]
Mp 165.5-166°.

Bedoukian, P.Z. *et al., J.A.C.S.*, 1957, **79**, 889
Wheeler, J.W. *et al., Science (Washington, D.C.)*, 1964, **144**, 540
Naves, Y.R. *et al., Helv. Chim. Acta*, 1967, **50**, 1461 (*ir*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1983, **21**, 849 (*rev, tox*)
Chang, Y.H. *et al., Synthesis*, 1990, 1033 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXU280

2-Dodecenoic acid D-1023

[4412-16-2]

$H_3C(CH_2)_8CH{=}CHCOOH$

$C_{12}H_{22}O_2$ 198.305

(E)-form [32466-54-9]
Mp 13-18°. Bp_3 155-158° $Bp_{0.15}$ 127-130°.

Me ester: [6208-91-9]
$C_{13}H_{24}O_2$ 212.331
Occurs in volatile component of pears. Oil. Bp_3 105°.

Et ester: [28290-90-6]
$C_{14}H_{26}O_2$ 226.358
Occurs in pears.

(Z)-form [55928-65-9]

Org. Synth., Coll. Vol., 4, 1963, 398 (*synth*)
Creveling, R.K. *et al., J. Agric. Food Chem.*, 1970, **18**, 19 (*ir, pmr, ms, uv*)
Bus, J. *et al., Chem. Phys. Lipids*, 1976, **17**, 501; 1977, **18**, 130 (*cmr*)
Muto, S. *et al., Eur. J. Org. Chem.*, 2001, 4635-4638 (*Me ester*)
Popaj, K. *et al., Helv. Chim. Acta*, 2001, **84**, 180-186 (*Et ester, synth, ir, pmr, cmr*)

1-Dodecyl sulfate D-1024

[151-41-7]
Monododecyl sulfate, 9CI. Lauryl sulfate

$H_3C(CH_2)_{11}OSO_2OH$

$C_{12}H_{26}O_4S$ 266.401

Cryst. Sol. H_2O.

► LD_{50} (rat, orl) 1300 mg/kg. WT0700000

Na salt: [151-21-3] *Sodium lauryl sulfate. Sodium dodecyl sulfate. SDS. Numerous proprietary names*
Used in foods as an emulsifier, whipping agent, surfactant and wetting agent. Flakes (EtOH). Mp 204-207°.

► WT1050000

Glycine salt:
Mp 110°.

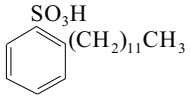
Urea salt:
Mp 110°.

[2044-56-6, 2235-54-3, 3097-08-3, 4706-78-9, 7423-32-7]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 805A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 904C (*ir*)
Sadtler Standard C-13 NMR Spectra, 4458 (*Na salt, cmr*)
Sadtler Standard Proton NMR Spectra, 16888 (*Na salt, pmr*)
Weber, K. *et al., J. Biol. Chem.*, 1969, **244**, 4406 (*use*)
Schulten, H.R. *et al., Anal. Chim. Acta*, 1976, **87**, 103 (*Na salt, ms*)
Jaeger, D.A. *et al., J.O.C.*, 1977, **42**, 3298 (*synth*)
Hung, S.C. *et al., Talanta*, 1982, **29**, 85 (*detn, Ag*)
Tan Zhe, *et al., Talanta*, 1984, **31**, 624 (*detn, Zn*)
Surfactants in Cosmetics, (eds., Rieger, M.M.) M. Dekker, New York, 1985, (*uses*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 281
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 448-450
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4557-4558 (*Na salt, use*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1534
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2567-2568 (*Na salt*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MRH250; SOM500; SIB600

2-Dodecylbenzenesulfonic acid, 9CI D-1025

[1330-69-4, 1886-81-3, 27176-87-0]



$C_{18}H_{30}O_3S$ 326.499
The Na salt is likely to be a minor component of sodium laurylbenzenesulfonate used as a detergent in food processing. See D-1026 and D-1027.

S-*Benzylisothiouronium salt:*
Mp 100-101°.

[1322-98-1, 25155-30-0, 26264-05-1, 26264-06-2, 27177-77-1, 27323-41-7]

Truce, W.E. *et al., J.A.C.S.*, 1951, **73**, 126 (*synth*)

3-Dodecylbenzenesulfonic acid, 9CI D-1026

[16577-13-2]

[1330-69-4, 1886-81-3, 27176-87-0]

$C_{18}H_{30}O_3S$ 326.499

Na salt: [19589-59-4] *Sodium dodecylbenzenesulfonate. Sodium laurylbenzenesulfonate*
Surfactant for use in washing or lye peeling of fruit and vegetables and in poultry scald solutions. White to light yellow flakes, granules or powder. The coml. prod. is a mixture of 1,2-, 1,3- and 1,4-isomers..

S-*Benzylisothiouronium salt:*
Mp 97-98°.

p-*Toluidine salt:*
Mp 103-104°.

[1322-98-1, 25155-30-0, 26264-05-1, 26264-06-2, 27176-87-0, 27177-77-1, 27323-41-7]

Truce, W.E. *et al., J.A.C.S.*, 1951, **73**, 126 (*synth*)
Chem. Eng. (N.Y.), 1954, **61**, 372-375 (*manuf*)
Merck Index, 12th edn., 1996, 8757 (*bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2553-2554 (*use*)

4-Dodecylbenzenesulfonic acid, 9CI D-1027

[1330-69-4, 1886-81-3, 27176-87-0]

$C_{18}H_{30}O_3S$ 326.499

Na salt: [121-65-3]

[1322-98-1]
Surfactant for use in washing or lye peeling of fruit and vegetables and poultry scald solutions. Mp 144-145°. The commercial prod. is a mixt. of 1,2-, 1,3- and 1,4-isomers. See also, D-1026 and refs. given there.

S-*Benzylisothiouronium salt:*
Mp 117-118°.

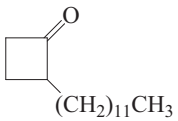
p-*Toluidine salt:*
Mp 144-145° (138-139.5°).

[25155-30-0, 26264-05-1, 26264-06-2, 27177-77-1, 27323-41-7]

Ogawa, M. *et al., Nippon Kagaku Kaishi*, 1951, **54**, 779; *CA*, **48**, 3918 (*synth*)
Truce, W.E. *et al., J.A.C.S.*, 1951, **73**, 126 (*synth*)
Pueschel, F. *et al., Tenside Deterg.*, 1970, **7**, 249; *CA*, **74**, 99561 (*synth, ir*)

2-Dodecylcyclobutanone, 9CI D-1028

[35493-46-0]
2-DCB



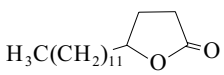
$C_{16}H_{30}O$ 238.412

(±)-*form*
Marker for γ-irradiation of foodstuffs esp. chicken, formed by dec. of palmitic acid triglycerides. Mp 25-27°. $Bp_{0.075}$ 88-96°.
► Possesses genotoxic and cytotoxic activity *in vitro*.

Boyd, D.R. *et al., J. Agric. Food Chem.*, 1991, **39**, 789-792 (*formn, detn, synth, ms, pmr, cnmr*)
Delincee, H. *et al., Radiat. Phys. Chem.*, 1998, **52**, 39-42 (*tox*)
Horvatovich, P. *et al., J. Chromatogr., A*, 2000, **897**, 259-268 (*detn, glc*)
Stewart, E.M. *et al., J. Sci. Food Agric.*, 2000, **80**, 121-130 (*detn*)

5-Dodecyldihydro-2(3*H*)-furanone, 9CI D-1029

[730-46-1]
4-Hexadecanolide. γ-Palmitolactone. 4-Dodecyl-γ-butyrolactone

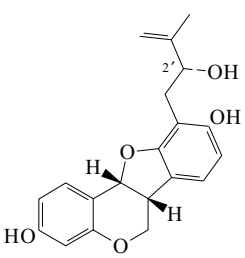


$C_{16}H_{30}O_2$ 254.412
Found in pineapple essence and essential oil of parsnip (*Pastinaca sativa*). Mp 54°.

Näf-Müller, R. *et al., Helv. Chim. Acta*, 1971, **54**, 1880 (*isol*)
Kubeczka, K.H. *et al., Planta Med.*, 1977, **31**, 173; *CA*, **86**, 177157 (*isol*)

Dolichin D-1030

3,9-Dihydroxy-10-(2-hydroxy-3-methyl-3-butenyl)pterocarpan



(2′*R*)-*form*

$C_{20}H_{20}O_5$ 340.375

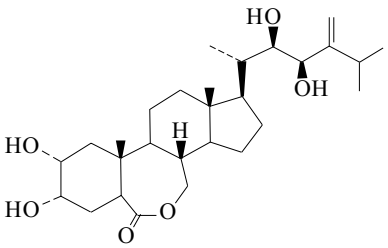
(2′*R*)-*form* [78919-15-0]
Dolichin A
Isol. from bacteria-inoculated leaves of *Dolichos biflorus* (papadi). $[\alpha]_D$ -265 (c, 0.05 in MeOH). λ_{max} 212 ; 282 ; 288 (EtOH) (Berdy). λ_{max} 215 ; 249 ; 298 (EtOH-NaOH) (Berdy).

(2′*S*)-*form* [78859-49-1]
Dolichin B
From *Dolichos biflorus* (papadi). $[\alpha]_D$ -235 (c, 0.04 in MeOH). λ_{max} 213 ; 282 ; 288 (EtOH) (Berdy). λ_{max} 216 ; 248 ; 298 (EtOH-NaOH) (Berdy).

Ingham, J.L. *et al., Phytochemistry*, 1981, **20**, 807 (*struct, uv, nmr, ms*)

Dolicholide D-1031

[85228-11-1]
*2α,3α,22*R,*23*R-*Tetrahydroxy-B-homo-7-oxa-5α-ergost-24(28)-en-6-one, 9CI*

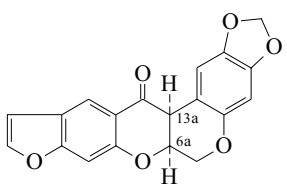


$C_{28}H_{46}O_6$ 478.668
Constit. of *Dolichos lablab* (hyacinth bean). Cryst. (MeCN aq. or MeOH). Mp 234-238°. $[\alpha]_D^{22}$ +56.3 (c, 0.405 in MeOH).

Yokota, T. *et al., Tet. Lett.*, 1982, **23**, 4965 (*isol, struct*)
Okada, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 925 (*synth*)
Takasuto, S. *et al., Tet. Lett.*, 1983, **24**, 773 (*synth*)
Mori, K. *et al., Tetrahedron*, 1984, **40**, 1767 (*synth*)
Singh, H. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 989 (*rev*)
Adam, G. *et al., Phytochemistry*, 1986, **25**, 1787 (*rev*)
Takatsuto, S. *et al., Agric. Biol. Chem.*, 1988, **52**, 2361 (*synth*)

Dolineone D-1032

[10065-28-8]
6a,13a-Dihydro-1,3-dioxolo[6,7][1]benzopyrano[3,4-b]furo[3,2-g][1]benzopyran-13(6H)-one, 9CI. Dolichone



$C_{19}H_{12}O_6$ 336.3
CA numbering shown. Isol. from roots of *Pachyrrhizus erosus* (yam bean). Needles (MeOH). Mp 233-235°. $[\alpha]_D^{20}$ +135 (c, 1.3 in $CHCl_3$).

13a-Hydroxy: [28617-71-2]

[28753-27-7] ***13a-Hydroxydolineone***. *12a-Hydroxydolineone*
Constit. of *Pachyrrhizus erosus* (yam bean). Needles ($CHCl_3$/MeOH). Mp 194-195° (180-181°). $[\alpha]_D$ +137 ($CHCl_3$). λ_{max} 237 (4.54); 276 (3.84); 304 (3.66); 338 (sh) (3.64) (EtOH).

13a-Methoxy: [54534-96-2] ***13a-Methoxydolineone***. *12a-Methoxydolineone*
$C_{20}H_{14}O_7$ 366.326

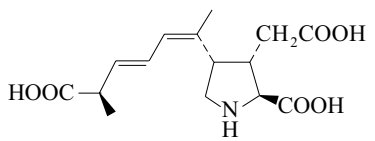
Oil. $[\alpha]_D$ +58.

6a,13a-Didehydro: [28570-72-1] ***Dehydrodolineone***
$C_{19}H_{10}O_6$ 334.284
Yellow needles. Mp 290-292°. Poss. artifact.

Crombie, L. *et al., J.C.S.*, 1963, 1569 (*isol, struct*)
Krishnamurti, M. *et al., Tetrahedron*, 1970, **26**, 3023 (*12a-Hydroxydolineone*)
Oberholzer, M.E. *et al., Tet. Lett.*, 1974, 2211 (*Dehydrodolineone, 12a-Methoxydolineone*)
Kalra, A.J. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 1084 (*12a-Hydroxydolineone*)
Van Puyvelde, L. *et al., J. Nat. Prod.*, 1987, **50**, 349 (*isol, pmr, cmr, ms*)
Phrutivoraponkgul, A. *et al., Chem. Pharm. Bull.*, 2002, **50**, 534-537 (*isol, pmr, cmr*)

Domoic acid D-1033

[14277-97-5]
2-Carboxy-4-(5-carboxy-1-methyl-1,3-hexadienyl)-3-pyrrolidineacetic acid, 9CI



$C_{15}H_{21}NO_6$ 311.334
Constit. of the red algae *Chondria armata* and *Alsidium corallinum*. Also isol. from toxin contaminated edible mussels (*Mytilus edulis*). Needles + $2H_2O$. Sol. H_2O, AcOH; fairly sol. MeOH, EtOH; poorly sol. Me_2CO, C_6H_6. Mp 213° dec. $[\alpha]_D^{12}$ -109.6 (H_2O). λ_{max} 242 (ϵ 24300) (H_2O at pH 2) (Derep). λ_{max} 242 (ϵ 26100) (H_2O pH 7) (Derep). λ_{max} 242 (ϵ 17500) (H_2O) (Berdy).

▶ UX9665100

(1′E)-Isomer: [126872-96-6] ***Isodomoic acid E***
$C_{15}H_{21}NO_6$ 311.334
Isol. from mussel (*Mytilus edulis*). $[\alpha]_D^{25}$ -19.5 (H_2O).

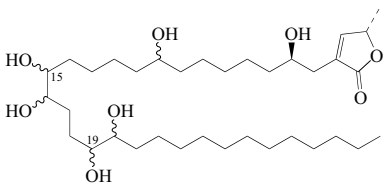
(3′Z)-Isomer: [101977-26-8] ***Isodomoic acid D***
$C_{15}H_{21}NO_6$ 311.334
Isol. from mussel (*Mytilus edulis*). $[\alpha]_D^{25}$ -72 (H_2O). λ_{max} 213 (ϵ 5030) (MeOH) (Berdy).

(1′E,3′Z)-Isomer: [127761-30-2] ***Isodomoic acid F***
$C_{15}H_{21}NO_6$ 311.334
Isol. from mussels. $[\alpha]_D^{25}$ -85 (H_2O).

Daigo, K. *et al., Yakugaku Zasshi*, 1959, **79**, 350; 353; 356; 365; *CA*, **53**, 14218d (*isol, algae*)
Takemoto, T. *et al., Yakugaku Zasshi*, 1966, **86**, 874 (*pmr, struct*)
Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549 (*isol, algae*)
Ohfune, Y. *et al., J.A.C.S.*, 1982, **104**, 3511 (*synth, struct*)
Thibault, P. *et al., Biomed. Mass Spectrom.*, 1989, **18**, 373 (*ms*)
Falk, M. *et al., Can. J. Chem.*, 1989, **67**, 1421 (*uv*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1990, **68**, 22 (*Isodomoic acids, isol, mussels*)
Tryphonas, L. *et al., Toxicol. Pathol.*, Pt. 2, 1990, **18**, 165 (*rev, tox*)
Walter, J.A. *et al., Can. J. Chem.*, 1992, **70**, 1156 (*pmr, cmr*)
Parsons, A.F. *et al., Tetrahedron*, 1996, **52**, 4149-4174 (*rev*)

Donhexocin D-1034

3-(2,8,13,14,17,18-Hexahydroxytriacontyl)-5-methyl-2(5H)-furanone



$C_{35}H_{66}O_8$ 614.902
Constit. of the seeds of *Annona muricata* (soursop). Amorph. powder. Mp 120-122° (96-98°). $[\alpha]_D$ +8 (c, 0.1 in MeOH). $[\alpha]_D$ +11.7 (c, 0.2 in $CHCl_3$). C-15:C-16 and C-19:C-20 are *threo*-configs..

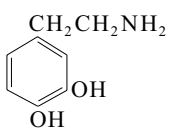
Stereoisomer: ***Murihexol***
$C_{35}H_{66}O_8$ 614.902
Constit. of the seeds of *Annona muricata* (soursop). Powder. Mp 116-118°. $[\alpha]_D^{16}$ +7.2 (c, 0.1 in $CHCl_3$). C-15:C-16 has *threo*-config. and C-19:C-20 has *erythro*-config..

19,20-Dideoxy:5-Methyl-3-(2,8,13,14-tetrahydroxytriacontyl)-2(5H)-furanone. ***Donbutocin***
$C_{35}H_{66}O_6$ 582.903
Amorph. Mp 90-92°. $[\alpha]_D^{18}$ +16.3 (c, 0.1 in MeOH).

Jiang, Z. *et al., Phytochemistry*, 1998, **49**, 769-775 (*isol, ir, pmr, cmr, ms*)
Yu, J.-G. *et al., Phytochemistry*, 1998, **49**, 1689-1692 (*isol, ir, pmr, cmr, ms*)

Dopamine, BAN, INN D-1035

[51-61-6]
4-(2-Aminoethyl)-1,2-benzenediol, 9CI. 2-(3,4-Dihydroxyphenyl)ethylamine. 3,4-Dihydroxyphenethylamine. Hydroxytyramine. Oxytyramine. Cardiosteril. Dopastat. Intropin. NSC 169105. ASL 279. Many other names



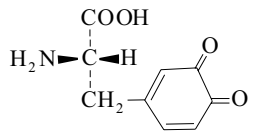
$C_8H_{11}NO_2$ 153.18
Occurs in several higher plants, such as banana (*Musa sapientum*). Log P 0.02 (calc). Autoxidises very readily as free base.

▶ LD_{50} (rat, ipr) 163 mg/kg. Exp. reprod. and teratogenic effects. UX1088000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1294A; 1294B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 622B; 622C (*nmr*)
Waalkes, T.P. *et al., Science (Washington, D.C.)*, 1958, **127**, 648-650 (*isol*)
Keppe, T. *et al., J. Med. Chem.*, 1965, **8**, 368-374 (*uv*)
Lundström, J. *et al., Acta Chem. Scand.*, 1971, **25**, 3489-3499 (*biosynth*)
Milne, G.W. *et al., Anal. Chem.*, 1973, **45**, 1952-1954 (*ms*)
Lambert, F. *et al., Org. Magn. Reson.*, 1975, **7**, 266-273 (*pmr*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9-18 (*occur, bibl*)
Scratchley, G.A. *et al., J. Chromatogr.*, 1979, **169**, 313-319 (*hplc*)
Carter, J.E. *et al., Anal. Profiles Drug Subst.*, 1982, **11**, 257-272 (*rev, uv, ir, pmr, cmr, ms, anal*)
Carey, R.M. *et al., Recent Prog. Horm. Res.*, 1986, **42**, 251-296 (*rev*)
Mueller, D.D. *et al., Bioconjugate Chem.*, 1993, **4**, 47-53 (*pmr, cmr*)
Volin, P. *et al., J. Chromatogr., B: Biomed. Appl.*, 1994, **655**, 121-126 (*hplc*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 1113 (*synonyms*)
Merck Index, 12th edn., 1996, 3479
Hay, M. *et al., J. Chromatogr., B: Biomed. Appl.*, 1997, **703**, 15-23 (*hplc*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DYC400; DYC600

Dopaquinone D-1036

[4430-97-1]
α-Amino-3,4-dioxo-1,5-cyclohexadiene-1-propanoic acid, 9CI



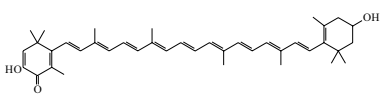
$C_9H_9NO_4$ 195.174

(S)-form
L-form
Implicated in food discolouration (enzymatic browning).

Young, T.E. *et al., J.O.C.*, 1974, **39**, 1980
Pelizzetti, E. *et al., J.C.S. Perkin 2*, 1976, 1651
Graham, D.G. *et al., CA*, 1978, **88**, 115920j (*tox*)

β-Doradecin D-1037

[31460-54-5]
3′-Hydroxy-β,β-carotene-3,4-dione. 3′-Hydroxy-3,4-diketo-β-carotene. Dehydroadonixanthin. 3-Hydroxyeuglenanone

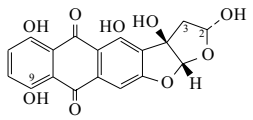


$C_{40}H_{52}O_3$ 580.849
Isol. as an ester from Pacific salmon. λ_{max} 465 (EtOH). λ_{max} 455 (hexane).

Egger, K. *et al., Phytochemistry*, 1965, **4**, 609
Katayama, T. *et al., Int. J. Biochem.*, 1970, **1**, 438 (*isol*)
Kitahara, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1984, **78**, 859 (*isol*)

Dothistromin D-1038

[31456-72-1]



Absolute configuration

$C_{18}H_{12}O_9$ 372.287

CA numbering shown.Red solid. Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 229 (ϵ 27100); 280 (ϵ 20400); 480 (ϵ 6230); 491 (ϵ 7050); 510 (ϵ 5580); 525 (ϵ 4740) (MeOH) (Berdy).

▶CB1753000

Penta-Ac: [31456-73-2]
Cryst. ($CHCl_3$/hexane). Mp 196-198°. $[\alpha]_D$ -142 (c, 0.17 in $CHCl_3$).

2-Me ether: ***2-O-Methyldothistromin***
$C_{19}H_{14}O_9$ 386.314

2-Deoxy: ***4′-Deoxydothistromin***
$C_{18}H_{12}O_8$ 356.288
Named acc. to alternative numbering system.

2-Deoxy, 2,3-didehydro: ***3′,4′-Dehydro-4′-deoxydothistromin***
$C_{18}H_{10}O_8$ 354.272
Mp 211-213° (as tetra-Ac).

*2,3*a*-Dideoxy:* [52997-52-1] ***Bisdeoxydothistromin***
$C_{18}H_{12}O_7$ 340.289
Red cryst. (C_6H_6). Mp 269-270°. Rel. config. only detd..

2,9-Dideoxy: ***4′,5-Bisdeoxydothistromin***
$C_{18}H_{12}O_7$ 340.289
Cryst. ($CHCl_3$). Mp 254-258°.

3-Hydroxy: ***3-Hydroxydothistromin***
$C_{18}H_{12}O_{10}$ 388.287

2-Epimer: ***2-Epidothistromin***
$C_{18}H_{12}O_9$ 372.287
Shows antibiotic props.

Gallacher, R.T. *et al., Aust. J. Chem.*, 1972, **25**, 2399 (*isol*)
Bear, C.A. *et al., J.C.S. Perkin 2*, 1972, 2375 (*struct*)
Danks, A.V. *et al., Aust. J. Chem.*, 1974, **27**, 1603 (*Bisdeoxydothistromin*)
Assante, G. *et al., Phytochemistry*, 1977, **16**, 125-126; 243-247 (*Dothistromin, 2-Epidothistromin*)
Shaw, G.J. *et al., Phytochemistry*, 1978, **17**, 1743-1745 (*biosynth*)
Stoessl, A. *et al., Mycopathologia*, 1984, **86**, 165 (*isol*)
Stoessl, A. *et al., Can. J. Chem.*, 1985, **63**, 1258 (*derivs*)

Dotriacontane, 9CI D-1039

[544-85-4]
Dicetyl. Lacceran. Bicetyl

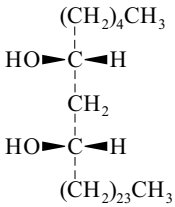
$H_3C(CH_2)_{30}CH_3$

$C_{32}H_{66}$ 450.873
Constit. of *Mentha aquatica* (water mint). Plates (Et_2O). Mp 74-75°. $Bp_{1.5}$ 245°.

▶JT2360000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 8B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 6D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 8D (*ir*)
Levene, P.A. *et al., J. Biol. Chem.*, 1915, **20**, 530 (*synth*)
Brown, I. *et al., J.C.S.*, 1960, 2783 (*isol*)
Razafindrazaka, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 1633 (*isol*)

6,8-Dotriacontanediol D-1040

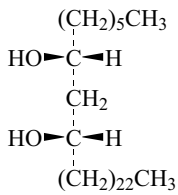


$C_{32}H_{66}O_2$ 482.872

(6*R,8*S**)-*form*** [155800-89-8]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 79-82°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

7,9-Dotriacontanediol D-1041



$C_{32}H_{66}O_2$ 482.872

(7*R,9*S**)-*form*** [193419-73-7]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 77-80°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

10,12-Dotriacontanedione D-1042

$H_3C(CH_2)_{19}COCH_2CO(CH_2)_8CH_3$

$C_{32}H_{62}O_2$ 478.841
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

11,13-Dotriacontanedione D-1043

$H_3C(CH_2)_{18}COCH_2CO(CH_2)_9CH_3$

$C_{32}H_{62}O_2$ 478.841
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

12,14-Dotriacontanedione D-1044

$H_3C(CH_2)_{17}COCH_2CO(CH_2)_{10}CH_3$

$C_{32}H_{62}O_2$ 478.841
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Dotriacontanol D-1045

[6624-79-9]
Laccerol

$H_3C(CH_2)_{30}CH_2OH$

$C_{32}H_{66}O$ 466.873
Plates (C_6H_6). Mp 89°.

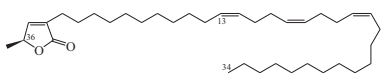
Ac: [23811-94-1]
$C_{34}H_{68}O_2$ 508.91
Mp 76-77°.

p-*Hydroxycinnamoyl:* [92533-57-8] ***Randilongin***
$C_{41}H_{72}O_3$ 613.018
Isol. from *Cinnamomum cassia* (Chinese cinnamon). Cryst. ($CHCl_3$/petrol). Mp 82°.

Octacosanoyl: [117611-65-1] *Dotriacontyl octacosanoate*
$C_{60}H_{120}O_2$ 873.607

Gascard, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1914, **159**, 258 (*isol*)
Sosa, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1950, **230**, 995 (*isol*)
Cocker, W. *et al., J.C.S.*, 1962, 5194 (*isol*)
Kuo, Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 1984, **31**, 159 (*Randilongin*)
Bhakuni, R.S. *et al., Fitoterapia*, 1988, **59**, 45 (*Dotriacontyl octacosanoate*)
Talapatra, S.K. *et al., J. Indian Chem. Soc.*, 1989, **66**, 694 (*Randilongin*)
Misra, T.N. *et al., Phytochemistry*, 1992, **31**, 1809 (*isol, ir, pmr*)
Parmar, V.S. *et al., Phytochemistry*, 1998, **49**, 1069-1078 (*isol, pmr, cmr, ms*)

3-(11,15,19-Dotriacontatrienyl)-5-methyl-2(5*H*)-furanone D-1046



$C_{37}H_{64}O_2$ 540.911
Acetogenin numbering shown.

(13*Z*,17*Z*,21*Z*,36*S*)-*form* ***Chatenaytrienin 3***
Constit. of *Annona muricata* (soursop).

13,14-Dihydro: [206131-79-5] *3-(15,19-Dotriacontadienyl)-5-methyl-2(5*H*)-furanone.* ***Muridienin 4***
$C_{37}H_{66}O_2$ 542.927
Constit. of *Annona muricata* (soursop).

21,22-Dihydro: [206131-78-4] *3-(11,15-Dotriacontadienyl)-5-methyl-2(5*H*)-furanone.* ***Muridienin 3***
$C_{37}H_{66}O_2$ 542.927
Constit. of *Annona muricata* (soursop).

Gleye, C. *et al., Phytochemistry*, 1998, **47**, 749-754 (*isol, pmr, cmr, ms*)

3-(13,17,21-Dotriacontatrienyl)-5-methyl-2(5*H*)-furanone D-1047

$C_{37}H_{64}O_2$ 540.911

(15*Z*,19*Z*,23*Z*,36*S*)-*form* [206131-76-2] ***Chatenaytrienin 4***
Constit. of *Annona muricata* (soursop).

23,24-Dihydro: [185502-81-2] *3-(13,17-Dotriacontadienyl)-5-methyl-2(5*H*)-furanone.* ***Muridienin 2***
$C_{37}H_{66}O_2$ 542.927
Constit. of *Annona muricata* (soursop). Oil. $[\alpha]_D$ +10 (c, 0.1 in MeOH). λ_{max} 215 (log ϵ 3.65) (MeOH).

Gleye, C. *et al., Tet. Lett.*, 1996, **37**, 9301-9304 (*isol, uv, pmr, cmr*)
Gleye, C. *et al., Phytochemistry*, 1998, **47**, 749-754 (*isol, pmr, cmr, ms*)

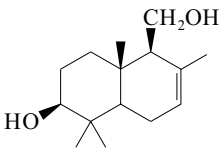
8-Dotriacontenoic acid D-1048

[182141-52-2]
$H_3C(CH_2)_{22}CH{=}CH(CH_2)_6COOH$
$C_{32}H_{62}O_2$ 478.841
Constit. of *Centella asiatica* (Asiatic pennywort). Config. not detd..

Srivastava, R. *et al., Indian Drugs*, 1996, **33**, 233-234 (*isol*)

7-Drimene-3,11-diol D-1049

[124987-04-8]

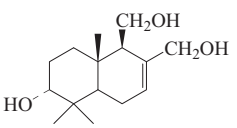


$C_{15}H_{26}O_2$ 238.369

3β-*form*
Constit. of *Marasmius oreades* (fairy ring mushroom). Oil.

Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371 (*isol, pmr, cmr*)

7-Drimene-3,11,12-triol D-1050



(3α,9β)-*form*

$C_{15}H_{26}O_3$ 254.369

(3α,9β)-*form*

11,12-Dialdehyde, 3-Ac: [160668-33-7] *3-Acetoxy-7-drimene-11,12-dial.* ***3α-Acetoxypolygodial***
$C_{17}H_{24}O_4$ 292.374
Oil.

11,12-Dialdehyde, 3-Ac, 12-di-Me acetal: [160668-34-8]
$C_{19}H_{30}O_5$ 338.443
Oil.

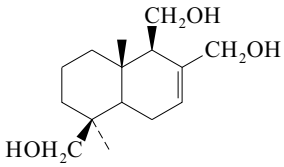
(3β,9β)-*form* [101470-79-5]
Constit. of *Marasmius oreades* (fairy ring mushroom). Cryst. (EtOAc). Mp 165-166°. $[\alpha]_D^{20}$ -10.9 (c, 1.1 in MeOH).

11,12-Dialdehyde, 3-Ac: [128718-16-1] ***3β-Acetoxypolygodial***
$C_{17}H_{24}O_4$ 292.374
Cryst. Mp 131-132°. $[\alpha]_D$ -58 (c, 0.05 in $CHCl_3$).

Sierra, J.R. *et al., Phytochemistry*, 1986, **25**, 253-254 (*synth*)
Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371-1380 (*Marasmius oreades metab*)
Al-Said, M.S. *et al., Phytochemistry*, 1990, **29**, 975-977 (*Canella winterana constit*)
Ying, B.P. *et al., Phytochemistry*, 1995, **38**, 909-915 (*3-Acetoxypolgodial*)

7-Drimene-11,12,14-triol D-1051

[124869-11-0]

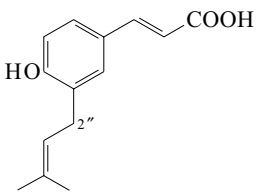


$C_{15}H_{26}O_3$ 254.369
Metab. of *Marasmius oreades* (fairy ring mushroom). Cryst. (EtOAc). Mp 178-180°. $[\alpha]_D^{24}$ -10.7 (c, 0.15 in MeOH).

Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371 (*isol, pmr, cmr*)

Drupanin D-1052

[53755-58-1]
3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenoic acid, 9CI. 4-Hydroxy-3-prenylcinnamic acid



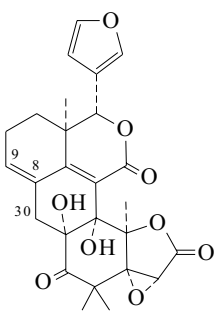
$C_{14}H_{16}O_3$ 232.279
Acicular cryst. Mp 147-148°.

Aldehyde:3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenal. 4-Hydroxy-3-prenylcinnamaldehyde
$C_{14}H_{16}O_2$ 216.279
Prod. by injured peel of grapefruit (*Citrus paradisi*) and orange (*Citrus sinensis*). Mp 144.5-146°.

Stange, R.R. *et al., J. Nat. Prod.*, 1993, **56**, 1627 (*isol, aldehyde*)

Dukunolide A D-1053

[97804-04-1]



$C_{26}H_{26}O_9$ 482.486
Constit. of *Lansium domesticum* (langsat). Cryst. Mp 279-281°. $[\alpha]_D^{20}$ +166 (c, 0.9 in $CHCl_3$). λ_{max} 292 (ε 14600) (possibly MeOH, not reported) (Derep).

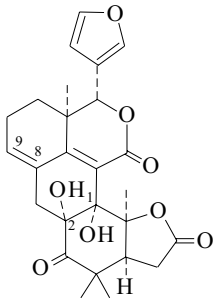
8α,9α-Epoxide: [99343-73-4] ***Dukunolide B***
$C_{26}H_{26}O_{10}$ 498.485
From *Lansium domesticum* (langsat). Cryst. (CH_2Cl_2/hexane). Mp 248.5-251°. $[\alpha]_D^{20}$ +82.2 (c, 0.9 in $CHCl_3$).

30α-Acetoxy: [99343-74-5] ***Dukunolide C***
$C_{28}H_{28}O_{11}$ 540.523
From *Lansium domesticum* (langsat). Cryst. (EtOAc/hexane). Mp 217-218°. $[\alpha]_D^{20}$ +206 (c, 0.89 in $CHCl_3$).

Nishizawa, M. *et al., J.O.C.*, 1985, **50**, 5487

Dukunolide D D-1054

[101560-02-5]



$C_{26}H_{28}O_8$ 468.502
Constit. of *Lansium domesticum* (langsat). Cryst. (EtOAc/hexane). Mp 295.5-298°. $[\alpha]_D^{14.5}$ +175.3 (c, 0.57 in $CHCl_3$).

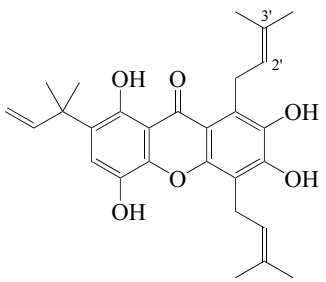
8α,9α-Epoxide: [101559-97-1] ***Dukunolide E***
$C_{26}H_{28}O_9$ 484.502
Constit. of *Lansium domesticum* (langsat). Cryst. Mp 270-272°. $[\alpha]_D^{13}$ +189 (c, 0.68 in $CHCl_3$).

8α,9α-Epoxide, 1,2-diepimer: [113625-61-9] ***Dukunolide F***
$C_{26}H_{28}O_9$ 484.502
Constit. of *Lansium domesticum* (langsat). Cryst. Mp 268-269°. $[\alpha]_D^{14}$ +167 (c, 0.73 in $CHCl_3$).

Nishizawa, M. *et al., Phytochemistry*, 1988, **27**, 237

Dulciol B D-1055

[175617-24-0]
*7-(1,1-Dimethyl-2-propenyl)-2,3,5,8-tetrahydroxy-1,4-diprenylxanthone. 7-(1,1-Dimethyl-2-propenyl)-2,3,5,8-tetrahydroxy-1,4-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one*



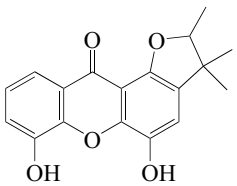
$C_{28}H_{32}O_6$ 464.557
Constit. of *Garcinia dulcis* (mundu). Yellow needles (MeOH). Mp 109°. λ_{max} 206 ; 231 ; 260 ; 285 ; 342 ; 380 (sh) (MeOH).

2′,3′-Dihydro, 3′-hydroxy: [175617-25-1] ***Dulciol C***
$C_{28}H_{34}O_7$ 482.572
Constit. of *Garcinia dulcis* (mundu).

Amorph. yellow solid. λ_{max} 206 ; 230 ; 261 ; 285 ; 308 ; 342 (MeOH).

Iinuma, M. *et al., J. Nat. Prod.*, 1996, **59**, 472 (*isol, uv, ir, pmr, cmr, ms*)

Dulciol E D-1056



$C_{18}H_{16}O_5$ 312.321

(±)-*form* [175617-27-3]

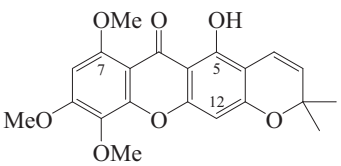
Constit. of *Garcinia dulcis* (mundu). Amorph. yellow solid. λ_{max} 207 ; 230 (sh) ; 248 ; 265 (sh) ; 317 ; 396 (MeOH).

Iinuma, M. *et al., J. Nat. Prod.*, 1996, **59**, 472 (*isol, uv, ir, pmr, cmr, ms*)

Dulxanthone F D-1057

[263249-30-5]

*5-Hydroxy-7,9,10-trimethoxy-2,2-dimethyl-2*H*,6*H*-pyrano[3,2-*b*]xanthen-6-one*



$C_{21}H_{20}O_7$ 384.385

Constit. of *Garcinia dulcis* (mundu). Yellow needles (EtOAc). Mp 152-153°. λ_{max} 216 (log ε 4.9); 235 (log ε 4.83); 276 (log ε 5.05); 333 (log ε 4.77) (MeOH).

12-Methoxy: [263249-33-8] ***Dulxanthone G***

$C_{22}H_{22}O_8$ 414.411

Constit. of *Garcinia dulcis* (mundu). Yellow needles (EtOAc). Mp 182.5-184°. λ_{max} 222 (log ε 5.38); 276 (log ε 5.65); 342 (log ε 5.39) (MeOH).

*12-Methoxy, 7-*O*-de-Me, 5-Me ether:* [263249-36-1] ***Dulxanthone H***

$C_{22}H_{22}O_8$ 414.411

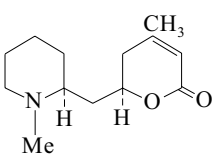
Constit. of *Garcinia dulcis* (mundu). Yellow cubes (EtOAc). Mp 195.9-196.5°. λ_{max} 207 (log ε 5.78); 274 (log ε 6.04); 286 (log ε 5.97); 327 (log ε 5.57) (MeOH).

Kosela, S. *et al., J. Nat. Prod.*, 2000, **63**, 406-407

Dumetorine D-1058

[96552-67-9]

*5,6-Dihydro-4-methyl-6-[(1-methyl-2-piperidinyl)methyl]-2*H*-pyran-2-one, 9CI*



$C_{13}H_{21}NO_2$ 223.314

Alkaloid from the tubers of the famine food *Dioscorea dumetorum*. Oil. $[\alpha]_D^{28}$ +40 (c, 0.021 in $CHCl_3$).

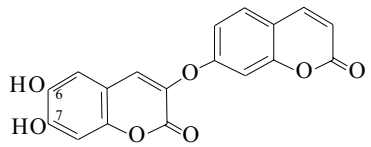
Corley, D.G. *et al., Tet. Lett.*, 1985, **26**, 1615 (*isol, ir, pmr, cmr, struct, abs config*)

Amarasekara, A.S. *et al., Tet. Lett.*, 1987, **28**, 3151 (*synth*)

Edgeworthin E-1

[53947-90-3]

*6,7-Dihydroxy-3-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-2*H*-1-benzopyran-2-one, 9CI. 6,7-Dimethoxy-3,7′-bicoumarin. Demethyldaphnoretin*



$C_{18}H_{10}O_7$ 338.273

Cryst. (THF). Mp 280-282° dec.

7-O-β-D-Glucopyranoside:Edgeworthin 7-glucoside

$C_{24}H_{20}O_{12}$ 500.415

Mp 224-226° dec. $[\alpha]_D^{20}$ -21.4 (c, 0.7 in MeOH/$CHCl_3$). λ_{max} 258 (log ϵ 3.37); 320 (log ϵ 4.03); 349 (log ϵ 3.96) (MeOH/$CHCl_3$).

Di-Ac:

Mp 189°.

6-Me ether: [2034-69-7] ***Daphnoretin**. Thymelol*

$C_{19}H_{12}O_7$ 352.3

Yellow needles (THF/MeOH) or long rods. Mp 244-247°. λ_{max} 222 (ϵ 11000); 266 (ϵ 7100); 323 (ϵ 19100); 345 (ϵ 19500) (MeOH) (Berdy). λ_{max} 228 (ϵ 14700); 264 (ϵ 9100); 325 (ϵ 16200); 342 (ϵ 17800) (EtOH) (Berdy).

► GN6940000

6-Me ether, 7-Ac: [17064-09-4] ***7-O-Acetyldaphnoretin***

$C_{21}H_{14}O_8$ 394.337

Cryst. (MeOH). Mp 230-232°.

6-Me ether, 7-O-β-D-glucopyranoside: [55806-40-1] ***Daphnorin***

$C_{25}H_{22}O_{12}$ 514.442

Fine needles (MeOH aq.). Mp 202-204° dec. $[\alpha]_D^{20}$ -78 (c, 0.6 in H_2O).

6-Me ether, 7-O-β-D-galactopyranoside: [163318-72-7] ***Chamaejasmoside***

$C_{25}H_{22}O_{12}$ 514.442

Cryst. (MeOH). Mp 204-205°.

6-Me ether, 7-O-[3-hydroxy-3-methylglutaroyl-(→6)-β-D-glucopyranoside]: [119179-04-3] ***Rutarensin***

$C_{31}H_{30}O_{16}$ 658.568

Needles. Mp 220° dec.

Di-Me ether: [3749-38-0] *Daphnoretin methyl ether. Isodaphnoretin (incorr.)*

$C_{20}H_{14}O_7$ 366.326

Constit. of *Ruta graveolens* (rue). Yellow needles (EtOH). Mp 240°. λ_{max} 224 ; 264 ; 322 ; 338 (MeOH).

*8-Hydroxy, 7-O-β-D-glucopyranoside:-**Daphsaifnin***

$C_{24}H_{20}O_{13}$ 516.414

Amorph. powder. λ_{max} 227 ; 285 ; 323 ; 334 (MeOH).

Tschesche, R. *et al., Annalen*, 1963, **662**, 113 (*struct*)

Tschesche, R. *et al., Naturwissenschaften*, 1963, **50**, 521 (*struct*)

Kirkiacharian, B. *et al., Bull. Soc. Chim. Fr.*, 1966, 770 (*synth*)

Reisch, J. *et al., Planta Med.*, 1968, **16**, 372 (*deriv*)

Majumder, P.L. *et al., Phytochemistry*, 1974, **13**, 1929 (*Edgeworthin*)

Tandon, S. *et al., Phytochemistry*, 1977, **16**, 1991 (*isol*)

Cordell, G.A. *et al., J. Nat. Prod.*, 1984, **47**, 84 (*pmr, cmr*)

Ulubelen, A. *et al., J. Nat. Prod.*, 1986, **49**, 692 (*Edgeworthin*)

Chakrabarti, R. *et al., Phytochemistry*, 1986, **25**, 557 (*isol*)

Fisher, H. *et al., Planta Med.*, 1988, **54**, 398-400 (*Rutarensin*)

Baba, K. *et al., Phytochemistry*, 1990, **29**, 247-249 (*Rutarensin*)

Narantuya, S. *et al., Khim. Prir. Soedin.*, 1994, **30**, 216; *Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 197 (*Chamaejasmoside*)

Liu, G.F. *et al., J. Chin. Pharm. Sci.*, 1997, **6**, 125-128 (*Isodaphnoretin*)

Ke, H. *et al., Planta Med.*, 2000, **66**, 564-567 (*isol, activity*)

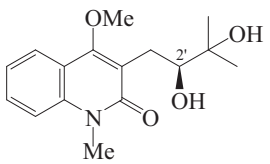
Riaz, M. *et al., Heterocycles*, 2001, **55**, 769-773 (*Daphsaifnin*)

Riaz, M. *et al., Eur. J. Org. Chem.*, 2002, 1436-1438 (*7-glucoside*)

Edulinine E-2

[13849-56-4]

*3-(2,3-Dihydroxy-3-methylbutyl)-4-methoxy-1-methyl-2(1*H*)-quinolinone*



$C_{16}H_{21}NO_4$ 291.346

Abs. config. revised in 2000.

(S)-form [27495-36-9]

Alkaloid from the bark of *Casimiroa edulis* (Mexican apple). Plates (EtOAc). Mp 140° (synthetic). $[\alpha]_D$ -32 ($CHCl_3$) (synthetic). The alkaloid is probably partly racemic. Lower Mps. around 114° have been reported for natural isolates.

2′-Ac: [207603-52-9] ***2′-O-Acetyledulinine**. Acetoxyedulinine (incorr.)*

$C_{18}H_{23}NO_5$ 333.383

Amorph. light brown solid. $[\alpha]_D^{29}$ -40 (c, 0.02 in $CHCl_3$). Synonym is misleading λ_{max} 229 (log ϵ 4.55); 231 (log ϵ 4.57) (MeOH).

3′-Deoxy, 2′-ketone: [123613-75-2] *4-Methoxy-1-methyl-3-(3-methyl-2-oxobutyl)-2(1*H*)-quinolinone, 9CI. **Orixiarine**. Orijanone*

$C_{16}H_{19}NO_3$ 273.331

Needles (cyclohexane) (synthetic). Mp 80-81° (synthetic). λ_{max} 232 (log ϵ 4.24); 236 (log ϵ 4.25) (MeOH).

*3′-Deoxy, 3′,4′-didehydro:**Ptelefoliarine***

$C_{16}H_{19}NO_3$ 273.331

Light brown gum. $[\alpha]_D^{29}$ -8 (c, 0.12 in $CHCl_3$). λ_{max} 232 (log ϵ 4.39) (MeOH).

*3′-Deoxy, 3′,4′-didehydro, Ac:**O-Acetylptelefoliarine**. Acetoxyptelefoliarine (incorr.)*

$C_{18}H_{21}NO_4$ 315.368

Amorph. light brown solid. $[\alpha]_D^{29}$ -8 (c, 0.13 in $CHCl_3$). λ_{max} 230 (log ϵ 4.16) (MeOH).

Iriarte, J. *et al., J.C.S.*, 1956, 4170 (*isol, uv, ir, struct*)

Toube, T.P. *et al., Tetrahedron*, 1967, **23**, 2061 (*pmr, ms*)

Boyd, D.R. *et al., J.C.S.(C)*, 1970, 556 (*synth, struct*)

Naito, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 366 (*synth*)

Gaston, J.L. *et al., J.C.S. Perkin 1*, 1989, 905-908 (*Orixiarine, synth*)

Barr, S.A. *et al., Chem. Comm.*, 1994, 153 (*synth*)

Atta-ur-Rahman, *et al., J. Nat. Prod.*, 1998, **61**, 713-717 (*Orixiarine, Acetoxyedulinine, Ptelefoliarine, Acetoxyptelefoliarine*)

Boyd, D.R. *et al., J.C.S. Perkin 1*, 2000, 3379-3405 (*abs config*)

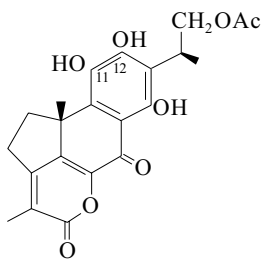
Noshita, T. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 710-713 (*Orixiarine*)

Kumar, R.N. *et al., Heterocycles*, 2002, **57**, 357-360 (*Orixiarine, synth*)

Funayama, S. *et al., CA*, **132**, 262617w (*isol, activity*)

Edulone A E-3

[68421-12-5]



$C_{22}H_{22}O_8$ 414.411

Constit. of *Plectranthus edulis* (oromo dinich). Powder. Mp 153-159° dec.

11,12-Di-Ac:

Yellow cryst. Mp 216-217°.

Buchbauer, G. *et al., Helv. Chim. Acta*, 1978, **61**, 1969 (*isol*)

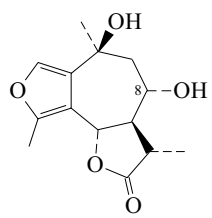
Künzle, J.M. *et al., Helv. Chim. Acta*, 1986, **69**, 1513 (*cryst struct*)

Ef 108 B E-4

Anti-listerial bacteriocin-like substance. Prod. by *Enterococcus faecium* 108.

Dallas, H.L. *et al., J. Food Saf.*, 1996, **16**, 183-199 (*isol*)

Egelolide E-5



$C_{14}H_{18}O_5$ 266.293

8-Ac: [142449-62-5] ***8-Acetylegelolide**. 3-Oxaachillicin*

$C_{16}H_{20}O_6$ 308.33

Constit. of *Achillea millefolium* (yarrow). Cryst. (Et_2O). Mp 219-221°.

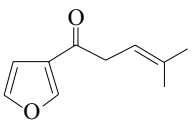
8-Angeloyl: [142449-63-6] ***8-Angeloylege-***

lolide. *8α-Angeloyloxy-3-oxaartabsin*
$C_{19}H_{24}O_6$ 348.395
Constit. of *Achillea millefolium* (yarrow). Cryst. (Et_2O). Mp 152-154°. $[\alpha]_D^{20}$ +5.8 (c, 0.34 in $CHCl_3$).

8-Tigloyl: [158649-42-4] ***8α-Tigloyloxy-3-oxaartabsin***
$C_{19}H_{24}O_6$ 348.395
Ochir, G. *et al., Phytochemistry*, 1991, **30**, 4163-4165 (*isol, pmr, cmr*)
Schröder, H. *et al., Phytochemistry*, 1994, **36**, 1449-1451 (*struct, bibl*)

Egomaketone E-6

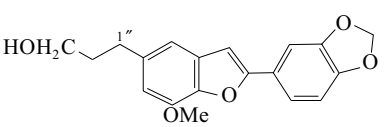
[59204-74-9]
1-(3-Furanyl)-4-methyl-3-penten-1-one, 9CI. 3-(4-Methyl-3-pentenoyl)furan



$C_{10}H_{12}O_2$ 164.204
Constit. of *Perilla frutescens* (perilla).
Cryst. Mp 17°. Bp_{13} 116-117°.
▶ LD_{50} (mus, ipr) 10 mg/kg. JX2580000
Hoppmann, A. *et al., Tetrahedron*, 1978, **34**, 1723 (*synth*)
Gosselin, P. *et al., J.O.C.*, 1979, **44**, 2807 (*synth*)
Koyangi, J. *et al., J. Nat. Prod.*, 1995, **58**, 1955 (*synth*)

Egonol E-7

[530-22-3]
2-(1,3-Benzodioxol-5-yl)-7-methoxy-5-benzofuranpropanol, 9CI. 5-(2-Hydroxypropyl)-7-methoxy-2-(3,4-methylenedioxyphenyl)benzofuran



$C_{19}H_{18}O_5$ 326.348
Norneolignans. Prod. by *Laetiporus sulphureus* var. *miniatus*. Plates (butanol). Mp 117.5-118°.

O-*β*-D-*Glucopyranoside:* [77690-83-6] *Egonol glucoside*
$C_{25}H_{28}O_{10}$ 488.49
Prod. by *Laetiporus sulphureus* var. *miniatus*. Brown needles (EtOH). Mp 169-170°. $[\alpha]_D^{22}$ -15.2 (c, 0.6 in MeOH).

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Matsutakeside I.*** *Egonol primeveroside*
$C_{30}H_{36}O_{14}$ 620.606
Isol. from the fungus *Laetiporus sulphureus* var. *miniatus*. Amorph. powder. $[\alpha]_D^{25}$ -19.9 (c, 2.6 in MeOH). λ_{max} 210 (log ϵ 4.49); 233 (log ϵ 4.46); 278 (log ϵ 4.17) (MeOH).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:Egonol gentiobioside*
$C_{31}H_{38}O_{15}$ 650.632
Prod. by *Laetiporus sulphureus* var. *miniatus*. Cryst. (EtOAc/petrol) (as hepta-Ac). Mp 147-149° (hepta-Ac).
Poss. identical with an egonol glycoside Mp 143°, $[\alpha]_D^{21}$ -29.8°, earlier isol. from *S. formosanus*.

Demethoxy: [53279-35-9] ***Demethoxyegonol.*** *2-(1,3-Benzodioxol-5-yl)-5-benzofuranpropanol. 5-(3-Hydroxypropyl)-2-(3,4-methylenedioxyphenyl)benzofuran*
$C_{18}H_{16}O_4$ 296.322
Prod. by *Laetiporus sulphureus* var. *miniatus*. Needles (MeOH aq.). Mp 124-125° (118-119°). λ_{max} 214 (ϵ 35200); 317 (ϵ 32300); 331 (ϵ 26200) (EtOH).
Takanashi, M. *et al., Chem. Lett.*, 1974, 869-871 (*Demethoxyegonol*)
Anil, H. *et al., Phytochemistry*, 1980, **19**, 2784 (*glycosides*)
Takanashi, M. *et al., Phytochemistry*, 1988, **27**, 1224 (*derivs*)
Aoyagi, Y. *et al., Heterocycles*, 1995, **41**, 1077 (*synth*)
Mali, R.S. *et al., J. Chem. Res., Synop.*, 1998, 230-231 (*synth*)
Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 327-329 (*Matsutakeside I*)

2,4-Eicosadienoic acid, 9CI E-8

[25448-01-5, 32839-28-4]
2,4-Icosadienoic acid
$H_3C(CH_2)_{14}CH{=}CHCH{=}CHCOOH$
$C_{20}H_{36}O_2$ 308.503

(E,E)-form [38225-16-0]
2-Methylpropylamide: [54794-71-7] N-*(2-Methylpropyl)-2,4-eicosadienamide, 9CI. 2,4-Eicosadienoic acid isobutylamide. 2,4-Icosadienoic acid isobutylamide.* **N-*Isobutyl-2,4-eicosadienamide***
$C_{24}H_{45}NO$ 363.626
Cryst. (EtOAc). Mp 68° Mp 89-90°.

Piperidide: [74267-84-8] *1-(1-Oxo-2,4-eicosadienyl)piperidine, 9CI.* **N-*(2,4-Eicosadienoyl)piperidine.*** *2,4-Eicosadienoic acid piperidide*
$C_{25}H_{45}NO$ 375.637
Alkaloid from *Piper retrofractum* (Javanese long pepper). λ_{max} 265 (log ϵ 4.1) (MeOH).

Pyrrolidide: See Trichonine in *The Combined Chemical Dictionary.*

[38306-23-9]
Vig, B. *et al., Indian J. Chem.*, 1972, **10**, 564; 1975, **13**, 1358-1359 (*synth*)
Okogun, J.I. *et al., J.C.S. Perkin 1*, 1974, 2195-2198 (*2-methylpropylamide, isol*)
Addae-Mensah, I. *et al., Phytochemistry*, 1977, **16**, 483-485 (*isol, ir, pmr, ms, struct, 2-methylpropylamide*)
Vig, B. *et al., J. Indian Chem. Soc.*, 1979, **56**, 935-937 (*synth, piperidide*)
Kikuzaka, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1329-1333 (*isol, piperidide*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419-432 (*synth*)

2,14-Eicosadienoic acid E-9

$H_3C(CH_2)_4CH{=}CH(CH_2)_{10}CH{=}CHCOOH$
$C_{20}H_{36}O_2$ 308.503

(2E,14Z)-form
Piperidide: [151391-74-1] **N-*(2,14-Eicosadienoyl)piperidine.*** *2,14-Eicosadienoic acid piperidide*
$C_{25}H_{45}NO$ 375.637
Alkaloid from *Piper retrofractum* (Javanese long pepper). Oil. λ_{max} 212 (log ϵ 3.81) (MeOH).
Kikuzaki, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1329-1333

11,14-Eicosadienoic acid E-10

[60362-00-7]
[2091-39-6, 25448-01-5, 32839-28-4]
11,14-Icosadienoic acid
$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_9COOH$
$C_{20}H_{36}O_2$ 308.503
Sol. Me_2CO, hexane; poorly sol. H_2O.
$Bp_{0.08}$ 198°.

(Z,Z)-form [5598-38-9]
Isol. from lipids of *Ginkgo biloba* (ginkgo).

14S,15R-Epoxide: [64019-95-0] *13-(3-Pentyloxiranyl)-11-tridecenoic acid, 9CI. 14,15-Epoxy-11-eicosenoic acid.* ***Alchornoic acid***
Karrer, P. *et al., Helv. Chim. Acta*, 1943, **26**, 619 (*synth*)
Ito, S. *et al., Bull. Chem. Soc. Jpn.*, 1963, **36**, 1439 (*isol, uv, ir, struct*)
Williams, M.A. *et al., Biochem. Biophys. Res. Commun.*, 1973, **54**, 1560 (*isol*)
Spener, F. *et al., Chem. Phys. Lipids*, 1973, **11**, 215 (*synth*)
Sung-Kee, C. *et al., Tet. Lett.*, 1974, 3023 (*synth*)
Bardyshev, I.I. *et al., CA*, 1975, **83**, 166073q (*isol*)
Kleiman, R. *et al., Lipids*, 1977, **12**, 610 (*Alchornoic acid*)

1,20-Eicosanediol, 9CI E-11

[7735-43-5]
1,20-Icosanediol
$HOCH_2(CH_2)_{18}CH_2OH$
$C_{20}H_{42}O_2$ 314.551
Occurs in Carnauba wax and apple wax.
Cryst. (C_6H_6 or EtOH). Mp 111-112° (103°). $Bp_{1.5}$ 215-217°.

Di-Ac:
$C_{24}H_{46}O_4$ 398.625
Mp 64.5°.
Chuit, P. *et al., Helv. Chim. Acta*, 1929, **12**, 850 (*synth*)
Kimura, K. *et al., Chem. Pharm. Bull.*, 1960, **8**, 1059 (*di-Ac*)
Nakaya, T. *et al., Makromol. Chem.*, 1987, **188**, 265 (*synth*)
Percec, V. *et al., Macromolecules*, 1990, **23**, 3509 (*synth, pmr*)
Weiper-Idelmann, A. *et al., Acta Chem. Scand.*, 1998, **52**, 672-682 (*synth, ir, pmr, ms*)

4,6-Eicosanedione E-12

4,6-Icosanedione
$H_3C(CH_2)_{13}COCH_2COCH_2CH_2CH_3$
$C_{20}H_{38}O_2$ 310.519
Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-eicosanone
$C_{20}H_{40}O_2$ 312.535
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

5,7-Eicosanedione E-13

5,7-Icosanedione

$H_3C(CH_2)_{12}COCH_2CO(CH_2)_3CH_3$

$C_{20}H_{38}O_2$ 310.519

Constit. of the pollen of *Helianthus annuus* (sunflower).

5-Alcohol:5-Hydroxy-7-eicosanone

$C_{20}H_{40}O_2$ 312.535

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

6,8-Eicosanedione E-14

6,8-Icosanedione

$H_3C(CH_2)_{11}COCH_2CO(CH_2)_4CH_3$

$C_{20}H_{38}O_2$ 310.519

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

Eicosanoic acid E-15

[506-30-9]

Arachidic acid. Icosanoic acid. Arachic acid

$H_3C(CH_2)_{18}COOH$

$C_{20}H_{40}O_2$ 312.535

Constit. of arachis (*Arachis hypogaea*) (ground-nut) oil glycerides. Cryst. (EtOH). Sol. $CHCl_3$, hexane; poorly sol. H_2O. Mp 77°. Bp_1 203-205°.

►JX3780000

Me ester: [1120-28-1]

$C_{21}H_{42}O_2$ 326.562

Mp 45.8-46.3°. Bp_{10} 215-216° Bp_2 188°.

Et ester: [18281-05-5]

$C_{22}H_{44}O_2$ 340.588

Mp 41.4-42°. Bp_{100} 295-297° Bp_2 186-187°.

Amide:

$C_{20}H_{41}NO$ 311.55

Mp 109°.

Nitrile:

$C_{20}H_{39}N$ 293.535

Mp 49.5°.

Hexacosyl ester: [17318-45-5] *Hexacosyl eicosanoate*

$C_{46}H_{92}O_2$ 677.232

Heptadecyl ester: [36610-58-9] *Heptadecyl eicosanoate*

$C_{37}H_{74}O_2$ 550.99

Mp 62.8-63.2°.

[14923-81-0]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 758A (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 486A; 610A (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 632B (*ir*)

Adam, N.K. *et al., J.C.S.*, 1925, **127**, 72 (*synth*)

Sy, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **239**, 1813 (*synth*)

Radler, F. *et al., Aust. J. Chem.*, 1965, **18**, 1059 (*isol*)

Marosi, L. *et al., Annalen*, 1973, 584 (*props, cryst struct*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAF000

5,8,11,14,17-Eicosapentaenoic acid E-16

[1553-41-9]

[25378-27-2, 32839-30-8]

5,8,11,14,17-Icosapentaenoic acid. EPA

$H_3CCH_2(CH{=}CHCH_2)_5CH_2CH_2COOH$

$C_{20}H_{30}O_2$ 302.456

Component of Omega-3 Marine Triglycerides, O-156.

►JX3830000

(all-Z)-form [10417-94-4]

Timnodonic acid. *Icosapent, INN*

Present in fish oils as an acylglycerol and in animal phospholipids. Nutriceutical with antioxidation props.. Oil. Launched 1990

Et ester: [86227-47-6] *Ethyl icosapentate, JAN. Ethyl EPA. MND 21*

$C_{22}H_{34}O_2$ 330.509

Isol. from fish oils.

[2734-47-6, 84494-70-2]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 786A (*nmr*)

Teshima, S. *et al., CA*, 1978, **89**, 193306 (*isol, nmr*)

Von Schacky, C. *et al., J. Clin. Invest.*, 1985, **76**, 2446 (*metab, pharmacol*)

Eur. Pat., 1988, 292 846; *CA*, **111**, 63962 (*isol, Et ester*)

Corey, E.J. *et al., J.O.C.*, 1988, **53**, 5980 (*synth, ir, pmr, ms*)

Viala, J. *et al., Tet. Lett.*, 1992, **33**, 4897 (*synth*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 991

Vatele, J.-M. *et al., Chem. Phys. Lipids*, 1995, **78**, 65 (*synth*)

Sandri, J. *et al., J.O.C.*, 1995, **60**, 6627 (*synth, ir*)

Suzuki, M. *et al., Phytochemistry*, 1996, **43**, 63 (*isol*)

5,8,11,14-Eicosatetraenoic acid E-17

[7771-44-0]

[27400-91-5]

5,8,11,14-Icosatetraenoic acid

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_3COOH$

$C_{20}H_{32}O_2$ 304.472

►JX3850000

(all-Z)-form [506-32-1]

[31152-45-1]

Arachidonic acid

Essential fatty acid. Constit. of many animal phospholipids. Mp -49.5°. Bp_1 163°.

►Potentially explosive. LD_{50} (mus, ivn) 33 mg/kg. CE6675000

[6610-25-9, 77297-91-7]

Osbond, J.M. *et al., J.C.S.*, 1961, 2779 (*synth*)

Schlenk, H. *et al., J. Am. Oil Chem. Soc.*, 1965, **42**, 481 (*occur*)

Wagner, H. *et al., Naturwissenschaften*, 1965, **52**, 305 (*occur*)

Frost, D.J. *et al., Chem. Phys. Lipids*, 1975, **15**, 53 (*pmr*)

Fryer, R.I. *et al., J.O.C.*, 1975, **40**, 348 (*synth*)

Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1976, **17**, 1 (*cmr*)

Corey, E.J. *et al., Tet. Lett.*, 1984, **25**, 2729 (*purifn*)

Tanaka, Y. *et al., Arch. Biochem. Biophys.*, 1988, **263**, 178 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQS750

2,4,8-Eicosatrienoic acid E-18

[27070-56-0]

2,4,8-Icosatrienoic acid

$H_3C(CH_2)_{10}CH{=}CHCH_2CH_2(CH{=}CH)_2COOH$

$C_{20}H_{34}O_2$ 306.487

(2E,4E,8Z)-form

2-Methylpropylamide: [64543-30-2] ***2,4,8-Eicosatrienoic acid isobutylamide***. N-*Isobutyl-2,4,8-eicosatrienamide*

$C_{24}H_{43}NO$ 361.61

Alkaloid from *Piper officinarum* (Javanese long pepper). Mp 67-67.5°.

Gupta, O.P. *et al., Phytochemistry*, 1977, **16**, 1436 (*uv, ir, pmr, ms, isol, struct*)

2,4,14-Eicosatrienoic acid E-19

2,4,14-Icosatrienoic acid

$H_3C(CH_2)_4CH{=}CH(CH_2)_8CH{=}CHCH{=}CHCOOH$

$C_{20}H_{34}O_2$ 306.487

(2E,4E,14Z)-form

2-Methylpropylamide: [151391-70-7] ***2,4,14-Eicosatrienoic acid isobutylamide***. N-*Isobutyl-2,4,8-eicosatrienamide*

$C_{24}H_{43}NO$ 361.61

Alkaloid from *Piper retrofractum* (Javanese long pepper). Oil. λ_{max} 264 (log ϵ 4.19) (MeOH).

Kikuzaki, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1329-1333

2,4,16-Eicosatrienoic acid E-20

[27070-56-0]

2,4,16-Icosatrienoic acid

$H_3CCH_2CH_2CH{=}CH(CH_2)_{10}CH{=}CHCH{=}CHCOOH$

$C_{20}H_{34}O_2$ 306.487

(2E,4E,16Z)-form

Piperidide: [145237-20-3] ***Pipereicosalidine***

$C_{25}H_{43}NO$ 373.621

Alkaloid from fruits of *Piper retrofractum* (Javanese long pepper). Oil.

Ahn, J.W. *et al., Phytochemistry*, 1992, **31**, 3609

5,11,14-Eicosatrienoic acid E-21

[15541-36-3]

[27070-56-0]

5,11,14-Icosatrienoic acid

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_4CH{=}CH(CH_2)_3COOH$

$C_{20}H_{34}O_2$ 306.487

(all-Z)-form [7019-85-4]

[80558-45-8]

Sciadonic acid. *Podocarpic acid (obsol.)*

Isol. from tall oil (*Pinus sylvestris*) and from *Ginkgo biloba* (ginkgo).

[20182-93-8]

Ito, S. *et al., Bull. Chem. Soc. Jpn.*, 1963, **36**, 1439 (*isol, uv, ir*)

Gellerman, J.L. *et al., Experientia*, 1963, **19**, 522 (*isol*)
Takagi, T. *et al., Lipids*, 1982, **17**, 716 (*occur, glc, cmr*)
Wolff, R.L. *et al., J. Am. Oil Chem. Soc.*, 1999, **76**, 1515-1516 (*rev*)

10-Eicosene E-22

[66587-45-9]
10-Icosene
$H_3C(CH_2)_8CH{=}CH(CH_2)_8CH_3$
$C_{20}H_{40}$ 280.536
Isol. from *Rosa damascena* (Bulgarian rose oil). Oil.

[78999-41-4, 78999-42-5]

Kovats, E. *et al., J. Chromatogr.*, 1987, **406**, 185 (*isol*)
Collazo, L.R. *et al., J.O.C.*, 1993, **58**, 43 (*synth, ir, ms, pmr, cmr*)

11-Eicosenoic acid, 9CI E-23

[2462-94-4]

[26764-41-0]
11-Icosenoic acid
$H_3C(CH_2)_7CH{=}CH(CH_2)_9COOH$
$C_{20}H_{38}O_2$ 310.519
(*E*)-*form* [62322-84-3]
Mp 49-51°.
(Z)-*form* [5561-99-9]

[28933-89-3]
Gondoic acid
Constit. of rape oil and fish oils as glyceride. Also in other plant oils, e.g. false flax (*Camelina sativa*), and swede (*Brassica napobrassica*). Cryst. (Me_2CO/hexane). Mp 24-25°.

Me ester: [2390-09-2]
$C_{21}H_{40}O_2$ 324.546
Mp -45°.
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 783C; 988B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 686A (*ir*)
Fieser, L.F. *et al., J.A.C.S.*, 1948, **70**, 71 (*synth*)
Argoudelis, C.J. *et al., Lipids*, 1968, **3**, 379 (*struct, ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 742 (*occur*)
Spencer, F. *et al., Chem. Phys. Lipids*, 1973, **11**, 215 (*synth*)

13-Eicosenoic acid, 9CI E-24

[14134-51-1]

[26764-41-0]
13-Icosenoic acid
$H_3C(CH_2)_5CH{=}CH(CH_2)_{11}COOH$
$C_{20}H_{38}O_2$ 310.519
(*Z*)-*form* [17735-94-3]

[28933-89-3]
Paullinic acid
Isol. from herring oil and rapeseed oil and from various Sapindaceae.

[69119-92-2, 69120-02-1, 82683-17-8]

Kishimoto, Y. *et al., J. Lipid Res.*, 1964, **5**, 98 (*isol, struct*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Richter, I. *et al., Z. Naturforsch., C*, 1978, **33**, 629 (*synth*)
Yu, Q.T. *et al., Lipids*, 1989, **24**, 79 (*ms*)
Spitzer, V. *et al., Phytochemistry*, 1996, **42**, 1357 (*isol*)

11-Eicosen-1-ol, 9CI E-25

[87268-65-3]
11-Icosen-1-ol
$H_3C(CH_2)_7CH{=}CH(CH_2)_9CH_2OH$
$C_{20}H_{40}O$ 296.535
(*E*)-*form* [68760-58-7]
Cryst. (hexane). Mp 43-44°.
(*Z*)-*form* [62442-62-0]
Present in seeds of *Simmondsia chinensis* (jojoba). Plates (pentane at -10°). Mp 25-26°.

Ac:
$C_{22}H_{42}O_2$ 338.573
Cryst. (pentane at -10°). Mp 19.5°.
Kobayashi, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1973 (*synth, ir, glc, pmr, acetate*)
Shani, A. *et al., J. Chem. Ecol.*, 1979, **5**, 557 (*pmr*)
Pickett, J.A. *et al., J. Chem. Ecol.*, 1982, **8**, 163 (*glc, ms*)
Tagabi, T. *et al., Lipids*, 1985, **20**, 675 (*glc*)
Andersen, J.F. *et al., J. Chem. Ecol.*, 1988, **14**, 1153-1162 (*Z-form, isol, pmr, ms*)
Pederson, R.L. *et al., Adv. Synth. Catal.*, 2002, **344**, 728-735 (*synth*)

3-Eicosyne E-26

[61886-66-6]
3-Icosyne
$H_3C(CH_2)_{15}C{\equiv}CCH_2CH_3$
$C_{20}H_{38}$ 278.52
Constit. of *Basella rubra* (Malabar spinach).

Kameoka, H. *et al., J. Food Compos. Anal.*, 1991, **4**, 315 (*isol*)
Jiang, Z. *et al., CA*, 1994, **121**, 5163g (*isol*)

5-Eicosyne E-27

[74685-31-7]
5-Icosyne
$H_3C(CH_2)_{13}C{\equiv}C(CH_2)_3CH_3$
$C_{20}H_{38}$ 278.52
Constit. of the essential oil of *Basella rubra* (Malabar spinach).

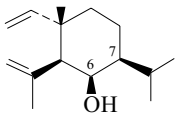
Kameoka, H. *et al., J. Food Compos. Anal.*, 1991, **4**, 315; *CA*, **116**, 127288u (*isol, ir, ms*)

9-Eicosyne E-28

[71899-38-2]
9-Icosyne
$H_3C(CH_2)_9C{\equiv}C(CH_2)_7CH_3$
$C_{20}H_{38}$ 278.52
Constit. of *Basella rubra* (Malabar spinach).

Busker, E. *et al., Org. Mass Spectrom.*, 1979, **14**, 222 (*ms*)
Kameoka, H. *et al., J. Food Compos. Anal.*, 1991, **4**, 315 (*isol*)
Jiang, Z. *et al., CA*, 1994, **121**, 5163g (*isol*)

1,3-Elemadien-6-ol E-29



Absolute configuration

$C_{15}H_{26}O$ 222.37
6β-*form* [35727-45-8]
Shyobunol
Constit. of a *Galbanum* absolute. Oil. $[\alpha]_D^{20}$ -9.3 (c, 1.1 in $CHCl_3$).

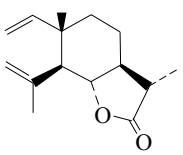
Ac:
$C_{17}H_{28}O_2$ 264.407
Constit. of *Galbanum* absolute. Oil. $[\alpha]_D^{20}$ +7.4 (c, 2.1 in $CHCl_3$).

6-Ketone: [21698-44-2] *1,3-Elemadien-6-one.* ***Shyobunone***
$C_{15}H_{24}O$ 220.354
Constit. of the rhizome of *Acorus calamus* (sweet flag). Oil.

Ketone, 7-epimer: [39020-72-9] ***Epishyobunone***. epi-*Shyobunone*
$C_{15}H_{24}O$ 220.354
Constit. of the rhizome of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D^{20}$ -179 (c, 1.4 in $CHCl_3$).

Yamamura, S. *et al., Tetrahedron*, 1971, **27**, 5419; 5987 (*isol, struct, synth*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1978, **61**, 2671 (*isol, struct*)
Frater, G. *et al., Helv. Chim. Acta*, 1978, **61**, 2709 (*synth, struct*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)

1,3-Elemadien-12,6-olide E-30

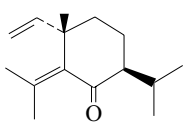


$C_{15}H_{22}O_2$ 234.338
(6α,11α)-*form* [23527-07-3]
Saussurea lactone
From costus root oil (*Saussurea lappa*), probably formed by pyrolysis of Dihydrocostunolide. Cryst. (MeOH). Mp 148-149°. $[\alpha]_D$ +66 ($CHCl_3$).

Rao, A.S. *et al., Tetrahedron*, 1961, **13**, 319 (*struct*)
Masayoshi, A. *et al., Chem. Lett.*, 1978, 617, (*synth*)
Ando, M. *et al., J.O.C.*, 1983, **48**, 1210 (*synth*)
Blay, G. *et al., Can. J. Chem.*, 1992, **70**, 817 (*synth*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)

1,4-Elemadien-6-one E-31

[21698-46-4]
Isoshyobunone



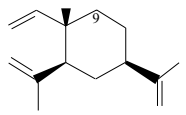
Absolute configuration

$C_{15}H_{24}O$ 220.354
Constit. of the rhizomes of *Acorus calamus* (sweet flag). Oil.

Iguchi, M. *et al., Tet. Lett.*, 1968, 5315 (*isol, struct*)
Alexandre, C. *et al., Bull. Soc. Chim. Fr.*, 1977, 117 (*synth*)
Niwa, M. *et al., Chem. Lett.*, 1977, 1415 (*abs config*)

1,3,11-Elematriene E-32

[33880-83-0]
β-Elemene



(−)-*form*

$C_{15}H_{24}$ 204.355

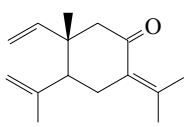
(+)-*form*
Poorly sol. hexane. $[\alpha]_D$ +14.2. n_D^{20} 1.4945.
▶ LD_{50} (mus, ipr) 278.7 mg/kg.

(-)-*form* [515-13-9]
Constit. of sweet-flag and juniper oils, *Mentha* spp.. Oil. $Bp_{15.5}$ 117-124°. $[\alpha]_D^{20}$ -11.1 ($CHCl_3$).
▶ GU9660000

Pigulevskii, G.V. *et al., J. Org. Chem. USSR (Engl. Transl.)*, 1962, **32**, 3054 (*isol*)
Irie, T. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 1053 (*isol, ir, pmr*)
Hunter, G.L.K. *et al., J. Food Sci.*, 1964, **29**, 25 (*isol*)
Patil, L.J. *et al., Tet. Lett.*, 1967, 2273 (*synth*)
McMurry, J.E. *et al., Tet. Lett.*, 1985, **26**, 2171 (*synth*)
Wang, X.-W. *et al., Drugs of the Future*, 1998, **23**, 266-270 (*rev*)
Duh, C.Y. *et al., J. Nat. Prod.*, 1999, **62**, 1518 (*isol, activity*)
Kozmin, S.A. *et al., J.A.C.S.*, 1999, **121**, 9562-9573 (*synth*)
Kim, D. *et al., Tetrahedron*, 2001, **57**, 1247-1252 (*synth*)

1,3,7(11)-Elematrien-8-one E-33

[20303-60-0]
β-Elemenone

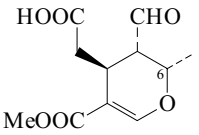


$C_{15}H_{22}O$ 218.338
Constit. of *Myrica gale* (bog myrtle). Oil. $[\alpha]_D$ +46 (c, 0.8 in $CHCl_3$).

Naya, Y. *et al., Heterocycles*, 1978, **10**, 29 (*isol*)
Fujisawa, T. *et al., Chem. Lett.*, 1983, 1533 (*synth*)
Yoshikoshi, A. *et al., Chem. Lett.*, 1990, 151 (*synth*)
Kato, M. *et al., J.O.C.*, 1991, **56**, 7071 (*synth, pmr*)

Elenaic acid E-34

[34422-12-3]
*3-Formyl-3,4-dihydro-5-(methoxycarbonyl)-2-methyl-2*H*-pyran-4-acetic acid, 9CI. Elenolic acid*



$C_{11}H_{14}O_6$ 242.228
Isol. from olives (*Olea europaea*) leaves and fruits. $[\alpha]_D$ -77.7 ($CHCl_3$). λ_{max} 239 (ε 10729) (EtOH) (Berdy).

Me ester: [58865-06-8]
Oil. $[\alpha]_D^{25}$ -121 (c, 0.68 in $CHCl_3$).

(3,4-Dihydroxyphenylethyl) ester: [50915-70-3]
$C_{19}H_{22}O_8$ 378.378
Isol. from leaves of *Olea europaea* (olive).

6-Epimer: [119816-62-5]
Oil (as Me ester). $[\alpha]_D^{25}$ +78.9 (c, 0.3 in $CHCl_3$) (Me ester).

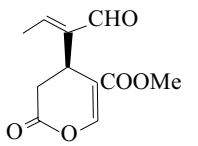
6-Epimer, 2-(3,4-dihydroxyphenylethyl) ester: [102734-62-3]
$C_{19}H_{22}O_8$ 378.378
Isol. from olive leaves (*Olea europaea*).

[58865-08-0]

U.S. Pat., 1962, 3 033 877; *CA*, **58**, 554d (*isol*)
Renis, H.E. *et al., Antimicrob. Agents Chemother.*, 1969, 167 (*pharmacol*)
Kelly, R.C. *et al., J.A.C.S.*, 1973, **95**, 7156 (*synth*)
Brown, R.T. *et al., J.C.S. Perkin 1*, 1976, 160 (*synth*)
Hatakeyama, S. *et al., Tet. Lett.*, 1985, **26**, 865 (*synth*)
Gariboldi, P. *et al., Phytochemistry*, 1986, 865 (*3,4-dihydroxyphenethyl esters, isol, struct*)
Baggiolini, E.G. *et al., Tetrahedron*, 1988, **44**, 3203 (*synth, pmr, ms*)
Takano, S. *et al., Heterocycles*, 1990, **30**, 583 (*synth, bibl*)

Elenolide E-35

[24582-91-0]

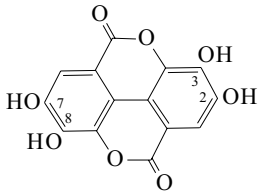


$C_{11}H_{12}O_5$ 224.213
Constit. of olive oil. Cryst. (EtOH). Mp 155-156°. $[\alpha]_D$ +367 ($CHCl_3$).

Tietze, L.F. *et al., Angew. Chem., Int. Ed.*, 1979, **19**, 539 (*isol, struct*)
Brown, R.T. *et al., Chem. Comm.*, 1986, 1818 (*synth*)

Ellagic acid, INN E-36

[476-66-4]
2,3,7,8-Tetrahydroxy[1]benzopyrano[5,4,3-cde][1]benzopyran-5,10-dione, 9CI. Benzoaric acid. Elagostasine. Lagistase. Alizarin yellow. Kajidin. Gallogen†



$C_{14}H_6O_8$ 302.197
CAS numbering shown, other systems freq. used. Parent compd. has 2-fold symmetry with 2 ≡ 7 and 3 ≡ 8. Widely distributed in higher plants esp. dicotyledons. Intestinal astringent, dietary role disputed. Nutriceutical with anticancer and antioxidation props.. No longer marketed. Yellow needles + 2Py (Py). Spar. sol. H_2O, EtOH; insol. Et_2O; sol. hot Py. Mp 360°. Log P 0.26 (calc). λ_{max} 257 (ε 10000); 292 (ε 20000) (EtOH/NaOH) (Derep). λ_{max} 255 (ε 39800); 362 (ε 8510) (EtOH) (Derep). λ_{max} 235 (ε 39800); 366 (ε 8511) (MeOH) (Berdy).
▶ Exp. reprod. effects. DJ2620000

2-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [2455-85-8] ***Amritoside***
$C_{26}H_{26}O_{18}$ 626.481
Isol. from guava (*Psidium guajava*). Platelets (EtOH). Mp 248-250°. $[\alpha]_D^{25}$ -41.4 (Py).

3-Me ether, 8-O-α-L-rhamnopyranoside:
$C_{21}H_{18}O_{12}$ 462.366
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Yellow powder. λ_{max} 246 (log ε 4.6); 260 (sh) (log ε 4.5); 285 (sh) (log ε 4); 360 (sh) (log ε 3.9); 375 (log ε 4) (MeOH).

3-Me ether, 8-O-(2-O-acetyl-α-L-rhamnopyranoside):
$C_{23}H_{20}O_{13}$ 504.403
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Yellow powder. Possible artifact.

3-Me ether, 8-O-(3-O-acetyl-α-L-rhamnopyranoside):
$C_{23}H_{20}O_{13}$ 504.403
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Yellow powder. Possible artifact.

3-Me ether, 8-O-(4-O-acetyl-α-L-rhamnopyranoside):
$C_{23}H_{20}O_{13}$ 504.403
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Yellow powder. Possible artifact λ_{max} 246 (log ε 4.6); 260 (sh) (log ε 4.5); 285 (sh) (log ε 4); 360 (sh) (log ε 4); 375 (log ε 4) (MeOH).

2,3-Di-Me ether: [52600-48-3] ***2,3-Di-O-methylellagic acid***
$C_{16}H_{10}O_8$ 330.25
Constit. of the Chinese tallowtree (*Sapium sebiferum*). Cryst. (DMF). Mp >360°.

2,8-Di-Me ether: [57499-59-9] ***2,8-Di-O-methylellagic acid***
$C_{16}H_{10}O_8$ 330.25
Constit. of the Java plum (*Eugenia jambolana*).

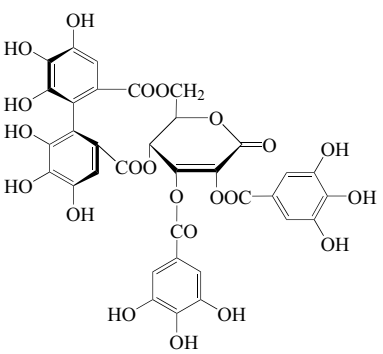
3,8-Di-Me ether, 2-O-[β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:
[113963-57-8]

$C_{28}H_{30}O_{18}$ 654.534
Constit. of the stem bark of *Diospyros discolor* (mabolo).

Perkin, A.G. *et al., J.C.S.*, 1905, **87**, 1412-1430 (*synth*)
Zetzsche, F. *et al., Helv. Chim. Acta*, 1931, **14**, 240-242 (*synth*)
Nierenstein, M. *et al., Helv. Chim. Acta*, 1931, **14**, 912 (*synth*)
Bate-Smith, E.C. *et al., Chem. Ind. (London)*, 1956, R32-R33 (*occur*)
Okuda, T. *et al., Chem. Pharm. Bull.*, 1961, **9**, 178-181 (*isol, deriv*)
Row, L.R. *et al., Tetrahedron*, 1962, **18**, 357-360 (*2,8-di-Me glucoside, isol*)
Seshadri, T.R. *et al., Phytochemistry*, 1965, **4**, 317; 989-992 (*Amritoside*)
Arthur, H.R. *et al., Aust. J. Chem.*, 1969, **22**, 597-600 (*isol*)
Press, R.E. *et al., J. Appl. Chem.*, 1969, **19**, 247 (*props*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1143 (*occur*)
Pradhan, B.P. *et al., Indian J. Chem.*, 1973, **11**, 1220-1221 (*2,3-di-Me ether*)
Yazaki, Y. *et al., Phytochemistry*, 1976, **15**, 1180-1182 (*3-Me ether rhamnoside*)
Doyle, B. *et al., Xenobiotica*, 1980, **10**, 247-256 (*metab*)
Nawwar, M.A.M. *et al., Phytochemistry*, 1982, **21**, 1755-1758; 1994, **36**, 793-798 (*isol, struct, uv, ir, pmr, cmr, 3,8-di-Me ether glucoside*)
Srivastava, S.K. *et al., J. Indian Chem. Soc.*, 1986, **63**, 1004 (*3,8-di-Me ether 2-galactosylglucoside*)
Sato, T. *et al., Phytochemistry*, 1987, **26**, 2124-2125 (*synth, cmr*)
Food and Cancer Prevention: Chemical and Biological Aspects, (ed. Waldron, K.W.), Royal Society of Chemistry, 1993, (*biochem*)
Sato, T. *et al., J. Het. Chem.*, 1997, **34**, 665-667 (*uv, struct*)
Li, X.-C. *et al., Magn. Reson. Chem.*, 1999, **37**, 856-859 (*pmr, cmr*)
Kim, J.-P. *et al., Phytochemistry*, 2001, **57**, 587-591 (*3-Me 8-rhamnoside*)

Emblicanin A E-37

[180465-44-5]

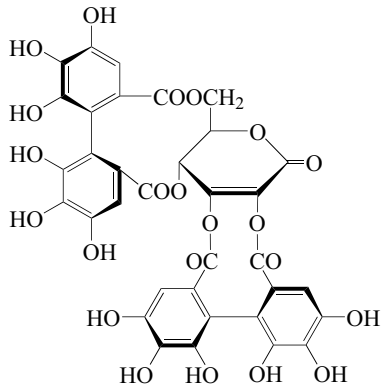


$C_{34}H_{22}O_{22}$ 782.535
Constit. of the fruit of *Emblica officinalis* (emblic). Amorph. powder + $2H_2O$. $[\alpha]_D^{28}$ -5.3 (H_2O). λ_{max} 216 (log ϵ 3.53); 278 (log ϵ 4.02) (MeOH).

Ghosal, S. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 941 (*isol, uv, ir, pmr, ms*)

Emblicanin B E-38

[180465-45-6]



$C_{34}H_{20}O_{22}$ 780.519
Constit. of the fruit of *Emblica officinalis* (emblic). Tan powder + $2H_2O$. $[\alpha]_D^{28}$ -2.8 (H_2O). λ_{max} 218 (log ϵ 3.44); 294 (log ϵ 4.16) (MeOH).

Ghosal, S. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 941 (*isol, uv, ir, pmr, ms*)

Emitanins E-39

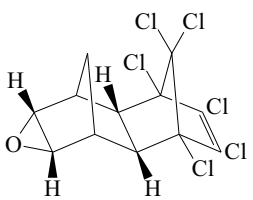
[64641-39-0]

Structs. unknown. A group of antitumour agents prod. by such fungi as *Tricholoma* sp., *Volvariella* sp., *Flammulina* sp., *Pholiota* sp. and *Pleurotus* sp..

Japan. Pat., 1977, 77 79 087; *CA*, **87**, 199155
Ger. Pat., 1978, 2 809 092; *CA*, **90**, 37625
Japan. Pat., 1979, 79 113 495; *CA*, **92**, 92699
Japan. Pat., 1980, 80 68 293; *CA*, **93**, 148116

Endrin, BSI, ESA, ISO, JMAF E-40

[72-20-8]
3,4,5,6,9,9-Hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-2,7:3,6-dimethanonaph[2,3-b]oxirene, 9CI. Hexadrin. Nendrin. OMS 197. ENT 17251

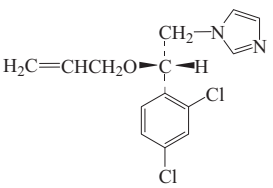


$C_{12}H_8Cl_6O$ 380.911
Stereoisomeric with Dieldrin. Has been found as a contaminant throughout the environment, including foodstuffs, fish, human milk, etc.. Cryst. Sol. Me_2CO, C_6H_6, xylene, spar. sol. CCl_4, hexane.
▶ LD_{50} (rat, orl) 3 mg/kg. LD_{50} (rat, skn) 12 mg/kg. Very toxic if swallowed and in contact with skin. Exp. reprod. and teratogenic effects. OES: long-term 0.1 mg m^{-3}; short-term 0.3 mg m^{-3} (sk). IO1575000

U.K. Pat., 1954, 714 688; *CA*, **50**, 401
U.S. Pat., 1955, 2 705 236; *CA*, **50**, 2680 (*synth*)
Keith, L.H. *et al., Tet. Lett.*, 1971, 3 (*pmr*)
DeLacy, T.P. *et al., J.C.S. Perkin 2*, 1972, 2153 (*cryst struct*)
Biros, F.J. *et al., Org. Mass Spectrom.*, 1972, **6**, 1161; 1171 (*ms*)
IARC Monog., 1974, **5**, 157; *Suppl.* 7, 63 (*rev, tox*)
Roberts, R.L. *et al., J. Agric. Food Chem.*, 1974, **22**, 542 (*cmr*)
Korte, F. *et al., CA*, 1978, **89**, 209992 (*metab*)
Runhaar, E.A. *et al., Hum. Toxicol.*, 1985, **4**, 241 (*tox*)
Handbook of Environmental Fate and Exposure Data for Organic Chemicals, (eds. Howard, P.H.), Lewis Publishers, 1991, **3**, 349 (*environ*)
Pesticide Manual, 9th edn., 1991, No. 5560
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1127
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAT500
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 840 (*tox*)

Enilconazole, BAN, INN E-41

[35554-44-0]
1-[2-(2,4-Dichlorophenyl)-2-(2-propenyloxy)ethyl]-1H-imidazole, 9CI. Imazalil, ANSI, BSI, ISO. Fecundal. Fungaflor. Fungazil. Fung-azil. Imaversol. Nuzone. Deccozil S75. Flo Pro IMZ. R 23979



(*R*)-*form*

$C_{14}H_{14}Cl_2N_2O$ 297.183
Agricultural fungicide. Log P 3.54 (calc).
▶ Eye and skin irritant. LD_{50} (rat, orl) 227 mg/kg. Exp. reprod. effects. NI4776000
(*R*)-*form* [166734-81-2]
$[\alpha]_D^{22}$ -77.9 (c, 9.5 in MeOH).
(*S*)-*form* [166734-82-3]
$[\alpha]_D^{22}$ +81 (c, 13.7 in MeOH). Active isomer.
(±)-*form* [73790-28-0]
Yellow-brown oil. Sl. sol. H_2O. d^{23} 1.24. n_D^{20} 1.5643.
▶ LD_{50} (rat, orl) 227-343 mg/kg.
Sulfate: [60534-80-7] *Imazalil hydrogen sulfate*
Powder. Sol. H_2O.

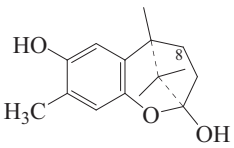
[33586-66-2, 58594-72-2, 61144-39-6, 94659-50-4]

Ger. Pat., 1970, 1 940 388; *CA*, **72**, 90466 (*synth, props*)
Dobrat, W. *et al., Gesunde Pflanz.*, 1979, **31**, 66 (*rev*)
Thienpont, D. *et al., Arzneim.-Forsch.*, 1981, **31**, 309 (*pharmacol, tox*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A230
Chankvetadze, B. *et al., J. Chromatogr., A*, 1995, **700**, 43-49 (*sepn, enantiomers*)
Pesticide Manual, 11th edn., 1997, No. 410
Cabras, P. *et al., J. Agric. Food Chem.*, 1999, **47**, 3352-3354 (*activity*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 377
Pat. Coop. Treaty (WIPO), 2000, 00 38 521, (*Celgene*); *CA*, **133**, 70187e (*synth, isomers*)
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1458

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FPB875

Enokipodin A E-42

[306951-07-5]



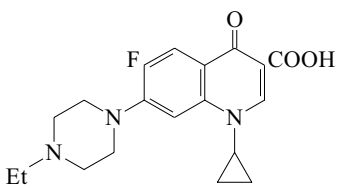
$C_{15}H_{20}O_3$ 248.321
Constit. of *Flammulina velutipes* (velvet shank). Cryst. Mp 138.5-138.9°. $[\alpha]_D^{23}$ +48 (c, 0.5 in MeOH).

8α-Hydroxy: [359701-26-1] ***Enokipodin C***
$C_{15}H_{20}O_4$ 264.321
Constit. of *Flammulina velutipes* (velvet shank). Oil. $[\alpha]_D^{24}$ -9.4 (c, 1 in MeOH). λ_{max} 209 (log ϵ 4.24); 299 (log ϵ 3.63) (MeOH).

Ishikawa, N.K. *et al., Phytochemistry*, 2000, **54**, 777-782 (*isol, pmr, cmr*)
Ishikawa, N.K. *et al., J. Nat. Prod.*, 2001, **64**, 932-934 (*Enokipodin C*)

Enrofloxacin, BAN, INN, USAN E-43

[93106-60-6]
1-Cyclopropyl-7-(4-ethyl-1-piperazinyl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid, 9CI. Baytril. Bay VP 2674



$C_{19}H_{22}FN_3O_3$ 359.399
Vet. antibacterial agent, used in poultry. Mp 219-221°. Log P -0.36 (calc).
▶ LD_{50} (mus, orl) 4336 mg/kg. LD_{50} (mus, ivn) 200 mg/kg. Mutagenic props.. VB1993650

Hydrochloride:
Mp 334-336° dec. (328° dec.).

Grohe, K. *et al., Annalen*, 1987, 29 (*synth*)
Altreuther, P. *et al., Vet. Med. Rev.*, 1987, 87 (*rev, pharmacol, tox*)
Drugs of the Future, 1988, **13**, 305 (*rev*)
Tyczkowska, K. *et al., J. Chromatogr.*, 1989, **493**, 337 (*hplc*)
Tarbin, J.A. *et al., Food Addit. Contam.*, 1992, **9**, 345 (*hplc*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 161
Tyczkowska, K.L. *et al., J. Chromatogr., B: Biomed. Appl.*, 1994, **658**, 341 (*hplc*)
Rutgers, H.C. *et al., Vet. Rec.*, 1994, **135**, 357 (*activity*)

Enterocin CTC 492 E-44

Peptide containing 35 amino acid residues. Bacteriocin active against *Listeria monocytogenes*; can be used in food. Prod. by *Enterococcus faecium* CTC 492.

Pat. Coop. Treaty (WIPO), 1995, 95 06 663; *CA*, **123**, 52160e (*isol*)

Enterocin EL1 E-45

Protein MW, approx. 2300. Prod. by *Enterococcus faecium* EL1 isol. from meat. Bacteriocin.

Lyon, W.J. *et al., J. Food Prot.*, 1995, **58**, 890-898 (*isol*)

Enterocins E-46

Peptides. Prod. by *Enterococcus faecium*. Bacteriocins with food uses.

Enterocin A [194739-76-9]
Prod. by *Enterococcus faecium* T136. Contains 47 amino acid residues.

Enterocin B [194739-77-0]
Prod. by *Enterococcus faecium* T136. Contains 53 amino acid residues.

Enterocin CCM 4231 [208996-20-7]
Prod. by *Enterococcus faecium* CCM 4231.

Enterocin CRL 35 [160829-93-6]
Prod. by *Enterococcus faecium* CRL 35.

Enterocin EJ97 [221191-09-9]
Prod. by *Enterococcus faecium* isol. from municipal waste water.

Enterocin EIA
Prod. by *Enterococcus faecium* EI.

Enterocin L50 [214899-00-0]
Prod. by *Enterococcus faecium* isol. from Spanish dried sausages.

Enterocin P [200359-22-4]
Prod. by *Enterococcus faecium* P13 from a Spanish dry sausage. Contains 44 amino acid residues.

Enterocin 01 [162430-14-0]
Prod. by *Enterococcus faecium* NA01 from fermented skimmed cows' milk products.

Enterocin 4

Enterocin 226NWC [146239-60-3]
Prod. by *Enterococcus faecium* 226NWC from fermented whey cultures.

Enterocin 900 [179530-08-6]
Prod. by *Enterococcus faecium* BFE900 from black olives.

Enterocin 1146 [144377-24-2]
Prod. by *Enterococcus faecium* DPC 1146.

Kramer, J. *et al., J. Gen. Microbiol.*, 1975, **88**, 93-100 (*Enterocin EIA*)
Parente, E. *et al., J. Food Prot.*, 1992, **55**, 497-502 (*Enterocin 1146*)
Viliani, F. *et al., J. Appl. Bacteriol.*, 1993, **74**, 380-387 (*Enterocin 226NWC*)
Olasupo, N.A. *et al., Lett. Appl. Microbiol.*, 1994, **19**, 438-441 (*Enterocin 01*)
Aymerich, T. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 1676-1682 (*Enterocin A*)
Joosten, H.M. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 4220-4223 (*Enterocin 4*)
Franz, C.M.A.P. *et al., Int. J. Food Microbiol.*, 1996, **29**, 255-270 (*Enterocin 900*)
Farias, M.E. *et al., Lett. Appl. Microbiol.*, 1996, **22**, 417-419 (*Enterocin CRL 35*)
Cintas, L.M. *et al., Appl. Environ. Microbiol.*, 1997, **63**, 4321-4330 (*Enterocin P*)
Nunez, M. *et al., J. Appl. Microbiol.*, 1997, **83**, 671-677 (*food use*)
Causus, P. *et al., Microbiology (Reading, U.K.)*, 1997, **143**, 2287-2294 (*Enterocins A, B*)
Galvez, A. *et al., Arch. Microbiol.*, 1998, **171**, 59-65 (*Enterocin EJ97*)
Cintas, L.M. *et al., Food Microbiol.*, 1998, **15**, 289-298 (*Enterocin L50*)
Nilsen, T. *et al., J. Bacteriol.*, 1998, **180**, 1848-1854 (*Enterocin B*)
Laukova, A. *et al., Lett. Appl. Microbiol.*, 1998, **26**, 215-218 (*Enterocin CCM 4231*)

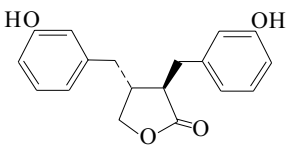
Enterococcin EFS2 E-47

[181186-58-3]
Polypeptide containing 67 amino acid residues. Prod. by *Enterococcus faecalis* EFS2 isol. from a cheese. Bacteriocin.

Maisnier-Patin, S. *et al., Int. J. Food Microbiol.*, 1996, **30**, 255-257 (*isol*)

Enterolactone E-48

[78473-71-9]
*Dihydro-3,4-bis(3-hydroxyphenyl)methyl-2(3*H*)-furanone, 9CI. 2,3-Bis(3-hydroxybenzyl)butyrolactone. HPMF*



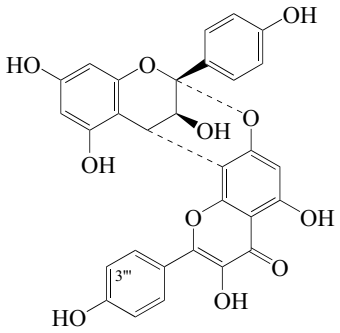
$C_{18}H_{18}O_4$ 298.338
Prod. of intestinal flora acting on lignans present in cereal. Gum. $[\alpha]_D^{20}$ -40.5 (c, 0.62 in $CHCl_3$).

[76721-88-5]

Setchell, K.D.R. *et al., Nature (London)*, 1980, **287**, 740 (*isol, struct, synth, ms, pmr*)
Ganeshpure, P.A. *et al., Chem. Ind. (London)*, 1981, 778 (*synth*)
Pelter, A. *et al., Tet. Lett.*, 1981, 1549 (*synth*)
Axelson, M. *et al., Nature (London)*, 1982, **298**, 659 (*isol*)
Mahalanabis, K.K. *et al., Tet. Lett.*, 1982, **23**, 3975 (*synth*)
Kirk, D.N. *et al., J.C.S. Perkin 1*, 1985, 35 (*synth*)
Bambagiotti-Alberti, M. *et al., Heterocycles*, 1987, **26**, 1735 (*synth*)
Yoda, H. *et al., Tetrahedron*, 1992, **48**, 3313 (*synth, bibl*)
Van Oeveren, A. *et al., J.O.C.*, 1994, **59**, 5999 (*synth*)
Srikrishna, A. *et al., Indian J. Chem., Sect. B*, 1995, **35**, 679 (*synth*)
Chenevert, R. *et al., Can. J. Chem.*, 1999, **77**, 223-226 (*synth*)
Sibi, M.P. *et al., J.O.C.*, 2002, **67**, 1738-1745 (*synth*)
Eklund, P. *et al., Org. Lett.*, 2003, **5**, 491-493 (*synth*)

Ephedrannin A E-49

[82001-39-6]
*3,5,11,13,15-Pentahydroxy-2,8-bis(4-hydroxyphenyl)-8,14-methano-4*H*,14*H*-1-benzopyrano[7,8-*d*][1,3]benzodioxocin-4-one, 9CI. 3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,4′,5,7-tetrahydroxyflavone.*
ent-*Epiafzelechin(2α→*O*-7,4α→8)kaempferol*



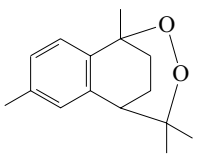
$C_{30}H_{20}O_{11}$ 556.481
Isol. from *Prunus armeniaca* (apricot). Mp 360°. $[\alpha]_D$ -357 (MeOH).

3‴-Hydroxy:3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavone. ent-*Epiafzelechin(2α→O-7,4α→8)quercetin*
$C_{30}H_{20}O_{12}$ 572.481
λ_{max} 232 ; 279 ; 332 ; 379 (MeOH).

Hikino, H. *et al., Tet. Lett.*, 1982, **23**, 673
Bilia, A.R. *et al., Phytochemistry*, 1996, **43**, 887 (*isol, deriv, uv, pmr, cmr, ms*)
Prasad, D. *et al., Fitoterapia*, 1997, **68**, 275-276 (*isol, pmr, cmr*)

10,11-Epidioxycalamene E-50

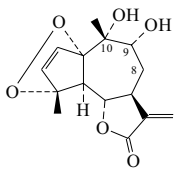
[168207-85-0]
10,12-Peroxycalamenene



$C_{15}H_{20}O_2$ 232.322
Constit. of *Cyperus rotundus* (nutgrass). Needles (hexane). Mp 67-68.5°. $[\alpha]_D^{20}$ -67.2 (c, 0.28 in $CHCl_3$).

Thebtaranonth, C. *et al., Phytochemistry*, 1995, **40**, 125 (*isol, pmr, cmr*)

1,4-Epidioxy-9,10-dihydroxy-2,11(13)-guaiadien-12,6-olide E-51

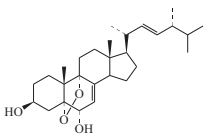


(1α,4α,5α,6α,9α,10α)-*form*

$C_{15}H_{18}O_6$ 294.304
(1α,4α,5α,6α,9α,10α)-*form*
*10-Tigloyl:***α-*Peroxyachifolide***
$C_{20}H_{24}O_7$ 376.405
Constit. of *Achillea millefolium* (yarrow). Needles (EtOH). Mp 154°.

Rücker, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1991, **324**, 979 (*Peroxyachifolides*)

5,9-Epidioxyergosta-7,22-diene-3,6-diol E-52

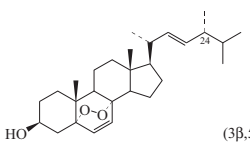


(3β,5α,6α,9α,22*E*,24*R*)-*form*

$C_{28}H_{44}O_4$ 444.653
(3β,5α,6α,9α,22*E*,24*R*)-*form* [348611-55-2]
Amorph. powder. $[\alpha]_D^{23}$ +8.8 (c, 0.1 in $CHCl_3$).
(3β,5α,6β,9α,22*E*,24*R*)-*form* [348611-57-4]
Constit. of *Tricholoma matsutake* (matsutake) and *Lepista nuda* (wood blewit). Amorph. powder. $[\alpha]_D^{19}$ -24.4 (c, 0.08 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2001, **49**, 589-594 (*isol, pmr, cmr*)

5,8-Epidioxyergosta-6,22-dien-3-ol E-53



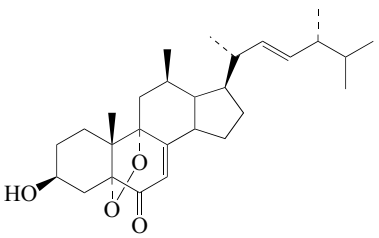
(3β,5α,8α,22*E*,24*R*)-*form*

$C_{28}H_{44}O_3$ 428.654
(3β,5α,8α,22*E*,24*R*)-*form* [2061-64-5]
Ergosterol peroxide. *5α,8α-Peroxyergosterol*
Obt. from leaves of *Ananas comosus* (pineapple). Cryst. (MeOH). Mp 181.5-183° (176-198°). $[\alpha]_D$ -29 (c, 0.8 in $CHCl_3$).
► KE7289000
3-O-β-D-Glucopyranoside: [140447-22-9]
$C_{34}H_{54}O_8$ 590.796
$[\alpha]_D^{25}$ -15.6.
Ac: [23869-16-1]
Cryst. (Me_2CO). Mp 202.5-203.5°. $[\alpha]_D$ -23 (c, 0.65 in $CHCl_3$).
*3-(2-Hydroxy-4-methoxy-6-propylbenzoyl):****5,8-Peroxyergosteryl divaricatinate***
$C_{39}H_{56}O_6$ 620.868
Cryst. (EtOAc). Mp 171-172°.
(3β,5α,8α,22*E*,24*S*)-*form* *5,8-Epidioxycampesta-6,22-dien-3-ol*
Oil.
(3β,5β,8β,22*E*,24*R*)-*form*
3-O-β-D-Glucopyranoside: [348144-81-0]
Constit. of *Lactarius volemus* (tawny milkcap mushroom).
[75197-39-6]

Windaus, A. *et al., Annalen*, 1928, **460**, 225 (*isol*)
Windaus, A. *et al., Z. Phys. Chem.*, 1942, **276**, 280 (*isol, struct*)
Wieland, P. *et al., Helv. Chim. Acta*, 1947, **30**, 1028 (*isol*)
Bauslaugh, G. *et al., Nature (London)*, 1964, **202**, 1218 (*isol*)
Takahashi, R. *et al., Phytochemistry*, 1972, **11**, 1850 (*isol*)
Fattorusso, G. *et al., Gazz. Chim. Ital.*, 1974, **104**, 409
Pakrashi, S.C. *et al., Indian J. Chem.*, 1975, **13**, 755
Gunatilaka, A.A.C. *et al., J.O.C.*, 1981, **46**, 3860
Matsueda, S. *et al., Chem. Ind. (London)*, 1985, 411 (*synth, props*)
Della Greca, M. *et al., Gazz. Chim. Ital.*, 1990, **120**, 391 (*isol, pmr, cmr, bibl*)
Bok, J.W. *et al., Phytochemistry*, 1999, **51**, 891-898 (*glucoside*)
Cantrell, C.L. *et al., Planta Med.*, 1999, **65**, 732-734 (*isol, activity*)
Yue, J.-M. *et al., Phytochemistry*, 2001, **56**, 801-806 (*Lactarius volemus constit*)

5,9-Epidioxy-3-hydroxyergosta-7,22-dien-6-one E-54

5,9-Epidioxy-3-hydroxy-24-methylcholesta-7,22-dien-6-one

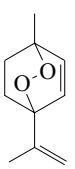


$C_{28}H_{42}O_4$ 442.637
(3β,5α,9α,22*E*,24*R*)-*form* [211486-16-7]
Constit. of *Hypsizygus marmoreus* (bunashimeji) and *Pleurotus ostreatus* (oyster mushroom). Unstable amorph. powder.
22,23-Dihydro: [211486-17-8] ***5,9-Epidioxy-3-hydroxyergost-7-en-6-one****. 5,9-Epidioxy-3-hydroxy-24-methylcholest-7-en-6-one*
$C_{28}H_{44}O_4$ 444.653
Constit. of *Hypsizygus marmoreus* (bunashimeji). Unstable amorph. powder.

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950 (*isol, pmr, cmr*)

1,4-Epidioxy-*p*-mentha-2,8-diene E-55

[120749-17-9]

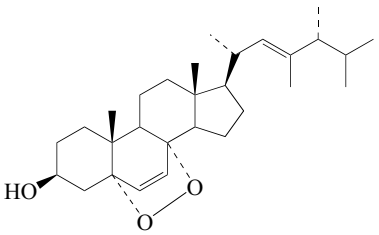


$C_{10}H_{14}O_2$ 166.219
Constit. of parsley leaves (*Petroselinum crispum*).

Nitz, S. *et al., Phytochemistry*, 1989, **28**, 3051 (*isol, pmr, ms, ir*)

5,8-Epidioxy-23-methylergosta-6,22-dien-3-ol E-56

5,8-Epidioxy-23,24-dimethylcholesta-6,22-dien-3-ol



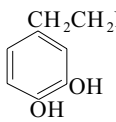
$C_{29}H_{46}O_3$ 442.681

(3β,22*E*,24*R*)-*form* [211486-11-2]
Constit. of *Lentinus edodes* (shiitake). Amorph. powder. $[\alpha]_D^{16}$ -37 (c, 0.05 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950 (*isol, pmr, cmr*)

Epinine E-57

[501-15-5]
4-[2-(Methylamino)ethyl]-1,2-benzenediol, 9CI. 4-[2-(Methylamino)ethyl]pyrocatechol, 8CI. 4-(β-Methylaminoethyl)catechol. N-*Methyl-2-(3,4-dihydroxyphenyl)ethylamine. Deoxyadrenaline. Desoxyepinephrine.* N-*Methyldopamine*



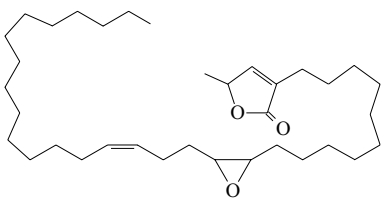
$C_9H_{13}NO_2$ 167.207
Alkaloid from *Vicia faba*. Cryst. (EtOH). Mp 188-189°. Log P 0.16 (calc).

Hydrochloride: [62-32-8]
Prisms (H_2O). Mp 179-180°.
► LD_{50} (mus, ipr) 212 mg/kg. UX1925000
O*4′*-*Phosphate:*N-*Methyldopamine 4*-O-*dihydrogen phosphate. Z 2055*
$C_9H_{14}NO_5P$ 247.187
Mp 175-178° (as hydrochloride).

Pyman, F.L. *et al., J.C.S.*, 1909, 95; 1266; 1610 (*synth*)
Buck, J.S. *et al., J.A.C.S.*, 1930, **52**, 4119 (*synth*)
Bretschneider, H. *et al., Monatsh. Chem.*, 1947, **76**, 335 (*synth*)
Dewhurst, W.G. *et al., Br. J. Pharmacol.*, 1965, **25**, 682 (*pharmacol*)
Path, P.N. *et al., J. Pharmacol. Exp. Ther.*, 1967, **155**, 1 (*pharmacol*)
Tocher, R.D. *et al., Phytochemistry*, 1972, **11**, 1161 (*isol*)
Borgman, R.J. *et al., J. Med. Chem.*, 1973, **16**, 630 (*synth*)
Giesecke, J. *et al., Acta Cryst. B*, 1976, **32**, 2337 (*cryst struct*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*rev, occur*)
Van Woerkens, L.J. *et al., Br. J. Pharmacol.*, 1992, **107**, 303 (*pharmacol*)
Boomsma, F. *et al., J. Chromatogr.*, 1992, **574**, 109 (*hplc*)
Schwinger, R.H.G. *et al., J. Pharmacol. Exp. Ther.*, 1993, **265**, 346 (*pharmacol*)
Ianelli, S. *et al., Acta Cryst. C*, 1995, **51**, 1338 (*cryst struct, phosphate*)
Daul, A. *et al., Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1995, **352**, 429 (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1578
Schwinger, R.H.G. *et al., Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1996, **354**, 343 (*pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAZ000

Epomuricenin B E-58

[152340-40-4]
*5-Methyl-3-[10-[3-(3-octadecenyl)oxiranyl]decyl]-2(5*H*)-furanone, 9CI*

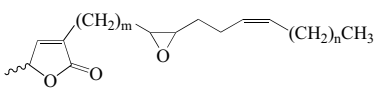


$C_{35}H_{62}O_3$ 530.873
Isol. from the seeds of *Annona muricata* (soursop). Obt. as a mixt. with Epomuricenin A (see Epoxymurin A, E-172).

Roblot, F. *et al., Phytochemistry*, 1993, **34**, 281-285 (*isol, uv, ir, pmr, cmr, ms*)

Epomusenin A E-59

[178330-55-7]



m = 14, n = 11

$C_{37}H_{66}O_3$ 558.927
Constit. of the fruit of *Rollinia mucosa* (biriba). Wax. Isol. as a mixt. with Epomusenin B, E-60 λ_{max} 210 (log ϵ 3.9) (EtOH). λ_{max} 210 (ϵ 7943) (MeOH) (Berdy).

Chen, Y.-Y. *et al., Phytochemistry*, 1996, **42**, 1081-1083 (*isol, uv, ir, pmr, cmr, ms*)

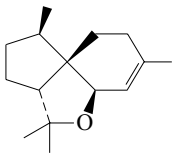
Epomusenin B E-60

[178330-56-8]
As Epomusenin A, E-59 with
m = 12, n = 13
$C_{37}H_{66}O_3$ 558.927
Constit. of the fruit of *Rollinia mucosa* (biriba). Isol. as a wax with Epomusenin A, E-59.

Chen, Y.-Y. *et al., Phytochemistry*, 1996, **42**, 1081-1083 (*isol, uv, ir, pmr, cmr, ms*)

6,11-Epoxy-4-acorene E-61

[104188-25-2]
Italicene ether

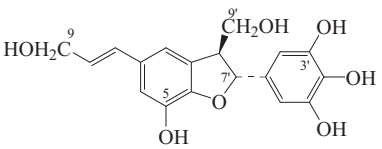


$C_{15}H_{24}O$ 220.354
Constit. of *Helichrysum italicum* (curry plant). Misleading trivial name.

Cool, L.G. *et al., Phytochemistry*, 1994, **36**, 1283 (*isol*)

4,7′-Epoxy-3,8′-bilign-7-ene-3′,4′,5,5′,9,9′-hexol E-62

4,7′-Epoxy-3′,4′,5,5′,9,9′-hexahydroxy-3,8′-bilign-7-ene



(7′*R*,8*E*,8′*S*)-*form*

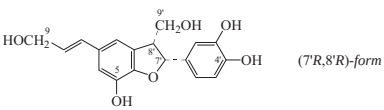
$C_{18}H_{18}O_7$ 346.336
Lignan numbering shown.

(7′*R*,8*E*,8′*S*)-*form*
3′,5,5′-Tri-Me ether, 4′-O-*β*-D-*glucopyranoside:* [217650-81-2] ***Scorzonoside***
$C_{27}H_{34}O_{12}$ 550.558
Constit. of *Scorzonera hispanica* (scorzonera).

Tolstikhina, V.V. *et al., Rastit. Resur.*, 1998, **34**, 77-80; *CA*, **130**, 63632f (*Scorzonoside*)

4,7′-Epoxy-3,8′-bilign-7-ene-3′,4′,5,9,9′-pentol E-63

4,7′-Epoxy-3′,4′,5,9,9′-pentahydroxy-3,8′-bilign-7-ene, 9CI



(7′*R*,8′*R*)-*form*

$C_{18}H_{18}O_6$ 330.337
Lignan numbering shown.

(7′*R*,8′*S*)-*form* [155836-29-6]
3′,5-Di-Me ether, 4′-O-*β*-D-*glucopyranoside:* [107870-87-1]
$C_{26}H_{32}O_{11}$ 520.532
Constit. of *Citrus* spp.. $[\alpha]_D^{20}$ -71.2 (c, 0.56 in MeOH).

(7′*S*,8′*S*)-*form*
3′,5-Di-Me ether, 4′-O-*β*-D-*glucopyranoside:* [96738-84-0]
Constit. of *Fortunella japonica* (round kumquat). Mp 125°.

(7′*R,8′*S**)-*form***
9-Carboxylic acid, 3′,5-di-Me ether, Me ester: [107296-48-0]
$C_{21}H_{22}O_7$ 386.401
Constit. of *Zizyphus jujuba* (Chinese date).

9,9′-Dicarboxylic acid, 3′,5-di-Me ether: [160169-55-1]

[151998-30-0, 180579-78-6] ***3-[3-Carboxy-2,3-***

dihydro-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-5-benzofuranyl]-2-propenoic acid, 9CI. *5-(2-Carboxyvinyl)-2,3-dihydro-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-3-benzofurancarboxylic acid*

$C_{20}H_{18}O_8$ 386.357

Isol. by saponification from wheat bran, cocksfoot, switch grass and cultured corn cells. Antioxidant. Fine cryst. Mp 169-174° dec.

(7′ξ,8′ξ)-*form*

3′,5-Di-Me ether:

$C_{20}H_{22}O_6$ 358.39

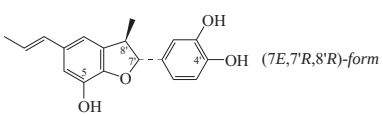
Isol. from *Silybum marianum* (milk thistle). Isolate was dextrorotatory, no stereochem. assigned.

[28199-68-0, 86363-02-2, 97465-82-2, 112835-77-5, 150407-42-4]

Freudenberg, K. *et al., Chem. Ber.*, 1960, **93**, 1354; 1963, **96**, 1265
Kovacik, V. *et al., Chem. Ber.*, 1969, **102**, 3623 (*ms*)
Weinges, K. *et al., Annalen*, 1970, **736**, 170 (*isol*)
Sih, C.J. *et al., J.A.C.S.*, 1976, **98**, 5412 (*synth*)
Arens, H. *et al., Planta Med.*, 1985, 52 (*glucosides*)
Fukuyama, Y. *et al., Planta Med.*, 1986, **501**, 502 (*carboxylic acid derivs*)
Binns, A.N. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1987, **84**, 980 (*glucosides*)
Yoshizawa, F. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1927 (*glucosides*)
Bardon, A. *et al., Phytochemistry*, 1993, **34**, 253-259 (*isol*)
Hirai, N. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1679 (*abs config, resoln*)
Hashimoto, Y. *et al., CA*, 1994, **121**, 251213h
Ralph, J. *et al., J.C.S. Perkin 1*, 1994, 3485-3498 (*diacid-di-Me ether, isol, synth, diacid-di-Me ether-di-Et ester, nmr*)
Garcia-Conesa, M.T. *et al., Biochem. Soc. Trans.*, 1998, **26**, 5166; 5168 (*diacid-di-Me ether, isol, props*)
Ralph, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 2531-2532 (***synth, diacid-di-Me ether-di-Et ester***)
Bolzacchini, E. *et al., Tet. Lett.*, 1998, **39**, 3291-3294 (*diacid-di-Me ether, synth*)
Yuen, M.S.M. *et al., Tetrahedron*, 1998, **54**, 12429-12444 (*abs config*)
Rummakko, P. *et al., Synlett*, 1999, 333-335 (*synth*)
Juhasz, L. *et al., Tet. Lett.*, 2000, **41**, 2491-2494 (*9-carboxylic acid, 9-acid 3,5 di-Me ether Me ester, synth*)

4,7′-Epoxy-3,8′-bilign-7-ene-3′,4′,5-triol E-64

2,3-Dihydro-2-(3,4-dihydroxyphenyl)-7-hydroxy-3-methyl-5-(1-propenyl)benzofuran



(7*E*,7′*R*,8′*R*)-*form*

$C_{18}H_{18}O_4$ 298.338

Lignan numbering shown.

(7*E*,7′*R*,8′*R*)-*form*

5′-Methoxy, 3′,4′,5-tri-Me ether: [60297-83-8] ***Licarin C***

$C_{22}H_{26}O_5$ 370.444

Isol. from nutmeg. Cryst. (MeOH). Mp 100-101°.

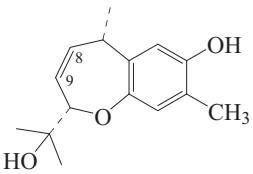
[23342-98-5, 42016-15-9, 56353-18-5]

Braz, R. *et al., Tet. Lett.*, 1976, 1157 (*Licarin C, pmr*)
Davis, D.V. *et al., J. Agric. Food Chem.*, 1982, **30**, 495 (*Licarin C, ms*)

5,10-Epoxy-1,3,5,8-bisabolatetraene-2,11-diol E-65

[161730-07-0]

Heliannuol B



$C_{15}H_{20}O_3$ 248.321

Constit. of *Helianthus annuus* (sunflower). Oil. $[\alpha]_D^{25}$ -18 (c, 0.1 in $CHCl_3$).

8,9-Dihydro: [161730-09-2] *5,10-Epoxy-1,3,5-bisabolatriene-2,11-diol.* ***Heliannuol D***

$C_{15}H_{22}O_3$ 250.337

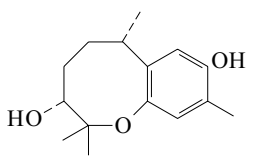
Constit. of *Helianthus annuus* (sunflower). Cryst. ($CHCl_3$). Mp 59-61°. $[\alpha]_D^{25}$ +16 (c, 0.1 in $CHCl_3$).

Macías, F.A. *et al., J.O.C.*, 1994, **59**, 8261-8266 (*isol, pmr, cmr*)
Takabatake, K. *et al., J.C.S. Perkin 1*, 2000, 1807-1808 (*synth, abs config*)
Vyvyan, J.R. *et al., Tet. Lett.*, 2000, **41**, 1151-1154 (*synth*)
Macías, F.A. *et al., Tetrahedron*, 2003, **59**, 1679-1683 (*synth*)

5,11-Epoxy-1,3,5-bisabolatriene-2,10-diol E-66

[148054-17-5]

Heliannuol A



$C_{15}H_{22}O_3$ 250.337

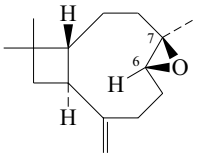
Constit. of *Helianthus annuus* (sunflower). Cryst. ($CHCl_3$). Mp 80-81°. $[\alpha]_D$ -55.4 (c, 0.3 in MeOH). λ_{max} 280 (ϵ) (EtOH) (Derep).

Macías, F.A. *et al., Tet. Lett.*, 1993, **34**, 1999-2002 (*isol, pmr, cmr, cryst struct*)
Grimm, E.L. *et al., Tet. Lett.*, 1994, **35**, 6847-6850 (*(±)-form, synth*)
Takabatake, K. *et al., J.C.S. Perkin 1*, 2000, 1807-1808 (*synth, abs config*)

6,7-Epoxy-3(15)-caryophyllene E-67

[17627-43-9]

Epoxycaryophyllene. Caryophyllene oxide. Epoxydihydrocaryophyllene



(6*R*,7*R*)-*form*

$C_{15}H_{24}O$ 220.354

(6*R*,7*R*)-*form* [1139-30-6]

Caryophyllene α-oxide

Constit. of oil of cloves (*Eugenia caryophyllata*). Also in oils of *Betula alba, Mentha piperita* (peppermint) and others. Cryst. Mp 63.5-64°. $[\alpha]_D^{20}$ -79.4 (c, 2.32 in $CHCl_3$).

▶ Skin irritant. LD_{50} (rat, orl) >5000 mg/kg. RP5530000

(6*S*,7*S*)-*form*

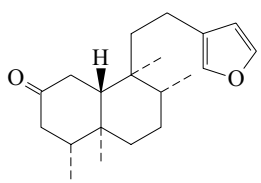
Caryophyllene β-oxide

Mp 29-31° approx. $[\alpha]_D$ 0 (c, 2.46 in $CHCl_3$). Warnhoff appears to show the wrong configs..

[13877-94-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 237C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 380A (*nmr*)
Treibs, W. *et al., Chem. Ber.*, 1947, **80**, 56 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1930 (*occur*)
Warnhoff, E.W. *et al., Can. J. Chem.*, 1973, **51**, 3955 (*synth, pmr*)
Gatilov, Yu.A. *et al., Khim. Prir. Soedin.*, 1982, **18**, 715; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 677 (*cryst struct, bibl*)
Nishiya, K. *et al., Phytochemistry*, 1992, **31**, 3511 (*isol, pmr, cmr*)
Heymann, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 138 (*isol, pmr, cmr*)
Thebtaranonth, C. *et al., Phytochemistry*, 1995, **40**, 125 (*isol, pmr, cmr*)
Sakar, M.K. *et al., Fitoterapia*, 1999, **70**, 103-105 (*pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCN100

15,16-Epoxy-13(16),14-clerodadien-2-one E-68



$C_{20}H_{30}O_2$ 302.456

Struct. revised in 1989.

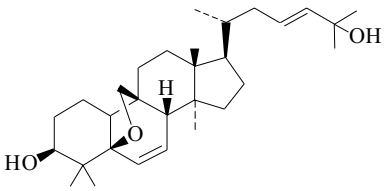
(*ent*-4α*H*)-*form* [59742-40-4]

Cascarillone

Constit. of oil of *Croton eleuteria* (cascarilla). Oil.

Claude-Lafontaine, A. *et al., Bull. Soc. Chim. Fr.*, 1976, 88 (*isol*)
Iio, H. *et al., J.C.S. Perkin 1*, 1989, 1360 (*struct, synth*)
McChesney, J.D. *et al., Fitoterapia*, 1990, **61**, 172 (*isol*)

5,19-Epoxycucurbita-6,23-diene-3,25-diol E-69



$C_{30}H_{48}O_3$ 456.707

(3β,5β,23*E*)-*form*

3-O-*β*-D-*Glucopyranoside:* [81371-55-3] ***Momordicoside I***
$C_{36}H_{58}O_8$ 618.849
Constit. of *Momordica charantia* (bitter melon). Mp 210-216°. $[\alpha]_D$ -110.2.

3-O-*β*-D-*Allopyranoside:* [81348-82-5] ***Momordicoside F₂***
$C_{36}H_{58}O_8$ 618.849
Constit. of *Momordica charantia* (bitter melon). Cryst. Mp 155-158°. $[\alpha]_D$ -96.5.

3-O-*β*-D-*Allopyranoside, 25*-O-*β*-D-*glucopyranoside:* [333333-12-3] ***Goyaglycoside e***
$C_{42}H_{68}O_{13}$ 780.991
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{28}$ -75.6 (c, 0.7 in EtOH).

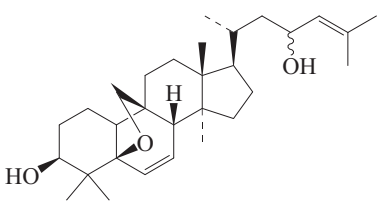
O^{25}-*Me:*
$C_{31}H_{50}O_3$ 470.734
Cryst. Mp 139-140°. $[\alpha]_D$ -90.6.

O^{25}-*Me, 3*-O-*β*-D-*glucopyranoside:* [81348-81-4] ***Momordicoside F₁***
$C_{37}H_{60}O_8$ 632.876
Constit. of *Momordica charantia* (bitter melon). Cryst. Mp 198-203°. $[\alpha]_D$ -111.

O^{25}-*Me, 3*-O-*β*-D-*allopyranoside:* [81371-54-2] ***Momordicoside G***
$C_{37}H_{60}O_8$ 632.876
Constit. of *Momordica charantia* (bitter melon). Cryst. Mp 183-187°. $[\alpha]_D$ -107.3.

Okabe, H. *et al., Tet. Lett.*, 1982, **23**, 77
Mulholland, D.A. *et al., Phytochemistry*, 1997, **45**, 391 (*isol, pmr, cmr*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 54-63 (*Goyaglycoside e*)

5,19-Epoxycucurbita-6,24-diene-3,23-diol E-70



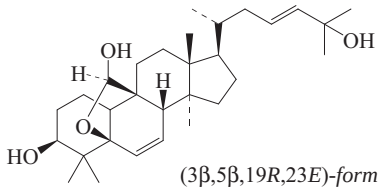
$C_{30}H_{48}O_3$ 456.707

(3β,5β,23ξ)-*form*

3-O-*β*-D-*Glucopyranoside, 23*-O-*β*-D-*allopyranoside:* [333333-13-4] ***Goyaglycoside f***
$C_{42}H_{68}O_{13}$ 780.991
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{28}$ -75.6 (c, 0.7 in EtOH).

Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 54-63 (*isol, pmr, cmr*)

5,19-Epoxycucurbita-6,23-diene-3,19,25-triol E-71



(3β,5β,19*R*,23*E*)-*form*

$C_{30}H_{48}O_4$ 472.707

(3β,5β,19*R*,23*E*)-*form*

19-Me ether, 3-O-*β*-D-*allopyranoside:* [333332-48-2] ***Goyaglycoside b***
$C_{37}H_{60}O_9$ 648.876
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{23}$ -110.7 (c, 0.5 in MeOH).

19-Me ether, 3-O-*β*-D-*allopyranoside, 25*-O-*β*-D-*glucopyranoside:* [333333-14-5] ***Goyaglycoside g***
$C_{43}H_{70}O_{14}$ 811.018
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{27}$ -79.2 (c, 0.5 in MeOH).

19-Me ether, 3-O-*β*-D-*glucopyranoside:* [333332-41-5] ***Goyaglycoside a***
$C_{37}H_{60}O_9$ 648.876
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{26}$ -101.4 (c, 0.5 in MeOH).

19,25-Di-Me ether, 3-O-*β*-D-*allopyranoside:* [333332-50-6] ***Goyaglycoside d***
$C_{38}H_{62}O_9$ 662.902
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{26}$ -141.1 (c, 0.1 in MeOH).

19,25-Di-Me ether, 3-O-*β*-D-*glucopyranoside:* [333332-49-3] ***Goyaglycoside c***
$C_{38}H_{62}O_9$ 662.902
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{26}$ -110.8 (c, 0.5 in MeOH).

(3β,5β,19ξ,23*E*)-*form* [191097-54-8]
$[\alpha]_D$ -93.2 (c, 0.278 in $CHCl_3$).

19-Me ether: [191097-55-9] *5,19-Epoxy-19-methoxycucurbita-6,23-diene-3,25-diol*
$C_{31}H_{50}O_4$ 486.734
Cryst. Mp 102-104°. $[\alpha]_D$ -52.8 (c, 0.036 in $CHCl_3$).

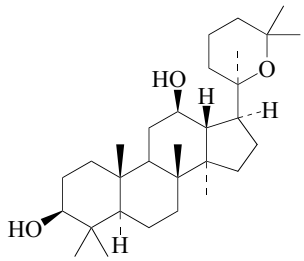
25-Me ether: [191097-53-7] *5,19-Epoxy-9,25-methoxycucurbita-6,23-diene-3,19-diol*
$C_{31}H_{50}O_4$ 486.734
Cryst. Mp 182-184°. $[\alpha]_D$ -55.9 (c, 0.102 in $CHCl_3$).

19,25-Di-Me ether: [85372-70-9] *5,19-Epoxy-9,25-dimethoxycucurbita-6,23-dien-3-ol*
$C_{32}H_{52}O_4$ 500.76
$[\alpha]_D$ -37.1 (c, 0.054 in $CHCl_3$).

Mulholland, D.A. *et al., Phytochemistry*, 1997, **45**, 391-395 (*isol, pmr, cmr*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 54-63 (*Goyaglycosides*)

20,25-Epoxydammarane-3,12-diol E-72

[19666-76-3]



$C_{30}H_{52}O_3$ 460.739

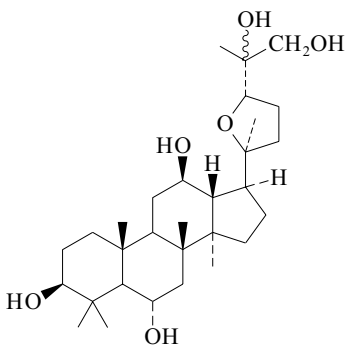
(3β,12β,20*R*)-*form*

Panaxadiol. *Ginsengenin II. Panaxol*
Present in ginseng. Cryst. (MeOH). Mp 250°. $[\alpha]_D^{18.5}$ +1 (c, 1 in $CHCl_3$).

3-O-*β*-D-*Glucopyranoside:* [60431-52-9] *Ginsenoside Rh₂'*
$C_{36}H_{62}O_8$ 622.881

Shibata, S. *et al., Chem. Pharm. Bull.*, 1963, **11**, 759; 762 (*ir, ms, pmr*)
Tanaka, O. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1204 (*struct*)
Uvarova, N.I. *et al., Zh. Org. Khim.*, 1976, **12**, 984 (*synth*)
Liu, W. *et al., CA*, 1988, **109**, 6831 (*Ginsenodide Rh₂'*)

20,24-Epoxydammarane-3,6,12,25,26-pentol E-73



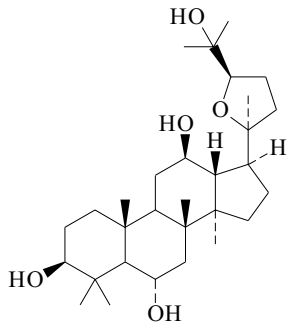
$C_{30}H_{52}O_6$ 508.737

(3β,6α,12β,20*S*,24*S*,25ξ)-*form* [156006-36-9]
Cryst. (MeOH aq.). Mp 143-145°. $[\alpha]_D^{28}$ +17.9 (c, 0.67 in $CHCl_3$).

6-O-*[β*-D-*Xylopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [156398-73-1] ***Vinaginsenoside R14***
$C_{41}H_{70}O_{15}$ 802.995
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{18}$ -13.7 (c, 0.7 in MeOH).

Duc, N.M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 634 (*isol, pmr, cmr*)

20,24-Epoxydammarane-3,6,12,25-tetrol E-74



$C_{30}H_{52}O_5$ 492.738

(3β,6α,12β,20*S*,24*R*)-*form*

6-O-*β*-D-*Glucopyranoside:* [98474-78-3] ***Pseudoginsenoside RT$_5$***
$C_{36}H_{62}O_{10}$ 654.88
Needles (MeOH aq.). Mp 211-213°. $[\alpha]_D^{25}$ +24.2 (c, 1.05 in MeOH).

6-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [69884-00-0] ***Ginsenoside A$_1$***. *Pseudoginsenoside F$_{11}$*
$C_{42}H_{72}O_{14}$ 801.022
Constit. of *Panax quinquefolium* (American ginseng). Amorph. powder. $[\alpha]_D^{24}$ -12 (c, 0.43 in MeOH).

6-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside]:* [98474-76-1] ***Pseudoginsenoside RT$_2$***
$C_{41}H_{70}O_{14}$ 786.996
Amorph. powder. $[\alpha]_D^{24}$ +11.1 (c, 0.85 in MeOH).

(3β,6α,12β,20*S*,24*S*)-*form*

6-O-*β*-D-*Glucopyranoside:* [98474-77-2] ***Pseudoginsenoside RT$_4$***
$C_{36}H_{62}O_{10}$ 654.88
Needles (MeOH aq.). Mp 247-249°. $[\alpha]_D^{25}$ +14.4 (c, 1 in MeOH).

6-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside]:* [81534-63-6] ***Majonoside R2***
$C_{41}H_{70}O_{14}$ 786.996
Constit. of *Panax japonicus* (Japanese ginseng). Amorph. powder. $[\alpha]_D^{15}$ -2.4 (c, 1.13 in MeOH).

6-O-*[β-D-Xylopyranosyl-(1→2)-6*-O-*acetyl-β-D-glucopyranoside]:* [156980-42-6] ***Vinaginsenoside R2***
$C_{43}H_{72}O_{15}$ 829.033
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Needles (MeOH aq.). Mp 186-189°. $[\alpha]_D^{25}$ -17.4 (c, 0.69 in MeOH).

6-O-*[α-L-Rhamnopyranosyl-(1→2)-6*-O-*acetyl-β-D-glucopyranoside]:* [156980-41-5] ***Vinaginsenoside R1***
$C_{44}H_{74}O_{15}$ 843.06
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Powder. $[\alpha]_D^{25}$ -23.1 (c, 1.08 in MeOH).

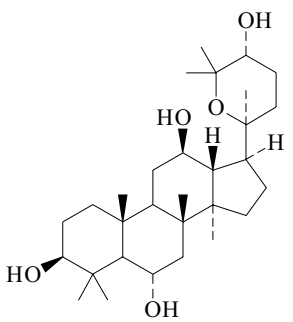
6-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [81534-62-5] ***Majonoside R1***
$C_{42}H_{72}O_{15}$ 817.022
Constit. of *Panax japonicus* (Japanese ginseng). Amorph. powder. $[\alpha]_D^{15}$ +1 (c, 1.13 in MeOH).

6-O-*[α-D-Glucopyranosyl-(1→4)-β-D-xylopyranosyl-(1→2)-β-D-glucopyranoside]:* [156009-81-3] ***Vinaginsenoside R5***
$C_{47}H_{80}O_{19}$ 949.138
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{18}$ +38 (c, 1 in MeOH).

6-O-*[α-D-Glucopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranoside]:* [156009-82-4] ***Vinaginsenoside R6***
$C_{47}H_{80}O_{19}$ 949.138
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Amorph. powder. $[\alpha]_D^{25}$ +20 (c, 0.4 in MeOH).

Tanaka, O. *et al., Phytochemistry*, 1978, **17**, 1353 (*Pseudoginsenoside F$_{11}$*)
Chen, S.E. *et al., Planta Med.*, 1981, **42**, 406 (*Pseudoginsenoside F$_{11}$*)
Morita, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4341 (*Majonosides*)
Tanaka, O. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2323 (*Pseudoginsenoside RT$_2$, Pseudoginsenoside RT$_4$, Pseudoginsenoside RT$_5$*)
Minh Duc, N. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2010-2014 (*Vinaginsenosides R1 and R2*)
Minh Duc, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 115-122 (*Vinaginsenosides R5 and R6*)

20,25-Epoxydammarane-3,6,12,24-tetrol E-75



$C_{30}H_{52}O_5$ 492.738

(3β,6α,12β,20*S*,24*R*)-*form* [156042-09-0]
Cryst. (MeOH aq.). Mp 237-239°. $[\alpha]_D^{26}$ +13.3 (c, 0.9 in $CHCl_3$).

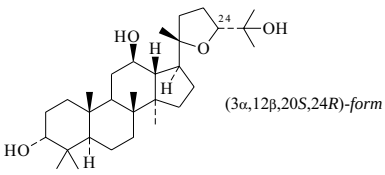
6-O-*β*-D-*Glucopyranoside:* [156398-69-5] ***Vinaginsenoside R10***
$C_{36}H_{62}O_{10}$ 654.88
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Needles (MeOH aq.). Mp 257-259°. $[\alpha]_D^{28}$ +105.5 (c, 0.67 in MeOH).

6-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside]:* [156398-70-8] ***Vinaginsenoside R11***
$C_{41}H_{70}O_{14}$ 786.996
Constit. of *Panax vietnamensis* (Vietnamese ginseng). Needles (MeOH aq.). Mp 251-253°. $[\alpha]_D^{18}$ +3.8 (c, 1 in MeOH).

Duc, N.M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 634 (*isol, pmr, cmr*)

20,24-Epoxydammarane-3,12,25-triol E-76

[19942-07-5, 88195-75-9, 166021-03-0, 166021-04-1]



(3α,12β,20*S*,24*R*)-*form*

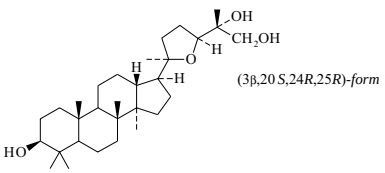
$C_{30}H_{52}O_4$ 476.738

(3β,12β,20*S*,24*R*)-*form* [162062-88-6] ***Protopanaxadiol oxide I***
Powder. $[\alpha]_D^{15}$ +19.7 (c, 1.07 in $CHCl_3$).

3-Malonyl, 12-Ac: [151890-02-7] ***3-Epipapyriferic acid***
$C_{35}H_{56}O_8$ 604.823
Constit. of silver birch (*Betula pendula*) bark resin, used in manuf. of sweet birch oil.

Yamauchi, H. *et al., Tet. Lett.*, 1969, 4245 (*cryst struct*)
Taipale, H.T. *et al., Phytochemistry*, 1993, **34**, 755 (*3-Epipapyriferic acid*)

20,24-Epoxydammarane-3,25,26-triol E-77



(3β,20*S*,24*R*,25*R*)-*form*

$C_{30}H_{52}O_4$ 476.738

(3β,20*S*,24*R*,25*R*)-*form* ***Neoalsogenin H***
Powder.

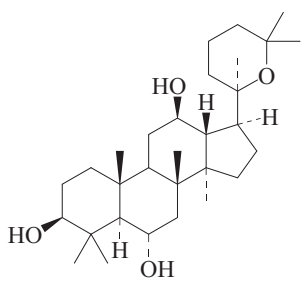
3-O-*[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucopyranoside]:* ***Neoalsoside H1***
$C_{48}H_{82}O_{17}$ 931.166
Powder. $[\alpha]_D^{20}$ -10.4 (c, 0.48 in MeOH).

(20*S*,24*R*,25ξ)-*form*

3-Ketone: [146830-04-8] *20,24-Epoxy-25,26-dihydroxydammaran-3-one*
$C_{30}H_{50}O_4$ 474.723
Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 143-144°. $[\alpha]_D^{30}$ +34 (c, 0.5 in $CHCl_3$).

Anjaneyulu, V. *et al., Phytochemistry*, 1993, **32**, 469 (*isol, pmr, cmr*)
Fujita, S. *et al., Phytochemistry*, 1995, **38**, 465 (*isol, pmr, cmr*)

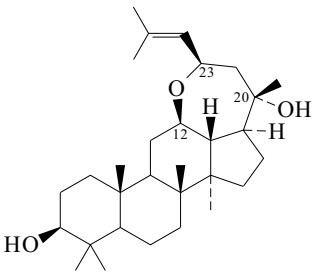
20,25-Epoxydammarane-3,6,12-triol E-78



$C_{30}H_{52}O_4$ 476.738

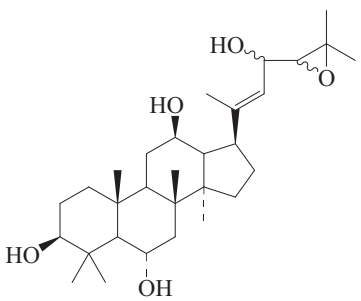
(3β,6α,12β,20*R*)-*form*
Panaxatriol
Present in ginseng. Cryst. Mp 238-239°. $[\alpha]_D^{22}$ +14.2 ($CHCl_3$).
Nagai, Y. *et al., Tetrahedron*, 1971, **27**, 881

12,23-Epoxydammar-24-ene-3,20-diol E-79



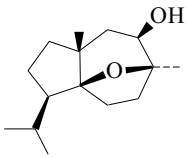
$C_{30}H_{50}O_3$ 458.723
(3β,12β,20*S*,23*R*)-*form*
3,20-Di-O-*β*-D-*glucopyranoside:* [123617-34-5] ***Ginsenoside La***
$C_{42}H_{70}O_{13}$ 783.007
Isol. from ginseng. Needles (MeOH). Mp 179-180°. $[\alpha]_D$ -18.4 (Py).
Zhang, S. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1966

24,25-Epoxydammar-20(22)-ene-3,6,12,23-tetrol E-80



$C_{30}H_{50}O_5$ 490.722
(3β,6α,12β,20(22)*E*,23ξ,24ξ)-*form*
6-O-*β*-D-*Glucopyranoside:* [343962-53-8] ***Notoginsenoside T_1***
$C_{36}H_{60}O_{10}$ 652.864
Constit. of *Panax notoginseng* (sanchi) roots. Solid. $[\alpha]_D^{26}$ +14.49 (c, 0.5 in MeOH).
23-Me ether, 6-O-*β*-D-*glucopyranoside:* [343962-54-9] ***Notoginsenoside T_2***
$C_{37}H_{62}O_{10}$ 666.891
Constit. of *Panax notoginseng* (sanchi) roots. Solid. $[\alpha]_D^{25}$ +28.38 (c, 0.41 in MeOH).
Teng, R.W. *et al., Chin. Chem. Lett.*, 2001, **12**, 239-242 (*isol, pmr, cmr*)

5,8-Epoxy-9-daucanol E-81

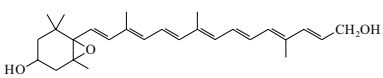


Absolute configuration

$C_{15}H_{26}O_2$ 238.369
(5β,8β,9β)-*form* [887-08-1]
Daucol
Constit. of carrot (*Daucus carota*) seed oil. Cryst. (petrol at -30°). Mp 113-115°. Bp_2 124-132°. $[\alpha]_D^{20}$ -16.9 (c, 2.8 in EtOH).
Deoxy: [56484-24-3] ***5,8-Epoxydaucane. Carota-1,4-oxide***
$C_{15}H_{26}O$ 222.37
Constit. of carrot *Daucus carota*. Oil.
Sykora, V. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 788 (*struct*)
Zalkov, L.H. *et al., J.O.C.*, 1961, **26**, 981 (*struct*)
de Broissia, H. *et al., Bull. Soc. Chim. Fr.*, 1972, 4314 (*synth*)
Dhillon, R.S. *et al., Phytochemistry*, 1989, **28**, 639 (*deriv*)

5,6-Epoxy-5,6-dihydro-10′-apo-β,ψ-carotene-3,10′-diol, 9CI E-82

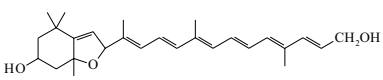
[68378-37-0]



$C_{27}H_{38}O_3$ 410.595
Isol. from the peel of the ripe Golden Delicious apple. Prob. a metab. of in the mature fruit. λ_{max} 372 ; 394 ; 418 (no solvent reported).
Gross, J. *et al., Phytochemistry*, 1978, **17**, 1803

5,8-Epoxy-5,8-dihydro-10′-apo-β,ψ-carotene-3,10′-diol E-83

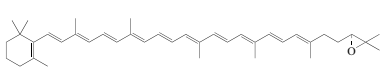
[53905-15-0]



$C_{27}H_{38}O_3$ 410.595
Struct. assignment should be considered tentative. Isol. from *Persea americana* (avocado) and from Valencia orange juice. λ_{max} 397 ; 423 ; 452 (no solvent reported).
Gross, J. *et al., Phytochemistry*, 1974, **13**, 1917; 1975, **14**, 249

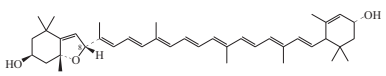
1′,2′-Epoxy-1′,2′-dihydro-β,ψ-carotene E-84

[58556-43-7]
1′,2′-Epoxy-1′,2′-dihydro-γ-carotene



$C_{40}H_{56}O$ 552.882
λ_{max} 433 ; 461 ; 492 (petrol). λ_{max} 444 ; 459 ; 490 (hexane).
(*S*)-*form* [92008-21-4]
Isol. from fruits of Delta tomato mutant (*Lycopersicon esculentum*). Red cryst. (CH_2Cl_2/MeOH). Mp 142-143°.
[91464-08-3, 92075-73-5]
Britton, G. *et al., Phytochemistry*, 1975, **14**, 2530 (*isol*)
Pfander, H. *et al., Helv. Chim. Acta*, 1980, **63**, 1792-1796 (*synth*)
Kamber, M. *et al., Helv. Chim. Acta*, 1984, **67**, 968-985 (*synth, abs config*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 215

5,8-Epoxy-5,8-dihydro-β,ε-carotene-3,3′-diol E-85

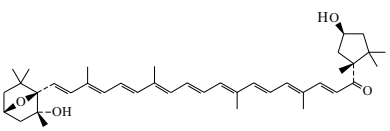


(3*S*,3′*R*,5*R*,6′*R*,8*R*)-*form*

$C_{40}H_{56}O_3$ 584.881
(3*S*,3′*R*,5*R*,6′*R*,8*R*)-*form* [512-29-8]
Flavoxanthin
Constit. of *Taraxacum officinale* (dandelion). Red cryst. (MeOH). Mp 175.5-177.5°. $[\alpha]_D^{23}$ +265.
(3*S*,3′*R*,5*R*,6′*R*,8*S*)-*form* [27780-11-6]
Chrysanthemaxanthin
Yellow cryst. Mp 178.5-180°. $[\alpha]_D^{23}$ +104.
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1847
Cadosch, H. *et al., Helv. Chim. Acta*, 1978, **61**, 783 (*isol, cd, pmr, cmr*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 248; 249 (*bibl*)

3,6-Epoxy-5,6-dihydro-3′,5-dihydroxy-β,κ-caroten-6′-one E-86

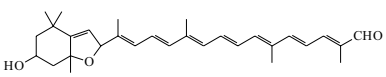
[103955-76-6]



$C_{40}H_{56}O_4$ 600.88
Constit. of paprika. Red prisms. Mp 169-170°. $[\alpha]_D$ +3.2 (C_6H_6).
Parkes, K.E.B. *et al., Tet. Lett.*, 1986, **27**, 2535 (*occur*)

5,8-Epoxy-5,8-dihydro-3-hydroxy-8′-apo-β,ψ-carotenal, 9CI E-87

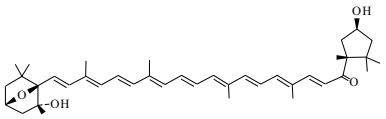
[54899-35-3]



$C_{30}H_{40}O_3$ 448.644
Isol. from Valencia orange juice. λ_{max} 430 (EtOH). λ_{max} 445 ($CHCl_3$). λ_{max} 406 ; 428 ; 452 (hexane).
Gross, J. *et al., Phytochemistry*, 1975, **14**, 249

3,6-Epoxy-5,6-dihydro-5-hydroxy-β,κ-caroten-6′-one E-88

Capsanthin 3,6-epoxide

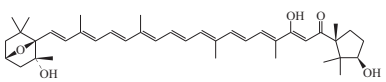


$C_{40}H_{56}O_4$ 600.88

Incorrectly named. Constit. of red paprika (*Capsicum annuum*). Red prisms. Mp 169-170°. $[\alpha]_D$ +3.2 (C_6H_6).

Parkes, K.E.B. *et al., Tet. Lett.*, 1986, **27**, 2535
Deli, J. *et al., Helv. Chim. Acta*, 1996, **79**, 1435 (*isol, pmr, cmr, cd*)

3,6-Epoxy-5,6-dihydro-3′,5,8′-trihydroxy-β,κ-caroten-6′-one E-89

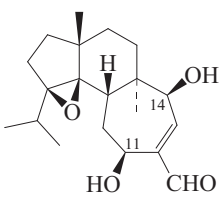


$C_{40}H_{56}O_5$ 616.879

(3*S*,3′*S*,5*R*,5′*R*,6*R*)-*form* [256505-53-0]
Constit. of the oyster *Crassostrea gigas*. Red amorph. solid. λ_{max} 464 (Et_2O).

Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr, cmr*)

3,4-Epoxy-11,14-dihydroxy-12-cyathen-15-al E-90



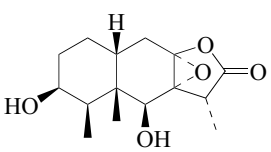
$C_{20}H_{30}O_4$ 334.455

(3β,4β,11β,14β)-*form*

*11-Et ether, 14-*O-*β*-D-*xylopyranoside:* [178120-49-5]
$C_{27}H_{42}O_8$ 494.624
Constit. of *Hericium erinaceum* (lions mane). Sol. MeOH, Me_2CO, $CHCl_3$.

Japan. Pat., 1996, 96 73 486; *CA*, **125**, 56399

7,8-Epoxy-3,6-dihydroxy-12,8-eremophilanolide E-91



(3β,6β,7α,8α,10β,11α)-*form*

$C_{15}H_{22}O_5$ 282.336

(3β,6β,7α,8α,10β,11α)-*form*

6-Angeloyl: [71047-01-3] ***Eremopetasitenin A1***
$C_{20}H_{28}O_6$ 364.438
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D$ -23.2.

3-(3-Methylthiopropenoyl)(Z-), 6-Me ether: [189100-11-6] ***Eremopetasitenin A2***
$C_{20}H_{28}O_6S$ 396.504
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D$ -27.8.

(3β,6β,7β,8β,10β,11β)-*form*

6-Angeloyl: [189100-13-8] ***Eremopetasitenin B1***
$C_{20}H_{28}O_6$ 364.438
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D$ -55.6.

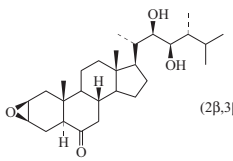
3-(3-Methylthiopropenoyl)(Z-), 6-angeloyl: [189100-15-0] ***Eremopetasitenin B2***
$C_{24}H_{32}O_7S$ 464.579
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D$ -66.9.

6-Me ether: [270902-91-5] *7,8-Epoxy-3-hydroxy-6-methoxy-12,8-eremophilanolide.* ***Eremopetasitenin B3***
$C_{16}H_{24}O_5$ 296.363
$[\alpha]_D^{22}$ -15.8 (c, 1.2 in $CHCl_3$).

Tori, M. *et al., Phytochemistry*, 1998, **47**, 401-409 (*isol, pmr, cmr*)
Tori, M. *et al., Tet. Lett.*, 2000, **41**, 1797-1799 (*Eremopetasitenin B3*)

2,3-Epoxy-22,23-dihydroxyergostan-6-one E-92

2,3-Epoxy-22,23-dihydroxy-24-methylcholestan-6-one



(2β,3β,5α,22*R*,23*R*,24*R*)-*form*

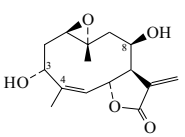
$C_{28}H_{46}O_4$ 446.669

(2β,3β,5α,22*R*,23*R*,24*R*)-*form* [167075-97-0] ***24-Episecasterone***

(2β,3β,5α,22*R*,23*R*,24*S*)-*form* [164321-81-7] ***Secasterone***
Constit. of *Secale cerale* seeds (rye).

Schmidt, J. *et al., Phytochemistry*, 1995, **38**, 1095 (*Secasterone*)
Friebe, A. *et al., Phytochemistry*, 1999, **52**, 1607-1610 (*24-Episecasterone*)

1,10-Epoxy-3,8-dihydroxy-4,11(13)-germacradien-12,6-olide E-93



(1β,3α,4*Z*,6α,8β,10α)-*form*

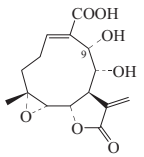
$C_{15}H_{20}O_5$ 280.32

(1β,3β,4*Z*,6α,8β,10α)-*form* [73035-83-3] ***Heliangin***
Cryst. Mp 232-235°.

8-Tigloyl: [13323-48-3] ***Heliangin***
$C_{20}H_{26}O_6$ 362.422
Isol. from *Helianthus tuberosus* (Jerusalem artichoke). Cryst. (MeOH). Mp 227-229°. $[\alpha]_D^{23}$ -110 (c, 0.5 in $CHCl_3$).

Morimoto, H. *et al., Tetrahedron*, 1966, **22**, 3173 (*Heliangin*)
Nishikawa, M. *et al., Tetrahedron*, 1966, **22**, 3601 (*cryst struct, Heliangin*)
Neidle, S. *et al., Chem. Comm.*, 1972, 140 (*abs config, Heliangin*)

4,5-Epoxy-8,9-dihydroxy-1(10),11(13)-germacradien-12,6-olid-14-oic acid E-94



(1(10)*E*,4α,5α,6α,8α,9α)-*form*

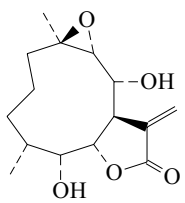
$C_{15}H_{18}O_7$ 310.303

(1(10)*E*,4α,5α,6α,8α,9α)-*form*

*8-*O*-(2,3-Epoxy-2-methylbutanoyl), 9-Ac, Me ester:PSF-A*
$C_{23}H_{28}O_{10}$ 464.468
Constit. of *Polymnia sonchifolia* (yacon). Cryst. Mp 146-148°.

Japan. Pat., 1995, 95 61 980; *CA*, **123**, 3368 (*PSF-A*)

9,10-Epoxy-5,8-dihydroxy-11(13)-germacren-12,6-olide E-95



$C_{15}H_{22}O_5$ 282.336

(4β*H*,5α,6α,8α,9α,10β)-*form*

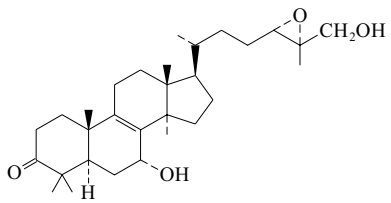
5-Ac: [111545-48-3] ***Blumealactone C***
$C_{17}H_{24}O_6$ 324.373
Constit. of *Blumea balsamifera* (sambong). Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 247-250°. $[\alpha]_D$ -4.85 (c, 1.55 in $CHCl_3$).

8-(2-Methyl-2-butenoyl): [111545-46-1] ***Blumealactone A***
$C_{20}H_{28}O_6$ 364.438
Constit. of *Blumea balsamifera* (sambong). Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 205-208°. $[\alpha]_D$ -45.9 (c, 0.88 in $CHCl_3$).

8-(3-Methyl-2-butenoyl): [111545-47-2] ***Blumealactone B***
$C_{20}H_{28}O_6$ 364.438
Constit. of *Blumea balsamifera* (sambong). Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 221-222°. $[\alpha]_D$ -34.2 (c, 0.58 in $CHCl_3$).

Fujimoto, Y. *et al., Phytochemistry*, 1988, **27**, 1109

24,25-Epoxy-7,26-dihydroxylanost-8-en-3-one E-96

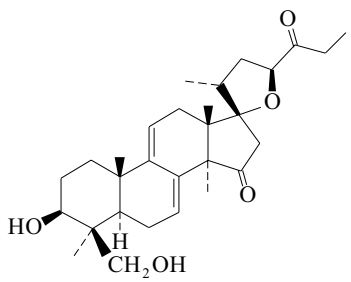


$C_{30}H_{48}O_4$ 472.707

(7α,24*S*,25*S*)-*form* [114020-56-3]
Epoxyganoderiol A
Metab. of *Ganoderma lucidum* (reishi). Gummy solid. $[\alpha]_D^{23}$ +65 (c, 0.2 in $CHCl_3$).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 211

17,23-Epoxy-3,29-dihydroxy-27-norlanosta-7,9(11)-diene-15,24-dione E-97

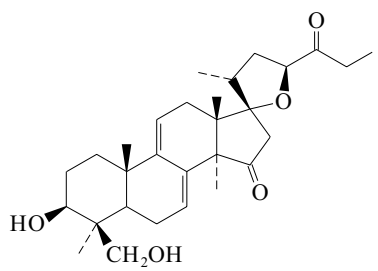


$C_{29}H_{42}O_5$ 470.648

(3β,17α,23*S*)-*form*
Constit. of *Muscari comosum* (tassel hyacinth). Cryst. (MeOH). Mp 221-224°.

Adinolfi, M. *et al., J. Nat. Prod.*, 1984, **47**, 544

17,23-Epoxy-3,29-dihydroxy-27-norlanost-8-ene-15,24-dione E-98



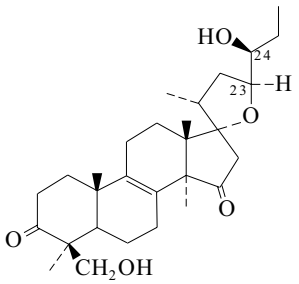
$C_{29}H_{44}O_5$ 472.664

(3β,17α,23*R*)-*form*
Constit. of *Muscari comosum* (tassel hyacinth). Cryst. (Me_2CO). Mp 196-198°.

3-Ketone:17,23-Epoxy-29-hydroxy-27-norlanost-8-ene-3,15,24-trione
$C_{29}H_{42}O_5$ 470.648
From *Muscari comosum* (tassel hyacinth). Cryst. (EtOH). Mp 184-186°.

Adinolfi, M. *et al., J. Nat. Prod.*, 1984, **47**, 101

17,23-Epoxy-24,29-dihydroxy-27-norlanost-8-ene-3,15-dione E-99

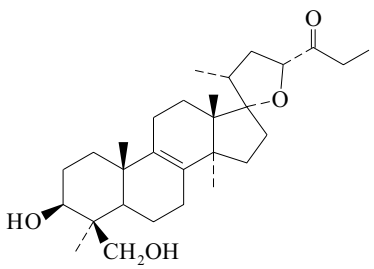


$C_{29}H_{44}O_5$ 472.664

(23*S*,24*S*)-*form*
Constit. of *Muscari comosum* (tassel hyacinth). Cryst. (C_6H_6). Mp 194-195°. $[\alpha]_D$ +67.2 (c, 0.2 in $CHCl_3$).

Adinolfi, M. *et al., J. Nat. Prod.*, 1983, **46**, 559

17,23-Epoxy-3,29-dihydroxy-27-norlanost-8-en-24-one E-100

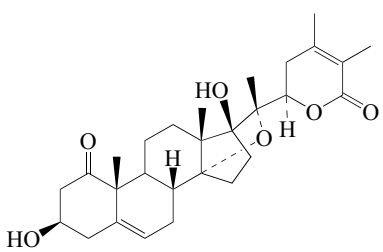


$C_{29}H_{46}O_4$ 458.68

(3β,17α,23*S*)-*form*
Constit. of *Muscari comosum* (tassel hyacinth). Cryst. (MeOH). Mp 195-197°. $[\alpha]_D$ -22 (c, 0.3 in $CHCl_3$).

Adinolfi, M. *et al., J. Nat. Prod.*, 1984, **47**, 721

14,20-Epoxy-3,17-dihydroxy-1-oxowitha-5,24-dienolide E-101



$C_{28}H_{38}O_6$ 470.605

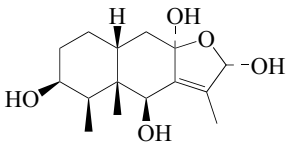
(3β,14α,17β,20*S*,22*R*)-*form* [261637-27-8]
Coagulin R
Amorph. powder. $[\alpha]_D$ +35 (c, 0.37 in MeOH). λ_{max} 225 (log ϵ 3.87) (MeOH).

3-O-β-D-Glucopyranoside: [221695-66-5]
$C_{34}H_{48}O_{11}$ 632.747
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. Mp 210-211°. $[\alpha]_D^{25}$ +78 (c, 0.0077 in MeOH). λ_{max} 222 (log ϵ 3.98) (MeOH).

Ahmad, S. *et al., J. Nat. Prod.*, 1999, **62**, 493-494 (*isol, pmr, cmr*)

Atta-ur-Rahman, *et al., Phytochemistry*, 1999, **52**, 1361-1364 (*Coagulin R*)

8,12-Epoxy-7(11)-eremophilene-3,6,8,12-tetrol E-102



$C_{15}H_{24}O_5$ 284.352

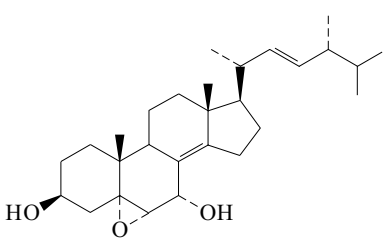
(3β,6β,8α,12α)-*form*
6,8,12-Tri-Me ether:
$C_{18}H_{30}O_5$ 326.432
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{20}$ -39 (c, 0.21 in $CHCl_3$). Possibly an artifact.

(3β,6β,8β,12α)-*form*
8,12-Di-Me ether, 6-angeloyl:
$C_{22}H_{34}O_6$ 394.507
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{20}$ +0.62 ($CHCl_3$). Possibly an artifact.

Tori, M. *et al., Phytochemistry*, 1988, **47**, 401-409 (*isol, pmr, cmr*)

5,6-Epoxyergosta-8(14),22-diene-3,7-diol E-103

5,6-Epoxy-24-methylcholesta-8(14),22-diene-3,7-diol



$C_{28}H_{44}O_3$ 428.654

(3β,5α,6α,7α,22*E*,24*R*)-*form* [22259-18-3]
$[\alpha]_D$ -83 (c, 0.9 in $CHCl_3$).

Di-Ac:
Cryst. (MeOH). Mp 126-129°. $[\alpha]_D$ -133.

(3β,5α,6α,7β,22*E*,24*R*)-*form*
Constit. of *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{18}$ -52.4 (c, 0.2 in $CHCl_3$).

(3β,5α,6α,7α,22*E*,24ξ)-*form*

Della Greca, M. *et al., Nat. Prod. Lett.*, 1993, **2**, 27 (*isol, pmr, cmr*)

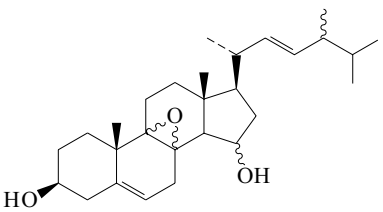
Migliuolo, A. *et al., Steroids*, 1993, **58**, 134 (*isol, pmr, cmr*)

Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*isol, pmr, cmr*)

Yue, J.-M. *et al., Phytochemistry*, 2001, **56**, 801-806 (*isol, pmr, cmr*)

8,9-Epoxyergosta-5,22-diene-3,15-diol E-104

8,9-Epoxy-24-methylcholesta-5,22-diene-3,15-diol



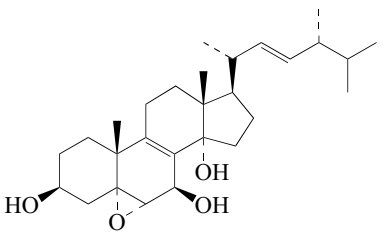
$C_{28}H_{44}O_3$ 428.654

(3β,8ξ,9ξ,15ξ,24ξ)-*form* [133587-90-3]
Constit. of *Ganoderma lucidum* (reishi). Powder. Mp 228-230°.

Chiang, H.-C. *et al., J. Chin. Chem. Soc. (Taipei)*, 1991, **38**, 71 (*isol, pmr, cmr*)

5,6-Epoxyergosta-8,22-diene-3,7,14-triol E-105

5,6-Epoxy-24-methylcholesta-8,22-diene-3,7,14-triol



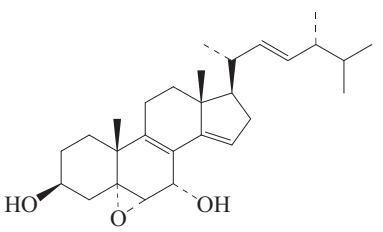
$C_{28}H_{44}O_4$ 444.653

(3β,5α,6α,7β,14α,22*E*,24*R*)-*form* [211486-18-9]
Constit. of *Lentinus edodes* (shiitake). Amorph. powder. $[\alpha]_D^{21}$ -19.6 (c, 0.05 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950 (*isol, pmr, cmr*)

5,6-Epoxyergosta-8,14,22-triene-3,7-diol E-106

5,6-Epoxy-24-methylcholesta-8,14,22-triene-3,7-diol



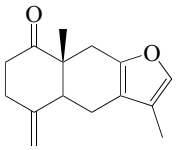
$C_{28}H_{42}O_3$ 426.638

(3β,5α,6α,7α,22*E*,24*R*)-*form* [276864-98-3]
Constit. of *Tricholoma matsutake* (matsutake). Amorph. powder. $[\alpha]_D^{33}$ -61.9 (c, 0.1 in $CHCl_3$).

Ohnuma, N. *et al., Chem. Pharm. Bull.*, 2000, **48**, 749-751 (*isol, pmr, cmr*)

8,12-Epoxy-4(15),7,11-eudesmatrien-1-one E-107

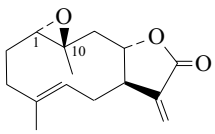
[220289-78-1]



$C_{15}H_{18}O_2$ 230.306
Constit. of *Smyrnium olusatrum* (alexanders).

Mölleken, U. *et al., Phytochemistry*, 1998, **49**, 1709-1714 (*isol, pmr, cmr*)

1,10-Epoxy-4,11(13)-germacradien-12,8-olide E-108



$C_{15}H_{20}O_3$ 248.321

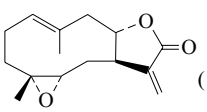
(1α,4*E*,8α,10β)-*form*
Oil.

(1β,4*E*,8β,10α)-*form*
Constit. of *Inula helenium* (elecampane). Cryst. (Et_2O/petrol). Mp 156°. $[\alpha]_D^{24}$ -20 (c, 0.2 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172 (*isol, pmr*)

Jakupovic, J. *et al., Phytochemistry*, 1987, **26**, 451

4,5-Epoxy-1(10),11(13)-germacradien-12,8-olide E-109



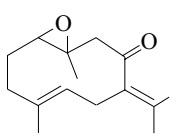
(1(10)*E*,4α,5α,8α)-*form*

$C_{15}H_{20}O_3$ 248.321

(1(10)*E*,4β,5α,8β)-*form* [68776-52-3]
Constit. of *Inula helenium* (elecampane). Cryst. (Et_2O). Mp 131°. $[\alpha]_D^{24}$ -14.4 (c, 1 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172 (*isol, pmr*)

1,10-Epoxy-4,7(11)-germacradien-9-one E-110

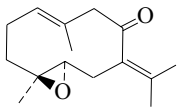


$C_{15}H_{22}O_2$ 234.338

(1ξ,4*E*,10ξ)-*form* [52061-45-7]
1,10-Epoxygermacrone
Constit. of the roots of *Smyrnium olusatrum* (alexanders). Oil. $[\alpha]_D^{24}$ +313 (c, 0.8 in $CHCl_3$).

Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 3614

4,5-Epoxy-1(10),7(11)-germacradien-8-one E-111



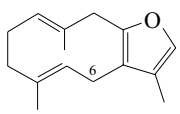
$C_{15}H_{22}O_2$ 234.338

(1(10)*E*,4β,5α)-*form* [92691-35-5]
Germacrone 4,5-epoxide
Constit. of essential oil of *Curcuma zedoaria* (zedoary). Prisms (hexane). Mp 59-60°. $[\alpha]_D^{16}$ +399 (c, 1.05 in $CHCl_3$).

Yoshihara, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2059-2062; 1986, **34**, 434-437 (*isol, cryst struct*)

8,12-Epoxy-1(10),4,7,11-germacratetraene E-112

[19912-61-9]



$C_{15}H_{20}O$ 216.322

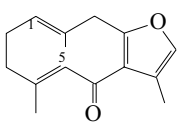
(1(10)*E*,4*E*)-*form*
Furanodiene. Isofuranodiene
Constit. of *Curcuma zedoaria* (zedoary). Cryst. Mp 66°.

Hikino, H. *et al., Chem. Pharm. Bull.*, 1970, **18**, 752-755 (*isol, struct*)

Rücker, G. *et al., Phytochemistry*, 1971, **10**, 221 (*isol*)

Phan, M.G. *et al., Tap Chi Hoa Hoc*, 2000, **38**, 91-94 (*activity*)

8,12-Epoxy-1(10),4,7,11-germacratetraen-6-one E-113



(1(10)*E*,4*E*)-*form*

$C_{15}H_{18}O_2$ 230.306

(1(10)*E*,4*E*)-*form* [24268-41-5]
Furanodienone
Constit. of *Curcuma zedoaria* (zedoary). Cryst. Mp 89.5-90.5°. λ_{max} 241 (log ε 2.98); 248 (log ε 3.95) (EtOH).

(1(10)*E*, 4*Z*)-*form* [24268-42-6]
Isofuranodienone
Constit. of *Curcuma zedoaria* (zedoary). Cryst. (petrol). Mp 70-71°. λ_{max} 223 (log ε 4.17); 248 (log ε 3.95) (EtOH).

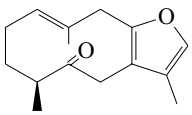
*4,5-Dihydro:**8,12-Epoxy-1(10),7,11-germacratrien-6-one***
$C_{15}H_{20}O_2$ 232.322
Liq.

(1(10)*Z*,4*Z*)-*form*
Liq.

Hikino, H. *et al., J.C.S. Perkin 1*, 1975, 478-484 (*Furanodienone, Isofuranodienone*)

Brieskorn, C.H. *et al., Phytochemistry*, 1983, **22**, 1207-1211 (*Commiphora molmol constit*)
Dolara, P. *et al., Planta Med.*, 2000, **66**, 356-358 (*isol, activity*)
Phan, M.G. *et al., Tap Chi Hoa Hoc*, 2000, **38**, 91-94 (*activity*)
Dakebo, A. *et al., Tet. Lett.*, 2000, **41**, 9875-9878 (*Furanodienone, bibl, cryst struct*)

8,12-Epoxy-1(10),7,11-germacratrien-5-one E-114



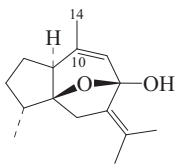
$C_{15}H_{20}O_2$ 232.322

(1(10)*E*,4α*H*)-*form* [81678-18-4]
Furanogermenone
Constit. of *Curcuma zedoaria* (zedoary). Cryst. Mp 46.5-47.5°. $[\alpha]_D^{22}$ +135 ($CHCl_3$).

► LU3420000

Shibuya, H. *et al., Heterocycles*, 1982, **17**, 215
Shibuya, H. *et al., Yakugaku Zasshi*, 1986, **106**, 212-216

5,8-Epoxy-7(11),9-guaiadien-8-ol E-115



(1α,4α,5β,8β)-*form*

$C_{15}H_{22}O_2$ 234.338

The incorrect abs. configs. for Curcumenol and Isocurcumenol have appeared in the lit. The cryst. struct. paper gives the incorrect sterochem. in the text.

(1α,4α,5β,8β)-*form* [350602-21-0]
4-Epicurcumenol
Constit. of rhizomes of *Curcuma zedoaria* (zedoary). Oil. $[\alpha]_D^{26}$ +120 (c, 1.8 in $CHCl_3$).

(1α,4β,5β,8β)-*form* [19431-84-6]
Curcumenol
Constit. of *Curcuma zedoaria* (zedoary) and *Curcuma longa* (turmeric). Cryst. (EtOAc). Mp 118.5-119.5°. $[\alpha]_D$ +397 (c, 5.1 in $CHCl_3$).

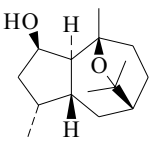
11β,12-Epoxide: [119205-46-8] ***Oxycurcumenol***
$C_{15}H_{22}O_3$ 250.337
Prisms (MeOH). Mp 114-116°. $[\alpha]_D^{20}$ -133 (c, 0.1 in $CHCl_3$).

$\Delta^{10(14)}$-Isomer: [24063-71-6] *5,8-Epoxy-7(11),10(14)-guaiadien-8-ol.* ***Isocurcumenol***
$C_{15}H_{22}O_2$ 234.338
The stereochem. of Curcumenol and Isocurcumenol has been given wrongly in some refs.. Constit. of *Curcuma zedoaria* (zedoary). Cryst. (EtOAc). Mp 139-141°. $[\alpha]_D$ +34 (c, 1.0 in $CHCl_3$).

(1β,4β,5β,8β)-*form*
Epicurcumenol
Constit. of *Curcuma longa* (turmeric). Viscous oil. $[\alpha]_D$ -20 (c, 0.4 in MeOH).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 39-42; 1969, **17**, 959-960
Shiobara, Y. *et al., Phytochemistry*, 1985, **24**, 2629-2633 (*isol, struct*)
Shiobara, Y. *et al., Tet. Lett.*, 1985, 913-916 (*synth*)
Shibuya, H. *et al., Yakugaku Zasshi*, 1986, **212**, 216 (*isol*)
Firman, K. *et al., Phytochemistry*, 1988, **27**, 3887-3891 (*Oxycurcumenol*)
Bats, J.W. *et al., Acta Cryst. C*, 1999, **55**, 1595-1598 (*abs config, bibl, Isocurcumenol*)
Matsuda, H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1558-1566 (*4-Epicurcumenol*)
Matsuda, H. *et al., Heterocycles*, 2001, **55**, 841-846 (*4-Epicurcumenol*)

10,11-Epoxy-2-guaianal E-116



$C_{15}H_{26}O_2$ 238.369

(1α,2β,4α,5β,10β)-*form* [3321-65-1]
α-Kessyl alcohol
Constit. of *Valeriana officinalis* (valerian) and other spp.. Cryst. (EtOH or petrol). Mp 85-86°. $[\alpha]_D$ -38.4 (c, 10 in $CHCl_3$).

2-Ac: ***α-Kessyl acetate***
$C_{17}H_{28}O_3$ 280.406
Oil. $[\alpha]_D$ -73.5 (c, 1.22 in $CHCl_3$).

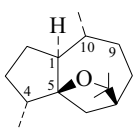
2-Ketone: [7637-95-8] *10,11-Epoxy-2-guaianone. α-Kessyl ketone*
Cryst. (EtOH). Mp 105°. $[\alpha]_D^{26}$ +239 (c, 10 in $CHCl_3$).

(1β,2β,4α,5β,10β)-*form* *Isokessyl alcohol*
Cryst. (EtOH). Mp 118-119°.

2-Ketone: [7663-37-8] *Isokessyl ketone*
Cryst. (EtOH). Mp 56°. $[\alpha]_D$ -133.5.

Ito, S. *et al., Tetrahedron*, 1967, **23**, 553 (*struct*)
Nishiya, K. *et al., Phytochemistry*, 1992, **31**, 3511 (*isol, pmr, cmr*)

5,11-Epoxyguaiane E-117



(1α,4α,5β,7β,10α)-*form*

$C_{15}H_{26}O$ 222.37

(1α,4α,5β,7β,10α)-*form*
Oil. $[\alpha]_D$ -45 (c, 2 in $CHCl_3$).

(1β,4α,5β,7β,10β)-*form* [21764-22-7]
Liguloxide
Cryst. Mp 36°. $[\alpha]_D^{23}$ -58.2 (c, 1 in $CHCl_3$).

9β-Hydroxy: [21764-23-8] ***Liguloxidol***
$C_{15}H_{26}O_2$ 238.369
Oil. $[\alpha]_D^{22}$ -36.8 (c, 1 in $CHCl_3$).

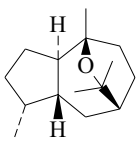
9β-Acetoxy: [18680-79-0] ***Liguloxidol acetate***
$C_{17}H_{28}O_3$ 280.406
Cryst. Mp 85°. $[\alpha]_D$ -52.

3β-Hydroxy:5,11-Epoxy-3β-guaianol. ***3β-Hydroxyliguloxide***
$C_{15}H_{26}O_2$ 238.369
Oil. $[\alpha]_D^{23}$ -22.2 ($CHCl_3$).

(1β,4β,5β,7β,10β)-*form* [20149-50-2] ***Guaioxide***
Constit. of guaiac wood oil (*Bulnesia sarmienti*). Oil. $[\alpha]_D^{26}$ -40 (c, 1 in $CHCl_3$).

Ishii, H. *et al., Tetrahedron*, 1970, **26**, 2751; 2911
Hirota, H. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 785
San Feliciano, A. *et al., Phytochemistry*, 1989, **28**, 2717 (*3β-Hydroxyliguloxide*)
Lee, E. *et al., Tet. Lett.*, 1992, **33**, 6673 (*synth*)

10,11-Epoxyguaiane E-118



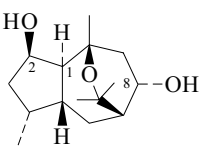
$C_{15}H_{26}O$ 222.37

(1α,4α,5β,10β)-*form* [3321-66-2]
Kessane
Constit. of *Valeriana officinalis* (valerian). Oil. Bp_6 110-112°. $[\alpha]_D$ -7.2 (c, 10 in $CHCl_3$).

(1β,4α,5β,10β)-*form* [177019-46-4]
Isokessane. β-Kessane
Constit. of *Rubus rosifolius* (Mauritius raspberry). Oil. $[\alpha]_D^{26}$ +19.2 (c, 1.7 in $CDCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1963, **11**, 547-549 (*Kessane*)
Gijsen, H.J.M. *et al., Tetrahedron*, 1991, **47**, 4409-4416 (*synth*)
Nishiya, K. *et al., Phytochemistry*, 1992, **31**, 3511-3514 (*isol, pmr, cmr*)
Southwell, I.A. *et al., Phytochemistry*, 1993, **33**, 857-862 (*pmr, cmr*)
Southwell, I.A. *et al., J. Essent. Oil Res.*, 1996, **8**, 143-148 (*Isokessane*)

10,11-Epoxy-2,8-guaianediol E-119



$C_{15}H_{26}O_3$ 254.369

(1α,2β,4α,5β,8α,10β)-*form* [6894-57-1]
Kessyl glycol. *Kessoglycol*
Constit. of the rhizomes of *Valeriana officinalis* (valerian). Cryst. Mp 128°. Bp_4 130-135°. $[\alpha]_D$ -19.3 (c, 3.4 in $CHCl_3$).

8-O-β-D-Glucopyranoside:
$C_{21}H_{36}O_8$ 416.511
Amorph. powder. Mp 112-114°. $[\alpha]_D$ -36 (c, 0.82 in MeOH).

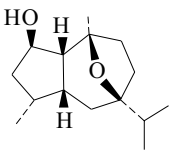
2-Ac: ***Kessyl glycol 2-acetate***
$C_{17}H_{28}O_4$ 296.406
Prisms. Mp 63-65°. $[\alpha]_D$ -60.6 (c, 0.42 in $CHCl_3$).

8-Ac: ***Kessyl glycol 8-acetate***
$C_{17}H_{28}O_4$ 296.406
Oil. $[\alpha]_D$ -36.8 (c, 0.52 in $CHCl_3$).

Di-Ac:
$C_{19}H_{30}O_5$ 338.443
Cryst. (petrol). Mp 117°. $[\alpha]_D$ -78.5 (c, 10.4 in $CHCl_3$).

Ito, S. *et al., Tetrahedron*, 1967, **23**, 553 (*struct*)
Hikino, H. *et al., Tetrahedron*, 1968, **24**, 3147 (*synth*)
Nishiya, K. *et al., Phytochemistry*, 1992, **31**, 3511 (*isol, pmr, cmr*)

7,10-Epoxy-2-guaianol E-120

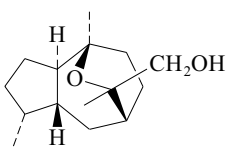


$C_{15}H_{26}O_2$ 238.369
(1β,2β,4α,5β,7β,10β)-*form* [3466-70-4]
***β*-Kessyl alcohol**
Constit. of *Valeriana officinalis* (valerian). Cryst. (EtOH or petrol). Mp 150.5-151°. $[\alpha]_D$ -15.1 (c, 5.3 in $CHCl_3$).

2-Ketone: [3466-16-8] *7,10-Epoxy-2-guaianone.* ***β*-Kessyl ketone**
$C_{15}H_{24}O_2$ 236.353
Constit. of *Valeriana officinalis* (valerian). Cryst. (EtOH). Mp 109-110°. $[\alpha]_D$ -182.7 (c, 5.0 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 485

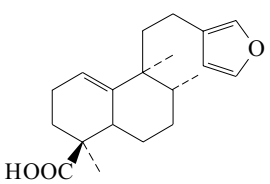
10,11-Epoxy-12-guaianol E-121



$C_{15}H_{26}O_2$ 238.369
(1α,4α,5β,10β,11*S*)-*form*
Ac: [173693-49-7] ***Valeracetate***
$C_{17}H_{28}O_3$ 280.406
Constit. of *Valeriana officinalis* (valerian). $[\alpha]_D^{24}$ +1 (c, 1.4 in $CHCl_3$).

Tori, M. *et al., Phytochemistry*, 1996, **41**, 977 (*isol, pmr, cmr*)

15,16-Epoxy-1(10),13(16),14-halimatrien-19-oic acid E-122



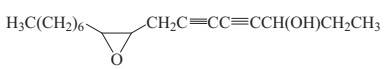
$C_{20}H_{28}O_3$ 316.439
ent*-*form
Isol. (as Me ester) from seed-pod resin of *Hymenaea courbaril* (copinol).

[52591-99-8]

Khoo, S.F. *et al., Tetrahedron*, 1973, **29**, 3379 (*isol*)

9,10-Epoxy-4,6-heptadecadiyn-3-ol E-123

[138828-83-8]
8-(3-Heptyloxiranyl)-4,6-octadiyn-3-ol, 9CI

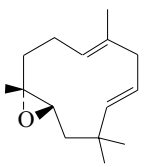


$C_{17}H_{26}O_2$ 262.391
Isol. from *Panax ginseng* (ginseng).

Hirakura, K. *et al., Phytochemistry*, 1991, **30**, 3327-3333 (*isol*)

2,3-Epoxy-6,9-humuladiene E-124

[19888-33-6]
Humulene epoxide I

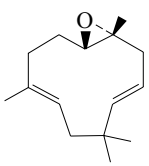


$C_{15}H_{24}O$ 220.354
Constit. of hops and wild ginger (*Zingiber zerumbet*). Oil. d_4^{30} 0.95. $Bp_{1.5}$ 104-105°. $[\alpha]_D^{30}$ -22.8 (c, 3.6 in $CHCl_3$). n_D^{30} 1.4953.

Damodaran, N.P. *et al., Tetrahedron*, 1968, **24**, 4123

6,7-Epoxy-2,9-humuladiene E-125

[19888-34-7]
Humulene epoxide II

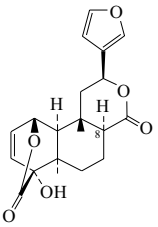


$C_{15}H_{24}O$ 220.354
Constit. of hops and wild ginger (*Zingiber zerumbet*). Oil. d_4^{30} 0.95. $Bp_{1.5}$ 105-106°. $[\alpha]_D^{30}$ -31.2 (c, 4.2 in $CHCl_3$). n_D^{30} 1.4962.

Damodaran, N.P. *et al., Tetrahedron*, 1968, **24**, 4123 (*isol*)
Picket, J.A. *et al., Chem. Ind. (London)*, 1977, 30 (*synth*)
Tsui, W.-Y. *et al., J. Nat. Prod.*, 1996, **59**, 1084 (*isol, pmr, cmr*)
Sakar, M.K. *et al., Fitoterapia*, 1999, **70**, 103-105 (*pmr, cmr*)

15,16-Epoxy-4-hydroxy-2,13(16),14-clerodatriene-17,12:18,1-diolide E-126

Isocolumbin

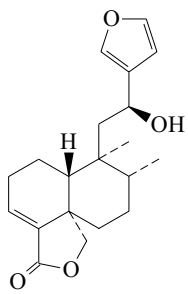


(1β,4α,5α,8α*H*,12α*H*)-*form*

$C_{20}H_{22}O_6$ 358.39
(1β,4α,5α,8α*H*,12α*H*)-*form* [471-54-5]
Isocolumbin
Isol. from *Dioscoreophyllum cumminsii* (serendipity berry). Cryst. (MeOH). Mp 190°. λ_{max} 210 (log ε 3.73) (EtOH).

Cheung, K.K. *et al., J.C.S.(B)*, 1966, 583 (*cryst struct, Isocolumbin*)
Ramstad, E. *et al., Phytochemistry*, 1975, **14**, 2719 (*isol, Isocolumbin*)
Sarma, D.N.K. *et al., Fitoterapia*, 1998, **69**, 541-542 (*Isocolumbin, cmr*)

15,16-Epoxy-12-hydroxy-3,13(16),14-clerodatrien-18,19-olide E-127

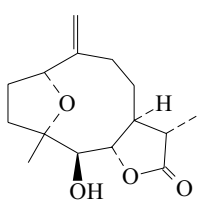


$C_{20}H_{26}O_4$ 330.423
(*ent*-12*R*)-*form*
Ac: [172548-61-7] ***Tanabalin***
$C_{22}H_{28}O_5$ 372.46
Constit. of *Tanacetum balsamita* (costmary). Cryst. ($MeOH/CHCl_3$). Mp 150-152°. $[\alpha]_D$ -124 (c, 5 in $CHCl_3$). $[\alpha]_D$ -132 (c, 0.1 in EtOH).

Kubo, I. *et al., Chem. Lett.*, 1996, 441 (*Tanabalin, isol, pmr, cmr, cryst struct*)
Lima, M.A.S. *et al., Phytochemistry*, 1996, **41**, 217 (*isol, pmr, cmr, cryst struct*)
Watanabe, H. *et al., Tet. Lett.*, 1999, **40**, 2545-2548 (*synth*)

1,4-Epoxy-5-hydroxy-10(14)-germacren-12,6-olide E-128

[131966-27-3]
Achillifolin



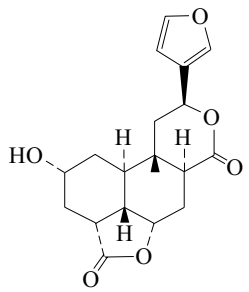
$C_{15}H_{22}O_4$ 266.336

(1α,4α,5β,6α,11β*H*)-*form*

Constit. of *Achillea millefolium* (yarrow).

Ulubelen, A. *et al., Phytochemistry*, 1990, **29**, 3948 (*isol, pmr*)

15,16-Epoxy-2-hydroxy-19-nor-13(16),14-clerodadiene-17,12:18,6-diolide E-129



$C_{19}H_{22}O_6$ 346.379

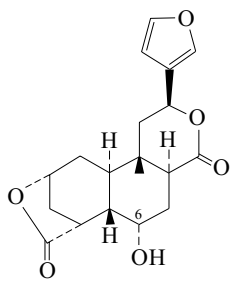
(2α,4β*H*,5β,6α,12α*H*)-*form* [67567-15-1]

Diosbulbin G

Isol. from *Dioscorea bulbifera* (air potato). Cryst. (MeOH). Mp 215-217°. $[\alpha]_D$ -36 (c, 0.26 in MeOH).

Ida, Y. *et al., Annalen*, 1978, 818; 834 (*isol, cryst struct*)

15,16-Epoxy-6-hydroxy-19-nor-13(16),14-clerodadiene-17,12:18,2-diolide E-130



$C_{19}H_{22}O_6$ 346.379

(2α,4β*H*,5β,6α,8α*H*,12α*H*)-*form* [67567-14-0]

Diosbulbin E

Constit. of *Dioscorea bulbifera* (air potato). Cryst. (MeOH). Mp 235-237°. $[\alpha]_D$ +16 (c, 0.16 in MeOH).

6-Ketone: [66756-57-8] *15,16-Epoxy-19-nor-6-oxo-13(16),14-clerodadiene-17,12:18,2-diolide.* ***Diosbulbin D***

$C_{19}H_{20}O_6$ 344.363

Constit. of *Dioscorea bulbifera* (air potato). Cryst. (MeOH). Mp 229-230°. $[\alpha]_D$ -49 (c, 0.11 in MeOH).

(2α,4β*H*,5β,6α,8β*H*,12α*H*)-*form*

*Ac:**8-Epidiosbulbin E acetate***

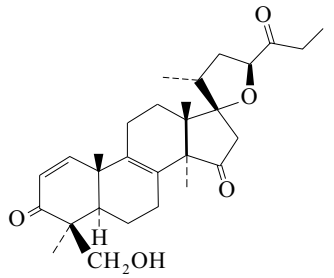
$C_{21}H_{24}O_7$ 388.416

Isol. from *Dioscorea bulbifera* (air potato). Cryst. Mp 223-225°. $[\alpha]_D^{20}$ +46 (c, 0.145 in MeOH).

Ida, Y. *et al., Annalen*, 1978, 818 (*isol, struct*)

Murray, R.D.H. *et al., Phytochemistry*, 1984, **23**, 623 (*isol*)

17,23-Epoxy-29-hydroxy-27-norlanosta-1,8-diene-3,15,24-trione E-131



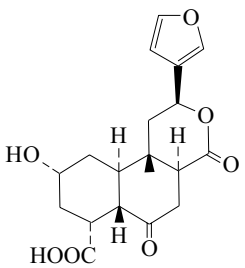
$C_{29}H_{40}O_5$ 468.632

(17α,23*S*)-*form*

Constit. of *Muscari comosum* (tassel hyacinth). Cryst. (Me_2CO). Mp 181-183°.

Adinolfi, M. *et al., J. Nat. Prod.*, 1984, **47**, 544

15,16-Epoxy-2-hydroxy-19-nor-6-oxo-13(16),14-clerodadien-17,12-olid-18-oic acid E-132



$C_{19}H_{22}O_7$ 362.379

(2α,4β*H*,5β,12α*H*)-*form* [66835-37-8]

Me ester: ***Diosbulbin F***

$C_{20}H_{24}O_7$ 376.405

Isol. from *Dioscorea bulbifera* (air potato). Cryst. (MeOH). Mp 211-212°. $[\alpha]_D$ +31 (c, 0.19 in MeOH).

Butyl ester: [67567-13-9] ***Diosbulbin H***

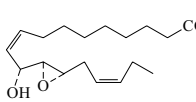
$C_{23}H_{30}O_7$ 418.486

Isol. from *Dioscorea bulbifera* (air potato). Cryst. (MeOH). Mp 176-178°. $[\alpha]_D$ +59 (c, 0.24 in MeOH).

Ida, Y. *et al., Annalen*, 1978, 818

12,13-Epoxy-11-hydroxy-9,15-octadecadienoic acid E-133

11-Hydroxy-1-[3-(2-pentenyl)oxiranyl]-9-undecenoic acid, 9CI



(9Z,11*R*,12*S*,13*S*,15Z)-*form*

$C_{18}H_{30}O_4$ 310.433

(9*Z*,11*R*,12*S*,13*S*,15*Z*)-*form* [106034-49-5]

Isol. from leaves of rice plants with rice blast disease (*Pyricularia oryzae*). Oil. $[\alpha]_D^{27}$ +40.3 (c, 1.2 in $CHCl_3$).

O-(p-*Bromobenzoyl):* $[\alpha]_D$ +26 (c, 0.493 in $CHCl_3$).

(9*Z*,11*S*,12*S*,13*S*,12*Z*)-*form* [105977-35-3]

Isol. from leaves of rice plants with rice blast disease (*Pyricularia oryzae*). Oil. $[\alpha]_D^{27}$ +65.2 (c, 0.8 in $CHCl_3$). $[\alpha]_D$ +65.2 ($CHCl_3$) (synthetic).

O-(p-*Bromobenzoyl):* $[\alpha]_D$ -41.2 (c, 0.131 in $CHCl_3$).

(9*Z*,11*R*,12*S*,13*S*,15*Z*)-*form*

$[\alpha]_D$ -54.2 ($CHCl_3$) (synthetic).

Me ester: [130931-06-5]

$C_{19}H_{32}O_4$ 324.459

$[\alpha]_D^{25}$ -48 (c, 0.63 in Me_2CO).

15,16-Dihydro, Me ester:Methyl 12,13-epoxy-11-hydroxy-9-octadecenoic acid

$C_{19}H_{34}O_4$ 326.475

[106034-56-4, 106034-57-5]

Kato, T. *et al., Chem. Comm.*, 1986, 743 (*isol, ms, pmr, abs config*)

Haynes, R.K. *et al., Chem. Comm.*, 1990, 1102 (*synth*)

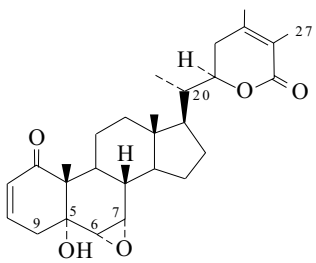
Bernart, M.W. *et al., J. Nat. Prod.*, 1993, **56**, 245 (*isol*)

Wu, W. *et al., Tetrahedron*, 1993, **49**, 4665 (*synth*)

Honda, T. *et al., Heterocycles*, 1997, **46**, 137-140 (*synth*)

Honda, T. *et al., J.C.S. Perkin 1*, 1999, 23-29 (*synth, ir, pmr, cmr*)

6,7-Epoxy-5-hydroxy-1-oxowitha-2,24-dienolide E-134



$C_{28}H_{38}O_5$ 454.605

(5α,6α,7α,20*S*,22*R*)-*form* [56973-41-2]

Withanolide B

Constit. of the leaves of *Lycium chinense* (Chinese boxthorn). Cryst. Mp 260-265°.

20β-Hydroxy: [32911-62-9] *6,7-Epoxy-5,20-dihydroxy-1-oxowitha-2,24-dienolide.* ***Withanolide A***

$C_{28}H_{38}O_6$ 470.605

Isol. from *Lycium chinense* (Chinese boxthorn). Cryst. (EtOAc). Mp 282-284°. $[\alpha]_D$ +88 (c, 0.02 in $CHCl_3$). C-20 has *R*-config.

27-Hydroxy: [60124-17-6] *6,7-Epoxy-5,27-dihydroxy-1-oxowitha-2,24-dienolide.* ***27-Hydroxywithanolide B***

$C_{28}H_{38}O_6$ 470.605

Cryst. (EtOAc) (as 27-Ac). Mp 230-232° (27-Ac). $[\alpha]_D$ +73 (c, 0.11 in $CHCl_3$) (27-Ac).

*20β,27-Dihydroxy:6α,7α-Epoxy-5,20*R*,27-trihydroxy-1-oxowitha-2,24-dienolide.* ***Withasomniferol A***

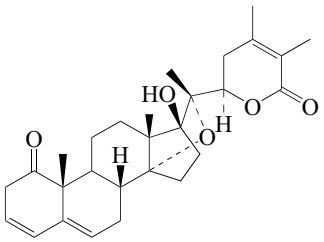
$C_{28}H_{38}O_7$ 486.604

Needles ($CHCl_3$/MeOH). Mp 271-273°. $[\alpha]_D$ +74.9 (c, 0.4 in MeOH). λ_{max} 225 (log ε 4.19) (EtOH).

Haensel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1975, **308**, 653

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 424-433 (*isol, pmr, cmr*)

14,20-Epoxy-17-hydroxy-1-oxowitha-3,5,24-trienolide E-135



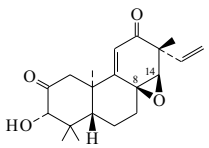
$C_{28}H_{36}O_5$ 452.589

(14α,17β,20*S*,22*R*)-*form*

Constit. of *Physalis peruviana* (Cape gooseberry). Light yellow amorph. solid. Mp 192-193°. $[\alpha]_D^{25}$ -11 (c, 0.0062 in $CHCl_3$/MeOH). λ_{max} 226 (MeOH).

Ahmad, S. *et al., Fitoterapia*, 1998, **69**, 433-436 (*isol, pmr, cmr*)

8,14-Epoxy-3-hydroxy-9(11),15-pimaradiene-2,12-dione E-136



(*ent*-3β,8α,14α)-*form*

$C_{20}H_{26}O_4$ 330.423

(*ent*-3β,8α,14α)-*form* [119626-47-0]

Yucalexin P8

Constit. of cassava roots (*Manihot esculenta*).

(*ent*-3β,8β,14β)-*form* [119626-48-1]

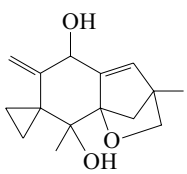
Yucalexin P10

Constit. of cassava *Manihot esculenta*.

Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769

2,12-Epoxy-7(14)-illudadiene-3,8-diol E-137

[141940-50-3]



$C_{15}H_{20}O_3$ 248.321

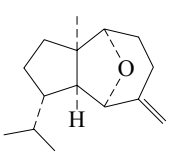
Metab. of *Agrocybe aegerita*.

Stránsky, K. *et al., Coll. Czech. Chem. Comm.*, 1992, **57**, 590 (*isol, pmr, cmr*)

6,10-Epoxy-7(14)-isodaucene E-138

[88395-47-5]

1,5-Epoxy-4(14)-salvialene

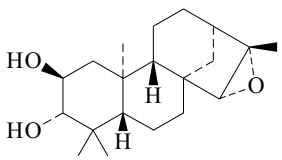


$C_{15}H_{24}O$ 220.354

Constit. of Clary sage oil (*Salvia sclarea*). Cryst. Mp 61-62°. $[\alpha]_D^{20}$ +40.5 (c, 1 in $CHCl_3$).

Maurer, B. *et al., Helv. Chim. Acta*, 1983, **66**, 2223

15,16-Epoxy-2,3-kauranediol E-139



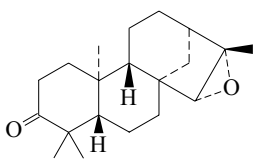
$C_{20}H_{32}O_3$ 320.471

(*ent*-2α,3β,15β,16β)-*form* [140636-08-4]

Isol. from leaves of a blight-resistant rice cultivar. Needles (EtOAc/hexane). Mp 179-180°. $[\alpha]_D^{22}$ +1 (c, 0.32 in MeOH).

Watanabe, M. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 113 (*isol, pmr, cmr*)

15,16-Epoxy-3-kauranone E-140



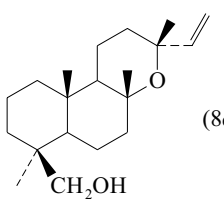
$C_{20}H_{30}O_2$ 302.456

(*ent*-15β,16β)-*form* [140636-10-8]

Isol. from leaves of a blight-resistant rice cultivar. Needles. Mp 134-136°. $[\alpha]_D^{22}$ -35 (c, 0.06 in MeOH). λ_{max} 278 (ϵ 130) (MeOH) (Berdy).

Watanabe, M. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 113 (*isol, pmr, cmr*)

8,13-Epoxy-14-labden-19-ol E-141



(8α,13*R*)-*form*

$C_{20}H_{34}O_2$ 306.487

(8α,13*R*)-*form*

19-Hydroxymanoyl oxide

Cryst. Mp 47-48°. $[\alpha]_D$ +13.1 (c, 0.013 in $CHCl_3$).

19-Carboxylic acid: [56687-75-3] ***8α,13R-Epoxy-14-labden-19-oic acid***

Isol. from *Pinus sylvestris* (Scotch pine). Cryst. (as Me ester). Mp 83-85° (Me ester). $[\alpha]_D$ -43.2 (c, 1.2 in EtOH) (Me ester).

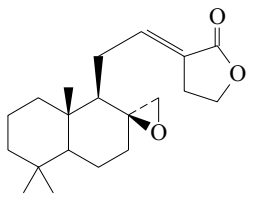
San Martin, A. *et al., Phytochemistry*, 1980, **19**, 1985

Bardyshev, I.I. *et al., Khim. Prir. Soedin.*, 1982, **18**, 480; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 447

Stierle, D.B. *et al., Phytochemistry*, 1988, **27**, 517

Zdero, C. *et al., Phytochemistry*, 1992, **31**, 1631 (*deriv*)

8,17-Epoxy-12-labden-16,15-olide E-142



$C_{20}H_{30}O_3$ 318.455

(8β,12*E*)-*form* [115753-79-2]

Galanolactone

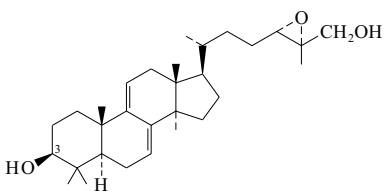
Constit. of *Alpinia galanga* (greater galangal). Needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 125.5-126°. $[\alpha]_D$ +28 (c, 0.26 in $CHCl_3$). λ_{max} 226 (ϵ 11400) (EtOH) (Berdy).

Morita, H. *et al., Planta Med.*, 1988, **54**, 117 (*isol, pmr, cmr*)

Jung, M. *et al., Tet. Lett.*, 1997, **38**, 2871 (*synth*)

Singh, M. *et al., Planta Med.*, 1999, **65**, 2-8 (*rev*)

24,25-Epoxylanosta-7,9(11)-diene-3,26-diol E-143



$C_{30}H_{48}O_3$ 456.707

(3β,24*S*,25*S*)-*form* [114020-58-5]

Epoxyganoderiol C

Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ +43 (c, 0.2 in EtOH).

3-Ketone: [114020-57-4] *24*S,*25*S-*Epoxy-26-hydroxylanosta-7,9(11)-dien-3-one.*

Epoxyganoderiol B

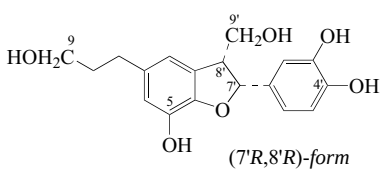
$C_{30}H_{46}O_3$ 454.692

Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ +35 (c, 0.4 in EtOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 211

4,7′-Epoxy-3′,4′,5,9,9′-lignanepentol E-144

2-(3,4-Dihydroxyphenyl)-2,3-dihydro-7-hydroxy-3-hydroxymethyl-5-benzofuranpropanol. 3′,4′,5,9,9′-Pentahydroxy-4,7′-epoxylignan



(7′*R*,8′*R*)-*form*

$C_{18}H_{20}O_6$ 332.352

Lignan numbering shown.Numerous derivs. have been isol. with unspecified

stereochem. - some as mixts. of stereoisomers.

(7′*R*,8′*R*)-*form*

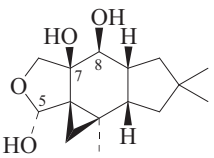
*3′-Me ether, 9′-*O*-β-D-glucopyranoside:*
$C_{25}H_{32}O_{11}$ 508.521
Isol. from Riesling wine. λ_{max} 207 ; 282 (MeOH).

*3′,5-Di-Me ether, 9′-*O*-β-D-glucopyranoside:*
$C_{26}H_{34}O_{11}$ 522.548
Isol. from Riesling wine. λ_{max} 213 ; 282 (MeOH).

[14049-57-1, 57687-35-1, 57687-37-3, 60536-58-5, 73135-77-0, 75775-36-9, 85115-04-4, 106543-53-7, 125874-71-7, 131723-83-6]

Baderschneider, B. *et al., J. Agric. Food Chem.*, 2001, **49**, 2788-2798 (*3′-Me 9′-glucoside, 3′,5-di-Me 9′-glucoside*)

5,14-Epoxy-5,7,8-marasmanetriol E-145



$C_{15}H_{24}O_4$ 268.352

(5α,7β,8β)-*form*

5-Me ether: [243447-93-0] ***Lactapiperanol C***
$C_{16}H_{26}O_4$ 282.379
Constit. of *Lactarius piperatus*.
Amorph. powder. $[\alpha]_D^{22}$ -52.6 (c, 0.04 in $CHCl_3$).

5-Me ether, 8-Ac: [243447-94-1] ***Lactapiperanol D***
$C_{18}H_{28}O_5$ 324.416
Constit. of *Lactarius piperatus*. Oil. $[\alpha]_D^{21}$ -105.3 (c, 0.04 in $CHCl_3$).

(5β,7β,8β)-*form*

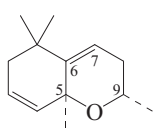
5-Me ether: [243447-91-8] ***Lactapiperanol A***
$C_{16}H_{26}O_4$ 282.379
Constit. of *Lactarius piperatus*.
Amorph. powder. $[\alpha]_D^{21}$ +26.3 (c, 0.04 in $CHCl_3$).

5-Me ether, 8-Ac: [243447-92-9] ***Lactapiperanol B***
$C_{18}H_{28}O_5$ 324.416
Constit. of *Lactarius piperatus*. Oil. $[\alpha]_D^{20}$ +33.3 (c, 0.06 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 894-896 (*isol, pmr, cmr*)

5,9-Epoxy-3,6-megastigmadiene E-146

*3,5,6,8*a*-Tetrahydro-2,5,5,8*a*-tetramethyl-2*H*-1-benzopyran, 9CI*



(5α,9α)-*form*

$C_{13}H_{20}O$ 192.3

(5α,9α)-*form* [41678-30-2]
[162488-96-2]
Edulan II
Key flavour constit. in purple passion fruit (*Passiflora edulis*). Oil. $[\alpha]_D$ +73.4 (c, 0.39 in CH_2Cl_2).

6α,7-Dihydro: [41678-32-4] ***Dihydroedulan II***
$C_{13}H_{22}O$ 194.316

(5β,9α)-*form* [41678-29-9]
[162488-97-3]
Edulan I
Key flavour constit. in purple passion fruit (*Passiflora edulis*). Oil. $[\alpha]_D$ +82.8 (c, 0.39 in CH_2Cl_2).

6β,7-Dihydro: [63335-66-0] *5,9-Epoxy-3-megastigmene.* ***Dihydroedulan I***
$C_{13}H_{22}O$ 194.316

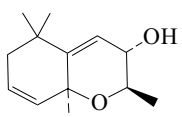
6α,7α-Epoxide: [69979-86-8] *5,9:6,7-Diepoxy-3-megastigmene.* ***6,7-Epoxyedulan.*** *Riesling acetal*
$C_{13}H_{20}O_2$ 208.3
Oil.

[58116-28-2, 58116-29-3]

Prestwich, G.D. *et al., Tetrahedron*, 1970, **32**, 2945 (*Dihydroedulans*)
Adams, D.R. *et al., J.C.S. Perkin 1*, 1975, 1736 (*synth*)
Whitfield, F.B. *et al., Aust. J. Chem.*, 1977, **30**, 1073 (*struct*)
Winter, M. *et al., Helv. Chim. Acta*, 1979, **62**, 131 (*epoxide*)
Etoh, H. *et al., Agric. Biol. Chem.*, 1980, **44**, 2871
Winterhalter, P. *et al., Chem. Ind. (London)*, 1990, 463 (*isol*)
Sugai, T. *et al., Tetrahedron*, 1991, **47**, 7227 (*synth*)
Weyerstahl, P. *et al., Annalen*, 1994, 415 (*synth*)
Schmidt, G. *et al., J. Agric. Food Chem.*, 1995, **43**, 185-188 (*synth, pmr, abs config*)
Honda, T. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 837 (*synth, abs config*)

5,9-Epoxy-3,6-megastigmadien-8-ol E-147

8-Hydroxyedulan. *3-Hydroxyedulan*



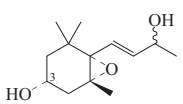
$C_{13}H_{20}O_2$ 208.3

(5α,8β,9β)-*form* [69927-26-0]
Constit. of *Passiflora edulis* (passion fruit). Oil.

Winter, M. *et al., Helv. Chim. Acta*, 1979, **62**, 131

5,6-Epoxy-7-megastigmene-3,9-diol E-148

5,6-Epoxy-3-hydroxy-β-ionol



(3α,5α,6α,7*E*,9ξ)-*form*

$C_{13}H_{22}O_3$ 226.315

(3α,5α,6α,7*E*,9ξ)-*form*
Cryst. (MeOH) (as di-Ac). Mp 72-74° (di-Ac).

*3-*O*-β-D-Glucopyranoside:* [143775-71-7]
$C_{19}H_{32}O_8$ 388.457
Isol. from sloe tree (*Prunus spinosa*). Characterised as penta-Ac.

(3β,5α,6α,7*E*,9*R*)-*form*

*9-*O*-β-D-Glucopyranoside:*
$C_{19}H_{32}O_8$ 388.457
Constit. of *Premna subscandens*, *Bunias orientalis* (hill mustard). Amorph. powder. $[\alpha]_D^{19}$ -35.2 (c, 1.08 in MeOH).

(3β,5α,6α,7*E*,9*S*)-*form* [189351-22-2]
Corchoionol A
Powder. $[\alpha]_D^{27}$ -56.1 (c, 0.3 in MeOH).

*3-*O*-β-D-Glucopyranoside:* [189351-14-2]
Corchoionoside A
$C_{19}H_{32}O_8$ 388.457
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{28}$ -24.8 (c, 0.1 in MeOH).

(3β,5α,6α,7*E*,9ξ)-*form*

*9-*O*-β-D-Glucopyranoside:* [172823-80-2]
$C_{19}H_{32}O_8$ 388.457
Constit. of *Malus domestica* (apple). Maybe identical to 9-*O*-β-D-glucopyranoside above.

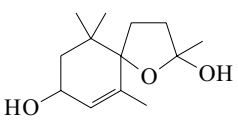
(5α,6α,7*E*,9ξ)-*form*

3-Ketone: [155418-97-6] *5,6-Epoxy-9-hydroxy-7-megastigmen-3-one.* ***Annuionone C***
$C_{13}H_{20}O_3$ 224.299
Constit. of *Helianthus annuus* (sunflower). Oil. $[\alpha]_D^{25}$ -8 (c, 0.1 in $CHCl_3$).

Humpf, H.-U. *et al., J. Agric. Food Chem.*, 1992, **40**, 1898 (*isol, glucoside*)
Winterhalter, P. *et al., Nat. Prod. Lett.*, 1994, **4**, 57 (*isol, pmr, cmr*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 464-469 (*Corchoionoside A*)
Marcías, F.A. *et al., Phytochemistry*, 1998, **48**, 631-636; 1999, **52**, 613-621 (*Annuionones*)

6,9-Epoxy-4-megastigmene-3,9-diol E-149

Riesling acetal

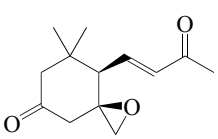


$C_{13}H_{22}O_3$ 226.315
Constit. of Riesling wine.

Winterhalter, P. *et al., Chem. Ind. (London)*, 1990, 463 (*isol, pmr, cmr*)

5,13-Epoxy-7-megastigmene-3,9-dione E-150

[211183-73-2]
Annuionone B

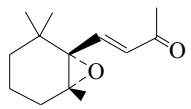


$C_{13}H_{18}O_3$ 222.283
Constit. of *Helianthus annuus* (sunflower). Oil. $[\alpha]_D^{25}$ -13.5 (c, 0.1 in $CHCl_3$).

7,8-Dihydro: [201288-96-2] *5,13-Epoxy-3,9-megastigmanedione.* ***Annuionone A***
$C_{13}H_{20}O_3$ 224.299
Constit. of *Helianthus annuus* (sunflower). Oil. $[\alpha]_D^{25}$ +12.3 (c, 0.4 in $CHCl_3$).
Marcías, F.A. *et al., Phytochemistry*, 1998, **48**, 631-636 (*isol, pmr, cmr*)

5,6-Epoxy-7-megastigmen-9-one E-151

[23267-57-4]
4-(2,2,6-Trimethylbicyclo[4.1.0]hept-1-yl)-3-buten-2-one, 9CI. 5,6-Epoxy-5,6-dihydro-β-ionone

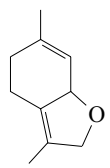


Absolute configuration

$C_{13}H_{20}O_2$ 208.3
(5R,6S)-form
Constit. of tomatoes and carrots. Cryst. (Et_2O/hexane). Mp 48.5-49.5°. $[\alpha]_D$ -85 (c, 0.64 in EtOH).
Acemoglu, M. *et al., Helv. Chim. Acta*, 1981, **64**, 2691 (*synth, bibl*)

3,9-Epoxy-*p*-mentha-1,4(8)-diene E-152

[132437-74-2]
Linden ether



$C_{10}H_{14}O$ 150.22
Constit. of linden honey.

[125811-37-2]

Blank, I. *et al., Helv. Chim. Acta*, 1990, **73**, 1250 (*isol, pmr, cmr*)

1,4-Epoxy-*p*-menthane, 8CI E-153

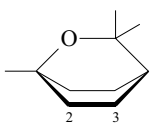
[470-67-7]
1-Methyl-4-(1-methylethyl)-7-oxabicyclo[2.2.1]heptane, 9CI. 1-Isopropyl-4-methylbicyclo[2.2.1]heptane. ***1,4-Cineole****. Isocineole*



$C_{10}H_{18}O$ 154.252
Constit. of *Piper cubeba* (cubeb pepper). d^{20} 0.9. Bp 173-174°. n_D^{20} 1.4470.
▶ OS9274000
Wallach, O. *et al., Annalen*, 1907, **356**, 197 (*isol, struct*)
Austerweil, M.G. *et al., Bull. Soc. Chim. Fr.*, 1929, **45**, 862 (*synth*)
Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1950, 673 (*isol*)
Matsubara, Y. *et al., Nippon Kagaku Zasshi*, 1970, **91**, 762; *CA*, **73**, 120762a (*isol, purifn*)
Takahashi, H. *et al., Chem. Lett.*, 1979, 373 (*synth, pmr*)

1,8-Epoxy-*p*-menthane E-154

[470-82-6]
1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane, 9CI. ***1,8-Cineole****. Eucalyptol. Eucapur. Soledum. Terpane. Zineol. Cineole. Cyneol. Cajeputol. FEMA 3658*



$C_{10}H_{18}O$ 154.252
Occurs in eucalyptus, lavender, sage and many other oils. Flavouring ingredient. Oil with camphoraceous odour. Mp 1.5°. Bp 176-177°. n_D^{20} 1.4550. Log P 2.76 (calc).
▶ Flammable, fl. p. 50°. LD_{50} (rat, orl) 2480 mg/kg. Exp. reprod. effects (large dose). OS9275000

2,3-Didehydro: [92760-25-3] ***Dehydro-1,8-cineole****. 1,8-Epoxy*-p-*menth-2-ene*
$C_{10}H_{16}O$ 152.236
Isol. from *Laurus nobilis* (bay laurel) oil. Oil. Bp_{40} 78-80°. $[\alpha]_D^{20}$ -53 (c, 3 in EtOH). Props. refer to synthetic material. Opt. rotn. and abs. config. of nat. isolates not reported.

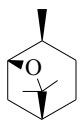
3-Oxo: [101221-23-2] *1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octan-2-one, 9CI.* ***3-Oxo-1,8-cineole****. 1,8-Epoxy*-p-*methan-3-one*
$C_{10}H_{16}O_2$ 168.235

[58264-16-7, 63025-72-9, 66113-06-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 245C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 395A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 323D (*ir*)
Coxen, J.M. *et al., Chem. Ind. (London)*, 1968, **652**, (*synth*)
Achilladelis, B. *et al., Phytochemistry*, 1968, **7**, 1317 (*biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 570 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Hogg, J.W. *et al., Phytochemistry*, 1974, **13**, 868 (*Dehydrocineole, isol*)
Zenin, V.S. *et al., Khim. Prir. Soedin.*, 1975, **11**, 15; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 13 (*ir, anal*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Bondavalli, F. *et al., J.C.S. Perkin 1*, 1977, 430; 1978, 804 (*synth*)
Orsini, F. *et al., Gazz. Chim. Ital.*, 1980, **110**, 553 (*biosynth*)
Ayorinde, F.O. *et al., Tet. Lett.*, 1984, **25**, 3525 (*isol, synth, Dehydrocineole*)
Kumar, N. *et al., Phytochemistry*, 1986, **25**, 250 (*3-Oxocineole*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CAL000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1354
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 113 (*rev*)
Brecknell, D.J. *et al., Aust. J. Chem.*, 1997, **50**, 35 (*synth*)
Rieder, C. *et al., Helv. Chim. Acta*, 2000, **83**, 2504-2513 (*biosynth*)
Bond, A.D. *et al., Aust. J. Chem.*, 2001, **54**, 683-684 (*cryst struct*)
Wise, M.L. *et al., J.A.C.S.*, 2002, **124**, 8546-8547 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAL000

6,8-Epoxy-*p*-menthane E-155

[5718-77-4]
4,7,7-Trimethyl-6-oxabicyclo[3.2.1]octane. Dihydropinol



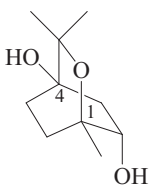
$C_{10}H_{18}O$ 154.252
Minor constit. of caraway oil. Oil. Bp 186-188°. $[\alpha]_D$ +104.

[55822-05-4]

Schmidt, H. *et al., Ber.*, 1955, **88**, 453
Siemieniuk, A. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1974, **22**, 1009

1,8-Epoxy-*p*-menthane-2,4-diol E-156

[161168-81-6, 161168-82-7, 161168-83-8]
1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane-4,6-diol, 9CI. 2,4-Dihydroxy-1,8-cineole



(1*R*,2*R*,4*R*)-*form*

$C_{10}H_{18}O_3$ 186.25

(1R,2R,4R)-form [176896-61-0]
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 158-159°. $[\alpha]_D^{26}$ -23 (c, 0.2 in MeOH).

2-O-*β*-*D*-*Glucopyranoside:* [174390-07-9]
Foeniculoside VI
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Powder. $[\alpha]_D^{27}$ -59.5 (c, 0.1 in MeOH).

4-O-*β*-*D*-*Glucopyranoside:* [174285-77-9]
Foeniculoside VII
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Powder. $[\alpha]_D^{27}$ -15.6 (c, 1.2 in MeOH).

(1S,2R,4S)-form [219546-81-3]
Constit. of *Foeniculum vulgare* (fennel). Powder. $[\alpha]_D^{26}$ -31.2 (c, 0.2 in MeOH).

2-O-*β*-*D*-*Glucopyranoside:* [174232-47-4]
Foeniculoside V

$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Powder. $[\alpha]_D^{29}$ -56.9 (c, 3.6 in MeOH).

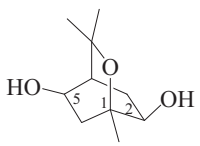
(1*S*,2*S*,4*S*)-*form*

2-O-*β*-D-*Glucopyranoside:* [219583-09-2]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -23.5 (c, 0.1 in MeOH).

Carman, R.M. *et al., Aust. J. Chem.*, 1994, **47**, 2087 (*isol, pmr, cmr, synth*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 337-342 (*Foeniculosides*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1738-1742 (*Foeniculum vulgare constits*)

1,8-Epoxy-*p*-menthane-2,5-diol E-157

2,5-Dihydroxy-1,8-cineole



(1*S*,2*R*,4*S*,5*R*)-*form*

$C_{10}H_{18}O_3$ 186.25

(1*S*,2*R*,4*S*,5*R*)-*form* [219546-82-4]
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH) or powder. Mp 151-153°. $[\alpha]_D^{26}$ -62.2 (c, 0.5 in MeOH).

2-O-*β*-D-*Glucopyranoside:* [174232-48-5]
Foeniculoside IX
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Powder. $[\alpha]_D^{29}$ -65.9 (c, 2.5 in MeOH).

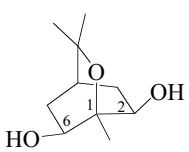
(1*S*,2*S*,4*S*,5*R*)-*form* [219546-83-5]
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -13 (c, 0.3 in MeOH).

2-O-*β*-D-*Glucopyranoside:* [219583-17-2]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -24.7 (c, 0.3 in MeOH).

Ono, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 337-342 (*isol, pmr, cmr*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1738-1742 (*isol, pmr, cmr*)

1,8-Epoxy-*p*-menthane-2,6-diol E-158

2,6-Dihydroxy-1,8-cineole



$C_{10}H_{18}O_3$ 186.25

(1*RS*,2*RS*,4*SR*,6*SR*)-*form* [38223-98-2]
exo,exo-*form*
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH) or powder. Mp 164-165°. Parent compound is *meso*-. Monoglycosylation at O^2 or O^6 produces diastereoisomeric compounds.

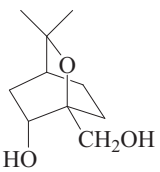
2-O-*β*-D-*Glucopyranoside:* [174285-76-8]
Foeniculoside VIII
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Powder. $[\alpha]_D^{29}$ -34.9 (c, 1.6 in MeOH). Abs. config. is (1*S*,2*R*,4*R*,6*S*)-.

6-O-*β*-D-*Glucopyranoside:* [219583-13-8]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -23.5 (c, 0.1 in MeOH). Abs. config. is (1*R*,2*R*,4*S*,6*S*)-. Can also be descr. as the 2-glucoside with abs. config. (1*R*,2*S*,4*S*,6*R*).

Ono, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 337-342 (*isol, pmr, cmr*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1738-1742 (*isol, pmr, cmr*)

1,8-Epoxy-*p*-menthane-2,7-diol E-159

2,7-Dihydroxy-1,8-cineole



(1*S*,2*R*,4*S*)-*form*

$C_{10}H_{18}O_3$ 186.25

(1*S*,2*R*,4*S*)-*form* [176794-61-9]

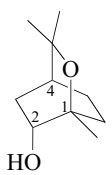
(1*S*,2*S*,4*S*)-*form*

2-O-*β*-D-*Glucopyranoside:* [219546-80-2]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -18 (c, 0.1 in MeOH).

Carman, R.M. *et al., Aust. J. Chem.*, 1996, **49**, 741-749 (*isol, synth*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1738-1742 (*2-glucoside*)

1,8-Epoxy-*p*-menthan-2-ol E-160

2-Hydroxy-1,8-cineole



(1*R*,2*R*,4*S*)-*form*

$C_{10}H_{18}O_2$ 170.251

(1*R*,2*R*,4*S*)-*form*

O-*β*-D-*Glucopyranoside:* [155836-26-3]
$C_{16}H_{28}O_7$ 332.393
Constit. of *Alpinia galanga* (greater galangal) and *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 85-86°. $[\alpha]_D^{23}$ -66.3 (c, 1 in MeOH).

(1*R*,2*S*,4*S*)-*form*

O-*β*-D-*Glucopyranoside:* [219583-06-9]
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 94-95°. $[\alpha]_D^{21}$ -7.2 (c, 1 in MeOH).

(1*S*,2*R*,4*R*)-*form*

O-*β*-D-*Glucopyranoside:* [168038-89-9]
Constit. of *Foeniculum vulgare* (fennel). Isol from the leaves of *Salvia officinalis* (Dalmatian sage). Amorph. solid. Mp 92-94°. $[\alpha]_D^{21}$ -46.3 (c, 1.5 in MeOH).

(1*S*,2*S*,4*R*)-*form*

O-*β*-D-*Glucopyranoside:* [113270-15-8]
Constit. of *Alpinia galanga* (greater galangal), *Citrus unshiu* (satsuma mandarin) and *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 83-84°. $[\alpha]_D^{23}$ +5.5 (c, 1.6 in MeOH).

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [217975-07-0]
$C_{21}H_{36}O_{11}$ 464.509
Amorph. powder. $[\alpha]_D^{23}$ -24.1 (c, 1.6 in MeOH).

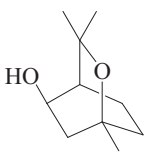
(1*R*,2*S*,4*S*)-*form*

O-*β*-D-*Glucopyronoside:* [259875-20-2] ***Bucharioside***
$[\alpha]_D^{25}$ -25.5 (c, 2.3 in MeOH).

Manns, D. *et al., Phytochemistry*, 1995, **39**, 1115-1118 (*Cunila spicata glucoside*)
Yoshikawa, Y. *et al., Nat. Med. (Tokyo)*, 1996, **50**, 176-178 (*Citrus unshiu glucoside*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1583-1586 (*apiosylglucoside*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1738-1742 (*Foeniculum vulgare glucosides*)
Wang, M. *et al., J. Agric. Food Chem.*, 1998, **46**, 2509-2511 (*glucoside, isol, nmr*)
Ahmad, V.U. *et al., Phytochemistry*, 1999, **52**, 1319-1322 (*Bucharioside*)
Someya, Y. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 950-953 (*Alpinia galanga glucosides*)

1,8-Epoxy-*p*-menthan-3-ol E-161

[98920-24-2]
1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octan-5-ol, 9CI. 3-Hydroxy-1,8-cineole



(1*R*,3*R*,4*S*)-*form*

$C_{10}H_{18}O_2$ 170.251

(1*R*,3*R*,4*S*)-*form* [76793-04-9]
Cryst. (pentane). Mp 90-91°. $[\alpha]_D^{22}$ +50.5 (c, 2.5 in EtOH).

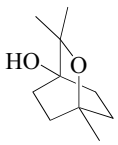
(1*R*,3*S*,4*S*)-*form* [76735-22-3]
Cryst. (pentane). Mp 68-69°. $[\alpha]_D^{22}$ -19 (c, 2.7 in EtOH).

O-*β*-D-*Glucopyranoside:* [155836-27-4]
$C_{16}H_{28}O_7$ 332.393
Constit. of fresh ginger (*Zingiber officinale*) and *Alpinia galanga* (greater galangal). $[\alpha]_D^{23}$ -22.7 (c, 0.42 in MeOH).

[81801-58-3, 83860-14-4, 107133-88-0, 118013-28-8, 118013-29-9]

Bondavalli, F. *et al., J.C.S. Perkin 1*, 1980, 2626-2630 (*synth*)
de Boggiatto, M.V. *et al., J.O.C.*, 1987, **52**, 1505-1511 (*synth*)
Asakawa, Y. *et al., Phytochemistry*, 1988, **27**, 3861-3869 (*synth, cmr*)
Sekiwa, Y. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 384-389 (*glucoside*)
Someya, Y. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 950-953 (*glucoside*)

1,8-Epoxy-*p*-menthan-4-ol E-162



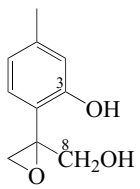
$C_{10}H_{18}O_2$ 170.251

Parent compd. is achiral.

O-*β*-D-*Glucopyranoside:* [219546-79-9]
$C_{16}H_{28}O_7$ 332.393
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{21}$ -18 (c, 1.3 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1738-1742 (*isol, pmr, cmr*)

9,10-Epoxy-*p*-mentha-1,3,5-triene-3,8-diol E-163



$C_{10}H_{12}O_3$ 180.203

Bis(2-methylpropanoyl): [22518-06-5]
$C_{18}H_{24}O_5$ 320.385
Constit. of various plant spp. including *Madia sativa* (Chile tarweed).

3-(2-Methylpropanoyl), 8-(2-methylbutanoyl): [22518-07-6]
$C_{19}H_{26}O_5$ 334.411
Constit. of various plant spp. incl. *Madia sativa* (Chile tarweed).

3-(2-Methylpropanoyl), 8-(3-methylbutanoyl): [71939-56-5]
$C_{19}H_{26}O_5$ 334.411
Constit. of *Madia sativa* (Chile tarweed).

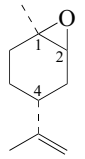
Bis(3-methylbutanoyl): [97745-11-4]
$C_{20}H_{28}O_5$ 348.438
Oil.

3-Tigloyl: [361541-55-1]
$C_{15}H_{18}O_4$ 262.305
$[\alpha]_D^{23}$ -32 (c, 1.1 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1103-1107 (*Madia sativa esters*)
Metwally, M.A. *et al., Phytochemistry*, 1985, **24**, 1377-1378 (*bis-3-methylbutanoyl*)
Tori, M. *et al., J. Nat. Prod.*, 2001, **64**, 1048-1051 (*Eupatorium fortunei ester*)

1,2-Epoxy-*p*-menth-8-ene, 8CI E-164

[1195-92-2]
1-Methyl-4-(1-methylethenyl)-7-oxabicyclo[4.1.0]heptane, 9CI. Limonene oxide



(1*R*,2*S*,4*R*)-*form*

$C_{10}H_{16}O$ 152.236
Isol. from oil of *Cymbopogon* spp., orange (*Citrus sinensis*), Japanese pepper tree (*Zanthoxylum piperitum*) and others. Stereoisomers mostly not differentiated; occurs as mixts., difficult to separate. Undergoes radiation-induced cationic homopolym. to give low-mol. wt. polymers.

► Mutagenic. RN8761000

(1*R*,2*S*,4*R*)-*form* [4680-24-4]
Oil. Bp_{26} 96-98°. $[\alpha]_D^{23.5}$ +36 (neat). $n_D^{23.5}$ 1.4683.

(1*S*,2*R*,4*R*)-*form* [6909-30-4]
Oil. Bp_{10} 78.5-80.5°. $[\alpha]_D^{24}$ +83.22 (neat). n_D^{24} 1.4657.

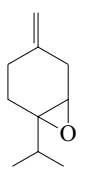
(1*S*,2*R*,4*S*)-*form* [32543-51-4]
Oil. $[\alpha]_D$ -30.4 (c, 0.56 in MeOH).

[10373-59-8, 13837-75-7, 26767-54-4]

Newhall, W.F. *et al., J.O.C.*, 1964, **29**, 185 (*synth, config*)
Nigam, M.C. *et al., Can. J. Chem.*, 1965, **43**, 521 (*isol*)
Royals, E.E. *et al., J.O.C.*, 1966, **31**, 1937 (*synth*)
Sakai, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1945 (*isol*)
Aikens, J.A. *et al., ACS Symp. Ser.*, 1985, **286**, 335 (*polym*)
Baptistella, L.H.B. *et al., Annalen*, 1994, 785 (*1S2R4S-form: synth, pmr*)
dos Santos, A.G. *et al., Synth. Commun.*, 1996, **26**, 2651 (*1S2R4R-form: synth, ir, pmr, cmr, ms*)
Van Der Werf, M.J. *et al., Tet. Lett.*, 2001, **42**, 5521-5524 (*synth*)

3,4-Epoxy-*p*-menth-1(7)-ene E-165

[21391-86-6]
4-Methylene-1-(1-methylethyl)-7-oxabicyclo[4.1.0]heptane

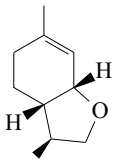


$C_{10}H_{16}O$ 152.236
Isol. from *Zanthoxylum piperitum* (Japanese pepper tree).

Sakai, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1945 (*isol*)
Ashraf, M. *et al., Pak. J. Sci. Ind. Res.*, 1980, **23**, 70

3,9-Epoxy-*p*-menth-1-ene, 8CI E-166

[70786-44-6]
2,3,3a,4,5,7a-Hexahydro-3,6-dimethylbenzofuran, 9CI. ***Anethofuran****. Dill ether*



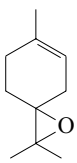
$C_{10}H_{16}O$ 152.236
Isol. from the leaf oil of *Anethum graveolens* (dill).

[13955-47-0, 13955-48-1, 74410-10-9, 88764-44-7, 88764-45-8, 118015-24-0, 118015-25-1]

Ohloff, G. *et al., Helv. Chim. Acta*, 1966, **49**, 2135 (*synth*)
Groeckeritz, D. *et al., Pharmazie*, 1979, **34**, 846 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2639 (*synth*)
Brunke, E.J. *et al., J. Essent. Oil Res.*, 1991, **3**, 257

4,8-Epoxy-*p*-menth-1-ene E-167

[4584-23-0]
Terpinolene oxide

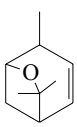


$C_{10}H_{16}O$ 152.236
Isol. from *Zanthoxylum piperitum* (Japanese pepper tree).

Sakai, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1945 (*isol*)
Roy, A. *et al., J. Sci. Ind. Res.*, 1997, **56**, 513-517 (*rev*)

6,8-Epoxy-*p*-menth-2-ene E-168

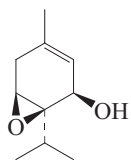
[52812-45-0]
4,7,7-Trimethyl-6-oxabicyclo[3.2.1]oct-2-ene



$C_{10}H_{16}O$ 152.236
Isol. from *Laurus nobilis* (bay laurel).

Hogg, J.W. *et al., Phytochemistry*, 1974, **13**, 868 (*isol, ms, pmr*)

4,5-Epoxy-*p*-menth-1-en-3-ol E-169



$C_{10}H_{16}O_2$ 168.235

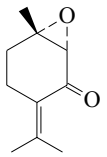
(3β,4β,5β)-*form* [359875-84-6]
Amorph. powder. $[\alpha]_D^{22}$ +53 (c, 0.1 in MeOH).

3-O-*β*-D-*Glucopyranoside:* [359875-79-9]
$C_{16}H_{26}O_7$ 330.377
Constit. of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{24}$ +45 (c, 0.5 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*isol, pmr, cmr*)

1,2-Epoxy-*p*-menth-4(8)-en-3-one E-170

[5945-46-0]
6-Methyl-3-(1-methylethylidene)-7-oxabicyclo[4.1.0]heptan-2-one, 9CI. 2,3-Epoxy-6-isopropylidene-3-methylcyclohexanone. ***Rotundifolone****. Piperitenone oxide*


Absolute configuration

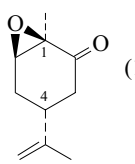
$C_{10}H_{14}O_2$ 166.219
Constit. of *Mentha rotundifolia* and other *Mentha* spp. Flavouring ingredient. Cryst. Mp 27.5°. Bp_1 86°. $[\alpha]_D^{10}$ +166.5 (MeOH).

[5056-08-6, 35178-55-3]

Shimizu, S. *et al., Agric. Biol. Chem.*, 1966, **30**, 89
Almeida, R.N. *et al., Fitoterapia*, 1996, **67**, 334 (*isol, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2230

1,6-Epoxy-*p*-menth-8-en-2-one E-171

[33204-74-9]
1-Methyl-4-(1-methylethenyl)-7-oxabicyclo[4.1.0]heptan-2-one, 9CI. ***Carvone oxide***


(1*S*,4*S*,6*S*)-*form*

$C_{10}H_{14}O_2$ 166.219
(1*R*,4*R*,6*R*)-*form* [18383-49-8]
$[\alpha]_D^{20}$ +87.6 ($CHCl_3$).
(1*S*,4*R*,6*S*)-*form*
$[\alpha]_D^{20}$ -88 ($CHCl_3$).
(1*S*,4*S*,6*S*)-*form*
Oil. $[\alpha]_D^{23}$ -44 (c, 0.002 in hexane).
(1ξ,4ξ,6ξ)-*form*
Isol. from spearmint oil.

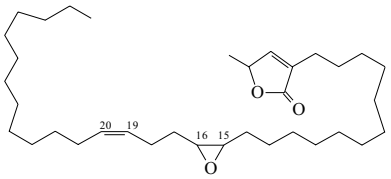
[36616-60-1, 39067-90-8, 39903-98-5, 74608-55-2]

Klein, E. *et al., Tetrahedron*, 1963, **19**, 1091 (*synth*)
Lindquist, N. *et al., Phytochemistry*, 1985, **24**, 863 (*isol*)

Epoxymurin A E-172

[151484-64-9]

[150670-81-8]
3-[12-[3-(3-Hexadecenyl)oxiranyl]dodecyl]-5-methyl-2(5H)-furanone, 9CI



$C_{35}H_{62}O_3$ 530.873
Isol. from the bark of *Annona muricata* (soursop). Obt. as a mixture with Epoxymarin B λ_{max} 210 (ϵ 6310) (EtOH) (Berdy).

19,20-Epoxide: [142733-57-1]

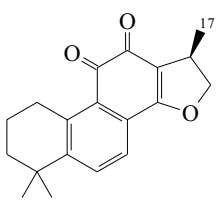
[129196-65-2] ***Diepomuricanin A****. Epoxyrollin B*
$C_{35}H_{62}O_4$ 546.872
Isol. from *Annona muricata* (soursop). Wax. Identity of Epoxyrollin B with Diepomuricanin A not certain.

19,20-Epoxide, 15,16-deepoxy: [151592-70-0]

[150670-81-8] *Epomuricenin A.* ***Epoxymurin B***
$C_{35}H_{62}O_3$ 530.873
From bark of *Annona muricata* (soursop).

Laprevote, O. *et al., Tet. Lett.*, 1990, **31**, 2283 (*Epoxyrollin B*)
Roblot, F. *et al., Phytochemistry*, 1993, **34**, 281 (*Epomuricenin A*)
Hisham, A. *et al., Tetrahedron*, 1993, **49**, 6913 (*isol, struct*)
Konno, H. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2355 (*pmr, cmr, ms*)
Konno, H. *et al., Tet. Lett.*, 1996, **37**, 5953 (*Diepomuricanin, synth*)

14,16-Epoxy-20-nor-5(10),6,8,13-abietatetraene-11,12-dione E-173



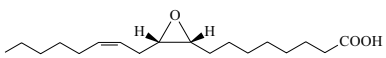
$C_{19}H_{20}O_3$ 296.365
(*R*)-*form* [35825-57-1]
Cryptotanshinone
Isol. from *Rosmarinus officinalis* (rosemary). Red cryst. Mp 182°. $[\alpha]_D^{21}$ -91.4 ($CHCl_3$). λ_{max} 263 (ϵ 29000); 271 (ϵ 25700); 292 (ϵ 8900); 293 (ϵ 8912); 353 (ϵ 2511); 355 (ϵ 2560); 445 (ϵ 2300); 460 (ϵ 3020) (MeOH) (Berdy). λ_{max} 221 ; 263 ; 272 ; 290 ; 355 ; 447 (EtOH) (Berdy).
17-Hydroxy: [145940-77-8] ***17-Hydroxycryptotanshinone***
$C_{19}H_{20}O_4$ 312.365
Reddish solid or red plates (MeOH). Mp 165-167°. $[\alpha]_D^{18}$ -17.9 (c, 0.11 in $CHCl_3$). Has (*S*)-config..
(±)-*form*
Orange-brown needles. Mp 174-175°.

[4783-35-1]

Takiura, K. *et al., Chem. Pharm. Bull.*, 1962, **10**, 112 (*isol*)
Baillie, A.C. *et al., J.C.S.(C)*, 1968, 48 (*synth*)
Inouye, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 3318 (*synth*)
Tateishi, M. *et al., Tetrahedron*, 1971, **27**, 237 (*synth*)
Brieskorn, C.H. *et al., Planta Med.*, 1973, **24**, 190 (*isol*)
Romanova, A.S. *et al., Khim. Prir. Soedin.*, 1977, **13**, 414; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 350 (*isol*)
Tomita, Y. *et al., Chem. Comm.*, 1987, 1311 (*biosynth, abs config*)
de la Torre, M.C. *et al., Phytochemistry*, 1992, **31**, 3953 (*17-Hydroxycryptotanshinone*)
Luis, J.G. *et al., Tetrahedron*, 1993, **49**, 6277 (*17-Hydroxycryptotanshinone*)
Danheiser, R.L. *et al., J.O.C.*, 1995, **60**, 8341 (*synth*)
Lee, D.-S. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 2236-2239 (*isol, activity*)
Jiang, Y.-Y. *et al., Tet. Lett.*, 2003, **44**, 2073-2075 (*synth*)

9,10-Epoxy-12-octadecenoic acid E-174

[65167-83-1]
3-(2-Octenyl)oxiraneoctanoic acid, 9CI. Leukotoxin A

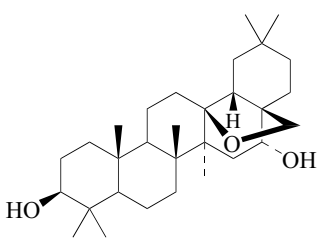


$C_{18}H_{32}O_3$ 296.449
(9*R*,10*S*,12*Z*)-*form* [16833-56-0]
Coronaric acid
Found in *Chrysanthemum coronarium* (chop-suey greens) and some other seed oil. Isol. from rice plant, Fukuyuki. $[\alpha]_D$ +3.44. $[\alpha]_{350}$ +8.94 (c, 9.54 in hexane). Racemic diastereoisomers known synthetically and characterised as the corresp. diols.

[61949-82-4, 126639-25-6]

Smith, C.R. *et al., J.O.C.*, 1960, **25**, 218 (*isol*)
Powell, R.G. *et al., Lipids*, 1967, **2**, 172 (*abs config*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1975, **15**, 174; 189; 198 (*synth, glc, tlc, pmr, ms*)
Sen Gupta, A.K. *et al., Chem. Ind. (London)*, 1976, 257
Kato, T. *et al., Tet. Lett.*, 1983, **24**, 4715 (*isol*)

13,28-Epoxy-3,16-oleananediol E-175



$C_{30}H_{50}O_3$ 458.723
See also refs. in 13,28-Epoxy-3,16,22-oleananetriol, E-176.
(3β,13β,16α)-*form* [2611-08-7]
Protoprimulagenin A
Cryst. (Me_2CO/hexane). Mp 272-273°. $[\alpha]_D$ +13 (c, 1.0 in $CHCl_3$).

3-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside]:
[126882-54-0]
$C_{52}H_{86}O_{21}$ 1047.239
Amorph. powder. Mp 205° dec. $[\alpha]_D$ -4.3 (c, 1 in MeOH).

3-O-[β-D-Rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside]:
[172615-58-6]
$C_{53}H_{88}O_{21}$ 1061.266
Amorph. powder. Mp 199° dec. $[\alpha]_D$ -23 (c, 1 in MeOH).

3-O-[α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)]-β-D-glucuronopyranoside]:
[208599-88-6] ***Primulasaponin 2***
$C_{59}H_{96}O_{27}$ 1237.391
Cryst. $[\alpha]_D$ -4 (c, 0.01 in MeOH). Mp >140° dec..

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [65312-86-9] ***Primulasaponin 1***. *Primulasaponin. Primulasaponin A*
$C_{54}H_{88}O_{23}$ 1105.275
Cryst. Mp 241-243°. $[\alpha]_D$ +3 (c, 0.01 in MeOH). $[\alpha]_D^{26}$ -29.9 (c, 1 in MeOH). Mp >140° dec..

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [86667-22-3]
$C_{54}H_{88}O_{23}$ 1105.275
No phys. props reported.

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-galactopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [137682-20-3]
$C_{54}H_{88}O_{23}$ 1105.275
Constit. of roots of Siberian ginseng (*Eleutherococcus (Acanthopanax) senticosus*). Mp 255-258°. $[\alpha]_D^{22}$ -45 (c, 0.4 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→?)-β-D-glucuronopyranoside]:
[137682-21-4]
$C_{60}H_{98}O_{26}$ 1235.419
Constit. of roots of Siberian ginseng (*Eleutherococcus (Acanthopanax) senticosus*). Mp 230° (dec.). $[\alpha]_D^{22}$ -15 (c, 0.5 in MeOH).

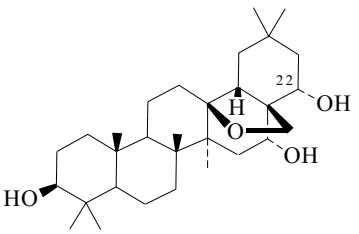
3-O-[α-L-Rhamnopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucuronopyranoside]:
[59527-84-3] ***Sakurasaponin***
$C_{60}H_{98}O_{27}$ 1251.418
Cryst. (MeOH). Mp 267-270° (266-268°). $[\alpha]_D^{22}$ -39 (c, 2 in MeOH).

16-Ketone: [2749-23-7] *13,28-Epoxy-3-hydroxy-16-oleananone*. ***Aegicerin***. *Egicerin*
$C_{30}H_{48}O_3$ 456.707
Needles (MeOH). Mp 254-256°. $[\alpha]_D^{28}$ -23.6 (c, 0.9 in $CHCl_3$).

Rao, K.V. *et al., Tetrahedron*, 1962, **18**, 461; 1964, **20**, 973 (*Aegicerin*)
Tschesche, R. *et al., Annalen*, 1964, **674**, 185-195; 1983, 993-1000 (*Primula saponins*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2226-2234; 1976, **24**, 2470-2479; 1980, **28**, 296-300 (*Sakurasaponin*)
Segiet-Kujawa, E. *et al., J. Nat. Prod.*, 1991, **54**, 1044-1048 (*Eleutherococcus senticosus saponins*)
Calis, I. *et al., J. Nat. Prod.*, 1992, **55**, 1299-1306 (*Primula saponin Me ester, cmr*)
Kazuhiro, O. *et al., Phytochemistry*, 1993, **33**, 83-86 (*activity, Sakurasaponin*)
Hegde, V.R. *et al., J. Nat. Prod.*, 1995, **58**, 1492 (*Myrsine australis saponins*)
Siems, K. *et al., Planta Med.*, 1998, **64**, 272-274 (*Primulasaponins*)

13,28-Epoxy-3,16,22-oleananetriol E-176

[20654-97-1]



$C_{30}H_{50}O_4$ 474.723

(3β,13β,16α,22α)-*form* [20054-97-1] ***Priverogenin B***
Sapogenin from *Primula veris* (cowslip). Cryst. (CCl_4/Me_2CO). Mp 265-269° Mp 280-283° (double Mp). $[\alpha]_D^{20}$ -7.9 (c, 0.33 in MeOH).

22-Ac: [26339-94-6]
$C_{32}H_{52}O_5$ 516.76
Saponin from *Primula veris* (cowslip). Mp 250-253°. $[\alpha]_D^{20}$ -23 (c, 0.62 in $CHCl_3$).

3-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-α-L-arabinopyranoside]: [160669-21-6] ***Anagallosaponin VI***
$C_{46}H_{76}O_{17}$ 901.096
Cryst. (MeOH). Mp 235-237°. $[\alpha]_D^{20}$ -8.7 (c, 1.82 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-α-L-arabinopyranoside]:
[160632-42-8] ***Anagallosaponin VII***
$C_{52}H_{86}O_{22}$ 1063.238
Cryst. (MeOH). Mp 258-259°. $[\alpha]_D^{20}$ -13.6 (c, 0.59 in MeOH).

3-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside], 22-Ac: [162763-02-2] ***Anagallosaponin IV***
$C_{54}H_{88}O_{23}$ 1105.275
Cryst. (MeOH). Mp 237-239°. $[\alpha]_D^{20}$ -19.4 (c, 1.39 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-α-L-arabinopyranoside], 22-Ac: [162763-03-3] ***Anagallosaponin V***
$C_{54}H_{88}O_{23}$ 1105.275
Needles (MeOH). Mp 253-255°. $[\alpha]_D^{20}$ -26.2 (c, 2.51 in Py).

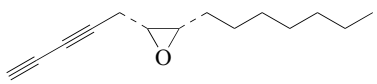
3-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-α-L-arabinopyranoside], 22-Ac: [162763-01-1] ***Anagallosaponin III***
$C_{48}H_{78}O_{18}$ 943.133
Cryst. (MeOH). Mp 246-247°. $[\alpha]_D^{20}$ -17.3 (c, 2.07 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside], 22-Ac: [114318-83-1] ***Anagalloside C***
$C_{60}H_{98}O_{28}$ 1267.417

Tschesche, R. *et al., Annalen*, 1966, **696**, 160 (*isol*)
Tschesche, R. *et al., Tet. Lett.*, 1968, 183 (*struct*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2226 (*isol*)
Narayanan, C.R. *et al., J.O.C.*, 1974, **39**, 2639 (*synth*)
Kitagawa, I. *et al., Tet. Lett.*, 1974, 469 (*struct*)
Gomblitza, K.W. *et al., Planta Med.*, 1987, **53**, 548-555 (*cmr, Anagalloside C*)
Kohda, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3304 (*cmr*)
Shoji, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1750 (*Anagallosaponin III, Anagallosaponin IV, Anagallosaponin V*)
Shoji, N. *et al., Phytochemistry*, 1994, **37**, 1397 (*Anagallosaponin VI, Anagallosaponin VII*)

6,7-Epoxy-1,3-tetradecadiyne E-177

2-Heptyl-3-(2,4-pentadiynyl)oxirane, 9CI. ***Panaquinquecol 8***. *PQ 8*



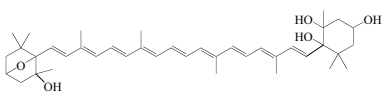
$C_{14}H_{20}O$ 204.311

(6*R*,7*S*)-*form* [155519-48-5]
Constit. of *Panax quinquefolium* (American ginseng). Oil. $[\alpha]_D$ -30.9 (c, 0.1 in $CHCl_3$).

Fujimoto, Y. *et al., Phytochemistry*, 1994, **35**, 1255 (*isol, pmr, cmr, ms*)
Satoh, M. *et al., Heterocycles*, 1997, **45**, 177 (*synth, abs config, pmr, cmr*)

3,6-Epoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3′,5,5′,6′-tetrol E-178

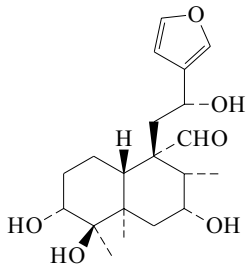
[181046-82-2]



$C_{40}H_{58}O_5$ 618.895
Constit. of red paprika pods of *Capsicum annuum* var. *longum*. λ_{max} 427 ; 453 ; 483 (C_6H_6).

Deli, J. *et al., Helv. Chim. Acta*, 1996, **79**, 1435-1443 (*isol, ms, uv, cd*)

15,16-Epoxy-3,4,7,12-tetrahydroxy-13(16),14-clerodadien-20-al E-179



$C_{20}H_{30}O_6$ 366.453

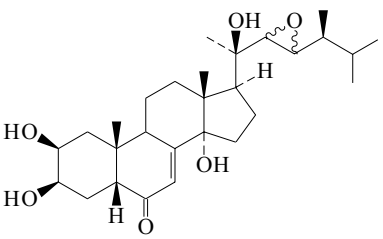
(*ent*-3β,4α,7β,12*S*)-*form*

7-Ac: [10118-56-6] ***Cascarillin***
$C_{22}H_{32}O_7$ 408.491
Constit. of *Croton eleuteria* (cascarilla). Cryst. (EtOH). Mp 203.5°.

McEachan, C.E. *et al., J.C.S.(B)*, 1966, 633

22,23-Epoxy-2,3,14,20-tetrahydroxyergost-7-en-6-one E-180

22,23-Epoxy-2,3,14,20-tetrahydroxy-24-methylcholest-7-en-6-one

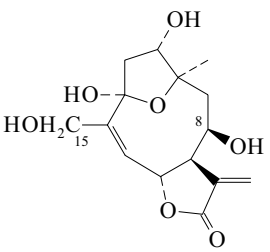


$C_{28}H_{44}O_6$ 476.652

(2β,3β,5β,14α,20*R*,22ξ,23ξ,24*R*)-*form*
[141360-90-9]
Polyporusterone C
Constit. of *Polyporus umbellatus* (zhu ling). Needles (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 250°. λ_{max} 241 (ε 10230) (MeOH) (Berdy).

Ohsawa, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 143 (*isol, pmr, cmr*)

3,10-Epoxy-1,3,8,15-tetrahydroxy-4,11(13)-germacradien-12,6-olide E-181



$C_{15}H_{20}O_7$ 312.319

(1α,3α*OH*,4*Z*,6α,8β,10β)-*form*

8-(2-Methyl-2-propenoyl): [326606-56-8]
$C_{19}H_{24}O_8$ 380.394

8-(2-Methylbutanoyl): [99274-78-9] ***2′,3′-Dihydroniveusin A***
$C_{20}H_{28}O_8$ 396.436
Gum.

8-Angeloyl: [75680-26-1] ***Niveusin A***
$C_{20}H_{26}O_8$ 394.421
Cryst. (EtOAc). Mp 127-128°.

1-Me ether, 8-(2-methylbutanoyl): [351416-98-3]
$C_{21}H_{30}O_8$ 410.463

1-Me ether, 8-angeloyl: [351345-21-6]
$C_{21}H_{28}O_8$ 408.447

3-Me ether, 8-angeloyl: ***3-O-Methylniveusin A***
$C_{21}H_{28}O_8$ 408.447
Constit. of *Helianthus annuus* (sunflower).

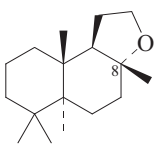
4ξ,5-Dihydro, 8-angeloyl: [98204-96-7] ***4,5-Dihydroniveusin A***
$C_{20}H_{28}O_8$ 396.436
Constit. of *Helianthus annuus* (sunflower). Needles ($CHCl_3$). Mp 95-96°.

[80482-71-9]

Ohno, N. *et al., Phytochemistry*, 1980, **19**, 609
Melek, F.R. *et al., Phytochemistry*, 1985, **24**, 1537-1539 (*4,5-Dihydroniveusin A*)
Gao, F. *et al., Phytochemistry*, 1986, **25**, 137-140 (*2′,3′-Dihydroniveusin A*)
Alfatafta, A.A. *et al., Phytochemistry*, 1992, **31**, 4109 (*isol, pmr, cmr*)
Spring, O. *et al., Phytochemistry*, 2000, **55**, 255-261 (*isol, pmr, cmr*)
Spring, O. *et al., Phytochemistry*, 2001, **57**, 267-272 (*Viguiera quinqueremis constits*)

8,12-Epoxy-13,14,15,16-tetranorlabdane E-182

*Dodecahydro-3*a*,6,6,9*a*-tetramethylnaphtho[2,1-*b*]furan, 9CI. 1,1,4*a*,6-Tetramethyl-5-ethyl-6,5-oxidodecahydronaphthalene. Norlabdane oxide*



8α-*form*

$C_{16}H_{28}O$ 236.397

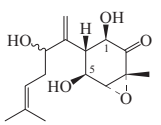
Terpenoid numbering shown.

8α-*form* [6790-58-5]
Ambrox. *Bicyclofarnesyl epoxide. Ambronide.* n-*Epoxide. Amberlyn. Ambroxan. FEMA 3471*
Flavouring ingredient. Cryst. (petrol). Mp 75-76°. $[\alpha]_D$ -25 (c, 1 in $CHCl_3$) (>99%ee). The (+)-enantiomer has a much weaker odour.

8β-*form* [68365-88-8]
Isoambrox. Isoepoxide
Mp 60°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 383A (*nmr*)
Stoll, M. *et al., Helv. Chim. Acta*, 1950, **33**, 1251; 1951, **34**, 1664 (*synth, config*)
Hinder, M. *et al., Helv. Chim. Acta*, 1953, **36**, 1995 (*synth, ir*)
Lucius, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1958, **291**, 57; *CA*, **52**, 14635e (*config*)
Torii, S. *et al., J.O.C.*, 1978, **43**, 4600 (*synth*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1985, **68**, 2022
Gonzalez-Sierra, M. *et al., Heterocycles*, 1987, **26**, 2801 (*synth*)
Koyama, H. *et al., Tet. Lett.*, 1987, **28**, 2863 (*synth*)
Decorzaut, R. *et al., Tetrahedron*, 1987, **43**, 1871 (*synth*)
Büchi, G. *et al., Helv. Chim. Acta*, 1989, **72**, 996 (*synth, ir, pmr*)
Mori, K. *et al., Annalen*, 1990, 361 (*synth*)
Escher, S. *et al., Helv. Chim. Acta*, 1990, **73**, 1935
Snowden, R.L. *et al., Tet. Lett.*, 1991, **32**, 4119 (*synth*)
Martnes, P. *et al., Tet. Lett.*, 1993, **34**, 629 (*synth*)
Barrero, A.F. *et al., Tetrahedron*, 1993, **49**, 6251; 9325 (*synth*)
Barton, D.H.R. *et al., Tet. Lett.*, 1994, **35**, 5801 (*synth*)
Verstegen-Haaksma, A.A. *et al., Tetrahedron*, 1994, **50**, 10095 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 748
Barco, A. *et al., Tetrahedron*, 1995, **51**, 8333 (*synth*)
Barrero, A.F. *et al., J.O.C.*, 1996, **61**, 2215 (*synth*)
Tanimoto, H. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 1695 (*synth*)
Kutney, J.P. *et al., Can. J. Chem.*, 1997, **75**, 1136-1150 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2768-2769
Hashimoto, T. *et al., Heterocycles*, 1998, **49**, 315-326 (*synth*)
Zoretic, P.A. *et al., J.O.C.*, 1998, **63**, 4779-4785 (*synth*)
Koga, T. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 3819-3823 (*synth*)
Moulines, J. *et al., Synth. Commun.*, 2001, **31**, 749-758 (*synth*)
Bolster, M.G. *et al., Tetrahedron*, 2001, **57**, 5657-5662 (*synth*)
Ishihara, K. *et al., J.A.C.S.*, 2002, **124**, 3647-3655 (*synth*)
Castro, J.M. *et al., Tetrahedron*, 2002, **58**, 5941-5949 (*synth*)

3,4-Epoxy-1,5,8-trihydroxy-7(14),10-bisaboladien-2-one E-183



(1*R*,3*R*,4*R*,5*S*,6*S*,8ξ)-*form*

$C_{15}H_{22}O_5$ 282.336

(1*R*,3*R*,4*R*,5*S*,6*S*,8ξ)-*form*

8-Angeloyl, 1-Ac: [348113-03-1]
$C_{22}H_{30}O_7$ 406.475
Constit. of flower buds of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D^{23}$ -32 (c, 0.4 in $CHCl_3$). λ_{max} 213 (log ε 4.17) (MeOH).

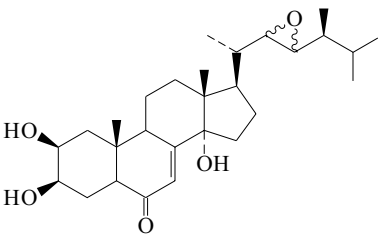
(1*S*,3*S*,4*S*,5*R*,6ξ,8ξ)-*form*

8-Angeloyl, 1,5-di-Ac: [246024-91-9]
$C_{24}H_{32}O_8$ 448.512
Constit. of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D$ +4.64 (c, 0.22 in $CHCl_3$). λ_{max} 203 (log ε 4.2) (EtOH).

Ryu, J.-H. *et al., J. Nat. Prod.*, 1999, **62**, 1437-1438 (*isol, pmr, cmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2001, **49**, 645-648 (*isol, pmr, cmr*)

22,23-Epoxy-2,3,14-trihydroxyergost-7-en-6-one E-184

22,23-Epoxy-2,3,14-trihydroxy-24-methylcholest-7-en-6-one



$C_{28}H_{44}O_5$ 460.653

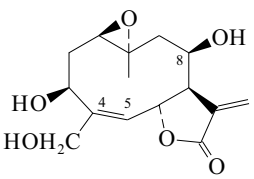
(2β,3β,5β,14α,22ξ,23ξ,24*R*)-*form* [141360-92-1]

Polyporusterone E

Constit. of *Polyporus umbellatus* (zhu ling). Needles (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 232°. λ_{max} 242 (ϵ 10470) (MeOH) (Berdy).

Ohsawa, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 143 (*isol, pmr, cmr*)

1,10-Epoxy-3,8,15-trihydroxy-4,11(13)-germacradien-12,6-olide E-185



$C_{15}H_{20}O_6$ 296.319

(1β,3β,4*Z*,6α,8β,10α)-*form*

8-Angeloyl: [121541-07-9] ***15-Hydroxyleptocarpin***

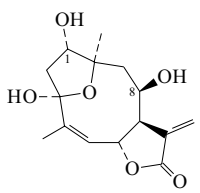
$C_{20}H_{26}O_7$ 378.421

Constit. of *Helianthus annuus* (sunflower). Gum. $[\alpha]_D$ -84.5 (c, 0.24 in MeOH).

Pérez, C.A.L. *et al., Phytochemistry*, 1984, **23**, 823 (*15-Hydroxyleptocarpin*)

Macias, F.A. *et al., Phytochemistry*, 1996, **43**, 1205 (*isol, angeloyl*)

3,10-Epoxy-1,3,8-trihydroxy-4,11(13)-germacradien-12,6-olide E-186



(1α,3α,4*Z*,6α,8β)-*form*

$C_{15}H_{20}O_6$ 296.319

(1α,3α,4*Z*,6α,8β)-*form*

8-Angeloyl: [75680-27-2] ***Niveusin C***. *Annuithrin*

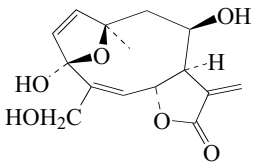
$C_{20}H_{26}O_7$ 378.421

Constit. of *Helianthus annuus* (sunflower). Cryst. (EtOAc) or oil. Mp 88-89° Mp 125-126°. $[\alpha]_D$ -148 (c, 0.28 in MeOH).

► EM9252300

Ohno, N. *et al., Phytochemistry*, 1980, **19**, 609 (*Niveusin C*)

3,10-Epoxy-3,8,15-trihydroxy-1,4,11(13)-germacratrien-12,6-olide E-187



$C_{15}H_{18}O_6$ 294.304

(3β,6α,8β,10β)-*form*

8-(2-Methylbutanoyl): [351417-00-0]

[351417-01-1]

$C_{20}H_{26}O_7$ 378.421

8-Angeloyl: [121519-08-2] ***1,2-Anhydridoniveusin***

$C_{20}H_{24}O_7$ 376.405

Constit. of *Helianthus annuus* (sunflower).

3-Me ether, 8-angeloyl: [200274-02-8] ***3-Methyl-1,2-anhydridoniveusin***. *3-Methoxy-1,2-anhydridoniveusin (incorr.)*

$C_{21}H_{26}O_7$ 390.432

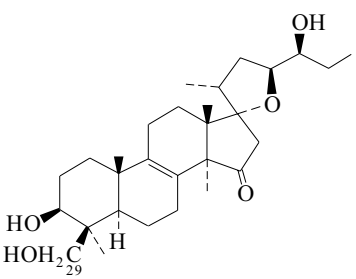
Oil.

Spring, O. *et al., Phytochemistry*, 1989, **28**, 745-749 (*1,2-Anhydridoniveusin*)

Meragelman, K.M. *et al., J. Nat. Prod.*, 1998, **61**, 105-107 (*3-Methyl-1,2-anhydridoniveusin*)

Spring, O. *et al., Phytochemistry*, 2001, **57**, 267-272 (*isol, pmr, cmr*)

17,23-Epoxy-3,24,29-trihydroxy-27-norlanost-8-en-15-one E-188



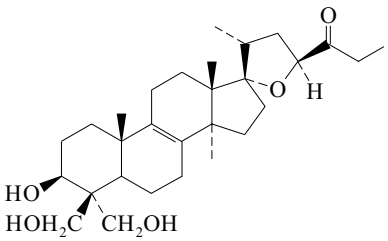
$C_{29}H_{46}O_5$ 474.679

(3β,17α,23*S*,24*S*)-*form*

Constit. of *Muscari comosum* (tassel hyacinth). Cryst. (Me_2CO). Mp 234-236°.

Adinolfi, M. *et al., J. Nat. Prod.*, 1984, **47**, 721

17,23-Epoxy-3,28,29-trihydroxy-27-norlanost-8-en-24-one E-189



$C_{29}H_{46}O_5$ 474.679

(3β,17α,23*S*)-*form*

Aglycone from *Muscari comosum* (tassel hyacinth). Amorph. $[\alpha]_D$ -27 (c, 0.5 in $CHCl_3$).

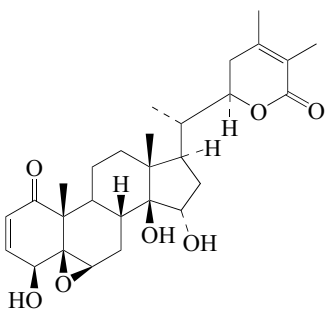
*3-Ketone:17α,23*S*-Epoxy-28,29-dihydroxy-27-norlanost-8-ene-3,24-dione*

$C_{29}H_{44}O_5$ 472.664

Aglycone from *Muscari comosum* (tassel hyacinth). Cryst. (EtOH). Mp 156-158°. $[\alpha]_D$ -33 (c, 0.5 in $CHCl_3$).

Parrilli, M. *et al., Tetrahedron*, 1980, **36**, 3591

5,6-Epoxy-4,14,15-trihydroxy-1-oxowitha-2,24-dienolide E-190



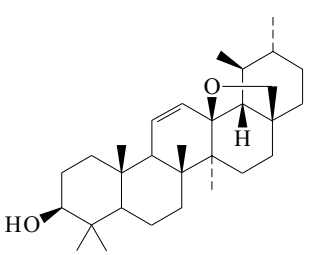
$C_{28}H_{38}O_7$ 486.604

(4β,5β,6β,14β,15α,20*S*,22*R*)-*form* [222609-98-5]

Constit. of *Physalis peruviana* (Cape gooseberry). Needles. Mp 142-144°. $[\alpha]_D$ +68 (c, 0.2 in MeOH). λ_{max} 224 (log ϵ 4.15) (MeOH).

Ahmad, S. *et al., Phytochemistry*, 1999, **50**, 647-651 (*isol, pmr, cmr*)

13,28-Epoxy-11-ursen-3-ol E-191



$C_{30}H_{48}O_2$ 440.708

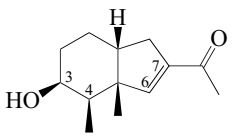
(3β,13β)-*form* [35959-06-9]

Needles (EtOAc). Mp 250-252°. $[\alpha]_D^{20}$ +43 ($CHCl_3$).

3-Ketone: [128529-78-2] ***13β,28-Epoxy-11-ursen-3-one. Momordicinin***
$C_{30}H_{46}O_2$ 438.692
Constit. of *Momordica charantia* (bitter melon). Cryst. Mp 146-147° (136-137°). $[\alpha]_D$ +115 (c, 0.11 in $CHCl_3$). $[\alpha]_D$ +54 ($CHCl_3$).
Mezzetti, T. *et al., Planta Med.*, 1971, **20**, 244 (*synth*)
González, A.G. *et al., Phytochemistry*, 1990, **29**, 1691 (*isol, pmr, cmr*)
Begum, S. *et al., Phytochemistry*, 1997, **44**, 1313 (*Momordicinin*)

Eremopetasinorol E-192

[182127-77-1]



$C_{13}H_{20}O_2$ 208.3
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D$ -28.4 (c, 1.1 in MeOH). λ_{max} 241 (log ϵ 3.9) (MeOH).

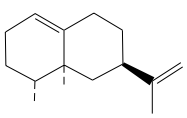
3-Ketone: [182127-76-0] ***Eremopetasinorone A***
$C_{13}H_{18}O_2$ 206.284
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{18}$ -118 (c, 0.3 in MeOH). λ_{max} 235 (log ϵ 3.8) (MeOH).

3-Ketone, 4-epimer: [182266-15-5] ***Eremopetasinorone B***
$C_{13}H_{18}O_2$ 206.284
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{18}$ +8.8 (c, 0.1 in MeOH). λ_{max} 228 (log ϵ 3.8) (MeOH).

6α,7α-Epoxide: [182127-78-2] ***Epoxyeremopetasinorol***
$C_{13}H_{20}O_3$ 224.299
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{20}$ -10.5 (c, 0.1 in MeOH).

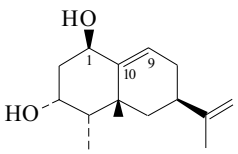
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1731 (*isol, pmr, cmr*)

1(10),11-Eremophiladiene E-193



$C_{15}H_{24}$ 204.355
(4α,5α,7β)-*form* [4630-07-3]
Valencene
Constit. of orange oil. Oil. Bp_{11} 123°. $[\alpha]_D$ +79.2.
(4β,5β,7β)-*form* [10219-75-7]
Eremophilene
Oil. Bp_{13} 129.5°. $[\alpha]_D^{24}$ -142.5.
Křepinský, J. *et al., Tet. Lett.*, 1968, 3315 (*isol*)
Coates, R.M. *et al., J.O.C.*, 1970, **35**, 2597 (*synth*)
Ishida, T. *et al., Chem. Ind. (London)*, 1970, 312 (*isol, struct*)
McGuire, H.M. *et al., J.C.S. Perkin 1*, 1974, 1879 (*synth*)
Miller, C.A. *et al., Chem. Comm.*, 1977, 230 (*biosynth*)
Naf, F. *et al., Helv. Chim. Acta*, 1982, **65**, 2212 (*synth*)
Torii, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 887 (*synth*)
Majetich, G. *et al., J.O.C.*, 1985, **50**, 3615 (*synth*)

9,11-Eremophiladiene-1,3-diol E-194



$C_{15}H_{24}O_2$ 236.353
(1β,3α,4α,5β)-*form* [37208-05-2]
Capsidiol
Phytoalexin of infected sweet pepper fruits (*Capsicum annuum*). Cryst. (Et_2O). Sol. MeOH, EtOH; fairly sol. Et_2O, $CHCl_3$; poorly sol. H_2O. Mp 152-153°. $[\alpha]_D^{22}$ +21 (c, 2.1 in $CHCl_3$).

1-Ketone: [41720-93-8] *3-Hydroxy-9,11-eremophiladien-1-one. Capsenone*
$C_{15}H_{22}O_2$ 234.338

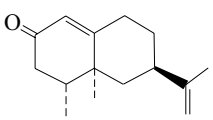
9,10β-Dihydro, 1-ketone: [109986-01-8] *3-Hydroxy-11-eremophilen-1-one.* ***Dihydrocapsenone***
$C_{15}H_{24}O_2$ 236.353

[109986-02-9]

Ward, G.W.B. *et al., Phytopathology*, 1972, **62**, 1186 (*Capsenone*)
Gordon, M. *et al., Can. J. Chem.*, 1973, **51**, 748 (*struct*)
Baker, F.C. *et al., Phytochemistry*, 1976, **15**, 689 (*biosynth*)
Hoyano, Y. *et al., Can. J. Chem.*, 1980, **58**, 1894 (*biosynth*)
Stillman, M.J. *et al., Can. J. Chem.*, 1981, **59**, 2303 (*abs config*)
Whitehead, I.M. *et al., Phytochemistry*, 1987, **26**, 1367 (*Dihydrocapsenone*)
Whitehead, I.M. *et al., Phytochemistry*, 1989, **28**, 775 (*biosynth*)
Yoshiazwa, Y. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 305 (*biosynth*)

1(10),11-Eremophiladien-2-one E-195

[4674-50-4]
Nootkatone. FEMA 3166

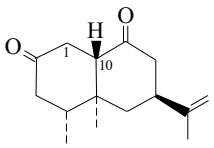


$C_{15}H_{22}O$ 218.338
Constit. of grapefruit oil and juice. Flavouring ingredient. Cryst. (petrol). Mp 36-37°. $[\alpha]_D$ +195.5 (c, 1.5 in $CHCl_3$).

Semicarbazone:
Cryst. Mp 195-197° dec. $[\alpha]_D$ +384 (c, 0.5 in $CHCl_3$).

MacLeod, W.D. *et al., Tet. Lett.*, 1965, 4779 (*struct*)
McGuire, H.M. *et al., J.C.S. Perkin 1*, 1974, 1879 (*synth*)
Takagi, Y. *et al., Tetrahedron*, 1978, **34**, 517 (*synth*)
Hiyama, T. *et al., Tet. Lett.*, 1979, 3529 (*synth*)
Yanami, T. *et al., J.O.C.*, 1980, **45**, 607 (*synth*)
Torii, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 887 (*synth*)
Inokuchi, T. *et al., J.O.C.*, 1982, **47**, 4622 (*synth*)
Majetich, G. *et al., J.O.C.*, 1985, **50**, 3615 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 607
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1987-1988

11-Eremophilene-2,9-dione E-196

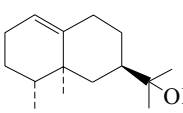


$C_{15}H_{22}O_2$ 234.338
(4α,5α)-*form*
Constit. of grapefruit (*Citrus paradisi*) juice. Cryst. (Et_2O/pentane). Mp 60-61°. $[\alpha]_D^{20}$ +30.6 (c, 0.75 in $CHCl_3$).

1,10-Didehydro:1(10),11-Eremophiladiene-2,9-dione
$C_{15}H_{20}O_2$ 232.322
Constit. of grapefruit (*Citrus paradisi*) juice. Cryst. (pentane). Mp 71-72.5°. $[\alpha]_D^{20}$ +45.7 (c, 1.29 in $CHCl_3$).

Demole, E. *et al., Helv. Chim. Acta*, 1983, **66**, 1381

1(10)-Eremophilen-11-ol E-197



(4α,5α,7β)-*form*

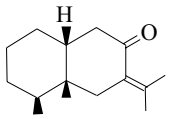
$C_{15}H_{26}O$ 222.37
(4α,5α,7β)-*form* [20489-45-6]
Valerianol. Kusunol
Constit. of the root of *Valeriana officinalis* (valerian). Oil. $Bp_{0.01}$ 120°. $[\alpha]_D^{20}$ +134 ($CHCl_3$).

3,5-Dinitrobenzoyl:
Cryst. (hexane). Mp 148°.

(4β,5β,7β)-*form* [10219-71-3] ***Eremoligenol***
Oil. Bp_2 120°. $[\alpha]_D^{23}$ -93.5 (c, 0.675 in $CHCl_3$).

Ishii, H. *et al., J.C.S.(C)*, 1966, 1545 (*isol, struct*)
Jommi, G. *et al., Tet. Lett.*, 1967, 677 (*isol, struct*)
Coates, R.M. *et al., J.O.C.*, 1970, **35**, 2597 (*synth*)
Odom, H.C. *et al., J.C.S. Perkin 1*, 1972, 2193 (*synth*)
Naf, F. *et al., Helv. Chim. Acta*, 1982, **65**, 2212 (*synth*)

7(11)-Eremophilen-8-one E-198



$C_{15}H_{24}O$ 220.354

(4β,5β,10β)-*form* [19593-06-7]

Fukinone

Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $Bp_{0.8}$ 97°. $[\alpha]_D^{24}$ +67.5 (c, 1 in MeOH). λ_{max} 251 (ϵ 6800) (EtOH).

Naya, K. *et al., Tetrahedron*, 1968, **24**, 5871-5879 (*isol, uv, pmr, ord, struct*)

Piers, E. *et al., J.O.C.*, 1970, **35**, 3997-3999 (*synth*)

Pinder, A.R. *et al., J.C.S.(C)*, 1971, 3410-3414 (*synth*)

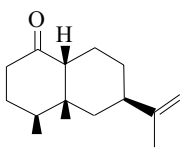
Hayashi, K. *et al., Phytochemistry*, 1973, **12**, 2931-2933 (*isol*)

Sato, T. *et al., Chem. Lett.*, 1977, 1191-1194 (*struct, pmr, cd*)

11-Eremophilen-1-one E-199

[35943-99-8]

Eremofukinone



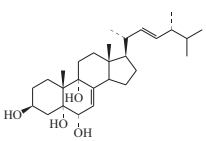
$C_{15}H_{24}O$ 220.354

Constit. of rhizomes of wild *Petasites japonicus* (sweet coltsfoot). Oil. $Bp_{0.15}$ 75-100° (bath). $[\alpha]_D^{24}$ +24.6 (c, 1.1 in $CHCl_3$).

Naya, K. *et al., Chem. Lett.*, 1972, 241

Ergosta-7,22-diene-3,5,6,9-tetrol, 9CI E-200

24-Methylcholesta-7,22-diene-3,5,6,9-tetrol



(3β,5α,6α,9α,22*E*,24*R*)-*form*

$C_{28}H_{46}O_4$ 446.669

(3β,5α,6α,9α,22*E*,24*R*)-*form* [211486-15-6]

Constit. of edible mushrooms including *Lentinus edodes* (shiitake), *Flammulina velutipes* (enokitake), *Hypsizygus marmoreus* (bunashimeji), *Pleurotus ostreatus* (tree oyster) and *Pholiota nameko* (nameko). Amorph. powder. $[\alpha]_D^{24}$ -28.8 (c, 0.1 in $CHCl_3$).

22,23-Dihydro, 6-ketone: [211486-13-4] ***3,5,9-Trihydroxyergost-7-en-6-one***. *3,5,9-Trihydroxy-24-methylcholest-7-en-6-one*

$C_{28}H_{46}O_4$ 446.669

Isol. from the fungi *Lentinus edodes* (shiitake), *Hypsizygus marmoreus* (bunashimeji), *Pleurotus ostreatus* (tree oyster) and *Pholiota nameko* (nameko). Amorph. powder. $[\alpha]_D^{28}$ -21.5 (c, 0.09 in $CHCl_3$). Has 24*S*-config. (change of Cahn-Ingold-Prelog priorities) λ_{max} 236 (log ϵ 3.8) (MeOH).

(3β,5α,6α,9α,22*E*,24ξ)-*form*

6-O-Sulfate: [168982-46-5]

$C_{28}H_{46}O_7S$ 526.733

22,23-Dihydro, 6-O-sulfate: [168982-47-6]

$C_{28}H_{48}O_7S$ 528.749

(3β,5α,6β,9α,22*E*,24*R*)-*form* [88191-06-4]

Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 225-227°. $[\alpha]_D$ -141 (c, 0.032 in Py).

6-Me ether: [88191-15-5] ***6-Methoxyergosta-7,22-diene-3,5,9-triol***

$C_{29}H_{48}O_4$ 460.696

Cryst. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 178-180°. $[\alpha]_D$ -117 (c, 0.75 in $CHCl_3$). λ_{max} (EtOH) (Berdy).

6-Ketone: [88191-14-4] ***3,5,9-Trihydroxyergosta-7,22-dien-6-one***. *3,5,9-Trihydroxy-24-methylcholesta-7,22-dien-6-one*

$C_{28}H_{44}O_4$ 444.653

Cryst. Mp 225-228°. $[\alpha]_D$ -64 (c, 0.056 in $CHCl_3$).

(3β,5α,6β,9α,22*E*,24*S*)-*form* [133161-20-3]

Cryst. (MeOH aq.). Mp 252-254°. $[\alpha]_D^{25}$ -25 (c, 0.08 in MeOH).

22,23-Dihydro: [243449-56-1] ***Ergost-7-ene-3,5,6,9-tetrol***

$C_{28}H_{48}O_4$ 448.685

Amorph. powder.

Valisolalao, J. *et al., Tetrahedron*, 1983, **39**, 2779-2785 (*Polyporus versicolor metabs*)

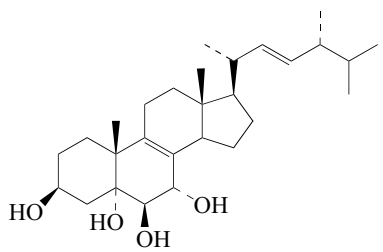
Migliuolo, A. *et al., J. Nat. Prod.*, 1990, **53**, 1414-1424 (*Spongia officinalis metab, isol, pmr, cmr*)

Aiello, A. *et al., Steroids*, 1995, **60**, 666-673 (*6-sulfates, isol, pmr, cmr*)

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950; 1999, **47**, 847-851 (*mushroom constits*)

Ergosta-8,22-diene-3,5,6,7-tetrol E-201

24-Methylcholesta-8,22-diene-3,5,6,7-tetrol



$C_{28}H_{46}O_4$ 446.669

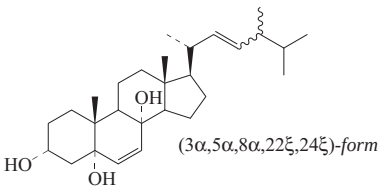
(3β,5α,6β,7α,22*E*,24*R*)-*form* [200942-15-0]

Constit. of *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{20}$ +50 (c, 0.1 in $CHCl_3$).

Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*isol, pmr, cmr*)

Ergosta-6,22-diene-3,5,8-triol E-202

[76420-88-7]



(3α,5α,8α,22ξ,24ξ)-*form*

$C_{28}H_{46}O_3$ 430.67

(3α,5α,8α,22ξ,24ξ)-*form*

Cryst. (EtOAc). Mp 178-181°. $[\alpha]_D$ -23 (c, 1.7 in $CHCl_3$).

(3β,5α,8α,22*E*,24ξ)-*form* [7001-69-6]

Cryst. (petrol/Me_2CO). Mp 178-180°. $[\alpha]_D$ -2.1 (c, 1 in $CHCl_3$). $[\alpha]_D$ -16.8 (Py).

(3β,5β,8β,22*E*,24ξ)-*form* [288847-52-9]

Constit. of *Gyroporus castaneus* (chestnut bolete).

[40691-24-5]

Clayton, R.B. *et al., J.C.S.*, 1953, 2015-2021 (*synth*)

Dalton, F. *et al., J.C.S.*, 1961, 1880-1884 (*synth*)

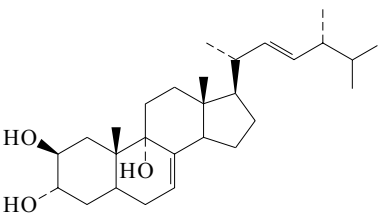
Dannenberg, H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1965, **342**, 199-213 (*synth*)

Hou, Z.-F. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 293-296 (*isol, ir, pmr, cmr, ms*)

Wan, H. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 1999, **11**, 18-21; *CA*, **133**, 190274c (*Gyroporus castaneus constit*)

Ergosta-7,22-diene-2,3,9-triol E-203

24-Methylcholesta-7,22-diene-2,3,9-triol



$C_{28}H_{46}O_3$ 430.67

(2β,3α,9α,24*R*)-*form*

Metab. of *Ganoderma lucidum* (reishi). Needles (MeOH). Mp 253°. $[\alpha]_D^{25}$ -7.2 (c, 0.125 in MeOH).

2-Me ether:

$C_{29}H_{48}O_3$ 444.696

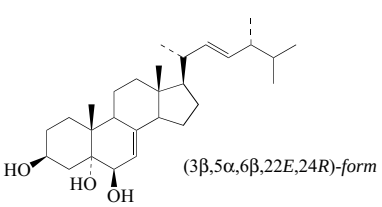
Powder (MeOH) (as di-Ac). Mp 197-198° (di-Ac). $[\alpha]_D^{25}$ +40 (c, 0.5 in $CHCl_3$) (di-Ac).

Lin, C.-N. *et al., J. Nat. Prod.*, 1991, **54**, 998 (*isol, pmr, cmr*)

Lin, C.-N. *et al., Phytochemistry*, 1993, **32**, 1549 (*isol, pmr, cmr*)

Ergosta-7,22-diene-3,5,6-triol E-204

24-Methylcholesta-7,22-diene-3,5,6-triol



(3β,5α,6β,22*E*,24*R*)-*form*

$C_{28}H_{46}O_3$ 430.67

(3β,5α,6β,22*E*,24*R*)-*form* [516-37-0]

Cerevisterol
Cryst. (MeOH). Mp 254-256°. $[\alpha]_D^{21}$ -79.9 (c, 1.35 in Py).

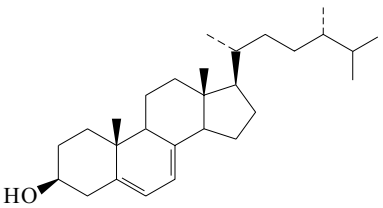
3-O-β-D-Glucopyranoside: [140447-21-8]
Tuberoside
$C_{34}H_{56}O_8$ 592.812
Constit. of Chinese truffles (*Tuber indicum*). Amorph. powder (MeOH). Mp 245-247°. $[\alpha]_D^{26}$ -95.5 (c, 0.22 in Py).

6-Ketone: ***3,5-Dihydroxyergosta-7,22-dien-6-one****. 3,5-Dihydroxy-24-methylcholesta-7,22-dien-6-one*
$C_{28}H_{44}O_3$ 428.654
Constit. of *Grifola frondosa* (maitake). Amorph. solid. $[\alpha]_D^{25}$ +9.1 (c, 0.1 in $CHCl_3$). λ_{max} 248 (log ϵ 3.9) (MeOH).

Aiello, A. *et al., Steroids*, 1991, **56**, 337 (*isol, pmr, ketone*)
Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*6-ketone*)
Jinming, G. *et al., Steroids*, 2001, **66**, 771-775 (*Cerevisterol, pmr, cmr, Tuberoside*)

Ergosta-5,7-dien-3-ol E-205

24-Methylcholesta-5,7-dien-3-ol



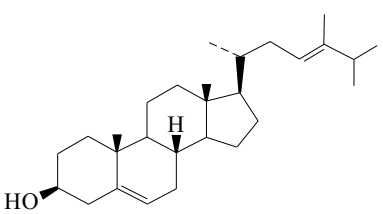
$C_{28}H_{46}O$ 398.671

(3β,24*S*)-*form* [516-79-0]
22,23-Dihydroergosterol*. Provitamin D_4*
Constit. of seed oil of *Vitis vinifera* (wine grape). Cryst. + H_2O (EtOAc/MeOH). Mp 152-153°. $[\alpha]_D$ -128.7 (c, 0.4 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1974, 1326 (*isol*)
Kircher, H.W. *et al., Lipids*, 1975, **10**, 517 (*synth*)
Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1976, 821 (*synth*)
Brynjolffssen, J. *et al., J.C.S. Perkin 1*, 1976, 826 (*synth*)
Mercer, E.I. *et al., Phytochemistry*, 1976, **15**, 283 (*biosynth*)
Curry, D.J. *et al., J.C.S. Perkin 1*, 1977, 822 (*synth*)

Ergosta-5,23-dien-3-ol E-206

24-Methylcholesta-5,23-dien-3-ol



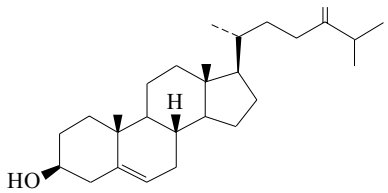
$C_{28}H_{46}O$ 398.671

3β-*form* [72962-53-9]
Constit. of *Zea mays* (sweet corn).

Ac:
$C_{30}H_{48}O_2$ 440.708
Cryst. Mp 122-124°. $[\alpha]_D$ -41.
Scheid, F. *et al., Phytochemistry*, 1979, **18**, 1207

Ergosta-5,24(28)-dien-3-ol E-207

24-Methylenecholest-5-en-3-ol



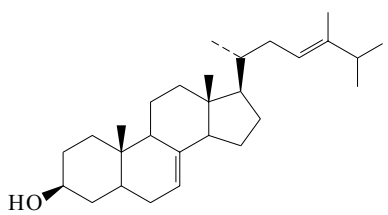
$C_{28}H_{46}O$ 398.671

3β-*form* [474-63-5]
Ostreasterol*. 24-Methylenecholesterol. Chalinasterol. Oestreasterol. Campestadienol*
Constit. of clams and oysters. Cryst. Mp 142-143°. $[\alpha]_D^{20}$ -43.6 ($CHCl_3$).

Bergmann, W. *et al., Annalen*, 1957, **603**, 36 (*struct, ir*)
Devys, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1965, **261**, 4901 (*isol*)
Popplestone, C.R. *et al., Phytochemistry*, 1973, **12**, 1131 (*isol*)
Adler, G. *et al., Phytochemistry*, 1975, **14**, 723 (*biosynth*)
Bu'lock, J.D. *et al., Phytochemistry*, 1975, **15**, 1249 (*biosynth*)
Heble, M.R. *et al., Phytochemistry*, 1976, **15**, 681 (*biosynth*)
Anastasia, M. *et al., J.C.S. Perkin 1*, 1985, 595 (*synth*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1997, **45**, 224 (*cmr, biosynth*)
Sheu, J.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 253-257 (*isol, activity*)

Ergosta-7,23-dien-3-ol E-208

24-Methylcholesta-7,23-dien-3-ol

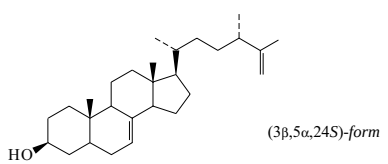


$C_{28}H_{46}O$ 398.671

(3β,5α)-*form* [72982-05-9]
Constit. of *Zea mays* (sweet corn).
Scheid, F. *et al., Phytochemistry*, 1979, **18**, 1207

Ergosta-7,25-dien-3-ol E-209

24-Methylcholesta-7,25-dien-3-ol



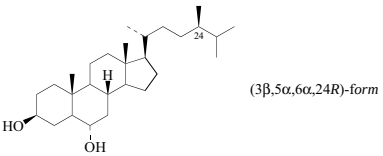
$C_{28}H_{46}O$ 398.671

(3β,5α,24*S*)-*form* [95043-18-8]
25-Dehydrofungisterol
Isol. from seeds of *Cucurbita maxima*.

(3β,5α,24ξ)-*form* [91811-31-3]
Prahl, F.G. *et al., J. Mar. Biol. Assoc. U.K.*, 1984, **64**, 317; 1986, **66**, 1
Garg, V.K. *et al., Phytochemistry*, 1984, **23**, 2919; 1986, **25**, 2591
Norton, R.A. *et al., Lipids*, 1991, **26**, 247 (*isol*)

Ergostane-3,6-diol E-210

24-Methylcholestane-3,6-diol



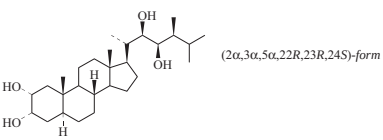
$C_{28}H_{50}O_2$ 418.702

(3β,5α,6α,24*R*)-*form*
Diketone: [88662-00-4] *Ergostane-3,6-dione. Campestane-3,6-dione*
$C_{28}H_{46}O_2$ 414.67
Constit. of *Phoenix dactylifera* (date).

(3β,5α,6α,24ξ)-*form*
6-Ketone: [134982-58-4] *3-Hydroxy-24-methylcholestan-6-one. 3-Hydroxyergostan-6-one, 9CI*
$C_{28}H_{48}O_2$ 416.686
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087-2088 (*Ergostane-3,6-dione*)
Cabrera, G. *et al., Phytochemistry*, 1991, **30**, 1239 (*isol, pmr, cmr, ketone*)
Suzuki, H. *et al., Phytochemistry*, 1995, **40**, 1391 (*isol, pmr, cmr, biosynth*)

Ergostane-2,3,22,23-tetrol E-211

24-Methylcholestane-2,3,22,23-tetrol



$C_{28}H_{50}O_4$ 450.701

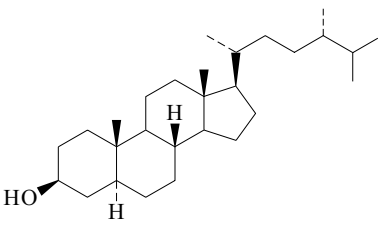
(2α,3α,5α,22*R*,23*R*,24*S*)-*form* [87833-54-3]
6-Deoxocastasterone
Isol. from *Phaseolus vulgaris* (kidney bean).

(2α,3α,22*R*,23*R*,24*R*)-*form*
6-Deoxo-24-epicastasterone
Cryst. (EtOAc/hexane). Mp 216-217°. $[\alpha]_D^{25}$ -6.6 (c, 3.5 in MeOH).

(2α,3β,5α,22*R*,23*R*,24*S*)-*form*
6-Deoxo-3-epicastasterone
Cryst. Mp 237-239°.
Schneider, J.A. *et al., Tet. Lett.*, 1983, **24**, 3859
Spengler, B. *et al., Phytochemistry*, 1995, **40**, 907 (*isol, pmr, ms, synth*)
Fujioka, S. *et al., Phytochemistry*, 2000, **53**, 549-553 (*isol, pmr, cmr, synth*)

Ergostan-3-ol E-212

24-Methylcholestan-3-ol



$C_{28}H_{50}O$ 402.702

(3β,5α,24*S*)-*form* [474-60-2]

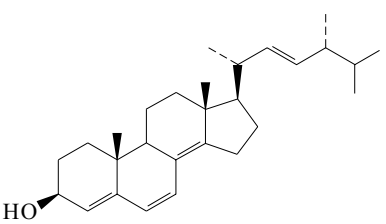
[17105-72-5]

Ergostanol. *Chalinastanol*. *γ-Ergostanol*
Constit. of coffee and of pot marigold (*Calendula officinalis*). Cryst. (MeOH/Et_2O). Mp 144-145°. $[\alpha]_D$ +15.94 ($CHCl_3$).

Karrer, P. *et al., Helv. Chim. Acta*, 1951, **34**, 832 (*isol*)
Nagasampagi, B.A. *et al., Phytochemistry*, 1971, **10**, 1101 (*isol*)
Adler, G. *et al., Phytochemistry*, 1975, **14**, 627 (*isol*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1978, **56**, 1898 (*pmr*)
Bohlin, L. *et al., Phytochemistry*, 1981, **20**, 2397 (*isol*)

Ergosta-4,6,8(14),22-tetraen-3-ol E-213

24-Methylcholesta-4,6,8(14),22-tetraen-3-ol



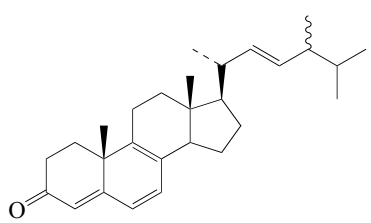
$C_{28}H_{42}O$ 394.639

(3β,22*E*,24*R*)-*form* [104729-39-7]
Constit. of *Marasmius oreades* (fairy ring mushroom). Cryst. Mp 118-120°. $[\alpha]_D^{20}$ +174 (c, 2 in $CDCl_3$).

Pang, Z. *et al., Nat. Prod. Lett.*, 1993, **3**, 193 (*isol, pmr, cmr*)

Ergosta-4,6,8,22-tetraen-3-one E-214

24-Methylcholesta-4,6,8,22-tetraen-3-one



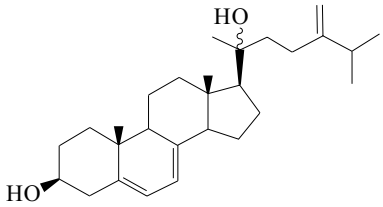
$C_{28}H_{40}O$ 392.623

(22*E*, 24ξ)-*form* [194721-75-0]
Constit. of *Pleurotus ostreatus* (oyster fungus). λ_{max} 349 (log ε 4.13) (EtOH).

Chobot, V. *et al., Phytochemistry*, 1997, **45**, 1669-1671 (*isol, pmr, cmr*)

Ergosta-5,7,24(28)-triene-3,20-diol E-215

24-Methylenecholesta-5,7-diene-3,20-diol, 9CI



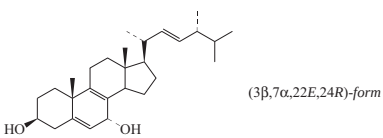
$C_{28}H_{44}O_2$ 412.654

(3β,20ξ)-*form* [85643-78-3]
Amasterol
Isol. from *Amaranthus viridis* (calalu). Cryst. (C_6H_6/petrol). Sol. Me_2CO, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 170°. $[\alpha]_D$ +42 ($CHCl_3$). λ_{max} 262 (ε 5630); 271 (ε 8700); 281 (ε 10000); 294 (ε 5370) (MeOH) (Berdy).

Roy, S. *et al., Phytochemistry*, 1982, **21**, 2417 (*isol, struct*)

Ergosta-5,8,22-triene-3,7-diol E-216

24-Methylcholesta-5,8,22-triene-3,7-diol



(3β,7α,22*E*,24*R*)-*form*

$C_{28}H_{44}O_2$ 412.654

(3β,7α,22*E*,24*R*)-*form*

5α,6α:8α,9α-Diepoxide: [243449-51-6]
5,6:8,9-Diepoxyergost-22-ene-3,7-diol. *5,6:8,9-Diepoxy-24-methylcholest-22-ene-3,7-diol*
$C_{28}H_{44}O_4$ 444.653
Isol. form *Hypsizygus marmoreus* (bunashimeji). Amorph. powder. $[\alpha]_D$ -53.6 (c, 0.06 in $CHCl_3$).

(3β,7α,22*E*,24*S*)-*form*

5α,6α-Epoxide: [16250-61-6] *5,6-Epoxyergosta-8,22-diene-3,7-diol*. ***Melithasterol B***
$C_{28}H_{44}O_3$ 428.654
Cryst. (MeOH). Mp 184.5-186° (174-175°). $[\alpha]_D^{20}$ -51 (c, 0.76 in $CHCl_3$).

5α,6α-Epoxide, di-Ac:
Cryst. (MeOH). Mp 150-152°. $[\alpha]_D$ -86.

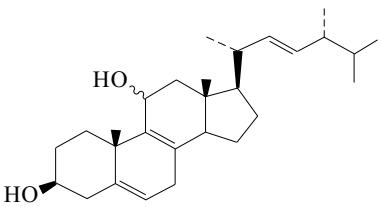
(3β,7β,22*E*,24*R*)-*form*

5α,6α-Epoxide: [243449-53-8]
$C_{28}H_{44}O_3$ 428.654
Constit. of *Tricholoma portentosum*. Amorph. powder. $[\alpha]_D^{26}$ -37 (c, 0.05 in $CHCl_3$).

5α,6α:8α,9α-Diepoxide: [243449-52-7]
Isol. from *Hypsizygus marmoreus* (bunashimeji). Amorph. powder. $[\alpha]_D^{20}$ -17.2 (c, 0.06 in $CHCl_3$).

Petzoldt, K. *et al., Annalen*, 1969, **724**, 194 (*Melithasterol*)
Kobayashi, M. *et al., J.C.S. Perkin 1*, 1991, 1177 (*isol, pmr, cmr, Melithasterol*)
Della Greca, M. *et al., Nat. Prod. Lett.*, 1993, **2**, 27 (*isol, pmr, cmr, Melithasterol*)
Migliuolo, A. *et al., Steroids*, 1993, **58**, 134 (*isol, pmr, cmr, Melithasterol*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 847-851 (*diepoxides*)
Yue, J.-M. *et al., Phytochemistry*, 2001, **56**, 801-806 (*isol, pmr, cmr*)

Ergosta-5,8,22-triene-3,11-diol E-217



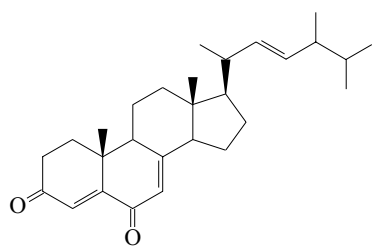
$C_{28}H_{44}O_2$ 412.654

(3β,11ξ,22*E*)-*form* [62005-66-7]
Portensterol
Constit. of *Tricholoma portentosum* and *Clitocybe nebularis* (clouded agaric). Cryst. (EtOH). Mp 250°. $[\alpha]_D^{20}$ -53 (c, 0.01 in $CHCl_3$/MeOH).

Regerat, F. *et al., Ann. Pharm. Fr.*, 1976, **34**, 323

Ergosta-4,7,22-triene-3,6-dione, 9CI E-218

[19698-66-9]
Ganodosterone. *6-Ketoergosterone*

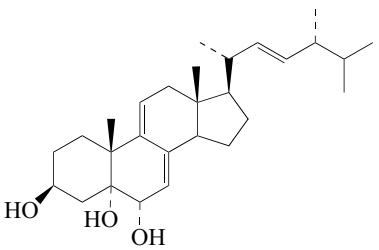


$C_{28}H_{40}O_2$ 408.623
Isol. from the fungus *Ganoderma lucidum* (reishi). Cryst. Mp 156-159° dec Mp 176-177°.

Malhotra, S.K. *et al., J.A.C.S.*, 1968, **90**, 6565-6566 (*synth*)
Malorni, A. *et al., Nouv. J. Chim.*, 1978, **2**, 351-354 (*isol, synth*)
Hirotani, M. *et al., Phytochemistry*, 1987, **26**, 2797-2803 (*isol, pmr*)
Kovganko, N.V. *et al., Khim. Prir. Soedin.*, 1999, **35**, 354-358; *Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 320-323 (*synth*)

Ergosta-7,9(11),22-triene-3,5,6-triol E-219

24-Methylcholesta-7,9(11),22-triene-3,5,6-triol



$C_{28}H_{44}O_3$ 428.654

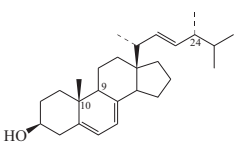
(3β,5α,6α,22*E*,24*R*)-*form* [71097-07-9]
Constit. of *Grifola frondosa* (maitake).

(3β,5α,6β,22*E*,24*R*)-*form* [200942-16-1]
Constit. of *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{20}$ -3.7 (c, 0.3 in $CHCl_3$). λ_{max} 244 (log ϵ 4) (MeOH).

Chen, R. *et al., Acta Bot. Sin. (Engl. Transl.)*, 1991, **33**, 65-68 (*isol, pmr, cmr*)
Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*isol, pmr, cmr*)

Ergosta-5,7,22-trien-3-ol E-220

24-Methylcholesta-5,7,22-trien-3-ol



(3β,22*E*,24*R*)-*form*

$C_{28}H_{44}O$ 396.655

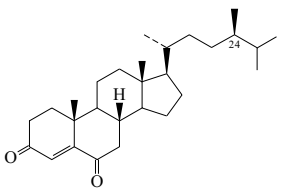
(3β,22*E*,24*R*)-*form* [57-87-4]
Ergosterol. *Ergosterin*. *Provitamin D_2*. *Ertron*
Indicator of fungal contamination, esp. in cereals. Occurs in yeast and fungi. The main fungal steroid. Also found in small amts. in higher plant prods., e.g. palm oil. Small hydrated plates (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 168° (165°). $[\alpha]_D$ -133 ($CHCl_3$). Log P 9.01 (uncertain value) (calc). λ_{max} 280 (MeOH) (Berdy). λ_{max} 262 ; 271 ; 282 ; 293 (EtOH) (Berdy).

5ξ,6ξ-Epoxide: [216302-95-3]
Constit. of *Armillaria mellea* (honey mushroom). Cryst. Mp 229-231°. Stereochem. at C5 and C6 not clear from ref..

(3β,9β,10α,22*E*,24*R*)-*form* [474-69-1]
Lumisterol
Cryst. (Me_2O/MeOH). Mp 118°. $[\alpha]_D^{18}$ +197 ($CHCl_3$).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1049C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 570B (*nmr*)
Kennedy, T. *et al., J.C.S.*, 1939, 250-253 (*struct*)
Jacobs, H.J.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 932-941 (*ord*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2060 (*occur*)
Fryberg, M. *et al., J.A.C.S.*, 1973, **95**, 5747-5757 (*Ergosterol, biosynth*)
Hull, S.E. *et al., Acta Cryst. B*, 1976, **32**, 2370-2373 (*cryst struct, Ergosterol*)
Mercer, E.I. *et al., Phytochemistry*, 1976, **15**, 283-286 (*biosynth*)
Adler, J.H. *et al., Lipids*, 1977, **12**, 364-366 (*pmr, struct*)
Smith, W.B. *et al., Org. Magn. Reson.*, 1977, **9**, 644-648 (*cmr*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567-1594 (*pmr*)
Young, J.C. *et al., J. Agric. Food Chem.*, 1993, **41**, 577-581; 1995, **43**, 2904-2910 (*Ergosterol, detn*)
Zhou, W. *et al., Tet. Lett.*, 1996, **37**, 1339-1342; 2000, **41**, 2791-2796 (*biosynth*)
Shi, L. *et al., Chem. Res. Chin. Univ.*, 1998, **14**, 270-272; *CA*, **130**, 22611e (*epoxide*)
Bok, J.W. *et al., Phytochemistry*, 1999, **51**, 891-898 (*5,6-epoxide*)

Ergost-4-ene-3,6-dione E-221



(24*R*)-*form*

$C_{28}H_{44}O_2$ 412.654

(24*R*)-*form* [85081-02-3]
Isol. from the stems of *Phoenix dactylifera* (date). Cryst. (MeOH). Mp 162-163°.

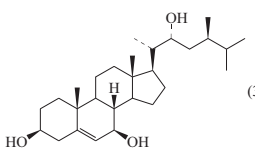
(24*S*)-*form* [50868-50-3]
Isol. from *Glycine max* (soybean). No phys. props. reported.

[59092-26-1, 90486-33-2]

Itokawa, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1386 (*isol*)
Weber, N. *et al., Phytochemistry*, 1977, **16**, 1849 (*isol*)
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087 (*isol*)

Ergost-5-ene-3,7,22-triol E-222

24-Methylcholest-5-ene-3,7,22-triol



(3β,7β,22*R*,24*R*)-*form*

$C_{28}H_{48}O_3$ 432.685

(3β,7β,22*R*,24*R*)-*form*

7-Me ether: [256445-53-1] *7-Methoxyergost-5-ene-3,22-diol*. ***Schleicherastatin 3***
$C_{29}H_{50}O_3$ 446.712
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 178-180°. $[\alpha]_D$ +44 (c, 0.3 in $CHCl_3$).

7-Ketone: [256445-61-1] *3,22-Dihydroxyergost-5-en-7-one. 3,22-Dihydroxy-24-methylcholest-5-en-7-one*. ***Schleicherastatin 6***
$C_{28}H_{46}O_3$ 430.67
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 209-212°. $[\alpha]_D$ -94 (c, 0.2 in $CHCl_3$). λ_{max} 235 (log ϵ 3.79) (EtOH).

(3β,7β,22*R*,24*S*)-*form*

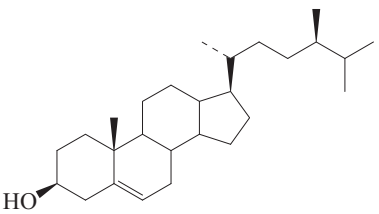
7-Me ether: [256445-55-3] ***Schleicherastatin 4***
$C_{29}H_{50}O_3$ 446.712
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 148-151°. $[\alpha]_D$ -36 (c, 0.2 in $CHCl_3$).

7-Ketone: [256445-64-4] ***Schleicherastatin 7***
$C_{28}H_{46}O_3$ 430.67
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 148-152°. $[\alpha]_D$ -112 (c, 0.1 in $CHCl_3$). λ_{max} 235 (log ϵ 3.56) (EtOH).

Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 72-78 (*isol, pmr, cmr*)

Ergost-5-en-3-ol, 9CI E-223

24-Methylcholest-5-en-3-ol



$C_{28}H_{48}O$ 400.687

(3β,24*R*)-*form* [474-62-4]

[4651-51-8, 23929-42-2]
Campesterol. *Mieyajunsu A*. *EB 82A*
Constit. of rapeseed oil (*Brassica napa*), soybean oil (*Glycine max*) and wheatgerm oil (*Triticum* spp.). Found in virtually all plant oils. Cryst. (Me_2CO). Mp 157-158°. $[\alpha]_D^{23}$ -33 ($CHCl_3$).

O-*β-D-Glucopyranoside:* [32214-82-7]
$C_{34}H_{58}O_6$ 562.829

O-*(6-O-Hexadecanoyl-β-D-glucopyranoside):* [59252-88-9]
$C_{50}H_{88}O_7$ 801.241
Constit. of peach seeds.

O-*[6-O-(9Z-Octadecenoyl)-β-D-glucopyranoside]:* [87168-08-9]
$C_{52}H_{90}O_7$ 827.279
Constit. of peach seeds.

O-*Sulfate:* [24815-92-7]
$C_{28}H_{48}O_4S$ 480.751

Ac: [1900-53-4] *Campesteryl acetate*
$C_{30}H_{50}O_2$ 442.724
Cryst. (EtOH). Mp 139°. $[\alpha]_D$ -38 ($CHCl_3$).

Tetradecanoyl: [87189-08-0] *Campesteryl myristate*
$C_{42}H_{74}O_2$ 611.045

Hexadecanoyl: [74240-46-3]

[84354-48-3, 104113-00-0] *Campesteryl palmitate*
$C_{44}H_{78}O_2$ 639.099

Octadecanoyl: [55064-20-5] *Campesteryl stearate*
$C_{46}H_{82}O_2$ 667.153
Constit. of corn oil.

9Z-Octadecenoyl: [64144-49-6]

[120663-71-0] *Campesteryl elaidate*
$C_{46}H_{80}O_2$ 665.137

Constit. of corn oil and soybean oil.

9Z,12Z-Octadecadienoyl: [86248-87-5] *Campesteryl linoleate*
$C_{46}H_{78}O_2$ 663.121
Constit. of corn oil and soybean oil.

9Z,12Z,15Z-Octadecatrienoyl: [94365-87-4]

[120707-25-7] *Campesteryl α-linolenate*
$C_{46}H_{76}O_2$ 661.105
Constit. of soybean oil and corn pollen.

Docosanoyl: [81053-28-3] *Campesteryl behenate*
$C_{50}H_{90}O_2$ 723.26
Cryst. (hexane). Mp 95-96°.

*13*E-*Docosenoyl:* [110671-73-3] *Campesteryl brassidate*
$C_{50}H_{88}O_2$ 721.244
Constit. of rapeseed oil.

4-Hydroxycinnamoyl: [156297-95-9] *Campesteryl* p-*coumarate*
$C_{37}H_{54}O_3$ 546.832
Isol. from corn bran.

3,4-Dihydroxycinnamoyl: [75873-74-4] *Campesteryl caffeate*
$C_{37}H_{54}O_4$ 562.831
Constit. of canary grass (*Phalaris canariensis*). Antioxidant.

4-Hydroxy-3-methoxycinnamoyl: [20972-07-0]

[97860-21-4] *Campesteryl ferulate*
$C_{38}H_{56}O_4$ 576.858
Constit. of various cereal grains.

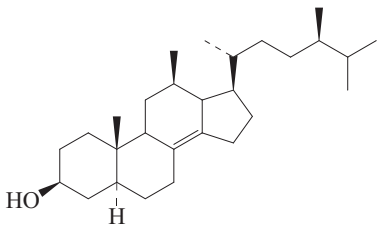
(3β,24*S*)-*form*

[4651-51-8, 23929-42-2]
Dihydrobrassicasterol
Occurs in *Physalis peruviana* (Cape gooseberry). Needles (Me_2CO). Mp 157-158°. $[\alpha]_D^{24}$ -46.3 (c, 1.2 in $CHCl_3$).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 567B (*nmr*)
Thompson, M.J. *et al., Steroids*, 1965, **5**, 745 (*synth*)
Fedeli, E. *et al., J. Am. Oil Chem. Soc.*, 1966, **43**, 254 (*occur*)
Tarzia, G. *et al., Gazz. Chim. Ital.*, 1967, **97**, 102 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2053 (*occur*)
Thompson, M.J. *et al., Phytochemistry*, 1972, **11**, 1781 (*pmr*)
Lenton, J.R. *et al., Phytochemistry*, 1975, **14**, 1523 (*biosynth*)
Lin, T.D. *et al., Chem. Pharm. Bull.*, 1976, **24**, 253-261 (*6-hexadecanoylglucoside*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*cmr*)
Takagi, T. *et al., J. Am. Oil Chem. Soc.*, 1980, **57**, 326-330 (*caffeate*)
Benes, I. *et al., Phytochemistry*, 1981, **20**, 2438 (*docosanoyl*)
Morishige, H. *et al., CA*, 1983, **99**, 145987f (*isol, glucosides*)
Uomori, A. *et al., Chem. Comm.*, 1984, 1176 (*biosynth*)
Trost, V.W. *et al., J. Am. Oil Chem. Soc.*, 1989, **66**, 325-333 (*isol, esters*)
Seo, S. *et al., J.C.S. Perkin 1*, 1992, 569 (*biosynth*)
Rogers, E.J. *et al., J. Am. Oil Chem. Soc.*, 1993, **70**, 301-307 (*isol, ferulate*)
Yamada, J. *et al., Tetrahedron*, 1997, **53**, 877 (*biosynth*)
Nasu, K. *et al., Phytochemistry*, 2000, **54**, 381-385 (*biosynth*)

Ergost-8(14)-en-3-ol E-224

24-Methylcholest-8(14)-en-3-ol



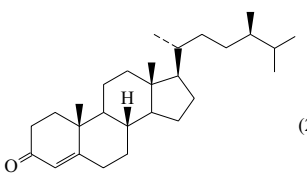
$C_{28}H_{48}O$ 400.687

(3β,5α,24*R*)-*form*
Constit. of *Dioscorea batatas* (Chinese yam).

(3β,5α,24*S*)-*form* [632-32-6]
Isol. from *Dioscorea batatas* (Chinese yam). Cryst. (MeOH). Mp 130-131°. $[\alpha]_D$ +17.9 ($CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1949, 214 (*synth*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*pmr, struct*)
Akihisa, T. *et al., Phytochemistry*, 1991, **30**, 2369 (*isol, pmr, ms*)

Ergost-4-en-3-one E-225



(24*R*)-*form*

$C_{28}H_{46}O$ 398.671

(24*R*)-*form* [22260-46-4]
4-Campesten-3-one
Isol. from *Phoenix dactylifera* (date). Cryst. (Et_2O/EtOH). Mp 86-87°. $[\alpha]_D^{25}$ +77.5 ($CHCl_3$).

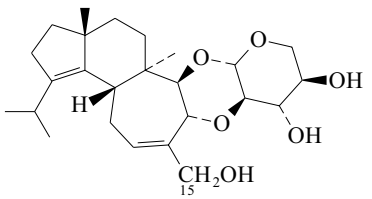
(24*S*)-*form* [51014-22-3]
Isol. from *Glycine max* (soybean).

[61949-21-1]

Hayashi, S. *et al., Chem. Pharm. Bull.*, 1969, **17**, 163 (*isol*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 3186 (*isol*)
Slatkin, D.J. *et al., Phytochemistry*, 1975, **14**, 580 (*isol*)
Smith, A.G. *et al., Biomed. Mass Spectrom.*, 1976, **3**, 81 (*synth, ms*)
Weber, N. *et al., Phytochemistry*, 1977, **16**, 1849 (*isol*)
Schulte, K.E. *et al., Planta Med.*, 1979, **35**, 76 (*isol*)
Subramanian, P.S. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 331 (*isol*)
Conner, A.H. *et al., Phytochemistry*, 1980, **19**, 1121 (*isol*)
Kokke, W.C.M.C. *et al., Steroids*, 1982, **40**, 307 (*isol*)
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087 (*isol*)

Erinacine C E-226

[156101-09-6]



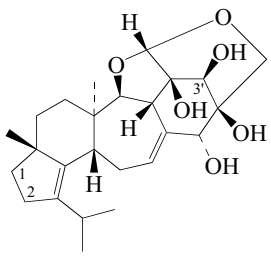
$C_{25}H_{38}O_6$ 434.572
Metab. of *Hericium erinaceum* (lions mane). Cryst. Sol. MeOH, EtOAc, Me_2CO, $CHCl_3$; fairly sol. EtOH; poorly sol. H_2O. Mp 115-118°. λ_{max} 203 (ϵ 8100) (MeOH) (Berdy).

15-Aldehyde: [156101-08-5] ***Erinacine B***
$C_{25}H_{36}O_6$ 432.556
Metab. of *Hericium erinaceum* (lions mane). Cryst. Sol. MeOH, Me_2CO, EtOAc, $CHCl_3$; fairly sol. EtOH; poorly sol. H_2O. Mp 125-127°. λ_{max} 200 (ϵ 20800); 230 (ϵ 8400) (MeOH) (Berdy).

Kawagishi, H. *et al., Tet. Lett.*, 1994, **35**, 1569 (*isol, pmr, cmr*)
Kenmoku, H. *et al., Tet. Lett.*, 2000, **41**, 4389-4393 (*synth*)

Erinacine E E-227

[178120-47-3]



$C_{25}H_{36}O_6$ 432.556
Metab. of *Hericium erinaceum* (lions mane) and *Hericium ramosum*. Cryst. Mp 161-163°. $[\alpha]_D^{25}$ -144 (c, 0.5 in MeOH). λ_{max} 207 (ϵ 7100) (MeOH).

3′-Ketone: ***Antibiotic CJ 15544***. *CJ 15544*
$C_{25}H_{34}O_6$ 430.54
Metab. of *Hericium ramosum*. Powder. $[\alpha]_D^{25}$ -78.6 (c, 0.06 in MeOH).

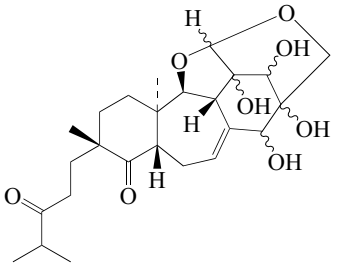
1,2-Didehydro: ***Antibiotic CP 412065***. *CP 412065*
$C_{25}H_{34}O_6$ 430.54
Metab. of *Hericium ramosum*. Powder. λ_{max} 256 (ϵ 5714) (MeOH).

Diastereoisomer: [178232-25-2] ***Erinacine F***
$C_{25}H_{36}O_6$ 432.556
Metab. of *Hericium erinaceum* (lions mane). Sol. MeOH, $CHCl_3$, Me_2CO. $[\alpha]_D^{25}$ -31 (c, 0.2 in MeOH). λ_{max} 203 (ϵ 8000) (MeOH).

Kawagishi, H. *et al., Tet. Lett.*, 1996, **37**, 7399-7402 (*isol, pmr, cmr, cryst struct*)
Saito, T. *et al., J. Antibiot.*, 1998, **51**, 983-990 (*isol, derivs*)

Erinacine G E-228

[182927-59-9]



$C_{25}H_{36}O_8$ 464.555

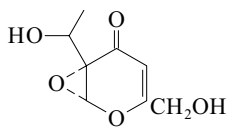
Metab. of *Hericium erinaceum* (lions mane). $[\alpha]_D^{25}$ -13 (c, 0.25 in MeOH). λ_{max} 204 (ε 13000) (MeOH).

Kawagishi, H. *et al., Tet. Lett.*, 1996, **37**, 7399-7402 (*isol, pmr, cmr*)

Erinapyrone C E-229

[157207-53-9]

*6-(1-Hydroxyethyl)-3-(hydroxymethyl)-2,7-dioxabicyclo[4.1.0]hept-3-en-5-one, 9CI. 5,6-Epoxy-5,6-dihydro-5-(1-hydroxyethyl)-2-(hydroxymethyl)-4*H*-pyran-4-one*



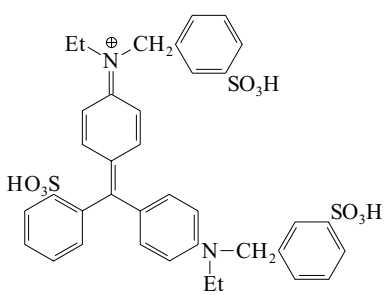
$C_8H_{10}O_5$ 186.164

Prod. by the fungus *Hericium erinaceus* (lions mane). Solid. Sol. MeOH, EtOAc. Mp 72°. $[\alpha]_D^{25}$ +141 (c, 1 in MeOH). λ_{max} 280 (ε 9700) (EtOH) (Berdy).

Arnone, A. *et al., J. Nat. Prod.*, 1994, **57**, 602 (*isol, pmr, cmr*)

Erioglaucine A E-230

N-*Ethyl*-N-*[4-[[4-[ethyl[(3-sulfophenyl)-methyl]amino]phenyl](2-sulfophenyl)-methylene]-2,5-cyclohexadien-1-ylidene]-3-sulfobenzenemethanaminium(1+). Alphazurine. Brilliant blue 9. Disulphine lake blue EG. Eriosky blue. FD and C Blue No. 1. Food blue 1. C.I. Acid blue 9. C.I. Food blue 2. C.I. 42090. E133. Many other names*



$C_{37}H_{37}N_2O_9S_3^{\oplus}$ 749.905

Strictly, the name Erioglaucine A applies to the diammonium salt. FDA permitted food colour for food and food contact paper or board (also as lakes). Used also as Ca and Al lakes.

Di-Na salt: [3844-45-9]

Reddish-violet powder with metallic lustre. Sol. H_2O, EtOH.

▶ Carcinogen. BQ4725000

Di-NH_4 salt: [2650-18-2]

Dark blue cryst. powder. Sol. H_2O. E° +1.13 V (1*M* H_2SO_4).

▶ BQ4550000

[25305-78-6, 53026-57-6, 68921-42-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1033B (*ir*)

Hansen, W.H. *et al., Toxicol. Appl. Pharmacol.*, 1966, **8**, 29 (*tox*)

Bishop, E. *et al., Indicators*, Oxford, Pergamon, 1972, 634

Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1530C

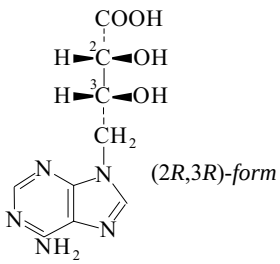
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1062-1065; 1067-1069; 1070-1071 (*use*)

Sigma-Aldrich Library of Stains, Dyes and Indicators, 312

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAE000; FMU059

Eritadenine E-231

*6-Amino-α,β-dihydroxy-9*H*-purine-9-butanoic acid, 9CI. 4-(6-Amino-9*H*-purin-9-yl)-4-deoxyerythronic acid, 8CI. 4-(9-Adeninyl)-2,3-dihydroxybutanoic acid. Lentysine. Lentinacin*



(2*R*,3*R*)-*form*

$C_9H_{11}N_5O_4$ 253.217Log P -2.76 (calc).

(2*R*,3*R*)-*form* [23918-98-1]

D-erythro-*form*

Isol. from the edible shitake mushroom. Mp 261-263° dec. (279° dec.). $[\alpha]_D$ +50 (0.1*M* NaOH). $[\alpha]_D$ +16 (1*M* HCl). λ_{max} 259 (ε 14129) (HCl) (Berdy). λ_{max} 261 (ε 14508) (H_2O) (Berdy). λ_{max} 262 (ε 14300) (NaOH) (Berdy).

Me ester: [25616-63-1]

Mp 231° dec.

2,3-Di-Ac, Me ester: [25616-64-2]

Mp 225° dec.

*2,3-*O*-Isopropylidene, Me ester:* [28991-46-0]

Mp 181°.

3-Deoxy: [31701-90-3] ***Deoxyeritadenine***

$C_9H_{11}N_5O_3$ 237.218

Constit. of the edible shitake mushroom. Mp 270-271° dec. $[\alpha]_D$ +18.4 (c, 1.0 in 0.1N NaOH). λ_{max} 262 (ε 14300) (0.1 M NaOH). λ_{max} 262 (ε 13900) (0.1 M HCl).

(2*R*,3*S*)-*form* [28617-17-6]

D-threo-*form*

Mp 297° dec. $[\alpha]_D$ +82 (0.1*M* NaOH).

(2*S*,3*R*)-*form* [28617-16-5]

L-threo-*form*

Mp 297° dec. $[\alpha]_D$ -81 (0.1*M* HCl).

Chibata, I. *et al., Experientia*, 1969, **25**, 1237 (*isol*)

Rokujo, T. *et al., Life Sci.*, 1970, **9**, 379 (*pharmacol*)

Hashimoto, M. *et al., Tet. Lett.*, 1970, 1359 (*synth*)

Saito, Y. *et al., Tet. Lett.*, 1970, 4863 (*Deoxyeritadenine*)

Okumura, K. *et al., J.O.C.*, 1971, **36**, 1573

Kamiya, T. *et al., Tetrahedron*, 1972, **28**, 899 (*synth, abs config*)

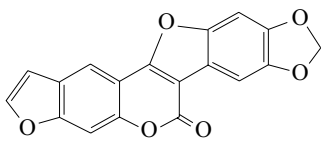
Kawazu, M. *et al., J.O.C.*, 1973, **38**, 2887 (*synth, pmr*)

Okumura, K. *et al., J. Med. Chem.*, 1974, **17**, 846

Tensho, A. *et al., Yakugaku Zasshi*, 1974, **94**, 708 (*Deoxyeritadenine*)

Holy, A. *et al., Coll. Czech. Chem. Comm.*, 1982, **47**, 1392 (*synth, pharmacol*)

Erosnin E-232



$C_{18}H_8O_6$ 320.258

Constit. of the yam bean (*Pachyrrhizus erosus*). Yellow needles. Mp 350° dec. approx.

Norton, L.B. *et al., J.A.C.S.*, 1945, **67**, 1609 (*isol*)

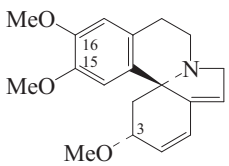
Chatterjea, J.N. *et al., J. Indian Chem. Soc.*, 1957, **32**, 97 (*isol*)

Eisenbeiss, J. *et al., Helv. Chim. Acta*, 1959, **42**, 61 (*isol*)

Chatterjea, J.N. *et al., Chem. Ber.*, 1964, **97**, 1252 (*isol*)

Fukui, K. *et al., Tet. Lett.*, 1965, 2559 (*synth*)

Erysotrine E-233



$C_{19}H_{23}NO_3$ 313.396

(+)-*form* [27740-43-8]

Alkaloid from *Etrythrina fusca* (gallito). Yellow cryst. (petrol). Mp 95-97°. $[\alpha]_D^{22}$ +264.3 (c, 0.8 in EtOH).

O^{16}-*De-Me:* [7290-03-1] ***Erysodine***. *1,2,6,7-Tetradehydro-3,15-dimethoxyerythrinan-16-ol*

$C_{18}H_{21}NO_3$ 299.369

Alkaloid from *Erythrina fusca* (gallito). Cryst. (EtOH). Mp 204-205°. $[\alpha]_D^{27}$ +248 (c, 0.311 in EtOH). $[\alpha]_D^{20}$ +239 (c, 0.50 in $CHCl_3$). Erysocine was a complex of Erysodine with Erysovine.

O^{15},O^{16}-*Di-de-Me:* [545-68-6] ***Erysopine***. *1,2,6,7-Tetradehydro-3-methoxyerythrinan-15,16-diol*

$C_{17}H_{19}NO_3$ 285.342

Alkaloid from *Erythrina fusca* (gallito). Cryst. (EtOH). Mp 241-242°. $[\alpha]_D^{25}$ +265.2 (EtOH/glycerol). $[\alpha]_D^{25}$ +225 (morpholine). $[\alpha]_D^{25}$ +276 (HCl aq.).

O^{15},O^{16}*-Di-de-Me,* O^{16}*-(carboxymethylsulfonyl):* ***Erysothiopine***

$C_{19}H_{21}NO_7S$ 407.443

Alkaloid from the seeds of *Erythrina glauca* (gallito). Cryst. (H_2O). Mp 168-169°. $[\alpha]_D^{25}$ +193 (c, 0.183 in EtOH). Hydrol. to Erysopine, and sulfoacetic acid.

Folkers, K. *et al., J.A.C.S.*, 1940, **62**, 1677-1683; 1941, **63**, 15444-1549; 1942, **64**, 1892-1896; 1944, **66**, 1083 (*Erysodine, Erysovine, Erysopine, Erysonine, Erysothiovine, Erysothiopine, isol*)

Delofeu, V. *et al., J.O.C.*, 1947, **12**, 486-489 (*Erysodine, isol*)

Prelog, V. *et al., Helv. Chim. Acta*, 1949, **32**, 453-461 (*Erysodine, isol*)

Prelog, V. *et al., Helv. Chim. Acta*, 1956, **39**, 498-504 (*Erysodine, Erysovine, Erysopine, struct*)

Weiss, U. *et al., Experientia*, 1963, **19**, 108-112 (*Erysodine, Ersopine, ord, config*)

Barton, D.H.R. *et al., J.C.S.(C)*, 1968, 1529-1537 (*struct, stereochem, biosynth*)

Boar, R.B. *et al., J.C.S.(B)*, 1970, 1591-1595 (*Erysodine, Erysopine, Erysovine, ms*)

Miana, G.A. *et al., J. Nat. Prod.*, 1972, **35**, 92 (*isol, uv, pmr, ms*)

Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1973, 874-880 (*Erysodine*)

Hargreaves, R.T. *et al., J. Nat. Prod.*, 1974, **37**, 569-580 (*Erysodine, Erysovine, Erythravine, Erysopine, Erysonine, Erysoline, occur*)

Games, D.E. *et al., J. Nat. Prod.*, 1974, **37**, 581-588 (*Erysodine, Erysovine, Erythravine, Erysopine, Erysonine, occur*)

Ito, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 52-55 (*isol, uv, pmr, ms, Erysodine*)

Mondon, A. *et al., Chem. Ber.*, 1979, **112**, 1329-1347 (*synth, uv, ir, bibl*)

Sarragiotto, M.H. *et al., Can. J. Chem.*, 1981, **59**, 2771-2775 (*isol, uv, ir, pmr, cmr, ms, oxide*)

Jackson, A.H. *et al., Allertonia*, 1982, **3**, 39; *CA*, **98**, 50334f (*Erysonine, Erysopine, Erysovine, occur*)

Chawla, A.S. *et al., Org. Magn. Reson.*, 1983, **21**, 39-41 (*cmr*)

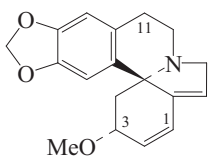
Tsuda, Y. *et al., Chem. Comm.*, 1984, 1216-1217 (*synth*)

Tsuda, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1365-1373; 1993, **41**, 2087-2095 (*(±)-form, (+)-form, synth*)

Wandji, J. *et al., Phytochemistry*, 1995, **39**, 677-681 (*Erysodine, Glucoerysodine*)

Erythraline E-234

1,2,6,7-Tetradehydro-3-methoxy-15,16-[methylenebis(oxy)]erythrinan, 9CI



$C_{18}H_{19}NO_3$ 297.353

(+)-*form* [466-77-3]

Alkaloid from *Erythrina glauca* (gallito). Mp 120° (106-107°). $[\alpha]_D^{21.5}$ +228 (c, 1.35 in EtOH).

Folkers, K. *et al., J.A.C.S.*, 1940, **62**, 436; 1673 (*isol, uv*)

Deulofeu, V. *et al., J.O.C.*, 1947, **12**, 486 (*isol*)

Prelog, V. *et al., Helv. Chim. Acta*, 1949, **32**, 453 (*isol, uv*)

Nowacki, W. *et al., Z. Kristallogr.*, 1958, **110**, 89; *CA*, **52**, 15185c (*cryst struct*)

Weiss, U. *et al., Experientia*, 1963, **19**, 108 (*ord*)

Barton, D.H.R. *et al., J.C.S.(C)*, 1970, 1213 (*biosynth*)

Hargreaves, R.T. *et al., J. Nat. Prod.*, 1974, **37**, 569 (*occur*)

Ito, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 52 (*Erythraline, Erythrinine, isol, uv, pmr, ms*)

Barakat, I. *et al., J. Nat. Prod.*, 1977, **40**, 471 (*occur*)

El-Olemy, M.M. *et al., J. Nat. Prod.*, 1978, **41**, 342 (*abs config*)

Jackson, A.H. *et al., Allertonia*, 1982, **3**, 39; *CA*, **98**, 50334f (*occur*)

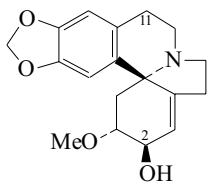
Chawla, A.S. *et al., Org. Magn. Reson.*, 1983, **21**, 39 (*cmr*)

Sano, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 479 (*synth, Erythraline, 8-Oxoerythraline*)

Erythratine E-235

[5550-20-9]

1,6-Didehydro-3-methoxy-15,16-[methylenebis(oxy)]erythrinan-2-ol, 9CI



$C_{18}H_{21}NO_4$ 315.368

Alkaloid from the seeds of *Erythrina glauca* (gallito). Cryst. + 0.5 H_2O (EtOH). Mp 170°. $[\alpha]_D^{28}$ +145.5 (c, 0.371 in EtOH).

Folkers, K. *et al., J.A.C.S.*, 1939, **61**, 1232; 3053; 1940, **62**, 436; 1673; 1942, **64**, 2146; 1951, **73**, 589 (*Erythratine, Erythramine, isol, uv, struct*)

Deulofeu, V. *et al., J.O.C.*, 1947, **12**, 486 (*Erythratine, Erythramine, isol*)

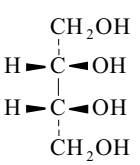
Barton, D.H.R. *et al., J.C.S.(C)*, 1968, 1529 (*Erythratine, Erythramine, 2-Epierythratine, Erythratinone, struct, stereochem, synth, biosynth*)

Ghosh, D.K. *et al., Curr. Sci.*, 1972, **41**, 578 (*Erythramine, Erythratine, Erythratinone, isol, ms*)

Erythritol, 9CI, 8CI E-236

[149-32-6]

(R,S)-1,2,3,4-Butanetetrol, 9CI, 8CI. Mesoerythritol. Phycitol. Erythroglucin



$C_4H_{10}O_4$ 122.121

For (*R*,*R*)-form see Threitol, T-386. Opt. inactive (*meso*-): some derivs. may be chiral (see for example 5-Hydroxy-2-phenyl-1,3-dioxane-4-methanol). Bulk sweetener with good taste props. Not metabolised, excreted unchanged in urine. Less sweet than sucrose. Use not yet permitted in most countries (1997). GRAS status for use as a sweetener, thickener, stabiliser, humectant, etc. in food. Cryst. (MeOH). Mp 121.5°. Bp 329-331° Bp_{200} 294-296°. Sweetness ca. 0.7 x sucrose.

▶ KF2000000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 184C (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 287A (*nmr*)

Trenner, N.R. *et al., J.A.C.S.*, 1949, **71**, 2352 (*synth*)

Jeanes, A. *et al., J.O.C.*, 1955, **20**, 1565 (*synth*)

Sonogashira, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2616 (*synth, ir*)

Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 144 (*occur*)

Ceccarelli, C. *et al., Acta Cryst. B*, 1980, **36**, 3079 (*cryst struct*)

Angyal, S.J. *et al., Carbohydr. Res.*, 1980, **84**, 201 (*cmr*)

Hawkes, G.E. *et al., J.C.S. Perkin 2*, 1984, 2073 (*pmr, conformn*)

Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)

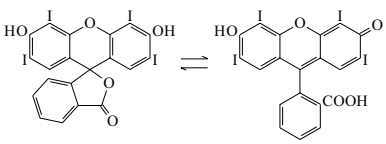
Food Chem. News, 2001, **43(36)**, 26-27 (*use*)

Erythrosine E-237

[15905-32-5]

[568-63-8, 16423-68-0]

3′,6′-Dihydroxy-2′,4′,5′,7′-tetraiodospiro[isobenzofuran-1(3H),9′(9H)-xanthen]-3-one, 9CI. Tetraiodofluorescein. Iodofluorescein. C.I. Food red 14. Aizen erythrosine. Cogilor orange 211.10. Cogilor orange 312.42. Dianthine B. Iodeosine B. Pyrosine B. Red 1427. FD and C Red No. 3. C.I. 45430. Food red no. 3. C.I. Acid red 51. E127. Ceplac. Felumin. Trace



$C_{20}H_8I_4O_5$ 835.898

Tautomeric (?) between spiro and open-chain forms. CA data refers to spiro-form. Strictly the name Erythrosine refers to the disodium salt. Dye used in food and feed additives. Prohibited in U.S.A. and Norway. Brown powder (as di-Na salt). Na salt sol. H_2O. Log P 7.69 (uncertain value) (calc).

▶ LD_{50} (mus, orl) 4000 mg/kg.LD_{50} (rat, ivn) 200 mg/kg, as di-Na salt. Exp. carcinogen at high doses. LM5940000

Al salt (3:2): [12227-78-0]

[39290-73-8, 53026-61-2] *C.I. Pigment red 172*

Former food dye prohibited from use in foods.

[49746-10-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1014C; 1014D (*ir*)

Dolinksy, M. *et al., J. Assoc. Off. Agric. Chem.*, 1951, **34**, 114 (*synth*)

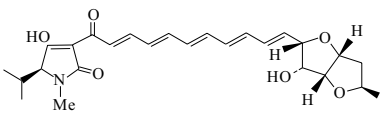
Machwe, H.K. *et al., Curr. Sci.*, 1967, **36**, 261; 1973, **42**, 786 (*spectra*)

Seybold, P.G. *et al., CA*, 1969, **71**, 8201c (*props*)

Iwachido, T. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 1835 (*use*)
Canadian Pat., 1974, 953 624; *CA*, **83**, 15670f (*use*)
Marmino, D.M. *et al., J. Assoc. Off. Anal. Chem.*, 1974, **57**, 495 (*nmr*)
Collins, T.F.X. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 233 (*tox*)
Matveets, M.A. *et al., Zh. Anal. Khim.*, 1979, **34**, 1049 (*props*)
Tananaiko, M.M. *et al., Zh. Anal. Khim.*, 1979, **34**, 1899 (*detn, Cd, Pb*)
Hoshi, S. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1983, **32**, 287
Mchedlov-Petrosyan, N.O. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1989, **59**, 611 (*tautom*)
Poulsen, E. *et al., Food Addit. Contam.*, 1993, **10**, 315 (*tox*)
Soedjak, H.S. *et al., Anal. Biochem.*, 1994, **220**, 142 (*use*)
Andree, H.A.M. *et al., Anal. Biochem.*, 1994, **222**, 465 (*use*)
Zijno, A. *et al., Food Chem. Toxicol.*, 1994, **32**, 159 (*tox*)
Suzuki, S. *et al., J. Chromatogr., A*, 1994, **680**, 541 (*anal*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1001
Sigma-Aldrich Library of Stains, Dyes and Indicators, 314; 316
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG040

Erythroskyrin E-238

[4987-27-3]



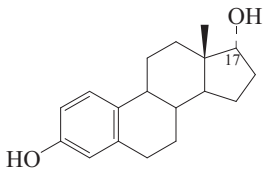
$C_{26}H_{33}NO_6$ 455.55

Mycotoxin prod. by the common food storage mould *Penicillium islandicum*. Orange-red cryst. (EtOH). Sol. MeOH, Py, bases, AcOH; fairly sol. Et_2O; poorly sol. H_2O, hexane. Mp 130-133°. $[\alpha]_D$ +46.9 ($CHCl_3$). λ_{max} 260 (ϵ 13800); 392 (ϵ 60300) (EtOH/NaOH) (Derep). λ_{max} 260 (ϵ 8910); 409 (ϵ 28200) (EtOH) (Derep).

▶ LD_{50} (mus, ipr) 60 mg/kg. UY7600000

Howard, B.H. *et al., Biochem. J.*, 1954, **57**, 212 (*isol*)
Shoji, J. *et al., Chem. Pharm. Bull.*, 1965, **13**, 1240 (*isol, uv, ir, pmr, struct*)
Shibata, S. *et al., Chem. Pharm. Bull.*, 1966, **14**, 474 (*biosynth*)
Ueno, Y. *et al., Jpn. J. Exp. Med.*, 1975, **45**, 525 (*tox*)
Beutler, J.A. *et al., J. Nat. Prod.*, 1988, **51**, 562 (*abs config, pmr, cmr*)
Dixon, D.J. *et al., J.C.S. Perkin 1*, 1999, 839-841 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 688

Estra-1,3,5(10)-triene-3,17-diol E-239



17α-*form*

$C_{18}H_{24}O_2$ 272.386

Estradiol is the accepted U.S. and IUPAC spelling.

Marketed drug**17β-*form*** [50-28-2] ***Estradiol, INN, USAN***. *Oestradiol, BAN. α-Estradiol (obsol., misleading). Almediol. Alora. Climara. Climaval. Compudose. Dermestril. Elleste-solo. Estrace. Estraderm. Evoral. Fermatrix. FemSeven. Menorest. Oestrogel. Ovocyclin. Progynova. Sandrena. Vagifem. Zumenon. Many other names*

Growth promoter for livestock. Permitted in the USA. Leaflets or needles (EtOH aq.). Mp 178°. $[\alpha]_D^{18}$ +78 (EtOH). Log P 3.78 (uncertain value) (calc).

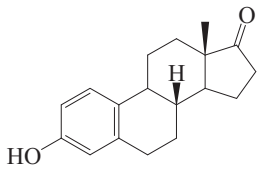
▶ Exp. carcinogen. Human and exp. reprod. effects. Exp. teratogenic effects. Semisynthetic esters should be considered to have similar toxicological properties.
KG2975000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1055C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 565A; 589B; 600B (*nmr*)
Marker, R.E. *et al., J.A.C.S.*, 1938, **60**, 2927 (*synth*)
Miki, T. *et al., Proc. Chem. Soc., London*, 1963, 139 (*synth*)
Gibson, H. *et al., Tet. Lett.*, 1966, 2321 (*synth*)
Tsukuda, Y. *et al., J.C.S.(B)*, 1968, 1387 (*cryst struct*)
Wittstruck, T.A. *et al., J.O.C.*, 1973, **38**, 1542 (*cmr*)
Busetta, B. *et al., Acta Cryst. B*, 1976, **32**, 1290 (*cryst struct*)
Eder, U. *et al., Chem. Ber.*, 1976, **109**, 2948 (*synth*)
IARC Monog., 1979, **21**, 279 (*tox, rev*)
Quinkert, G. *et al., Annalen*, 1981, 2335; 1982, 1999 (*synth*)
Hylarides, M.D. *et al., J.O.C.*, 1984, **49**, 2744 (*synth*)
Larner, J.M. *et al., Endocrinology (Baltimore)*, 1985, **117**, 1209 (*metab*)
Salole, E.G. *et al., Anal. Profiles Drug Subst.*, 1986, **15**, 283 (*rev*)
Collins, M.A. *et al., Tet. Lett.*, 1995, **36**, 4467 (*synth*)

Estrone, INN E-240

[53-16-7]

3-Hydroxyestra-1,3,5(10)-trien-17-one, 9CI. Oestrone, BAN. Follicular hormone. Menformon. Oestrin. Oxohydroxyoestrin. Progynon. Theelin. Many other names



$C_{18}H_{22}O_2$ 270.371

A trace constit. of plant tissues, e.g. seeds of date (*Phoenix dactylifera*) and pomegranate (*Punica granatum*). Cryst. (EtOH) (trimorphic). Mp 254° (triple Mp) Mp 256° Mp 259°. $[\alpha]_D$ +165 ($CHCl_3$). Log P 3.38 (uncertain value) (calc).

▶ Exp. neoplastic agent and teratogen. Adverse male reproductive effects.
KG8575000

[6891-91-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1055D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 589C (*nmr*)
Douglas, G.H. *et al., J.C.S.*, 1963, 5072 (*synth, ir*)
Kuo, C.H. *et al., Chem. Ind. (London)*, 1966, 1340 (*synth*)
Heftmann, E. *et al., Phytochemistry*, 1966, **5**, 231; 1337 (*isol*)
Rufer, C. *et al., Annalen*, 1967, **705**, 211 (*synth*)
Busetta, B. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1972, **274**, 153 (*cryst struct*)
Wittstruck, T.A. *et al., J.O.C.*, 1973, **38**, 1542 (*cmr*)
Sergeev, P.V. *et al., Zh. Fiz. Khim.*, 1973, **47**, 1643 (*ms*)
Cohen, N. *et al., J.O.C.*, 1975, **40**, 681 (*synth*)
Kametani, T. *et al., J.A.C.S.*, 1976, **98**, 3378; 1977, **99**, 3461 (*synth*)
Danishefsky, S. *et al., J.A.C.S.*, 1976, **98**, 4975 (*synth*)
Duax, W.L. *et al., Acta Cryst. B*, 1979, **35**, 2656 (*cryst struct*)
IARC Monog., 1979, **21**, 343 (*tox, rev*)
Nicolaou, K.C. *et al., J.O.C.*, 1980, **45**, 1403 (*synth*)
Grieco, P.A. *et al., J.O.C.*, 1980, **45**, 2247 (*synth*)
Quinkert, G. *et al., Annalen*, 1981, 2335 (*synth*)
Ziegler, F.E. *et al., Tet. Lett.*, 1981, 1179 (*synth*)
Posner, G.H. *et al., Tetrahedron*, 1981, **37**, 3921 (*synth*)
Both, D. *et al., Anal. Profiles Drug Subst.*, 1983, **12**, 135 (*rev*)
Hutchinson, J.H. *et al., Can. J. Chem.*, 1987, **65**, 1 (*synth*)
Taber, D.F. *et al., J.O.C.*, 1987, **52**, 28 (*synth*)
Caspi, E. *et al., Chem. Comm.*, 1989, 1302 (*biosynth*)
Sunder, N.M. *et al., J.C.S. Perkin 1*, 1990, 1331 (*synth*)
Barlaam, B. *et al., Tet. Lett.*, 1991, **32**, 623 (*synth*)
Subba Rao, G.S.R. *et al., Aust. J. Chem.*, 1992, **45**, 187 (*synth*)
Takano, S. *et al., Tet. Lett.*, 1992, **33**, 1909 (*synth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 153 (*bibl, synth*)
Brito, M. *et al., Synth. Commun.*, 1996, **26**, 623 (*synth, Me ether*)
Sugahara, T. *et al., Tet. Lett.*, 1996, **37**, 7403 (*synth*)
Smales, C.M. *et al., Acta Cryst. C*, 1997, **53**, 1082-1084 (*cryst struct*)
Tanaka, K. *et al., Org. Lett.*, 2000, 1915-1917 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EDV000; EDV600

1,2-Ethanediamine, 9CI E-241

[107-15-3]

Ethylenediamine, 8CI. 1,2-Diaminoethane

$H_2NCH_2CH_2NH_2$

$C_2H_8N_2$ 60.099

Microbial agent used in cane-sugar and beet-sugar mills. Clear, thick, strongly alkaline liq. with ammoniacal odour. Sol. EtOH, H_2O (with hydration); insol. C_6H_6; sl. sol. Et_2O. d_{20}^{20} 0.9. Mp 11°. Bp 118°. n_D^{20} 1.4565. pK_a 6.85. Steam-volatile. Forms compds. with metallic salts. Vp 10.7 mmHg (20°). Readily absorbs CO_2 from the air.

▶ Flammable, fl. p. 34°, autoignition temp. 385°. Reacts violently with many materials. Eye, skin and respiratory tract irritant. Conc. solns. corrosive. An allergen and sensitiser. LD_{50} (rat, orl) 500 mg/kg. Exp. reprod. effects. ACGIH TLV: long-term 10 ppm (Sk). KH8575000

N,N,N′,N′-*Tetra-Ac:* [10543-57-4] *Tetraacetylethylenediamine.* N,N′-*1,2-Ethanediylbis[*N-*acetylacetamide], 9CI.* N,N′-*Ethylenebis(diacetamide), 8CI*

$C_{10}H_{16}N_2O_4$ 228.247

Bleach activator used in food-contact paper and paperboard. Mp 149-150°.

N-*Nitro:* [58130-90-8]

$C_2H_7N_3O_2$ 105.096

Isol. from *Agaricus silvaticus* (red staining mushroom).

[20829-66-7, 25723-52-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 289C; 289D; 303A; 303B; 304A; 304B; 304C; 304D; 305B; 1271D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 463B; 463C; 488B; 488C; 489A; 490A; 490B; 491A; 491C; 492A; 492C; 1234B; **2**, 573C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 374D; 387D; 388A; 388B; 389B; 389C; 390D; 391B; 1165C; 1167C; 390A-390C (*ir*)
Johnson, T.B. *et al., J.A.C.S.*, 1916, **38**, 2135 (*deriv*)
Ing, H.R. *et al., J.C.S.*, 1926, 2348 (*synth, deriv*)
Bloom, M.S. *et al., J.A.C.S.*, 1945, **67**, 539 (*deriv*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 239; **4**, 231
Matsuura, T. *et al., Kogyo Kagaku Zasshi*, 1969, **72**, 179; *CA*, **70**, 96703
Mariella, R.P. *et al., J.O.C.*, 1971, **36**, 735 (*synth, tetra-Ac*)
Jamet-Deleroix, S. *et al., Acta Cryst. B*, 1973, **29**, 977 (*cryst struct*)
Austin, G.R. *et al., Chem. Eng. (N.Y.)*, 1974, **81**, 143; 148; 150 (*rev, manuf*)
Chilton, W.S. *et al., Phytochemistry*, 1975, **14**, 2291 (*isol, deriv, ir, uv*)
Ivin, K.J. *et al., Makromol. Chem.*, 1978, **179**, 591 (*synth, pmr*)
Nilsson, L. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 929 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 970
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0899
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 376
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DJI400; EIW000; DPK400; EEA500

1,1-Ethanedithiol E-242

1,1-Dimercaptoethane

$H_3CCH(SH)_2$

$C_2H_6S_2$ 94.201

S,S′-*Di-Ac:* [20266-80-2] S,S′-*Ethylidene dithioacetate*

$C_6H_{10}O_2S_2$ 178.276

Isol. from orange juice. Oil. $Bp_{0.002}$ 41°.

S,S′-*Di-Et:* See 1,1-Bis(ethylthio)ethane in *The Combined Chemical Dictionary.*

Sternson, L. *et al., J.O.C.*, 1978, **43**, 4532-4533 (*di-Ac, synth*)
Naaf, R. *et al., J. Essent. Oil Res.*, 1996, **8**, 587-595 (*di-Ac, isol*)

1,2-Ethanedithiol E-243

[540-63-6]

1,2-Dimercaptoethane. Dithioethylene glycol. FEMA 3484

$HSCH_2CH_2SH$

$C_2H_6S_2$ 94.201

Present in cooked chicken and beef. Flavouring ingredient. Liq. Bp 146° Bp_{150} 76-81°. pK_{a1} 9.05; pK_{a2} 10.56 (25°).

▶ LD_{50} (mus, orl) 342 mg/kg. KI3325000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 513A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 418C; **2**, 1609B (*nmr*)
Hall, W.P. *et al., J.A.C.S.*, 1943, **65**, 1466 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 401 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 189; **5**, 290
Hargittai, I. *et al., Chem. Comm.*, 1972, 323 (*struct*)
Org. Synth., Coll. Vol., 5, 1973, **54**, 33
DeSimone, R.E. *et al., Org. Magn. Reson.*, 1974, **6**, 583 (*cmr*)
Bittell, J.E. *et al., J.O.C.*, 1978, **43**, 1687 (*synth, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 210
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 935-936
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EEB000

Ethanethioic acid, 9CI E-244

[507-09-5]

Thioacetic acid. Thiolacetic acid†

$H_3CCOSH \Leftrightarrow H_3CC(S)OH$

C_2H_4OS 76.119

Tautomeric. Forms 2 series of esters.Liq. with pungent odour. Sol. H_2O, EtOH, Et_2O. d^{20} 1.07. Mp -17°. Bp 93°. n_D^{20} 1.4630. pK_a 3.33 (25°).

▶ LD_{50} (mus, ipr) 75 mg/kg. Flammable, fl. p. < 23°. AJ5600000

SH-form

Me ester: [1534-08-3] S-*Methyl thioacetate. FEMA 3876*

C_3H_6OS 90.146

Found in melon, strawberry, passion fruit, onion, cheese, cooked meats, beer, whiskies, wines and coffee. Flavouring agent. Bp 95-96°.

Et ester: [625-60-5] S-*Ethyl thioacetate. FEMA 3282*

C_4H_8OS 104.173

Flavouring ingredient. Insol. H_2O; v. sol. EtOH, Et_2O. d^{20} 0.98. Bp 116-117°. n_D^{21} 1.4583.

Propyl ester: [2307-10-0] S-*Propyl thioacetate. FEMA 3385*

$C_5H_{10}OS$ 118.199

Flavouring ingredient. Bp 135-137°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 528A; 827B; **2**, 312C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 817C; 1165B; **2**, 1285C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 597A; 760D; 1379C (*ir*)
Sadtler Standard C-13 NMR Spectra, 14404 (*cmr*)
Clarke, H.T. *et al., J.A.C.S.*, 1924, **46**, 1731 (*synth*)
Baker, R.B. *et al., J.A.C.S.*, 1929, **51**, 1568 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 928 (*synth*)
Harris, S.J. *et al., Chem. Comm.*, 1976, 1008 (*synth*)
Randhawa, H.S. *et al., J. Mol. Struct.*, 1977, **37**, 187 (*ir, Raman*)
Caserio, M.C. *et al., J.A.C.S.*, 1983, **105**, 6896 (*ms*)
Juaristi, E. *et al., J.O.C.*, 1988, **53**, 3334 (*synth*)
Nomura, R. *et al., Chem. Ber.*, 1990, **123**, 2081 (*synth*)
Bordwell, F.G. *et al., J.O.C.*, 1991, **56**, 4218 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 268; 706
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1042; 2374
Ayers, J.T. *et al., Synth. Commun.*, 1999, **29**, 351-358 (*S-esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFA000; TFA500

Ethanol, 9CI E-245

[64-17-5]

Ethyl alcohol. Hydroxyethane. Alcohol. FEMA 2419

H_3CCH_2OH

C_2H_6O 46.069

Intoxicating constit. of all alcoholic beverages. Used as a solvent and vehicle for food dressings and flavourings. Antimicrobial agent, e.g for pizza crusts prior to baking. extraction solvent for foodstuffs. Widely distributed in fruits and other foods. Very mobile liq., with pleasant odour and burning taste. Misc. H_2O, most org. solvs. d_4^{20} 0.79. Fp -117.3 (-112.3°). Bp 78.5° Bp_{130} 39.8° Bp_{16} 4°. $n_D^{20.5}$ 1.3610. pK_a 15.93 (25°). Hygroscopic, forming an azeotrope contg. 4.43% wt H_2O, Bp 78.15°. Crit. point 243° (62.7 atm.). Mol. Bp elevation 11.7°. Is obt. anhyd. by azeotropic distillation with C_6H_6 or by dehydration with K_2CO_3, CaO, $CaSO_4$, etc..

▶ Human and exp. reprod. effects. Highly flammable, fl. p. 12°. Reacts violently with a wide range of oxidants. Eye and skin irritant. Prolonged or repeated exposure can damage liver and brain. LD_{50} (rat, orl)

7060 mg/kg. OES: long-term 1000 pm. Ethanol for duty-free use (methylated spirit) contains MeOH and/or pyridine and is highly toxic. KQ6300000

[925-93-9, 1516-08-1, 1759-87-1, 2154-50-9, 16331-64-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 109C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 163B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 155C (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 928
Jönsson, P.-G. *et al., Acta Cryst. B*, 1976, **32**, 232 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **9**, 338 (*rev, bibl*)
Kricka, L.J. *et al., Biochemistry of Alcohol and Alcoholism*, Ellis Horwood, 1979, (*book*)
Goldstein, D.B. *et al., Pharmacology of Alcohol*, Oxford Univ. Press, 1983, (*book*)
Holford, N.H.G. *et al., Clin. Pharmacokinet.*, 1987, **13**, 273 (*rev*)
Pohorecky, L.A. *et al., Pharmacol. Ther.*, 1988, **36**, 335 (*rev, pharmacol*)
Molecular Mechanisms of Alcohol: Neurobiology and Metabolism, (eds. Sun, G.Y. *et al*), Humona Press, Clifton, NJ, 1989, (*book*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 7-9
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1114
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 946-948 (*use, occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0866
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 21
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 577
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EFU000

Ethenol, 9CI E-246

[557-75-5]
Vinyl alcohol
$H_2C{=}CHOH$
C_2H_4O 44.053

The enol tautomer of Acetaldehyde, A-20, not known in the free state. Keto/enol equilib. = 3×10^{-7} at 25°.

▶ YZ0495000

Ac: [108-05-4] *Ethenyl acetate, 9CI. Vinyl acetate*
$C_4H_6O_2$ 86.09
Esterification agent for modification of food starch. Liq. with a characteristic odour. Misc. EtOH, Et_2O; spar. sol. H_2O. d^{20} 0.93. Fp -100 (-93°). Bp 72°. n_D^{20} 1.3959. Vp 89 mmHg (20°). Radical polym. gives poly(vinyl acetate); copolymers with acrylates, maleates and ethylene are also produced. Q/e for copolym., Q 0.026, e -0.88. Coml. samples are stabilised with hydroquinone or diphenylamine. Rate for radical polym., k_p 1012 L mol^{-1} s^{-1}, k_t 5.9×10^{5} L mol^{-1} s^{-1} (25°). Copolym. with vinyl chloride: r_{VAC} 0.23, r_{VC} 1.68 (typical values, 60°); Q 0.026; e -0.22. Also copolym with vinylidene chloide: r_{VOC} 6.0, r_{VAC} 0.1 (typical values); Q 0.026; e -0.22.

▶ Highly flammable, fl. p. -8°, autoignition temp. 385°. May polymerise violently. Skin and eye irritant. LD_{50} (rat, orl) 2920 mg/kg. Exp. reprod. effects. OES: long-term 10 ppm; short-term 20 ppm. AK0875000

Benzoyl: [769-78-8] *Ethenyl benzoate, 9CI. Vinyl benzoate*
$C_9H_8O_2$ 148.161
Liq. d_4^{20} 1.07. Bp 203° Bp_{20} 95-96°. Q/e values for copolym., Q 0.030, e -0.77. Rate for radical polym., k_p 185 L mol^{-1} s^{-1}, k_t 4.02×10^{-4} L mol^{-1} s^{-1} (C_6H_6, 30°).

▶ Skin and eye irritant. LD_{50} (rat, orl) 3250 mg/kg. DI1050000

Me ether: See Methyl vinyl ether in *The Combined Chemical Dictionary.*

Et ether: See Ethyl vinyl ether in *The Combined Chemical Dictionary.*

Vinyl ether: See Divinyl ether in *The Combined Chemical Dictionary.*

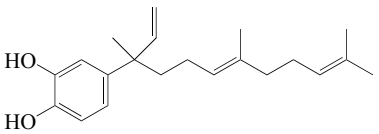
Ph ether: See Phenoxyethylene in *The Combined Chemical Dictionary.*

Isobutyl ether: See 1-(Ethenyloxy)-2-methylpropane in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 632D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 963A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 155C; 663B (*ir*)
Lewis, F.M. *et al., J.A.C.S.*, 1945, **67**, 1701 (*Ac, copolym, reactivity ratios*)
Matheson, M.S. *et al., J.A.C.S.*, 1949, **71**, 2610 (*polym kinetics, Ac*)
Kainer, F. *et al., CA*, 1950, **44**, 3739 (*synth, use*)
Foster, D.J. *et al., J.A.C.S.*, 1961, **83**, 851 (*derivs*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1271
Lindemann, M.K. *et al., Encycl. Polym. Sci. Technol.*, Interscience, N.Y., 1971, 531 (*rev*)
Finch, C.A. *et al., Polyvinyl Alcohol*, Wiley-Interscience, New York, 1973,
U.K. Pat., 1975, 1 396 703 (*Ac, copolym, reactivity ratios*)
Komachi, M. *et al., Macromolecules*, 1977, **10**, 501 (*polym kinetics, benzoate*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 817; 848; 910 (*rev, uses*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Capon, B. *et al., J.A.C.S.*, 1981, **103**, 1761 (*synth, pmr*)
Capon, B. *et al., J.A.C.S.*, 1982, **104**, 7567 (*tautom*)
Albrecht, B. *et al., Helv. Chim. Acta*, 1984, **67**, 216 (*synth, pe*)
IARC Monog., 1986, **39**, 113; *Suppl.* 7, 73 (*rev, tox*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 1989, **17**, 167; 393 (*rev, polymers*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **8**, 5485-5488 (*Ac, use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2916
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1434
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1317
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VLU250; VMK000

4-(1-Ethenyl-1,5,9-trimethyl-4,8-decadienyl)-1,2-benzenediol, 9CI E-247

[74683-11-7]
3-(3,4-Dihydroxyphenyl)-3,7,11-trimethyl-1,6,10-dodecatriene. 4-Nerolidylcatechol

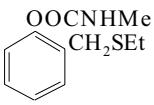


$C_{21}H_{30}O_2$ 314.467
Constit. of *Pothomorphe umbellata* (pariparoba) and *Pothomorphe peltata* (Piperaceae). Light yellow oil. $[\alpha]_D$ +3.3 (c, 4 in CH_2Cl_2). λ_{max} 216 (ε 4700); 282 (ε 2000) (MeOH).

Gustafson, K.R. *et al., J.O.C.*, 1992, **57**, 2809-2811 (*isol, uv, ir, pmr, cmr*)
Desmarchelier, C. *et al., Planta Med.*, 1997, **63**, 561-563 (*isol, props*)

Ethiofencarb, BSI E-248

[29973-13-5]
2-(Ethylthiomethyl)phenyl methylcarbamate, 9CI. N-*Methyl*-O-*(2-ethylthiomethyl) phenylcarbamate. Croneton*



$C_{11}H_{15}NO_2S$ 225.311
Systemic agricultural insecticide. Used for control of aphids on hard and soft fruits, vegetables and sugar beet. Yellow oil or solid. Sl. sol. H_2O. d_4^{20} 1.15. Mp 33.4°.

▶ LD_{50} (rat, orl) 200 mg/kg. LD_{50} (rat, skn) 1000 mg/kg. FC2628000

S-*Oxide:* [53380-22-6] *2-(Ethylsulfinylmethyl)phenyl methylcarbamate*
$C_{11}H_{15}NO_3S$ 241.31
Ethiofencarb metabolite.

▶ SL4506000

S,S-*Dioxide:* [53380-23-7] *2-(Ethylsulfonylmethyl)phenyl methylcarbamate*
$C_{11}H_{15}NO_4S$ 257.31
Ethiofencarb metabolite.

▶ SL4506500

U.K. Pat., 1969, 1 298 515; *CA*, **73**, 109533j
Ger. Pat., 1974, 2 258 805; *CA*, **81**, 77701j (*oxides*)
Draeger, G. *et al., Pflanzenschutz-Nachr.*, 1974, **27**, 144 (*glc*)
Nye, D.E. *et al., J. Agric. Food Chem.*, 1976, **24**, 371 (*metab, oxides*)
Konecny, V. *et al., Chem. Pap.*, 1985, **39**, 413 (*synth, activity*)
Olek, M. *et al., J. Chromatogr.*, 1985, **325**, 231 (*hplc*)
Pesticide Manual, 11th edn., 1997, No. 282
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EPR000

Ethoxyacetic acid, 9CI, 8CI E-249

[627-03-2]
Glycolic acid ethyl ether

$EtOCH_2COOH$

$C_4H_8O_3$ 104.105

Component of perilla leaf extract (*Perilla frutescens*). Liq. d_4^{20} 1.1. Bp 206-207° Bp_{16} 104.5-105°. Bp also recorded as 156-157°/16 mm.

▶ Exp. reprod. effects. Testicular toxin. AH3600000

Sommelet, M. *et al., Ann. Chim. Phys.*, 1906, **9**, 484 (*synth, derivs*)
Sommelet, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1906, **143**, 827 (*synth, derivs*)
Rothstein, B. *et al., Bull. Soc. Chim. Fr.*, 1932, **51**, 838 (*synth*)

1-Ethoxy-1-butoxyethane E-250

[57006-87-8]
1-(1-Ethoxyethoxy)butane, 9CI. Acetaldehyde butyl ethyl acetal

$H_3C(CH_2)_3OCH(OEt)CH_3$

$C_8H_{18}O_2$ 146.229

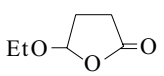
(±)-*form*
Aromatic-smelling liq. d_4^{20} 0.83. Bp 151-152° Bp_{28} 58-60°. n_D^{20} 1.3975.

(ξ)-*form*
Detected in strawberry volatiles by gc-ms.

Shostakovskii, M.F. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1946, **16**, 937; 1948, **18**, 451 (*synth*)
Deschamps, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 911 (*synth*)
Reppe, W. *et al., Annalen*, 1956, **601**, 81 (*synth*)
McFadden, W.H. *et al., J. Chromatogr.*, 1965, **18**, 10 (*isol*)

5-Ethoxy-4,5-dihydro-2(3*H*)furanone, 9CI E-251

[932-85-4]
4-Ethoxy-4-hydroxybutyric acid γ-lactone. 4-Ethoxy-γ-butyrolactone



$C_6H_{10}O_3$ 130.143

An aroma component of Ruby Cabernet wine from the European grape *Vitis vinifera*.

Muller, C.J. *et al., J. Agric. Food Chem.*, 1972, **20**, 193 (*isol, synth, ir, ms*)
Lukehart, C.M. *et al., J. Organomet. Chem.*, 1976, **105**, 231 (*synth, ir, pmr*)

2-Ethoxyethanol, 9CI E-252

[110-80-5]
Ethylene glycol ethyl ether. 2-Ethoxyethyl alcohol. Ethyl 2-hydroxyethyl ether. Ethyl cellosolve. Cellosolve. Oxitol. Bikanol E1

$EtOCH_2CH_2OH$

$C_4H_{10}O_2$ 90.122

Diluent in colour additive mixts. for marking food. Prac. odourless liq. Misc. H_2O, EtOH, Et_2O, Me_2CO. Fp -70. Bp_{743} 134.8°.

▶ Eye and skin irritant. LD_{50} (rat, orl) 2125 mg/kg. Exp. reprod. effects. MEL: long-term 10 ppm (Sk). KK8050000

Ac: [111-15-9] *2-Ethoxyethyl acetate*
$C_6H_{12}O_3$ 132.159
Mp -61°. Bp 156° Bp_{12} 51°. n_D^{20} 1.4040.
▶ Flammable, fl. p. 47/51°, autoignition temp. 380°. Eye and skin irritant. LD_{50} (rat, orl) 2900 mg/kg. Exp. reprod. and teratogenic effects. MEL: long-term 10 ppm (Sk). KK8225000

Benzoyl: [5451-72-9]
$C_{11}H_{14}O_3$ 194.23
$Bp_{738.5}$ 260-261°.

4-Methylbenzenesulfonyl: [17178-11-9]
$C_{11}H_{16}O_4S$ 244.311
Cryst. or oil. Mp 18.5°. Bp_3 186-187°.

tert-*Butyl ether:* [51422-54-9] *1-tert-Butoxy-2-ethoxyethane*
$C_8H_{18}O_2$ 146.229
Mp 148°. n_D^{20} 1.4015.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 223A; 666D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 337B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 293B; 722B (*ir*)
Cretcher, L.H. *et al., J.A.C.S.*, 1924, **46**, 1503 (*synth*)
U.S. Pat., 1927, 1 732 356; *CA*, **24**, 127 (*synth*)
Conn, R.C. *et al., J.A.C.S.*, 1932, **54**, 4370 (*derivs*)
Ger. Pat., 1973, 2 262 318; *CA*, **79**, 78088k (*manuf*)
Barrelle, M. *et al., Org. Magn. Reson.*, 1982, **19**, 102 (*cmr*)
Illing, H.P.A. *et al., HSE Toxicity Review 10: Glycol Ethers*, HMSO, London, 1985, (*tox, rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 973-974
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 598
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EES350; EES400

1-(1-Ethoxyethoxy)-3-hexene, 9CI E-253

[88683-94-7]
1-Ethoxy-1-(3-hexenyloxy)ethane. Acetaldehyde ethyl 3-hexenyl acetal

H_3CCH_2CH
$=CHCH_2CH_2OCH(OEt)CH_3$

$C_{10}H_{20}O_2$ 172.267

(*Z*)-*form* [28069-74-1]
Constit. of the volatile components of strawberries and victoria plums. Flavouring ingredient.
▶ MP6795000

[60763-40-8]

McFadden, W.H. *et al., J. Chromatogr.*, 1965, **18**, 10 (*isol*)
Ismail, H.M. *et al., J. Sci. Food Agric.*, 1981, **32**, 613 (*isol*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 275 (*rev*)

2-(1-Ethoxyethoxy)propanoic acid, 9CI E-254

[162845-25-2]

$EtOCH(CH_3)OCH(CH_3)COOH$

$C_7H_{14}O_4$ 162.185

K salt: [100743-68-8] *FEMA 3752*
Acetaldehyde generating agent, used to impart a fresh flavour to orange drinks and other foodstuffs. Yellowish viscous liq.

[37101-80-7]

Oser, B.L. *et al., Food Technol. (Chicago)*, 1985, **39**, 108; **39(11)**, 110; 112; 114; 116-117 (*use*)
Eur. Pat., 1987, 217 581; *CA*, **107**, 96337s (*synth, use, Et ester*)
U.S. Pat., 1992, 5 349 047; *CA*, **122**, 266257v (*synth*)
Giles, R.G.F. *et al., J.C.S. Perkin 1*, 1999, 3029-3038 (*synth*)

1-Ethoxy-1-hexyloxyethane E-255

[54484-73-0]
1-(1-Ethoxyethoxy)hexane, 9CI. Acetaldehyde ethyl hexyl acetal

$H_3C(CH_2)_5OCH(OEt)CH_3$

$C_{10}H_{22}O_2$ 174.283

▶ MO3650000

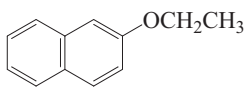
(±)-*form*
Liq. d_4^{20} 0.83. Bp_{27} 90-91° Bp_{13} 65-66°. n_D^{20} 1.4101.

(ξ)-*form*
Detected as a volatile component of strawberries.

Deschamps, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 911 (*synth*)
McFadden, W.H. *et al., J. Chromatogr.*, 1965, **18**, 10 (*isol*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 277 (*rev*)

2-Ethoxynaphthalene, 9CI, 8CI E-256

[93-18-5]
Ethyl 2-naphthyl ether. β-Naphthyl ethyl ether. Bromelia. Nerolin II. FEMA 2768



$C_{12}H_{12}O$ 172.226

Flavouring ingredient. Plates. Mp 37.5°. Bp 282° (274-275°).

▶ Skin irritant. LD_{50} (rat, orl) 3110 mg/kg. QJ6900000

Picrate:
Mp 101-101.5°.

Davis, W.A. *et al., J.C.S.*, 1900, 33
Werner, R.L. *et al., Aust. J. Chem.*, 1955, **8**, 364 (*ir*)
Yokoyama, M. *et al., Yakugaku Zasshi*, 1958, **78**, 123; *CA*, **52**, 10986c
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 587
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1935
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EEY500

1-Ethoxy-1-pentyloxyethane E-257

[13442-89-2]
1-(1-Ethoxyethoxy)pentane, 9CI. Acetaldehyde ethyl pentyl acetal

$H_3C(CH_2)_4OCH(OEt)CH_3$

$C_9H_{20}O_2$ 160.256

(±)-*form*
Liq. d_4^{20} 0.83. Bp 169°. n_D^{20} 1.4047.

(ξ)-*form*
Detected in strawberry volatiles.
Deschamps, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 911 (*synth*)
McFadden, W.H. *et al., J. Chromatogr.*, 1965, **18**, 10 (*isol*)

(4-Ethoxyphenyl)urea, 9CI E-258

[150-69-6]
p-*Ureidophenetole. Dulcin. Sucrol. Valzin*



$C_9H_{12}N_2O_2$ 180.206
Sweetening agent ca. 250 times sweeter than sucrose. Prohibited from human food use in U.S.A. and other countries. Plates (H_2O). Mp 173-174°.
▶ Adverse CNS effects by ingestion. LD_{50} (rat, orl) 1900 mg/kg. YT2275000
N-*Ac:*
$C_{11}H_{14}N_2O_3$ 222.243
Mp 220°.
N-*Benzoyl:*
$C_{16}H_{16}N_2O_3$ 284.314
Mp 215-217°.
Uhthoff, J. *et al., CA*, 1929, **23**, 1889 (*synth*)
Sah, P.P.T. *et al., Ber.*, 1936, **69**, 2762 (*synth*)
Roura, V.C. *et al., CA*, 1942, **36**, 2845 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 52
Asabe, Y. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 3482 (*nmr*)
Sen Gupta, A.K. *et al., J. Indian Chem. Soc.*, 1972, **49**, 727 (*synth*)
IARC Monog., 1976, **12**, 97; *Suppl.* 7, 63 (*rev, tox*)
Goldsmith, R.H. *et al., J. Chem. Educ.*, 1987, **64**, 954 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EFE000
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Ethyl acetate, 9CI E-259

[141-78-6]
Ethyl ethanoate. Acetic ester. FEMA 2414
$H_3CCOOEt$
$C_4H_8O_2$ 88.106
Found in cereal crops, radishes, fruit juices, beer, wine, spirits etc. and produced by *Anthemis nobilis* (Roman chamomile) and *Rubus* spp. Used in artificial fruit essences. Used as a solvent in the manufacture of modified hop extract and decaffeinated tea or coffee. Also used for colour and inks used to mark fruit or vegetables. A volatile flammable liq. with characteristic, fruity odour. Misc. most org. solvs., sol. 13 parts H_2O at 15°, less sol. at higher temps. Slowly hydrol. by H_2O. Forms azeotrope with H_2O, 6.1% w/w, Bp 70.4°.
▶ Highly flammable, fl. p. -4°, autoignition temp. 426°. May ignite or explode with $LiAlH_4$. Irritant to eyes, skin and mucous membranes. High vapour conc. narcotic and can damage liver and kidneys. Prolonged or repeated exposure causes conjunctival irritation and corneal clouding. LD_{50} (rat, orl) 5620 mg/kg. OES: long-term 400 ppm. AH5425000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 600B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 898B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 607C (*ir*)
Wade, J. *et al., J.C.S.*, 1905, **87**, 1656 (*synth*)
Guest, R.J. *et al., Anal. Chem.*, 1955, **27**, 931 (*use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 711 (*rev, tox*)
Caswell, L.R. *et al., J.O.C.*, 1976, **41**, 3312 (*uv*)
Minato, H. *et al., Chem. Lett.*, 1977, 1095 (*synth, pmr*)
Nefedov, B.K. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1977, 614; *CA*, **87**, 38814 (*manuf*)
Sandell, E.B. *et al., Photometric Determination of Traces of Metals, General Aspects*, Wiley, New York, 1977, (*use*)
Couperus, P.A. *et al., Org. Magn. Reson.*, 1978, **11**, 590 (*cmr*)
Bews, J.R. *et al., J. Mol. Struct.*, 1981, **71**, 297 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EFR000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1102
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 940 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1518
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 233
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 582
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EFR000

Ethyl acetoacetate, 8CI E-260

Ethyl 3-oxobutanoate, 9CI. Acetoacetic ester. Ethyl 3-hydroxy-2-butenoate. FEMA 2415
$H_3CCOCH_2COOEt \Leftrightarrow H_3CC(OH)=CHCOOEt$
$C_6H_{10}O_3$ 130.143
Equilibrium mixt. consists of approx. 92.3% oxo and 7.7% enol forms at r.t. Both forms have been obt. at low temps.. Flavouring agent. Present in strawberry, yellow passion fruit juice and coffee. Liq. with characteristic agreeable/irritant odour. pK_a 11.8 (50% dioxan). pK_a 10.68 (25°).
▶ Flammable, fl. p. 57/68/84°, autoignition temp. 295°.
Oxo-*form* [141-97-9]
Liq. Misc. most org. solvents, sol. dil. alkalis, pptd. with CO_2, spar. sol. H_2O. d^{20} 1.03. Bp_{14} 74° Bp_1 28.5°. n_D^{20} 1.4190.
▶ Mod. toxic. Eye and skin irritant. LD_{50} (rat, orl) 3980 mg/kg. AK5250000
Semicarbazone: [5982-65-0]
Needles (Et_2O). Sol. hot H_2O. Mp 129° dec.
Phenylhydrazone: [6078-46-2]
Needles. Sol. EtOH. Mp 50°. Oxidised by air.
Enol-*form* [1522-29-8]
Oil. n_D^{20} 1.4480.
Me ether: [3510-99-4] *Ethyl 3-methoxy-2-butenoate, 9CI. Ethyl 3-methoxycrotonate, 8CI*
Bp 188-193° Bp_{13} 70-72°.
Et ether: [998-91-4] *Ethyl 3-ethoxy-2-butenoate, 9CI. Ethyl 3-ethoxycrotonate, 8CI*
Mp 31°. Bp 195-200° Bp_7 70-72°. Probably *E*- or *cis*-form.
[19232-39-4, 22157-27-3, 22157-28-4, 57031-90-0, 57592-45-7]
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 687B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 743B (*ir*)
Knorr, L. *et al., Ber.*, 1911, **44**, 1138 (*tautomers*)
Snell, J.M. *et al., J.A.C.S.*, 1931, **53**, 2310 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 235 (*synth*)
Kundu, P.C. *et al., Fresenius' Z. Anal. Chem.*, 1961, **184**, 255 (*use*)
Reed, R.I. *et al., Tetrahedron*, 1967, **23**, 2807; 4425 (*ms*)
Markov, P. *et al., Tet. Lett.*, 1972, 4017 (*uv*)
Carlson, R.M. *et al., Tet. Lett.*, 1973, 4819 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 713 (*rev, tox*)
Kato, T. *et al., Yakugaku Zasshi*, 1974, **94**, 884 (*synth*)
Schimelpfenig, C.W. *et al., J. Chem. Educ.*, 1977, **54**, 446 (*synth*)
Bauer, S.H. *et al., J. Phys. Chem.*, 1983, **87**, 2411 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EFS000
Cook, W.M. *et al., Food Chem. Toxicol.*, 1992, **30**, 567 (*tox*)
Fanizzi, F.P. *et al., J.C.S. Dalton*, 1992, 309 (*pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2381-2384 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EFS000

Ethyl carbamate, 9CI E-261

[51-79-6]
Urethane, INN. *Ethyl aminoformate. Ethyl urethane. Leucethane. Pracarbamin. NSC 746*
$H_2NCOOEt$
$C_3H_7NO_2$ 89.094
Common contaminant of fermented beverages. Prisms (C_6H_6 or toluene) with cooling, saline taste. V. sol. H_2O, EtOH, Et_2O, $CHCl_3$, C_6H_6; spar. sol. petrol. Mp 48.5-50°. Bp 182-184° Bp_{54} 103°. Log P -0.18 (calc). Aq. solution at 130° → Urea.
▶ Possible human carcinogen. Exp. carcinogen and teratogen. LD_{50} (mus, orl) 2500 mg/kg. FA8400000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 771D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1257C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 786D (*ir*)
Guerci, L. *et al., CA*, 1922, **16**, 2481 (*synth*)
Mirvish, S.S. *et al., Adv. Cancer Res.*, 1968, **11**, 1 (*rev, pharmacol*)
Tartler, G. *et al., CA*, 1969, **70**, 37331 (*synth*)
Vishnyakova, T.P. *et al., CA*, 1969, **71**, 101267 (*synth*)

Fuks, R. *et al., Bull. Soc. Chim. Belg.*, 1973, **82**, 23 (*synth*)
IARC Monog., 1974, **7**, 111; *Suppl*. 7, 73 (*rev, tox*)
Tatsumi, K. *et al., Chem. Pharm. Bull.*, 1980, **28**, 351 (*metab*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 1877
Maggi, C.A. *et al., Experientia*, 1986, **42**, 109; 292; 531 (*rev, pharmacol*)
Lawrence, J.F. *et al., Food Contam. Environ. Sources, 1990*, (eds. Nriagu, J.O. *et al*), J. Wiley, New York, 1990, (*alcoholic beverages*)
Marstokk, K.-M. *et al., Acta Chem. Scand.*, 1999, **53**, 329-334 (*microwave*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACL000; UVA000

O-Ethyl *S,S*-diphenyl phosphorodithioate, 9CI, 8CI E-262

[17109-49-8]
Edifenphos, BSI. Hinosan

$(PhS)_2P(O)OEt$

$C_{14}H_{15}O_2PS_2$ 310.377

Rice fungicide. Yellowish liq. Prac. insol. H_2O. d_4^{20} 1.23. $Bp_{0.01}$ 154°. n_D^{22} 1.6112. Hydrol. in strongly acid or alk. media.

▶ LD_{50} (rat, orl) 100 mg/kg. TE3850000

U.K. Pat., 1965, 1 083 377; *CA*, **68**, 49297v (*synth, use*)
Umeda, Y. *et al., Jpn. Pestic. Inf.*, 1972, 85; 1973, 25 (*rev, props, metab*)
Tomizawa, C. *et al., J. Environ. Sci. Health, Part B*, 1976, **11**, 231 (*metab*)
Agrochemicals Handbook, Royal Society of Chemistry, 1983, A174
Pesticide Manual, 11th edn., 1997, No. 267
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EIM000

Ethyl 1-(ethylthio)ethyl disulfide, 9CI E-263

[94944-48-6]
5-Methyl-3,4,6-trithiaoctane

$EtSCH(CH_3)–S–SEt$

$C_6H_{14}S_3$ 182.375

Constit. of the fruit of *Durio zibethinus* (durian).

[137839-22-6]

Hwang, S.S. *et al., J. Agric. Food Chem.*, 1986, **34**, 538-542 (*synth*)
Weenen, H. *et al., J. Agric. Food Chem.*, 1996, **44**, 3291-3293 (*isol*)

Ethyl (ethylthio)methyl disulfide, 9CI E-264

[183554-16-7]
3,4,6-Trithiaoctane

$EtSCH_2–S–SEt$

$C_5H_{12}S_3$ 168.348

Constit. of the fruit of *Durio zibethinus* (durian).

Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

Ethyl 1-(ethylthio)propyl disulfide E-265

[183554-18-9]

$EtSCH(CH_2CH_3)–S–SEt$

$C_7H_{16}S_3$ 196.401

Constit. of the fruit of *Durio zibethinus* (durian).

Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

Ethyl formate, 9CI E-266

[109-94-4]
FEMA 2434

HCOOEt

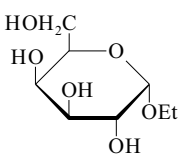
$C_3H_6O_2$ 74.079

Found in various foods, e.g. cooked apple, orange juice, pineapple, other fruits, raw cabbage, coffee, black tea, wheat bread, white clover, sorghum. Used as a flavouring agent. Mobile, flammable liq. with pleasant aroma. Misc. EtOH, Et_2O, C_6H_6, spar. sol. in and gradually hyd. by H_2O. d^{20} 0.92. Mp -80.5°. Bp 54°. n_D^{20} 1.3598.

▶ Extremely flammable, fl. p.-20°, autoignition temp. 440/455°. Eye, skin and respiratory skin irritant, high vapour conc. narcotic. LD_{50} (rat, orl) 1850 mg/kg. OES: long-term 100 ppm; short-term 150 ppm. LQ8400000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 599B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 895B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 605B (*ir*)
Young, S. *et al., J.C.S.*, 1893, **63**, 1202 (*synth*)
Bishop, W.B.S. *et al., J. Soc. Chem. Ind., London*, 1923, **42**, 401T (*synth*)
Gravin, A.I. *et al., J. Appl. Chem. USSR (Engl. Transl.)*, 1943, **16**, 105; *CA*, **38**, 1239 (*synth*)
Kantlehner, W. *et al., Chem. Ber.*, 1971, **104**, 3711 (*synth*)
Wagenknecht, J.H. *et al., Synth. Commun.*, 1972, **2**, 215 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 233
Dorman, D.E. *et al., J.O.C.*, 1975, **40**, 3729 (*cmr*)
Harrison, A.G. *et al., Can. J. Chem.*, 1976, **54**, 2029 (*ms*)
Caswell, L.R. *et al., J.O.C.*, 1976, **41**, 3312 (*uv*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 737 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EKL000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 982-984 (*use, occur*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 310
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 602
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Ethyl galactoside E-267



α-D-Pyranose-*form*

$C_8H_{16}O_6$ 208.211

α-D-Pyranose-*form* [15486-24-5]
Eleutheroside C

Constit. of *Glycine max* (soybean). Cryst. (EtOH). Mp 140°. $[\alpha]_D^{20}$ +186 (H_2O).

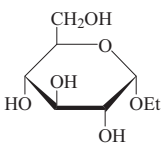
Tetra-O-*Ac:* [31281-90-0] *Ethyl 2,3,4,6-tetra*-O-*acetyl*-α-D-*galactopyranoside*
$C_{16}H_{24}O_{10}$ 376.36
Cryst. (pentane). Mp 87-88°. $[\alpha]_D^{20}$ +136 ($CHCl_3$).

β-D-Pyranose-*form* [18997-88-1]
Cryst. (EtOH). Mp 159-161°. $[\alpha]_D^{21}$ -6 (c, 2 in H_2O).

Overend, W.G. *et al., J.C.S.*, 1962, 3429 (*synth*)
Ovodov, Y.S. *et al., Khim. Prir. Soedin.*, 1967, **3**, 63; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 53 (*isol*)
Kulshrestha, D.K. *et al., Chem. Ber.*, 1968, **101**, 2096 (*isol*)
Bruyne, C.K. *et al., Carbohydr. Res.*, 1972, **25**, 59 (*synth*)
Sishandri, T.R. *et al., Curr. Sci.*, 1973, **42**, 421 (*isol*)
Schroeder, L.R. *et al., Carbohydr. Res.*, 1974, **37**, 368 (*synth*)
Zamojski, A. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1975, **49**, 2113 (*synth*)
Van Heeswijk, W.A.R. *et al., Carbohydr. Res.*, 1977, **58**, 494 (*synth*)
Jain, M.P. *et al., Phytochemistry*, 1980, **19**, 1880 (*isol*)
Khan, K.M. *et al., Nat. Prod. Lett.*, 2002, **16**, 283-290 (*isol, pmr, cmr*)

Ethyl glucoside, 8CI E-268

[27214-60-4]



α–D-Pyranose-*form*

$C_8H_{16}O_6$ 208.211

β-D-Pyranose-*form* [3198-49-0]
Constit. of Citrus peels, the fresh root cortex of *Manihot esculenta* (cassava) and other plant spp.. Cryst. with bitter taste. Mp 90.4° Mp 98-100°. $[\alpha]_D^{20}$ -36.7 (H_2O).

Ferguson, J.H. *et al., J.A.C.S.*, 1932, **54**, 4086 (*α-D-pyr, α-D-pyr tetra-Ac, β-D-pyr, β-D-pyr tetra-Ac*)
Rowell, R.M. *et al., Carbohydr. Res.*, 1972, **23**, 417 (*β-D-pyr, β-D-pyr tri-Ac, β-D-pyr tri-Ac derivs, β-D-pyr Me*)
Matsubera, Y. *et al., CA*, **113**, 17474g (*β-D-pyr, isol, props*)

Ethyl hydrogen sulfate E-269

[540-82-9]
Monoethyl sulfate, 9CI. Sulfovinic acid. Ethylsulfuric acid

$EtOSO_2OH$

$C_2H_6O_4S$ 126.133

Has not been obt. pure. Found in wines. Pale amber, oily liq. Misc. and slowly hyd. H_2O. d^{17} 1.32. Dec. on heating → C_2H_4. Forms salts which are readily sol. in H_2O and dec. on boiling in soln..

▶ Highly irritant. Emits highly toxic fumes on heating to dec.. WT1101700

Evans, F.N. *et al., J.A.C.S.*, 1917, **39**, 456 (*synth, salts*)
Popelier, F. *et al., Bull. Soc. Chim. Belg.*, 1926, **35**, 264 (*synth, derivs*)

Hamid, M.A. *et al., J.C.S.*, 1926, 1098 (*synth, salts*)
Breslow, D.S. *et al., J.A.C.S.*, 1954, **76**, 5361 (*synths*)
Page, R. *et al., Ethylene Its Ind. Deriv.*, Ernest Benn Ltd, London, 1969, 787 (*rev, bibl*)
Masaki, M. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3174 (*synth, derivs*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 674

Ethyl isopropyl disulfide E-270

[53966-36-2]
Ethyl 1-methylethyl disulfide, 9CI

EtS–S–$CH(CH_3)_2$

$C_5H_{12}S_2$ 136.282

Constit. of *Allium cepa* (onion) juice. Bp_9 49°.

Alonso, M.E. *et al., J.O.C.*, 1978, **43**, 4491-4495 (*synth, ms*)
Org. Synth., 1978, **58**, 147-152
Gupta, D. *et al., Can. J. Chem.*, 1981, **59**, 543-548 (*ms*)
Talyzin, V.V. *et al., Zh. Anal. Khim.*, 1988, **43**, 911-916 (*isol*)

Ethyl methyl disulfide, 9CI E-271

[20333-39-5]
2,3-Dithiapentane

Et–S–S–Me

$C_3H_8S_2$ 108.228

Constit. of *Allium* spp. and *Durio zibethinus* (durian). Liq. d^{20} 1.02. Bp 135° Bp_{57} 58°. n_D^{20} 1.5130.

Brintzinger, H. *et al., Chem. Ber.*, 1953, **86**, 557-563 (*synth*)
Birch, S.F. *et al., J. Inst. Pet.*, 1953, **39**, 206-219 (*synth*)
Milligan, B. *et al., J.C.S.*, 1963, 6008-6012 (*synth*)
Allum, K.G. *et al., Spectrochim. Acta A*, 1968, **24**, 927-941 (*ir, Raman*)
Dauphin, G. *et al., Org. Magn. Reson.*, 1979, **12**, 557-560 (*cmr*)
Gupta, D. *et al., Can. J. Chem.*, 1981, **59**, 543-548 (*ms*)
Barony, G. *et al., J.O.C.*, 1983, **48**, 4750-4761 (*pmr*)
Ohsaku, M. *et al., J. Phys. Chem.*, 1988, **92**, 4591-4594 (*mol struct, conformn*)

Ethyl methyl sulfide E-272

[624-89-5]
(Methylthio)ethane, 9CI. 2-Thiabutane. FEMA 3860

EtSMe

C_3H_8S 76.162

Flavouring ingredient. Aroma constit. of cooked meats, canned salmon, tomato, coffee and leek oil. Food additive listed in the EAFUS Food Additive Database (Jan 2001). Fp -104.8. Bp 66.9°.

▶ Highly flammable, fl. p. < 21°/-15°.

S-*Oxide:* See Ethyl methyl sulfoxide in *The Combined Chemical Dictionary.*

S,S-*Dioxide:* [594-43-4] *(Methylsulfonyl)ethane, 9CI. Ethyl methyl sulfone, 8CI*
$C_3H_8O_2S$ 108.161
Needles (Et_2O). Sol. H_2O, EtOH, spar. sol. Et_2O. Mp 36°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 265C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 426C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 348B (*ir*)
Beckmann, E.O. *et al., J. Prakt. Chem.*, 1878, **17**, 439 (*dioxide*)
Klason, P. *et al., Ber.*, 1887, **20**, 3413 (*synth*)
Brozozowski, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1963, **37**, 1069; *CA*, **60**, 5323 (*synth*)
Ohsaka, M. *et al., J. Mol. Sci. (Int. Ed)*, 1977, **42**, 31 (*ir*)
Moesch, C. *et al., Ann. Pharm. Fr.*, 1992, **49**, 286 (*synth*)
Eberlin, M.N. *et al., J.A.C.S.*, 1992, **114**, 2884 (*ms*)
Girard, B. *et al., J. Food Sci.*, 2000, **65**, 34-39 (*detn, salmon*)

Ethyl methyl trisulfide E-273

[31499-71-5]
2,3,4-Trithiahexane. FEMA 3861

EtS-S-SMe

$C_3H_8S_3$ 140.294

Found in durian fruit, cooked beef, crucifers, pork, Chinese chive (*Allium tuberosum*), Rakkyo (*Allium chinense*), coffee and roasted peanut aroma. Flavouring for meat products. Pale yellow liq. with powerful odour.

Naef, R. *et al., Flavour Fragrance J.*, 1996, **11**, 295-303 (*occur, durian*)
Nedjma, M. *et al., J. Agric. Food Chem.*, 1996, **44**, 3935-3938 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1119 (*use, occur*)
Pino, J.A. *et al., J. Agric. Food Chem.*, 2001, **49**, 1328-1330 (*detn, alliums*)

Ethyl 1-(methylthio)ethyl disulfide E-274

[183554-13-4]

[137818-68-9]

$MeSCH(CH_3)$–S–SEt

$C_5H_{12}S_3$ 168.348

Constit. of the fruit of *Durio zibethinus* (durian).

Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

Ethyl (methylthio)methyl disulfide E-275

[183554-12-3]
2,4,5-Trithiaheptane

$MeSCH_2$–S–SEt

$C_4H_{10}S_3$ 154.321

Constit. of the fruit of *Durio zibethinus* (durian).

Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

Ethyl 1-(methylthio)propyl disulfide, 9CI E-276

[53897-67-9]

H_3CCH_2CH(SMe)-S-S-Et

$C_6H_{14}S_3$ 182.375

Constit. of shallots (*Allium cepa*) and Chinese chives (*Allium tuberosum*). Characterised spectroscopically.

Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*synth, ms*)
Wu, J.L. *et al., J. Food Sci.*, 1982, **47**, 606-608 (*occur, ms*)
Lopes, D. *et al., Flavour Fragrance J.*, 1997, **12**, 237-239 (*occur*)

Ethyl nitrite, 9CI, 8CI E-277

[109-95-5]
Nitrosyl ethoxide. FEMA 2446

EtONO

$C_2H_5NO_2$ 75.067

Flavouring ingredient. Very volatile liq. or gas with a characteristic ether-like odour. V. sl. sol. H_2O, sol. EtOH. Bp 17°.

▶ High vapour conc. narcotic. LC_{50} (rat, ihl) 160 ppm (4h exposure). Explodes if heated or shocked. Extremely flammable; fl. p. -35°, autoignition temp. 90°. RA0810000

Chrétien, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1943, **217**, 504 (*synth*)
Adickes, F. *et al., J. Prakt. Chem.*, 1943, **161**, 271 (*synth*)
Krueger, J.R. *et al., J.O.C.*, 1978, **43**, 2877 (*ir, pmr, cmr*)
Macdonald, J.C. *et al., Acta Chem. Scand., Ser. B*, 1981, **35**, 485 (*tox*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 156 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 256
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1021
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0814
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 613
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ENN000

Ethyl oxyhydrate E-278

[1338-05-2]

[8030-89-5]
Rum ether. FEMA 2996

A mixture of 22 components by glc, consisting principally of water, ethanol, ethyl acetate, methanol, ethyl formate, acetaldehyde and formaldehyde. Flavouring ingredient. Liq. with rum-like odour and flavour. Bp 65-87°.

Fenaroli, G. *et al., Perfum. Essent. Oil Res.*, 1966, **57**, 293-300 (*props, manuf, glc*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 721 (*props, use*)

Ethyl propyl disulfide E-279

[30453-31-7]
3,4-Dithiaheptane

EtS–S–$CH_2CH_2CH_3$

$C_5H_{12}S_2$ 136.282

Constit. of *Allium* spp., *Durio zibethinus* (durian) and *Nigella sativa* (black cumin). Bp_{80} 104-106° Bp_7 47-48°.

Brois, S.J. *et al., J.A.C.S.*, 1970, **92**, 7629-7631 (*synth*)
Harpp, D.N. *et al., J.O.C.*, 1979, **44**, 4140-4144 (*synth*)
Gupta, D. *et al., Can. J. Chem.*, 1981, **59**, 543-548 (*ms*)
Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

Ethyl 1-(propylthio)propyl disulfide E-280

[183554-24-7]

[137867-56-2]

$H_3CCH_2CH_2SCH(CH_2CH_3)–S–SEt$

$C_8H_{18}S_3$ 210.428

Constit. of the fruit of *Durio zibethinus* (durian).

Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

Ethyl vinyl disulfide, 8CI E-281

[24298-49-5]

Ethenyl ethyl disulfide, 9CI. 3,4-Dithia-1-hexene

$EtS–S–CH=CH_2$

$C_4H_8S_2$ 120.239

Constit. of the fruit of *Durio zibethinus* (durian). Bp_{10} 36-40°.

Wijers, H.E. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 519-529 (*synth*)

Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

N-Ethylacetamide, 9CI, 8CI E-282

[625-50-3]

N-*Ethylethanamide*

$H_3CCONHEt$

C_4H_9NO 87.121

Found in tea and wine. Oily liq. Sol. H_2O, EtOH, Et_2O. Bp 205° $Bp_{0.15}$ 66°.

▶ LD_{50} (rat, ipr) 3130 mg/kg. Fl. p. 106/110°. AB8500000

Hydrochloride:
Deliquescent needles. Mp 60°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1229B (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 779D (*ir*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 441D (*ir*)

Wallach, O. *et al., Annalen*, 1873, **184**, 108 (*synth*)

Titherley, A.W. *et al., J.C.S.*, 1901, **79**, 391 (*synth*)

Fr. Pat., 1971, 2 067 629; *CA*, **77**, 4977 (*purifn*)

Schreier, P. *et al., Z. Lebensm.-Unters. -Forsch.*, 1975, **157**, 34 (*isol, ms*)

Kisfaludy, L. *et al., J.O.C.*, 1979, **44**, 654 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EFM000

Ethylamine, 8CI E-283

[75-04-7]

Ethanamine, 9CI

$H_3CCH_2NH_2$

C_2H_7N 45.084

Found in foods and drinks. Flammable gas with ammoniacal odour. Misc. EtOH, Et_2O, H_2O, salted out by NaOH. Fp -80. Bp 16.6°. pK_a 10.7.

▶ Extremely flammable, fl. p. < -18°, autoignition temp. 580°. Skin, respiratory tract and severe eye irritant. High vapour conc. may affect CNS. LD_{50} (rat, orl) 400 mg/kg. LD_{50} (rbt, skn) 390 mg/kg. OES: long-term 10 ppm. KH2100000

[16999-99-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 279D; 364D (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 449B; 449C (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 364B (*ir*)

Watt, G.W. *et al., J.A.C.S.*, 1947, **69**, 836 (*synth*)

Lerch, B. *et al., Z. Naturforsch., B*, 1966, **21**, 216 (*occur*)

Steiner, M. *et al., Planta*, 1968, **79**, 113 (*isol*)

Gallant, R.W. *et al., Hydrocarbon Process.*, 1969, **48**, 143 (*rev, bibl, props*)

Neurath, G.B. *et al., Food Cosmet. Toxicol.*, 1979, **15**, 275 (*isol*)

Wagner, W. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1980, **36**, 125 (*ms*)

Faure, R. *et al., Org. Magn. Reson.*, 1980, **14**, 20 (*cmr*)

Altona, C. *et al., Magn. Reson. Chem.*, 1989, **27**, 564 (*pmr*)

Wolff, H. *et al., Spectrochim. Acta A*, 1991, **47**, 165 (*conformn, ir*)

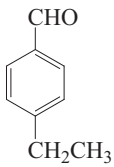
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 95

Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 585

4-Ethylbenzaldehyde, 9CI E-284

[4748-78-1]

FEMA 3756



$C_9H_{10}O$ 134.177

Present in roasted chicken, cider, tea and roasted peanuts. Flavouring ingredient. Liq. with a bitter almond odour. Bp 221° Bp_{10} 109-110°.

Oxime: [61946-88-1]
$C_9H_{11}NO$ 149.192
Mp 29°.

2,4-Dinitrophenylhydrazone:
Mp 216°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 109C (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 939A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1289A (*ir*)

v. Braun, J. *et al., Annalen*, 1924, **436**, 299 (*synth*)

Edmund, I. *et al., J.A.C.S.*, 1941, **63**, 1462 (*synth*)

Baker, J.W. *et al., J.C.S.*, 1956, 404 (*synth*)

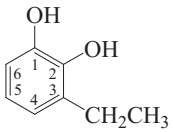
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 218

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 950-951

3-Ethyl-1,2-benzenediol E-285

[933-99-3]

3-Ethylcatechol. 3-Ethylpyrocatechol



$C_8H_{10}O_2$ 138.166

Pyrolysis prod. of coffee. Oil. Bp_{15} 132-134°.

Bis(4-nitrobenzoyl):
Pale yellow needles (Me_2CO). Mp 139.6-140.4°.

1-Me ether: [90534-46-6] *2-Ethyl-6-methoxyphenol. 6-Ethylguaiacol*
$C_9H_{12}O_2$ 152.193

2-Me ether: [97678-77-8] *3-Ethyl-2-methoxyphenol. 3-Ethylguaiacol*
$C_9H_{12}O_2$ 152.193
No phys. props. reported.

Mosimann, W. *et al., Ber.*, 1916, **49**, 1261 (*synth*)

Stern, R. *et al., J.A.C.S.*, 1957, **79**, 5792 (*synth*)

Silar, J. *et al., Chem. Prum.*, 1970, **20**, 521; *CA*, **74**, 31607k (*synth*)

Ger. Pat., 1971, 2 031 712; *CA*, **76**, 59212 (*synth*)

Ansell, M.F. *et al., J.C.S.(C)*, 1971, 1401 (*synth, ir*)

Arnarp, J. *et al., Acta Chem. Scand.*, 1989, **43**, 44 (*mono-Me ethers*)

4-Ethyl-1,2-benzenediol E-286

[1124-39-6]

4-Ethylpyrocatechol, 8CI. 4-Ethylcatechol

$C_8H_{10}O_2$ 138.166

Constit. of roasted coffee. Also isol. from eggplant leaves (*Solanum melongena*). Mp 41°. Bp_{10} 145°.

1-Me ether: [2785-88-8] *5-Ethyl-2-methoxyphenol. 5-Ethylguaiacol.* ***Locustol***
$C_9H_{12}O_2$ 152.193Later work (Obeng-Ofori, *et al.*) failed to confirm its occurrence in locusts or its claimed pheromonal activity.

2-Me ether: [2785-89-9] *4-Ethyl-2-methoxyphenol. 4-Ethylguaiacol. FEMA 2436*
$C_9H_{12}O_2$ 152.193
Constit. of numerous plant spp. and cooked foods. Flavouring agent. Liq. with smoky bacon-like odour. Bp 234-236° Bp_{46} 140-146°.

2-Me ether, benzoyl:
$C_{16}H_{16}O_3$ 256.301
Cryst. (EtOH). Mp 58-60°.

2-Me ether, 3,5-dinitrobenzoyl:
Cryst. (EtOH). Mp 127° (121.5°).

Di-Me ether: [5888-51-7] *4-Ethyl-1,2-dimethoxybenzene. 4-Ethylveratrole*
$C_{10}H_{14}O_2$ 166.219
Constit. of tea and coffee aroma. Oil. Bp_{15} 122-124° Bp_1 112°.

Clemmensen, E. *et al., Ber.*, 1914, **47**, 51-63 (*synth*)

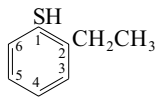
Tsukervanik, I.P. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1947, **17**, 1009-1014 (*synth*)

Coscia, C.J. *et al., J.O.C.*, 1961, **26**, 5085-5091 (*4-Ethylguaiacol*)

Potts, K.T. *et al., J.O.C.*, 1963, **28**, 3202-3205 (*4-Ethylveratrole*)
Ansell, M.F. *et al., J.C.S.(C)*, 1971, 1401-1414 (*synth*)
Nolte, D.J. *et al., J. Insect Physiol.*, 1976, **22**, 833 (*Locustol*)
Yadav, J.S. *et al., Tetrahedron*, 1988, **44**, 7243-7254 (*di-Me ether*)
Arnarp, J. *et al., Acta Chem. Scand.*, 1989, **43**, 44-50 (*Locustol*)
Sreng, L. *et al., J. Chem. Ecol.*, 1990, **16**, 2899-2912 (*2-Me ether, isol*)
Obeng-Ofori, D. *et al., J. Chem. Ecol.*, 1994, **20**, 2077-2087 (*Locustol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 986-987 (*2-Me ether, use, occur*)

2-Ethylbenzenethiol, 9CI E-287

[4500-58-7]
2-Ethylthiophenol. FEMA 3345



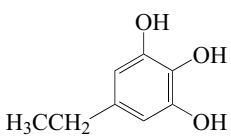
$C_8H_{10}S$ 138.233
Flavouring ingredient esp. for instant coffee. Liq. with pungent, roasted odour. d_4^{20} 1.04. Bp 203-205° (210°). n_D^{20} 1.5700.

S-*Me:*
$C_9H_{12}S$ 152.26
d 1.03. Bp_{772} 228.2-228.6°. n_D^{20} 1.5708.

Fricke, R. *et al., Ber.*, 1925, **58**, 24 (*synth*)
Adv. Chem. Ser., 1955, **15**, 329 (***props***)
Hansch, C. *et al., J.O.C.*, 1956, **21**, 265-270 (*synth*)
U.S. Pat., 1976, 3 968 264; *CA*, **85**, 122119w (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1042-1043
Bianchini, C. *et al., Chem. Comm.*, 2001, 479-480 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 600 (*use*)

5-Ethyl-1,2,3-benzenetriol, 9CI E-288

[66125-16-4]
5-Ethylpyrogallol



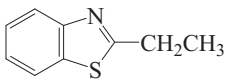
$C_8H_{10}O_3$ 154.165
Mp 86-87°.

1,3-Di-Me ether: [14059-92-8] *4-Ethyl-2,6-dimethoxyphenol, 9CI. Ethylsyringol. FEMA 3671*
$C_{10}H_{14}O_3$ 182.219
Component of smoked food flavourings. $Bp_{0.02}$ 160-170° (bath temp.). n_D^{25} 1.5335.

Pepper, J.M. *et al., J.A.C.S.*, 1948, **70**, 67-71; 1951, **73**, 3316-3320 (*1,3-di-Me ether, synth, formn*)
Loubinoux, B. *et al., Tet. Lett.*, 1980, **21**, 4991-4994 (*1,3-di-Me ether, formn, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 227
Guillen, M.D. *et al., J. Agric. Food Chem.*, 1995, **43**, 463-468 (*1,3-di-Me ether, detn, glc*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 966 (*1,3-di-Me ether*)

2-Ethylbenzothiazole, 9CI E-289

[936-77-6]



C_9H_9NS 163.243
Claimed food uses not well documented. Liq. d_4^{25} 1.14. Mp -2.5°. Bp 252°. n_D^{25} 1.6004.

Picrate:
Mp 135°.

Metzger, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 1692-1696 (*synth*)
Elderfield, R.C. *et al., J.A.C.S.*, 1960, **82**, 1982-1988 (*synth*)
Jenkins, G.L. *et al., J.O.C.*, 1961, **26**, 274 (*synth*)
Guglielmetti, R. *et al., Bull. Soc. Chim. Fr.*, 1967, 4195-4205 (*pmr*)
Salmona, G. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1970, **271**, 1416-1419 (*ms*)
Davidovics, G. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1974, **71**, 659-665 (*ir, Raman*)
Faure, R. *et al., Org. Magn. Reson.*, 1978, **11**, 617-621 (*cmr*)
Quast, H. *et al., Annalen*, 1996, 1541-1549 (*synth*)

2-Ethylbutanal, 9CI E-290

[97-96-1]
2-Ethylbutyraldehyde, 8CI. Diethylacetaldehyde. FEMA 2426
$(H_3CCH_2)_2CHCHO$
$C_6H_{12}O$ 100.16
Occurs in canned foods, bread crusts, melon, french fries, maize and scallops. Flavouring ingredient. Liq. d^{20} 0.81. Mp -89°. Bp 117-119°.
▶ Highly flammable, fl. p. 21°. Skin irritant. LD_{50} (rat, orl) 3980 mg/kg. ES2625000

2,4-Dinitrophenylhydrazone: [14086-21-6] Orange plates (petrol). Mp 94.5-95° (129-130°, 137°).

Semicarbazone: [33861-38-0] Prisms (C_6H_6/petrol). Mp 97.5-99.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 466D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 728C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 552C (*ir*)
Brunner, H. *et al., J.C.S.*, 1937, 1039 (*synth, derivs*)
Wiechert, K. *et al., Z. Chem.*, 1967, **7**, 229 (*synth*)
Pallaud, R. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **273**, 418 (*synth*)
Sultanov, N.T. *et al., CA*, 1972, **77**, 4817 (*synth*)
Mueller, E. *et al., Chem. Ber.*, 1975, **108**, 1475 (*derivs*)
Cornils, B. *et al., Chem.-Ztg.*, 1977, **101**, 107 (*rev, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 221
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 955-956
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DHI000

2-Ethylbutanoic acid, 9CI E-291

[88-09-5]
2-Ethylbutyric acid, 8CI. Pentane-3-carboxylic acid. Diethylacetic acid. FEMA 2429
$(H_3CCH_2)_2CHCOOH$
$C_6H_{12}O_2$ 116.16
Occurs in bread crusts and geranium oil. Also found in tobacco vapours. Misc. EtOH, Et_2O; sl. sol. H_2O. d^{20} 0.92. Fp -15. Bp 194-195° (190°) Bp_{13} 90°. n_D^{20} 1.4132. pK_a 4.73 (25°,H_2O at).
▶ Skin, eye and respiratory tract irritant. LD_{50} (rat, orl) 2200 mg/kg. ET1400000

Me ester: [816-11-5]
$C_7H_{14}O_2$ 130.186
Liq. Bp_{736} 135-137°.

Et ester: [2983-38-2]
$C_8H_{16}O_2$ 144.213
Bp 152°.

Isopropyl ester: [5129-47-5]
$C_9H_{18}O_2$ 158.24
Bp 161-162°.

2-Propenyl ester: [7493-69-8] *2-Propenyl 2-ethylbutanoate. Allyl 2-ethylbutyrate*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient. Liq. Mp 165-167°. n_D^{15} 1.4240.

Chloride: [2736-40-5]
$C_6H_{11}ClO$ 134.605
Liq. Bp 134-137°.

Amide: [1114-38-1]
$C_6H_{13}NO$ 115.175
Needles (EtOH). Sol. H_2O. Mp 107°. Bp 230-235°.
▶ Exp. teratogen.

Nitrile: [617-80-1] *2-Ethylbutanenitrile, 9CI. Diethylacetonitrile. 3-Cyanopentane*
$C_6H_{11}N$ 97.16
Liq. Misc. EtOH, Et_2O. Bp 144-146°.

Anhydride: [54502-37-3]
$C_{12}H_{22}O_3$ 214.304
Liq. Bp 230° Bp_{12} 120°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 489A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 759C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 579C (*ir*)
Fittig, W. *et al., Annalen*, 1880, **200**, 24 (*synth*)
Fr. Pat., 1935, 790 213; *CA*, **30**, 2992 (*synth*)
Koch, H. *et al., Ber.*, 1940, **73**, 1171 (*ester*)
Breusch, F.L. *et al., Fette, Seifen, Anstrichm.*, 1971, **73**, 635 (*props*)
Cornils, B. *et al., Chem.-Ztg.*, 1977, **101**, 107 (*rev, bibl*)
McAdoo, D.J. *et al., J.A.C.S.*, 1977, **99**, 7265 (*ms*)
Wahlberg, I. *et al., Phytochemistry*, 1977, **16**, 1217 (*isol*)
Marr, D.H. *et al., Org. Magn. Reson.*, 1980, **13**, 28 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 23; **2**, 222
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 88; 958-959

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DHI400

2-Ethyl-1-butanol, 9CI E-292

[97-95-0]

$(H_3CCH_2)_2CHCH_2OH$

$C_6H_{14}O$ 102.176

Bp 144-146°.

▶ Skin and severe eye irritant. LD_{50} (rat, orl) 1850 mg/kg. LD_{50} (rbt, skn) 1260 mg/kg. EL3850000

Ac: [10031-87-5] *2-Ethylbutyl acetate. FEMA 2425*

$C_8H_{16}O_2$ 144.213

Flavouring ingredient. d^{20} 0.88. Bp_{20} 64.5-65.5°. n_D^{20} 1.4109.

2-Propenoyl: [3953-10-4] *2-Ethylbutyl acrylate*

$C_9H_{16}O_2$ 156.224

Bp_{20} 79-81°.

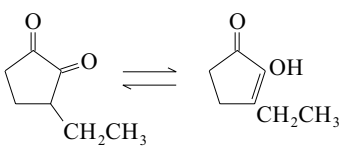
3,5-Dinitrobenzoyl:

Cryst. (petrol). Mp 35°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 116A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 171C; 903A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 163A; 610A (*ir*)
Whitmore, F.C. *et al., J.A.C.S.*, 1941, **63**, 643 (*synth*)
Harper, S.H. *et al., J.C.S.*, 1955, 1512 (*synth*)
U.S. Pat., 1962, 3 031 493; *CA*, **59**, 3776e (*2-propenoyl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 220 (*Ac*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 955 (*Ac*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4611
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 176
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EGW000

3-Ethyl-1,2-cyclopentanedione, 9CI E-293

3-Ethyl-2-hydroxy-2-cyclopenten-1-one, 9CI. FEMA 3152



$C_7H_{10}O_2$ 126.155

The two tautomers are apparently capable of separate isolation. Isol. from coffee and tobacco. Flavouring material, with caramel flavour and flavour enhancing props.

Oxo-*form* [13494-08-1]

Oil. Sol. Et_2O. Fp 20. Bp_1 65-68°. λ_{max} 259 (log ϵ 4.04) (EtOH).

Enol-*form* [21835-01-8]

Cryst. (hexane) with caramel-like odour. Sol. Et_2O. Mp 38-40° (42-44°). Bp_4 78-80°. Dec. in air.

2,4-Dinitrophenylhydrazone: [26103-86-6]

Cryst. (EtOH). Mp 135-138°. Believed to be the 1-DNP of the enol tautomer.

Semicarbazone: [26103-87-7]

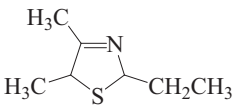
Cryst. (EtOH). Mp 232° dec. Believed to be the 1-semicarbazone of the enol tautomer.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 689C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 534D (*ir*)
Leir, C.M. *et al., J.O.C.*, 1970, **35**, 3203 (*synth, pmr, uv*)
Kende, A.S. *et al., Tet. Lett.*, 1973, 697 (*synth*)
Barco, A. *et al., Synthesis*, 1975, 104 (*synth*)
Maignon, C. *et al., Bull. Soc. Chim. Fr.*, 1976, 550 (*synth*)
Ito, S. *et al., Yakugaku*, 1976, **25**, 326 (*synth*)
Ishiguro, S. *et al., Agric. Biol. Chem.*, 1978, **42**, 1527 (*isol*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*detn, ms, coffee*)

2-Ethyl-2,5-dihydro-4,5-dimethylthiazole, 9CI E-294

[76788-46-0]

2-Ethyl-4,5-dimethyl-3-thiazoline. FEMA 3620



$C_7H_{13}NS$ 143.252

Maillard prod. in foods. Flavouring agent for meats and soups, doubtless as a mixt. of *cis*- and *trans*-forms.

Picrate:

Mp 114.5-115°.

(±)-*form*

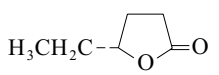
Bp_3 63-64°.

Asinger, F. *et al., Annalen*, 1958, **615**, 70-76 (*synth*)
Shu, C.K. *et al., J. Agric. Food Chem.*, 1988, **36**, 801-803 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 177 (*use*)

5-Ethyldihydro-2(3*H*)-furanone, 9CI E-295

[695-06-7]

4-Hexanolactone. 4-Caprolactone. 4-Ethylbutyrolactone. 4-Hydroxyhexanoic acid lactone. 4-Hexanolide. γ-Hexalactone. FEMA 2556



(*R*)-*form*

$C_6H_{10}O_2$ 114.144

▶ Skin irritant. LU4220000

(*R*)-*form* [63357-95-9]

$[\alpha]_D^{20}$ +53.2 (c, 1 in MeOH).

(*S*)-*form* [41035-07-8]

$[\alpha]_D^{20}$ -53.2 (c, 1 in MeOH).

(±)-*form* [57129-70-1]

Flavouring ingredient. Sol. aq. alkalis. Bp 215-216° $Bp_{0.2}$ 50-60° (bath).

(ξ)-*form*

Constit. of fruits, e.g. apple, raspberry, strawberry, wine grapes, quince etc. Also present in French fried potato, wheat bread, crispbread, butter, red or white wine and cooked beef.

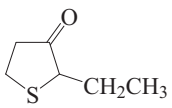
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1128C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 750C (*ir*)
Windaus, A. *et al., Ber.*, 1921, **54**, 586
Meyers, A.I. *et al., J.O.C.*, 1974, **39**, 2783
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 48
Ravid, U. *et al., Tetrahedron*, 1978, **34**, 1449
Fuganti, C. *et al., Tet. Lett.*, 1983, **24**, 3753 (*synth*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 919 (*synth*)
Högberg, H.-E. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 694 (*synth*)
Bestmann, H.J. *et al., Tet. Lett.*, 1987, **28**, 2111 (*synth*)
Yadav, J.S. *et al., Synth. Commun.*, 1989, **19**, 705 (*synth*)
Nuñez, M.T. *et al., J.O.C.*, 1990, **55**, 1928 (*synth, pmr, cmr, ms, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1292-1293 (*occur, props*)
Bertus, P. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 1369-1380 (*R-form, synth, pmr, cmr*)

2-Ethyldihydro-3(2*H*)-thiophenone, 9CI E-296

[52662-38-1]

[123698-30-6]

2-Ethyltetrahydrothiophen-3-one



$C_6H_{10}OS$ 130.21

Cysteine-derived Maillard product. Bp_1 73°.

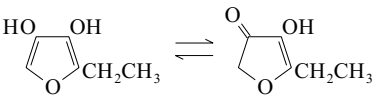
[76780-78-4]

Durden, J.A. *et al., J. Agric. Food Chem.*, 1974, **22**, 396-400 (*synth*)
Farmer, L.J. *et al., J. Sci. Food Agric.*, 1989, **49**, 347-368; 1990, **53**, 505-525 (*occur*)
Whitfield, F.B. *et al., J. Agric. Food Chem.*, 2001, **49**, 816-822 (*occur*)

2-Ethyl-3,4-dihydroxyfuran E-297

[27402-93-3]

5-Ethyl-4-hydroxy-3(2H)-furanone, 8CI. 2-Ethyl-3,4-furandiol



$C_6H_8O_3$ 128.127

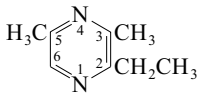
Flavour ingredient.

Ger. Pat., 1978, 2 812 713; *CA*, **90**, 38775 (*synth*)

2-Ethyl-3,5-dimethylpyrazine E-298

[13925-07-0]

FEMA 3150



$C_8H_{12}N_2$ 136.196
Isol. from coffee aroma. Also present in raw asparagus, wheat bread, other breads, smoked fatty fish, roast chicken, roast beef, lamb and mutton liver, black tea, hydrolyzed soy protein and other foods. Organoleptic agent. Flavouring agent. Bp_{19} 80-81° Bp_8 64-66°. n_D^{22} 1.4975.

▶ UQ3155000

Klein, B. *et al., J.A.C.S.*, 1951, **73**, 2949 (*synth*)
Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 968-969 (*use, occur*)

3-Ethyl-2,5-dimethylpyrazine E-299

[13360-65-1]

$C_8H_{12}N_2$ 136.196
Isol. from coffee. Constit. of numerous cooked foods. Organoleptic agent with nutty roasted odour. Bp_{11} 72-73°. n_D^{24} 1.4945.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694
Gelas, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1968, **266**, 625 (*synth, uv, ir, pmr*)
Ohta, A. *et al., Heterocycles*, 1987, **26**, 2449 (*synth*)
Buechi, G. *et al., J.O.C.*, 1991, **56**, 2605 (*synth*)

5-Ethyl-2,3-dimethylpyrazine E-300

[15707-34-3]

$C_8H_{12}N_2$ 136.196
Constit. of Galbanum oil. Liq. Bp_{14} 72°. n_D^{24} 1.4982.

Gelas, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1968, **266**, 625 (*synth*)
Rizzi, G.P. *et al., J.O.C.*, 1968, **33**, 1333 (*synth*)
Netherlands Pat., 1969, 68 121 899; *CA*, **71**, 61421 (*synth*)
Burrell, J.W.K. *et al., Chem. Ind. (London)*, 1970, 1409 (*isol*)
von Stralendorff, F. *et al., J. Chem. Ecol.*, 1987, **13**, 655

Ethylene, 8CI E-301

[74-85-1]
Ethene, 9CI. Elayl
$H_2C{=}CH_2$
C_2H_4 28.054
Occurs naturally in ripening fruit and is used artificially to accelerate fruit ripening, e.g in banana transportation. Colourless, odourless, flammable gas. V. sol. EtOH, Et_2O; sol. Me_2CO, C_6H_6; sl. sol. H_2O. Mp -169°. Bp -103.7° Bp_{50} 8.9° Bp_{10} -52.8°. Crit. point 9.5° (50.65 atm). Polymerises at high press. to give a range of solid polymers known as polythene, a saturated straight chain hydrocarbon of chain length about 1000, Mp *ca.* 115°. It has valuable mechanical and electrical properties, is highly resistant to H_2O, acids, and alkalis, and is insol. in cold org. solvs.; it dissolves in some hydrocarbon solvs. at higher temps. Radical polym. gives low-density polyethylene (LDPE); Ziegler-Natta polym. gives high-density polyethylene (HDPE). Rates for radical polym., k_p = 242 L mol^{-1} s^{-1}; k_t = 5.4 × 10^{-4} L mol^{-1} s^{-1} (83°); k_p 1800 L mol^{-1} s^{-1}, k_t = 5.8 × 10^{-4} L mol^{-1} s^{-1} (132°, 10^8 Pa). Q/e values for copolym., Q 0.016, e 0.05. Copolym. with vinyl chloride: r_E 0.21, r_{VC} 3.21 (typical values, 50°); Q 0.015; e -0.20.

▶ Extremely flammable, autoignition temp. 425°. Explosive reacn. with many materials. An asphyxiant. High conc. cause anaesthesia. KU5340000

[683-73-8, 1517-53-9, 2669-89-8, 2680-00-4, 2813-62-9, 6755-54-0, 9002-88-4, 34470-02-5]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 17C (*ir*)
Newth, G.S. *et al., J.C.S.*, 1901, **79**, 915 (*synth*)
Senderens, J.-B. *et al., Bull. Soc. Chim. Fr.*, 1911, **9**, 370 (*synth*)
Kesting, W. *et al., Angew. Chem.*, 1925, **38**, 362 (*synth*)
U.S. Pat., 1949, 2 476 474; *CA*, **43**, 8742g (*copolym, reactivity ratios*)
Richards, R.B. *et al., J. Appl. Chem.*, 1951, **1**, 370 (*polythene*)
Gattermann, L. *et al., Die Praxis des Organischen Chemikers*, De Gruyter and Co., Berlin, 1962, 41st Ed.; 98; *CA*, **60**, 382 (*rev*)
Rabel, W. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1963, **67**, 710 (*polym, kinetics*)
Miller, S.A. *et al., Ethylene Its Ind. Deriv.*, E. Benn, London, 1969,
Spencer, M. *et al., Prog. Chem. Org. Nat. Prod.*, 1969, **27**, 31 (*rev, biochem*)
IARC Monog., 1979, **19**, 157; *Suppl.* 7, 63 (*rev, tox*)
Wunder, F.G. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 126 (*synth*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Adlington, R.M. *et al., Chem. Comm.*, 1982, 1086 (*biosynth*)
Lim, P.C. *et al., Makromol. Chem.*, 1983, **184**, 207 (*polym, kinetics*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1986, **6**, 383; 522 (*rev, polym*)
de Reuck, K.M. *et al., Ethylene: IUPAC International Thermodynamic Tables of the Fluid State*, Blackwell, 1988, **10**, (*thermodyn*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **9**, 877 (*rev*)
Kieber, J.J. *et al., Trends Genet.*, 1993, **9**, 356 (*rev, biosynth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2439-2442 (*use*)
Stella, L. *et al., Bull. Soc. Chim. Fr.*, 1996, **133**, 441 (*rev, biosynth, biochem*)
Gibson, G.G. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 339 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0733
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 593
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EIO000

[Ethylenebis(dithiocarbamato)]manganese, 8CI E-302

[12427-38-2]
[1,2-Ethanediylbis[carbamodithioato](2-)]manganese(II), 9CI. Maneb, BSI, ISO. Dithiane M-22. Farmaneb. Manzate. MEB. Many other names
$[MnS_2CNHCH_2CH_2NHCS_2]_n$
$C_4H_6MnN_2S_4$ 265.307
Polymeric chain struct., geometry about Mn not known. Fungicide esp. for protection of potatoes and tomatoes. Yellow cryst., slow dec. on prolonged exp. to air, rapid dec. in acid. May be stabilised by presence of formaldehyde or various other compds. Insol. H_2O, common org. solvs. Mp 131° (dec.). Forms a dihydrate, adducts with NH_3 and dodecylamine.

▶ OP0700000

Kozlov, G.A. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 396 (*synth, ir, dihydrate*)
Kwoka, W. *et al., J. Inorg. Nucl. Chem.*, 1975, **37**, 1889 (*synth, magnetism, ir*)
Schmandke, H. *et al., CA*, 1985, **103**, 18079 (*tox*)
Gergely, S. *et al., Chem. Zvesti*, 1988, **42**, 229 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1990, **D7**, 180 (*rev, bibl*)
Pesticide Manual, 11th edn., 1997, 764-766
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAS500

Ethylenebisdithiocarbamic acid, 8CI E-303

[111-54-6]
1,2-Ethanediylbiscarbamodithioic acid, 9CI. Tetrathioethanedicarbamic acid
HSC(S)NHCH$_2$CH$_2$NHC(S)SH
$C_4H_8N_2S_4$ 212.385
Parent acid very unstable, not characterised.Dec. to CS_2 and ethylenethiourea.

▶ Salts are toxic.

Di-Na salt: [142-59-6] *Nabam, BSI, ISO. Parzate. Dithiane D-14. Nafun IPO*
$C_4H_6N_2Na_2S_4$ 256.348
Antimicrobial agent used in cane-sugar and beet sugar mills. Cryst. + $6H_2O$.

▶ LD_{50} (rat, orl) 395 mg/kg. Exp. reprod. and teratogenic effects. FA6825000

Di-NH_4 salt: [3566-10-7] *Ambis*
$C_4H_{14}N_4S_4$ 246.445

▶ LD_{50} (rat, orl) 395 mg/kg. BT6000000

Di-Me ester: [20721-48-6]
$C_6H_{12}N_2S_4$ 240.438
Light yellow needles (EtOH). Mp 105-107°.

▶ Forms an explosive dust.

Dibenzyl ester: [28249-26-5]
$C_{18}H_{20}N_2S_4$ 392.633
Cryst. (EtOH). Mp 114-116° (128-129°).

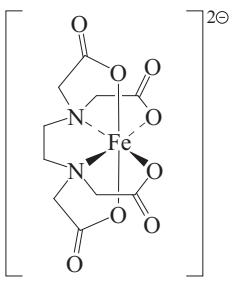
[6197-45-1, 10039-34-6]

Dimond, A.E. *et al., Phytopathology*, 1943, **33**, 1095 (*activity*)
Collins, A.P. *et al., J. Am. Pharm. Assoc.*, 1955, **44**, 310 (*synth, pharmacol*)
Kennard, K.C. *et al., J.O.C.*, 1959, **24**, 464 (*derivs*)
Dorsett, H.G. *et al., Bur. Mines Rep. Invest.*, No. 7132, 1968, (*haz*)
Wakamori, S. *et al., Agric. Biol. Chem.*, 1969, **33**, 1367 (*ester, synth, use*)
Engst, R. *et al., Nahrung*, 1971, **15**, 815 (*rev, bibl, metab*)
Yamamoto, D. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1980, **29**, 396 (*detn, Ni*)
Yokoyama, M. *et al., Synthesis*, 1981, 908 (*Di-Me ester*)

Clyde, D.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 646 (*Nabam, synth, detn*)
Mak, T.C.W. *et al., Can. J. Chem.*, 1984, **62**, 808 (*Nabam, synth, cryst struct, pmr, cmr*)
Vrabel, V. *et al., Acta Cryst. C*, 1987, **43**, 2293 (*Nabam, cryst struct*)
Dangerous Prop. Ind. Mater. Rep., 1987, **7**, 44 (*Nabam, rev, tox*)
Katritzky, A.R. *et al., J. Polym. Sci., Part A: Polym. Chem.*, 1987, **25**, 3205 (*synth*)
Pesticide Manual, 9th edn., 1991, No. 8740
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 891-892 (*di-Na salt*)
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1436 (*dithiocarbamates, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANZ000; DXD200

(Ethylenediaminetetraacetato)ferrate(*II*)(2-) E-304

[15651-72-6]
*[[*N,N′*-1,2-Ethanediylbis[*N*-(carboxymethyl)glycinato]](4-)*-N,N′,O,O′,O^N,$O^{N'}$*]ferrate(2-), 9CI. [(Ethylenedinitrilo)tetraacetato]ferrate(2-)*



$C_{10}H_{12}FeN_2O_8^{\ominus}$ 344.06

Di-H compd: [21393-59-9]
$C_{10}H_{14}FeN_2O_8$ 346.076
Solid not isol.; stable for up to 6 h as aq. soln.

Di-Na salt: [14729-89-6] *Sodium iron versenate*
$C_{10}H_{12}FeN_2Na_2O_8$ 390.04
Listed in the EAFUS Food Additive Database (Jan 2001) but with no reported use. Cryst.

Polish Pat., 1982, 115 918; *CA*, **99**, 73116w (*manuf*)
Zang, V. *et al., Inorg. Chem.*, 1988, **27**, 3279 (*synth*)

Ethylenediaminetetraacetic acid E-305

[60-00-4]
N,N′*-1,2-Ethanediylbis[*N*-(carboxymethyl)]glycine, 9CI. Ethylenedinitrilotetraacetic acid, 8CI. EDTA. **Edetic acid, BAN, INN**. 3,6-Bis(carboxymethyl)-3,6-diazaoctanedioic acid. Versene acid. Sequestrene. Tetracemin. Complexone III. Versene. Clewat TAA. YD 30. Edathamil. Gluma Cleanser*

$(HOOCCH_2)_2NCH_2CH_2N(CH_2COOH)_2$
$C_{10}H_{16}N_2O_8$ 292.245
Dimorphic cryst. (H_2O). Prac. insol. H_2O; insol. common org. solvs. Mp 220° dec. pK_{a1} 0.26; pK_{a2} 0.96; pK_{a3} 2.02; pK_{a4} 2.66; pK_{a5} 6.21; pK_{a6} 10.31 (20°, 0.1*M* KNO_3). Log P -1.97 (calc). Starts to decarboxylate above 150°. Stable in boiling H_2O.

▶ LD_{50} (rat, ipr) 397 mg/kg. Exp. reprod. and teratogenic effects (large doses). AH4025000

Di-Na salt:

[139-33-3, 6381-92-6, 7379-28-4] ***Edetate disodium, USAN**. Disodium edetate, BAN. Chelaplex. Chelaplex III. Chelaton III. Chelest B*
$C_{10}H_{14}N_2Na_2O_8$ 336.209
Preservative and sequestrant in foods. Cryst. + $2H_2O$. Mp 252° dec. (dihydrate).

▶ LD_{50} (rat, orl) 2000 mg/kg. AH4375000

Tri-Na salt: [150-38-9]

[7379-28-4] ***Edetate trisodium, USAN**. Trisodium edetate. Limclair. Sequestrene NA 3. Versene 9. Clewat 300A*
$C_{10}H_{13}N_2Na_3O_8$ 358.191
Preservative. Cryst. + $1H_2O$ (H_2O). Mp 300° (monohydrate).

▶ LD_{50} (rat, orl) 2150 mg/kg. AH5275000

Tetra-Na salt: [64-02-8]

[7379-28-4, 13235-36-4] ***Edetate sodium, USAN**. Complexone II. Trilon B. Kutrilon CS. Celon E. Celon H. Tetralon A. Hampene 100*
$C_{10}H_{12}N_2Na_4O_8$ 380.173
Chelating agent used in food processing. Amorph. powder + $2H_2O$. Mp 300° (dihydrate).

▶ Skin and eye irritant. LD_{50} (mus, ipr) 330 mg/kg. AH5075000

Di-Na mono-Ca salt: [62-33-9]

[74011-06-6] ***Sodium calcium edetate, BAN, INN**. Edetate calcium disodium, USAN. Edathamil calcium disodium. Calcium disodium versenate. Mosatil. Antallin. Ledclair. Many other names. E385*
$C_{10}H_{12}CaN_2Na_2O_8$ 374.271
Preservative and sequestrant in foods. Powder. Forms a tetrahydrate.

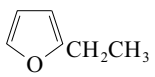
▶ Nephrotoxic and other adverse effects reported when used therapeutically. LD_{50} (rat, orl) 10000 mg/kg. EV7700000

[7379-26-2, 10378-23-1, 17572-97-3, 20824-56-0, 23411-34-9, 25102-12-9, 58167-76-3, 85715-60-2]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 484C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 567A (*ir*)
Smith, R. *et al., J.O.C.*, 1949, **14**, 355 (*synth*)
Biermans, J. *et al., Ind. Chim. (Rome)*, 1952, **39**, 6 (*rev, bibl*)
Přibil, R. *et al., Analytical Applications of EDTA and Related Compounds*, Pergamon Press, Oxford, 1972, (*use*)
Ladd, M.F.C. *et al., Acta Cryst. B*, 1973, **29**, 2973 (*cryst struct*)
Baisden, P.A. *et al., Inorg. Chem.*, 1977, **16**, 1367 (*pmr*)
Nuttall, R.H. *et al., J.C.S. Dalton*, 1977, 1884 (*Raman*)
Halstead, B.W. *et al., The Scientific Basis of EDTA Therapy*, Golden Quill Publ. Colton, Calif., 1979, (*book*)
Aime, S. *et al., Inorg. Chim. Acta*, 1987, **129**, L23 (*cmr*)
Gonzalez Vilchez, F. *et al., Spectrochim. Acta A*, 1987, **43**, 1039 (*ir, Raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 1607D (*haz*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EIV000; EIX500
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 176-179
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 981; 982
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 913-916; 916-920; 920-922
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EIV000; EIX000; EJB000; TNL250; EIX500

2-Ethylfuran E-306

[3208-16-0]
FEMA 3673



C_6H_8O 96.129
Constit. of numerous plant spp. and cooked foods e.g. chicken, beef, pork liver, coffee, tea, roasted filbert, soybean, rice, oats etc. Flavouring ingredient. Liq. with coffee-like flavour/odour on dilution. Bp 95° (91.5-92°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 580C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 14C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1450D (*ir*)
Shuikin, N.I. *et al., Chem. Ber.*, 1958, **91**, 948 (*synth*)
Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)
Camus, F. *et al., Synth. Commun.*, 1982, **12**, 647 (*synth*)
Huntsman, W.D. *et al., J.O.C.*, 1983, **48**, 3813 (*synth*)
Cormier, R.A. *et al., Synth. Commun.*, 1988, **18**, 677 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 984 (*occur, props*)

3-Ethylfuran E-307

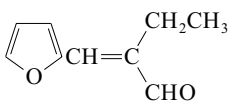
[67363-95-5]

C_6H_8O 96.129
Constit. of carob (*Ceratonia siliqua*) and coffee. Liq. Bp 92°.

Wiley, R.A. *et al., J.O.C.*, 1983, **48**, 1106 (*synth*)
MacLeod, G. *et al., Phytochemistry*, 1992, **31**, 3113 (*occur*)

2-Ethyl-4-(2-furanyl)-2-propenal E-308

[770-27-4]
α-Ethyl-β-2-furylacrolein. 2-Furfurylidenebutyraldehyde. FEMA 2492



$C_9H_{10}O_2$ 150.177

Synthetic flavouring ingredient. Bp 240°.

Thiosemicarbazone:
$C_{10}H_{13}N_3OS$ 223.298
Cryst. (EtOH). Mp 206-207°. pK_{a1} 0.92; pK_{a2} 11.85.

Kerentseva, V.P. *et al., Zh. Anal. Khim.*, 1971, **26**, 1144; 1972, **27**, 719 (*synth, pKa, detn, Pd, Pt*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 640 (*use, props*)

2-Ethylheptanoic acid E-309

[3274-29-1]
$H_3C(CH_2)_4CH(CH_2CH_3)COOH$
$C_9H_{18}O_2$ 158.24

(±)-*form*
Bp_{31} 153°. n_D^{27} 1.4255.

Me ester: [816-63-7]
$C_{10}H_{20}O_2$ 172.267
Bp 157° Bp_{45} 108°.

(ξ)-*form*
Constit. of starfruit (*Averrhoa carambola*).

[36414-42-3, 59415-02-0]

Royals, E.E. *et al., J.A.C.S.*, 1955, **77**, 3155 (*synth*)
Trent, F.M. *et al., J. Chem. Eng. Data*, 1960, **5**, 110
Zheng, Y. *et al., Zhiwu Xuebao*, 1989, **31**, 69 (*isol*)
MacLeod, G. *et al., Phytochemistry*, 1990, **29**, 165 (*isol*)

2-Ethyl-2-heptenal, 8CI E-310

[10031-88-6]

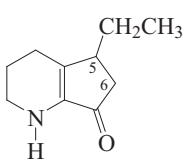
[34210-19-0]
FEMA 2438

$H_3C(CH_2)_3CH{=}C(CHO)CH_2CH_3$
$C_9H_{16}O$ 140.225
Flavouring ingredient. Present in walnut peel and ambarella fruits *Spondias cytherea*. Misnamed as 2-ethyl-2-hepten-1-ol by Bhalerao *et al*.

Bhalerao, U.T. *et al., J.A.C.S.*, 1971, **93**, 4835-4840 (*synth, pmr*)
Duhamel, L. *et al., Tet. Lett.*, 1993, **34**, 7745-7748 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 235 (*use*)
Jirovetz, L. *et al., Ernaehrungsforschung*, 1996, **20**, 286-287; *CA*, **125**, 113132n (*detn, walnut peel*)
Jirovetz, L. *et al., Z. Lebensm.-Unters. -Forsch.*, 1999, **208**, 74-76 (*detn, ambarella*)

5-Ethyl-1,2,3,4,5,6-hexahydro-7*H*-cyclopenta[*b*]pyridin-7-one, 13CI E-311

[104704-37-2]
*5-Ethyl-1,2,3,4,5,6-hexahydro-7*H*-1-pyrindin-7-one, 12CI*



$C_{10}H_{15}NO$ 165.235
Proline-derived Maillard product. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*isol, ir, ms, pmr*)

6-Ethyl-1,2,3,4,5,6-hexahydro-7*H*-cyclopenta[*b*]pyridin-7-one, 13CI E-312

[118355-69-4]
*6-Ethyl-1,2,3,4,5,6-hexahydro-7*H*-1-pyrindin-7-one, 12CI*

$C_{10}H_{15}NO$ 165.235
Proline-derived Maillard product. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*isol, ir, ms, pmr*)
Chen, C.W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

2-Ethyl-1-hexanethiol, 9CI E-313

[7341-17-5]
2-(Mercaptomethyl)heptane. FEMA 3833
$H_3CCH_2CH_2CH_2CH(CH_2CH_3)CH_2SH$
$C_8H_{18}S$ 146.296

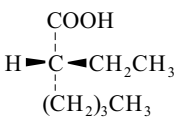
(±)-*form*
Food flavouring. Liq. d^{25} 0.85. Bp_{19} 80°. n_D^{25} 1.4541.

[110502-32-4]

U.K. Pat., 1946, 574 936; *CA*, **43**, 2630b (*synth*)
Farlow, M.W. *et al., Ind. Eng. Chem.*, 1950, **42**, 2547 (*synth*)
Levy, E.J. *et al., Anal. Chem.*, 1961, **33**, 707 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 545

2-Ethylhexanoic acid, 9CI E-314

2-Ethylcaproic acid. 3-Heptanecarboxylic acid



(*R*)-*form*

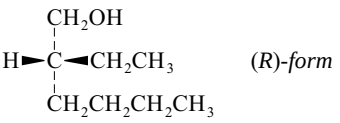
$C_8H_{16}O_2$ 144.213
Found in grapes.

[136-51-6, 136-52-7, 136-53-8, 2457-01-4, 2983-37-1, 3164-85-0, 3444-17-5, 13586-82-8, 19766-89-3]

Dolique, R. *et al., Ann. Chim. (Paris)*, 1931, **15**, 425 (*synth*)
Levene, P.A. *et al., J. Biol. Chem.*, 1936, **115**, 401 (*synth*)
Creger, P.L. *et al., J.A.C.S.*, 1970, **92**, 1397 (*synth*)
Grinevich, I.A. *et al., Zh. Org. Khim.*, 1976, **12**, 1655 (*synth*)
Miyazaki, S. *et al., J. Am. Oil Chem. Soc.*, 1978, **95**, 536 (*synth*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)

2-Ethyl-1-hexanol, 9CI E-315

[104-76-7]



(*R*)-*form*

$C_8H_{18}O$ 130.23
► Skin and eye irritant. LD_{50} (rat, orl) *ca.* 2000 mg/kg. Exp. reprod. and teratogenic effects. MP0350000

(*R*)-*form* [50373-29-0]
Liq. Bp_{55} 110°. $[\alpha]_D^{24}$ -0.22 (neat).

Ac: [50373-28-9]
$C_{10}H_{20}O_2$ 172.267
$[\alpha]_D^{24}$ +0.26 (neat).

(*S*)-*form* [128821-84-1]
Liq. Bp_{22} 92-94°. $[\alpha]_D^{20}$ +2.57 (C_6H_6).

(±)-*form* *FEMA 3151*
Flavouring ingredient. Liq. V. spar. sol. H_2O; misc. EtOH, Me_2CO, Et_2O. Bp_{15} 84-86°, 182-185°.
► Mod. toxic. MP0350000

Ac: [103-09-3]
Liq. Bp_{25} 95°.
► Skin and eye irritant. LD_{50} (rat, orl) 3000 mg/kg. AH5600000

O-*Nitrate:* [27247-96-7]
$C_8H_{17}NO_3$ 175.227
d 0.96. n_D^{20} 1.4320.

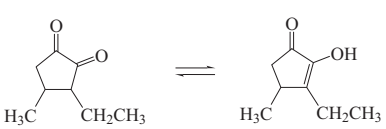
O-*Sulfate:* [126-92-1]
$C_8H_{18}O_4S$ 210.294CAS no. refers to Na salt. Props. not well documented.

(ξ)-*form*
Occurs in corn, olive oil, tobacco, tea, rice, tamarind, grapes, blueberries etc.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 117B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 174A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 164D (*ir*)
Weizmann, C. *et al., J.C.S.*, 1920, **117**, 324 (*synth*)
Levene, P.A. *et al., J. Biol. Chem.*, 1922, **54**, 351 (*synth*)
Orlandini, K.A. *et al., Anal. Chem.*, 1965, **37**, 1149 (*use*)
Wudl, F. *et al., J.A.C.S.*, 1971, **93**, 271-273 (*nitrate, synth*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 1923 (*resoln*)
Austin, G.T. *et al., Chem. Eng. (N.Y.)*, 1974, **81**, 143; 148; 150 (*rev manuf*)
Kito, T. *et al., CA*, 1978, **89**, 107947 (*synth*)
Lyon, P.A. *et al., Anal. Chem.*, 1984, **56**, 8-13 (*O-sulfate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EKQ000; OEE000

3-Ethyl-2-hydroxy-4-methyl-2-cyclopenten-1-one, 9CI E-316

[42348-12-9]
3-Ethyl-4-methyl-1,2-cyclopentanedione. FEMA 3453

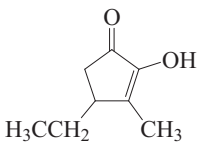


$C_8H_{12}O_2$ 140.182
Flavouring agent. $Bp_{0.06}$ 65°.

Maignan, C. *et al., Bull. Soc. Chim. Fr.*, 1973, 1454-1456 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 239 (*use*)

4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one E-317

[71387-71-8]



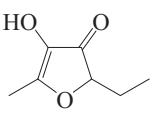
$C_8H_{12}O_2$ 140.182
Volatile constit. of roasted Arabica coffee beans and heated invert sugar solutions with sweet malty odour. Characterised spectroscopically.

Ito, H. *et al., Nippon Shokuhin Kogyo Gakkaishi*, 1978, **25**, 549-555; *CA*, **91**, 122355u (*occur, sugar*)
Arnarp, J. *et al., Acta Chem. Scand., Ser. B*, 1986, 839-854 (*synth, pmr*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*occur, ms, coffee*)

2-Ethyl-4-hydroxy-5-methyl-3(2*H*)-furanone, 9CI E-318

[27538-10-9]

[27538-09-6, 110516-60-4, 131222-79-2, 131222-80-5]
Homofureanol. *HEMF*



$C_7H_{10}O_3$ 142.154
Volatile flavour and aroma component of Japanese style soya sauce (shoyu) and fermented soya bean paste (miso). Antioxidant. Isol. from *Theobroma grandiforum* (cupuassu). Liq. with intense sweet odour and cooked fruit flavour. $Bp_{0.3}$ 85-90°.

Re, L. *et al., Helv. Chim. Acta*, 1973, **56**, 1882-1894 (*synth*)
Nonomura, N. *et al., Agric. Biol. Chem.*, 1976, **40**, 491-495 (*uv, ms, pmr, glc, detn in Shoyu*)
Wong, C.-H. *et al., J.O.C.*, 1983, **48**, 3493-3497 (*synth, pmr*)
Mosandl, A. *et al., J. High Resol. Chromatogr.*, 1990, **13**, 660-662 (*glc, hplc*)
Huber, U.A. *et al., Perfum. Flavor.*, 1992, **17**, 15-19 (*rev*)
Sugawara, E. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1134-1135 (*occur, miso*)

5-Ethyl-3-hydroxy-4-methyl-2(5*H*)-furanone, 9CI E-319

[698-10-2]
2,4-Dihydroxy-3-methyl-2-hexenoic acid γ-lactone. 5-Ethyl-4-methylisotetronic acid. Abhexone. 5-Ethylsotolone. FEMA 3153

$C_7H_{10}O_3$ 142.154
Prod. in protein hydrolysates. Hygroscopic yellow oil with intense odour of lovage.

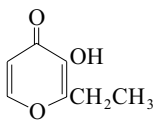
(±)-form
Flavouring for foodstuffs. Mp 21°. $Bp_{0.2}$ 92-94° $Bp_{0.003}$ 70-71°.

Ac:
$C_9H_{12}O_4$ 184.191
$Bp_{0.05}$ 90-92°.

Monnin, J. *et al., Helv. Chim. Acta*, 1957, **40**, 1983 (*synth*)
Sakan, T. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 1171 (*uv, ir*)
Ger. Pat., 1970, 1 955 390; *CA*, **73**, 77034 (*synth, use*)
Bonini, C.C. *et al., Org. Mass Spectrom.*, 1980, **15**, 516 (*ms*)
Stach, H. *et al., Helv. Chim. Acta*, 1987, **70**, 369 (*synth, ir, pmr, cmr, bibl*)

2-Ethyl-3-hydroxy-4*H*-pyran-4-one, 9CI E-320

[4940-11-8]
Ethyl maltol. Veltol plus. E637. FEMA 3487



$C_7H_8O_3$ 140.138
Flavour enhancer and flavouring agent, sweetener, 4-6 x potency of 3-Hydroxy-2-methyl-4*H*-pyran-4-one, H-609. Cryst. with sweet, fruity taste and caramel-like odour. Mp 90-91°. 3 Polymorphs known.
► LD_{50} (rat, orl) 1150 mg/kg. UQ0840000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 724B (*nmr*)
Aoyagi, N. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1008 (*isol, pharmacol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, (Suppl.), 1975, **13**, 805 (*tox, rev*)
Torii, S. *et al., Chem. Lett.*, 1976, 495 (*synth*)
Suzuki, R. *et al., Heterocycles*, 1977, **6**, 1575 (*synth*)
Brennan, T.M. *et al., Tet. Lett.*, 1978, 331 (*synth*)
Levey, J.A. *et al., Biochem. Pharmacol.*, 1988, **37**, 2051 (*pharmacol*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EMA600
Georgiadis, M. *et al., Org. Prep. Proced. Int.*, 1992, **24**, 95 (*synth*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 180-181
Brown, S.D. *et al., Acta Cryst. C*, 1995, **51**, 1335 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EMA600

2-Ethyl-3-hydroxypyrazine E-321

[25680-54-0]
3-Ethyl-2(1H)-pyrazinone, 9CI. 3-Ethylpyrazinol, 8CI



$C_6H_8N_2O$ 124.142
Mp 105°.

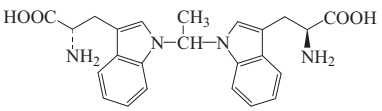
OH-form

Me ether: [25680-58-4] *3-Ethyl-2-methoxypyrazine*
$C_7H_{10}N_2O$ 138.169
Constit. of potato and wine must. Flavour enhancer for dehydrated potato. Component of FEMA 3280. Bp_{20} 95-98°. FEMA 3280 is an isomeric mixt. of ethylmethoxypyrazines and methylmethoxypyrazines.

U.S. Pat., 1973, 3 772 039; *CA*, **80**, 58618a (*synth, Me ether, use*)
Nursten, H.E. *et al., J. Sci. Food Agric.*, 1974, **25**, 643-663 (*Me ether, occur, ms*)
Sala, C. *et al., J. Chromatogr., A*, 2000, **880**, 93-99 (*Me ether, occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 563-564 (*FEMA 3280*)

1,1′-Ethylidenebistryptophan, 9CI E-322

[132685-02-0]
1,1-Di-1-tryptophylethane. Peak E. Peak 97. EBT

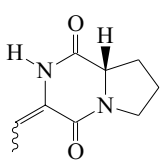


$C_{24}H_{26}N_4O_4$ 434.494
Impurity in synthetic L-tryptophan, linked to an outbreak of fatal eosinophilia myalgia syndrome in 1989 associated with dietary supplements containing tryptophan. Amorph. powder.

Mayeno, A.N. *et al., Science (Washington, D.C.)*, 1990, **250**, 1707-1708 (*isol, struct, pmr, ms*)
Smith, M.J. *et al., Tet. Lett.*, 1991, **32**, 991-994 (*synth, nmr, struct*)
Fu, T.J. *et al., J. Agric. Food Chem.*, 1996, **44**, 1224-1229 (*occur, bibl*)
Williamson, B.L. *et al., Toxicol. Lett.*, 1997, **92**, 139-148 (*detn*)

3-Ethylidenehexahydropyrrolo[1,2-*a*]pyrazine-1,4-dione, 9CI E-323

1,6-Propano-3-ethylidene-1,4-piperazine-2,5-dione



$C_9H_{12}N_2O_2$ 180.206

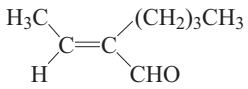
(S)-form [160706-82-1]
Isol. from cultured cells of *Aspidosperma quebracho-blanco* (quebracho). Amorph. powder.

Aimi, N. *et al., Heterocycles*, 1994, **38**, 2411 (*isol, pmr, cmr, struct*)

2-Ethylidenehexanal, 9CI, 8CI E-324

[25409-08-9]

2-Butyl-2-butenal. FEMA 3392



(*E*)-*form*

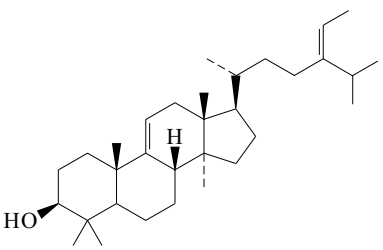
$C_8H_{14}O$ 126.198
Flavouring ingredient, imparting sweet nutty flavour. d_4^{20} 1.45. n_D^{20} 1.4540. Stereochemistry unspecified by FEMA.

2,4-Dinitrophenylhydrazone:
Mp 162°.

(*E*)-*form* [87745-65-1]
Bp_{16} 69°.

Gelin, R. *et al., Bull. Soc. Chim. Fr.*, 1972, 720-723 (*synth*)
U.S. Pat., 1975, 3 914 451; *CA*, **84**, 42231r (*synth, use*)
Barbot, F. *et al., Synthesis*, 1983, 651-654 (*E-form, synth, pmr*)

24-Ethylidenelanost-9(11)-en-3-ol E-325

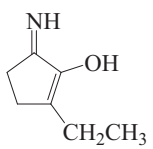


$C_{32}H_{54}O$ 454.778
(3β,24(24[1])*Z*)-*form* [155062-80-9]
Constit. of *Pisum sativum* (pea) seeds.

Akihisa, T. *et al., Phytochemistry*, 1994, **35**, 1309 (*isol, pmr, ms*)

2-Ethyl-5-imino-1-cyclopenten-1-ol, 9CI E-326

[90554-84-0]
3-Ethyl-2-hydroxy-2-cyclopentenimine



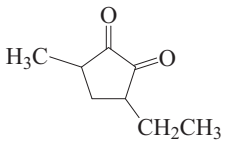
$C_7H_{11}NO$ 125.17
Maillard product, formed in model roast meat aroma systems. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*isol, ms, pmr, ir*)
Reese, G. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **194**, 417-421 (*formn, ms*)

3-Ethyl-5-methyl-1,2-cyclopentanedione E-327

[53263-58-4]

[58228-72-1]
5-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one, 9CI. 3-Ethyl-2-hydroxy-5-methyl-2-cyclopenten-1-one. FEMA 3454

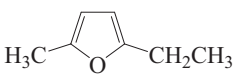


$C_8H_{12}O_2$ 140.182
Enolised α-diketone, obtained as a mixt of enol. tautomers. Present in roast Arabica coffeee bean volatiles. Flavouring agent.

Naoshima, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1393-1397 (*synth*)
Arnarp, J. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 839-854 (*synth, pmr, occur, tobacco*)
Niemola, K. *et al., Carbohydr. Res.*, 1988, **184**, 131-137 (*occur, kraft liquors*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*isol, coffee*)
U.S. Pat., 1990, 4 892 966; *CA*, **113**, 23189j (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 239 (*use*)

2-Ethyl-5-methylfuran E-328

[1703-52-2]

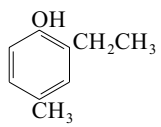


$C_7H_{10}O$ 110.155
Maillard product. Oil. d_4^{20} 0.89. Bp 118-119°. n_D^{20} 1.4473.

Fittig, R. *et al., Annalen*, 1889, **250**, 210 (*synth*)
Morizur, J.P. *et al., Bull. Soc. Chim. Fr.*, 1966, 2296 (*nmr*)

2-Ethyl-4-methylphenol E-329

[3855-26-3]
2-Ethyl-p-*cresol, 8CI*



$C_9H_{12}O$ 136.193
Constit. of coffee and hops. Bp 215-221° Bp_{50} 134° Bp_{10} 100°.

Phenylurethane:
Mp 101°.

Niederl, J.B. *et al., J.A.C.S.*, 1937, **59**, 1113 (*synth*)
Ungnade, H.E. *et al., J.A.C.S.*, 1944, **66**, 118 (*synth*)
Stroh, R. *et al., Angew. Chem.*, 1957, **69**, 699 (*synth*)
Kraus, M. *et al., Coll. Czech. Chem. Comm.*, 1963, **28**, 1877 (*synth*)
Givens, E.N. *et al., J. Chem. Eng. Data*, 1969, **14**, 392 (*synth, pmr, ms*)
Nishinaga, A. *et al., Tetrahedron*, 1979, **35**, 2493 (*synth*)
Fischer, A. *et al., Can. J. Chem.*, 1981, **59**, 2314 (*synth*)
Arnarp, R.E. *et al., Acta Chem. Scand.*, 1991, **45**, 529 (*isol, ms*)

2-Ethyl-5-methylphenol E-330

[1687-61-2]
6-Ethyl-m-*cresol, 8CI*

$C_9H_{12}O$ 136.193
Constit. of *Angelica* spp. Metab. of *Penicillium* spp. on barley. Cryst. Mp 42-44° (41-42°). Bp_{50} 134°.

▶ GP1100000

Phenylurethane:
Mp 154°.

Stroh, R. *et al., Angew. Chem.*, 1957, **69**, 699 (*synth*)
Clemens, A.H. *et al., Aust. J. Chem.*, 1977, **30**, 103 (*synth*)
Fischer, A. *et al., Aust. J. Chem.*, 1978, **31**, 1241 (*synth*)
Wilkins, C.K. *et al., Int. J. Food Microbiol.*, 1989, **8**, 11 (*occur*)
Arnarp, J. *et al., Acta Chem. Scand.*, 1991, **45**, 529 (*isol, ms*)

3-Ethyl-4-methylphenol E-331

[6161-67-7]
3-Ethyl-p-*cresol, 8CI*

$C_9H_{12}O$ 136.193
Constit. of wild rice grains (*Zizania aquatica*). Needles (petrol). Mp 35-36° (33-34°). Bp_4 100-101°.

3,5-Dinitrobenzoyl:
Mp 110°.

Newman, M.S. *et al., J.O.C.*, 1963, **28**, 2804 (*synth*)
Marx, J.N. *et al., J.A.C.S.*, 1974, **96**, 2121 (*synth*)
Pilkington, J.W. *et al., J.C.S. Perkin 2*, 1976, 1349 (*synth, pmr*)
Withycombe, D.A. *et al., J. Agric. Food Chem.*, 1978, **26**, 816 (*occur*)
Gesson, J.-P. *et al., Tetrahedron*, 1978, **34**, 1715 (*synth*)
Pons, A. *et al., Bull. Soc. Chim. Fr.*, 1979, 381 (*synth*)
Arnarp, R.E. *et al., Acta Chem. Scand.*, 1991, **45**, 529 (*occur, ms*)

3-Ethyl-5-methylphenol E-332

[698-71-5]
5-Ethyl-m-*cresol, 8CI*

$C_9H_{12}O$ 136.193
Isol. from grains of wild rice (*Zizania aquatica*). Mp 54° (50-51°). Bp 233° Bp_{20} 130°.

4-Nitrobenzoyl:
Mp 84°.

Kovavic, P. *et al., J.O.C.*, 1967, **32**, 585 (*synth*)
Sellier, N. *et al., Appl. Spectrosc.*, 1974, **28**, 60 (*ms*)
House, H.O. *et al., J.O.C.*, 1978, **43**, 3653 (*synth, bibl*)
Rajoharison, H.G. *et al., Synth. Commun.*, 1980, **10**, 195 (*synth*)
Arnarp, R.E. *et al., Acta Chem. Scand.*, 1991, **45**, 529 (*isol, ms*)

4-Ethyl-2-methylphenol E-333

[2219-73-0]
4-Ethyl-o-*cresol, 8CI*

$C_9H_{12}O$ 136.193
Constit. of coffee. Bp 222° Bp_{12} 110°.

4-Nitrobenzoyl:
Pale yellow leaflets (EtOH). Mp 70°.

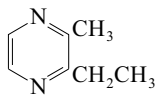
Phenylurethane:

Needles (EtOH). Mp 104°.

Kruber, O. *et al., Chem. Ber.*, 1948, **81**, 221 (*synth*)
Kraus, M. *et al., Coll. Czech. Chem. Comm.*, 1963, **28**, 1877 (*synth*)
Ansell, M.F. *et al., J.C.S.(C)*, 1971, 1401 (*synth*)
Fischer, A. *et al., Can. J. Chem.*, 1981, **59**, 2314 (*synth*)
Arnarp, R.E. *et al., Acta Chem. Scand.*, 1991, **45**, 529 (*isol, ms*)

2-Ethyl-3-methylpyrazine, 9CI E-334

[15707-23-0]
FEMA 3155



$C_7H_{10}N_2$ 122.169
Flavour component in cooked foods, e.g. baked potato, wheat bread, boiled egg, roast chicken, cooked beef, cooked pork, roasted barley, roasted sesame seed. Flavouring ingredient. Bp_{10} 57°. n_D^{20} 1.5030. Odour threshold 130 ppb in H_2O.

Flament, I. *et al., Helv. Chim. Acta*, 1967, **50**, 1754 (*synth*)
Rizzi, G.P. *et al., J.O.C.*, 1968, **33**, 1333 (*synth*)
Heynes, K. *et al., Chem. Ber.*, 1981, **114**, 240 (*synth*)
Schwaiger, W. *et al., Food Chem.*, 1984, **13**, 225 (*synth, uv*)
Roberts, J.D. *et al., Org. Magn. Reson.*, 1984, **22**, 201 (*N-15 nmr*)
Kuo, M. *et al., J. Agric. Food Chem.*, 1989, **37**, 1020 (*anal, glc*)
Liu, S.-Y. *et al., Life Sci.*, 1994, **55**, 1317 (*pharmacol*)

2-Ethyl-5-methylpyrazine, 9CI, 8CI E-335

[13360-64-0]
FEMA 3154
Found in roast peanuts, roast filberts, cooked beef, cooked lamb, wheat bread, bakesd or fried potato, coffee beans, cocoa butter, roast barley and other foodstuffs. Used in food flavouring. Bp_{56} 79-80°. n_D^{25} 1.4925. Odour threshold 100 ppb in H_2O.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694
U.S. Pat., 1976, 3 952 026; *CA*, **71**, 90131m (*manuf, uses*)
Shibamoto, T. *et al., J. Agric. Food Chem.*, 1979, **27**, 1027 (*formn*)
Milic, B.L. *et al., Food Chem.*, 1984, **13**, 165 (*gc*)

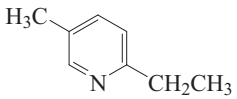
2-Ethyl-6-methylpyrazine, 9CI, 8CI E-336

[13925-03-6]
FEMA 3919
Found in roast peanuts, coffee beans, barley and cocoa butter. Flavouring agent for baked goods, confectionery and meat products. Bp_{11} 57-63°.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694 (*synth*)
Riezebos, G. *et al., J.C.S.*, 1971, 1627
U.S. Pat., 1976, 3 952 026; *CA*, **71**, 90131m (*manuf, uses*)
Shibamoto, T. *et al., J. Agric. Food Chem.*, 1979, **27**, 1027 (*formn*)
Milic, B.L. *et al., Food Chem.*, 1984, **13**, 165 (*gc*)

2-Ethyl-5-methylpyridine E-337

[18113-81-0]
6-Ethyl-3-picoline



$C_8H_{11}N$ 121.182
Constit. of coffee aroma and cooked shrimp (*Parapenaeus fissurus*). Maillard product. Bp 171-174° Bp_{10} 62-63°.

Picrate: [18113-82-1]
Cryst. (Me_2CO). Mp 144°.

Kazanskii, B.A. *et al., Zh. Org. Khim.*, 1970, **6**, 2203-2206; *J. Org. Chem. USSR (Engl. Transl.)*, 1970, **6**, 2212-2215 (*synth*)
Kutney, J.P. *et al., Can. J. Chem.*, 1975, **53**, 1796-1817 (*synth, ir, uv, pmr*)
Baltes, W. *et al., J. Agric. Food Chem.*, 1987, **35**, 340-346 (*occur, ms, coffee*)
Chye, S.C. *et al., CA*, 1988, **110**, 211196w (*occur, shrimp*)

5-Ethyl-2-methylpyridine E-338

[104-90-5]
5-Ethyl-α-picoline. Aldehydecollidine. FEMA 3546

$C_8H_{11}N$ 121.182
Present in dry red beans, cocoa, tea and whisky. Flavouring agent. Liq. Part misc. H_2O. d^0 0.94. Bp 178.3°. n_D^{20} 1.4978. pK_a 6.51 (20°). Steam-volatile.

► Violent reacn. with HNO_3. Severe skin and eye irritant. LD_{50} (rat, orl) 368 mg/kg; LD_{50} (rbt, skn) 1000 mg/kg. TJ6825000

Picrate:
Yellow plates or needles (H_2O or EtOH aq.). Mp 164-165°.

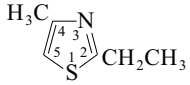
N-*Oxide:* [768-44-5]
$C_8H_{11}NO$ 137.181

► Mod. toxic, skin irritant. TJ7000000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 742D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 256A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1523A (*ir*)
Org. Synth., Coll. Vol., 4, 1963, 451 (*bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 253
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1015-1016
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2801
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EOS000

2-Ethyl-4-methylthiazole E-339

[15679-12-6]
FEMA 3680



C_6H_9NS 127.21
Organoleptic, occurring mainly in coffee aroma, also cooked uncured pork and fennel. Flavouring agent. Liq. d_4^4 1.03. $Bp_{728.5}$ 160.6-161°. n_D^{20} 1.5059.

Benbadjamian, A. *et al., Bull. Soc. Chim. Fr.*, 1968, 4878 (*synth, pmr, ir, uv*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210 (*isol*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511 (*ms*)

4-Ethyl-2-methylthiazole E-340

[32272-48-3]

C_6H_9NS 127.21
Organoleptic, present mainly in coffee aroma and cooked meat. Liq. Bp_{719} 169-171°.

Picrate:
Mp 114-115°.

Roussel, C. *et al., Bull. Soc. Chim. Fr.*, 1971, 1087 (*synth*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210 (*isol*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511 (*ms*)

5-Ethyl-4-methylthiazole E-341

[31883-01-9]

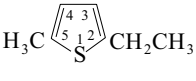
C_6H_9NS 127.21
Organoleptic, occurring in coffee aroma. Liq. d_4^{25} 1.04. Bp_{745} 169.5-170° Bp_{25} 78-79°.

Picrate:
Mp 164.7-165.1°.

Buchman, E.R. *et al., J.A.C.S.*, 1945, **67**, 395 (*synth*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264 (*synth, ms*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210 (*isol*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511 (*ms*)

2-Ethyl-5-methylthiophene, 9CI E-342

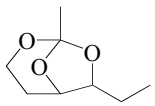
[40323-88-4]



$C_7H_{10}S$ 126.222
Maillard product. Organoleptic present in cooked meat aroma. Liq. d_4^{20} 0.97. Bp 159.8-160.4° Bp_{22} 153-155°. n_D^{20} 1.5073.

Shepard, A.F. *et al., J.A.C.S.*, 1932, **54**, 2952 (*synth*)
Adv. Chem. Ser., 1955, **15**, 199 (***props***)
McIntosh, J.M. *et al., Can. J. Chem.*, 1975, **53**, 209 (*synth*)
U.S. Pat., 1976, 3 952 026; *CA*, **85**, 94216 (*use, synth*)

6-Ethyl-1-methyl-2,7,8-trioxabicyclo[3.2.1]octane E-343

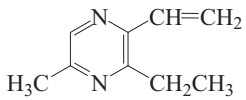


$C_8H_{14}O_3$ 158.197
Constit. of the flowers of *Jasminum sambac* (Arabian jasmine).

Knudsen, J.T. *et al., Phytochemistry*, 1993, **33**, 253 (*occur*)

3-Ethyl-5-methyl-2-vinylpyrazine E-344

[181589-32-2]
2-Ethenyl-3-ethyl-5-methylpyrazine, 9CI



$C_9H_{12}N_2$ 148.207
Odour constit. of roasted coffee and French fries. Odour threshold 0.014 ng/L in air.

Czerny, M. *et al., J. Agric. Food Chem.*, 1996, **44**, 3268-3272; 1999, **47**, 695-699 (*occur, synth, pmr, ms*)
Wagner, R.K. *et al., J. Am. Oil Chem. Soc.*, 1998, **75**, 1385-1392 (*occur*)

4-Ethyloctanoic acid, 9CI E-345

[16493-80-4]

[159223-87-7, 160173-76-2]
FEMA 3800

$H_3C(CH_2)_3CH(CH_2CH_3)CH_2CH_2COOH$
$C_{10}H_{20}O_2$ 172.267

(±)-*form*
Liq. d_4^{20} 0.91. Bp_2 109-110°. n_D^{20} 1.4388.

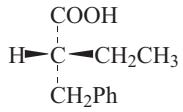
(ξ)-*form*
Present in raw and cooked goat meat, mutton and goat/sheep cheese. Food flavourant.

Schulte, K.E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1951, **288**, 69-82 (*synth*)
Petrov, A.D. *et al., Fette, Seifen, Anstrichm.*, 1959, **61**, 940-946; *CA*, **54**, 17251g (*synth*)
Ha, J.K. *et al., J. Dairy Sci.*, 1991, **74**, 3267-3274 (*occur*)
Brennand, C.P. *et al., Food Sci. Technol.*, 1992, **25**, 357-364 (*occur, meats*)
Karl, V. *et al., Chirality*, 1994, **6**, 420-426 (*synth*)
Attaie, R. *et al., J. Dairy Sci.*, 1996, **79**, 717-724 (*occur, goat cheese*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 585 (*use, occur*)

2-Ethyl-3-phenylpropanoic acid E-346

[5669-16-9]

[58635-83-9]
α-Ethylbenzenepropanoic acid, 9CI. α-Ethylhydrocinnamic acid, 8CI. 2-Benzylbutanoic acid



(R)-form

$C_{11}H_{14}O_2$ 178.23

(*R*)-*form* [56640-46-1]
Oil. $[\alpha]_D^{23}$ -40 (c, 1 in CH_2Cl_2) (>98% ee).

Benzyl ester:
$C_{18}H_{20}O_2$ 268.355
Oil. $[\alpha]_D^{23}$ -55 (c, 1 in CH_2Cl_2) (>98% ee).

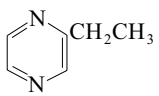
(±)-*form* [89496-36-6]
Bp_8 180° (bath temp.).

Et ester: [2983-36-0] *FEMA 3341*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. $Bp_{0.5}$ 78° (bath temp.).

House, H.O. *et al., J.A.C.S.*, 1960, **82**, 1452-1457 (*synth*)
Nakazaki, M. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 1380-1387 (*synth*)
Dehmlow, E.V. *et al., Annalen*, 1969, **729**, 64-68 (*Et ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 231 (*Et ester, use*)
Backes, B.J. *et al., J.O.C.*, 1999, **64**, 5472-5478 (*R-form, synth, pmr, cmr*)

2-Ethylpyrazine, 9CI E-347

[13925-00-3]
FEMA 3281

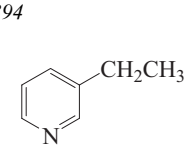


$C_6H_8N_2$ 108.143
Flavouring ingredient. Present in baked or French fried potato, wheat bread, crispbread, asparagus, cocoa, coffee, black or green tea, roasted filbert, roasted peanut, soybean, shoyu, malt, cooked shrimp and clam. Bp 152-153°.
▶ UQ3330000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 840B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 398A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1556A (*ir*)
Gainer, H. *et al., J.O.C.*, 1959, **24**, 691 (*synth*)
Cenker, M. *et al., Ind. Eng. Chem. Prod. Res. Dev.*, 1964, **3**, 11-14 (*synth*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123-126 (*ir*)

3-Ethylpyridine E-348

[536-78-7]
FEMA 3394



C_7H_9N 107.155
Present in cooked chicken, cooked beef, beer, coffee, black tea, and raw fish. Flavouring ingredient. Liq. with a tobacco flavour. Sl. sol. H_2O, sol. EtOH, Et_2O. d^0 0.95. Bp 162-165°. n_D^{20} 1.5020. pK_a 5.56 (25°).

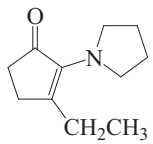
Picrate:
Mp 128-130°.

N-*Oxide:* [14906-62-8]
C_7H_9NO 123.154
Bp_4 100°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 735C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 244C (*nmr*)
Mijajima, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 429 (*cmr*)
Ferles, M. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 611 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 266
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1038
Bremner, D.H. *et al., Synth. Commun.*, 1997, **27**, 1535-1542 (*N-oxide*)

3-Ethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one E-349

[97826-61-4]



$C_{11}H_{17}NO$ 179.261
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*synth, ir, ms, pmr*)

5-Ethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one E-350

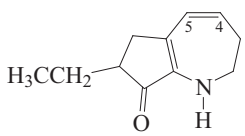
[97826-60-3]

$C_{11}H_{17}NO$ 179.261
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., Annalen*, 1985, 2017-2027 (*isol, pmr, cmr*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*synth, ir, ms, pmr*)

7-Ethyl-2,3,6,7-tetrahydrocyclopent[*b*]azepin-8(1*H*)-one E-351

[97826-69-2]



$C_{11}H_{15}NO$ 177.246
Proline-derived Maillard product. Characterised spectroscopically.

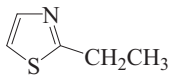
4,5-Dihydro: [97826-68-1] *7-Ethyl-2,3,4,5,6,7-hexahydrocyclopent[*b*]azepin-8(1*H*)-one*
$C_{11}H_{17}NO$ 179.261
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., Annalen*, 1985, 2017-2027 (*isol, ms, pmr*)

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*isol, ms, pmr*)

2-Ethylthiazole, 9CI E-352

[15679-09-1]



C_5H_7NS 113.183

Flavouring ingredient for coffee; Maillard product; volatile component of yeast extract; product of thermal dec. of Alliin, A-177. Liq. Mp 125.5-126° (as picrate). Bp_{70} 73-76°.

Erlenmeyer, H. *et al., Helv. Chim. Acta*, 1948, **31**, 1142-1158 (*synth*)
Chouteau, J, *et al., Bull. Soc. Chim. Fr.*, 1962, 1794-1804 (*ir*)
Vincent, E.J. *et al., Bull. Soc. Chim. Fr.*, 1966, 3524-3530 (*pmr*)
U.K. Pat., 1971, 127 829; *CA*, **76**, 2719j (*use*)
Garnier, R. *et al., Bull. Soc. Chim. Fr.*, 1972, 1040-1041 (*cmr*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264-269 (*synth, props*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511-524 (*ms*)
Silwar, R. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 112-119 (*occur*)
Yu, T.H. *et al., J. Agric. Food Chem.*, 1994, **42**, 146-153 (*occur*)
Ames, J.M. *et al., ACS Symp. Ser.*, 1995, **564**, 147-159 (*occur, yeast extract*)

1-(Ethylthio)ethyl methyl disulfide, 9CI E-353

[183554-17-8]
4-Methyl-2,3,5-trithiaheptane

$EtSCH(CH_3)–S–SMe$

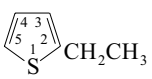
$C_5H_{12}S_3$ 168.348

Constit. of the fruit of *Durio zibethinus* (durian).

Naef, R. *et al., Fragrance J.*, 1996, **11**, 295-303 (*isol*)

2-Ethylthiophene E-354

[872-55-9]



C_6H_8S 112.195

Maillard product; present in roast meat aroma. Liq. d_4^{20} 0.99. Bp 134°. n_D^{20} 1.5122.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 44A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 592A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1467A (*ir*)
Buu-Hoi, N.P. *et al., J.O.C.*, 1950, **15**, 957 (*synth*)
Adv. Chem. Ser., 1955, **15**, 186 (***props***)
Jeffery, G.H. *et al., J.C.S.*, 1961, 570 (*uv*)
Bowie, J.H. *et al., J.C.S.(B)*, 1967, 616 (*ms*)
Peron, J.J. *et al., Spectrochim. Acta A*, 1970, **26**, 1651 (*ir*)
Fujieda, K. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1587 (*cmr*)

3-Ethylthiophene E-355

[1795-01-3]

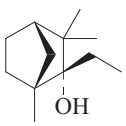
C_6H_8S 112.195

Maillard product; present in roast meat aroma. Liq. Fp -89.1. Bp 141-142° Bp_{160} 60°. n_D^{24} 1.5113.

Adv. Chem. Ser., 1955, **15**, 187 (***props***)
Gronowitz, S. *et al., Chem. Scr.*, 1974, **5**, 217
Pham, C.V. *et al., Synth. Commun.*, 1986, **16**, 689 (*synth, pmr*)
Wu, R. *et al., J.O.C.*, 1996, **61**, 6906 (*synth, ir, pmr, cmr*)

2-Ethyl-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol E-356

[67952-68-5]
2-Ethylfenchol. FEMA 3491



$C_{12}H_{22}O$ 182.305

(1*RS*,2*RS*,4*SR*)-*form* [70080-62-5]
(±)-endo-*form*

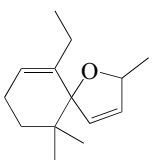
Flavouring agent with earthy tones.

[137255-07-3, 137255-09-5, 137255-11-9, 137255-15-3]

Pallaud, R. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1967, **265**, 1479-1482 (*synth*)
Gosselin, P. *et al., Tet. Lett.*, 1990, **31**, 3151-3154 (*synth*)
Finato, B. *et al., J. Agric. Food Chem.*, 1992, **40**, 857-859 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 270
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1044-1045

6-Ethyl-2,10,10-trimethyl-1-oxaspiro[4.5]deca-3,6-diene, 9CI E-357

[79893-63-3]
Etaspirene



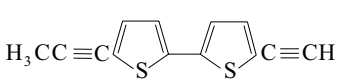
$C_{14}H_{22}O$ 206.327

Fragrance ingredient with a blackcurrant-like aroma.

Eur. Pat., 1981, 33 959; *CA*, **95**, 203728c (*synth, use*)

5-Ethynyl-5′-(1-propynyl)-2,2′-bithiophene, 9CI E-358

[17257-07-7]



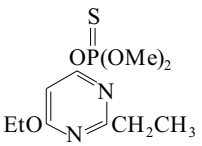
$C_{13}H_8S_2$ 228.338

Isol. from *Tagetes erecta* (African marigold). Yellow cryst. (petrol). Mp 75°.

Bohlmann, F. *et al., Chem. Ber.*, 1967, **100**, 2518; 1975, **108**, 2149 (*isol, struct, synth*)
Hogstad, S. *et al., Acta Chem. Scand., Ser. B*, 1984, **38**, 902 (*isol*)
D'Auria, M. *et al., Synth. Commun.*, 1987, **17**, 491 (*synth*)
Kagan, J. *et al., Prog. Chem. Org. Nat. Prod.*, 1991, **56**, 87 (*rev*)

Etrimfos E-359

[38260-54-7]
O-*(6-Ethoxy-2-ethyl-4-pyrimidinyl)* O,O-*dimethyl phosphorothioate, 9CI. Ekamet. Satisfar*



$C_{10}H_{17}N_2O_4PS$ 292.295

Agricultural insecticide. Oil. d_4^{20} 1.2. n_D^{20} 1.5068. Unstable when pure: stable in soln. in non-polar solvents.

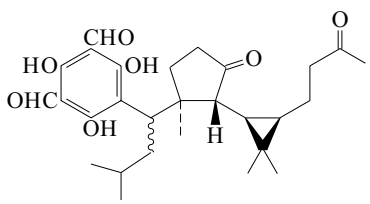
▶ LD_{50} (rat, orl) 1800 mg/kg. TF8350000

U.K. Pat., 1971, 1 387 661; *CA*, **77**, 152218e (*synth*)
Ioannou, Y.M. *et al., Pestic. Biochem. Physiol.*, 1978, **9**, 190 (*metab*)
Karapally, J.C. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1980, **11**, 125 (*rev, detn, props, synth*)
Stan, H.-J. *et al., J. Chromatogr.*, 1983, **279**, 173 (*glc*)
Bottomley, P. *et al., Analyst (London)*, 1984, **109**, 85 (*hplc*)
Pesticide Manual, 11th edn., 1997, No. 295

Eucalyptone E-360

[172617-99-1]

[168146-22-3]
Macrocarpal am1



$C_{28}H_{38}O_7$ 486.604

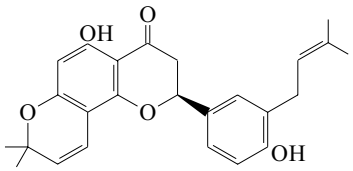
CAS name defective. Constit. of *Eucalyptus globulus* (Tasmanian bluegum). Powder. Mp 145-147°. $[\alpha]_D$ +44.6 (c, 0.19 in EtOH). $[\alpha]_D^{27}$ +70 (c, 0.21 in EtOH). No stereochem. indicated for Macrocarpal am1. λ_{max} 217 (ϵ 28000); 277 (ϵ 30000); 390 (ϵ 10000) (EtOH).

Singh, I.P. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2330-2332 (*Macrocarpal am 1*)
Osawa, K. *et al., Phytochemistry*, 1995, **40**, 183-184 (*Eucalyptone*)

Euchrenone a_2 E-361

[116310-62-4]
2,3-Dihydro-5-hydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-8,8-dimethyl-4H,8H-benzo[1,2-b:3,4-b′]dipyran-4-one,

9CI



$C_{25}H_{26}O_5$ 406.477

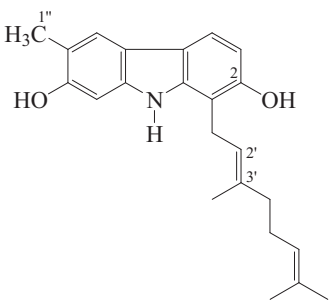
(*S*)-*form*
Pale yellow plates (hexane). Mp 145-146°.

5-Deoxy: [157414-03-4] ***Shinflavanone***
$C_{25}H_{26}O_4$ 390.478
Constit. of *Glycyrrhiza glabra* (licorice). Yellowish oil. $[\alpha]_D^{25}$ -14.7 (c, 0.53 in $CHCl_3$).

Mizuno, M. *et al., Phytochemistry*, 1988, **27**, 1831
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1056 (*Shinflavanone*)
Suh, H. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 1433-1436 (*Shinflavanone, synth*)

Euchrestine C E-362

[138822-95-4]
*1-Geranyl-2,7-dihydroxy-6-methylcarbazole. 1-(3,7-Dimethyl-2,6-octadienyl)-6-methyl-9*H*-carbazole-2,7-diol*



$C_{23}H_{27}NO_2$ 349.472
Powder.

2-Me ether: [138822-94-3] ***Euchrestine B***
$C_{24}H_{29}NO_2$ 363.499
Pale yellow oil.

7-Me ether: [144525-81-5] ***Murrayanol***†
$C_{24}H_{29}NO_2$ 363.499
Alkaloid from seeds of *Murraya koenigii* (curry leaf tree). Cryst. (CH_2Cl_2/petrol). Mp 161°.

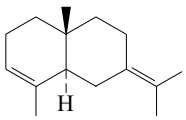
2′,3′-Epoxide: [139726-46-8] ***Euchrestine E***
$C_{23}H_{27}NO_3$ 365.471
Pale brown oil. Obt. as a racemate.

1″-Oxo, 2-Me ether: [139726-44-6] *6-Formyl-1-geranyl-7-hydroxy-2-methoxycarbazole.* ***Murrayaline D***
$C_{24}H_{27}NO_3$ 377.482
Pale brown oil. λ_{max} 243 ; 255 (sh) ; 287 ; 330 ; 357 ; 364 ; 368 (MeOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1668-1671 (*isol, pmr, cmr, struct*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2525-2528 (*Murrayaline D*)
Reisch, J. *et al., Phytochemistry*, 1992, **31**, 2877-2879 (*Murrayanol*)
Itoigawa, M. *et al., J. Nat. Prod.*, 2000, **63**, 893-897 (*activity*)

3,7(11)-Eudesmadiene E-363

[6813-21-4]
3,7(11)-Selinadiene

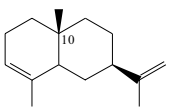


$C_{15}H_{24}$ 204.355
Constit. of essential oil of hops (*Humulus lupulus*). Oil.

Buttery, R.G. *et al., Chem. Ind. (London)*, 1966, 1225 (*isol, struct*)
Brown, E.D. *et al., J.C.S. Perkin 1*, 1975, 2326 (*synth*)
Wilson, S.R. *et al., J.A.C.S.*, 1978, **100**, 6289 (*synth*)
Banerjee, G.K. *et al., J. Chem. Res., Synop.*, 1984, 284 (*synth*)
Lee, S.-J. *et al., Chem. Comm.*, 1988, 1188 (*synth*)

3,11-Eudesmadiene E-364

[473-13-2]
3,11-Selinadiene



(5α,7β,10β)-*form*

$C_{15}H_{24}$ 204.355
$[\alpha]_D^{20}$ -14.5 (c, 1 in $CHCl_3$).

(5α,7β,10β)-*form*
α-Selinene. *α-Eudesmene*
Occurs in celery oil and hop (*Humulus lupulus*) oil. Oil. Bp 268-272°. $[\alpha]_D^{20}$ -14.5 (c, 1 in $CHCl_3$).

(5β,7α,10β)-*form* [66141-13-7]
α-Helmiscapene
Oil. $[\alpha]_D$ -100 ($CHCl_3$).

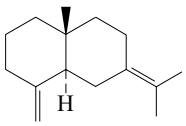
(5β,7β,10α)-*form* [28290-23-5]
Oil. $[\alpha]_D^{20}$ +2.1.

(5β,7β,10β)-*form* [83378-03-4]

Chetty, G.L. *et al., Tetrahedron*, 1966, **22**, 2311 (*α-form, synth*)
Klein, E. *et al., Tet. Lett.*, 1970, 279 (*5β,7β,10α-form, isol*)
Stevens, K.L. *et al., J.O.C.*, 1971, **36**, 2422 (*5β,7β,10α-form, synth*)
Maurer, B. *et al., Helv. Chim. Acta*, 1977, **60**, 2177 (*α-form, isol, pmr, ir*)
Anderson, N.H. *et al., Phytochemistry*, 1977, **16**, 1731 (*α-form, isol*)
Baker, R. *et al., Tet. Lett.*, 1978, 4073 (*isol*)
Naya, Y. *et al., Tet. Lett.*, 1982, **23**, 3047 (*isol*)
Kutney, J.P. *et al., Can. J. Chem.*, 1984, **62**, 1407 (*α-form, synth*)
Caine, D. *et al., Tetrahedron*, 1987, **43**, 5545 (*α-form, synth*)
Caine, D. *et al., J.O.C.*, 1988, **53**, 4124 (*α-form, synth*)
Schinzer, D. *et al., Annalen*, 1992, 139 (*5β,7α,10β-form, synth*)
Ando, M. *et al., J. Nat. Prod.*, 1994, **57**, 1189 (*synth*)
Williams, H.J. *et al., Phytochemistry*, 1995, **40**, 1633 (*α-form, pmr, cmr, ms*)
Zou, N. *et al., Chin. Chem. Lett.*, 1996, **7**, 1081 (*synth*)

4(15),7(11)-Eudesmadiene E-365

[515-17-3]
4(15),7(11)-Selinadiene. ***γ-Selinene***

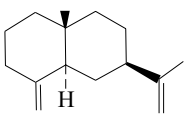


$C_{15}H_{24}$ 204.355
Constit. of essential oil of hops (*Humulus lupulus*). Oil. $[\alpha]_D$ +2.5 (c, 0.12 in $CHCl_3$).

Buttery, R.G. *et al., Chem. Ind. (London)*, 1966, 1225 (*isol*)
Andersen, N.H. *et al., Tet. Lett.*, 1970, 1759 (*struct*)
Brown, E.D. *et al., J.C.S. Perkin 1*, 1975, 2326 (*synth*)
Posner, G.H. *et al., Tet. Lett.*, 1975, 1373 (*synth*)
Morita, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1603 (*synth*)

4(15),11-Eudesmadiene E-366

4(15),11-Selinadiene



(5α,7β,10β)-*form*

$C_{15}H_{24}$ 204.355

(5α,7β,10β)-*form* [17066-67-0]
β-Selinene. *Cyperene II*
Constit. of celery oil. Also from *Cyperus rotundus* (nutgrass) and *Humulus lupulus* (hops). Oil. Bp_6 121-122°. $[\alpha]_D$ +61.

(5β,7α,10α)-*form* [473-12-1]
ent-*4(15),11-Eudesmadiene.* ent-*4(15),11-Selinadiene*
Oil. $Bp_{1.5}$ 70-115° (lit. gives a pressure range). $[\alpha]_D$ -46 (c, 10 in $CHCl_3$).

(5β,7β,10α)-*form* [29868-52-8]
Oil. $Bp_{0.3}$ 80-85°. $[\alpha]_D$ -71.63 (c, 4.61 in $CHCl_3$).

(5β,7β,10β)-*form* [83434-35-9]

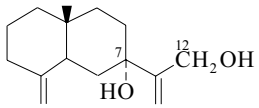
(5α,7β,10α)-*form* [66141-12-6]
β-Helmiscapene
Oil.

Trivedi, B. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 1675 (*isol*)
Marshall, J.A. *et al., J.O.C.*, 1966, **31**, 2933 (*synth*)
Dixit, S.M. *et al., Chem. Ind. (London)*, 1967, 1256 (*isol*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1968, **45**, 1033 (*synth*)
Stevens, K.L. *et al., J.O.C.*, 1971, **36**, 2422 (*synth*)
Govindachari, T.R. *et al., Indian J. Chem., Sect. B*, 1973, **11**, 971 (*isol, struct*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731 (*β-Helmiscapene*)
Naya, Y. *et al., Tet. Lett.*, 1982, **23**, 3047 (*isol*)
Wijnberg, J.B.P.A. *et al., J.O.C.*, 1983, **48**, 4380 (*synth*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2860 (*β-Selinene, pmr, cmr*)
Caine, D. *et al., J.O.C.*, 1988, **53**, 4124 (*synth*)
Williams, H.J. *et al., Phytochemistry*, 1995, **40**, 1633 (*pmr, cmr, ms*)
Morita, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1603 (*synth*)

Raharivelomanana, P. *et al., Phytochemistry*, 1998, **47**, 1085-1088 (*cmr*)

4(15),11(13)-Eudesmadiene-7,12-diol E-367

4(15),11(13)-Selinadiene-7,12-diol



$C_{15}H_{24}O_2$ 236.353

7α-*form* [86703-05-1]
7-Hydroxycostol
Phytoalexin from *Ipomoea batatas* (sweet potato) infected with *Ceratocystis fimbriata*. Oil. $[\alpha]_D$ +15 (c, 2 in CH_2Cl_2).

12-Aldehyde: [86703-04-0] *7α-Hydroxy-4(15),11(13)-eudesmadien-12-al.* ***7-Hydroxycostal***
$C_{15}H_{22}O_2$ 234.338
Phytoalexin from *Ipomoea batatas* (sweet potato). Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 123-124°. $[\alpha]_D$ +2 (c, 0.4 in CH_2Cl_2). λ_{max} 215 (ϵ 5400) (MeOH) (Berdy).

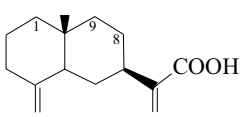
12-Carboxylic acid:7-Hydroxy-4(15),11(13)-eudesmadien-12-oic acid. ***7-Hydroxycostic acid***
$C_{15}H_{22}O_3$ 250.337
Cryst. Mp 220°. $[\alpha]_D^{24}$ +21 (c, 3.03 in $CHCl_3$).

[96479-42-4, 96479-43-5, 96647-97-1]

Schneider, J.A. *et al., Chem. Comm.*, 1983, 353 (*isol*)
Cuomo, J. *et al., J. Agric. Food Chem.*, 1985, **33**, 717 (*synth*)
Wijnberg, J.B.P.A. *et al., J.O.C.*, 1985, **50**, 2650 (*synth*)
Zdero, C. *et al., Phytochemistry*, 1987, **26**, 187 (*7-Hydroxycostic acid*)
Tanaka, A. *et al., Agric. Biol. Chem.*, 1988, **52**, 2043 (*synth*)

4(15),11(13)-Eudesmadien-12-oic acid E-368

[3650-43-9]
4(15),11(13)-Selinadien-12-oic acid. ***β-Costic acid****. Costus acid*



$C_{15}H_{22}O_2$ 234.338
Constit. of the root of costus (*Saussurea lappa*). Cryst. (EtOH aq.). Mp 87-88°. $[\alpha]_D$ +23.4 (c, 3 in $CHCl_3$). λ_{max} 210 (ϵ 5030) (MeOH) (Berdy).

4α,15-Epoxide:4α,15-Epoxy-11(13)-eudesmen-12-oic acid. ***4α,15-Epoxycostic acid***
$C_{15}H_{22}O_3$ 250.337
Oil (as Me ester). $[\alpha]_D^{24}$ -33 (c, 0.18 in $CHCl_3$) (Me ester).

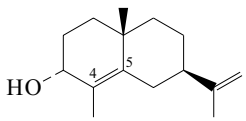
11ξ,13-Dihydro: [72944-20-8] *4(15)-Eudesmen-12-oic acid. 4(15)-Selinen-12-oic acid.* ***11,13-Dihydrocostic acid***
$C_{15}H_{24}O_2$ 236.353
$[\alpha]_D^{24}$ +55.1 (c, 1 in $CHCl_3$) (as Me ester).

(±)-*form*
Mp 115-116°.

Bawdekar, A.S. *et al., Tetrahedron*, 1965, **21**, 1521 (*isol, struct*)
Herz, W. *et al., J.O.C.*, 1966, **31**, 1632 (*isol*)
Marshall, J.A. *et al., J.O.C.*, 1966, **31**, 2933 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1189 (*11,13-Dihydrocostic acid*)
Zdero, C. *et al., Phytochemistry*, 1990, **29**, 3201 (*epoxide*)
Marco, J.A. *et al., Magn. Reson. Chem.*, 1992, **30**, 678 (*cmr*)

4,11-Eudesmadien-3-ol E-369

4,11-Selinadien-3-ol



$C_{15}H_{24}O$ 220.354

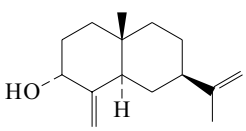
3α-*form* [20084-99-5]
Cyperol*. α-Cyperol*
Constit. of *Cyperus rotundus* (nutgrass). Cryst. (petrol). Mp 111.5-112°. $[\alpha]_D$ +131.4 (c, 6.2 in $CHCl_3$).

4α,5α-Epoxide: [61248-42-8] ***4α,5α-Epoxy-11-eudesmen-3α-ol***
Constit. of *Cyperus rotundus* (nutgrass). Cryst. (petrol). Mp 61.5°. $[\alpha]_D$ +37.3 (c, 4.7 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1929
Hikino, H. *et al., Phytochemistry*, 1976, **15**, 1265 (*epoxide*)

4(15),11-Eudesmadien-3-ol E-370

4(15),11-Selinadien-3-ol



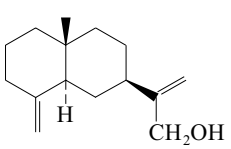
$C_{15}H_{24}O$ 220.354

3α-*form* [20085-00-1]
Isocyperol
Constit. of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D$ -5.4 (c, 4.5 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1929

4(15),11(13)-Eudesmadien-12-ol E-371

[515-20-8]
4(15),11(13)-Selinadien-12-ol



$C_{15}H_{24}O$ 220.354

(5α,7β,10β)-*form*
β-Costol*. Sesquibenihiol*
Constit. of the essential oil of costus (*Saussurea lappa*). Oil. $Bp_{0.5}$ 145° (bath). $[\alpha]_D$ +32.8 (c, 4.3 in $CHCl_3$).

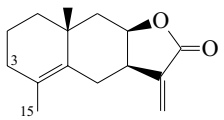
12-Aldehyde: [3650-40-6] *4(15),11(13)-Eudesmadien-12-al.* ***β-Costal***
$C_{15}H_{22}O$ 218.338
Oil. Bp_{15} 164-166°. $[\alpha]_D$ +24. Originally called α-Costal.

12-Aldehyde, semicarbazone:
Cryst. (EtOH). Mp 223°.

Bawdekar, A.S. *et al., Tetrahedron*, 1965, **21**, 1521; 1967, **23**, 1993 (*isol, struct*)
Marshall, J.A. *et al., J.O.C.*, 1966, **31**, 2933 (*synth*)
Klein, E. *et al., CA*, 1969, **70**, 4301 (*synth*)
Maurer, B. *et al., Helv. Chim. Acta*, 1977, **60**, 2177 (*isol, pmr, ir*)
Garratt, P.J. *et al., J.O.C.*, 1986, **51**, 5450 (*synth*)
Raharivelomanana, P. *et al., Phytochemistry*, 1995, **41**, 243 (*cmr*)

4,11(13)-Eudesmadien-12,8-olide E-372

4,11(13)-Selinadien-12,8-olide



$C_{15}H_{20}O_2$ 232.322

(7β,8β,10β)-*form* [64340-41-6]
Alloalantolactone
Constit. of *Inula helenium* (elecampane). Oil. Poorly sol. hexane. $[\alpha]_D$ +35.2 (c, 0.5 in $CHCl_3$).

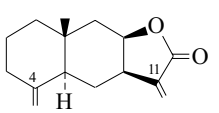
*4β,5β-Epoxide:****4β,5β-Epoxy-11(13)-eudesmen-12,8β-olide***
$C_{15}H_{20}O_3$ 248.321
Cryst. (Et_2O/petrol). Mp 115°.

(7α,8α,10α)-*form* ent-*4,11(13)-Eudesmadien-12,8β-olide.* ent-*Alloalantolactone.* ***Diplophyllin***
Cryst. Mp 30-31.5°. $[\alpha]_D$ -108 (pentane).

11α,13-Dihydro: [73039-16-4] ent-*4-Eudesmen-12,8β-olide.* **ent-*Dihydrodiplophyllin***
$C_{15}H_{22}O_2$ 234.338
Oil. $[\alpha]_D$ -43.8 (c, 1.8 in $CHCl_3$). The name *ent*-Dihydrodiplophyllin is misleading.

Ohta, Y. *et al., Tetrahedron*, 1977, **33**, 617 (*Diplophyllin*)
Ananthasubramanian, L. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 191 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165 (*Alloalantolactone*)
Asakawa, Y. *et al., Phytochemistry*, 1979, **18**, 1007 (ent-*Dihydrodiplophyllin*)
Bohlmann, F. *et al., Annalen*, 1983, 2227 (*epoxide*)
Bhandari, P. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 286 (*Alloalantolactone*)
Nishitani, K. *et al., Heterocycles*, 1994, **39**, 43 (*synth*)

4(15),11(13)-Eudesmadien-12,8-olide E-373



$C_{15}H_{20}O_2$ 232.322

(5α,8β)-*form* [470-17-7]
Isoalantolactone. *Isohelenin*
Constit. of the essential oil of *Inula helenium* (elecampane). Cryst. (EtOH aq.). Sol. EtOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 115° (109-110°). $[\alpha]_D$ +172 ($CHCl_3$).

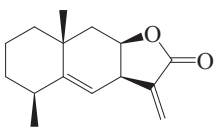
► LE3130000

4α,15-Epoxide:4α,15-Epoxy-4(15),11(13)-eudesmadien-12,8β-olide. ***4α,15-Epoxyisoalantolactone***
$C_{15}H_{20}O_3$ 248.321
Oil.

11α,13-Dihydro:4(15)-Eudesmen-12,8β-olide. ***Dihydroisoalantolactone***
$C_{15}H_{22}O_2$ 234.338
Isol. from roots of *Inula helenium* (elecampane). Needles (EtOH). Mp 172-173°.

Asselineau, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1958, **246**, 1874 (*struct*)
Ukita, T. *et al., J.A.C.S.*, 1960, **82**, 2224 (*Dihydroisoalantolactone*)
Marshall, J.A. *et al., J.O.C.*, 1964, **29**, 3727 (*pmr, struct*)
Miller, R.B. *et al., Tetrahedron*, 1974, **30**, 2961 (*synth*)
Jakupovic, J. *et al., Phytochemistry*, 1988, **27**, 3551 (*epoxide*)
Blay, G. *et al., Tetrahedron*, 1990, **48**, 5265 (*synth*)
Tada, M. *et al., J.C.S. Perkin 1*, 1993, 239 (*synth*)
Tan, R.X. *et al., Phytochemistry*, 1998, **49**, 157-161 (*activity*)
Cantrell, C.L. *et al., Planta Med.*, 1999, **65**, 351-355 (*activity*)

5,11(13)-Eudesmadien-12,8-olide E-374



$C_{15}H_{20}O_2$ 232.322Log P 3.27 (calc).

8β-*form* [546-43-0]
Alantolactone. *Helenine†. Alantic anhydride*
Constit. of *Inula helenium* (elecampane). Cryst. (pentane). Mp 78-80°. $[\alpha]_D$ +175 ($CHCl_3$). $[\alpha]_D$ +220 (c, 1 in MeOH). λ_{max} 211 (ϵ 9470) (MeOH) (Berdy). λ_{max} 212 (EtOH) (Berdy).

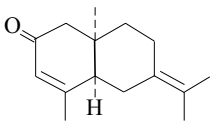
► Irritant, cytotoxic substance.

11α,13-Dihydro: [40285-97-0] *5-Eudesmen-12,8-olide.* ***11α,13-Dihydroalantolactone***
$C_{15}H_{22}O_2$ 234.338
$[\alpha]_D^{24}$ -35 (c, 0.2 in $CHCl_3$). λ_{max} 204 (log ϵ 3.86) (MeOH).

Tsuda, K. *et al., J.A.C.S.*, 1957, **79**, 5721 (*struct*)
Marshall, J.A. *et al., J.O.C.*, 1964, **29**, 3727 (*pmr, struct*)
Marshall, J.A. *et al., J.A.C.S.*, 1966, **88**, 3408 (*synth*)
Khvorost, P.P. *et al., Khim. Prir. Soedin.*, 1976, **12**, 820; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 740 (*isol*)
Schmalle, H.W. *et al., Acta Cryst. C*, 1986, **42**, 705 (*cryst struct*)
Milman, I.A. *et al., Khim. Prir. Soedin.*, 1990, **26**, 307; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 251 (*rev*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995, (*bibl*)
Su, B.-N. *et al., J. Nat. Prod.*, 2001, **64**, 466-471 (*11α,13-dihydro*)

3,7(11)-Eudesmadien-2-one E-375

3,7(11)-Selinadien-2-one



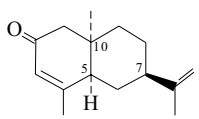
$C_{15}H_{22}O$ 218.338

(5α,10α)-*form* [86917-82-0]
Constit. of grapefruit (*Citrus paradisi*). Cryst. (pentane). Mp 92-92.5°. $[\alpha]_D^{20}$ +83 (c, 0.82 in $CHCl_3$).

Demole, E. *et al., Helv. Chim. Acta*, 1983, **66**, 1381

3,11-Eudesmadien-2-one E-376

3,11-Selinadien-2-one



(5α,7β,10α)-*form*

$C_{15}H_{22}O$ 218.338

(5α,7β,10α)-*form* [86941-63-1]
Constit. of grapefruit (*Citrus paradisi*). Oil. $[\alpha]_D^{20}$ +128 (c, 0.6 in $CHCl_3$).

(5β,7β,10α)-*form* [86917-81-9]
Constit. of grapefruit (*Citrus paradisi*). Oil. $[\alpha]_D^{20}$ -70 (c, 0.64 in $CHCl_3$).

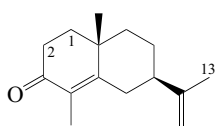
(5β,7β,10β)-*form* [86917-80-8]
Constit. of grapefruit (*Citrus paradisi*). Cryst. Mp 38°. $[\alpha]_D^{20}$ -61 (c, 0.87 in $CHCl_3$).

[86917-79-5]

Demole, E. *et al., Helv. Chim. Acta*, 1983, **66**, 1381

4,11-Eudesmadien-3-one E-377

4,11-Selinadien-3-one. ***α-Cyperone***



(+)-*form*

$C_{15}H_{22}O$ 218.338

(+)-*form* [473-08-5]
Constit. of *Cyperus rotundus* (nutgrass). Bp 177°. $[\alpha]_D$ +138. λ_{max} 248 (EtOH) (Berdy).

Semicarbazone:
Cryst. Mp 216°.

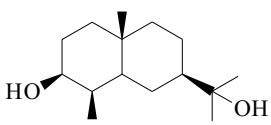
13-Hydroxy: [56423-80-4] *12-Hydroxy-4,11(13)-eudesmadien-3-one.* ***12-Hydroxy-α-cyperone***
$C_{15}H_{22}O_2$ 234.338
Oil.

1,2-Didehydro: [17081-85-5] *1,4,11-Eudesmatrien-3-one. 1,4,11-Selinatrien-3-one.* ***1,2-Dehydro-α-cyperone***
$C_{15}H_{20}O$ 216.322
Constit. of *Lycium chinense* (Chinese boxthorn). Oil. $[\alpha]_D$ -172.4 (c, 0.003 in MeOH).

(-)-*form* [23665-61-4]
ent-α-*Cyperone*
$[\alpha]_D$ -138 ($CHCl_3$).

Adamson, P.S. *et al., J.C.S.*, 1937, 1576 (*struct*)
Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1954, 332 (*isol*)
Howe, R. *et al., J.C.S.*, 1955, 2423 (*synth*)
Caine, D. *et al., J.O.C.*, 1974, **39**, 2154 (*synth*)
Sannai, A. *et al., Phytochemistry*, 1982, **21**, 2986 (*Dehydro-α-cyperone*)
Jakupovic, J. *et al., Phytochemistry*, 1988, **27**, 1129 (*12-Hydroxy-α-cyperone*)
Asakawa, Y. *et al., Phytochemistry*, 1990, **29**, 1577 (*ent-α-Cyperone*)
Haaksma, A.A. *et al., Tetrahedron*, 1992, **48**, 3121 (*synth*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)
Xiong, Z. *et al., J. Chem. Res., Synop.*, 1996, 477 (*synth*)
Xiong, Z. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 2607 (*synth*)

3,11-Eudesmanediol E-378



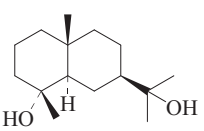
$C_{15}H_{28}O_2$ 240.385

(3β,4β)-*form* [102490-02-8]
Auberganol
Constit. of *Solanum melongena* (aubergine). Cryst. (EtOAc/hexane). Mp 173-173.5°. $[\alpha]_D$ -2.7.

(3α,4α)-*form*
Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1191 (*synth*)
Stressl, A. *et al., Can. J. Chem.*, 1986, **64**, 611 (*isol, pmr, cmr*)
Raharivelomanana, P. *et al., Phytochemistry*, 1996, **43**, 243 (*isol, pmr, cmr*)

4,11-Eudesmanediol E-379

4,11-Selinanediol



(4α,5α)-*form*

$C_{15}H_{28}O_2$ 240.385

(4α,5α)-*form* [4666-84-6]
Cryptomeridiol. *Proximadiol*
Cryst. Mp 138° (134.5-135.5°). $[\alpha]_D$ -33.3 ($CHCl_3$). Log P 2.98 (calc).

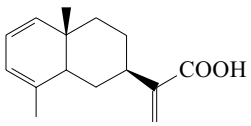
11-O-α-L-Rhamnopyranoside: [349112-30-7]
$C_{21}H_{38}O_6$ 386.528
Constit. of fruits of *Cananga odorata* (ylang ylang). Cryst. (EtOAc). Mp 189-190°. $[\alpha]_D^{25}$ -13.3 (c, 0.03 in $CHCl_3$).

[108006-39-9]

Hsieh, T.-J. *et al., J. Nat. Prod.*, 2001, **64**, 616-619 (*11-rhamnoside*)

1,3,11(13)-Eudesmatrien-12-oic acid E-380

[96383-98-1]

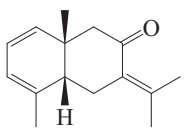


$C_{15}H_{20}O_2$ 232.322
Constit. of *Helianthus annuus* (sunflower).

Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 192 (*isol*)
Alfatafta, A.A. *et al., Phytochemistry*, 1992, **31**, 4109 (*isol, pmr, cmr*)

1,3,7(11)-Eudesmatrien-8-one E-381

1,3,7(11)-Selinatrien-8-one



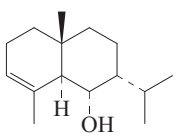
$C_{15}H_{20}O$ 216.322

5β-*form* [120216-95-7]
Constit. of *Eugenia uniflora* (Surinam cherry). Oil. $[\alpha]_D$ -258 (c, 1 in $CHCl_3$).

Weyerstahl, P. *et al., Planta Med.*, 1988, **54**, 546-549 (*isol, pmr, cmr*)
Kanazawa, A. *et al., J. Nat. Prod.*, 2000, **63**, 1292-1294 (*synth*)

3-Eudesmen-6-ol E-382

3-Selinen-6-ol



(5α,6α,7β*H*)-*form*

$C_{15}H_{26}O$ 222.37

(5α,6α,7β*H*)-*form* [260793-01-9]
7-Epiisojunenol

(5α,6β)-*form* [74144-55-1]
Isojunenol
Oil. $[\alpha]_D$ -35 (c, 1.1 in $CHCl_3$).

6-Ketone:3-Eudesmen-6-one. 3-Selinen-6-one. ***Isoacolamone***
$C_{15}H_{24}O$ 220.354
Constit. of the rhizomes of *Acorus calamus* (sweet flag). Oil.

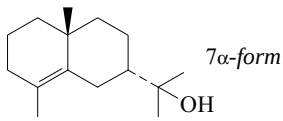
(5β,6α)-*form*
α-Verbesinol
Liq. $Bp_{0.2}$ 82-83°. $[\alpha]_D^{21}$ -15.3.

4-Hydroxycinnamoyl:
$C_{24}H_{32}O_3$ 368.515
Mp 116-122°. $[\alpha]_D^{16}$ +49. Data refers to mixt. with the deriv. of β-Verbesinol.

Gardner, P.D. *et al., J.A.C.S.*, 1961, **83**, 1511 (*isol*)
Niwa, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2930 (*Isoacolamone*)
Niwa, M. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3145 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1751 (*isol, config*)
Toyota, M. *et al., Phytochemistry*, 1988, **27**, 2155 (*isol*)
Cardona, L. *et al., Tetrahedron*, 1992, **48**, 851 (*synth*)
Warmers, U. *et al., Phytochemistry*, 1999, **52**, 1519-1524 (*7-Epiisojunenol*)

4-Eudesmen-11-ol E-383

4-Selinen-11-ol



$C_{15}H_{26}O$ 222.37

7β-*form* [1209-71-8]
γ-Eudesmol. *Uncineol*
Oil. $Bp_{0.1}$ 83-86°. $[\alpha]_D^{25}$ +66.7 (neat). n_D^{20} 1.5087.

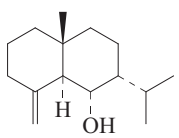
O-α-L-*Rhamnopyranoside:* [349112-31-8]
$C_{21}H_{36}O_5$ 368.512
Constit. of fruits of *Cananga odorata* (ylang ylang). Gum. $[\alpha]_D^{25}$ -11.5 (c, 0.24 in $CHCl_3$).

[13902-07-3, 51317-08-9, 72173-98-9]

Barrero, A.F. *et al., J. Nat. Prod.*, 1997, **60**, 1026-1030 (*glycosides*)

4(15)-Eudesmen-6-ol E-384

4(15)-Selinen-6-ol



(5α,6α,7α,10β)-*form*

$C_{15}H_{26}O$ 222.37

(5α,6α,7β,10α)-*form* [62358-38-7]
10-Epijunenol
Constit. of galbanum resin. Cryst. Mp 31°. $[\alpha]_D$ +85.7 (c, 6 in EtOH).

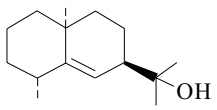
(5α,6α,7β,10β)-*form* [472-07-1]
Junenol
Constit. of the juniper berry (*Juniperus communis*). Cryst. (petrol or by subl.). Mp 62.5-63°. Bp_1 121-122°. $[\alpha]_D$ +52 (c, 3.35 in $CHCl_3$).

6-Ketone: [39012-14-1] *4(15)-Eudesmen-6-one. 4(15)-Selinen-6-one.* ***Acolamone***
$C_{15}H_{24}O$ 220.354
Constit. of *Acorus calamus* (sweet flag). Liq.

Shaligram, A.H. *et al., Tetrahedron*, 1962, **18**, 969 (*isol*)
Theobald, D.W. *et al., Tetrahedron*, 1964, **20**, 2593 (*struct*)
Hinge, V.K. *et al., Tetrahedron*, 1965, **21**, 3197 (*isol*)
Schwartz, M.A. *et al., J.A.C.S.*, 1972, **94**, 4361 (*synth*)
Niwa, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2930 (*Acolamone*)
Thomas, A.F. *et al., Tetrahedron*, 1976, **32**, 2261 (*isol, struct*)
Wender, P.A. *et al., J.A.C.S.*, 1978, **100**, 4321 (*synth*)
Banerjee, A.K. *et al., J.C.S. Perkin 1*, 1982, 2547 (*synth*)
Cardona, L. *et al., Tetrahedron*, 1992, **48**, 851 (*synth*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)

5-Eudesmen-11-ol E-385

5-Selinen-11-ol



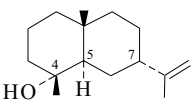
$C_{15}H_{26}O$ 222.37

(4α,7β,10α)-*form* [63891-61-2]
Rosifoliol
Constit. of *Rubus rosifolius* (Mauritius raspberry). Cryst. Mp 84°. $[\alpha]_D$ +105. $[\alpha]_D^{20}$ -17.1 (c, 0.66 in $CHCl_3$).

Southwell, I.A. *et al., Tet. Lett.*, 1977, 873
Beagley, B. *et al., Acta Cryst. B*, 1982, **38**, 1391 (*cryst struct*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1997, **60**, 1026-1030 (*isol, pmr, cmr*)

11-Eudesmen-4-ol E-386

11-Selinen-4-ol



(4α,5α,7α,10β)-*form*

$C_{15}H_{26}O$ 222.37

(4α,5α,7α,10β)-*form* [71963-78-5]
Isointermedeol
Constit. of *Cymbopogon flexuosus* (East Indian lemongrass). Solid. Mp 40-41°. $[\alpha]_D$ +2 (c, 3.3 in MeOH).

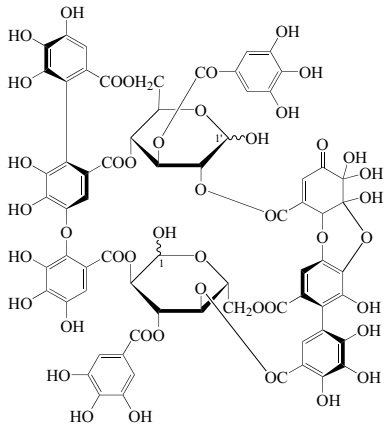
(4β,5β,7β,10α)-*form* [6168-59-8]
Intermedeol. *Paradisiol*
Constit. of *Citrus* spp.. Cryst. Mp 47-48°. $[\alpha]_D^{35}$ +10.7 (c, 0.957 in EtOH).

[41664-11-3]

Chetty, G.L. *et al., Tet. Lett.*, 1968, 3223 (*synth, struct*)
Hoffmann, J.W. *et al., J.O.C.*, 1976, **41**, 3705 (*synth*)
Zalkow, V.B. *et al., J.O.C.*, 1976, **41**, 3710 (*synth*)
Thappa, R.K. *et al., Phytochemistry*, 1979, **18**, 671 (*Isointermedeol*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2860 (*Intermedeol, pmr*)
Kawamata, T. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3770 (*synth*)
Kesselmans, R.P.W. *et al., J.O.C.*, 1991, **56**, 7237 (*synth*)
Wassmuth-Wagner, I. *et al., Planta Med.*, 1995, **61**, 196 (*pmr, cmr*)
Raharivelomanana, P. *et al., Phytochemistry*, 1998, **47**, 1085-1088 (*cmr, ms*)
Sakar, M.K. *et al., Fitoterapia*, 1999, **70**, 103-105 (*Intermedeol, pmr, cmr*)
Park, H.-J. *et al., Planta Med.*, 2000, **66**, 783-784 (*Intermedeol, activity*)

Eugeniflorin D_2 E-387

[189276-85-5]

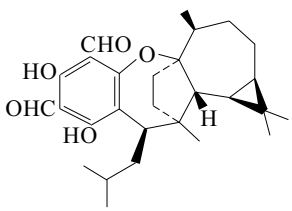


$C_{68}H_{48}O_{45}$ 1585.1
Constit. of *Eugenia uniflora* (Surinam cherry). Pale yellow powder +9 H_2O. $[\alpha]_D$ +37 (c, 1 in MeOH). Related to Oenothein B, O-117. λ_{max} 216 (log ϵ 4.89); 272 (log ϵ 4.48) (MeOH).

Lee, M.-H. *et al., Phytochemistry*, 1997, **44**, 1343-1349 (*isol, uv, cd, pmr, cmr*)

Euglobal V E-388

[77809-89-3]

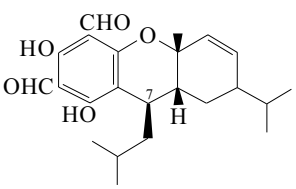


$C_{28}H_{38}O_5$ 454.605
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Prisms (EtOH). Mp 184-185°. $[\alpha]_D^{20}$ -206 (c, 1 in $CHCl_3$).

Amano, T. *et al., J. Chromatogr.*, 1981, **208**, 347 (*isol*)
Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1964 (*cryst struct*)
Takasaki, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2113 (*isol, pmr, cmr*)

Euglobal Ia_1 E-389

[77844-93-0]



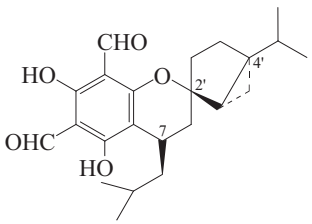
$C_{23}H_{30}O_5$ 386.487
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Oil. $[\alpha]_D^{20}$ -216.7 (c, 1.0 in $CHCl_3$). λ_{max} 277 (ϵ 32000); 340 (sh) (ϵ 4000) (EtOH) (Derep).

7-Epimer: [77794-63-9] *Euglobal Ia_2*
$C_{23}H_{30}O_5$ 386.487
Constit. of *Eucalyptus globulus* (tasmanian blue gum). Oil. $[\alpha]_D^{20}$ +31.8 (c, 1.0 in $CHCl_3$). λ_{max} 277 (ϵ 32000); 340 (sh) (ϵ 4000) (EtOH) (Derep).

Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1952

Euglobal Ic E-390

[77794-60-6]



$C_{23}H_{30}O_5$ 386.487
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Prisms (EtOH). Mp 108-110°. $[\alpha]_D^{20}$ -3.12 (c, 1.0 in $CHCl_3$). λ_{max} 277 (ϵ 32000); 340 (sh) (ϵ 4000) (EtOH) (Derep).

7-Epimer: [77844-92-9] ***Euglobal IIa***
$C_{23}H_{30}O_5$ 386.487
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Prisms (EtOH). Mp 130-132°. $[\alpha]_D^{20}$ +9.24 (c, 1.0 in $CHCl_3$). λ_{max} 277 (ϵ 32000); 340 (sh) (ϵ 4000) (EtOH) (Derep).

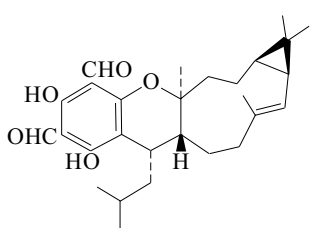
2′,4′-Diepimer: [163437-53-4] *Euglobal Bl 1*
$C_{23}H_{30}O_5$ 386.487
Prisms ($CHCl_3$). Mp 98-100°. $[\alpha]_D$ +11.3 (c, 1 in $CHCl_3$). λ_{max} 277 (ϵ 36000); 340 (ϵ 4300) (EtOH).

2′,4′,7-Triepimer: [77844-94-1] ***Euglobal Ib***
$C_{23}H_{30}O_5$ 386.487
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Needles (EtOH). Mp 119-121°. $[\alpha]_D^{20}$ -1.94 (c, 1.0 in $CHCl_3$). λ_{max} 277 (ϵ 32000); 340 (sh) (ϵ 4000) (EtOH) (Derep).

Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1952 (*cryst struct*)
Takasaki, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2177-2179 (*isol, pmr, cmr*)

Euglobal III E-391

[76449-26-8]

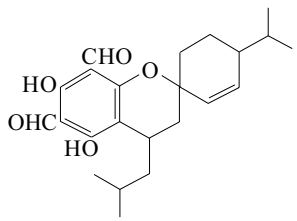


$C_{28}H_{38}O_5$ 454.605
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. (EtOH). Mp 169-171°. $[\alpha]_D$ +229 (c, 1 in $CHCl_3$). λ_{max} 278 (ϵ 32200); 345 (sh) (ϵ 4880) (EtOH) (Derep).

Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1964 (*struct, abs config*)

Euglobal IIb E-392

[77794-61-7]

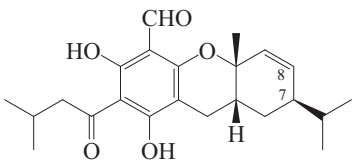


$C_{23}H_{30}O_5$ 386.487
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Oil. $[\alpha]_D^{20}$ +12.2 (c, 1 in $CHCl_3$). λ_{max} 277 (ϵ 32000); 340 (sh) (ϵ 4000) (EtOH) (Derep).

Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1952

Euglobal IIc E-393

[77794-62-8]



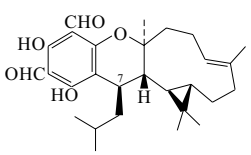
$C_{23}H_{30}O_5$ 386.487
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Oil. $[\alpha]_D^{20}$ -144 (c. 1.0 in $CHCl_3$). λ_{max} 277 (ϵ 32000); 340 (sh) (ϵ 4000) (EtOH) (Derep).

Δ^7-Isomer: [208182-90-5] ***Euglobal G6***
$C_{23}H_{30}O_5$ 386.487Racemic
λ_{max} 275 (log ϵ 4.33); 341 (log ϵ 3.25) (hexane).

Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1952-1963 (*Euglobal IIc*)
Chiba, K. *et al., J.C.S. Perkin 1*, 1998, 2939-2942 (*synth*)
Singh, I.P. *et al., Phytochemistry*, 1998, **47**, 1157-1159 (*Euglobal G6*)

Euglobal IVb E-394

[82864-79-7]



Absolute configuration

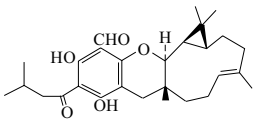
$C_{28}H_{38}O_5$ 454.605
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Prisms. Mp 187-190°. $[\alpha]_D^{20}$ -230 (c, 1.0 in $CHCl_3$).

7-Epimer: [77794-65-1] ***Euglobal IVa***
Constit. of *Eucalyptus globulus* (Tasmanian blue gum).

Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1964

Euglobal VII E-395

[77794-64-0]

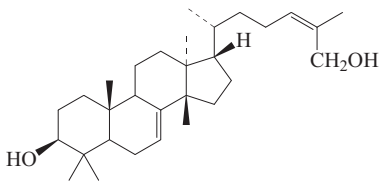


Absolute configuration

$C_{28}H_{38}O_5$ 454.605
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). $[\alpha]_D^{20}$ -137 (c, 1.0 in $CHCl_3$).

Kozuka, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1964

Eupha-7,24-diene-3,26-diol E-396



$C_{30}H_{50}O_2$ 442.724

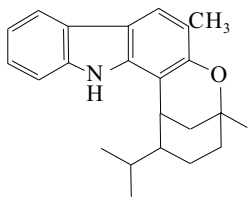
(3β,24*Z*)-*form* [6138-94-9]
Masticadienediol
Constit. of *Pistacia vera* (pistachio). Cryst. (C_6H_6). Mp 186-187°. $[\alpha]_D^{23}$ -59.6 (c, 0.7 in $CHCl_3$). λ_{max} 205 (ϵ 9700) (no solvent reported).

3-Ketone: [121063-66-9] *26-Hydroxyeupha-7,24-dien-3-one*
$C_{30}H_{48}O_2$ 440.708
Mp 137-138°. $[\alpha]_D^{20}$ -75.6 (c, 1 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1956, 4150-4157 (*synth, struct*)
Niimi, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 57-60 (*isol, pmr, cmr*)

Exozoline E-397

[70561-79-4]
1,2,3,4,5,13-Hexahydro-5,7-dimethyl-2-(1-methylethyl)-1,5-methanooxocino[3,2-a]carbazole, 9CI



$C_{23}H_{27}NO$ 333.472
Cryst. (C_6H_6/petrol). Mp 180-182°.

1′-Hydroxy: [49620-01-1] ***Murrayazolinine***. *1,2,3,4,5,13-Hexahydro-α,α,5,7-tetramethyl-1,5-methanooxocino[3,2-a]carbazole-2-methanol, 9CI*
$C_{23}H_{27}NO_2$ 349.472
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Mp 184°. Hydroxylated at the α-position of the isopropyl group.

Chakraborty, D.P. *et al., Chem. Ind. (London)*, 1973, 322 (*uv, ir, pmr, ms, struct, Murrayazolinine*)
Ganguly, S.N. *et al., Phytochemistry*, 1978, **17**, 1816 (*isol, uv, ir, pmr, ms, struct*)

Fabatin F-1

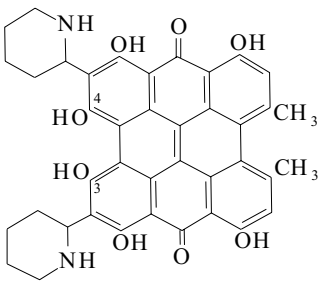
Large peptide antibiotic containing 47 AA residues. Constit. of *Vicia faba*.

Zhang, Y. *et al., FEMS Microbiol. Lett.*, 1997, **149**, 59-64 (*isol, struct*)

Fagopyrine F-2

[72393-03-4]

[72393-46-5, 72393-47-6]
1,3,4,6,8,13-Hexahydroxy-10,11-dimethyl-2,5-di-2-piperidinylphenanthro[1,10,9,8-opqra]perylene-7,14-dione, 9CI

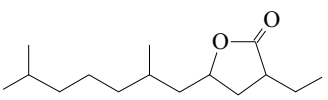


$C_{40}H_{34}N_2O_8$ 670.717
Photodynamic pigment of *Fagopyrum esculentum* (buckwheat). Violet powder. Sol. Py, to give red solns. Free base not obt. in pure state. tetra-Ac and tetrabenzoyl derivs. obt. chromatographically pure.

Brockmann, H. *et al., Annalen*, 1952, **575**, 53 (*isol*)
Brockmann, H. *et al., Tet. Lett.*, 1979, 1575 (*uv, pmr, cmr, struct*)

15,5-Farnesanolide F-3

[160775-28-0]
5-(2,6-Dimethylheptyl)-3-ethyl-3,4-dihydro-2(5H)-furanone

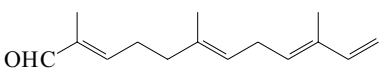


$C_{15}H_{28}O_2$ 240.385
Constit. of *Mangifera indica* (mango).

Sharma, S.K. *et al., Indian J. Nat. Prod.*, 1993, **9**, 3 (*isol*)

1,3,6,10-Farnesatetraen-12-al F-4

[17909-77-2]
2,6,10-Trimethyl-2,6,9,11-dodecatetraenal. ***α-Sinensal***†. *β-Sinensal (obsol.)*†



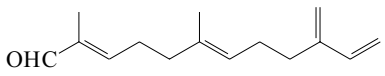
$C_{15}H_{22}O$ 218.338

The prefixes α and β originally applied to indicate order of discovery, were interchanged to correspond to β- and α-Farnesene. Constit. of orange oil. Oil. Rapidly polymerises on exp. to light and air λ_{max} 231 (log ϵ 4.57) (no solvent reported).

Flath, R.A. *et al., Tet. Lett.*, 1966, 295 (*isol, struct*)
Baumann, M. *et al., Annalen*, 1976, 1626 (*synth*)

1,3(15),6,10-Farnesatetraen-12-al F-5

[60066-88-8]
2,6-Dimethyl-10-methylene-2,6,11-dodecatrienal



$C_{15}H_{22}O$ 218.338

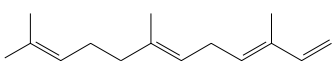
(6E,10E)-form [3779-62-2]
β-Sinensal†. *FEMA 3141*
Constit. of orange oil (*Citrus sinensis*) and mandarin oil (*Citrus reticulata*). Flavour ingredient. Oil. $Bp_{0.05}$ 92-95°. n_D^{20} 1.5077. λ_{max} 227 (ϵ 31000) (no solvent reported).

[4955-32-2, 59677-09-7]

Stevens, K.L. *et al., J.O.C.*, 1965, **30**, 1690 (*isol, struct*)
Bertele, E. *et al., Helv. Chim. Acta*, 1967, **50**, 2445 (*synth*)
Baumann, M. *et al., Annalen*, 1976, 1626 (*synth*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1979, **18**, 33 (*synth*)
Sato, K. *et al., J.C.S. Perkin 1*, 1981, 2411 (*synth*)
Mandai, T. *et al., J.O.C.*, 1983, **48**, 5183 (*synth*)
Fujisawa, T. *et al., Tet. Lett.*, 1984, **25**, 3213 (*synth*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 4051 (*synth*)

1,3,6,10-Farnesatetraene F-6

[125037-13-0]
3,7,11-Trimethyl-1,3,6,10-dodecatetraene. ***α-Farnesene****. Sesquicitronellene*



(3E,6E)-form

$C_{15}H_{24}$ 204.355
A mixt. with 1,3(15),6,10-Farnesatetraene, F-7 has been isol. from many plant sources and is used as a food flavourant (FEMA 3839).

(3E,6E)-form [502-61-4]

[21499-64-9]
Constit. of the natural coating of apples and pears and other fruit. Flavouring ingredient. Oil.

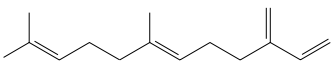
(3Z,6E)-form [26560-14-5]
Constit. of the oil of perilla (*Perilla frutescens*). Oil.

[28973-98-0, 28973-99-1]

Murray, K.E. *et al., Aust. J. Chem.*, 1969, **22**, 197 (*isol, synth*)
Brieger, G. *et al., J.O.C.*, 1969, **34**, 3789 (*synth*)
Anet, E.F.L.J. *et al., Aust. J. Chem.*, 1970, **23**, 2101 (*synth*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1970, **47**, 851 (*synth*)
Sutherland, O.R.W. *et al., J. Insect Physiol.*, 1973, **19**, 723 (*isol*)
Detrain, C. *et al., Experientia*, 1987, **43**, 345
Van der Meer, R.K. *et al., J. Chem. Ecol.*, 1988, **14**, 825 (*isol*)
Ramaiah, P. *et al., J.O.C.*, 1995, **60**, 6211 (*synth*)
Yarden, G. *et al., Bioorg. Med. Chem.*, 1996, **4**, 283 (*synth, ms*)

1,3(15),6,10-Farnesatetraene F-7

7,11-Dimethyl-3-methylene-1,6,10-dodecatriene. ***β-Farnesene***



(E)-form

$C_{15}H_{24}$ 204.355
A mixt. with 1,3,6,10-Farnesatetraene, F-6 has been isol. from many plant sources and is used as a food flavourant (woody-green flavour).

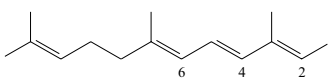
(E)-form [18794-84-8]
Constit. of hop, camomile and other essential oils. Oil. Bp_9 121-122°.

(Z)-form [28973-97-9]
Oil.

Naves, Y.R. *et al., Helv. Chim. Acta*, 1966, **49**, 1029 (*uv, ir, pmr*)
Brieger, G. *et al., J.O.C.*, 1969, **34**, 3789 (*synth*)
Anet, E.F.L.J. *et al., Aust. J. Chem.*, 1970, **23**, 2101 (*synth*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1975, **13**, 1244 (*synth*)
Tanaka, S. *et al., J.A.C.S.*, 1975, **97**, 3252 (*synth*)
Mandai, T. *et al., J.O.C.*, 1983, **48**, 2601 (*isol*)
Harvey, S. *et al., J. Chem. Ecol.*, 1989, **15**, 2061
Baeckström, P. *et al., Synth. Commun.*, 1990, **20**, 423 (*synth*)
Khallouki, F. *et al., Fitoterapia*, 2000, **71**, 544-546 (*activity*)

2,4,6,10-Farnesatetraene F-8

3,7,11-Trimethyl-2,4,6,10-dodecatetraene. ***Allofarnesene***



(2E,4E,6E)-form

$C_{15}H_{24}$ 204.355
Isol. (without stereochemical distinction) from oil of *Cymbopogon nardus* (citronella), *Cananga odorata* (ylang ylang) and others. $Bp_{4.4}$ 121-122°.

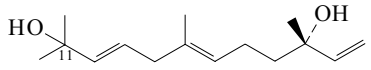
(2E,4E,6E)-form [6980-88-7]
Constit. of *Perilla frutescens* (perilla). Oil.

(2Z,4E,6E)-form [26560-15-6]
Constit. of *Perilla frutescens* (perilla). Oil.

Naves, Y.R. *et al., Helv. Chim. Acta*, 1966, **49**, 1029 (*synth, uv, ir, pmr*)
Sakai, T. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 3615 (*isol*)
Brieger, G. *et al., J.O.C.*, 1969, **34**, 3789 (*synth*)
Miyaura, N. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2221 (*synth*)

1,6,9-Farnesatriene-3,11-diol F-9

[58865-89-7]
2,6,10-Trimethyl-3,6,11-dodecatriene-2,10-diol



$C_{15}H_{26}O_2$ 238.369
Constit. of *Solanum melongena* (aubergine). Oil. $[\alpha]_D^{23}$ +14 (c, 1.0 in CCl_4).

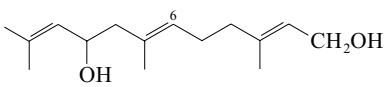
11-Me ether: [145385-71-3] ***11-Methoxy-3,7,11-trimethyl-1,6,9-dodecatrien-3-ol***
$C_{16}H_{28}O_2$ 252.396
$[\alpha]_D$ +9.9 (c, 0.6 in $CHCl_3$).

[54877-98-4]

Stoessl, A. *et al., Can. J. Chem.*, 1975, **53**, 3351 (*isol, uv, ms, pmr*)
Zdero, C. *et al., Phytochemistry*, 1989, **28**, 3105 (*isol, pmr*)
Grande, M. *et al., J. Nat. Prod.*, 1992, **55**, 1074 (*isol, pmr, cmr*)

2,6,10-Farnesatriene-1,9-diol F-10

3,7,11-Trimethyl-2,6,10-dodecatriene-1,9-diol, 9CI. 9-Hydroxyfarnesol



$C_{15}H_{26}O_2$ 238.369
(2*E*,6*E*,9ξ)-*form* [79421-77-5]
Stress metab. of *Ipomoea batatas* (sweet potato).

1-Ac: [152100-12-4]
$C_{17}H_{28}O_3$ 280.406
Oil.

9-Ac: [74323-51-6] ***9-Acetoxyfarnesol***
$C_{17}H_{28}O_3$ 280.406
Oil.

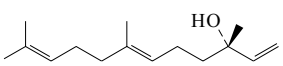
(2*Z*,6*E*,9ξ)-*form*
6,7-Dihydro, 1-(9-octadecenoyl):9-Hydroxyfarnesyl oleate
$C_{33}H_{60}O_3$ 504.835
Gum.

[74323-52-7, 79465-43-3]

Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 149 (*9-Acetoxyfarnesol*)
Burka, L.T. *et al., Phytochemistry*, 1981, **20**, 647 (*isol, synth, ir, pmr, cmr*)
Appendino, G. *et al., Phytochemistry*, 1993, **34**, 1171 (*isol, pmr, cmr*)
De Gutiérrez, A.N. *et al., Phytochemistry*, 1995, **39**, 795 (*Oleate*)

1,6,10-Farnesatrien-3-ol F-11

[7212-44-4]
3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol. ***Nerolidol****. Peruviol. Melaleucol. Humbertiol*†



(*S*)-*form*

$C_{15}H_{26}O$ 222.37
Identity of Humbertiol with Nerolidol shown in 1992. A component of many essential oils. The (*S*)-enantiomer is the commoner and occurs mostly as the (*S*)-(*E*)-isomer. Flavouring agent.
(*S*)-*form* [142-50-7]
Flavouring agent. Constit. of Peru balsam and from many other sources. Oil. $Bp_{0.2}$ 97° Bp 276°. $[\alpha]_D$ +10.7 (c, 0.9 in $CHCl_3$). $[\alpha]_D$ +15.5.

O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [130466-30-7]
$C_{27}H_{46}O_{10}$ 530.654
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ -25.4 (c, 1 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{33}H_{56}O_{14}$ 676.797
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ -41 (c, 1 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [130466-33-0]
$C_{33}H_{56}O_{14}$ 676.797
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ -40 (c, 1 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [130466-32-9]
$C_{39}H_{66}O_{18}$ 822.94
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ -50 (c, 1 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[4-(4-hydroxy-3-methoxycinnamoyl)-(E)-α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [143376-48-1]
$C_{49}H_{74}O_{21}$ 999.111
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ -70 (c, 1 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [116174-69-7] ***Loquatifolin A***
$C_{39}H_{66}O_{18}$ 822.94
Constit. of *Eriobotrya japonica* (loquat). Cryst. + $1\frac{1}{2}H_2O$. Mp 128-130°. $[\alpha]_D^{22}$ -79.7 (EtOH).

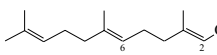
Ac: [2306-78-7] ***Nerolidyl acetate***
$C_{17}H_{28}O_2$ 264.407
Found in clary sage oil. Colourless to pale yellow liq. d_4^{20} 0.9 d_{25}^{25} 0.9.
► Skin irritant. JR4980000
(±)-*form* [40716-66-3]
Bp_{12} 145-146°. n_D^{20} 1.4790.

[2211-29-2, 3790-78-1, 28625-25-4, 56001-43-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 149A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 223C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 219C (*ir*)
Naves, Y.R. *et al., Helv. Chim. Acta*, 1947, **30**, 278 (*synth*)
Vlad, P. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 1726 (*abs config*)
Naves, Y.R. *et al., Helv. Chim. Acta*, 1963, **46**, 2551 (*uv*)
Borges, J. *et al., Tet. Lett.*, 1966, 3731 (*isol*)
Hill, H.C. *et al., J.C.S.(C)*, 1968, 93 (*ms*)
Raulais, D. *et al., Bull. Soc. Chim. Fr.*, 1970, 2401 (*Humbertiol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 124 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 887 (*rev, tox*)
Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1976, 513 (*synth*)
Care, D.E. *et al., J.A.C.S.*, 1981, **103**, 914 (*pmr*)
Yanagisawa, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1270 (*Loquatifolin A*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NCN700
De Tommasi, N. *et al., J. Nat. Prod.*, 1990, **53**, 810; 1992, **55**, 1025 (*glycosides*)
Weyerstahl, P. *et al., Annalen*, 1992, 1325 (*struct*)
Donath, J. *et al., Phytochemistry*, 1995, **39**, 785 (*biosynth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1288 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NCN800

2,6,10-Farnesatrien-1-ol F-12

[4602-84-0]
3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol. ***Farnesol****. FEMA 2478*



(2*E*,6*E*)-*form*

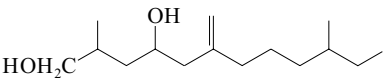
$C_{15}H_{26}O$ 222.37
► LD_{50} (rat, orl) 6000 mg/kg. JR4979000
(2*E*,6*E*)-*form* [106-28-5]
Flavouring ingredient. Liq. with a characteristic flowery odour. Bp_3 137°.

[24163-97-1, 40266-29-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 149B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 226B; 226C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 219D; 220A (*ir*)
Bates, R.B. *et al., J.O.C.*, 1963, **28**, 1086 (*isol, struct*)
Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1967, **89**, 4245 (*synth*)
Hill, H.C. *et al., J.C.S.(C)*, 1968, 93 (*ms*)
Nilles, G. *et al., J. Agric. Food Chem.*, 1973, **21**, 342 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1975, 913 (*cmr*)
Cardillo, C.R. *et al., Chem. Comm.*, 1976, 190 (*synth*)
Pauling, H. *et al., Helv. Chim. Acta*, 1976, **59**, 1233 (*synth*)
Org. Synth., 1977, **56**, 112-117 (*synth, ir*)
Pickett, J.A. *et al., J. Chem. Ecol.*, 1980, **6**, 425 (*isol*)
Van Tamelen, E.E. *et al., Bioorg. Chem.*, 1982, **11**, 133-170 (*synth*)
Wheller, J.W. *et al., J. Chem. Ecol.*, 1982, **8**, 821 (*isol*)
Amin, C *et al., Helv. Chim. Acta*, 1984, **67**, 1540-1546 (*synth, ir, pmr, ms*)
Yamagisawa, A. *et al., Chem. Lett.*, 1988, 1899-1902 (*synth*)
Andersen, J.F. *et al., J. Chem. Ecol.*, 1988, **14**, 1153 (*isol*)
Christensen, D.J. *et al., Bioorg. Med. Chem.*, 1994, **2**, 631 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 277
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1059-1060
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAB800

7(14)-Farnesene-9,12-diol F-13

[160775-29-1]
2,10-Dimethyl-6-methylene-1,4-dodecanediol

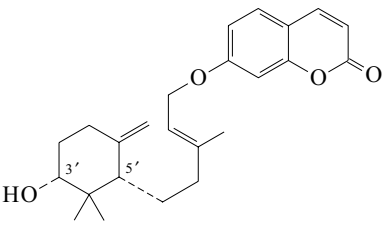


$C_{15}H_{30}O_2$ 242.401
Constit. of *Mangifera indica* (mango).

Sharma, S.K. *et al., Indian J. Nat. Prod.*, 1993, **9**, 3 (*isol*)

Farnesiferol B F-14

[54990-68-0]
7-[[3-Methyl-5-(3-hydroxy-2,2-dimethyl-6-methylene)cyclohexyl-2-pentenyl]oxy]-2H-1-benzopyran-2-one, 9CI. Kopeodin



$C_{24}H_{30}O_4$ 382.499
Constit. of *Ferula assa-foetida* (asafoetida). Prisms (EtOH aq.). Mp 112.5-113.5°. $[\alpha]_D$ +10 (c, 1.20 in $CHCl_3$).

Ac:
Needles (Et_2O/petrol). Mp 70.5-71.5°. $[\alpha]_D$ -18 (c, 1.1 in $CHCl_3$).

3′-Epimer: [70878-84-1] ***Latilobinol***
$C_{24}H_{30}O_4$ 382.499
Cryst. Mp 121-122°. $[\alpha]_D^{18}$ -63 (c, 0.92 in $CHCl_3$).

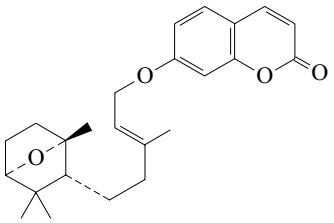
$\Delta^{5'}$-Isomer (1): [81800-58-0] ***Lehmferin***
$C_{24}H_{30}O_4$ 382.499
Cryst. Mp 118-119°.

$\Delta^{5'}$-Isomer (2): [115361-83-6] ***Assafoetidin***
Constit. of *Ferula assa-foetida* (asafoetida). Needles. Mp 112°. $[\alpha]_D$ +11.25 ($CHCl_3$). 3′-Config. not detd. May be identical with Lehmferin or may be the 3′-epimer (i.e. enantiomer).

Caglioti, L. *et al., Helv. Chim. Acta*, 1958, **41**, 2278; 1959, **42**, 2557
Kamilov, K.M. *et al., Khim. Prir. Soedin.*, 1973, **9**, 308; 1974, **10**, 442; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 294; 1974, **10**, 450 (*isol*)
Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1979, **15**, 90; 1984, **20**, 712; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 75; 1984, **20**, 674 (*Latilobinol*)
Sagitdinova, G.V. *et al., Khim. Prir. Soedin.*, 1983, **19**, 709; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 672 (*Lehmferin*)
Banerji, A. *et al., Tet. Lett.*, 1988, **29**, 1557 (*Assafoetidin*)
Nassar, M.I. *et al., Pharmazie*, 1994, **49**, 542 (*pmr, cmr, ms*)

Farnesiferol C F-15

7-[[3-Methyl-5-(1,3,3-trimethyl-7-oxabicyclo[2.2.1]hept-2-yl)-2-pentenyl]oxy]-2H-1-benzopyran-2-one, 9CI



$C_{24}H_{30}O_4$ 382.499

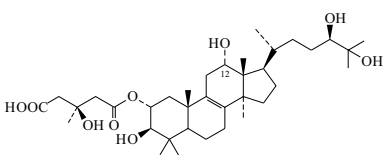
(-)-*form* [512-17-4]
Constit. of *Ferula assa-foetida* (asafoetida). Needles (Et_2O/hexane). Mp 83.5-84.5°. $[\alpha]_D$ -29.6 (c, 0.78 in $CHCl_3$).

(±)-*form*
Mp 85-87.5°.

Caglioti, L. *et al., Helv. Chim. Acta*, 1958, **41**, 2278; 1959, **42**, 2557
v. Tamelen, E.E. *et al., Chem. Comm.*, 1966, 413 (*synth*)
Bagirov, A.Yu. *et al., Khim. Prir. Soedin.*, 1977, **13**, 279; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 240
Mukaiyama, T. *et al., Chem. Lett.*, 1981, 29 (*synth*)
van Tamelen, E.E. *et al., Bioorg. Chem.*, 1982, **11**, 171 (*synth*)
Demnitz, F.W.J. *et al., J.O.C.*, 1995, **60**, 5114 (*synth, ir, pmr, cmr, ms*)

Fasciculic acid B F-16

[126882-55-1]



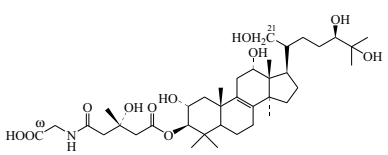
$C_{36}H_{60}O_9$ 636.865
Isol. from the toxic sulphur tuft mushroom *Naematoloma fasciculare*. Powder. Mp 98-103°. $[\alpha]_D^{26}$ +19.3 (c, 1 in MeOH). λ_{max} 202 (ε 7940) (MeOH) (Berdy).

12-Deoxy: [126906-00-1] ***Fasciculic acid A***
$C_{36}H_{60}O_8$ 620.865
From the toxic sulphur tuft mushroom *Naematoloma fasciculare*. Needles (MeOH/$CHCl_3$). Mp 177-179°. $[\alpha]_D^{27}$ +8.3 (c, 1 in MeOH). λ_{max} 201 (ε 13780) (MeOH) (Berdy).

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3247 (*isol*)
Nozoe, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1738 (*als config*)

Fasciculic acid C F-17

[126882-56-2]



$C_{38}H_{63}NO_{11}$ 709.916
Complex acyl deriv. of Lanost-8-ene-2,3,12,21,24,25-hexol, L-43. Isol. from the toxic sulphur tuft mushroom *Naematoloma fasciculare*. Pale yellow powder. Mp 141-144°. $[\alpha]_D^{28}$ +36.3 (c, 1 in MeOH). λ_{max} 201 (ε 13500) (MeOH) (Berdy).

ω-Me ester: [65694-20-4] ***Fasciculol E***
$C_{39}H_{65}NO_{11}$ 723.943
Constit. of mushroom *Naematoloma fasciculare*. Amorph. solid. λ_{max} 208 (ε 5000) (MeOH) (Berdy).

▶ Toxic ; LD_{50} (mus, ipr) 5O mg/kg.

2-Acyl isomer: [261638-74-8] ***Fasciculic acid D***
$C_{38}H_{63}NO_{11}$ 709.916

2-Acyl isomer, ω-Me ester: [65694-21-5] ***Fasciculol F***
$C_{39}H_{65}NO_{11}$ 723.943
Constit. of mushrooms *Naematoloma fasciculare* and *Naematoloma sublateritum*. Cryst. Mp 103-105°. $[\alpha]_D^{20}$ +20.4 (c, 0.27 in MeOH). λ_{max} 208 (ε 5000) (MeOH) (Berdy).

▶ Toxic ; LD_{50} (mus, ipr) 168 mg/kg.

21-Deoxy, ω-Me ester: [69770-64-5] ***Fasciculol G***
$C_{39}H_{65}NO_{10}$ 707.943

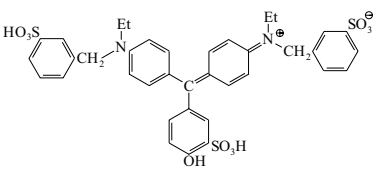
21-Deoxy, 2-acyl isomer: [261638-75-9] ***Fasciculic acid E***
$C_{38}H_{63}NO_{10}$ 693.916

21-Deoxy, 2-acyl isomer, ω-Me ester: [64971-23-9] ***Fasciculol D***
$C_{39}H_{65}NO_{10}$ 707.943
Sol. MeOH. Mp 95-97°. $[\alpha]_D$ +14.1 (MeOH). λ_{max} 208 (ε 3900) (MeOH) (Berdy).

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3247 (*isol*)
Kleinwachter, P. *et al., J. Basic Microbiol.*, 1999, **39**, 345-349 (*Fasciculic acids*)

Fast green FCF F-18

[2353-45-9]
N-*Ethyl*-N-*[4-[[4-[ethyl[(3-sulfophenyl)-methyl]amino]phenyl](4-hydroxy-2-sulfophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-3-sulfobenzenemethanaminium hydroxide inner salt, 9CI. C.I. Food green 3. C.I. 42053. FD and C Green No. 3*



$C_{37}H_{36}N_2O_{10}S_3$ 764.897
Strictly, the name Fast green FCF refers to the disodium salt. FDA permitted food colourant used in beverages, desserts, candies, baking goods, dairy products and maraschino cherries. Dark green cryst. (as di-Na salt). Sol. H_2O, EtOH, acids (di-Na salt). Mp 290° dec. (di-Na salt). CAS no. refers to di-Na salt λ_{max} 622 (no solvent reported).

Al salt:
FDA permitted colourant for foods and

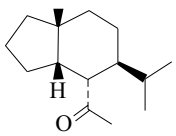
food contact paper or board. Lake.

Ca salt:
FDA permitted colourant for food and food contact paper or board. Lake.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1033C (*ir*)
Johnson, H. *et al., Ind. Eng. Chem.*, 1927, **19**, 497 (*synth*)
Dutt, V.V.S.E. *et al., Fresenius' Z. Anal. Chem.*, 1972, **258**, 32 (*use*)
Dutt, V.V.S.E. *et al., Indian J. Chem.*, 1972, **10**, 560 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1072-1075 (*use*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 345
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG000

Faurinone F-19

[21682-87-1]

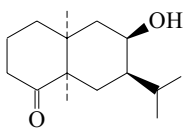


$C_{15}H_{26}O$ 222.37
Constit. of essential oil of *Valeriana officinalis* (valerian). Oil.

Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1779 (*isol*)
Bos, R. *et al., Phytochemistry*, 1983, **22**, 1505 (*struct*)

Fauronol F-20

[25146-17-2]



$C_{15}H_{26}O_2$ 238.369

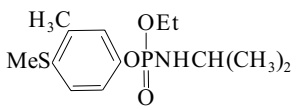
Ac: [2658-82-4] ***Fauronyl acetate***
$C_{17}H_{28}O_3$ 280.406
Constit. of root of *Valeriana officinalis* var. *latifolia*. Mp 85-86°. $[\alpha]_D$ -77.6.

Ac, semicarbazone:
Mp 218.5-220°.

Hikino, H. *et al., Chem. Pharm. Bull.*, 1965, **13**, 631; 1966, **14**, 735 (*isol, struct, abs config*)
Sammes, P.G. *et al., J.C.S. Perkin 1*, 1986, 281 (*synth*)

Fenamiphos, BSI F-21

[22224-92-6]
*Ethyl 3-methyl-4-(methylthio)phenyl 1-methylethylphosphoramidate, 9CI. Ethyl 4-methylthio-*m*-tolyl isopropylphosphoramidate, 8CI. Nemacur. Phenamiphos*

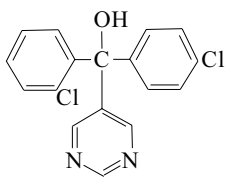


$C_{13}H_{22}NO_3PS$ 303.361
Systemic agricultural nematocide. Cholinesterase inhibitor.
▶ LD_{50} (rat, orl) 8 mg/kg. LD_{50} (rbt, skn) 178 mg/kg. ACGIH TLV 0.1 mg m^{-3} (Sk). TB3675000
(±)-form
Solid. Spar. sol. H_2O. Mp 49°.
S-*Oxide:* [31972-43-7]
$C_{13}H_{22}NO_4PS$ 319.361
n_D^{19} 1.5274.
S,S-*Dioxide:* [31972-44-8]
$C_{13}H_{22}NO_5PS$ 335.36
Mp 77°.

Ger. Pat., 1971, 1 934 001; *CA*, **74**, 141266f (*oxides*)
Waggoner, T.B. *et al., J. Agric. Food Chem.*, 1972, **20**, 157-160 (*metab*)
Waggoner, T.B. *et al., Residue Rev.*, 1974, **53**, 79-97 (*rev, pharmacol*)
Ripley, B.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 1084-1095 (*glc*)
Bowman, B.T. *et al., J. Environ. Sci. Health, Part B*, 1983, **18**, 221-227 (*props*)
Wilkins, J.P.G. *et al., Analyst (London)*, 1985, **110**, 1045-1051 (*glc-ms*)
Prinsloo, S.M. *et al., J. Assoc. Off. Anal. Chem.*, 1985, **68**, 1100-1108 (*glc*)
Bellar, T.A. *et al., Anal. Chem.*, 1988, **60**, 2076-2083 (*ms, hplc, oxides*)
Singh, R. *et al., Analyst (London)*, 1989, **114**, 425-427 (*hplc, oxides*)
Lacorte, S. *et al., J. Chromatogr., A*, 1995, **712**, 103-112 (*hplc, ms, detn*)
Terreni, M. *et al., Tetrahedron*, 1995, **51**, 7981-7992 (*S-oxide, S,S-dioxide*)
Pesticide Manual, 11th edn., 1997, No. 299
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAK000

Fenarimol, ANSI, BSI, ISO F-22

[60168-88-9]
α-(2-Chlorophenyl)-α-(4-chlorophenyl)-5-pyrimidinemethanol, 9CI. 2,4′-Dichloro-α-(5-pyrimidinyl)benzhydryl alcohol. Bloc. Rimidin. Rubigan

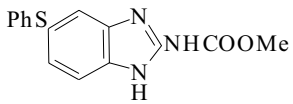


$C_{17}H_{12}Cl_2N_2O$ 331.2
▶ UV9279400
(±)-form
Agricultural and horticultural fungicide. Cryst. Mp 117-119°.
▶ LD_{50} (rat, orl) 2500 mg/kg. Exp. reprod. effects.

U.K. Pat., 1967, 1 218 623; *CA*, **72**, 100745b
Day, E.W. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1984, **13**, 173 (*detn*)
Sisler, H.D. *et al., Pestic. Sci.*, 1984, **15**, 167 (*rev, activity*)
Taylor, H.M. *et al., J. Med. Chem.*, 1987, **30**, 1359 (*synth*)
Albinati, A. *et al., Acta Cryst. C*, 1988, **44**, 1782 (*cryst struct*)
Gardyan, C. *et al., Z. Lebensm.-Unters. - Forsch.*, 1991, **192**, 40 (*hplc*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A193
Pesticide Manual, 11th edn., 1997, No. 300
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAK100

Fenbendazole, BAN, INN, USAN F-23

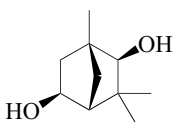
[43210-67-9]
*Methyl 5-phenylthio-1*H*-benzimidazol-2-ylcarbamate. Axilur. Panacur. Pancacur. Safe-Guard. Worm-A-Rest. Hoe 881*



$C_{15}H_{13}N_3O_2S$ 299.353
Veterinary anthelmintic. FDA approved for use in cattle, pigs and goats. Powder. Mp 233° dec. Log P 4.6 (calc).
▶ Mutagenic props.. DD6520500

Baeder, C. *et al., Experientia*, 1974, **30**, 753
Ger. Pat., 1974, 2 332 486; *CA*, **83**, 43324q
Averkin, E.A. *et al., J. Med. Chem.*, 1975, **18**, 1164 (*synth, pharmacol*)
Duewel, D. *et al., Pestic. Sci.*, 1977, **8**, 550 (*props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 43
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAL100

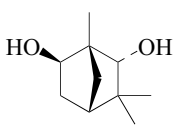
2,5-Fenchanediol F-24



$C_{10}H_{18}O_2$ 170.251
(1R,2S,4R,5S)-form
2-O-*β*-D-*Glucopyranoside:* [217960-83-3]
$C_{16}H_{28}O_7$ 332.393
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -3.5 (c, 0.4 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

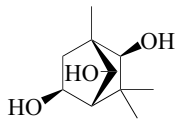
2,6-Fenchanediol F-25



$C_{10}H_{18}O_2$ 170.251
(1R,2R,4S,6R)-form
2-O-*β*-D-*Glucopyranoside:* [217960-81-1]
$C_{16}H_{28}O_7$ 332.393
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -34.8 (c, 0.6 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

2,5,7-Fenchanetriol F-26



$C_{10}H_{18}O_3$ 186.25

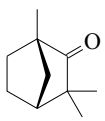
(1*S*,2*S*,4*R*,5*S*,7*S*)-*form*

2-O-β-D-Glucopyranoside: [217960-85-5]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 211-213°. $[\alpha]_D^{23}$ -6.5 (c, 0.3 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

Fenchone F-27

[1195-79-5]
1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one, 9CI. Fenchol (obsol.). FEMA 2479



(+)-*form*

$C_{10}H_{16}O$ 152.236

► Skin irritant. LD_{50} (rat, orl) 4400 mg/kg. Fl. p. 65°. RB7875000

(+)-*form* [7787-20-4]
Widespread in plants, e.g. found in fennel (*Foeniculum vulgare*). Flavouring ingredient. Oil with camphoraceous odour. Prac. insol. H_2O, v. sol. EtOH; Sol. MeOH, hexane. Mp 3-5° Fp 5-6. Bp 193.5°. $[\alpha]_D^{29}$ +63. $[\alpha]_D^{21}$ +48 (c, 0.2 in CCl_4).

(-)-*form* [4695-62-9]
Isol. from various essential oils. Flavouring ingredient. $[\alpha]_D$ -67.

► RB7875200

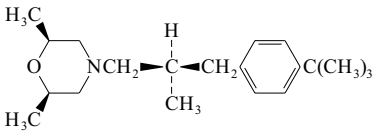
(±)-*form* [18492-37-0]
Bp 192-194°.

[74163-80-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 442B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 678B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 527C (*ir*)
Komppa, G. *et al., Ber.*, 1935, **68**, 2001 (*synth*)
Bays, D.E. *et al., J.C.S.(B)*, 1966, 885 (*cd*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1967, **50**, 826 (*ms*)
Baker, K.M. *et al., Tetrahedron*, 1968, **24**, 1663 (*pmr*)
Lipman, E. *et al., Org. Magn. Reson.*, 1970, **2**, 581 (*cmr*)
Boyle, P.H. *et al., J.C.S.(C)*, 1971, 2136 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 769 (*rev, tox*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 228
Buchbauer, G. *et al., Annalen*, 1981, 2093 (*synth*)
Wijekoon, W.M.D. *et al., J. Phys. Chem.*, 1983, **87**, 3034 (*pmr, cmr, uv, cd*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 278 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLW250

Fenpropimorph, BSI, ISO F-28

[67306-03-0]
*4-[3-[4-(1,1-Dimethylethyl)phenyl]-2-methylpropyl]-2,6-dimethylmorpholine, 9CI. 4-[3-(4-*tert*-Butylphenyl)-2-methylpropyl]-2,6-dimethylmorpholine. Corbel*



(*R*)-*form*

$C_{20}H_{33}NO$ 303.487
Agricultural fungicide used against powdery mildews on sugar beet, beans and leeks.

► QE2060000

(R)*-*form [67564-91-4]

► QE1940000

(S)*-*form [186691-34-9]
Mp 173-174° (as hydrochloride). Obt. aqs hydrochloride with 95.1% ee. No opt. rotn. reported. CAS no. refers to hydrochloride.

(±)-*form*
Oil. $Bp_{0.05}$ 120°. pK_a 7.02 (basic).

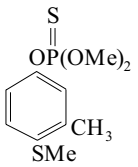
► LD_{50} (rat, orl) 3000 mg/kg.

[67564-92-5, 67564-93-6, 76492-89-2, 76492-90-5, 76492-92-7, 127738-75-4, 128141-83-3, 130462-20-3]

Bohnen, K. *et al., Meded. Fac. Landbouwwet., Rijksuniv. Gent*, 1979, **44**, 487; 499 (*rev, props, tox, use*)
Himmele, W. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 184
Ger. Pat., 1980, 2 907 614; *CA*, **94**, 65703s (*synth, resoln*)
Polak, A. *et al., Ann. N.Y. Acad. Sci.*, 1988, **544**, 221 (*rev*)
Jensen, J.S. *et al., Acta Cryst. C*, 1990, **46**, 779 (*cryst struct*)
Basarab, G.S. *et al., ACS Symp. Ser.*, 1992, **504**, 414 (*synth, activity*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A201
Sandholm Jensen, J. *et al., Pestic. Sci.*, 1992, **36**, 309 (*conformn*)
Avdagić, A. *et al., Synthesis*, 1995, 1427 (*S-form*)
Pesticide Manual, 11th edn., 1997, No. 314
Vinković, V. *et al., Tetrahedron*, 1997, **53**, 689-696; 1998, **54**, 9123-9128 (*S-form, synth, hplc*)

Fenthion, BAN, BSI F-29

[55-38-9]
O,O-*Dimethyl* O-*[(3-methyl-4-methylthio)phenyl] phosphorothioate, 9CI.* O,O-*Dimethyl*-O-*(4-methylthio*-m-*tolyl) phosphorothioate, 8CI. 4-Methylmercapto-3-methylphenyl dimethyl thiophosphate. Mercaptophos. Baytex. Lebaycid. Quelethox. Spotton. Talodex. Bayer 29493. ENT 25540. S 1752*



$C_{10}H_{15}O_3PS_2$ 278.332
Insecticide with low mammalian toxicity. Used in agriculture and against mosquito larvae in tropical fresh waters. Liq. with slight garlic odour. V. spar. sol. H_2O. d_4^{20} 1.25. $Bp_{0.01}$ 87°. n_D^{20} 1.5698. Log P 3.91 (calc). Thermally stable to 210°, alkali-resistant to pH 9. Metab. *via* sulfoxide and sulfone. Component of Tiguvon.

► LD_{50} (rat, orl) 180 mg/kg; LD_{50} (rat, skn) 330 mg/kg. Can cause delayed neurotoxic symptoms and retinal changes. Occup. exposure can cause numbness, tingling of extremities and muscle weakness. ACGIH TLV: long-term 0.2 mg m^{-3} (sk). TF9625000

S-*Oxide:* [3761-41-9] O,O-*Dimethyl* O-*[(3-methyl-4-methylsulfinyl)phenyl] phosphorothioate. Fenthion sulfoxide*
$C_{10}H_{15}O_4PS_2$ 294.332Stereochem. not detd..

► TF9400000

S,S-*Dioxide:* [3761-42-0] O,O-*Dimethyl* O-*[(3-methyl-4-methylsulfonyl)phenyl] phosphorothioate. Fenthion sulfone*
$C_{10}H_{15}O_5PS_2$ 310.331

► TF9420000

Ger. Pat., 1961, 1 116 656; *CA*, **56**, 14170 (*synth, props*)
Ibrahim, F.B. *et al., J. Agric. Food Chem.*, 1966, **14**, 369 (*uv*)
Keith, L.H. *et al., J. Assoc. Off. Anal. Chem.*, 1968, **51**, 1063 (*pmr*)
Getz, M.E. *et al., J. Assoc. Off. Anal. Chem.*, 1968, **51**, 1101 (*tlc*)
Ross, R.T. *et al., Anal. Chim. Acta*, 1970, **52**, 139 (*P nmr*)
Stan, H.-J. *et al., Fresenius' Z. Anal. Chem.*, 1977, **287**, 271 (*glc*)
Rainsford, K.D. *et al., Pestic. Biochem. Physiol.*, 1978, **8**, 302 (*tox, metab*)
Stan, H.-J. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 483 (*ms*)
Agrochemicals Handbook, Royal Society of Chemistry, 1983, A203
Ripley, B.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 1084 (*derivs, glc*)
Stan, H.-J. *et al., J. Chromatogr.*, 1983, **279**, 173 (*glc*)
Pesticide Manual, 9th edn., 1991, No. 6280
Ballantyne, B. *et al., Clinical and Experimental Toxicology of Organophosphates and Carbamates*, Butterworth-Heineman, Oxford, 1992,
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1127
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 301
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1023
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DSS400; DSS800; FAQ900

Fenugreekine F-30

[55069-02-8]

C_{27} steroid sapogenin peptide ester. Isol. from the seeds of *Trigonella foenum-*

graecum (fenugreek). Cryst. Mp 202-208°. $[\alpha]_D^{25}$ +43 (c, 0.528 in AcOH).

Ghosal, S. *et al., Phytochemistry*, 1974, **13**, 2247 (*isol*)

Totte, J. *et al., Farm. Tijdschr. Belg.*, 1983, **60**, 203 (*rev*)

Fenugrin B F-31

[70896-47-8]

Struct. unknown. Isol. from seeds of *Trigonella foenum-graecum* (fenugreek).

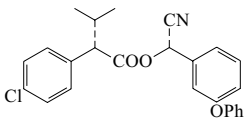
[70896-48-9]

Gangrade, H. *et al., Indian Drugs Pharm. Ind.*, 1979, **16**, 149; *CA*, **91**, 52711f (*isol*)

Fenvalerate, BAN, BSI, ISO F-32

[51630-58-1]

Cyano(3-phenoxyphenyl)methyl 4-chloro-α-(1-methylethyl)benzeneacetate, 9CI. α-Cyano-3-phenoxybenzyl 2-(4-chlorophenyl)-3-methylbutyrate. Belmark. Pydrin. Sumicidin. Ectrin. Fenval. Fenkill



(*S,S*)-*form*

$C_{25}H_{22}ClNO_3$ 419.906

Agricultural, public health and animal husbandry insecticide. Viscous yellow liq. d_{25}^{25} 1.18. Bp_{37} 300°.

►LD_{50} (rat, orl) 451 mg/kg. CY1576350

(*S,S*)-*form* [66230-04-4]

Esfenvalerate, BSI, ISO. *Sumi-alpha. Asana. Fenvalerate α*

Cryst. d_4^{26} 1.26. Mp 59-60°. $[\alpha]_D^{25}$ -15 (c, 2.0 in MeOH).

►CY1576367

[66267-77-4, 67614-32-8, 67614-33-9, 67890-39-5, 67890-40-8, 73367-17-6, 73367-18-7]

U.K. Pat., 1972, 1 439 615; *CA*, **80**, 120746w

Hattori, J. *et al., Jpn. Pestic. Inf.*, 1977, **33**, 13 (*rev, props*)

Aketa, K. *et al., Agric. Biol. Chem.*, 1978, **42**, 895 (*synth, pmr, activity*)

Ger. Pat., 1978, 2 737 297; *CA*, **88**, 152268y (*esfenvalerate*)

Yoshioka, H. *et al., Rev. Plant. Prot. Res.*, 1978, **11**, 39 (*rev, synth, tox*)

Horiba, M. *et al., Agric. Biol. Chem.*, 1982, **46**, 3041 (*abs config, bibl*)

Papadopoulou-Mourkidou, E. *et al., Residue Rev.*, 1983, **89**, 179 (*rev, detn*)

Wheeler, T.N. *et al., J. Agric. Food Chem.*, 1984, **32**, 1125 (*synth, activity*)

U.S. Pat., 1984, 4 432 908; *CA*, **100**, 209428y (*cryst struct*)

Oo'uchi, H. *et al., Jpn. Pestic. Inf.*, 1985, **46**, 21 (*esfenvalerate*)

Mikami, N. *et al., Pestic. Sci.*, 1985, **16**, 46 (*metab*)

Miyamoto, J. *et al., ACS Symp. Ser.*, 1986, **299**, 268 (*rev, tox*)

Lidgard, R.O. *et al., Biomed. Environ. Mass Spectrom.*, 1986, **13**, 677 (*ms*)

Papadopoulou-Mourkidou, E. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1988, **16**, 31 (*hplc*)

IARC Monog., 1991, **53**, 309 (*rev, tox*)

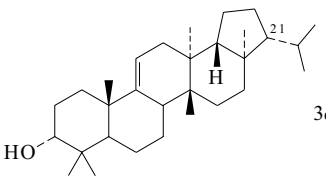
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A990; A207

Pesticide Manual, 11th edn., 1997, No. 319; *Pesticide Manual, 9th edn.*, 1991, 6340

Luzzio, F.A. *et al., J. Prakt. Chem.*, 2000, **342**, 498-501 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAR100

9(11)-Fernen-3-ol F-33



3α-*form*

$C_{30}H_{50}O$ 426.724

3α-*form* [29291-51-8]

3-Epifernenol

Cryst. ($CHCl_3$/MeOH). Mp 219-222°. $[\alpha]_D$ -15.6 (c, 0.64 in $CHCl_3$).

3β-*form* [4966-00-1]

Fernenol. *α-Fernenol*

Constit. of *Artemisia vulgaris* (mugwort). Cryst. Mp 192-193°. $[\alpha]_D$ -19.4 (c, 0.8 in $CHCl_3$).

Ac: [17884-58-1]

$C_{32}H_{52}O_2$ 468.762

Mp 218-220° Mp 222-223°. $[\alpha]_D^{26}$ -9.5 (c, 1 in $CHCl_3$).

Hexadecanoyl:Fernenol palmitate

$C_{46}H_{80}O_2$ 665.137

Mp 160-174°. $[\alpha]_D^{26}$ -10.5 (c, 1 in $CHCl_3$).

Me ether: [4555-56-0] *3β-Methoxy-9(11)-fernene.* ***Arundoin***

$C_{31}H_{52}O$ 440.751

Cryst. (hexane). Mp 242-243°. $[\alpha]_D$ -5.3 (c, 0.8 in $CHCl_3$).

3-Ketone: [6090-29-5] *9(11)-Fernen-3-one.* ***Fernenone***. *α-Fernenone*

$C_{30}H_{48}O$ 424.709

Cryst. (MeOH). Mp 198-199°. $[\alpha]_D^{23}$ -41.2 (c, 0.4 in $CHCl_3$).

(3β,21α*H*)-*form* [64554-36-5] ***Trematol***

Cryst. ($CHCl_3$/MeOH). Mp 215-216°. $[\alpha]_D$ -27.8 ($CHCl_3$).

3-Ketone: ***Trematone***. *β-Fernenone*

$C_{30}H_{48}O$ 424.709

Mp 219-220°. $[\alpha]_D$ -55.4 ($CHCl_3$).

Nishimoto, K. *et al., Tetrahedron*, 1968, **24**, 735 (*struct*)

Ohmoto, T. *et al., Chem. Comm.*, 1969, 601 (*struct*)

Sunder, R. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 599 (*3-Epifernenol*)

Ogunkoya, L. *et al., Phytochemistry*, 1977, **16**, 1606 (*isol*)

Anderson, C. *et al., J. Nat. Prod.*, 1979, **42**, 168 (*acetate, palmitate*)

Obafemi, C.A. *et al., Phytochemistry*, 1979, **18**, 496 (*isol*)

Blunt, J.W. *et al., Org. Magn. Reson.*, 1980, **13**, 26 (*cmr*)

Nes, W.D. *et al., Chem. Comm.*, 1984, 223 (*struct*)

Tanaka, R. *et al., Phytochemistry*, 1988, **27**, 3529 (*Arundoin*)

Hemmers, H. *et al., Z. Naturforsch., C*, 1989, **44**, 193 (*Trematone*)

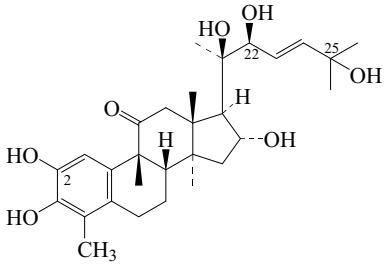
Wu, F.-E. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2282 (*Fernenone, pmr, cmr*)

Chakravarty, A.K. *et al., Tetrahedron*, 1994, **50**, 2865 (*cmr*)

Nakane, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 543-547 (*3-Epiternenol, pmr, cmr*)

Fevicordin F F-34

2,3,16,20,22,25-Hexahydroxy-4,9,14-trimethyl-19-norcholesta-1,3,5(10),23-tetraen-11-one, 9CI. 2,3,16,20,22,25-Hexahydroxy-29-norcucurbita-1,3,5(10),23-tetraen-11-one



$C_{29}H_{42}O_7$ 502.647

23,24-Dihydro, 22-ketone, 25-Ac, 2-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [151589-22-9] *Fevicordin B 2-gentiobioside*

$C_{43}H_{64}O_{18}$ 868.968

Constit. of *Cyclanthera pedata* (achoccha). Cryst. Mp 165-167°. $[\alpha]_D^{21}$ -36 (c, 0.4 in MeOH). $[\alpha]_D^{25}$ -36 (c, 1 in MeOH).

23,24-Dihydro, 22-ketone, 25-Ac, 2-O-[α-L-rhamnopyranoyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [178062-93-6]

$C_{49}H_{74}O_{22}$ 1015.11

Constit. of *Cyclanthera pedata* (achoccha). $[\alpha]_D^{25}$ -70 (c, 1 in MeOH).

6,7-Didehydro, 3-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [178062-90-3]

$C_{41}H_{60}O_{17}$ 824.915

Constit. of *Cyclanthera pedata* (achoccha). $[\alpha]_D^{25}$ -45 (c, 1 in MeOH).

6,7-Didehydro, 25-Ac, 3-O-β-D-glucopyranoside: [178062-92-5]

$C_{37}H_{52}O_{13}$ 704.81

Constit. of *Cyclanthera pedata* (achoccha). Cryst. Mp 140-145°. $[\alpha]_D^{25}$ -30 (c, 1 in MeOH).

6,7-Didehydro, 25-Ac, 3-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [178062-91-4]

$C_{43}H_{62}O_{18}$ 866.952

Constit. of *Cyclanthera pedata* (achoccha). $[\alpha]_D^{25}$ -40 (c, 1 in MeOH).

Himeno, E. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2885-2887; 1994, **42**, 2295; 2370 (*Cayaponosides*)

Achenbach, H. *et al., J. Nat. Prod.*, 1993, **56**, 1506 (*Fevicordins*)

De Tommasi, N. *et al., J. Agric. Food Chem.*, 1996, **44**, 2020-2025 (*Cyclanthera pedata constits*)

FIC F-35

Low-MW polar substance. Isol. from *Lactobacillus casein rhamnosus*. Inhibits the growth of *Penicillium* spores. Sol. EtOH, butanol, Me_2CO; poorly sol. hexane, $CHCl_3$. λ_{max} 269 (EtOH) (Berdy).

Eur. Pat., 1989, 302 300; *CA*, **111**, 172460b (*isol*)

Ficin F-36

[9001-33-6]

Ficus protease. Higueroxyl delabarre

Proteolytic sulfhydryl-requiring enzyme. Chillproofing agent for beer, meat tenderiser, dough conditioner, rennet substitute, processing aid for precooked cereals. GRAS approved. The name Ficin is used to describe both the enzyme itself and the crude dried latex.

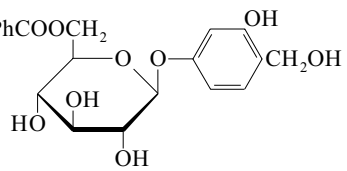
► Skin irritant.

Monter, B. *et al., Biotechnol. Appl. Biochem.*, 1991, **14**, 183-191 (*use, aminoacid coupling*)
Fed. Regist., 1995, **60**, 32904-2; *CA*, **123**, 81 896e
Merck Index, 12th edn., 1996, No. 4121 (*props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1114 (*food use*)
Iizuka, K. *et al., J. Sci. Food Agric.*, 2000, **80**, 1413-1420 (*use*)

Flacourtin F-37

[113270-18-1]

3-Hydroxy-4-(hydroxymethyl)phenyl β-D-glucopyranoside 6-benzoate, 9CI



$C_{20}H_{22}O_9$ 406.388

Isol. from the bark of an Indian medicinal plant, *Flacourtia indica*. Needles (EtOAc/Me_2CO). Mp 212°.

Penta-Ac:

Needles (Et_2O/petrol). Mp 105-106°.

Bhaumik, P.K. *et al., Phytochemistry*, 1987, **26**, 3090 (*isol, struct, pmr*)

Flammulin F-38

Basic polypeptide, MW approx. 24 kDa; struct. unknown. Isol. from *Flammulina velutipes* (velvet shank). Sol. H_2O; poorly sol. MeOH, hexane. λ_{max} 277 (H_2O) (Berdy).

► LD_{50} (mus, ipr) 25 mg/kg.

Watanabe, Y. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 747-750 (*isol*)

Flammutoxin F-39

[55599-71-8]

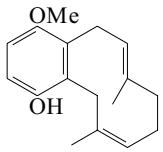
Comprises a single polypeptide chain, MW 32 kDa, with unusually large amounts of Trp, Ser and Gly. Isol. from the basidocorps of the edible mushroom *Flammulina velutipes* (velvet shank).

Lin, J.Y. *et al., Nature (London)*, 1974, **252**, 235-237 (*isol*)
Lin, J.Y. *et al., Toxicon*, 1975, **13**, 323-331 (*tox*)
Bernheimer, A.W. *et al., Toxicon*, 1987, **25**, 1145-1152 (*isol*)

Flavidulol A F-40

[117568-32-8]

5,8,9,12-Tetrahydro-4-methoxy-7,11-dimethyl-1-benzocyclodecenol, 9CI



$C_{17}H_{22}O_2$ 258.36

Stereochem. revised in 1993. Isol. from the edible but bitter tasting Japanese kihatsudake mushroom (*Lactarius flavidulus*). Oil.

► Allergenic.

Ac: [117568-35-1]

Needles (hexane). Mp 111-112°.

Octadecanoyl: [156980-40-4] ***Flavidulol D***

$C_{35}H_{56}O_3$ 524.826

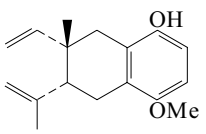
Constit. of *Lactarius flavidulus*. Waxy solid. Mp 40-41°.

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2366; 1993, **41**, 2032 (*isol, pmr, cmr, struct*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 1993, **41**, 654 (*isol, pmr, props*)

Flavidulol B F-41

[117568-33-9]

7-Ethenyl-5,6,7,8-tetrahydro-4-methoxy-7-methyl-6-(1-methylethenyl)-1-naphthalenol, 9CI



$C_{17}H_{22}O_2$ 258.36

Stereochem. revised in 1993. Isol. from the edible but bitter tasting Japanese kihatsudake mushroom (*Lactarius flavidulus*). Pale brown oil. Racemic.

Ac: [117568-36-2]

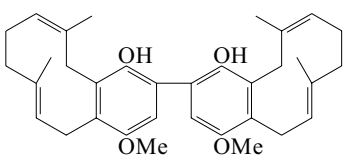
Needles (hexane). Mp 62-64°.

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2366; 1993, **41**, 2032 (*isol, pmr, cmr, struct*)

Flavidulol C F-42

[117568-34-0]

5,5′,8,8′,9,9′,12,12′-Octahydro-4,4′-dimethoxy-7,7′,11,11′-tetramethyl[2,2′-bibenzocyclodecene]-1,1′-diol, 9CI



$C_{34}H_{42}O_4$ 514.703

Stereochem. revised in 1993. Isol. from the edible, but bitter tasting Japanese kihatsudake mushroom (*Lactarius flavidulus*). Pale brown needles. Mp 185-186°. Stereochem. revised in 1993.

Di-Ac: [117608-81-8]

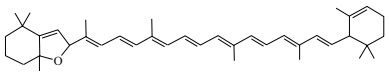
Needles (hexane). Mp 175-177°.

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2366; 1993, **41**, 2032 (*isol, pmr, cmr, struct*)

Flavochrome F-43

[473-05-2]

5,8-Epoxy-5,8-dihydro-β,ε-carotene

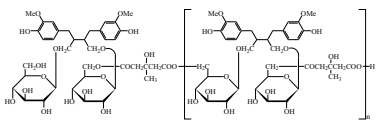


$C_{40}H_{56}O$ 552.882

Constit. of *Calendula officinalis* (pot marigold). Yellow cryst. (C_6H_6/MeOH). Mp 189°.

Karrer, P. *et al., Helv. Chim. Acta*, 1945, **28**, 471,1146 (*isol, struct*)
Goodwin, T.W. *et al., Biochem. J.*, 1954, **58**, 90 (*isol*)

Flaxseed lignan-HMGA oligomer F-44



$C_{190}H_{256}O_{100}$ 4140.052

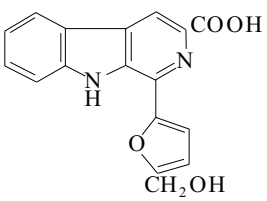
Oligomer consisting of secoisolariciresinol 9,9′-diglucosides and 3-hydroxy-3-methylglutaric acid residues. Major lignan has n = 4 to which MF refers. Constit. of the seeds of *Linum usitatissimum* (flax).

Kamal-Eldin, A. *et al., Phytochemistry*, 2001, **58**, 587-590

Flazine F-45

[100041-05-2]

1-[5-(Hydroxymethyl)-2-furanyl]-9H-pyrido[3,4-b]indole-3-carboxylic acid, 9CI



$C_{17}H_{12}N_2O_4$ 308.293

Alkaloid from Japanese soy sauce and sake. Cryst. (MeOH). Mp 231-233°. Fluorescent λ_{max} 217 (log ε 4.87); 275 (log ε 4.85); 365 (log ε 3.02); 379 (log ε 3.11) (MeOH).

Me ether: [159898-11-0] ***Flazine methyl ether. O-Methylflazine***

$C_{18}H_{14}N_2O_4$ 322.32

Alkaloid from freshly pressed juice of blackcurrant (*Ribes nigrum*)(Grossulariaceae). Mp 199-200°.

De(hydroxymethyl): [76135-36-9] *1-(2-Furanyl)-9H-pyrido[3,4-b]indole-3-carboxylic acid.* ***Dehydroxymethylflazine***

$C_{16}H_{10}N_2O_3$ 278.267

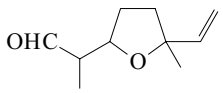
From blackcurrant (*Ribes nigrum*) (Grossulariaceae).

Nakatsuka, S. *et al., Tet. Lett.*, 1986, **27**, 3399-3402 (*isol, uv, ir, pmr, struct*)

Gessner, W.P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 95-98 (*synth, uv, pmr*)
Blech, S. *et al., Z. Naturforsch., C*, 1994, **49**, 540-544 (*Flazine methyl ether, Dihydroxymethylflazine*)
Su, B.-N. *et al., Planta Med.*, 2002, **68**, 730-733 (*isol, pmr, cmr, ms*)

Fliederaldehyde F-46

[81967-88-6]
5-Ethenyltetrahydro-α,5-dimethyl-2-furanacetaldehyde, 9CI. 2-(1-Formylethyl)-5-methyl-5-vinyltetrahydrofuran. Tetrahydro-α,5-dimethyl-5-vinyl-2-furanacetaldehyde. Lilac aldehyde



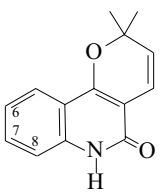
$C_{10}H_{16}O_2$ 168.235
Isol. from bergamot oil. Bp_{23} 99-101°. Mixture of four diastereoisomers incompletely separated.

[26863-72-9, 51685-39-3, 53447-48-6, 67920-63-2]

Naegeli, P. *et al., Tet. Lett.*, 1970, 959 (*synth, ir, uv, pmr*)
Wakayama, S. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3183; 1974, **47**, 1293 (*synth, ir, isol, pmr, ms*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1974, **57**, 2062 (*synth, pmr*)
Hattori, R. *et al., Agric. Biol. Chem.*, 1978, **42**, 1351 (*isol*)
Patt, J.M. *et al., Phytochemistry*, 1988, **27**, 91 (*isol*)
Misra, L.N. *et al., Phytochemistry*, 1991, **30**, 549 (*isol*)

Flindersine F-47

[523-64-8]
*2,6-Dihydro-2,2-dimethyl-5*H*-pyrano[3,2-c]quinolin-5-one, 9CI*



$C_{14}H_{13}NO_2$ 227.262
Mp 195-196° dec. λ_{max} 235 ; 333 ; 350 ; 365 (MeOH) (Berdy).

N-*(Acetoxymethyl):* [149998-45-8] **N-*Acetoxymethylflindersine***
$C_{17}H_{17}NO_4$ 299.326
Alkaloid from leaves of *Zanthoxylum simulans* (Szechuan pepper). Oil.

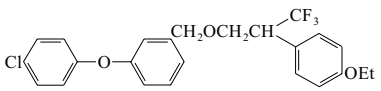
*8-Methoxy, 1′,2′-dihydro, 1′*R*,2′*R*-dihydroxy,* N-*Me:* [198336-59-3]

[193978-31-3] ***Zanthodioline***
$C_{16}H_{19}NO_5$ 305.33
Alkaloid from the bark of *Zanthoxylum simulans* (Szechuan pepper). Amorph. solid. $[\alpha]_D^{23}$ -20 (c, 0.05 in $CHCl_3$). λ_{max} 218 (log ε 4.14); 234 (log ε 4.21); 254 (log ε 4.11); 270 (sh) (log ε 3.56); 280 (log ε 3.59); 327 (log ε 3.23) (EtOH).

Brader, G. *et al., Annalen*, 1993, 355 (*N-Acetoxymethylflindersine*)
Watters, W.H. *et al., J. Chem. Res., Synop.*, 1997, 184-185 (*Zanthodioline, Veprisine, synth*)
Chen, I.S. *et al., Phytochemistry*, 1997, **46**, 525-529 (*Zanthodioline*)

Flufenprox F-48

[107713-58-6]
1-(4-Chlorophenoxy)-3-[[2-(4-ethoxyphenyl)-3,3,3-trifluoropropoxy]methyl]benzene, 9CI. ICI A5682



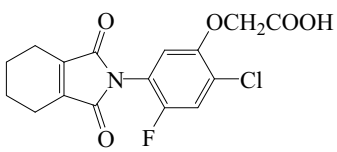
$C_{24}H_{22}ClF_3O_3$ 450.884
(±)-form
Insecticide for rice. Yellow-green liq. Bp 204-0.2°.

[118753-05-2]

Eur. Pat., 1987, 211 561, (*ICI*); *CA*, **106**, 175940r (*synth, activity*)
Gordon, R.F.S. *et al., Brighton Crop Prot. Conf. - Pests Dis.*, 1992, 81 (*activity*)
Pesticide Manual, 11th edn., 1997, No. 336 (*use, props*)

Flumiclorac, ANSI, BSI F-49

[87547-04-4]
*[2-Chloro-4-fluoro-5-(1,3,4,5,6,7-hexahydro-1,3-dioxo-2*H*-isoindol-2-yl)phenoxy]acetic acid, 9CI*



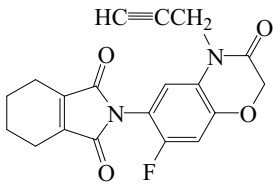
$C_{16}H_{13}ClFNO_5$ 353.734
Registered in 1994 for use in USA

Pentyl ester: [87546-18-7] ***Flumiclorac-pentyl, ANSI, BSI***. *Resource. Sumiverde. S 23031. V 23031*
$C_{21}H_{23}ClFNO_5$ 423.868
Post-emergence herbicide used against broad-leaved weeds in soybeans and maize. Beige solid. Mp 90°.

Eur. Pat., 1983, 83 055, (*Sumitomo*); *CA*, **99**, 175591q (*synth, activity*)
Eur. Pat., 1989, 305 826; *CA*, **111**, 194585y (*pentyl ester*)
Matsunaga, H. *et al., J. Agric. Food Chem.*, 1996, **44**, 1910-1914; 1997, **45**, 501-506 (*pentyl ester, metab*)
Birchfield, N.B. *et al., Pestic. Biochem. Physiol.*, 1997, **57**, 36-43 (*activity*)
Pesticide Manual, 12th edn., 2000, No. 367

Flumioxazin, ANSI, BSI F-50

[103361-09-7]
*2-[7-Fluoro-3,4-dihydro-3-oxo-4-(2-propynyl)-2*H*-1,4-benzoxazin-6-yl]-4,5,6,7-tetrahydro-1*H*-isoindole-1,3(2*H*)-dione, 9CI. Sumisoya. S 53482. V 53482*



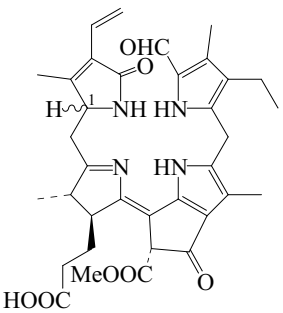
$C_{19}H_{15}FN_2O_4$ 354.337
Herbicide used on soybeans, peanuts, orchard fruits and other crops. Yellow-brown powder. Mp 201-204° (195-196°).

▶ LD_{50} (rat, orl) >5000 mg/kg.

Eur. Pat., 1986, 170 191, (*Sumitomo*); *CA*, **105**, 56350t (*synth, activity*)
Yoshida, R. *et al., Brighton Crop Prot. Conf. - Weeds*, 1991, 69-75 (*activity*)
Tomigahara, Y. *et al., J. Agric. Food Chem.*, 1999, **47**, 305-312 (*metab*)
Lyga, J.W. *et al., Pestic. Sci.*, 1999, **55**, 281-287 (*activity*)
Pesticide Manual, 12th edn., 2000, No. 368

Capsicum annuum Fluorescent chlorophyll catabolite F-51

Ca-*FCC-2*



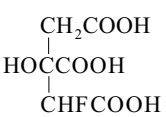
$C_{35}H_{40}N_4O_7$ 628.724
Chlorophyll catabolite isol. from *Capsicum annuum* (ripe sweet pepper). λ_{max} 221 ; 318 ; 358 (H_2O).

1-Epimer: Brassica napus *Fluorescent chlorophyll catabolite.* Bn-*FCC-2*
$C_{35}H_{40}N_4O_7$ 628.724
Chlorophyll catabolite isol. from *Brassica napus*. λ_{max} 264 (sh) ; 321 ; 361 (H_2O).

Muehlecker, W. *et al., Angew. Chem., Int. Ed.*, 1997, **36**, 401-404
Muehlecker, W. *et al., Helv. Chim. Acta*, 2000, **83**, 278-286

Fluorocitric acid, 8CI F-52

[357-89-1]
1-Fluoro-2-hydroxy-1,2,3-propanetricarboxylic acid, 9CI



$C_6H_7FO_7$ 210.115
Usually isol. as Ba salt. Stereoisomers not completely characterised.. Found in cattle bones, soybean leaves, other plants and foodstuffs (as the (2*R*,3*R*)-isomer). Important metab. of toxic

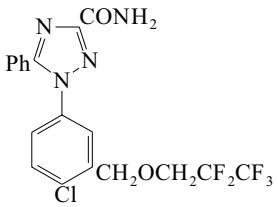
fluoroacetate. Hygroscopic solid.

Tri-Et ester: [309-98-8] *Ethyl fluorocitrate*
$C_{12}H_{19}FO_7$ 294.276
Needles. Mp 41°. $Bp_{0.1}$ 120°.

Rivett, D.E.A. *et al., J.C.S.*, 1953, 3710 (*synth*)
Fanshier, D.W. *et al., J. Biol. Chem.*, 1964, **239**, 425 (*synth, biosynth, ir, biochem*)
Dummel, R.J. *et al., J. Biol. Chem.*, 1969, **244**, 2966 (*resoln, pmr*)
Peters, R.A. *et al., Phytochemistry*, 1972, **11**, 1337 (*isol*)
Carrell, H.L. *et al., Acta Cryst. B*, 1973, **29**, 674 (*cryst struct*)
Glusker, J.P. *et al., Bioorg. Chem.*, 1973, **2**, 301 (*rev, stereochem*)
Eanes, R.Z. *et al., Mol. Pharmacol.*, 1974, **10**, 130 (*pharmacol*)
Harper, D.B. *et al., Nat. Prod. Rep.*, 1994, **11**, 123 (*rev*)

Flupoxam, BSI F-53

[119126-15-7]
*1-[4-Chloro-3-[(2,2,3,3,3-pentafluoropropoxy)methyl]phenyl]-5-phenyl-1*H*-1,2,4-triazole-3-carboxamide, 9CI. KNW-739. MON-18500*

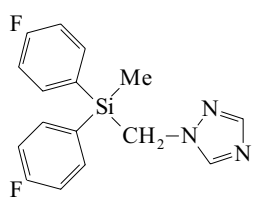


$C_{19}H_{14}ClF_5N_4O_2$ 460.79
Pre- and post emergence herbicide for broad-leaved weed control in winter cereals. Mp 144-148°.

Eur. Pat., 1988, 282 303, (*Kureha*); *CA*, **110**, 95247n (*synth, activity*)
O'Keeffe, M.G. *et al., Brighton Crop Prot. Conf. - Weeds*, 1991, **1**, 63 (*activity, tox*)
Pesticide Manual, 11th edn., 1997, no.583-584 (*use*)

Flusilazole F-54

[85509-19-9]
*1-[[Bis(4-fluorophenyl)methylsilyl]methyl]-1*H*-1,2,4-triazole, 9CI. Bis(4-fluorophenyl)methyl(1*H*-1,2,4-triazol-1-ylmethyl)silane. Flusilazol. DPD 78710F. PPX-H6573. DPX-N6573. Punch (pesticide). Punch 40EC. Nustar*



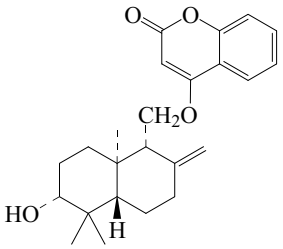
$C_{16}H_{15}F_2N_3Si$ 315.397
Highly potent broad-spectrum fungicide. Controls broad spectrum of diseases on economically important crops. Cryst. (Et_2O/petrol). Mp 48° (53°).

▶ LD_{50} (rat, orl) 1110 mg/kg. XZ4105000

Tacke, R. *et al., Appl. Organomet. Chem.*, 1989, **3**, 133 (*synth, cryst struct, pmr, cmr, ms use*)
Pesticide Manual, 9th edn., 1991, No. 6664

Foetidin F-55

[97165-40-7]

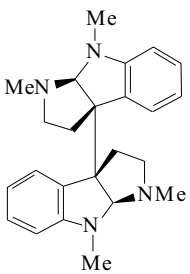


$C_{24}H_{30}O_4$ 382.499
Constit. of the roots of *Ferula assa-foetida* (asafoetida). Plates(MeOH). Mp 176-178°. $[\alpha]_D^{20}$ -39.8 (EtOH).

Buddrus, J. *et al., Phytochemistry*, 1985, **24**, 869-870 (*isol, pmr, ms*)

Folicanthine F-56

[6879-55-6]
1′-Methylcalycanthidine, 9CI



Absolute configuration

$C_{24}H_{30}N_4$ 374.528

(-)-*form*
Alkaloid from *Calycanthus floridus* (Carolina allspice) and *Calycanthus occidentalis* (Californian allspice). Mp 118-119°. $Bp_{0.1}$ 150-170°. $[\alpha]_D$ -364 (EtOH).

Picrate:
Mp 179°.

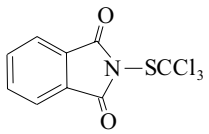
Picrolonate:
Needles (MeOH). Mp 176° dec.

(±)-*form*
Mp 168-169°.

Grant, I.J. *et al., Proc. Chem. Soc., London*, 1962, 148 (*cryst struct*)
Hino, T. *et al., Tet. Lett.*, 1963, 1757 (*synth, ms*)
O'Donovan, D.G. *et al., J.C.S.(C)*, 1966, 1570 (*biosynth*)
Hino, T. *et al., Tet. Lett.*, 1978, 4913 (*synth, pmr*)
Fang, C.-L. *et al., J.A.C.S.*, 1994, **116**, 9480 (*synth*)

Folpet, BSI F-57

[133-07-3]
*2-[(Trichloromethyl)thio]-1*H*-isoindole-1,3(2*H*)-dione, 9CI.* N-*(Trichloromethylthio)phthalimide. Folnit. Orthophaltan. Phaltan. Trifol. Vinicoll. Cosan T. Fungitrol 11. Intercide TMP*



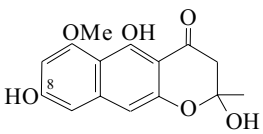
$C_9H_4Cl_3NO_2S$ 296.56
Agricultural fungicide. Cryst. Mp 177°.

▶ Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 7540 mg/kg. Mutagen. TI5685000

U.S. Pat., 1949, 2 553 770; *CA*, **45**, 6791i (*synth, activity*)
Kittleson, A.R. *et al., Science (Washington, D.C.)*, 1952, **115**, 84 (*synth, activity*)
Suzuki, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 1433 (*detn*)
Zupancic, B.G. *et al., Synthesis*, 1975, 169 (*synth*)
Carlstrom, A.A. *et al., J. Assoc. Off. Anal. Chem.*, 1978, **60**, 1157 (*ir*)
Pesticide Manual, 11th edn., 1997, No. 364
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TIT250

Fonsecin F-58

[3748-39-8]
*2,3-Dihydro-2,5,8-trihydroxy-6-methoxy-2-methyl-4*H*-naphtho[2,3-b]pyran-4-one, 9CI. Antibiotic TMC 256B1. TMC 256B1*



$C_{15}H_{14}O_6$ 290.272
Mycotoxin from a mutant of *Aspergillus fonsecaeus* also known as *Aspergillus carbonarius*. Bright yellow irregular prisms. Mp 198° dec. λ_{max} 233 (log ε 4.42); 275 (log ε 4.5); 321 (log ε 3.86); 332 (log ε 3.9); 400 (log ε 3.94) (MeOH).

8-Me ether: [1856-95-7] ***Fonsecin B**. Antibiotic TMC 256B2. TMC 256B2*
$C_{16}H_{16}O_6$ 304.299
Mycotoxin from a mutant of *Aspergillus fonsecaeus* also known as *Aspergillus carbonarius*. Yellow needles (Me_2CO aq.). Mp 176°. Dehydration gives, 6,8-Di-Me ether.

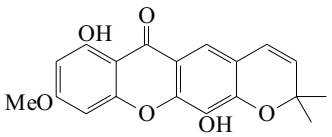
O-*De-Me:* ***De*-O-*methylfonsecin**. YWA 1*
$C_{14}H_{12}O_6$ 276.245
Pigment from a mutant of *Aspergillus fonsecaeus* also known as *Aspergillus carbonarius*. λ_{max} 229 ; 281 ; 323 ; 335 ; 411 (MeCN).

Raper, K.B. *et al., J. Elisha Mitchell Sci. Soc.*, 1953, **69**, 1 (*isol*)
Galmanini, O.L. *et al., Nature (London)*, 1962, **195**, 502 (*isol*)
Galmanini, O.L. *et al., Experientia*, 1974, **30**, 586 (*deriv*)
Ehrlich, K.C. *et al., Appl. Environ. Microbiol.*, 1984, **48**, 1 (*deriv*)
Bloomer, J.L. *et al., J.O.C.*, 1984, **49**, 5027 (*isol, cmr, biosynth*)
Priestap, H.A. *et al., Tetrahedron*, 1984, **40**, 3617 (*pmr*)
Watanabe, A. *et al., Tet. Lett.*, 1999, **40**, 91-94 (*De-O-methylfonsecin*)
Sakurai, M. *et al., J. Antibiot.*, 2002, **55**, 685-692 (*TMC 256B*)

Forbexanthone F-59

[150527-30-3]

7,12-Dihydroxy-9-methoxy-2,2-dimethyl-2H,6H-pyrano[3,2-b]xanthen-6-one, 9CI



$C_{19}H_{16}O_6$ 340.332

Yellow needles (EtOAc/hexane). Mp 222°.

Demethoxy: [82667-93-4] ***Rheediachromenoxanthone***

$C_{18}H_{14}O_5$ 310.306

Cryst. (Et_2O/hexane). Mp 223-224°.

O-*De-Me:* [92609-77-3] **O-*Demethylforbexanthone***

$C_{18}H_{14}O_6$ 326.305

Constit. of *Rheedia brasiliensis* (bakupari). Cryst. ($CHCl_3$/MeOH). Mp 315°. λ_{max} 273 (log ϵ 4.46); 330 (log ϵ 3.95); 366 (sh) (log ϵ 3.72) (MeOH).

Delle Monache, G. *et al., Phytochemistry*, 1983, **46**, 655 (*Rheediachromenoxanthone*)

Delle Monache, G. *et al., J. Nat. Prod.*, 1984, **47**, 620-625 (*O-Demethylforbexanthone*)

Harrison, L.J. *et al., Phytochemistry*, 1993, **33**, 727 (*Forbexanthone*)

Formic acid, 9CI, 8CI F-60

[64-18-6]

Methanoic acid. FEMA 2487

HCOOH

CH_2O_2 46.026

Used as a flavouring adjunct, an animal feed additive, a brewing antiseptic and as a food preservative. Liq. with pungent odour. Misc. H_2O, EtOH, Et_2O; mod. sol. C_6H_6. d_4^{20} 1.22. Mp 8.4°. Bp 100.5° Bp_{120} 50°. n_D^{20} 1.3714. Good solvent props. Strong reducing agent, burns with a blue flame.

► Fl. p. 69°, autoignition temp. 539°. Slow dec. can lead to build up of pressure in closed containers. Vapour is a skin and eye irritant. Liquid is corrosive to skin, eyes and mucous membranes. LD_{50} (rat, orl) 1100 mg/kg. OES: long-term 5 ppm. LQ4900000

Propyl ester: [110-74-7] *Propyl formate. FEMA 2943*

$C_4H_8O_2$ 88.106

Flavouring ingredient. Liq. with a characteristic fruity odour and bittersweeet flavour. Sl. sol. H_2O; misc. EtOH, Et_2O. d^{20} 0.91. Mp -92.9°. Bp 80-82°. n_D^{20} 1.3779.

► Fl. p. 27°. LR0175000

Butyl ester: [592-84-7] *Butyl formate. FEMA 2916*

$C_5H_{10}O_2$ 102.133

Flavouring agent. Liq. with a fruity odour and taste. Sl. sol. H_2O; misc. EtOH, Et_2O. d^{20} 0.89. Mp -91.5°. Bp 106-107°. n_D^{20} 1.3890.

► Fl. p. 64°. LQ5500000

[71-47-6, 917-71-5, 920-42-3, 925-94-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 481A; 545C; 599C; 768A (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 895C; 896A; 896C; 1254B (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 573A; 605C; 605D; 606B (*ir*)

Pryanishnikov, A.A. *et al., CA*, 1933, **27**, 2672 (*synth*)

Holsboer, D.H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1971, **90**, 556-561 (*esters*)

Nahringbauer, I. *et al., Acta Cryst. B*, 1978, **34**, 315-318 (*cryst struct*)

Benninghoven, A. *et al., Adv. Mass Spectrom.*, 1978, **7B**, 1433-1436 (*ms*)

Hefetz, A. *et al., Biochim. Biophys. Acta*, 1978, **543**, 484-495 (*biosynth, bibl*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **11**, 257 (*rev*)

Delseth, C. *et al., Helv. Chim. Acta*, 1980, **63**, 498-503 (*cmr, O-17 nmr*)

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, FNA 000

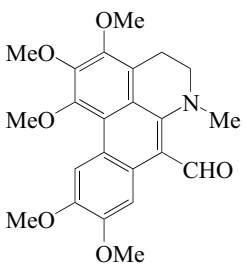
Jessop, P.G. *et al., Nature (London)*, 1994, **368**, 231-233 (*synth*)

Leitner, W. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 2207-2221 (*rev, synth, use*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 85; 280; 697

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 339-340; 1124-1126; 2357-2358

7-Formyldehydrothalicsimidine F-61

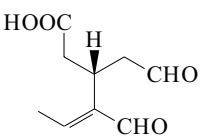


$C_{23}H_{25}NO_6$ 411.454

Alkaloid from *Annona purpurea* (soncoya). Yellow needles ($CHCl_3$). Mp 160-162°. λ_{max} 217 ; 268 ; 335 (sh) ; 432 (EtOH).

Chang, F.-R. *et al., Phytochemistry*, 1998, **49**, 2015-2018 (*isol, uv, ir, pmr*)

4-Formyl-3-(formylmethyl)-4-hexenoic acid F-62



$C_9H_{12}O_4$ 184.191

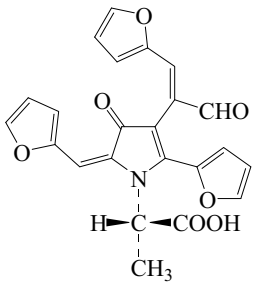
A secoiridoid. Constit. of the juice of ripe black olives (*Olea europaea*). Amorph. powder. $[\alpha]_D^{25}$ +6.5.

Lo Scalzo, R. *et al., J. Nat. Prod.*, 1993, **56**, 621 (*isol, pmr*)

[3-[1-Formyl-2-(2-furanyl)ethenyl]]-2-(2-furanyl)-5-(2-furanylmethylene)-4,5-dihydro-α-methyl-4-oxo-1*H*-pyrrole-1-acetic acid, 9CI F-63

[198414-08-3]

[198414-10-7]



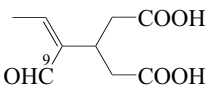
$C_{23}H_{17}NO_7$ 419.39

(*E,E*)-form predominates. Maillard product from reaction of L-alanine and 2-Furancarboxaldehyde, F-93. Deep red solid.

Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 932-940 (*occur, nmr, uv*)

3-(1-Formyl-1-propenyl)pentanedioic acid F-64

3-(1-Formyl-1-propenyl)glutaric acid



$C_9H_{12}O_5$ 200.191

(Z)-form

Constit. of olives (*Olea europaea*). Incorrectly stated as *E*-isomer in ref..

9-Alcohol:3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid. 3-(1-Hydroxymethyl-1-propenyl)glutaric acid

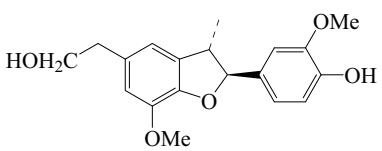
$C_9H_{14}O_5$ 202.207

Constit. of olives (*Olea europaea*).

Gil, M. *et al., Phytochemistry*, 1998, **49**, 1311-1315 (*isol, pmr, cmr, ms*)

Fragransol B F-65

[114394-20-6]



$C_{19}H_{22}O_5$ 330.38

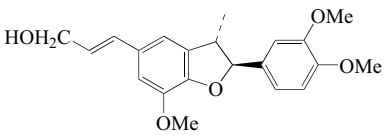
Constit. of *Myristica fragrans* (nutmeg). Oil.

Hada, S. *et al., Phytochemistry*, 1988, **27**, 563-568 (*isol*)

Juhasz, L. *et al., J. Nat. Prod.*, 2000, **63**, 866-870 (*synth, pmr, cmr*)

Fragransol C F-66

[114926-96-4]

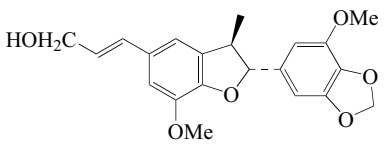


$C_{21}H_{24}O_5$ 356.418
Constit. of *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ -44 (c, 0.1 in $CHCl_3$).

Hattori, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 648-653 (*isol*)
Juhasz, L. *et al., J. Nat. Prod.*, 2000, **63**, 866-870 (*synth, pmr, cmr*)

Fragransol D F-67

[114892-43-2]

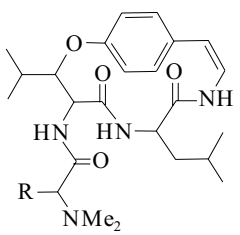


$C_{21}H_{22}O_6$ 370.401
Constit. of *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +47.6 (c,1 in $CHCl_3$). Closely related to Machilin B but appears to belong to the opposite enantiomeric series.

Hattori, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 648 (*Fragransol D*)

Frangulanine F-68

[25350-22-5]
2-(Dimethylamino)-3-methyl-N-*[3-(1-methylethyl)-7-(2-methylpropyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]pentanamide, 9CI. Ceanothamine A. Daechuine S2*



R = $H_3CCH_2CH(CH_3)$ —

$C_{28}H_{44}N_4O_4$ 500.68
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea), *Hovenia dulcis* (raisin tree) and *Zizyphus jujuba* var. *inermis*. Needles ($CHCl_3$/petrol, MeOH or CH_2Cl_2/EtOAc). Mp 276-279° (275-276°). $[\alpha]_D^{20}$ -288 (c, 0.1 in $CHCl_3$).

Dihydro:
Needles (MeOH/petrol). Mp 298°. $[\alpha]_D^{20}$ -7 (c, 0.1 in $CHCl_3$).

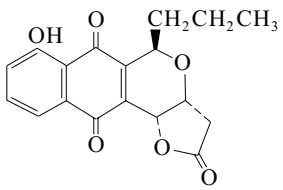
Tri-N-*Me; methiodide:*
Mp 242-244°.

N-*De-Me:* [52309-78-1] ***Hovenine A***. N-*Demethylfrangulanine*
$C_{27}H_{42}N_4O_4$ 486.653
Alkaloid from the root bark of *Hovenia dulcis* (raisin tree). Mp 215°. Opt. rotn. not reported.

Warnhoff, E.W. *et al., Can. J. Chem.*, 1965, **43**, 2594 (*isol, uv, pmr, ms*)
Tschesche, R. *et al., Chem. Ber.*, 1967, **100**, 3937 (*isol, uv, cd, ir, pmr, ms, struct*)
González Sierra, M. *et al., Chem. Comm.*, 1972, 915 (*pmr, stereochem*)
Mascaretti, O.A. *et al., Phytochemistry*, 1972, **11**, 1133 (*isol, ir*)
Bishay, D.W. *et al., Phytochemistry*, 1973, **12**, 693 (*uv, ir, pmr, ms*)
Takai, M. *et al., Phytochemistry*, 1973, **12**, 2985 (*isol, ir, pmr, ms, deriv*)
Chang, C.-J. *et al., Phytochemistry*, 1974, **13**, 1273 (*pmr*)
Otsuka, H. *et al., Phytochemistry*, 1974, **13**, 2016 (*occur*)
Takai, M. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2556; 1976, **24**, 2181 (*pmr, conformn, cryst struct*)
Haslinger, E. *et al., Tetrahedron*, 1978, **34**, 685 (*pmr, cmr, conformn*)
Haslinger, E. *et al., Monatsh. Chem.*, 1979, **113**, 95 (*pmr, cmr, conformn*)
Tschesche, R. *et al., Phytochemistry*, 1979, **18**, 702 (*isol*)
Han, B.H. *et al., Pure Appl. Chem.*, 1989, **61**, 443
Schmidt, U. *et al., Chem. Comm.*, 1991, 1002 (*synth*)

Frenolicin B F-69

[68930-68-7]
Antibiotic AM 3867I. AM 3867I. Antibiotic UCF76 C. UCF76 C



$C_{18}H_{16}O_6$ 328.321
Antibiotic feed additive esp. for poultry and pigs. Orange columns. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 157-159°. $[\alpha]_D^{24}$ +216 (c, 0.44 in $CHCl_3$). λ_{max} 278 (ε 8900); 540 (ε 4300) (MeOH/NaOH) (Derep). λ_{max} 260 (sh) (ε 16641); 268 (ε 16776); 426 (ε 562) (MeOH) (Derep). λ_{max} 260 (ε 8959); 270 (ε 9020); 425 (ε 4920) (MeOH) (Berdy). λ_{max} 260 ; 270 ; 425 (MeOH-HCl) (Berdy). λ_{max} 273 (ε 8500); 534 (ε 4300) (MeOH-NaOH) (Berdy).

Iwai, Y. *et al., J. Antibiot.*, 1978, **31**, 959 (*isol*)
Kraus, G.A. *et al., J.A.C.S.*, 1993, **115**, 5859 (*synth*)
Mazur, B. *et al., J. Agric. Food Chem.*, 1995, **43**, 3042-3045 (*anal*)
Kraus, G.A. *et al., J.O.C.*, 1995, **60**, 1154 (*synth, ir, pmr, ms*)
Masquelin, T. *et al., Helv. Chim. Acta*, 1997, **80**, 43-58 (*synth, ord*)
Contant, P. *et al., Synthesis*, 1999, 821-828 (*synth, cryst struct, ir, pmr*)
Hara, M. *et al., J. Antibiot.*, 2001, **54**, 182-186 (*UCF 76C, isol, activity*)

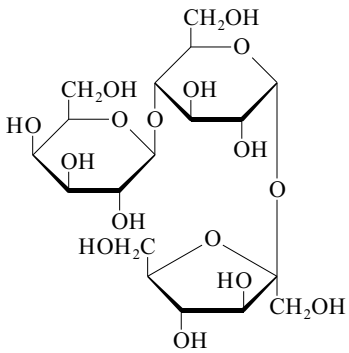
β-Fructofuranosidase F-70

[9001-57-4]
β-D-Fructofuranoside fructohydrolase. Invertase. Saccharase. E.C. 3.2.1.26. E1103
Enzyme. Used in production of invert sugar from sucrose. Hydrolyses terminal non-reducing β-D-fructofuranoside residues in β-D-fructofuranosides.

Myrback, K. *et al., The Enzymes*, (Boyer, P., Ed.), 2nd Edn., Academic Press, N.Y., 1960, **4**, 379-396 (*rev.*)
Neumann, N.P. *et al., Biochemistry*, 1967, **6**, 468-475 (*isol*)
Merck Index, 12th edn., 1996, 5025
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1396-1397 (*use*)

β-D-Fructofuranosyl β-D-galactopyranosyl-(1 → 4)-α-D-glucopyranoside, 9CI F-71

[87419-56-5]
Lactosucrose. 4-O-*β-D-Galactopyranosylsucrose*

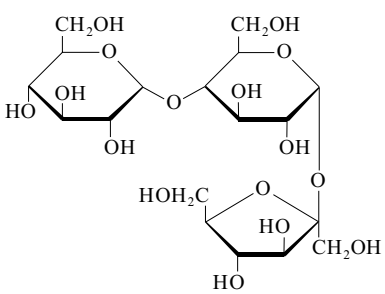


$C_{18}H_{32}O_{16}$ 504.441
Selectively enhances growth of bifidobacteria in human intestines. Cryst. V. sol. H_2O. Mp 181° (131°). $[\alpha]_D$ +59 (+44) (H_2O). Sweetness about 30% of sucrose.

Avigad, G. *et al., J. Biol. Chem.*, 1957, **229**, 121 (*enzymic synth*)
Tanaka, T. *et al., J. Biochem. (Tokyo)*, 1981, **90**, 521 (*enzymic synth*)
Minami, Y. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1688 (*metab*)
Hara, K. *et al., CA*, 1991, **115**, 181572z (*use*)
Fujita, K. *et al., CA*, 1991, **115**, 181751g (*manuf*)
Eur. Pat., 1991, 382 355; *CA*, **114**, 163008v (*use*)

β-D-Fructofuranosyl α-D-glucopyranosyl-(1 → 4)-D-glucopyranoside F-72

α-Maltosylfructose. 4-O-*α-D-Glucopyranosylsucrose. Erlose. Fructomaltose*



$C_{18}H_{32}O_{16}$ 504.441
Occurs in *Aphis pemi* honeydew. Isol. from a honey invertase digest of sucrose.

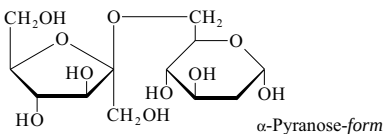
Monohydrate or trihydrate. Mp 118-124° dec. $[\alpha]_D^{25}$ +128.8 (c, 2.3 in H_2O).

Undeca-Ac:
Mp 68-73°. $[\alpha]_D^{25}$ +86 (c, 1.2 in $CHCl_3$).

White, J.W. *et al., J.A.C.S.*, 1953, **75**, 1259 (*synth*)
Taga, T. *et al., Carbohydr. Res.*, 1993, **240**, 39; 1994, **251**, 203 (*cryst struct*)

6-*O*-β-D-Fructofuranosyl-2-deoxy-D-glucose F-73

[57440-92-3]
6-O-*β-D-Fructofuranosyl-2-deoxy-D*-arabino-*hexose, 9CI*

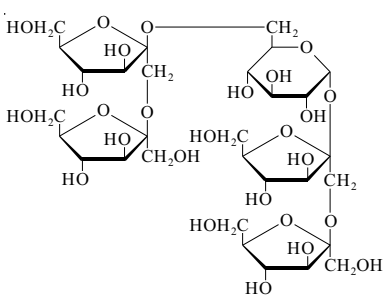

α-Pyranose-*form*

$C_{12}H_{22}O_{10}$ 326.3
Reducing disaccharide. Isolated from horseradish and peas which had been fed 2-deoxyglucose. $[\alpha]_D^{20}$ +28.2 (c, 0.91 in H_2O).

Barber, G.A. *et al., J.A.C.S.*, 1959, **81**, 3722 (*isol*)
Zemek, J. *et al., Z. Pflanzenphysiol.*, 1975, **76**, 114; *CA*, **84**, 13358g

β-D-Fructofuranosyl-(2→1)-β-D-fructofuranosyl β-D-fructofuranosyl-(2→1)-β-D-fructofuranosyl-(2→6)-α-D-glucopyranoside, 9CI F-74

[71231-05-5]
β-D-Fructofuranosyl-(2→1)-β-D-fructofuranosyl-(2→6)-α-D-glucopyranosyl-(1→2)-β-D-fructofuranosyl β-D-fructofuranoside

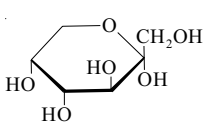


$C_{30}H_{52}O_{26}$ 828.725
Isol. from the roots of asparagus (*Asparagus officinalis*). $[\alpha]_D^{20}$ -6.6 (H_2O).

Shiomi, N. *et al., Agric. Biol. Chem.*, 1979, **43**, 1375 (*isol*)

Fructose, 9CI, 8CI F-75

[30237-26-4]
Levulose. arabino-*Hexulose. Fruit sugar. Laevulose. α-Acrose*


α-D-Pyranose-*form*

$C_6H_{12}O_6$ 180.157
α-Acrose was apparently an old synonym for the racemate.

D-*form* [57-48-7]
An aq. soln. at 30°C contains 2% α-pyr, 70% β-pyr, 5% α-fur, 23% β-fur, and 0.7% ketone. Occurs in honey and a large number of fruits, particularly apples and tomatoes. Fluid and nutrient replenisher, nutritive sweetener. Inulin from dandelion roots has also been used as a source. Present in polymeric form in the inulins, the energy reserve polysaccharides of many plants, e.g. dahlia and Jerusalem artichoke tubers. Mp 102-104°. $[\alpha]_D$ -133.5. $[\alpha]_D$ -92.4 (c, 4 in H_2O). pK_{a1} 12.03 (25°). Sweetness = 0.84 × sucrose (sometimes stated to be sweeter than sucrose).
▶ Gastrointestinal effects by ingestion (large dose).

1-O-(3,4,5-Trihydroxybenzoyl): [94356-19-1] ***1-O-Galloylfructose***
$C_{13}H_{16}O_{10}$ 332.263
Isol. from commercial rhubarb (*Rheum* sp.). Needles + ½H_2O (H_2O). Mp 168-169°. $[\alpha]_D^{25}$ -41.2 (c, 0.59 in MeOH). Exists as an equilibrated mixt. of α- and β-furanose and β-pyranose-forms.

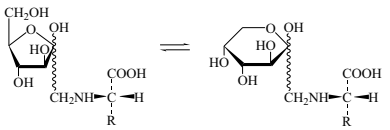
L-*form* [7776-48-9]
Mp 101-103°. $[\alpha]_D$ +128 → +98 (H_2O).

DL-*form*
Cryst. Mp 129-130°.

[8013-17-0, 25339-99-5, 27195-16-0, 41579-20-8, 41612-84-4, 41847-51-2, 92691-79-7, 92691-80-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 193D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 297A (*nmr*)
Barry, C.P. *et al., Adv. Carbohydr. Chem.*, 1952, **7**, 53 (*rev*)
Honeyman, J. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 116 (*β-D-form, isol*)
Wolfrom, M.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 118 (*synth*)
Verstraeten, L.M.J. *et al., Adv. Carbohydr. Chem.*, 1967, **22**, 229 (***rev***)
Kvernu, T.A.W. *et al., Carbohydr. Res.*, 1972, **21**, 455 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 617 (*occur, bibl*)
Kanters, J.A. *et al., Acta Cryst. B*, 1977, **33**, 665 (*cryst struct*)
Chen, M. *et al., Adv. Carbohydr. Chem. Biochem.*, 1977, **34**, 286 (*rev, metab*)
Mathlouthi, M. *et al., Carbohydr. Res.*, 1980, **78**, 225 (*Raman*)
Pfeffer, P.E. *et al., Carbohydr. Res.*, 1982, **102**, 11 (*cmr*)
Horton, D. *et al., Carbohydr. Res.*, 1982, **105**, 145 (*cmr*)
Morgenlie, S. *et al., Carbohydr. Res.*, 1982, **107**, 137 (*synth, DL-form*)
Geigert, J. *et al., Carbohydr. Res.*, 1983, **113**, 159 (*synth*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)
Steele, D. *et al., Carbohydr. Res.*, 1984, **133**, 313 (*ir, Raman*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461 (*1-O-Galloylfructose*)
Dhawale, M.R. *et al., Carbohydr. Res.*, 1986, **155**, 262 (*synth, L-form*)
Chen, C.C. *et al., Carbohydr. Res.*, 1988, **175**, 265 (*synth, bibl, L-form*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, LFI000
Krutosikova, A. *et al., Natural and Synthetic Sweet Substances*, Ellis Horwood, 1992, (*rev*)
Yaylayan, V.A. *et al., Carbohydr. Res.*, 1993, **248**, 355 (*equilib*)
Gizaw, Y. *et al., Carbohydr. Res.*, 1995, **266**, 81-85 (*synth, bibl, L-form*)
Flood, A.E. *et al., Carbohydr. Res.*, 1996, **288**, 45-46 (*equilib*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1363
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1127
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LFI000

Fructose aminoacids F-76



Naturally occurring compds. are derived from D-fructose and L-aminoacids. Amadori products resulting from sugar-aminoacid interactions in food products, esp. cooked foods.

Fructose-alanine [16124-24-6]

[71887-76-8, 86334-91-0, 87251-67-0, 87251-77-2, 87332-29-4]
1-[(1-Carboxyethyl)amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)alanine. 1-Deoxyalaninofructose*

$C_9H_{17}NO_7$ 251.236
Cryst. (MeOH aq./1-butanol). Mp 184° dec. $[\alpha]_D^{20}$ -61.2 (c, 2 in H_2O). α- and β-furanose and pyranose forms present in soln..

Fructose-glycine [60644-20-4]

[4429-05-4]
1-[(Carboxymethyl)amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)glycine*

$C_8H_{15}NO_7$ 237.209
Prisms. Mp 146.5-147.5°. $[\alpha]_D^{25}$ -66 (c, 1 in H_2O). β-Pyranose form predominates in aq. soln. and cryst. state.

Fructose-histidine [25020-13-7]
*1-[[1-Carboxy-2-(1*H*-imidazol-4-yl)ethyl]amino]-1-deoxyfructose, 9CI.* N-*(1-Deoxy-1-fructosyl)histidine*
$C_{12}H_{19}N_3O_7$ 317.298
Light yellow powder. Mp 130° dec. $[\alpha]_D^{20}$ -30.5 (c, 0.3 in H_2O).

Fructose-isoleucine [87304-79-8]

[34393-17-4]
1-[(1-Carboxy-2-methylbutyl)amino]-1-deoxyfructose. N-*(1-Deoxy-1-fructosyl)isoleucine*

$C_{12}H_{23}NO_7$ 293.316
Powder. Mp 120° dec. $[\alpha]_D^{20}$ -31 (c, 1.6 in H_2O).

Fructose-leucine [34393-18-5]
1-[(1-Carboxy-3-methylbutyl)amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)leucine*
$C_{12}H_{23}NO_7$ 293.316

Needles (butanol). Mp 145° dec. $[\alpha]_D^{20}$ -37 (c, 0.5 in H_2O). β-Pyranose form predominates in soln..

Fructose-methionine [20638-92-0]
1-[[1-Carboxy-3-(methylthio)propyl]amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)methionine*

$C_{11}H_{21}NO_7S$ 311.355
Cryst. (EtOH/butanol). Mp 95° dec. $[\alpha]_D^{20}$ -34 (c, 0.35 in H_2O).

Fructose-phenylalanine [87251-83-0]

[31105-03-0, 50826-04-5, 71887-77-9]
1-[(1-Carboxy-2-phenylethyl)amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)phenylalanine*

$C_{15}H_{21}NO_7$ 327.333
Cryst. (butanol aq.). Mp 143° dec Mp 170° (browning at 140°). $[\alpha]_D^{20}$ -34 (c, 2.2 in H_2O).

Fructose-proline [29118-61-4]

[5388-44-3]
1-(2-Carboxy-1-pyrrolidinyl)-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)proline. 1-Deoxyprolylfructose*

$C_{11}H_{19}NO_7$ 277.274
Needles (MeOH). Mp 145° dec. $[\alpha]_D^{20}$ -92.7 (c, 0.44 in H_2O).

Fructose-serine [87251-79-4]

[34393-26-5, 57288-23-0]
1-[(1-Carboxy-2-hydroxyethyl)amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)serine*

$C_9H_{17}NO_8$ 267.235
Needles. Mp 110° dec. $[\alpha]_D^{20}$ -46 (c, 2.3 in H_2O).

Fructose-threonine [70954-04-0]
1-[(1-Carboxy-2-hydroxypropyl)amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)threonine*

$C_{10}H_{19}NO_8$ 281.262
Monohydrate. Mp 108° dec. $[\alpha]_D^{20}$ -47 (c, 0.4 in H_2O).

Fructose-tryptophan [25020-15-9]
1-[[1-Carboxy-2-(1H-indol-3-yl)ethyl]amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)tryptophan*

$C_{17}H_{22}N_2O_7$ 366.37
Cryst. + $2H_2O$ (butanol aq.). Mp 143° dec (dihydrate). $[\alpha]_D^{20}$ -40 (c, 0.3 in H_2O).

Fructose-tyrosine [34393-22-1]
1-[[1-Carboxy-2-(4-hydroxyphenyl)ethyl]amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)tyrosine*

$C_{15}H_{21}NO_8$ 343.333
Mp 115° dec. $[\alpha]_D^{20}$ -16 (c, 0.5 in DMSO).

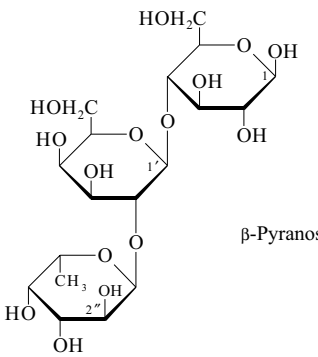
Fructose-valine
1-[(1-Carboxy2-methylpropyl)amino]-1-deoxyfructose, 9CI. N-*(1-Deoxy-1-fructosyl)valine*

$C_{11}H_{21}NO_7$ 279.289
Cryst. (MeOH aq.). Mp 156° dec. $[\alpha]_D^{20}$ -42.9 (c, 2 in H_2O). β-Pyranose form predominates in soln..

Heyns, K. *et al., Chem. Ber.*, 1958, **91**, 2750-2762 (*Fructosephenylalanine*)
Heyns, K. *et al., Annalen*, 1959, **622**, 160-174 (*Fructosealanine*)
Heyns, K. *et al., Tetrahedron*, 1961, **13**, 247 (*Fructoseproline*)
Heyns, K. *et al., Chem. Ber.*, 1964, **97**, 415-418 (*Fructosetryptophan*)
Tomita, H. *et al., Agric. Biol. Chem.*, 1965, **29**, 515; 959 (*isol, ir, synth*)
Hashiba, H. *et al., J. Agric. Food Chem.*, 1976, **24**, 70-73 (*synth, props*)
Nursten, H.E. *et al., Food Chem.*, 1980, **6**, 263 (*rev*)
Altena, J.H. *et al., Carbohydr. Res.*, 1981, **92**, 37-49 (*pmr, struct*)
Moll, N. *et al., J. Agric. Food Chem.*, 1982, **30**, 782-786 (*hplc, ms, cmr, purifn*)
Roeper, H. *et al., Carbohydr. Res.*, 1983, **116**, 183-195 (*synth, pmr, cmr*)
Walton, D.J. *et al., Carbohydr. Res.*, 1987, **167**, 123-130 (*synth, pmr*)
Yavlayan, V. *et al., Org. Mass Spectrom.*, 1988, **23**, 849 (*ms*)
Mossine, V.V. *et al., Carbohydr. Res.*, 1994, **262**, 257-270; 1995, **266**, 5-14 (*synth, pmr, cmr, ms, cryst struct*)

α-L-Fucopyranosyl-(1 → 2)-β-D-galactopyranosyl-(1 → 4)-D-glucose, 9CI, 8CI F-77

[41263-94-9]
2′-Fucosyllactose



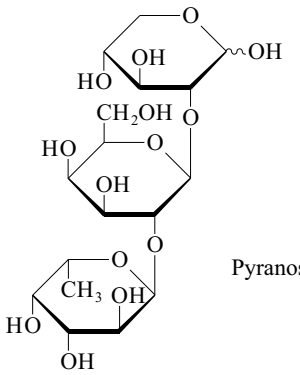
β-Pyranose-*form*

$C_{18}H_{32}O_{15}$ 488.442
Present in the free state in human milk. Solid (EtOH). Mp 230-231°. $[\alpha]_D$ -53.5 → -57.5 (72h) (c, 2.0 in H_2O). $[\alpha]_D$ -43 → -48 (c, 0.47 in H_2O).

Kuhn, R. *et al., Chem. Ber.*, 1955, **88**, 1135; 1956, **89**, 2513 (*isol*)
Biswas, M. *et al., Biopolymers*, 1980, **19**, 1555 (*conformn*)
Abbas, S.A. *et al., Carbohydr. Res.*, 1981, **88**, 51 (*synth, pmr*)
Hansson, G.C. *et al., Biochemistry*, 1989, **28**, 6672 (*gc-ms*)
Thurl, S. *et al., J. Chromatogr.*, 1991, **568**, 291 (*anal*)

α-L-Fucopyranosyl-(1 → 2)-β-D-galactopyranosyl-(1 → 2)-D-xylose F-78

[130136-27-5]
6-Deoxy-α-L-galactopyranosyl-(1 → 2)-β-D-galactopyranosyl-(1 → 2)-D-xylose, 9CI



Pyranose-*form*

$C_{17}H_{30}O_{14}$ 458.416
Constit. in the cell wall material of scarlet runner bean (*Phaseolus coccineus*). Syrup.

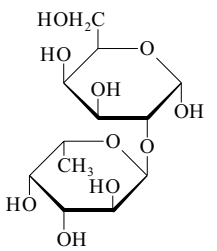
Octabenzyl: [130136-35-5]
$C_{73}H_{78}O_{14}$ 1179.411
Syrup.

[130136-79-7]

Kato, Y. *et al., Agric. Biol. Chem.*, 1980, **44**, 1751 (*constit*)
McDougall, G.J. *et al., Plant Physiol.*, 1989, **89**, 883 (*biol*)
Torgov, V.I. *et al., Bioorg. Khim.*, 1990, **16**, 854; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1990, **16**, 482 (*isol, pmr, cmr*)

2-*O*-α-L-Fucopyranosyl-D-galactose F-79

[24656-24-4]
2-O-(6-Deoxy-α-L-galactopyranosyl)-D-galactose, 9CI



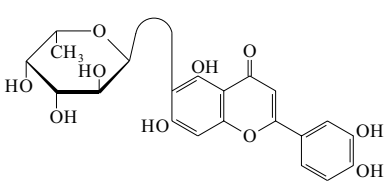
α-Pyranose-*form*

$C_{12}H_{22}O_{10}$ 326.3
Isol. from milk oligosaccharides. $[\alpha]_D^{22}$ -56 (c, 1.2 in H_2O).

Kuhn, R. *et al., Annalen*, 1958, **611**, 242-249 (*isol*)
Levy, A. *et al., Carbohydr. Res.*, 1967, **4**, 305-311 (*synth*)
Jacquinet, J.C. *et al., Tetrahedron*, 1976, **32**, 1693-1697 (*synth*)
Wegmann, B. *et al., Carbohydr. Res.*, 1988, **184**, 254-261 (*synth*)

6-*C*-Fucopyranosyl-3′,4′,5,7-tetrahydroxyflavone F-80

6-C-Fucosylluteolin

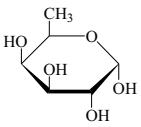


$C_{21}H_{20}O_{10}$ 432.383
Isol. from *Passiflora edulis* (passion fruit).

Mareck, U. *et al., Phytochemistry*, 1991, **30**, 3486-3487 (*isol, pmr, cmr*)

Fucose F-81

6-Deoxygalactose. Rhodeose. Galactomethylose



α-D-Pyranose-*form*

$C_6H_{12}O_5$ 164.158

An aq. soln. at 31°C contains 28% α-pyr, 67% β-pyr, =5% fur and 0.01% aldehyde.

L-*form* [2438-80-4]
A constit. of the polysaccharides obt. from gum tragacanth. Also found in glycoproteins obt. from milk. Prisms (EtOH). Mp 145° (140-141°). $[\alpha]_D^{17}$ -124 → -76 (c, 2.0 in H_2O).

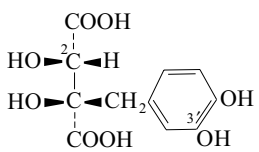
2-Me: [34299-00-8] *2*-O-*Methyl-*L*-fucose*
$C_7H_{14}O_5$ 178.185
Present in plant polysaccharides, e.g. of *Prunus domestica* (plum). Mp 150-152°. $[\alpha]_D^{23}$ -88 (c, 1.02 in H_2O).

[3713-31-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 188A; 190A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 291A (*nmr*)
Andrews, P. *et al., Chem. Ind. (London)*, 1957, 1453 (*2-O-Me, isol*)
Percival, E. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 195 (*L-form, synth*)
Izumi, K. *et al., Agric. Biol. Chem.*, 1971, **35**, 1816-1818 (*pmr*)
Dejter-Juszynski, M. *et al., Carbohydr. Res.*, 1971, **18**, 219-226; 1972, **23**, 41-45; 1973, **28**, 61-74; 144-146 (*L-form, α-L-pyr benzyl derivs*)
Gorin, P.J. *et al., Can. J. Chem.*, 1975, **53**, 1212-1223 (*pmr*)
Flowers, H.M. *et al., Adv. Carbohydr. Chem. Biochem.*, 1981, **39**, 279-345 (***rev***)
Defaye, J. *et al., Carbohydr. Res.*, 1981, **95**, 131-141 (*L-form, synth*)
Defaye, J. *et al., Carbohydr. Res.*, 1984, **126**, 165-169 (*L-form, synth*)
Sarbajna, S. *et al., Carbohydr. Res.*, 1995, **270**, 93-96 (*L-form, !synth*)
Takanashi, S. *et al., J.C.S. Perkin 1*, 1997, 607-612 (*L-form, synth, pmr, cmr*)

Fukiic acid F-82

2-[(3,4-Dihydroxyphenyl)methyl]-2,3-dihydroxybutanedioic acid, 9CI. 3,4-Dihydroxybenzyltartaric acid



$C_{11}H_{12}O_8$ 272.211

(2*S*,3*R*)-*form* [35388-56-8]
Hydrol. prod. from *Petasites japonicus* (sweet coltsfoot). Syrup. $[\alpha]_D^{25}$ +29.9 (c, 0.6 in MeOH). λ_{max} 248 (sh) (log ε 4.02); 291 (log ε 4.13); 332 (log ε 4.26) (MeOH).

1-Me ester:
$C_{12}H_{14}O_8$ 286.238
Cryst. + $1H_2O$. Mp 188-190°. $[\alpha]_D^{22}$ +40.5 (c, 1 in H_2O).

Di-Me ester: [56158-55-5]
$C_{13}H_{16}O_8$ 300.265
Isol. from *Petasites japonicus* (sweet coltsfoot).

*2-O-(3,4-Dihydroxy-*E*-cinnamoyl):*
[50982-40-6] ***Fukinolic acid***
$C_{20}H_{18}O_{11}$ 434.356
From *Petasites japonicus* (sweet coltsfoot). Amorph. powder. $[\alpha]_D^{20}$ +71.2 (c, 1 in H_2O). λ_{max} 248 (sh) (log ε 4.02); 291 (log ε 4.13); 332 (log ε 4.26) (MeOH).

*2-O-(3-Hydroxy-4-methoxy-*E*-cinnamoyl), 1-Me ester:*
$C_{22}H_{22}O_{11}$ 462.409
Pale yellow powder. $[\alpha]_D$ +36.4 (c, 0.37 in MeOH). λ_{max} 235 (sh) (log ε 4.3); 290 (log ε 4.19); 325 (log ε 4.22) (MeOH).

*2-O-(4-Hydroxy-3-methoxy-*E*-cinnamoyl), 1-Me ester:*
$C_{22}H_{22}O_{11}$ 462.409
Pale yellow powder. $[\alpha]_D$ +41.3 (c, 0.42 in MeOH). λ_{max} 235 (sh) (log ε 4.36); 291 (log ε 4.25); 327 (log ε 4.36) (MeOH).

3′-Me ether:
$C_{12}H_{14}O_8$ 286.238
Isol. from *Petasites japonicus* (sweet coltsfoot). Mp 137-138°.

*2-O-(4-Hydroxy-*E*-cinnamoyl):* ***Cimicifugic acid C***
$C_{20}H_{18}O_{10}$ 418.356
Pale yellow powder ($CHCl_3$/MeOH). $[\alpha]_D^{25}$ +38.7 (c, 0.3 in MeOH). λ_{max} 224 (log ε 4.23); 286 (sh) (log ε 4.16); 313 (log ε 4.27) (MeOH).

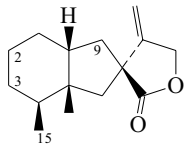
*2-O-(3-Hydroxy-4-methoxy-*E*-cinnamoyl):* ***Cimicifugic acid B***
$C_{21}H_{20}O_{11}$ 448.382
Pale yellow powder ($CHCl_3$/MeOH). $[\alpha]_D^{25}$ +42.5 (c, 0.5 in MeOH). λ_{max} 224 (log ε 4.23); 286 (sh) (log ε 4.16); 313 (log ε 4.27) (MeOH).

*2-O-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* ***Cimicifugic acid A***
$C_{21}H_{20}O_{11}$ 448.382
Pale yellow powder ($CHCl_3$/MeOH). $[\alpha]_D^{25}$ +47.8 (c, 0.9 in MeOH). λ_{max} 234 (log ε 4.16); 287 (sh) (log ε 4.08); 328 (log ε 4.28) (MeOH).

Sakamura, S. *et al., Agric. Biol. Chem.*, 1969, **33**, 1795; 1973, **37**, 1915 (*isol, struct, deriv*)
Yoshihara, T. *et al., Tet. Lett.*, 1971, 3809 (*stereochem*)
Matsumoto, T. *et al., Chem. Lett.*, 1972, 1 (*synth*)
Heller, W. *et al., Helv. Chim. Acta*, 1975, **58**, 974 (*isol*)
Kusano, G. *et al., Biol. Pharm. Bull.*, 1998, **21**, 997-999 (*activity, Fukinolic acid*)
Takahira, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 362-365 (*isol, uv, pmr, cmr, ms*)
Takahira, M. *et al., Phytochemistry*, 1998, **49**, 2115-2119 (*isol, uv, pmr, cmr, ms*)
Löser, B. *et al., Planta Med.*, 2000, **66**, 751-753 (*activity*)

Fukinanolide F-83

[19906-72-0]
Bakkenolide A



$C_{15}H_{22}O_2$ 234.338
Cryst. (pentane). Mp 80.5-80.6°. $[\alpha]_D^{22}$ +17 (c, 1 in MeOH).

2α-Hydroxy:2-Hydroxyfukinanolide. 2-Hydroxybakkenolide A
Cryst. Mp 91-93°.

2α-Hydroxy, 2-angeloyl: [133773-37-2] *2α-Angeloyloxybakkenolide A.* ***Homogynolide A***
$C_{20}H_{28}O_4$ 332.439
Cryst. Mp 62-65°.

3α-Hydroxy, 3-tigloyl:3α-Tigloyloxybakkenolide A. ***Homogynolide B***
$C_{20}H_{28}O_4$ 332.439
Oil.

9β-Hydroxy: [226711-43-9] ***Bakkenolide S.*** *9β-Hydroxyfukinanolide*
$C_{15}H_{22}O_3$ 250.337
Oil. $[\alpha]_D$ -87 (c, 0.037 in MeOH).

9β-Hydroxy, 9-Ac: [35945-70-1] ***9-Acetoxyfukinanolide***
$C_{17}H_{24}O_4$ 292.374
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. Mp 96-97°. $[\alpha]_D^{25}$ -28.5 (c, 1 in $CHCl_3$).

9β-Hydroxy, 9-(2-methylpropanoyl):
[226711-33-7] ***Bakkenolide I***
$C_{19}H_{28}O_4$ 320.428
Oil. $[\alpha]_D$ -32 (c, 0.079 in MeOH).

9β-Hydroxy, 9-(3-methylbutanoyl):
[226711-34-8] ***Bakkenolide J***
$C_{20}H_{30}O_4$ 334.455
Oil. $[\alpha]_D$ -140 (c, 0.013 in MeOH).

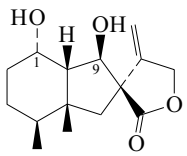
1,9-Dihydroxy: Fukinolidiol, F-84

Shirahata, K. *et al., Tetrahedron*, 1969, **25**, 3179; 4671 (*struct, ms*)
Naya, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3673 (*isol*)
Naya, K. *et al., Chem. Lett.*, 1972, 241 (*2-Acetoxyfukinanolide*)
Hayashi, K. *et al., Chem. Pharm. Bull.*, 1973, **21**, 2806 (*synth*)
Harmatha, J. *et al., Coll. Czech. Chem. Comm.*, 1976, **41**, 2047 (*isol, derivs*)
Evans, D.A. *et al., J.A.C.S.*, 1977, **99**, 5453 (*synth*)
Greene, A.E. *et al., J.O.C.*, 1985, **50**, 3943 (*synth*)
Crelho, F. *et al., Tet. Lett.*, 1989, **30**, 565 (*synth*)
Aclinou, P. *et al., Phytochemistry*, 1991, **30**, 2083 (*isol, pmr, cmr*)
Hartmann, B. *et al., Tet. Lett.*, 1991, **32**, 767; 1993, **34**, 3875 (*synth*)
Hamelin, O. *et al., Nat. Prod. Lett.*, 1997, **10**, 99-103 (*synth*)
Srikrishna, A. *et al., Tetrahedron*, 1998, **54**, 11517-11524 (*synth*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 375-382 (*Bakkenolides*)
Srikrishna, A. *et al., J.C.S. Perkin 1*, 1999, 2069-2076 (*synth*)
Back, T.G. *et al., J.O.C.*, 2001, **66**, 4361-4368 (*synth*)

Brocksom, T.J. *et al., J.A.C.S.*, 2002, **124**, 15313-15325. (*synth*)

Fukinolidiol F-84

[24909-95-3]



$C_{15}H_{22}O_4$ 266.336
Cryst. Mp 176.5-177.5°. $[\alpha]_D^{22}$ -62.6 (c, 1 in MeOH).

1-(2S-Methylbutanoyl), 9-Ac: [41059-95-4] ***Dihydrofukinolide***
$C_{22}H_{32}O_6$ 392.491
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (petrol). Mp 125-126°. $[\alpha]_D^{22}$ -105.5 (c, 1 in MeOH).

1-Angeloyl: [18456-00-3] ***Bakkenolide C***
$C_{20}H_{28}O_5$ 348.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (petrol). Mp 167-167.5°.

1-Angeloyl, 9-Ac: [18455-98-6] ***Bakkenolide B***. *Fukinolide. Petasilide*
$C_{22}H_{30}O_6$ 390.475
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (petrol). Mp 101-102°. $[\alpha]_D^{22}$ -126 (c, 1 in MeOH).

1,9-Diangeloyl: [41059-96-5] ***Homofukinolide***
$C_{25}H_{34}O_6$ 430.54
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (petrol). Mp 184-186°. $[\alpha]_D^{22}$ -127 (c, 1 in $CHCl_3$).

1-Tigloyl, 9-Ac: [21807-96-5] ***Bakkenolide E***
$C_{22}H_{30}O_6$ 390.475
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (EtOH). Mp 168°.

1-(3-Methylthio-2Z-propenoyl), 9-Ac: [18456-03-6] ***Bakkenolide D***. S-*Fukinolide*
$C_{21}H_{28}O_6S$ 408.515
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (petrol). Mp 200-201°. $[\alpha]_D^{22}$ -161 (c, 1 in $CHCl_3$).

Abe, N. *et al., Tet. Lett.*, 1968, 1993-1997 (*struct*)
Katayama, C. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 1976-1980 (*cryst struct*)
Naya, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3673-3685 (*isol*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 375-382 (*Bakkenolides*)
Wu, T.-S. *et al., Phytochemistry*, 1999, **52**, 901-905 (*Bakkenolides G and H, Deisobutyrylbakkenolide H*)
Brocksom, T.J. *et al., J.A.C.S.*, 2002, **124**, 15313-15325 (*synth*)

Fulvocin C F-85

[69865-50-5]

Peptide. Struct. consists of 45 amino acid residues including 8 half-cystines. Bacteriocin isol. from *Myxococcus fulvus*.

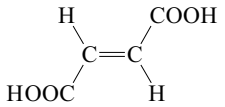
[76684-37-2]

Hirsch, H. *et al., Arch. Microbiol.*, 1978, **119**, 279 (*isol*)
Tsai, H. *et al., Biochim. Biophys. Acta*, 1981, **667**, 213 (*struct*)

Fumaric acid, 8CI F-86

[110-17-8]

[7704-73-6]
(E)-2-Butenedioic acid, 9CI. trans-*Ethylene-1,2-dicarboxylic acid. Paramaleic acid. Glaucic acid. Boletic acid. FEMA 2488. E297*



$C_4H_4O_4$ 116.073
Geometrical isomer of Maleic acid, M-34. Prod. industrially by fermentation of *Rhizopus nigricans*, or manuf. by catalytic or thermal isomerisation of maleic anhydride or maleic acid. Used as an antioxidant, acidulant, leavening agent and flavouring agent in foods. Present in raw lean fish. Dietary supplement. Used in powdered products since fumaric acid is less hygroscopic than other acids. Monoclinic, prismatic needles or leaflets (H_2O). Sol. EtOH; spar. sol. H_2O, Et_2O, Me_2CO; prac. insol. C_6H_6, $CHCl_3$. Mp 300-302° (sealed tube). pK_a 4.54 (25°). At 230° forms maleic anhydride.
▶ Skin and eye irritant. Nephrotoxic. LD_{50} (rat, orl) 10700 mg/kg. LS9625000

Na salt: [7704-73-6]

[17013-01-3] *Sodium fumarate*
Nutrient supplement.

K salt: [7704-72-5]

[4151-35-3] *Potassium fumarate*
Dietary supplement.

Ca salt: [7718-51-6]

[19855-56-2] *Calcium fumarate*
Nutrient supplement.

Mg salt: [7704-71-4]

[6880-23-5] *Magnesium fumarate*
Dietary supplement.

Mono-Me ester: [2756-87-8] *Methyl hydrogen fumarate. Monomethyl fumarate*
$C_5H_6O_4$ 130.1
Found in Mexican marigold *Tagetes minuta*. Prisms (EtOH). Mp 144.5°.

Di-Me ester: [624-49-7] *Dimethyl fumarate*
$C_6H_8O_4$ 144.127
Fungal growth inhibitor for tomato juice. Cryst. Insol. H_2O; sol. Me_2CO, $CHCl_3$. Mp 102°. Bp 192° Bp_{12} 88.5°.
▶ Eye and skin irritant. LD_{50} (rat, orl) 2240 mg/kg. EM6125000

Mono-Et ester: [2459-05-4] *Ethyl hydrogen fumarate. Monoethyl fumarate*
$C_6H_8O_4$ 144.127
Fungal growth inhibitor for tomato juice. Sol. EtOH, Me_2CO. Mp 66-68° (65°). Bp_{16} 147°.

Di-Et ester: [623-91-6] *Diethyl fumarate*
$C_8H_{12}O_4$ 172.18
Fungal growth inhibitor for tomato juice. Liq. Insol. H_2O; sol. Me_2CO, $CHCl_3$. d^{20} 1.05. Mp 1-2°. Bp 218-219° Bp_{10} 95-96°. n_D^{20} 1.4412. Q/e values for copolym., Q 0.25, e 2.26. Copolym. with vinyl chloride: r_{DE} 0.47, r_{VC} 0.12 (typical values, 60°); Q 0.61; e 1.25.
▶ LD_{50} (rat, orl) 1780 mg/kg. EM5950000

Monooctadecyl ester: [1741-93-1]

[4070-80-8] *Octadecyl fumarate. Monostearyl fumarate. Stearyl fumarate*
$C_{22}H_{40}O_4$ 368.556
Na salt is a dough conditioner, stabilising agent, conditioning agent for dehydrated potato and other processed foods. Mp 93-94°.

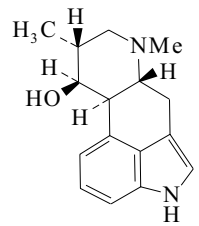
[5873-57-4, 6915-18-0, 17013-01-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 502D; 644D; 645A; 695A; 742C; 844A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 787B; 993B; 993C; 1119A; 1214A; 1360B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 689C; 690A; 746A; 773B; 803D (*ir*)
Anschütz, R. *et al., Annalen*, 1928, **461**, 155 (*isom*)
Justel, B. *et al., Angew. Chem.*, 1943, **56**, 157 (*detn, Th*)
Org. Synth., Coll. Vol., 2, 1943, 302 (*synth*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **2**, 41 (*synth, use*)
Spatz, S.M. *et al., J.O.C.*, 1958, **23**, 1559 (*monoester*)
U.S. Pat., 1958, 2 848 366; *CA*, **52**, 19023e
Christensen, E.A. *et al., J. Assoc. Off. Anal. Chem.*, 1972, **55**, 275 (*monooctadecyl ester*)
Devlin, C.J. *et al., J.C.S. Perkin 1*, 1972, 1249 (*di-Et ester*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 849
Junek, H. *et al., Tetrahedron*, 1972, **28**, 4083 (*synth, pmr, deriv*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Ito, A. *et al., Org. Mass Spectrom.*, 1973, **7**, 1279 (*ms*)
Kerr, R.O. *et al., Benzene Its Ind. Deriv.*, Wiley, N.Y., 1975, (*rev*)
Compton, D.A.C. *et al., J.C.S. Perkin 2*, 1975, 400 (*ir, Raman, diesters*)
Derissen, J.L. *et al., J. Mol. Struct.*, 1977, **38**, 177 (*struct, ed*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 910 (*di-Et ester, copolym, reactivity ratios*)
Dymicky, M. *et al., Org. Prep. Proced. Int.*, 1985, **17**, 121-131 (*monooctadecyl ester*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A16**, 53 (*rev*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1986, **4**, 779; 1987, **9**, 225
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **15**, 893 (*rev*)
Merwin, L.H. *et al., Magn. Reson. Chem.*, 1992, **30**, 440 (*cmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 197-198
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1086
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 386; 1129-1131; 1622; 2296; 2558-2559 (*props, use, salts*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand*

Reinhold, 1992, DEC600; FOU000; FOX000; FOY000; DSB600; DJJ800; DXD800

Fumigaclavine B F-87

6,8-Dimethylergolin-9-ol, 9CI



Absolute configuration

$C_{16}H_{20}N_2O$ 256.347

(-)-*form* [6879-93-2]
Mycotoxin from *Aspergillus fumigatus* and *Rhizopus arrhizus*. Mp 244-245° Mp 265-267° (double Mp). $[\alpha]_D$ -6.3 (c, 1.2 in MeOH).

Methiodide:
Cryst. (EtOH/Et_2O). Mp 309-310° dec.

O-*Ac:* [6879-59-0] ***Fumigaclavine A***
$C_{18}H_{22}N_2O_2$ 298.384
Alkaloid from *Aspergillus fumigatus*. Needles (MeOH aq.). Mp 84-85°.

▶ KE6345400

O-*Ac; hydrochloride:*
Prisms (EtOH). Mp 304-305° dec. (inserted at 300°). $[\alpha]_{Hg}^{22}$ -56.7 (c, 1.5 in MeOH).

8,9-Diepimer: See Isofumigaclavine A in *The Combined Chemical Dictionary.*

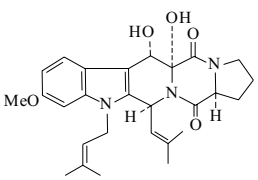
8,9-Diepimer, O-*Ac:* See Isofumigaclavine A in *The Combined Chemical Dictionary.*

(±)-*form*
Mp 199-200° dec.

Spilsbury, J.F. *et al., J.C.S.*, 1961, 2085 (*isol, uv, ir, struct*)
Bach, N.J. *et al., J.O.C.*, 1974, **39**, 1272 (*pmr, cmr, config*)
Kiguchi, T. *et al., Heterocycles*, 1985, **23**, 1925 (*synth, pmr*)
Ninomiya, I. *et al., Chem. Pharm. Bull.*, 1991, **39**, 23 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 545; 553

Fumitremorgin B F-88

[12626-17-4]
Lanosulin



Absolute configuration

$C_{27}H_{33}N_3O_5$ 479.575
Mycotoxin prod. by *Aspergillus fumigatus, Aspergillus caespitosus, Penicillium lanosum* and *Penicillium piscarium*. Isolated from *A. fumigatus* infected rice and miso. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 211-212° (204-206°). $[\alpha]_D^{25}$ +24 (c, 0.91 in $CHCl_3$). λ_{max} 228 (ϵ 39960); 278 (ϵ 11000); 295 (ϵ 12290) (MeOH) (Berdy). λ_{max} 226 (ϵ 31700); 278 (ϵ 7300); 295 (ϵ 7900) (EtOH) (Berdy).

▶ UY8709400

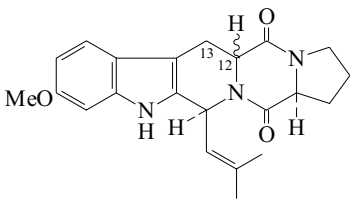
Tetrahydro:
Mp 97-100°.

13-Epimer:
Cotton-like needles (EtOAc). Mp 231.5-232° (226-227°).

Dix, D.T. *et al., Chem. Comm.*, 1972, 1168 (*uv, ir, pmr, ms*)
Yamazaki, M. *et al., Tet. Lett.*, 1975, 27 (*cryst struct*)
Yamazaki, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 245 (*isol, uv, ir, pmr, cd, ms*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Nakatsuka, S. *et al., Tet. Lett.*, 1986, **27**, 6361 (*synth, uv, ir, pmr*)
Kodato, S. *et al., Tetrahedron*, 1988, **44**, 359 (*synth, uv, ir, pmr, ms, cd*)
Hino, T. *et al., Heterocycles*, 1997, **46**, 673-704 (*rev, synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 360

Fumitremorgin C F-89

SM-Q



$C_{22}H_{25}N_3O_3$ 379.458
Struct. revised in 1988. Config. at C-12 not specified. Of the two synthetic epimers the one with 12α-*H* config. possessed spectroscopic characteristics identical with those reported for natural Fumitremorgin C. (Hino *et al*).However, complete identification was not possible and the Mp's were widely different. A cryst. struct. determination mentioned in 1985 has not been publ..λ_{max} 224 ; 272 ; 294 (MeOH) (Berdy). λ_{max} 225 ; 273 ; 299 (EtOH) (Berdy).

Natural-*form* [118974-02-0]
Mycotoxin from *Aspergillus fumigatus*. Cryst. (EtOAc). Mp 125-130°.

12,13-Epoxide: ***Epoxyfumitremorgin C***
$C_{22}H_{25}N_3O_4$ 395.457
From *Aspergillus fumigatus*.

12,13-Dihydroxy: [111427-99-7] ***Dihydroxyfumitremorgin C***
$C_{22}H_{25}N_3O_5$ 411.457
From *Aspergillus fumigatus*. Yellow cryst. Mp 197-198°. $[\alpha]_D$ +18.4.

Demethoxy: ***Demethoxyfumitremorgin C***
$C_{21}H_{23}N_3O_2$ 349.432
Prod. by *Aspergillus fumigatus*. Pale yellow needles. Sol. MeOH. Mp 210-212°. $[\alpha]_D^{30}$ +8 (c, 0.2 in $CHCl_3$). λ_{max} 226 (ϵ 24950); 282 (ϵ 9000); 291 (sh) (ϵ 7450) (MeOH).

12α-*form*
Powder (EtOAc). Mp 259.5-260.5° dec. $[\alpha]_D^{28}$ -13 (c, 0.53 in MeOH).

Demethoxy: [111768-16-2]
Cryst. (EtOH). Mp not reported.

12β-*form* [119066-64-7]
Pale yellow prisms (EtOH). Mp 240-247.5° dec. $[\alpha]_D^{28}$ +239 (c, 0.11 in MeOH).

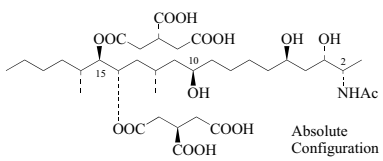
Demethoxy: [106211-91-0]
Cryst. + 1/3EtOAc (EtOAc). Mp 208-212°. $[\alpha]_D^{22}$ +281 (c, 0.1 in MeOH).

[118974-03-1, 119066-67-0, 119066-68-1, 119066-69-2]

Cole, R.J. *et al., J. Agric. Food Chem.*, 1977, **25**, 826-830 (*isol*)
Steyn, P.S. *et al., Prog. Chem. Org. Nat. Prod.*, 1985, **48**, 60 (*uv, pmr, cmr*)
Plate, R. *et al., J.O.C.*, 1987, **52**, 560-564 (*synth, uv, pmr, ms*)
O'Malley, G.J. *et al., Tet. Lett.*, 1987, **28**, 1131 (*synth, deriv*)
Hermkens, P.H.H. *et al., Tetrahedron*, 1988, **44**, 1991-2000 (*synth, uv, pmr, ms*)
Hino, T. *et al., Tetrahedron*, 1989, **45**, 1941-1944 (*synth, uv, ir, pmr, cmr, ms*)
Abraham, W.R. *et al., Phytochemistry*, 1990, **29**, 1025-1026 (*Dihydroxyfumitremorgin C*)
Cui, C.-B. *et al., J. Antibiot.*, 1996, **49**, 527-534; 534-540 (*pmr, cmr, demethoxy*)
Hino, T. *et al., Heterocycles*, 1997, **46**, 673-704 (*rev, synth*)
Bailey, P.D. *et al., Tet. Lett.*, 2001, **42**, 113-115 (*demethoxy, synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 364

Fumonisin A_1 F-90

[117415-48-2]
1,2,3-Propanetricarboxylic acid 1,1′-[1-[12-(acetylamino)-4,9,11-trihydroxy-2-methyltridecyl]-2-(1-methylpentyl)-1,2-ethanediyl] ester, 9CI



$C_{36}H_{61}NO_{16}$ 763.875
Prod. by *Fusarium moniliforme*. Sol. MeOH, H_2O; poorly sol. $CHCl_3$, hexane.

N-*De-Ac:* [116355-83-0] ***Fumonisin B_1.*** *Macrofusin*
$C_{34}H_{59}NO_{15}$ 721.838
From *Fusarium moniliforme*. Sol. MeOH, H_2O; poorly sol. $CHCl_3$, hexane.

▶ TZ8350000

N-*De(acetylamino),* N-*(3-hydroxy-1-pyridinyl):* [182063-58-7] *Fumonisin FP_1*
$C_{39}H_{62}NO_{16}^{\oplus}$ 800.916
Prod. by *Fusarium moniliforme*. Solid. λ_{max} 288 (ϵ 1320) (0.1M HCl). λ_{max} 288 (ϵ 1320) (HCl) (Berdy). λ_{max} 322 (ϵ 1170) (NaOH aq.) (Berdy).

15-Deacyl, 15-ketone: [170591-49-8] ***Fumonisin AK_1***
$C_{30}H_{53}NO_{11}$ 603.749
Prod. by *Fusarium proliferatum*.

5-Deoxy, N-*de-Ac:* [136379-59-4] ***Fumonisin B_3***
$C_{34}H_{59}NO_{14}$ 705.838

From *Fusarium moniliforme*. Sol. MeOH, H_2O.

5-Deoxy, N-*de(acetylamino),* N-*(3-hydroxy-1-pyridinyl):* [182063-60-1] ***Fumonisin FP$_3$***
$C_{39}H_{62}NO_{15}^{\oplus}$ 784.917
Prod. by *Fusarium moniliforme*. Solid. λ_{max} 288 (ϵ 1324) (0.1M HCl). λ_{max} 288 (ϵ 1324) (HCl) (Berdy). λ_{max} 322 (ϵ 1183) (NaOH) (Berdy).

10-Deoxy: [117415-47-1] ***Fumonisin A$_2$***
$C_{36}H_{61}NO_{15}$ 747.876
From *Fusarium moniliforme*. Sol. MeOH, H_2O; poorly sol. $CHCl_3$, hexane.

10-Deoxy, N-*de-Ac:* [116355-84-1] ***Fumonisin B$_2$***
$C_{34}H_{59}NO_{14}$ 705.838
From *Fusarium moniliforme*. Sol. MeOH, H_2O; poorly sol. $CHCl_3$, hexane.

▶ TZ8335000

10-Deoxy, N-*de(acetylamino),* N-*(3-hydroxy-1-pyridinyl):* [182063-59-8] ***Fumonisin FP$_2$***
$C_{39}H_{62}NO_{15}^{\oplus}$ 784.917
Prod. by *Fusarium moniliforme*. Solid. λ_{max} 288 (ϵ 1370) (0.1M HCl). λ_{max} 288 (ϵ 1370) (HCl) (Berdy). λ_{max} 320 (ϵ 1191) (NaOH aq.) (Berdy).

5,10-Dideoxy, N-*de-Ac:* [136379-60-7] ***Fumonisin B$_4$***
$C_{34}H_{59}NO_{13}$ 689.839
From *Fusarium moniliforme*. Sol. MeOH, H_2O.

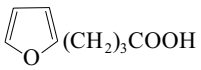
*4*R*-Hydroxy, 5-deoxy,* N-*de-Ac:* [203259-29-4] ***Isofumonisin B$_1$***
$C_{34}H_{59}NO_{15}$ 721.838
From *Fusarium moniliforme*.

[126254-17-9]

Bezuidenhout, S.C. *et al., Chem. Comm.*, 1988, 743 (*isol, struct*)
Laurent, D. *et al., Microbiol., Aliments, Nutr.*, 1989, **7**, 9 (*Macrofusin*)
Cawood, M.E. *et al., J. Agric. Food Chem.*, 1991, **39**, 1958 (*isol*)
Gelderblom, W.C.A. *et al., Mycopathologia*, 1992, **117**, 11 (*rev*)
Plattner, R.D. *et al., Mycopathologia*, 1992, **117**, 23 (*Fumonisin B$_3$*)
Hoye, T.R. *et al., J.A.C.S.*, 1994, **116**, 9409 (*abs config*)
Harmange, J.-C. *et al., Tet. Lett.*, 1994, **35**, 6819 (*abs config*)
Musser, S.M. *et al., J. Nat. Prod.*, 1995, **58**, 1392-1397 (*Fumonisin AK*)
Shier, W.T. *et al., Tet. Lett.*, 1995, **36**, 1571 (*abs config*)
Musser, S.M. *et al., J. Nat. Prod.*, 1996, **59**, 970-972 (*Fumonisin FP*)
Merrill, A.H. *et al., Trends Cell Biol.*, 1996, **6**, 218-223 (*rev*)
Musser, S.M. *et al., J. Agric. Food Chem.*, 1997, **45**, 1169-1173 (*Fumonisin FP*)
Shi, Y. *et al., J.O.C.*, 1997, **62**, 5666-5667 (*synth, Fumonisin B$_2$*)
MacKenzie, S.E. *et al., J. Nat. Prod.*, 1998, **61**, 367-369 (*Isofumonisin B$_1$*)
Hartl, M. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 1549-1556 (*abs config*)
Edwards, O.E. *et al., Tet. Lett.*, 1999, **40**, 4515-4518 (*abs config*)

2-Furanbutanoic acid, 9CI F-91

[92638-98-7]
2-(2-Furyl)butyric acid



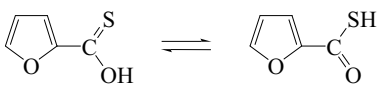
$C_8H_{10}O_3$ 154.165
Liq. $Bp_{0.005}$ 75-76°.

3-Methylbutyl ester: [7779-66-0] *3-Methylbutyl 2-furanbutanoate. Isoamyl 2-furylbutyrate. FEMA 2070*
$C_{13}H_{20}O_3$ 224.299
Flavouring ingredient. Pale yellow liq. with caramel-like flavour.

Föhlisch, B. *et al., Chem. Ber.*, 1984, **117**, 2580 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 378 (*3-methylbutyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1424 (*3-methylbutyl ester*)

2-Furancarbothioic acid, 9CI F-92

[4741-45-1]
Thio-2-furoic acid, 8CI



$C_5H_4O_2S$ 128.151
Liq. Bp_{16} 101°.

SH-form

Me ester: [13679-61-3] *Methyl 2-thiofuroate. FEMA 3311*
$C_6H_6O_2S$ 142.178
Flavouring ingredient with a fried, cooked onion odour. Bp_{11} 92-93°.

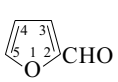
OH-form

Hydrazide: [68062-22-6] *2-Furanthiocarboxhydrazide*
$C_5H_6N_2OS$ 142.181
Cryst. (hot H_2O or C_6H_6). Sol. EtOH, C_6H_6; mod. sol. H_2O. Mp 130-131°.

Jensen, K.A. *et al., Acta Chem. Scand.*, 1961, **15**, 1097 (*synth, hydrazide*)
Niwa, E. *et al., CA*, 1968, **68**, 49377w (*synth*)
Shome, S.C. *et al., Mikrochim. Acta*, 1978, **2**, 343 (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 571 (*S-Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1869-1870 (*S-Me ester*)

2-Furancarboxaldehyde, 9CI F-93

[98-01-1]
2-Furaldehyde, 8CI. Furfural. 2-Formylfuran. Furfurole. α-Furfuraldehyde. Fural. α-Furole. FEMA 2489



$C_5H_4O_2$ 96.085
Flavour ingredient. Present in coffee, calamus, matsutake mushroom (*Tricholoma matsutake*), pumpkin, malt, peated malt, Bourbon vanilla, Lamb's lettuce, pimento leaf and various fruits, e.g. apple, apricot, sweet cherry, morello cherry, orange, grapefruit, Chinese quince and a common consit of essential oils. Liq. with odour of fresh-baked bread. Part. misc. H_2O. d_4^{20} 1.16. Mp -37°. Bp 162° Bp_{65} 90°. n_D^{20} 1.5261. Log P 0.67 (calc). Resinifies on keeping. Steam-volatile.

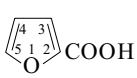
▶ Flammable, fl. p. 60°, autoignition temp. 316/391°. Skin, eye and mucous membrane irritant. May cause dermatitis. CNS depressant. Exp. hepatotoxic. LD_{50} (rat, orl) 65 mg/kg. Readily absorbed through skin. OES: long-term 2 ppm; short-term 10 ppm (Sk). LT7000000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 581B; 584A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 17A; 22C; 24C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1452C; 1456D; 1458A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 274 (*synth*)
Wacek, D.A. *et al., Angew. Chem.*, 1941, **54**, 453 (*rev*)
Barney, J.E. *et al., J. Chromatogr.*, 1969, **45**, 82 (*use*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1782 (*occur*)
Abraham, R.J. *et al., Tetrahedron*, 1972, **28**, 3015 (*pmr*)
Cano Pavon, J.M. *et al., Talanta*, 1973, **20**, 339 (*synth, detn, Pd*)
Fringuelli, F. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 175 (*pmr, cmr*)
Chadwick, D.J. *et al., J.C.S. Perkin 1*, 1974, 1141 (*pmr*)
Green, J.H.S. *et al., Spectrochim. Acta A*, 1977, **33**, 843 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 759 (*rev, tox*)
Hassan, R. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 844 (*uv*)
Casarini, D. *et al., J.C.S. Perkin 2*, 1985, 1839 (*cmr*)
Popelis, Y.Y. *et al., Zh. Obshch. Khim.*, 1985, **55**, 1615 (*O-17 nmr*)
Encyclopaedia of Polymer Science and Engineering, 2nd edn., Wiley-Interscience, New York, 1987, **7**, 454 (*rev, polymers*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 283
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1139-1140 (*occur, use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1720
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 308
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FPQ875

2-Furancarboxylic acid, 9CI F-94

[88-14-2]

[26447-28-9]
2-Furoic acid, 8CI. α-Furoic acid. Pyromucic acid



$C_5H_4O_3$ 112.085
Isol. from roots of *Phaseolus vulgaris* (kidney bean). Leaflets (H_2O). Mod. sol. cold H_2O; v. sol. hot. Mp 133-134°. Bp 230-232° Bp_{20} 141-144°.

▶ LD_{50} (mus, ipr) 100 mg/kg. LV1763000

Me ester: [611-13-2] *Methyl 2-furoate. FEMA 2703*
$C_6H_6O_3$ 126.112
Used in food flavouring. Found in cranberries, guava fruits, raisins and other fruits. Also present in baked potato, roasted filberts, roasted peanut, tomatoes, coffee, cocoa, okra (*Hibiscus esculentus*) and other foodstuffs. Oil or cryst. with fruity or mushroom odour. Bp 181.3°.

▶ Skin irritant. LV1950000

2-Phenylethyl ester: [7149-32-8] *2-Phenylethyl 2-furancarboxylate. Phenethyl 2-furoate. FEMA 2865*
$C_{13}H_{12}O_3$ 216.236
Flavouring ingredient. Liq.

Propyl ester: [615-10-1] *Propyl 2-furoate. FEMA 2946*
$C_8H_{10}O_3$ 154.165
Flavouring ingredient. Liq. Bp 211°. n_D^{20} 1.4737.

2-Propenyl ester: [4208-49-5] *2-Propenyl 2-furancarboxylate. Allyl 2-furoate. FEMA 2030*
$C_8H_8O_3$ 152.149
Flavouring ingredient. Liq. d^{25} 1.18. Bp 206-209° Bp 214-216°. n_D^{20} 1.4945.

Pentyl ester: [4996-48-9] *Amyl 2-furoate. FEMA 2072*
$C_{10}H_{14}O_3$ 182.219
Used in food flavouring. d_4^{20} 1.03. Bp 233° Bp_1 95-97°.

Hexyl ester: [39251-86-0] *Hexyl 2-furoate. FEMA 2571*
$C_{11}H_{16}O_3$ 196.246
Flavouring ingredient. Liq. Bp 252°. n_D^{20} 1.0170.

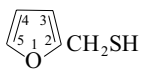
Octyl ester: [39251-88-2] *Octyl 2-furoate. FEMA 3518*
$C_{13}H_{20}O_3$ 224.299
Flavouring ingredient. d^{20} 0.99. Bp_7 158°. n_D^{20} 1.4693.

[1334-82-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 585A; 587A; 587B; 589B; 589D; 590B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 27A; 28C; 29B; 40A; 40C; 41A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1459A; 1459D; 1460A; 1465B; 1465C (*ir*)
Org. Synth., Coll. Vol., 4, 1963, 493 (*synth*)
Takasugi, M. *et al., Chem. Lett.*, 1973, 445
Borisova, N.N. *et al., Khim. Geterotsikl. Soedin.*, 1973, 590; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1973, 546 (*uv*)
Chadwick, D.J. *et al., J.C.S. Perkin 1*, 1974, 1141 (*pmr*)
Green, J.H.S. *et al., Spectrochim. Acta A*, 1977, **33**, 843 (*ir, Raman*)
Lukevits, E. *et al., Zh. Obshch. Khim.*, 1985, **55**, 2062; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 1830 (*cmr, pmr*)
Murahashi, S.-I. *et al., J.O.C.*, 1986, **51**, 898 (*synth, ir, pmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 24; 350; 625; 649; 698 (*esters*)
Hose, D.R.J. *et al., J.C.S. Perkin 1*, 1996, 691 (*synth, ir, pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 88-89; 161; 1763; 2032-2033; 2032-2033; 2161-2162; 2359 (*esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EKM000; FQF000; MKH600

2-Furanmethanethiol, 9CI F-95

[98-02-2]
2-Furfuryl mercaptan. 2-(Mercaptomethyl)furan. FEMA 2493



C_5H_6OS 114.168
Flavour ingredient used in coffee aroma. Formed by thermal treatment of cysteine/ribose mixtures. Present in cooked meats, popcorn, wheat bread, roasted coffee and roasted sesame seed oil. Liq. with v. disagreeable odour. d_4^{20} 1.14. Bp 160° Bp_{65} 84°. n_D^{25} 1.5280. Odour becomes coffee-like on dilution. Odour threshold 0.0025ng/L in air and 0.01 µg/kg in H_2O.

▶ LD_{50} (mus, ipr) 100 mg/kg. Exp. reprod. effects. LU2100000

S-*Formyl:* [59020-90-5] S-*(2-Furanylmethyl) methanethioate. Furfuryl thioformate. FEMA 3158*
$C_6H_6O_2S$ 142.178
Flavouring ingredient.

S-*Ac:* [13678-68-7] *Furfuryl thioacetate.* S-*(2-Furanylmethyl)ethanethioate, 9CI. FEMA 3162*
$C_7H_8O_2S$ 156.205
Present in roasted sesame seed oil, meat flavours and coffee. Liq. d 1.17. Bp_{12} 90-92°. n_D^{20} 1.5260.

S-*Propanoyl:* [59020-85-8] S-*(2-Furanylmethyl) propanethioate. Furfuryl thiopropionate. FEMA 3347*
$C_8H_{10}O_2S$ 170.232
Flavouring ingredient. Bp_{10} 95-97°.

S-*Me:* [1438-91-1] *2-(Methylthiomethyl)-furan. FEMA 3160*
C_6H_8OS 128.195
Minor constit. of aroma of coffee, also present in smoked cured pork and pork liver. Flavour ingredient. Bp_{28} 62-63°. $n_D^{22.5}$ 1.5210.

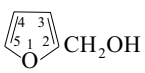
S-*Et:* [2024-70-6] *2-[(Ethylthio)methyl]-furan, 9CI. (2-Furfurylthio)ethane. Ethyl furfuryl sulfide*
$C_7H_{10}OS$ 142.221
Constit. of roast Arabica coffee aroma. Bp 152-154°. n_D^{20} 1.5136.

S-*Ph:* [3260-09-1] *2-(Phenylthiomethyl)-furan*
$C_{11}H_{10}OS$ 190.265
Oil. Bp 154°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 582C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 20B; 20C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1453D; 1454B (*ir*)
Kofod, H. *et al., Acta Chem. Scand.*, 1953, **7**, 1302 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 491 (*synth*)
Gianturco, M.A. *et al., Tetrahedron*, 1964, **20**, 2951 (*deriv*)
Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*S-Ac*)
Katritzky, A.R. *et al., Tetrahedron*, 1972, **28**, 2037 (*ir*)
Schreurs, P.H.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1976, **95**, 75-78 (*S-Et, synth*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1981, **29**, 1078-1082 (*S-Et, occur, ms*)
Molina, P. *et al., Synthesis*, 1982, 472-475 (*S-Et, synth*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*S-Ac, detn, sesame oil*)
Greeves, N. *et al., Synthesis*, 1993, 1109 (*S-Ph*)
Marstokk, K.M. *et al., Acta Chem. Scand.*, 1994, **48**, 298 (*microwave, struct*)
Blank, I. *et al., Dev. Food Sci.*, 1994, **35**, 271-276 (*S-Ac, detn, meat flavours*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 282; 287; 290-291 (*S-formyl, S-Ac*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1134-1135; 1144-1146; 1150-1151 (*S-formyl, S-Me, occur, use*)
Kerscher, R. *et al., J. Agric. Food Chem.*, 1998, **46**, 1954-1958 (*occur*)
Ayers, J.T. *et al., Synth. Commun.*, 1999, **29**, 351-358 (*S-Ac, synth, pmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FPM000

2-Furanmethanol, 9CI F-96

[98-00-0]
Furfuryl alcohol, 8CI. 2-(Hydroxymethyl)furan. FEMA 2491



$C_5H_6O_2$ 98.101
Isol. from coffee aroma, tea, wheat bread, crispbread, soybean, cocoa, rice, potato chips and other sources. Flavouring ingredient. Liq. Misc. H_2O; v. sol. EtOH, Et_2O. d_4^{23} 1.13. Bp 170-171° Bp_{10} 68-69°. n_D^{23} 1.4852. pK_a 9.55. Aq. solns. dec. on standing.

▶ Fl. p. 65°, autoignition temp. 390°. Mod. toxic, OES: long-term 5 ppm; short-term 15 ppm (Sk). Reacts violently with acids (e.g. formic acid). Eye, nose and throat irritant. CNS depressant. Can cause dermatitis. LD_{50} (rat, orl) 88.3 mg/kg. Exp. neurotoxic effects by inhalation. LU9100000

Ac: [623-17-6] *FEMA 2490*
$C_7H_8O_3$ 140.138
Flavouring ingredient. Present in wheat bread, crisp bread, roasted onion, pork liver, beer, rum, cocoa, coffee, roasted filbert, roasted peanut, roasted almond, shoyu, sukiyake, liquorice and Bourbon vanilla. Bp 175-177° Bp_{23} 85°.

▶ Fl. p. 85°. LU9120000

Propanoyl: [623-19-8] *2-Furanylmethyl propanoate. Furfuryl propionate. FEMA 3346*

$C_8H_{10}O_3$ 154.165
Flavouring ingredient. Oil. d^{20} 1.11. Bp 195-196°.

Butanoyl: [623-21-2] *2-Furanylmethyl butanoate. Furfuryl butyrate*
$C_9H_{12}O_3$ 168.192
Flavouring ingredient.

3-Methylbutanoyl: [13678-60-9] *Furfuryl isovalerate. Furfuryl 3-methylbutanoate. FEMA 3283*
$C_{10}H_{14}O_3$ 182.219
Flavouring ingredient. Constit. of coffee aroma. Liq. with ripe fruity aroma. Bp_{11} 97-98°.

Pentanoyl: [36701-01-6] *Furfuryl pentanoate. Furfuryl valerate. FEMA 3397*
$C_{10}H_{14}O_3$ 182.219
Flavouring ingredient. d^{20} 1.03. Bp_{764} 228-229°.

Octanoyl: [39252-03-4] *Furfuryl octanoate. FEMA 3396*
$C_{13}H_{20}O_3$ 224.299
Flavouring ingredient. Bp_{10} 139°.

Me ether: [13679-46-4] *2-(Methoxymethyl)furan, 9CI. Furfuryl methyl ether. FEMA 3159*
$C_6H_8O_2$ 112.128
Aroma constit. of roasted coffee and roasted almonds. Flavouring agent. d_4^{20} 1.02. Bp 134-135°. n_D^{20} 1.4570.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 581C; 588B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 18A; 32C; 36B (*nmr*)
Zanetti, J.E. *et al., J.A.C.S.*, 1925, **47**, 535 (*esters*)
Org. Synth., Coll. Vol., 1, 1932, 276 (*synth*)
Katayama, T. *et al., CA*, 1960, **54**, 11169; 1962, **53**, 15512; **56**, 7710 (*isol*)
Loughran, E.D. *et al., J. Het. Chem.*, 1972, **9**, 57 (*ms*)
Gronowitz, S. *et al., Chem. Scr.*, 1975, **7**, 211 (*pmr, cmr*)
Hearn, M.T.W. *et al., Aust. J. Chem.*, 1976, **29**, 107 (*cmr*)
Wong, H.N.C. *et al., Synthesis*, 1985, 1111 (*Me ether*)
Popelis, Y.Y. *et al., Zh. Obshch. Khim.*, 1985, **55**, 1615 (*O-17 nmr*)
Fodor, G. *et al., J.C.S. Perkin 1*, 1986, 545 (*Me ether*)
Marstokk, K.M. *et al., Acta Chem. Scand.*, 1994, **48**, 25 (*microwave, struct, conformn*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1141-1149 (*occur, use, derivs*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 638; 639; 641; 643; 644; 645 (*occur, use, derivs*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4653
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1763
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 309
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 636
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FPU000

3-Furanmethanol, 9CI F-97

[4412-91-3]
3-Furancarbinol. 3-Furfuryl alcohol. 3-(Hydroxymethyl)furan

$C_5H_6O_2$ 98.101
Liq. d_4^{20} 1.14. Bp_{17} 79-80°. n_D^{20} 1.4842.

Phenylurethane:
Fine needles. Mp 102.5-105.6°.

O-*β-D-Glucopyranoside:* [86425-28-7]
$C_{11}H_{16}O_7$ 260.243
Isol. from seeds of *Vigna angularis* (azuki bean). Hygroscopic powder. $[\alpha]_D^{26}$ +40 (c, 1.1 in MeOH).

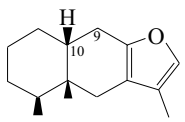
Benzoyl:
$C_{12}H_{10}O_3$ 202.209
$Bp_{0.75}$ 95-97°.

O-*(2-Pyrrolecarbonyl):* [119767-00-9] *3-Furfuryl 2-pyrrolecarboxylate*
$C_{10}H_9NO_3$ 191.186
Oil.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 581D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 18B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1453B (*ir*)
Sherman, E. *et al., J.A.C.S.*, 1950, **72**, 2195 (*synth*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 664 (*glucoside*)
Jurášek, A. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 2077 (*synth*)
Reinecke, M.G. *et al., J. Nat. Prod.*, 1988, **51**, 1236; 1989, **52**, 375 (*pyrrole-2-carboxylate*)
Marstokk, K.M. *et al., Acta Chem. Scand.*, 1993, **47**, 849 (*microwave, struct*)
Bures, E. *et al., J.O.C.*, 1997, **62**, 8741-8749 (*synth, ir, pmr, cmr*)

Furanoeremophilane F-98

[6750-13-6]

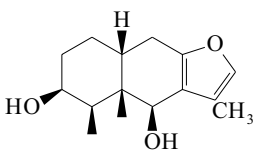


$C_{15}H_{22}O$ 218.338
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. Bp_{16} 148°. $[\alpha]_D$ -8.4. n_D^{20} 1.5172.

9,10-Didehydro: [62787-33-1] ***Furanoeremophil-9-ene***
$C_{15}H_{20}O$ 216.322
Oil. $Bp_{0.1}$ 130°. $[\alpha]_D^{24}$ +145 (c, 1.2 in $CHCl_3$).

Novotný, L. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 1400; 2462; 1965, **30**, 3579 (*isol, struct*)
Bohlmann, F. *et al., Chem. Ber.*, 1974, **107**, 1767 (*synth*)
Nayakura, I. *et al., Chem. Lett.*, 1975, 1143 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 135 (*isol*)

Furanoeremophilane-3,6-diol F-99



$C_{15}H_{22}O_3$ 250.337

(3β,6β)-*form* [34335-94-9] ***Furanofukinol***
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. Mp 178-180°.

6-Ac: [34335-95-0]
$C_{17}H_{24}O_4$ 292.374
Constit. of *Petasites japonicus* (sweet coltsfoot). Viscous oil.

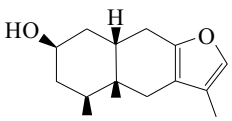
6-O-Angeloyl:
$C_{20}H_{28}O_4$ 332.439
Constit. of *Petasites japonicus* (sweet coltsfoot). Viscous oil.

6-O-Angeloyl, 3-(3-methylthio-2Z-propenoyl): [34335-97-2] **S-*Furanopetasitin***
$C_{24}H_{32}O_5S$ 432.58
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. Mp 107-108°. $[\alpha]_D$ -60.5.

Novotny, L. *et al., Phytochemistry*, 1968, **7**, 1349 (*Japonicin*)
Nagano, H. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1935 (*isol*)
Bohlmann, F. *et al., Chem. Ber.*, 1974, **107**, 3928; 1976, **109**, 1230-1238 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 774; 1978, **17**, 461-465; 1161-1164; 1980, **19**, 975; 1982, **21**, 2126-2127 (*isol, esters*)
Naya, K. *et al., Chem. Lett.*, 1978, 301 (*struct*)
Yamakawa, T. *et al., Chem. Pharm. Bull.*, 1979, **27**, 1747 (*synth*)
Guerriero, A. *et al., Phytochemistry*, 1982, **21**, 2887-2891 (*isol, uv, pmr, cmr*)
Jakupovic, J. *et al., Phytochemistry*, 1995, **40**, 1677 (*isol, pmr, cmr*)

Furanoeremophilan-2-ol F-100

2-Hydroxyfuranoeremophilane



$C_{15}H_{22}O_2$ 234.338

2β-*form*
λ_{max} 219 (log ε 4) (cyclohexane).

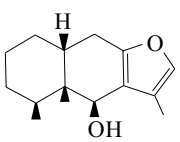
Angeloyl: [34335-98-3] ***Furanojaponin***
$C_{20}H_{28}O_3$ 316.439
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $Bp_{0.00005}$ 110-130°. $[\alpha]_D^{22}$ -33.5 (c, 1.2 in $CHCl_3$). λ_{max} 219 (log ε 4) (cyclohexane).

3-Methyl-2-butenoyl: [87339-52-4]
$C_{20}H_{28}O_3$ 316.439
Oil. $[\alpha]_D^{22}$ -51.3 (c, 0.8 in $CHCl_3$). λ_{max} 218 (log ε 4.01) (cyclohexane).

Naya, K. *et al., Tet. Lett.*, 1971, 2961
Guerriero, A. *et al., Phytochemistry*, 1982, **21**, 2887-2891 (*isol, pmr, cmr*)

Furanoeremophilan-6-ol F-101

6-Hydroxyfuranoeremophilane



$C_{15}H_{22}O_2$ 234.338

6β-*form* [4176-11-8]

Petasalbin. *Ligularol*
Constit. of coltsfoot and *Petasites japonicus* (sweet coltsfoot). Cryst. Mp 81-82°. $[\alpha]_D$ -11.2.

Ac: [4467-60-1]
$C_{17}H_{24}O_3$ 276.375
Oil.

Angeloyl: ***Albopetasin***
$C_{20}H_{28}O_3$ 316.439
Cryst. Mp 106-107°. $[\alpha]_D$ 0.

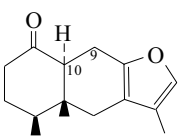
O-*(3-Methyl-2-butenoyl):*
$C_{20}H_{28}O_3$ 316.439
Oil.

Me ether: [34335-93-8] ***6β-Methoxyfuranoeremophilane***. *Furanofukinin*
$C_{16}H_{24}O_2$ 248.364
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $Bp_{0.0004}$ 90-100°. $[\alpha]_D$ -52.5.

6-Ketone: [4234-94-0] *Furanoeremophilan-6-one*. ***Ligularone***
$C_{15}H_{20}O_2$ 232.322
Mp 64-65°. $[\alpha]_D^{27}$ -57.7 (c, 1 in $CHCl_3$).

Novotný, L. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 2189-2193 (*Petasalbin, Albopetasin, struct*)
Ishii, H. *et al., Tetrahedron*, 1965, **21**, 2605-2610 (*Ligularol, Ligularone, isol, uv, ir, pmr, struct, synth*)
Novotný, L. *et al., Phytochemistry*, 1966, **5**, 1281-1287 (*Petasalbin, Albopetasin, occur*)
Naya, K. *et al., Tet. Lett.*, 1971, 2961-2964 (*isol, ether*)
Nagano, H. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2840-2845 (*3-methyl-2-butenoyl*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 1769-1771 (*Petasalbin, Petasalbin Ac*)
Sato, T. *et al., Tet. Lett.*, 1977, 3895-3898 (*cmr*)
Tada, M. *et al., Chem. Lett.*, 1979, 1441-1442 (*Ligularone, synth*)
Yamakawa, K. *et al., Chem. Pharm. Bull.*, 1979, **27**, 1747-1752 (*Furanofukinol, Petasalbin, synth*)
Miyashita, M. *et al., J.O.C.*, 1980, **45**, 2945-2950 (*Ligularone, synth*)
Jacobi, P.A. *et al., J.A.C.S.*, 1981, **103**, 4611-4613 (*Petasalbin, Ligularone, synth*)
Koike, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 897-899 (*Ligularone, synth*)

Furanoeremophilan-1-one F-102



10α*H-form*

$C_{15}H_{20}O_2$ 232.322

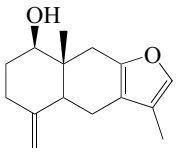
10α*H-form* [52061-43-5]
Furoeremophilone 1
Constit. of *Smyrnium olusatrum* (alexanders). Cryst. (petrol). Mp 72-73°. $[\alpha]_D^{24}$ -51.5 (c, 2.8 in $CHCl_3$).

9,10-Didehydro: [62787-34-2] *Furanoeremophil-9-en-1-one*
$C_{15}H_{18}O_2$ 230.306
Yellow oil. $Bp_{0.1}$ 130°.

10β*H-form* [105093-79-6] ***Senberginone***
$[\alpha]_D^{24}$ +31 (c, 1.7 in $CHCl_3$).

Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 3614 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 135 (*deriv*)
Bohlmann, F. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 707 (*Senberginone*)
Mölleken, U. *et al., Phytochemistry*, 1998, **49**, 1709-1714 (*Furoeremophilene 1, pmr, cmr*)

Furanoeudesm-4(15)-en-1-ol F-103



$C_{15}H_{20}O_2$ 232.322

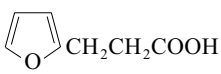
1β-*form*

Ac: [97456-36-5]
$C_{17}H_{22}O_3$ 274.359
Constit. of *Smyrnium olusatrum* (alexanders). Amorph. λ_{max} 220 (log ϵ 4.6) (MeOH).

Ulubelen, A. *et al., Phytochemistry*, 1985, **24**, 1105-1106 (*isol, struct*)

2-Furanpropanoic acid, 9CI F-104

[935-13-7]
Furfurylacetic acid. 3-(2-Furyl)propionic acid



$C_7H_8O_3$ 140.138
Cryst. ($CHCl_3$/petrol). Mp 58°. Bp_{16} 135° Bp_{10} 108-110°.

Me ester: [37493-31-5]
$C_8H_{10}O_3$ 154.165
Bp_{15} 89°.

Et ester: [10031-90-0] *FEMA 2435*
$C_9H_{12}O_3$ 168.192
Present in rum. Flavouring ingredient. Low-melting solid. Mp 24.5°. Bp 212° Bp_4 94-98°.

2-Methylpropyl ester: [105-01-1] *Isobutyl 2-furanpropionate. FEMA 2198*
$C_{11}H_{16}O_3$ 196.246
Flavouring ingredient with a sweet dry, brandy flavour at low levels. Colourless to pale straw-yellow liq. with sweet brandy flavour at low levels.

3-Methylbutyl ester: [7779-67-1] *Isoamyl 2-furonpropionate. FEMA 2071*
$C_{12}H_{18}O_3$ 210.272
Flavouring ingredient. Liq.

Amide:
$C_7H_9NO_2$ 139.154
Mp 107-108°.

Kirner, W.R. *et al., J.A.C.S.*, 1929, **51**, 3133 (*synth*)
Lambert, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1952, **235**, 626 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 379; 393; **2**, 232 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 985-986; 1424-1425; 1451-1452 (*esters*)
Robertson, A. *et al., Tetrahedron*, 1999, **55**, 11365-11384 (*synth*)

1-(2-Furanyl)-1,2-butanedione, 9CI F-105

[1438-90-0]
Ethyl 2-furanyl diketone



$C_8H_8O_3$ 152.149
Minor constit. of coffee aroma. Liq. Bp_6 95-96°. n_D^{22} 1.5172.

2-Oxime:
$C_8H_9NO_3$ 167.164
Cryst. (H_2O). Mp 78°.

Gianturco, M.A. *et al., Tetrahedron*, 1964, **20**, 2951 (*ir, uv, synth*)

1-(2-Furanyl)-1,3-butanedione, 9CI F-106

[25790-35-6]
1-(2-Furyl)-1,3-butanedione, 8CI



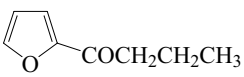
$C_8H_8O_3$ 152.149
Listed in the EAFUS Food Additive Database (Jan 2001) but with no current reported use. Bp_5 97-98°.

Cu salt (1:2):
Cryst. (EtOH). Mp 229-231°.

Rosenberg, D. *et al., Annalen*, 1976, 13 (*synth*)

1-(2-Furanyl)-1-butanone, 9CI, 8CI F-107

[4208-57-5]
2-Butanoylfuran. Propyl furyl ketone



$C_8H_{10}O_2$ 138.166
Constit. of coffee aroma and cocoa butter. Liq. Bp_7 76-78°. n_D^{16} 1.4992.

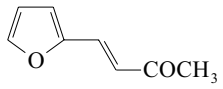
Semicarbazone:
Mp 190-191° (180-181°).

[138605-13-7]

Heid, J.V. *et al., J.O.C.*, 1948, **13**, 409-412 (*synth*)
Terentev, A.P. *et al., Zh. Obshch. Khim.*, 1958, **28**, 1167-1169; *CA*, **52**, 19967c (*synth*)
Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223-2225 (*ms*)
Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628-694 (*occur, coffee, glc, ms*)
Hashim, L. *et al., Food Res. Int.*, 1997, **30**, 163-169 (*occur, cocoa*)

4-(2-Furanyl)-3-buten-2-one, 9CI F-108

[623-15-4]
Furfurylideneacetone. Furfuralacetone. 2-Furalacetone. 2-(3-Oxobutenyl)furan. FEMA 2495



$C_8H_8O_2$ 136.15
Present in rum and coffee. Flavouring agent.

(*E*)-*form* [41438-24-8]
Needles. Mp 39-40°. Bp_{33} 135-137° Bp_{10} 112-115°.

Phenylhydrazone: [57337-21-0]
Needles (EtOH). Mp 131-132°.

2,4-Dinitrophenylhydrazone: [24414-36-6]
Mp 248°.

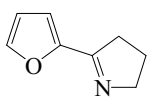
Thiosemicarbazone: [14673-53-1]
Mp 144°.

[108811-61-6]

v. Auwers, K. *et al., Ber.*, 1909, **42**, 4426
Chuit, C. *et al., Synthesis*, 1983, 294 (*synth*)
Hayakawa, K. *et al., J.A.C.S.*, 1984, **106**, 6735 (*synth, ir, pmr*)
Petrini, M. *et al., Tetrahedron*, 1986, **42**, 151 (*synth, pmr, ir*)
Nakano, T. *et al., J.O.C.*, 1987, **52**, 4855 (*synth, ir, pmr, cmr*)
Kasahara, A. *et al., J. Het. Chem.*, 1989, **26**, 597 (*synth, ir, pmr*)
Huang, Y.-Z. *et al., Synth. Commun.*, 1989, **19**, 501 (*synth*)
Komyagin, N.T. *et al., Zh. Obshch. Khim.*, 1991, **27**, 551 (*config*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 292
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1152-1153

5-(2-Furanyl)-3,4-dihydro-2*H*-pyrrole F-109

[104704-31-6]
2-(2-Furyl)-1-pyrroline

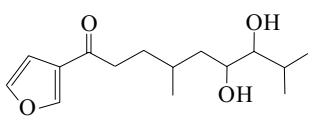


C_8H_9NO 135.165
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., Dev. Food Sci.*, 1986, **13**, 235-244 (*occur, ir, ms, pmr*)
Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, synth, ir, ms, pmr*)

1-(3-Furanyl)-6,7-dihydroxy-4,8-dimethyl-1-nonanone F-110

[66472-04-6]



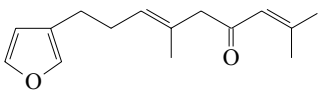
$C_{15}H_{24}O_4$ 268.352
Stress metab. from *Ipomoea batatas* (sweet potato). Cryst. (Et_2O/pentane). Mp 70-71°. $[\alpha]_D^{26}$ +17 (c, 1.6 in EtOH). λ_{max} 252 (ε 2550) (MeOH) (Berdy).

► RA8248000

Burka, L.T. *et al., Phytochemistry*, 1978, **17**, 317

9-(3-Furanyl)-2,6-dimethyl-2,6-nonadien-4-one, 9CI F-111

[69904-96-7]
6-Oxodendrolasin



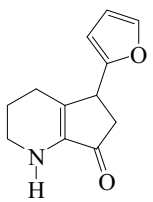
$C_{15}H_{20}O_2$ 232.322
Sol. $CHCl_3$, MeOH; poorly sol. H_2O.

(*E*)-*form* [53098-76-3]
Isol. from fungus-infected *Ipomoea batatas* (sweet potato). Oil. $Bp_{0.1}$ 120°.

Dimitriadis, E. *et al., Aust. J. Chem.*, 1980, **33**, 2729 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 587; 1982, **21**, 1309 (*isol*)
Burka, L.T. *et al., Phytochemistry*, 1981, **20**, 647 (*isol*)
Ito, I. *et al., Agric. Biol. Chem.*, 1984, **48**, 159 (*isol, pmr*)
Masaki, Y. *et al., J.C.S. Perkin 1*, 1984, 1289 (*synth, pmr*)

5-(2-Furanyl)-1,2,3,4,5,6-hexahydro-7*H*-cyclopenta[*b*]pyridin-7-one, 9CI F-112

[118355-71-8]
*5-(2-Furanyl)-1,2,3,4,5,6-hexahydro-7*H*-1-pyrindin-7-one*

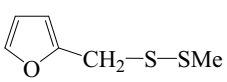


$C_{12}H_{13}NO_2$ 203.24
Proline-derived Maillard product. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*isol, ms, pmr*)

(2-Furanylmethyl) methyl disulfide F-113

[57500-00-2]
2-(Methyldithiomethyl)furan, 9CI, 8CI. Furfuryl methyl disulfide. FEMA 3362

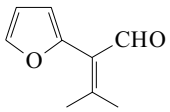


$C_6H_8OS_2$ 160.261
Flavouring ingredient. Constit. of wheat bread aroma, meat flavours, coffee and roasted sesame seed oil. d 1.08. $Bp_{0.8}$ 60-61°. n_D^{20} 1.5661.

Mulders, E.J. *et al., Chem. Ind. (London)*, 1976, 613-614 (*isol, pmr, cmr, bread*)
Dubs, P. *et al., Helv. Chim. Acta*, 1976, **59**, 1307-1310 (*synth, pmr*)
Harpp, D.N. *et al., J.O.C.*, 1978, **43**, 3481 (*synth*)
Ruther, J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2254-2259 (*occur, meat flavours*)
Leriverend, C. *et al., Synthesis*, 1994, 761-762 (*synth, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 502 (*use*)

2-(2-Furanyl)-3-methyl-2-butenal F-114

[31681-28-4]
α-(1-Methylethylidene)-2-furanacetaldehyde, 9CI. α-Isopropylidene-2-furanacetaldehyde



$C_9H_{10}O_2$ 150.177
Constit. of the oil of *Papaver somniferum* (opium poppy). Yellow liq. Bp_5 89°.

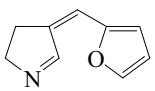
Semicarbazone: [31681-29-5]
Mp 170°. Subl. 164.

Dana, G. *et al., Bull. Soc. Chim. Fr.*, 1970, 3994 (*synth*)
Li, C. *et al., CA*, 1993, **118**, 165179 (*isol*)

4-(2-Furanylmethylene)-3,4-dihydro-2*H*-pyrrole F-115

[118248-28-5]

[118248-29-6]
3-Furfurylidene-1-pyrroline



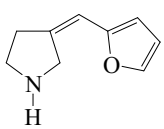
C_9H_9NO 147.176
Putative proline-derived Maillard product formed in model reactions with proline or pyrroline and ascorbic acid. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, ms, ir, pmr*)

3-(2-Furanylmethylene)pyrrolidine F-116

[118248-35-4]

[118248-34-3]
3-Furfurylidenepyrrolidine



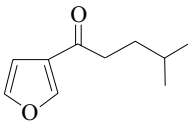
$C_9H_{11}NO$ 149.192
Putative proline-derived Maillard product formed in model reactions with proline or 1-pyrroline and ascorbic acid. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, ms, ir*)

1-(3-Furanyl)-4-methyl-1-pentanone, 9CI, 8CI F-117

[553-84-4]

Perilla ketone



$C_{10}H_{14}O_2$ 166.219
Isol. from the essential oil of *Perilla frutescens* (perilla). Light-yellow liq. Bp_{30} 130°.

▶ Potent lung toxin and cytotoxic agent. SA8935000

2,4-Dinitrophenylhydrazone:
Red-orange needles (EtOH). Mp 149.5°.

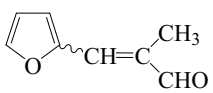
Oxime:
Needles (EtOH aq.). Mp 62-64°.

Kondo, K. *et al., Tet. Lett.*, 1976, 4363 (*synth*)
Kitamura, T. *et al., Synth. Commun.*, 1977, **7**, 521 (*synth*)
Abdulla, R.F. *et al., J.O.C.*, 1978, **43**, 4248 (*synth*)
Inomata, K. *et al., Chem. Lett.*, 1979, 709 (*synth*)
Boyd, M.R. *et al., Crit. Rev. Toxicol.*, 1980, **7**, 123 (*tox*)
Garst, J.E. *et al., J. Agric. Food Chem.*, 1984, **22**, 1083 (*synth*)
Koezuka, Y. *et al., Planta Med.*, 1985, 480 (*isol, props*)
Bailey, T.R. *et al., Synthesis*, 1991, 242 (*synth*)
Cahiez, G. *et al., Tet. Lett.*, 1992, **33**, 5245 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PCI750

3-(2-Furanyl)-2-methyl-2-propenal, 9CI F-118

[874-66-8]

[108576-21-2]
α-Methyl-2-furanacrolein, 8CI. FEMA 2704

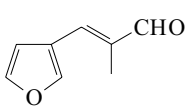


$C_8H_8O_2$ 136.15
Flavouring ingredient. Constit. of roasted sesame seed oil. Bp 225° Bp_{35} 126°. n_D^{22} 1.6093.

Francke, W. *et al., Annalen*, 1979, 1-10 (*synth, pmr*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*occur, glc*)
Burdock, G.A. *et al., Acute Toxic. Data*, 1990, **1**, 3 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1124-1125 (*use*)

3-(3-Furanyl)-2-methyl-2-propenal, 9CI F-119

[28043-36-9]
α-Methyl-3-furanacrolein, 8CI

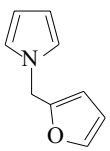


$C_8H_8O_2$ 136.15
Constit. of the aroma of carob bean (*Ceratonia siliqua*). Cryst. (pentane). Mp 41°.

Vu Moc Thuy, *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1970, **270**, 1039 (*synth*)
MacLeod, G. *et al., Phytochemistry*, 1992, **31**, 3113 (*occur*)

1-(2-Furanylmethyl)-1*H*-pyrrole, 9CI F-120

[1438-94-4]
N-*(2-Furfuryl)pyrrole. FEMA 3284*



C_9H_9NO 147.176
One of the constits. of the aroma of coffee also present in bread, roasted almond, popcorn, malt, roasted chicken, beer and sandalwood oil. Flavour ingredient. Bp_1 77-79°. n_D^{21} 1.5317.

▶ LD_{50} (mus, orl) 380 mg/kg. UX9631000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 42B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1466A (*ir*)
Gianturco, M.A. *et al., Tetrahedron*, 1964, **20**, 1763; 2951 (*isol, ir, pmr, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 290
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1149-1150

3-(2-Furanylmethyl)-1*H*-pyrrole F-121

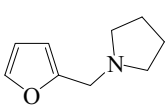
[118248-36-5]
3-Furfurylpyrrole

C_9H_9NO 147.176
Putative proline-derived Maillard product formed in model reactions with proline and ascorbic acid. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, ms, ir, pmr*)

1-(2-Furanylmethyl)pyrrolidine, 9CI F-122

[61893-12-7]
1-Furfurylpyrrolidine



$C_9H_{13}NO$ 151.208
Proline-derived Maillard product. Constit. of dried, roasted squid aroma. Bp_8 82-84°.

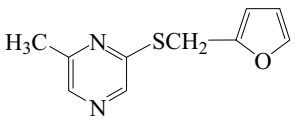
Picrate:
Mp 135-136°.

Erdtman, H. *et al., Acta Chem. Scand.*, 1963, **17**, 1717-1726 (*synth*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928; 1993, **41**, 547-553 (*occur, ms*)
Heaney, H. *et al., Chem. Comm.*, 1988, 1161-1163 (*synth*)
Kawai, T. *et al., J. Agric. Food Chem.*, 1991, **39**, 770-777 (*occur, squid*)

2-[(2-Furanylmethyl)thio]-6-methylpyrazine, 9CI F-123

[59021-05-5]

[59303-07-0, 59303-08-1, 59303-09-2]
6-Methyl-2-pyrazinyl 2-furfuryl sulfide. FEMA 3189

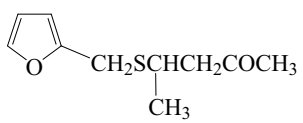


$C_{10}H_{10}N_2OS$ 206.268
The phys. props. given are for a mixt. of regioisomers (3-, 5- and 6-methylpyrazines), which are the coml. flavouring material FEMA 3189. Present in aroma of pumpkin seed oil. Flavouring ingredient. Liq. with roasted coffee-like taste. d_4^{20} 1.22. Bp_{10} 153-156°. n_D^{20} 1.5970. Synthesised as a mixt. of regioisomers (2,3-, 2,5- and 2,6-) to which the phys. props. refer. The FEMA no. refers to this mixt..

U.S. Pat., 1976, 3 989 713; *CA*, **86**, 43556d (*synth, use*)
Buchbauer, G. *et al., Ernaehrung (Vienna)*, 1998, **22**, 246-249; *CA*, **129**, 135437a (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1122-1123 (*use, props*)

4-[(2-Furanylmethyl)thio]-2-pentanone, 9CI F-124

[180031-78-1]
4-(Furfurylthio)pentan-2-one. FEMA 3840

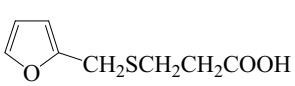


$C_{10}H_{14}O_2S$ 198.285
Odorous substance used in coffee compositions. Food flavouring agent. No phys. props. reported.

Eur. Pat., 1997, 811 618; *CA*, **128**, 61419b (*use, synth, ir*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 635 (*use*)

3-[(2-Furanylmethyl)thio]propanoic acid F-125

[83530-34-1]
3-(Furfurylthio)propanoic acid



$C_8H_{10}O_3S$ 186.231

Et ester: [94278-27-0] *FEMA 3674*
$C_{10}H_{14}O_3S$ 214.285

Flavouring ingredient with roasted, nutty-coffee taste at 10ppm. Liq. d_4^{23} 1.13. Bp 244°. n_D^{23} 1.5060.

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 542 (*Et ester, use*)

1-(2-Furanyl)-1-octanone, 9CI F-126

[5456-77-9]
2-Octanoylfuran

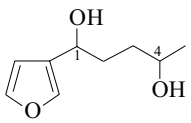


$C_{12}H_{18}O_2$ 194.273
Thermal degradn. product of laminated polyethylene terephthalate food packaging materials. $Bp_{0.075}$ 64-66°.

U.S. Pat., 1981, 4 254 043; *CA*, **95**, 24789b (*synth*)
De A. Freire, M.T. *et al., Food Addit. Contam.*, 1998, **15**, 473-480 (*detn*)

1-(3-Furanyl)-1,4-pentanediol F-127

[53011-73-7]
3-(1,4-Dihydroxypentyl)furan. ***1,4-Ipomeadiol***



$C_9H_{14}O_3$ 170.208
Prod. on *Fusarium solani*-infected sweet potatoes (*Ipomoea batatus*). $[\alpha]_D^{25}$ +1.27 (c, 1.21 in CCl_4).

▶ LD_{50} (mus, orl) 104 mg/kg. LD_{50} (mus, ipr) 67 mg/kg. SA0700000

1-Ketone: [32954-58-8]

[55659-41-1] *1-(3-Furanyl)-4-hydroxy-1-pentanone, 9CI. 3-(4-Hydroxypentanoyl)-furan.* ***4-Ipomeanol.*** *NSC 349438*
$C_9H_{12}O_3$ 168.192
Prod. on *Fusarium solani* and *Ceratocystis fimbriata*-damaged sweet potatoes (*Ipomoea batatus*). $[\alpha]_D^{25}$ +7.86 (c, 1.17 in $CHCl_3$). Log P 0.14 (calc). λ_{max} 211 (sh) (ε 6100); 251 (ε 2970) (MeOH) (Derep).

▶ Pulmonary toxin. Hepatotoxic in clin. trials. LD_{50} (rat, ipr) 17 mg/kg. SA9050000

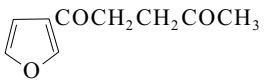
4-Ketone: [34435-70-6] *5-(3-Furanyl)-5-hydroxy-2-pentanone, 9CI.* ***1-Ipomeanol***
$C_9H_{12}O_3$ 168.192
Prod. on *Fusarium solani*-infected sweet potatoes (*Ipomoea batatus*). Light yellow solid. $[\alpha]_D^{24}$ +21.9 (c, 0.64 in $CHCl_3$).

▶ LD_{50} (mus, orl) 79 mg/kg. LD_{50} (mus, ipr) 49 mg/kg; LD_{50} (mus, ipr) 75 mg/kg. SA9060000

Boyd, M.R. *et al., Biochim. Biophys. Acta*, 1974, **337**, 184 (*isol*)
Burka, L.T. *et al., J.O.C.*, 1974, **39**, 2212 (*synth, ir, pmr*)
Wiben, B.J. *et al., Mycotoxins*, (I.F.H. Purchase Ed.), Elsevier, Amsterdam, 1974, 327 (*rev*)
Woessner, W.D. *et al., Synth. Commun.*, 1979, **9**, 147 (*synth*)
Christian, M.C. *et al., J. Natl. Cancer Inst.*, 1989, **81**, 1133; 1990, **82**, 1420 (*4-Ipomeanol, pharmacol*)
Gram, T.E. *et al., Pharmacol. Ther.*, 1989, **43**, 291 (*4-Ipomeanol, tox, rev*)
Rowinsky, E.K. *et al., Cancer Res.*, 1993, **53**, 1794 (*4-Ipomeanol, clin trial*)
Gram, T.E. *et al., Metabolic Activation and Toxicity of Chemical Agents to Lung Tissue and Cells*, (Ed. Gram, T.E.), Pergamon Press, 1993, 145 (*tox, rev*)
Plopper, C.G. *et al., J. Pharmacol. Exp. Ther.*, 1994, **269**, 867-880 (*4-Ipomeanol, pharmacol*)
Desai, D. *et al., Cancer Lett. (Shannon, Irel.)*, 1996, **108**, 263-270 (*4-Ipomeanol, synth, pharmacol*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 721; 725; 729
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FQL100; IGF200; IGF325

1-(3-Furanyl)-1,4-pentanedione, 9CI F-128

[496-06-0]
Ipomeanine



$C_9H_{10}O_3$ 166.176
Produced by *Ceratostomella fimbriata*; toxic substance in mouldy sweet potatoes. Oil or cryst. Mp 42-43°. $Bp_{0.001}$ 74-79°.

▶ SA1956000

2,4-Dinitrophenylhydrazone:
Red cryst. Mp 231-233°.

Kubota, T. *et al., Chem. Ind. (London)*, 1954, 902
Akazawa, T. *et al., Arch. Biochem. Biophys.*, 1962, **99**, 52 (*biosynth*)
Wilson, B.J. *et al., Nutr. Rev.*, 1973, **3**, 73 (*tox*)
Ito, Y. *et al., J.A.C.S.*, 1977, **99**, 1487 (*synth, pmr*)
Watanabe, E. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 3225 (*synth, ir, pmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 717
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IGF300

1-(2-Furanyl)-1-pentanone, 9CI F-129

[3194-17-0]
2-Pentanoylfuran. 2-Valeroylfuran. Butyl furyl ketone



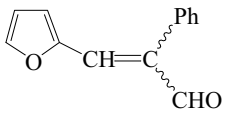
$C_9H_{12}O_2$ 152.193
Volatile constit. of rice smoke flavouring and roast beef. Liq. Bp_6 61°. n_D^{20} 1.4892.

Semicarbazone:
Mp 156-158°.

Vereshchagin, L.I. *et al., Zh. Org. Khim.*, 1965, **1**, 955-960; *J. Org. Chem. USSR (Engl. Transl.)*, 1965, **1**, 962-966 (*synth*)
Hsu, C.M. *et al., J. Food Sci.*, 1982, **47**, 2068-2069 (*occur*)
Miyakoshi, T. *et al., Synthesis*, 1990, 407-410 (*synth, pmr, ms*)
Han, Y. *et al., Tet. Lett.*, 1995, **36**, 1287-1290 (*synth*)
Pino, J.A. *et al., Alimentaria (Madrid)*, 1997, **283**, 49-51; *CA*, **127**, 80413r (*occur*)

3-(2-Furanyl)-2-phenyl-2-propenal F-130

[57568-60-2]
α-(2-Furanylmethylene)benzeneacetaldehyde, 9CI. FEMA 3586

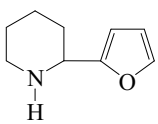


$C_{13}H_{10}O_2$ 198.221
Flavourant for tobacco and food products. Cryst. with sweet, honey-like taste/aroma. Mp 56-57°. $Bp_{0.001}$ 85-87°.

Ger. Pat., 1976, 2 614 797; *CA*, **86**, 2544e (*synth, use, props*)
Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-62; 64-66; 68-70 (*use*)
Baltes, W. *et al., Z. Lebensm.-Unters. -Forsch.*, 1987, **187**, 209-214; 1990, **190**, 9-13

2-(2-Furanyl)piperidine, 9CI F-131

[97073-24-0]
2-(2-Piperidinyl)furan

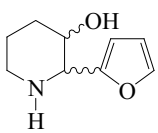


$C_9H_{13}NO$ 151.208
Proline-derived Maillard product. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*synth, ir, ms, pmr*)
Oh, Y.C. *et al., J. Agric. Food Chem.*, 1992, **40**, 1878-1880

2-(2-Furanyl)-3-piperidinol, 9CI F-132

2-(3-Hydroxy-2-piperidinyl)furan. 2-(2-Furanyl)-3-hydroxypiperidine



$C_9H_{13}NO_2$ 167.207
Proline-derived Maillard product.

[118248-22-9, 118248-23-0]

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*formn, ms*)

1-(2-Furanyl)-1,2-propanedione, 8CI F-133

[1438-92-2]
α-Furyl methyl diketone



$C_7H_6O_3$ 138.123
Constit. of coffee aroma. Cryst. (petrol). Mp 60-61°.

Oxime: [1196-47-0]
$C_7H_7NO_3$ 153.137
Cryst. (H_2O). Mp 114-115°.

Cosgrove, D.J. *et al., J.C.S.*, 1952, 4821 (*synth*)
Gianturco, M.A. *et al., Tetrahedron*, 1964, **20**, 2951 (*synth*)

1-(2-Furanyl)-1-propanone, 9CI, 8CI F-134

[3194-15-8]
Ethyl 2-furyl ketone. 2-Propanoylfuran



$C_7H_8O_2$ 124.139
Constit. of fruits of *Psidium guajava* (guava), *Zizania aquatica* seed (wild rice) and *Ceratonia siliqua* (carob bean), and of baked potato, and cooked meat (sukiyaki) volatiles. Mp 28-29°. Bp_{17} 79-80° Bp_6 63°.

Semicarbazone:
Mp 154°.

[69662-80-2, 75884-39-8, 116435-25-7]

Angelelli, J.M. *et al., Tetrahedron*, 1972, **28**, 2037-2050 (*ir*)
Carbateas, P.M. *et al., J. Het. Chem.*, 1974, **11**, 819-821 (*synth*)
Withycombe, D.A. *et al., J. Agric. Food Chem.*, 1978, **26**, 816-822 (*occur*)
Coleman, E.C. *et al., J. Agric. Food Chem.*, 1981, **29**, 42-48 (*occur*)
Shibamoto, T. *et al., J. Agric. Food Chem.*, 1981, **29**, 57-63 (*occur*)
Fayed, S. *et al., Synth. Commun.*, 1982, **12**, 1121-1126 (*synth*)
Casarini, D. *et al., J.C.S. Perkin 2*, 1985, 1839-1844 (*cmr*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1989, **37**, 139-142 (*occur*)
Kuo, Y.-H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 181-183 (*synth, ir, pmr*)
MacLeod, G. *et al., Phytochemistry*, 1992, **31**, 3113-3119 (*occur*)

1-(2-Furanyl)-2-propanone, 9CI F-135

[6975-60-6]
Acetonylfuran. Furfuryl methyl ketone. FEMA 2496

$C_7H_8O_2$ 124.139
Present in roasted onion, cooked potato, wheat bread, fried beef, pork liver, sherry and coffee. Flavouring ingredient. Liq. with an odour and taste suggestive of radish. d^{20} 1.1. Mp 29°. Bp 179-180° Bp_{10} 60-65°.

Oxime:
$C_7H_9NO_2$ 139.154
Liq. Bp_{25} 135-140°.

Semicarbazone:
Cryst. Mp 173-174°.

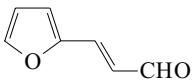
Thiosemicarbazone:
Mp 142-144°.

2,4-Dinitrophenylhydrazone:
Mp 223°.

Darzens, G. *et al., C. R. Hebd. Seances Acad. Sci.*, 1906, **142**, 215
Gerlach, H. *et al., Helv. Chim. Acta*, 1974, **57**, 2306 (*ir, pmr, ms, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 292
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1154-1155

3-(2-Furanyl)-2-propenal, 9CI F-136

[623-30-3]
Furfurylideneacetaldehyde. 2-Furanacrolein. FEMA 2494



(*E*)-*form*

$C_7H_6O_2$ 122.123
Present in rum and coffee. Flavouring ingredient.
► LT8528500
(*E*)-*form* [39511-08-5]
Needles with cinnamon odour. Sol. hot H_2O. Mp 54°. Bp_{14} 135°. Steam-volatile.

Phenylhydrazone:
Cryst. (petrol). Mp 132°.

Semicarbazone:
Mp 215-219°.

Thiosemicarbazone:
$C_8H_9N_3OS$ 195.245
Mp 157-158° (150-151°). pK_{a1} 0.46; pK_{a2} 11.7.

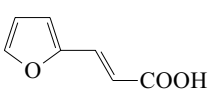
(*Z*)-*form* [71277-14-0]
$Bp_{0.1}$ 58°. 97% pure.

Di-Et acetal:2-(3,3-Diethoxy-1-propenyl)-furan
$C_{11}H_{16}O_3$ 196.246
$Bp_{0.2}$ 63°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 584D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 26C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1458D (*ir*)
König, R.H. *et al., J. Prakt. Chem.*, 1913, **88**, 193
Kerentseva, V.P. *et al., Zh. Anal. Khim.*, 1971, **26**, 1144; 1972, **27**, 719 (*synth, pKa, detn, Pd, Pt*)
Parr, W.J.E. *et al., Can. J. Chem.*, 1976, **54**, 3216 (*pmr*)
Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth*)
Bellassoued, M. *et al., J.O.C.*, 1993, **58**, 2517 (*synth, pmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 291
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1151-1152

3-(2-Furanyl)-2-propenoic acid, 9CI F-137

[539-47-9]
2-Furanacrylic acid, 8CI. Furfurylideneacetic acid. α-Furylacrylic acid



(*E*)-*form*

$C_7H_6O_3$ 138.123
► LT8560000
(*E*)-*form* [15690-24-1]
Needles (H_2O); cryst. (petrol). Mod. sol. hot H_2O. Mp 141°. Subl. in high vacuum at 112°. Steam-volatile.

Me ester: [58293-85-9]
$C_8H_8O_3$ 152.149
Mp 27.5°. Bp_{15} 112°.

Et ester: [53282-12-5]
$C_9H_{10}O_3$ 166.176
Mp 24.5°. Bp 230-233° Bp_{17} 120-121° Bp_5 94-98°.

Propyl ester: [623-22-3] *Propyl 2-furanacrylate. FEMA 2945*
Flavouring ingredient. Liq. d^{20} 1.07. Bp_7 119°. n_D^{20} 1.5229.

Chloride: [63485-67-6]
$C_7H_5ClO_2$ 156.568
Bp_{30} 126°.

Amide: [25525-85-3] *3-(2-Furanyl)-2-propenamide. 2-Furylacrylamide*
$C_7H_7NO_2$ 137.138
Plates. Mp 168-169°.

Hydrazide:
$C_7H_8N_2O_2$ 152.152
Mp 108-110°.

Nitrile: [6125-63-9] *3-(2-Furanyl)-2-propenenitrile. 2-Furylacrylonitrile. 1-Cyano-2-(2-furanyl)ethene*
C_7H_5NO 119.123
Liq. Bp_{10} 92°.

(*Z*)-*form* [25129-65-1]
Sol. hot H_2O. Mp 103-104°. Subl. in high vacuum at 95°. Changes slowly on boiling into the stable form with partial decarboxylation.

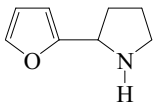
Et ester: [53282-26-1]
Bp_5 85°.

[623-16-5, 623-18-7, 623-20-1, 7187-01-1, 20689-54-7, 79148-89-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 586D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 28A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1459C (*ir*)
Liebermann, C. *et al., Ber.*, 1894, **27**, 284 (*isom*)
Org. Synth., Coll. Vol., 3, 1955, 425; *Org. Synth., Coll. Vol., 5*, 1973, 585
Fillippakis, S.E. *et al., J.C.S.(B)*, 1967, 229 (*cryst struct*)
Leiserowitz, L. *et al., J.C.S.(A)*, 1969, 2367 (*amide*)
Buddrus, J. *et al., Chem. Ber.*, 1974, **107**, 2050 (*nmr*)
Capron, B. *et al., Bull. Soc. Chim. Fr.*, 1975, 2575 (*synth*)
Hearn, M.T.W. *et al., Aust. J. Chem.*, 1976, **29**, 107 (*cmr*)
Sinisterra, J.V. *et al., Synthesis*, 1985, 1097 (*ester, nitrile*)
Dandarova, M. *et al., Coll. Czech. Chem. Comm.*, 1986, **51**, 889 (*pmr, cmr, conformn*)
Zheng, J. *et al., Synth. Commun.*, 1990, **20**, 3277 (*nitrile*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 697 (*propyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2358-2359 (*propyl ester*)

2-(2-Furanyl)pyrrolidine F-138

[90086-89-8]
2-(2-Pyrrolidinyl)furan



$C_8H_{11}NO$ 137.181

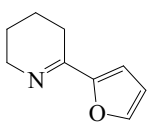
(±)-*form*
Putative proline-derived Maillard product formed in model reactions with 1-pyrroline and ascorbic acid.

4-Methylbenzenesulfonyl:
$C_{15}H_{17}NO_3S$ 291.37
Mp 58°.

Basha, F.Z. *et al., Tet. Lett.*, 1984, **25**, 5271-5274 (*synth*)
Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, synth, ms, ir, pmr*)
Pat. Coop. Treaty (WIPO), 2000, 00 58 285; *CA*, **133**, 266722v (*4-methylbenzenesulfonyl*)

2-(2-Furanyl)-3,4,5,6-tetrahydropyridine F-139

[104704-36-1]

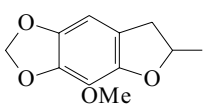


$C_9H_{11}NO$ 149.192
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., Dev. Food Sci.*, 1986, **13**, 235-244 (*occur, ms, ir, pmr*)
Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*synth, occur, ms, ir, pmr*)

Furapiole F-140

[70874-90-7]
6,7-Dihydro-4-methoxy-6-methylfuro-[2,3-f]-1,3-benzodioxole, 9CI. 2,3-Dihydro-7-methoxy-2-methyl-5,6-methylenedioxybenzofuran

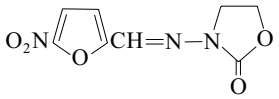


$C_{11}H_{12}O_4$ 208.213
Constit. of *Anethum sowa* (Indian dill). Viscous liq. $Bp_{0.3}$ 107°. $[\alpha]_D^{25}$ -0.23 (c, 5.2 in MeOH).

Saxena, V.S. *et al., J. Entomol. Res.*, 1978, **2**, 55 (*pharmacol*)
Tomar, S.S. *et al., Agric. Biol. Chem.*, 1979, **43**, 1479 (*synth, pmr, pharmacol*)
Ahmad, A. *et al., Phytochemistry*, 1990, **29**, 2035 (*isol, pmr, cmr*)

Furazolidone, BAN, INN F-141

[67-45-8]
3-[[(5-Nitro-2-furanyl)methylene]amino]-2-oxazolidinone, 9CI. 3-(5-Nitrofurylideneamino)-2-oxazolidinone. Furoxone. Nifulidone. Neftin. Many other names



$C_8H_7N_3O_5$ 225.16
Poultry food additive. Yellow cryst. Mp 275° dec. Log P -0.04 (uncertain value) (calc).

▶ Mutagenic props. LD_{50} (rat, orl) 2336 mg/kg. Exp. reprod. effects. Exp. carcinogenic data. RQ3675000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 40B (*nmr*)
Yurchenco, J.A. *et al., Antibiot. Chemother. (Washington, D.C.)*, 1953, **3**, 1035 (*pharmacol*)
Gever, G. *et al., J.A.C.S.*, 1955, **77**, 2277; 2282 (*synth*)
Rogers, G.S. *et al., Antibiot. Chemother. (Washington, D.C.)*, 1956, **6**, 231 (*pharmacol*)
Chamberlain, R.E. *et al., J. Antimicrob. Chemother.*, 1976, **2**, 325 (*rev*)
Cohen, S.M. *et al., Carcinog. - Compr. Surv.*, (ed. Bryan, G.T.), Raven Press, N.Y., 1978, 171-231 (*tox*)
Tatsumi, K. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3435 (*metab, tox*)
IARC Monog., 1983, **31**, 141; *Suppl.* 7, 63 (*rev, tox*)
Ali, B.H. *et al., Vet. Res. Commun.*, 1983, **6**, 1 (*rev, pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 837 (*synonyms*)
Ali, B.H. *et al., Gen. Pharmacol.*, 1989, **20**, 557 (*rev*)
Vroomen, L.H.M. *et al., Drug Metab. Rev.*, 1990, **22**, 663
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 514
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NGG500

Furcelleran F-142

[9000-21-9]
Furcelleran gum. Danish agar. Burtonitte 44

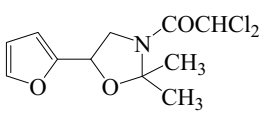
A sulfated polysaccharide, the dominant hexose units of which are galactose, anhydrogalactose and their half-ester sulfates. Emulsifier, stabiliser, thickening agent. Furcelleran 'salts' prepd. by increasing the concentration of the naturally occurring cations (ammonium, calcium, potassium or sodium) have similar utility.

Bjerre-Peterson, E *et al., Ind. Gums*, (ed. Whistler, R. L.), 2nd edn., Academic Press, 1973, 123-136 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1135-1139 (*use, props, salts*)

Furilazole, BSI F-143

[121776-33-8]

[121776-57-6]
3-(Dichloroacetyl)-5-(2-furanyl)-2,2-dimethyloxazolidine, 9CI. MON 13900



$C_{11}H_{13}Cl_2NO_3$ 278.134

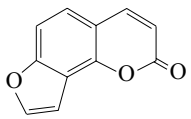
(±)-*form* [141980-03-2]
Herbicide safener for gramineous crops. Powder. Mp 97-98°.

▶ LD_{50} (rat, orl) 869 mg/kg.

Eur. Pat., 1989, 304 409; *CA*, **111**, 77993u (*synth, activity*)
Bussler, B.H. *et al., Brighton Crop Prot. Conf. - Weeds*, 1991, **1**, 39-44 (*activity*)
Bordás, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 926-931 (*sar*)
Pesticide Manual, 12th edn., 2000, No. 401

2*H*-Furo[2,3-*h*][1]benzopyran-2-one, 9CI F-144

[523-50-2]
***Angelicin*†**. *Isopsoralen. Furo[5′,4′:7,8]coumarin. Bakuchicin*



$C_{11}H_6O_3$ 186.167
Constit. of roots and leaves of angelica (*Angelica archangelica*). Found in roots and on surface of parsnips and diseased celery. Mp 138-139.5°. Log P 1.97 (calc). Struct. of Bakuchicin revised (1995).

▶ Prob. a weak photocarcinogen. LD_{50} (rat, orl) 322 mg/kg. LV0940000

5-Hydroxy: See Isobergaptol in *The Combined Chemical Dictionary.*

6-Hydroxy: See 6-Hydroxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one in *The Combined Chemical Dictionary.*

*3-Methoxy:3-Methoxy-2*H*-furo[2,3-*h*][1]benzopyran-2-one.* ***3-Methoxyangelicin***
$C_{12}H_8O_4$ 216.193
Cryst. Mp 138-140°.

*3,6-Dimethoxy:3,6-Dimethoxy-2*H*-furo[2,3-*h*][1]benzopyran-2-one.* ***3,6-Dimethoxyangelicin***
$C_{13}H_{10}O_5$ 246.219
Amorph. solid.

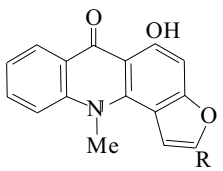
Barnes, C.S. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
Steck, W. *et al., Can. J. Chem.*, 1969, **47**, 2425 (*isol*)
Steck, W. *et al., Can. J. Biochem.*, 1970, **48**, 872 (*biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1388 (*occur*)
González, A.G. *et al., An. Quim.*, 1973, **69**, 1013 (*pmr*)
Reisch, J. *et al., Chem. Ber.*, 1979, **112**, 1491 (*synth*)
Desai, S.M. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 47 (*synth*)
Ceska, O. *et al., Experientia*, 1986, **42**, 1302 (*occur, tox*)
Wulff, W.D. *et al., J.A.C.S.*, 1988, **110**, 7419 (*synth*)
Zubia, E. *et al., Tetrahedron*, 1992, **48**, 4239 (*synth*)
McNab, H. *et al., J. Chem. Res., Synop.*, 1995, 116 (*Bakuchicin*)
Lee, Y.R. *et al., Tetrahedron*, 1995, **51**, 3087 (*synth, pmr*)
Amin, A.S. *et al., Pharm. Pharmacol. Commun.*, 2000, **6**, 455-458 (*activity*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FQC000

Furofoline F-145

[62541-22-4]

5-Hydroxy-11-methylfuro[2,3-c]acridin-6(11H)-one, 9CI. Furofoline I. Furacridone



R = H

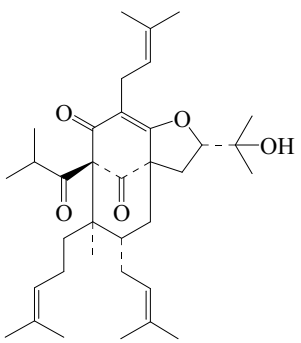
$C_{16}H_{11}NO_3$ 265.268

Alkaloid from the roots of *Ruta graveolens* (rue). Yellow plates (Me_2CO). Mp 245-246°.

Reisch, J. *et al., Phytochemistry*, 1977, **16**, 151 (*isol*)
Reisch, J. *et al., Annalen*, 1981, 85 (*synth*)
Wu, T.-S. *et al., J.C.S. Perkin 1*, 1983, 1681 (*isol, uv, ir, pmr, ms, struct*)

Furohyperforin F-146

[219793-20-1]



$C_{35}H_{52}O_5$ 552.793

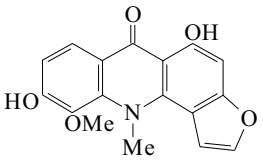
Constit. of *Hypericum perforatum* (St. John's Wort). Oil. $[\alpha]_D^{20}$ +62.4 (c, 0.9 in $CHCl_3$). λ_{max} 272 (log ϵ 4.06) (EtOH).

Hydroperoxide: ***33-Deoxy-33-hydroperoxyfurohyperforin***. *33-Hydroperoxyfurohyperforin*
$C_{35}H_{52}O_6$ 568.792
Constit. of *Hypericum perforatum* (St. John's Wort). Viscous oil. $[\alpha]_D^{20}$ +75 (c, 1.2 in $CHCl_3$). Has –OOH replacing –OH λ_{max} 272 (log ϵ 3.82) ($CHCl_3$).

Verotta, L. *et al., J. Nat. Prod.*, 1999, **62**, 770-772; 2000, **63**, 412-415 (*isol, pmr, cmr, uv, ir, cd, ms*)

Furoparadine F-147

[161161-72-4]



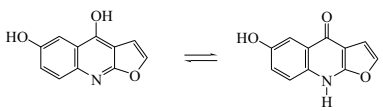
$C_{17}H_{13}NO_5$ 311.293

Alkaloid from roots of *Citrus paradisi* (grapefruit). Yellow oil.

Takemura, Y. *et al., Heterocycles*, 1995, **41**, 187 (*isol, uv, ir, pmr, cmr, ms, struct*)

Furo[2,3-*b*]quinoline-4,6-diol F-148

4,6-Dihydroxyfuro[2,3-b]quinoline. 6-Hydroxyfuro[2,3-b]quinolin-4(9H)-one



$C_{11}H_7NO_3$ 201.181

OH-form

Di-Me ether: [2221-41-2] *4,6-Dimethoxyfuro[2,3-b]quinoline, 9CI*. ***Pteleine***. *6-Methoxydictamnine*
$C_{13}H_{11}NO_3$ 229.235
Alkaloid tentatively identified in cells of *Ruta graveolens* (rue) grown in continuous light in liq. medium. Cubes (C_6H_6/petrol). Mp 134-135°.

▶ LV2708180

Di-Me ether, picrate:
Yellow needles (EtOH). Mp 195-196° dec.

Di-Me ether, picrolonate:
Mp 200-202° dec.

NH-form

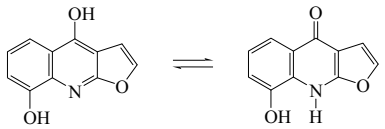
N-*Me:6-Hydroxy-9-methylfuro[2,3-b]quinolin-4(9H)-one, 9CI*. ***Dictangustine A***
$C_{12}H_9NO_3$ 215.208
Yellowish powder (Me_2CO). Mp >280°
λ_{max} 242 ; 255 ; 263 ; 348 ; 364 (MeOH).

6-Me ether, N-*Me:* [2181-84-2] *6-Methoxy-9-methylfuro[2,3-b]quinolin-4(9H)-one, 9CI*. ***Isopteleine***. *6-Methoxyisodictamnine*
$C_{13}H_{11}NO_3$ 229.235
Cryst. (EtOH/Me_2CO). Mp 214-216° (207-209°). Turns pink on standing.

Werny, F. *et al., Tetrahedron*, 1963, **19**, 1293 (*isol, uv, ir, struct, synth*)
Pai, B.R. *et al., Indian J. Chem.*, 1964, **2**, 491 (*synth, uv*)
Frolova, V.I. *et al., Zh. Obshch. Khim.*, 1964, **34**, 3499; *CA*, **62**, 2800f (*isol, struct*)
Kikvidze, I.M. *et al., Khim. Prir. Soedin.*, 1971, **7**, 675; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 659 (*Isopteleine*)
Steck, W. *et al., Phytochemistry*, 1971, **10**, 191 (*isol, uv, pmr*)
Sekiba, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 577 (*synth, uv*)
Narasimhan, N.S. *et al., Tetrahedron*, 1974, **30**, 4153 (*synth, uv, ir, pmr*)
Wu, T.-S. *et al., Phytochemistry*, 1999, **50**, 509-512 (*Dictangustine A*)

Furo[2,3-*b*]quinoline-4,8-diol F-149

4,8-Dihydroxyfuro[2,3-b]quinoline. 8-Hydroxyfuro[2,3-b]quinoline-4(9H)-one



$C_{11}H_7NO_3$ 201.181

OH-form

4-Me ether: [2255-50-7] *4-Methoxyfuro[2,3-b]quinolin-8-ol, 9CI. 8-Hydroxy-4-methoxyfuro[2,3-b]quinoline.* ***Robustine***†. *8-Hydroxydictamnine*
$C_{12}H_9NO_3$ 215.208
Cryst. (EtOH or C_6H_6). Mp 147-148° (142-143°).

4-Me ether, hydrochloride:
Cryst. (EtOH). Mp 199-200°.

4-Me ether, picrate:
Cryst. (EtOH). Mp 179-180°.

Di-Me ether: [524-15-2] *4,8-Dimethoxyfuro[2,3-b]quinoline.* ***γ-Fagarine***. *Haplopine. 8-Methoxydictamnine*
$C_{13}H_{11}NO_3$ 229.235
Alkaloid from *Aegle marmelos* (bael fruit). Pale-yellow prisms (petrol). Poorly sol. hexane. Mp 142°. λ_{max} 203 ; 243 ; 310 ; 325 (MeOH) (Berdy). λ_{max} 244 (ϵ 56210); 290 (ϵ 5250); 311 (ϵ 6610); 327 (ϵ 5750); 340 (ϵ 4900) (EtOH) (Berdy).

▶ LV2708200

Di-Me ether, picrate:
Yellow cryst. (EtOH). Mp 177°.

O^4-*Et,* O^8-*Me:* [105988-99-6] *4-Ethoxy-8-methoxyfuro[2,3-b]quinoline.* ***O-Ethyl-nor-γ-fagarine***
$C_{14}H_{13}NO_3$ 243.262

8-O-(3-Methyl-2-butenyl), O^4-*Me:* [55727-61-2] *4-Methoxy-8-[(3-methyl-2-butenyl)oxy]furo[2,3-b]quinoline, 9CI. 4-Methoxy-8-prenyloxyfuro[2,3-b]quinoline.* ***Haplophydine***. *Haplofidine. Haplophidine*
$C_{17}H_{17}NO_3$ 283.326
Cryst. (EtOH). Mp 111-112°.

NH-form

8-Me ether, N-*Me:8-Methoxy-9-methylfuro[2,3-b]quinolin-4(9H)-one.* ***Iso-γ-fagarine***
$C_{13}H_{11}NO_3$ 229.235
Needles (Me_2CO). Mp 160-161°. λ_{max} 246 ; 255 ; 301 ; 322 ; 336 ; 350 (MeOH).

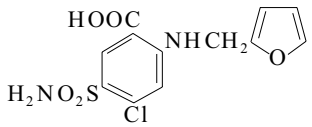
Fakhrutdinova, I.M. *et al., Khim. Prir. Soedin.*, 1965, **1**, 107; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 83 (*isol, struct*)
Faizutdinova, Z.S. *et al., Khim. Prir. Soedin.*, 1967, **3**, 260; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 218 (*ms*)
Collins, J.F. *et al., J.C.S. Perkin 1*, 1973, 94-97 (*synth*)
Abdullaeva, Kh.A. *et al., Khim. Prir. Soedin.*, 1974, **10**, 684; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 713 (*Haplophydine*)
Narasimhan, N.S. *et al., Tetrahedron*, 1974, **30**, 4153-4157 (*synth, uv, ir, pmr*)
Chang, P.T.O. *et al., J. Nat. Prod.*, 1976, **39**, 134 (*isol, ir, uv, ms, pmr*)
Lin, T.P. *et al., CA*, 1987, **106**, 30033n (*4-Ethoxy-8-methoxyfuroquinoline*)

Wu, T.S. *et al., Phytochemistry*, 1999, **50**, 509-512 (*Iso-γ-fagarine*)

Furosemide, INN, JAN, USAN F-150

[54-31-9]

5-(Aminosulfonyl)-4-chloro-2-[2-(furanylmethyl)amino]benzoic acid, 9CI. 4-Chloro-N-furfuryl-5-sulfamoylanthranilic acid. ***Frusemide, BAN****. Diurapid. Froop. Frumax. Frusid. Frusol. Fursemide. Lasix. Dryptal. Rusyde. Tenkafruse. Many other names*



$C_{12}H_{11}ClN_2O_5S$ 330.748

Potential contaminant in cow's milk arising from its use in dairy cattle for the treatment of physiological parturient edema. Marketed drug. Launched 1966. Cryst. (EtOH aq.). Mp 206°. Log P 1.77 (calc).

▶ LD_{50} (rat, orl) 2600 mg/kg. Exp. reprod. and teratogenic effects. CB2625000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 591A (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 41C (*nmr*)

Sturm, K. *et al., Chem. Ber.*, 1966, **99**, 328; 345 (*synth, props*)

Prandota, J. *et al., Eur. J. Drug Metab. Pharmacokinet.*, 1976, **1**, 177 (*rev, metab*)

Lamotte, J. *et al., Acta Cryst. B*, 1978, **34**, 1657 (*cryst struct*)

Benet, L.Z. *et al., J. Pharmacokinet. Biopharm.*, 1979, **7**, 1 (*rev*)

Rupp, W. *et al., Arch. Int. Pharmacodyn. Ther.*, Suppl., 1980, 119 (*rev, pharmacol*)

Brater, D.C. *et al., Annu. Rev. Pharmacol. Toxicol.*, 1983, **23**, 45 (*rev, pharmacol*)

Al-Obaid, A.M. *et al., Anal. Profiles Drug Subst.*, 1989, **18**, 153 (*rev*)

Ponto, L.L.B. *et al., Clin. Pharmacokinet.*, 1990, **18**, 460 (*rev, pharmacol*)

IARC Monog., 1990, **50**, 277 (*rev, tox*)

Du Souich, P. *et al., Prog. Pharmacol. Clin. Pharmacol.*, 1992, **9**, 147 (*rev*)

Aspects of Diuretic Therapy with Furosemide: an Update, Wells Medical, 1993, (*book*)

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 2766 (*synonyms*)

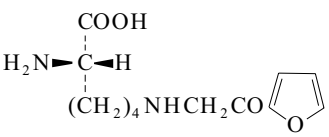
Stanker, L.H. *et al., J. Agric. Food Chem.*, 1996, **44**, 2455-2459 (*occur*)

Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 871

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CHJ750

Furosine F-151

N^6-[2-(2-Furanyl)-2-oxoethyl]lysine, 9CI. ε-N-(2-Furoylmethyl)lysine



$C_{12}H_{18}N_2O_4$ 254.285

(S)-form [19746-33-9]

L-form

Analytical indicator of heat treatment damage or storage deterioriation in milk, dried foods, pasta, tomato paste and eggs. Acid hydrolysis product of the Amadori compd.. Mp 97.5° dec.

Finot, P.A. *et al., Experientia*, 1968, **24**, 1097 (*struct, uv, pmr, ms*)

Nakai, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 2421-2422 (*synth, pmr*)

Hewedy, M.M. *et al., J. Dairy Res.*, 1991, **61**, 304-309 (*detn, milk*)

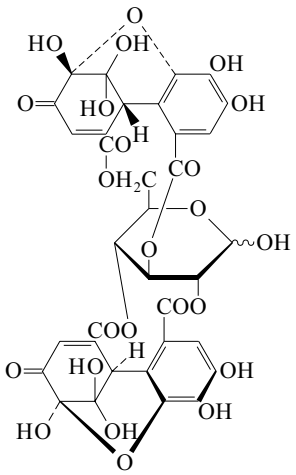
Hidalgo, A. *et al., J. Agric. Food Chem.*, 1995, **43**, 1673-1677; 1998, **46**, 4387-4390; 2000, **48**, 78-82 (*occur*)

Henle, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1995, **200**, 235-237 (*detn, occur*)

Guerra-Hernandez, E. *et al., Cereal Chem.*, 1996, **73**, 729-731 (*detn*)

Furosinin F-152

[81932-55-0]



$C_{34}H_{24}O_{24}$ 816.549

Exists as an equilibrated mixt. of many isomers of which one shown.Yellow amorph. powder + $3H_2O$. $[\alpha]_D$ -58 (c, 0.5 in Me_2CO aq.). Exists as a mixt. of cyclic acetals and hydrates.

1-O-(3,4,5-Trihydroxybenzoyl): [81967-70-6] ***Dehydrogeraniin***

$C_{41}H_{28}O_{28}$ 968.655

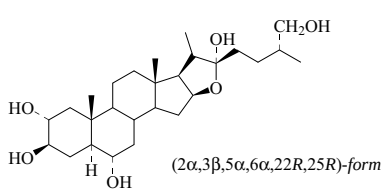
Yellow amorph. powder + $6H_2O$. $[\alpha]_D^{20}$ -137 (c, 0.5 in MeOH).

Okuda, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1113; 1983, **31**, 1625; 2497; 2501 (*isol, uv, pmr, cmr, struct, pharmacol*)

Okuda, T. *et al., Tet. Lett.*, 1982, **23**, 3941 (*cd*)

Yazaki, K. *et al., J.C.S. Perkin 1*, 1989, 2289 (*ir, uv, cd, pmr, cmr*)

Furostane-2,3,6,22,26-pentol F-153



(2α,3β,5α,6α,22*R*,25*R*)-*form*

$C_{27}H_{46}O_6$ 466.657

(2α,3β,5α,6α,22R,25R)-form

22-Me ether, 3-O-[β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-O-β-D-glucopyranoside: [256650-98-3]

$C_{57}H_{96}O_{30}$ 1261.367

Constit. of *Allium ampeloprasum* (greathead garlic).

(2α,3β,5α,6β,22R,25S)-form

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-O-β-D-glucopyranoside: [72947-92-3] ***Turoside C***

$C_{62}H_{104}O_{35}$ 1409.483

Amorph. powder. Mp 192-196°. $[\alpha]_D^{22}$ -69.5 (c, 0.46 in $CHCl_3$/MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-O-β-D-glucopyranoside: [118543-10-5] ***Ampeloside Bf2***

$C_{45}H_{76}O_{21}$ 953.083

Isol. from *Allium ampeloprasum* (greathead garlic). Powder + $3H_2O$ (Me_2CO aq.). $[\alpha]_D^{21}$ -40.7 (c, 1 in Py).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-O-β-D-glucopyranoside: [118524-13-3] ***Ampeloside Bf1***

$C_{51}H_{86}O_{26}$ 1115.225

Constit. of *Allium ampeloprasum* (greathead garlic). Powder + $2^1/_2$ H_2O (Me_2CO aq.). $[\alpha]_D^{21}$ -25.1 (c, 1 in Py).

(2α,3β,5α,6β,22ξ,25ξ)-form

22-Me ether, 3-O-[β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-O-β-D-glucopyranoside:

$C_{57}H_{96}O_{30}$ 1261.367

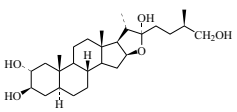
Pirtskhalava, G.V. *et al., Khim. Prir. Soedin.*, 1979, **15**, 514; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 446

Morita, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3480 (*Ampelosides*)

Lim, S.C. *et al., CA*, 1996, **126**, 4620v (*Allium victorialis saponin*)

Mimaki, Y. *et al., Nat. Med. (Tokyo)*, 1999, **53**, 134-137; *CA*, **132**, 134748c (*Allium ampeloprasum saponin*)

Furostane-2,3,22,26-tetrol F-154



(2α,3β,5α,22α,25*R*)-*form*

$C_{27}H_{46}O_5$ 450.657

(2α,3β,5α,22α,25R)-form

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-O-galactopyranoside], 26-β-D-glucopyranoside: [54999-56-3] ***Capsicoside A****. Capsicoside*

$C_{63}H_{106}O_{35}$ 1423.509

Constit. of the roots and seeds of *Capsicum annuum* var. *conides* and *Capsicum annuum* var. *fasciculatum*. Amorph. $[\alpha]_D^{28}$ -37.1 (c, 0.8 in Py). Struct. revised in 1994.

22-Me ether, 3-O-[β-D-glucopyranosyl-(1

*→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside:* [160219-66-9] ***Capsicoside C***
$C_{52}H_{88}O_{25}$ 1113.252
Constit. of the roots and seeds of *Capsicum annuum* var. *conides* and *Capsicum annuum* var. *fasciculatum*. Powder. $[\alpha]_D^{26}$ -42.9 (c, 0.53 in Py).

*22-Me ether, 3-*O*-[β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside:* [160219-65-8] ***Capsicoside B***
$C_{58}H_{98}O_{30}$ 1275.394
Constit. of the roots and seeds of *Capsicum annuum* var. *conides* and *Capsicum annuum* var. *fasciculatum*. Powder. $[\alpha]_D^{26}$ -49.3 (c, 0.73 in Py).

(2α,3β,5α,22ξ,25*R*)-*form*

*3-*O*-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [290347-58-9] ***Trigoneoside XI$_b$***
$C_{44}H_{74}O_{19}$ 907.057
Constit. of *Trigonella foenum-graecum* (fenugreek). Powder. $[\alpha]_D^{23}$ -24.7 (c, 0.2 in MeOH).

*3-*O*-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [290347-51-2] ***Trigoneoside X$_b$***
$C_{45}H_{76}O_{19}$ 921.084
Constit. of *Trigonella foenum-graecum* (fenugreek). Powder. $[\alpha]_D^{22}$ -51.5 (c, 0.6 in MeOH).

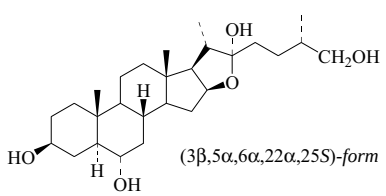
(2α,3β,5α,22ξ,25*S*)-*form*

*3-*O*-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [290347-38-5] ***Trigoneoside X$_a$***
$C_{45}H_{76}O_{19}$ 921.084
Constit. of *Trigonella foenum-graecum* (fenugreek). Powder. $[\alpha]_D^{22}$ -49.2 (c, 0.6 in MeOH).

*3-*O*-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [99753-11-4] ***Trigofoenoside B***
$C_{45}H_{76}O_{19}$ 921.084
Isol. from seeds of *Trigonella foenum-graecum* (fenugreek). Mp 198-200° dec. (as 22-Me ether).

Gupta, R.K. *et al., Phytochemistry*, 1986, **25**, 2205-2207 (*Trigofoenosides*)
Yahara, S. *et al., Phytochemistry*, 1994, **37**, 831 (*Capsicosides*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 994-1000 (*Trigoneosides*)

Furostane-3,6,22,26-tetrol F-155



(3β,5α,6α,22α,25*S*)-*form*

$C_{27}H_{46}O_5$ 450.657

(3β,5α,6α,22α,25*S*)-*form*

*22-Me ether, 6-*O*-[β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* ***Torvoside B***
$C_{45}H_{76}O_{18}$ 905.085
Constit. of *Solanum torvum* (pea eggplant). Amorph. powder. $[\alpha]_D^{27}$ -23.3 (c, 2.8 in MeOH).

*3-Ketone, 22-Me ether, 6-*O*-(6-deoxy-β-D-glucopyranoside), 26-*O*-β-glucopyranoside:* ***Torvoside E***
$C_{40}H_{66}O_{14}$ 770.953
Constit. of *Solanum torvum* (pea eggplant). Amorph. powder. $[\alpha]_D^{27}$ -27.2 (c, 0.7 in MeOH).

*3-Ketone, 22-Me ether, 6-*O*-[β-D-xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* ***Torvoside F***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of *Solanum torvum* (pea eggplant). Amorph. powder. $[\alpha]_D^{27}$ -18.8 (c, 0.5 in MeOH).

(3β,5α,6α,22ξ,25*R*)-*form*

*22-Me ether, 6-*O*-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [141360-81-8]
$C_{46}H_{78}O_{20}$ 951.11
Amorph. powder + $2H_2O$. $[\alpha]_D^{24}$ -21.8 (c, 0.33 in MeOH).

*22-Me ether, 6-*O*-[β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [141360-82-9]
$C_{52}H_{88}O_{25}$ 1113.252
Amorph. powder. $[\alpha]_D^{24}$ -18.7 (c, 0.31 in MeOH).

(3β,5α,6α,22ξ,25*S*)-*form*

*6-*O*-[α-L-Rhamnopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* ***Torvoside A***
$C_{45}H_{76}O_{18}$ 905.085
Constit. of *Solanum torvum* (pea eggplant). Amorph. powder. $[\alpha]_D^{27}$ -38.3 (c, 1 in MeOH).

(3β,5α,6β,22α,25*R*)-*form*

*22-Me ether, 3-*O*-[β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside:* [256642-48-5]
$C_{57}H_{96}O_{29}$ 1245.368
Constit. of *Allium ampeloprasum* (greathead garlic).

(3β,5α,6β,22ξ,25*R*)-*form*

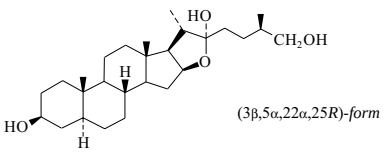
*3-*O*-[β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside:* [126594-42-1] ***Sativoside B1***
$C_{63}H_{106}O_{35}$ 1423.509
Constit. of *Allium sativum* (garlic) bulbs. Powder + $4H_2O$ (Me_2CO aq.). $[\alpha]_D^{26}$ -40 (c, 0.39 in H_2O).

*3-*O*-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside:* [186545-34-6] ***Protoisoeruboside B***
$C_{57}H_{96}O_{30}$ 1261.367
Constit. of fresh garlic bulbs (*Allium sativum*). Cryst. Mp 218-220°. $[\alpha]_D^{20}$ -26 (c, 0.1 in Py).

*6-Ketone, 3-*O*-[α-L-arabinopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→4)]-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [123941-66-2] ***Chinenoside I***
$C_{49}H_{80}O_{23}$ 1037.157
Constit. of *Allium chinense* (rakkyo). Powder + $3H_2O$ (Me_2CO aq.). $[\alpha]_D^{25}$ -42.2 (c, 0.7 in Py).

Matsuura, H. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1390; 2741; 3435 (*Sativoside, Chinenoside I*)
Mimaki, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 148-152 (*Camassia cusickii saponins*)
Yahara, S. *et al., Phytochemistry*, 1996, **43**, 1069 (*Torvosides*)
Peng, J.P. *et al., Yaoxue Xuebao*, 1996, **31**, 607-612 (*Protoisoeruboside B*)
Mimaki, Y. *et al., Nat. Med. (Tokyo)*, 1999, **53**, 134-137; *CA*, **132**, 134748c (*Allium ampeloprasum saponin*)

Furostane-3,22,26-triol F-156



(3β,5α,22α,25*R*)-*form*

$C_{27}H_{46}O_4$ 434.658

(3β,5α,22α,25*R*)-*form*

*3-*O*-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [98524-46-0] ***Melongoside N***
Constit. of *Solanum melongena* (aubergine). Cryst. Mp 187-189°. $[\alpha]_D^{20}$ -15 (c, 1 in MeOH).

*3-*O*-[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [98508-45-3] ***Melongoside P***
From *Solanum melongena* (aubergine). Cryst. Mp 179-180°. $[\alpha]_D^{20}$ -75 (c, 1 in H_2O).

(3β,5α,22α,25*S*)-*form*

*3-*O*-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside:* [75557-22-1] ***Tomatoside A***
$C_{51}H_{86}O_{24}$ 1083.226
Constit. of *Lycopersicon esculentum* (tomato). Cryst. Mp 247-250° dec. $[\alpha]_D^{20}$ -29.3 (c, 1.18 in Py).

*3-Ketone, 22-Me ether, 26-*O*-β-D-glucopyranoside:* [184777-22-8] ***Torvoside G***
$C_{34}H_{56}O_9$ 608.811
Constit. of *Solanum torvum* (pea eggplant). Amorph. powder. $[\alpha]_D^{27}$ -47.4 (c, 0.1 in MeOH).

(3β,5β,22α,25*S*)-*form*

*26-*O*-β-D-Glucopyranoside:* [60237-69-6] ***Asparagoside B***
$C_{33}H_{56}O_9$ 596.8
Constit. of *Asparagus officinalis* (asparagus).

*3-*O*-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [60267-25-6] ***Asparagoside E***
$C_{45}H_{76}O_{19}$ 921.084
Constit. of *Asparagus officinalis* (asparagus). Mp 254-260°. $[\alpha]_D^{20}$ -38 (c, 1 in H_2O).

*3-*O*-[β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:*

[60267-27-8] ***Asparagoside G***
$C_{51}H_{86}O_{24}$ 1083.226
From *Asparagus officinalis* (asparagus). Cryst. Mp 170-174°. $[\alpha]_D^{20}$ -200 (c, 0.6 in H_2O).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-[2,6-di*-O-*β-D-glucopyranosyl-β-D-glucopyranoside]], 26*-O-*β-D-glucopyranoside:* [24333-07-1] ***Sarsaparilloside***
$C_{57}H_{96}O_{28}$ 1229.369
Constit. of *Smilax aristolochiaefolia* (Mexican sarsaparilla). Amorph. powder. $[\alpha]_D^{20}$ -44.

3-O-*[β-D-Glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [60267-28-9] ***Asparagoside H***
$C_{56}H_{94}O_{28}$ 1215.342
From *Asparagus officinalis* (asparagus). Cryst. Mp 146-150°. $[\alpha]_D^{20}$ -200 (c, 0.6 in H_2O).

(3β,5α,22ξ,25*R*)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [126643-25-2] ***Protodegalactotigonin***
$C_{56}H_{94}O_{28}$ 1215.342
Constit. of *Capsicum annuum*. Powder. $[\alpha]_D^{30}$ -14.8 (c, 0.1 in Py).

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [160260-25-3] ***Capsicoside D***
$C_{62}H_{104}O_{33}$ 1377.484
Constit. of *Capsicum annuum*. Powder. $[\alpha]_D^{28}$ -53.9 (c, 0.5 in Py).

(3β,5α,22ξ,25*S*)-*form*

22-Me ether, 3-O-*[α-L-rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [74971-02-1]
$C_{52}H_{88}O_{23}$ 1081.253
Constit. of fenugreek seeds (*Trigonella foenum-graecum*). Amorph.

(3β,5β,22ξ,25*S*)-*form*

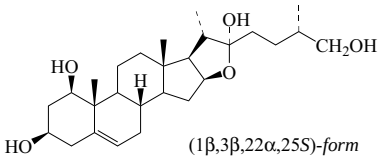
3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [126594-43-2] ***Sativoside R1***
$C_{62}H_{104}O_{33}$ 1377.484
Constit. of *Allium sativum* (garlic). Powder + $2H_2O$ (Me_2CO aq.). $[\alpha]_D^{26}$ -45 (c, 0.59 in Py).

(3β,5β,22α,25*R*)-*form*

22-Me ether, 3-O-*[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [244779-38-2]
$C_{46}H_{78}O_{19}$ 935.111
Constit. of the wild asparagus *Asparagus africanus*. Needles (Me_2CO). Mp 160-161°. $[\alpha]_D^{20}$ -29 (c, 0.14 in MeOH). λ_{max} 230 (MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1969, **102**, 1253-1269; 1972, **105**, 3397-3406 (*Sarsaparilloside, Lanatigoside*)
Sato, H. *et al., Agric. Biol. Chem.*, 1973, **37**, 225-231 (*Tomatoside A*)
Goryanu, G.M. *et al., Khim. Prir. Soedin.*, 1976, **12**, 400-401; 762-765; 823-824; 1977, **13**, 810-813; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 353-354; 684-686; 743-744; 1977, **13**, 682-684 (*Asparagosides B,E,G,H*)
Konishi, T. *et al., Chem. Pharm. Bull.*, 1979, **27**, 3086-3094 (*Asp IV, V, VI, VII*)
Shchelochkova, A.P. *et al., Khim. Prir. Soedin.*, 1980, **16**, 533-540; *Chem. Nat. Compd. (Engl. Transl.)*, 1980, **16**, 386-392 (*Tomatoside A*)
Hardman, R. *et al., Phytochemistry*, 1980, **19**, 698-700 (*isol, 3β,5α,22ξ,25S-form*)
Kintia, P.K. *et al., Phytochemistry*, 1982, **21**, 1447-1449; 1985, **24**, 1567-1569 (*Beshornoside, Melongosides*)
Sharma, S.C. *et al., Phytochemistry*, 1982, **21**, 1711-1714; 2075-2078; 1983, **22**, 1241-1244; 1996, **41**, 599-603; **43**, 1069-1074 (*Asparosides, Asparagus curillus glycosides, Uttrosides, Filicinosides*)
Sharma, S.C. *et al., Planta Med.*, 1982, **46**, 48-51 (*Asparoside C, Asparoside D*)
Matsuura, H. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2741-2743 (*Sativoside R1*)
Li, X.-C. *et al., Phytochemistry*, 1990, **29**, 3893-3898 (*Chloromaloside B*)
Yahara, S. *et al., Phytochemistry*, 1994, **37**, 831-835; 1996, **43**, 1069-1074 (*Capsicoside D, Protodegalactotigonin, Torvoside F*)
Debella, A. *et al., Phytochemistry*, 1999, **51**, 1069-1075 (*Asparagus africanus saponin*)

Furost-5-ene-1,3,22,26-tetrol F-157



(1β,3β,22α,25*S*)-*form*

$C_{27}H_{44}O_5$ 448.642

(1β,3β,22α,25*S*)-*form*

1-O-*[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranoside], 26*-O-*β-D-glucopyranoside:* [105798-62-7] ***Alliofuroside A***
$C_{44}H_{72}O_{18}$ 889.042
Constit. of *Allium cepa* (onion). Cryst. Mp 164-166°. $[\alpha]_D^{20}$ -63.7 (c, 1.11 in Py).

22-Me ether, 1,26-di-O-*β-D-glucopyranoside:* [294873-02-2]
$C_{40}H_{66}O_{15}$ 786.952
Amorph. solid. $[\alpha]_D^{25}$ -104 (c, 0.1 in $CHCl_3$/MeOH).

22-Me ether, 1-O-*[β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-fucopyranoside], 26*-O-*β-D-glucopyranoside:* [128397-48-8] ***Spicatoside B***
$C_{51}H_{84}O_{23}$ 1065.211

(1β,3β,22ξ,25*R*)-*form*

26-O-*β-D-Glucopyranoside, 1-sulfate:* [177747-12-5]
$C_{33}H_{54}O_{13}S$ 690.848
Amorph. powder (MeOH). $[\alpha]_D^{24}$ -86 (c, 0.01 in MeOH).

22-Me ether, 1-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [211379-08-7]
$C_{46}H_{76}O_{19}$ 933.095
Amorph. solid. $[\alpha]_D^{25}$ -36 (c, 0.1 in MeOH).

22-Me ether, 1-O-*[α-L-rhamnopyranosyl-(1→2)-6-O-acetyl-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [211379-11-2]
$C_{48}H_{78}O_{20}$ 975.132
Amorph. solid. $[\alpha]_D^{25}$ -46 (c, 0.1 in MeOH).

22-Me ether, 1-O-*[α-L-rhamnopyranosyl-(1→2)-3,4,6-tri*-O-*acetyl-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [211379-16-7]
$C_{52}H_{82}O_{22}$ 1059.207
Amorph. solid. $[\alpha]_D^{25}$ -160 (c, 0.1 in MeOH).

22-Me ether, 1-O-*[β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [211379-19-0]
$C_{52}H_{86}O_{24}$ 1095.237
Amorph. solid. $[\alpha]_D^{25}$ -98 (c, 0.1 in MeOH).

22-Me ether, 1-O-*[β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→2)-3,4,6-tri*-O-*acetyl-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [211379-22-5]
$C_{58}H_{92}O_{27}$ 1221.349
Amorph. solid. $[\alpha]_D$ -40 (c, 0.1 in MeOH).

Kravets, S.D. *et al., Khim. Prir. Soedin.*, 1986, **22**, 188; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 174 (*isol, ir*)
Yong, L.D. *et al., Arch. Pharmacal Res.*, 1989, 295 (*Spicatoside B*)
Qulad-Ali, A. *et al., Phytochemistry*, 1996, **42**, 895-897 (*isol, pmr, cmr*)
Mimaki, Y. *et al., Phytochemistry*, 1998, **48**, 485-493 (*Ruscus aculeatus saponins*)
Yokosuka, A. *et al., J. Nat. Prod.*, 2000, **63**, 1239-1243 (*Dracaena surculosa saponin*)

Furost-25(27)-ene-1,3,22,26-tetrol F-158

$C_{27}H_{44}O_5$ 448.642

(1β,3β,5β,22*R*)-*form*

1-[2-O-*(6-Deoxy-α-L-mannopyranosyl)-6-deoxy-β-D-glucopyranoside], 3-(6-deoxy-4*-O-*β-D-glucopyranosyl-α-L-mannopyranoside), 27*-O-*β-D-glucopyranoside:* [52591-05-6] ***Convallamaroside***. *Convallamarin*
$C_{57}H_{94}O_{27}$ 1211.353
Constit. of *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Amorph. powder.

(1β,3β,5α,22ξ)-*form*

22-Me ether, 1-O-*[α-L-rhamnopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-fucopyranoside], 26*-O-*β-D-glucopyranoside:* [202347-02-2]
$C_{51}H_{84}O_{22}$ 1049.211
Amorph. solid. $[\alpha]_D^{27}$ -20 (c, 0.11 in $CHCl_3$).

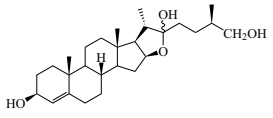
(1β,3α,5β,22*R*)-*form*

22-Me ether, 1-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranoside], 26*-O-*β-D-glucopyranoside:* [209848-39-5]
$C_{46}H_{76}O_{18}$ 917.096
Amorph. solid. $[\alpha]_D^{27}$ -45 (c, 0.12 in MeOH).

22-Me ether, 1-O-*[α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranoside], 26*-O-*β-D-glucopyranoside:*
$C_{45}H_{74}O_{18}$ 903.069
Amorph. solid. $[\alpha]_D^{27}$ -37.5 (c, 0.41 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1973, **106**, 3010
Mimaki, Y. *et al., Phytochemistry*, 1998, **47**, 79-85; 1351-1356 (*Cordyline saponin, Dracaena concinna saponins*)

Furost-4-ene-3,22,26-triol F-159



(3β,22ξ,25*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

(3β,22ξ,25*R*)-*form*

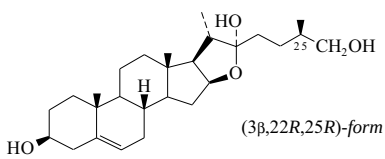
3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [290348-00-4] ***Trigoneoside XIIb***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of *Trigonella foenum-graecum* (fenugreek). Powder. $[\alpha]_D^{22}$ -48.2 (c, 0.5 in MeOH).

(3β,22ξ,25*S*)-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [290347-97-6] ***Trigoneoside XIIa***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of *Trigonella foenum-graecum* (fenugreek). Powder. $[\alpha]_D^{20}$ -48.8 (c, 0.6 in MeOH).

Murakami, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 994-1000 (*isol, pmr, cmr*)

Furost-5-ene-3,22,26-triol F-160



(3β,22*R*,25*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

(3β,22*R*,25*R*)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [98464-54-1] ***Melongoside O***
$C_{45}H_{74}O_{19}$ 919.068
Constit. of egg plant seeds (*Solanum melongena*). Cryst. Mp 183-184°. $[\alpha]_D^{20}$ -19 (c, 1 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [55056-80-9] ***Protodioscin***. *Saponin C*†. *NSC 698796*
$C_{51}H_{84}O_{22}$ 1049.211
From *Asparagus officinalis* (asparagus). Needles. Mp 190-192° dec. (188-190° dec). $[\alpha]_D^{13}$ -88.4 (c, 0.01 in Py). $[\alpha]_D$ -75.3 (c, 0.61 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [94714-56-4] ***Trigofoenoside F***
$C_{51}H_{84}O_{23}$ 1065.211
Isol. from fenugreek seeds. Amorph. solid. Mp 233-236°.

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→4)]-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [94714-57-5] ***Trigofoenoside G***
$C_{56}H_{92}O_{27}$ 1197.327
Isol. from fenugreek seeds. Amorph. solid. Mp 275-278°.

22-Me ether, 3-O-*[α-L-rhamnopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [101910-70-7] ***Trigofoenoside E1***
$C_{51}H_{84}O_{22}$ 1049.211
Isol. from fenugreek seeds. Amorph. powder ($MeOH/Me_2CO$). Mp 230-231°. $[\alpha]_D$ -57.9 (c, 1 in Py).

22-Me ether, 3-O-*[α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [55658-89-4] ***Protodioscin 22-methyl ether***
$C_{52}H_{86}O_{22}$ 1063.238
Isol. from seeds of *Trigonella caerulea* (sweet trefoil) and *Asparagus officinalis* (asparagus). Cryst. (MeOH/2-propanol). Mp 181-189°. $[\alpha]_D$ -59.8 (c, 0.56 in MeOH).

(3β,22*R*,25*S*)-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [99705-66-5] ***Trigofoenoside A***
$C_{45}H_{74}O_{18}$ 903.069
Isol. from seeds of fenugreek (*Trigonella foenum-graecum*). Amorph. powder. Mp 219-221° dec. $[\alpha]_D$ -90 (c, 1 in Py).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [60433-66-1] ***Asparasaponin II***
$C_{45}H_{74}O_{18}$ 903.069
From white asparagus shoots (*Asparagus officinalis*). Amorph.

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [60478-69-5] ***Asparasaponin I***. *Trigonelloside C. Yamogenintetroside C. Protoneodioscin*
$C_{51}H_{84}O_{22}$ 1049.211
Bitter principle from white asparagus shoots (*Asparagus officinalis*) and fenugreek (*Trigonella foenum-graecum*). Amorph. Mp 166-168° dec. $[\alpha]_D^{13}$ -70.1 (c, 0.01 in Py).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [99664-39-8] ***Trigofoenoside D***
$C_{51}H_{84}O_{23}$ 1065.211
Isol. from seeds of fenugreek (*Trigonella foenum-graecum*). Amorph. powder. Mp 246-248° (220° dec.). $[\alpha]_D$ -73.2 (c, 1 in Py).

22-Me ether, 3-O-*[α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [60478-70-8] ***Yamogenintetroside B***
$C_{52}H_{86}O_{22}$ 1063.238
From fenugreek *Trigonella foenum-graecum*. Amorph.

(3β,22ξ,25*R*)-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [145854-02-0] ***Balanitoside***
$C_{51}H_{84}O_{23}$ 1065.211
Constit. of the fruit of soapberry tree *Balanites aegyptiaca*.

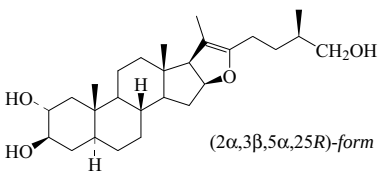
3-O-*[α-L-Rhamnopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→2)]-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside], 26*-O-*β-D-glucopyranoside:* [212369-13-6] ***Balanitesin***
$C_{60}H_{98}O_{29}$ 1283.417
Constit. of soapberry tree fruits (*Balanites aegyptiaca*). Amorph. powder. $[\alpha]_D^{23}$ +25.2 (c, 0.31 in MeOH).

(3β,22ξ,25*S*)-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [290348-13-9] ***Trigoneoside XIIIa***
$C_{57}H_{94}O_{28}$ 1227.353
Isol. from fenugreek. Powder. $[\alpha]_D^{26}$ -31.4 (c, 0.5 in MeOH).

Kawasaki, T. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2164 (*Protodioscin, Protogracillin*)
Hoyer, G.A. *et al., Phytochemistry*, 1975, **14**, 539 (*Protodioscin 22-methyl ether*)
Bogacheva, N.G. *et al., Khim. Prir. Soedin.*, 1976, **12**, 268; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 242 (*Trigonelloside C*)
Kawano, K. *et al., Agric. Biol. Chem.*, 1977, **41**, 1 (*Asparasaponins*)
Bogacheva, N.G. *et al., Khim.-Farm. Zh.*, 1977, **11**, 65 (*Yamogenintetrosides*)
Tomova, M. *et al., Planta Med.*, 1978, **34**, 188 (*Saponin C*)
Gupta, R.K. *et al., Phytochemistry*, 1984, **23**, 2605; 1985, **24**, 2399 (*Trigofoenosides*)
Gupta, R.K. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 1215 (*Trigofoenoside E1*)
Kintia, P.K. *et al., Phytochemistry*, 1985, **24**, 1567 (*Melongoside*)
Hosny, M. *et al., Phytochemistry*, 1992, **31**, 3565-3569 (*Balanitoside*)
Khodakov, G.V. *et al., Khim. Prir. Soedin.*, 1994, **30**, 766; *Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 713 (*Protodioscin, pmr, cmr*)
Shao, Y. *et al., Planta Med.*, 1997, **63**, 258-262 (*Protodioscin*)
Kamel, M.S. *et al., Phytochemistry*, 1998, **48**, 755-757 (*Balanitesin*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 994-1000 (*Trigoneoside XIIIa*)
Hu, K. *et al., Planta Med.*, 2002, **68**, 297-301 (*Protodioscin, activity*)

Furost-20(22)-ene-2,3,26-triol F-161



(2α,3β,5α,25*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

(2α,3β,5α,25*R*)-*form*

3-O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [425644-95-7] ***Trigoneoside VIII***
$C_{44}H_{72}O_{18}$ 889.042
Constit. of *Trigonella foenum-graecum* (fenugreek). Cryst. ($MeOH/CHCl_3$). Mp 173-175°. $[\alpha]_D$ -28.6 (c, 0.07 in MeOH).

(2α,3β,5α,25*S*)-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [259810-65-6] ***Tuberoside A***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of *Allium tuberosum* (Chinese chives). Amorph. solid. $[\alpha]_D^{22}$ -29.5 (c, 0.27 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [259810-67-8] ***Tuberoside B***
$C_{51}H_{84}O_{22}$ 1049.211
Constit. of *Allium tuberosum* (Chinese chives). Amorph. solid. $[\alpha]_D^{23}$ -29.5 (c, 0.3 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 26*-O-*β-D-glucopyranoside:* [259810-68-9] ***Tuberoside C***
$C_{51}H_{84}O_{23}$ 1065.211
Constit. of *Allium tuberosum* (Chinese chives). Amorph. solid. $[\alpha]_D^{23}$ -19.8 (c, 0.51 in MeOH).

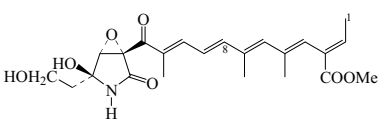
(2β,3β,5β,25*R*)-*form*

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside], 26*-O-*β-D-glucopyranoside:* [159935-11-2] ***Macrostemonoside L***
$C_{45}H_{74}O_{19}$ 919.068
Amorph. powder. Mp 206-208°.

Peng, J. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2180 (*Macrostemonoside L*)
Sang, S. *et al., Phytochemistry*, 1999, **52**, 1611-1615 (*Tuberosides*)
Shang, M.-Y. *et al., Yaoxue Xuebao*, 2001, **36**, 836-839 (*Trigoneoside VIII*)

Fusarin C F-162

[79748-81-5]



$C_{23}H_{29}NO_7$ 431.485
Prod. by many *Fusarium* spp. in infected corn.. λ_{max} 358 (ϵ 32000) (MeOH) (Derep).

► Mutagenic (comparable to Aflatoxin B_1). YQ2831500

1-Hydroxy: [145569-98-8] ***Fusarin X***
$C_{23}H_{29}NO_8$ 447.484

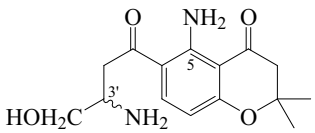
8Z-Isomer: [90987-21-6]
$C_{23}H_{29}NO_7$ 431.485
Cryst. (CH_2Cl_2). Mp 170-172° (synthetic). λ_{max} 350 (ϵ 25000) (MeOH) (Berdy).

6Z-Isomer: [194152-45-9]
$C_{23}H_{29}NO_7$ 431.485
Pale yellow oil.

Gelderblom, W.C.A. *et al., J. Agric. Food Chem.*, 1984, **32**, 1064 (*isol, struct*)
Gaddamidi, V. *et al., J. Agric. Food Chem.*, 1985, **33**, 652 (*cmr, conformn*)
Farber, J.M. *et al., J. Agric. Food Chem.*, 1986, **34**, 963 (*isol*)
Barrero, A.F. *et al., Phytochemistry*, 1991, **30**, 2259 (*isol*)
Lu, F.X. *et al., Chem. Res. Toxicol.*, 1993, **6**, 91-96; 97-101 (*Fusarin X*)
Eilbert, F. *et al., J. Antibiot.*, 1997, **50**, 443-445 (*6Z-isomer, 8Z-isomer*)

Fusarochromanone F-163

[104653-89-6]
*5-Amino-6-(3-amino-4-hydroxy-1-oxobutyl)-2,3-dihydro-2,2-dimethyl-4*H*-1-benzopyran-4-one, 9CI. TDP 1*



$C_{15}H_{20}N_2O_4$ 292.334
Mycotoxin prod. by *Fusarium roseum* and the cereal fungus *Fusarium equiseti* (*Fusarium graminearum*). Affects growth and development of poultry. Mp 132-134°. Fluor. in uv light.

$N^{3'}$-*Formyl:* [136685-28-4] ***Formylfusarochromanone***
$C_{16}H_{20}N_2O_5$ 320.344
Prod. by *Fusarium equiseti*. Yellow oil. λ_{max} 214 ; 248 ; 278 (MeOH) (Berdy).

3′-N-*Ac:* [120976-97-8] ***3′-N′-Acetylfusarochromanone. TDP 2***
$C_{17}H_{22}N_2O_5$ 334.371
Mycotoxin prod. by *Fusarium equiseti*.

$O^{4'}$, $N^{3'}$-*Di-Ac:* [104653-91-0]

[137623-88-2] ***Diacetylfusarochromanone***
$C_{19}H_{24}N_2O_6$ 376.408
Prod. by *Fusarium equiseti*. Needles (Me_2CO). λ_{max} 214 ; 248 ; 276 (MeOH) (Berdy).

4′-O-(9-Octadecenoyl), 3′-N-*Ac:* [136844-71-8]

[136536-85-1, 136599-17-2] ***3′-N-Acetyl-4′-O-(9-octadecenoyl)fusarochromanone***
$C_{35}H_{54}N_2O_6$ 598.821
Prod. by *Fusarium equiseti*.

4′-O-(14-Methylpentadecanoyl), 3′-N-*Ac:* [136762-45-3] ***3′-N-Acetyl-4′-O-(14-methylpentadecanoyl)fusarochromanone***
$C_{33}H_{52}N_2O_6$ 572.784
Prod. by *Fusarium equiseti*.

4′-O-(16-Methylheptadecanoyl), 3′-N-*Ac:* [136762-44-2] ***3′-N-Acetyl-4′-O-(14-methylheptadecanoyl)fusarochromanone***
$C_{35}H_{56}N_2O_6$ 600.837
Prod. by *Fusarium equiseti*.

4′-O-(10,12-Octadecadienoyl), 3′-N-*Ac:* [136536-84-0] ***3′-N-Acetyl-4′-O-(10,12-octadecadienoyl)fusarochromanone***
$C_{35}H_{52}N_2O_6$ 596.806
Prod. by *Fusarium equiseti*.

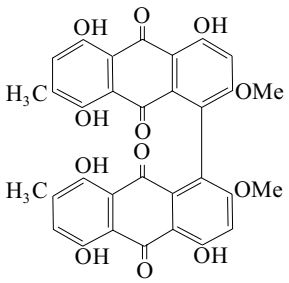
3′-Deamino: [162287-96-9] *5-Amino-6-(4-hydroxybutanoyl)-2,2-dimethyl-4-chromanone. **3′-Deaminofusarochromanone***
$C_{15}H_{19}NO_4$ 277.319
Prod. by *Fusarium equiseti*. Light yellow powder. λ_{max} 213 ; 246 ; 276 (MeOH) (Berdy).

3′-Deamino, 2′,3′-didehydro: [162287-97-0] *5-Amino-6-(4-hydroxy-2-butenoyl)-2,2-dimethyl-4-chromanone*
$C_{15}H_{17}NO_4$ 275.304
Prod. by *Fusarium equiseti*. Bright yellow powder. λ_{max} 210 ; 260 ; 390 (MeOH) (Berdy).

Pathre, S.V. *et al., Can. J. Chem.*, 1986, **64**, 1308 (*isol, cryst struct*)
Xie, W. *et al., Appl. Environ. Microbiol.*, 1989, **55**, 794 (*derivs*)
Xie, W. *et al., J. Agric. Food Chem.*, 1991, **39**, 1757 (*derivs*)
Xie, W. *et al., J. Nat. Prod.*, 1991, **54**, 1165; 1995, **58**, 124 (*derivs*)

Fusaroskyrin F-164

4,4′,5,5′,8,8′-Hexahydroxy-2,2′-dimethoxy-7,7′-dimethyl-1,1′-bianthraquinone



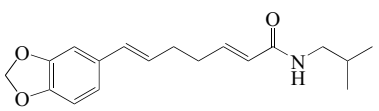
$C_{32}H_{22}O_{12}$ 598.519
Responsible for purple speck disease in soybean. Dark red powder. Mp 300°. λ_{max} 256 (ϵ 83000); 277 (ϵ 71000); 305 (ϵ 15900); 505 (ϵ 17800) (MeOH) (Berdy).

Hexa-Ac:
Mp 264-266°.

Matsueda, S. *et al., J.O.C.*, 1965, **30**, 744 (*isol, uv*)

Futoamide F-165

[114092-54-5]
7-(1,3-Benzodioxol-5-yl)-N-*(2-methylpropyl)-2,6-heptadienamide, 9CI.* N-*[7-(3,4-Methylenedioxyphenyl)-2,6-heptadienoyl]isobutylamine*



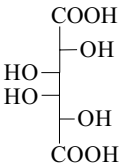
$C_{18}H_{23}NO_3$ 301.385Related to 1-[7-(3,4-Methylenedioxyphenyl)-2,6-heptadienoyl]-pyrrolidine, M-411.

(*E*,*E*)-*form* [23477-80-7]
Alkaloid from *Piper longum* (long pepper). Cryst. (Me_2CO/hexane). Mp 128-130°.

Takahashi, S. *et al., Phytochemistry*, 1969, **8**, 321 (*isol*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 458-460 (*synth*)
Blade, R.J. *et al., Tet. Lett.*, 1987, **28**, 3857-3860 (*synth*)
Li, S. *et al., Yaoxue Xuebao*, 1987, **22**, 196 (*isol*)
Das, B. *et al., Fitoterapia*, 1998, **69**, 548 (*isol, pmr, cmr*)

Galactaric acid, 9CI, 8CI G-1

[526-99-8]
1,2,3,4-Tetrahydroxy-1,4-butanedicarboxylic acid. Mucic acid. Tetrahydroxyadipic acid. Galactosaccharic acid



$C_6H_{10}O_8$ 210.14

A *meso*-compd., certain derivs. induce asymmetry. For stereoisomers see Glucaric acid, G-149, Allaric acid, Mannaric acid, Galactaric acid, G-1 and Idaric acid. Present in ripe fruits of peach and pear. Formed in grapes and grape must by the action of *Botrytis cinerea* on galacturonic acid. Cryst. Sol. alkalis; spar. sol. H_2O. Mp 213° Mp 225° Mp 230° dec.

► LD_{50} (mus, orl) 8000 mg/kg. LW5180000

Ca salt: [28380-80-5] *Calcium mucate*
Potential cause of turbidity in mucic acid rich wines. Mp 213°.

2-O-(3,4,5-Trihydroxybenzoyl): ***2-O-Galloylgalactaric acid***. *2-O-Galloylmucic acid*
$C_{13}H_{14}O_{12}$ 362.246
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. off-white powder + 1½ H_2O. $[\alpha]_D^{22}$ -25.3 (c, 0.28 in H_2O).

2-O-(3,4,5-Trihydroxybenzoyl), 1-Me ester:
$C_{14}H_{16}O_{12}$ 376.273
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 1 H_2O. $[\alpha]_D^{22}$ -38.1 (c, 0.22 in MeOH).

2-O-(3,4,5-Trihydroxybenzoyl), 6-Me ester:
$C_{14}H_{16}O_{12}$ 376.273
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 1½ H_2O. $[\alpha]_D^{22}$ -43.9 (c, 0.28 in MeOH).

2-O-(3,4,5-Trihydroxybenzoyl), di-Me ester:
$C_{15}H_{18}O_{12}$ 390.3
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 1¼ H_2O. $[\alpha]_D^{22}$ -51 (c, 0.41 in MeOH).

1,4-Lactone, 2-O-(3,4,5-trihydroxybenzoyl):2-O-Galloyl-1,4-galactarolactone
$C_{13}H_{12}O_{11}$ 344.231
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 1H_2O. $[\alpha]_D^{22}$ -9.5 (c, 0.26 in MeOH). This and the other *P. emblica* galactarolactones are chiral compds. but the information on their abs. config. in the lit. is confusing.

1,4-Lactone, 2-O-(3,4,5-trihydroxybenzoyl), Me ester:
$C_{14}H_{14}O_{11}$ 358.258
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 2 3/4 H_2O. $[\alpha]_D^{22}$ -13 (c, 0.19 in MeOH).

1,4-Lactone, 3-O-(3,4,5-trihydroxybenzoyl):3-O-Galloyl-1,4-galactarolactone
$C_{13}H_{12}O_{11}$ 344.231
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 2H_2O. $[\alpha]_D^{22}$ -30.3 (c, 0.16 in MeOH). See note under 2-galloyl isomer.

1,4-Lactone, 5-O-(3,4,5-trihydroxybenzoyl):5-O-Galloyl-1,4-galactarolactone
$C_{13}H_{12}O_{11}$ 344.231
Consist. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 1½H_2O. $[\alpha]_D^{22}$ -29.3 (c, 0.33 in MeOH). See note under 2-galloyl isomer.

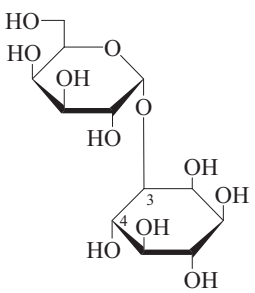
1,4-Lactone, 5-O-(3,4,5-trihydroxybenzoyl), Me ester:
$C_{14}H_{14}O_{11}$ 358.258
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 2½ H_2O. $[\alpha]_D^{22}$ -30.9 (c, 0.58 in MeOH).

1,4-Lactone, 3,5-bis-O-(3,4,5-trihydroxybenzoyl):3,5-Di-O-galloyl-1,4-galactarolactone
$C_{20}H_{16}O_{15}$ 496.337
Constit. of the fruit of emblic (*Phyllanthus emblica*). Amorph. powder + 2½H_2O. $[\alpha]_D^{22}$ -96.5 (c, 0.2 in MeOH). See note under 2-*O*-galloyl deriv..

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 458B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 524A (*ir*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 359 (*rev, derivs*)
Anet, E.F.L.J. *et al., Nature (London)*, 1954, **174**, 930 (*isol*)
Togasawa, Y. *et al., CA*, 1955, **49**, 7064 (*isol*)
Tanner, H. *et al., CA*, 1961, **72**, 77441p (*Ca salt*)
Schormuellar, J. *et al., Z. Lebensm.-Unters. -Forsch.*, 1967, **132**, 270-276 (*formn, grapes*)
Burden, I.J. *et al., J.C.S. Perkin 1*, 1974, 863 (*pmr*)
Jeffrey, G.A. *et al., Carbohydr. Res.*, 1982, **108**, 205 (*cryst struct*)
Zhang, Y.-J. *et al., Chem. Pharm. Bull.*, 2001, **49**, 537-540 (*2-galloyl derivs*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GAR000

Galactinol G-2

[3687-64-7]
3-O-α-D-Galactopyranosyl-myo-*inositol, 8CI. 1-O-α-D-Galactopyranosyl*-myo-*inositol (incorr.)*



$C_{12}H_{22}O_{11}$ 342.299

Frequently named as 1-*O*-galactosyl; see under *myo*-Inositol I-41 for correct numbering. Constit. of sugar-beet juice, castor-oil seed meal and potatoes after cold storage. Mp 113-114° (closed tube) Mp 220-222° (open tube) (dihydrate). $[\alpha]_D^{20}$ +135.6 (c, 2.0 in H_2O).

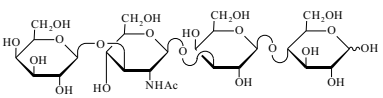
4-Me: [75589-40-1] *3-O-α-D-Galactopyranosyl-4-O-methyl-D*-myo-*inositol. 3-O-α-D-Galactopyranosylononitol.* ***4-O-Methylgalactinol***
$C_{13}H_{24}O_{11}$ 356.326
Constit. of the seeds of azuki bean (*Vigna angularis*). Powder. $[\alpha]_D^{20}$ +129.6 (c, 0.5 in H_2O). Struct. revised in 1997.

Nona-Me:
Cryst. (pentane). Mp 96.5-98°. $[\alpha]_D$ +119 (c, 2.0 in H_2O).

Brown, R.J. *et al., J.A.C.S.*, 1953, **75**, 1040 (*synth*)
Kabat, E.A. *et al., J.A.C.S.*, 1953, **75**, 4507 (*struct, nona-Me*)
Senser, M. *et al., Phytochemistry*, 1967, **6**, 1533 (*occur*)
Schweizer, T.F. *et al., Carbohydr. Res.*, 1981, **95**, 61-71 (*cmr, ms*)
Kuo, T.M. *et al., J. Am. Oil Chem. Soc.*, 1992, **69**, 569-574 (*isol, hplc, bibl*)
Richter, A. *et al., J. Nat. Prod.*, 1997, **60**, 749-751 (*4-O-Methylgalactinol*)
Mayer, T.G. *et al., Liebigs Ann./Recl.*, 1997, 859 (*synth, pmr, cmr*)
Marinone, F. *et al., Phytochemistry*, 1999, **51**, 499-505 (*isol, pmr*)
Noguchi, K. *et al., Carbohydr. Res.*, 2000, **328**, 241-248 (*cryst struct*)

β-D-Galactopyranosyl-(1→3)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1→3)-β-D-galactopyranosyl-(1→4)-D-glucose G-3

[14116-68-8]
*Lacto-*N-*tetraose. 3²-β-Galactosyllacto-*N-*triose II*



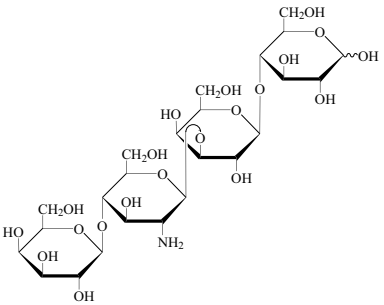
Pyranose-*form*

$C_{26}H_{45}NO_{21}$ 707.636
Present in the free state in human milk. $[\alpha]_D$ +25.5 (H_2O).

Phenylosazone:
Mp 222-223°.

Kuhn, R. *et al., Chem. Ber.*, 1954, **87**, 289; 1553; 1956, **89**, 504; 1027; 2514; 1958, **91**, 364; 1960, **93**, 647 (*isol, struct*)
Malpress, F.H. *et al., Biochem. J.*, 1958, **68**, 708
Dua, V.K. *et al., Anal. Biochem.*, 1983, **133**, 1 (*isol, hplc*)
Subramaniam, S. *et al., J.A.C.S.*, 1986, **108**, 2068 (*pmr, cmr*)
Aly, M.R.E. *et al., Carbohydr. Res.*, 1999, **316**, 121-132 (*synth*)

β-D-Galactopyranosyl-(1 → 4)-2-amino-2-deoxy-β-D-glucopyranosyl-(1 → 3)-β-D-galactopyranosyl-(1 → 4)-D-glucose G-4

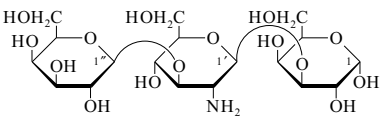


$C_{24}H_{43}NO_{20}$ 665.598

N-*Ac:* [13007-32-4] *Lacto*-N-*neotetraose. LNNT*
$C_{26}H_{45}NO_{21}$ 707.636
Isol. from human milk. Mp 214-218°. $[\alpha]_D^{22}$ +33 (6 min) → +27 (17 h) (c, 1.0 in H_2O).

Kuhn, R. *et al., Chem. Ber.*, 1962, **95**, 513-517; 518-522 (*isol*)
Sabesan, S. *et al., J.A.C.S.*, 1986, **108**, 2068-2080 (*N-Ac, synth, pmr, cmr, bibl*)
Yuen, C.T. *et al., J. Biol. Chem.*, 1994, **269**, 1595-1598 (*activity*)
Aly, M.R.E. *et al., Carbohydr. Res.*, 1999, **316**, 121-132 (*synth*)

β-D-Galactopyranosyl-(1 → 3)-2-amino-2-deoxy-β-D-glucopyranosyl-(1 → 3)-D-galactose G-5



α-Pyranose-*form*

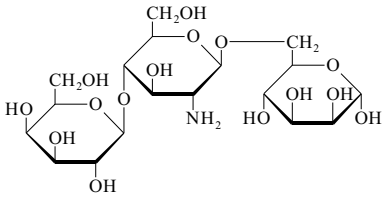
$C_{18}H_{33}NO_{15}$ 503.456

2′-N-*Ac:β-D-Glucopyranosyl-(1 → 3)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1 → 3)-D-galactose. Lacto*-N-*triose I*
$C_{20}H_{35}NO_{16}$ 545.494
Isol. from the partial acid hydrol. of human milk. Cryst. + $2H_2O$. Mp 202° (139-141° dec., 183-185°). $[\alpha]_D$ +19.3 (c, 2.0 in H_2O) (+13.6).

[93303-80-1]

Kuhn, R. *et al., Chem. Ber.*, 1954, **87**, 289; 1553; 1956, **89**, 504; 1027; 2514; 1958, **91**, 364; 1960, **93**, 647 (*isol*)
Auge, C. *et al., J.C.S. Perkin 1*, 1977, 1343 (*N-Ac synth, α-pyr deriv synth, pmr*)

β-D-Galactopyranosyl-(1 → 4)-2-amino-2-deoxy-β-D-glucopyranosyl-(1 → 6)-D-mannose, 9CI G-6



$C_{18}H_{33}NO_{15}$ 503.456
Constit. of blood group substance of human milk.

N-*Ac:* [82184-65-4]
$C_{20}H_{35}NO_{16}$ 545.494
Amorph. powder. $[\alpha]_D^{21}$ -10 (c, 1.0 in H_2O).

α-Pyranose-*form*

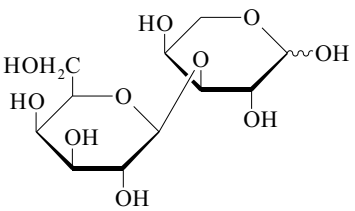
Benzyl glycoside, 2,3,4-tribenzyl, 2′N,2″,3′,3″,4″,6′,6″-hepta-Ac: [78561-23-6]
$C_{60}H_{71}NO_{22}$ 1158.214
Syrup. $[\alpha]_D^{21}$ +8 (c, 1.0 in $CHCl_3$).

[78561-25-8]

Arnarp, J. *et al., Carbohydr. Res.*, 1981, **98**, 154 (*N-Ac, α-benzyl pyr deriv, pmr, cmr*)
Bock, K. *et al., Eur. J. Biochem.*, 1982, **129**, 171 (*N-Ac, pmr, cmr, conformn*)
Gooi, H.C. *et al., Carbohydr. Res.*, 1983, **120**, 293 (*occur*)
Townsend, R.R. *et al., Anal. Biochem.*, 1988, **174**, 459 (*chromatog, anal*)

3-*O*-β-D-Galactopyranosyl-L-arabinose, 9CI, 8CI G-7

[6055-00-1]



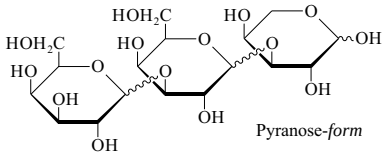
Pyranose-*form*

$C_{11}H_{20}O_{10}$ 312.273
Isol. from partial acid hydrolysates of *Aegle marmelos* gum (bael fruit) and from the mucilage of *Opuntia ficus-indica* (Indian fig). Cryst. (MeOH/EtOH). Mp 202-204° (192-194°). $[\alpha]_D$ +62 (in H_2O). $[\alpha]_D$ +57 (c, 0.2 in H_2O).

Aspinall, G.O. *et al., J.C.S.*, 1958, 4408; 1961, 3461 (*isol*)
Drummond, D.W. *et al., J.C.S.*, 1961, 3908
Gorin, P.A.J. *et al., Can. J. Chem.*, 1966, **44**, 2083 (*synth*)
Roy, A. *et al., Carbohydr. Res.*, 1975, **41**, 219
Audichya, T.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 601
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol, struct*)

D-Galactopyranosyl-(1 → 3)-D-galactopyranosyl-(1 → 3)-L-arabinose, 9CI G-8

[79043-15-5]



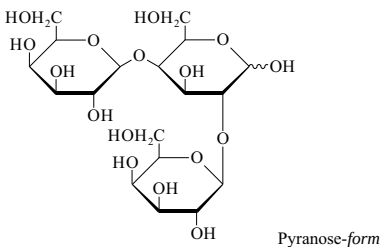
Pyranose-*form*

$C_{17}H_{30}O_{15}$ 474.415
Isol. from the hydrolysate of the gum of *Spondias dulcis* (ambarella). $[\alpha]_D^{24}$ +56 (c, 0.5 in H_2O).

Basu, S. *et al., Carbohydr. Res.*, 1981, **94**, 215

β-D-Galactopyranosyl-(1 → 2)-[β-D-galactopyranosyl-(1 → 4)]-D-galactose, 9CI G-9

[83788-45-8]

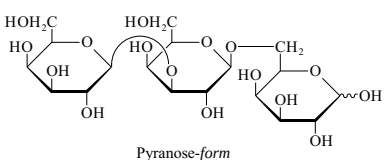


Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Isolated from the partial acid hydrolysate of cambium polysaccharides of Bael (*Aegle marmelos*). $[\alpha]_D^{24}$ +45.4 (H_2O).

Basak, R.K. *et al., Carbohydr. Res.*, 1982, **110**, 145

β-D-Galactopyranosyl-(1 → 3)-β-D-galactopyranosyl-(1 → 6)-D-galactose, 9CI G-10



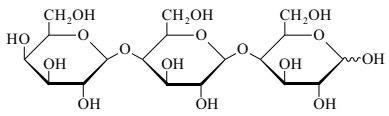
Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Isol. from the partial acid hydrolysates of the gums of *Prunus persica* and *Opuntia ficus-indica* (Indian fig). $[\alpha]_D$ +27.9 (c, 0.5 in H_2O).

Kubala, J. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 2809
Kardosova, A. *et al., Coll. Czech. Chem. Comm.*, 1978, **43**, 3428 (*isol, glc, ms*)
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57
Difabio, J.L. *et al., Carbohydr. Res.*, 1982, **99**, 41 (*isol*)

β-D-Galactopyranosyl-(1→4)-β-D-galactopyranosyl-(1→4)-D-galactose, 9CI G-11

[6118-87-2]



Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441

Isolated from the partial acid hydrolysate from the cambium polysaccharides of Bael (*Aegle marmelos*). $[\alpha]_D$ +58 (+50) (H_2O).

α-Pyranose-*form*

Allyl glycoside, 3,3′,3″,6,6′,6″-hexabenzyl, 2,2′,2″-tribenzoyl, 4″-Ac: [93495-79-5]
$C_{86}H_{86}O_{20}$ 1439.613
Mp 126-127°. $[\alpha]_D$ +70.5 ($CHCl_3$).

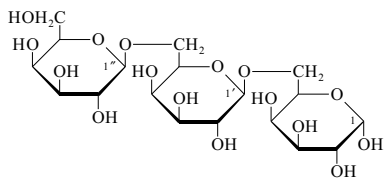
β-Pyranose-*form*

tert-*Butyldiphenylsilyl glycoside, 2,2′,2″,3,3′,3″,4″-heptabenzyl, 6,6′,6″-tri-Ac:* [129729-22-2]
$C_{89}H_{98}O_{19}Si$ 1499.827
Syrup + H_2O. $[\alpha]_D^{24}$ +22.5 (c, 0.5 in $CHCl_3$).

Bouveng, H.O. *et al., Acta Chem. Scand.*, 1959, **13**, 1884
Basak, R.K. *et al., Carbohydr. Res.*, 1982, **110**, 145
El Shenawy, H.A. *et al., Carbohydr. Res.*, 1984, **131**, 239 (*α-allyl pyr, pmr, cmr*)
Nakano, H. *et al., Agric. Biol. Chem.*, 1986, **50**, 3005 (*enzymic synth*)
Nakahara, Y. *et al., Carbohydr. Res.*, 1990, **200**, 363 (*β-silyl pyr, pmr, cmr*)

β-D-Galactopyranosyl-(1→6)-β-D-galactopyranosyl-(1→6)-D-galactose, 9CI G-12

[28245-12-7]



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441

Isolated from partial acid hydrolysates of *Opuntia ficus-indica* (Indian fig) gums. Needles (MeOH aq.). Mp 158-163° (137-142°, 152-155°). $[\alpha]_D^{18}$ +22 (c, 0.5 in H_2O) (+13).

β-Pyranose-*form*

Me glycoside: [77735-11-6]
$C_{19}H_{34}O_{16}$ 518.468
Cryst. (EtOH aq.). Mp 203-205°. $[\alpha]_D$ +38.1 (c, 1.0 in H_2O). $[\alpha]_D$ -10 (c, 0.8 in H_2O).

Me glycoside, decabenzoyl: [109022-60-8]
$C_{89}H_{74}O_{26}$ 1559.548
Mp 250-251°. $[\alpha]_D$ +115 ($CHCl_3$).

Me glycoside, 6″-bromoacetyl, nonabenzoyl: [101802-84-0]
$C_{84}H_{71}BrO_{26}$ 1576.373
Cryst. (CH_2Cl_2/MeOH). Mp 233-234°. $[\alpha]_D$ +162 (c, 0.8 in $CHCl_3$).

Me glycoside, 6″-chloroacetyl, nona-Ac: [100741-00-2]
$C_{39}H_{53}ClO_{26}$ 973.285
Foam. $[\alpha]_D$ -9 (c, 0.8 in $CHCl_3$).

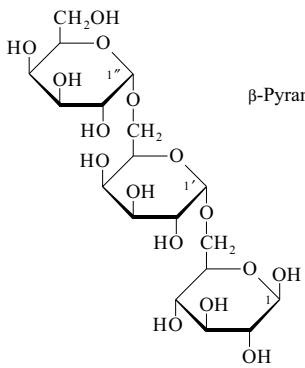
Allyl glycoside, deca-Ac: [110236-46-9]
$C_{41}H_{56}O_{26}$ 964.878
Syrup. $[\alpha]_D$ -18.2 (c, 0.9 in $CHCl_3$).

Allyl glycoside, 6″-bromoacetyl, nona-Ac: [110236-47-0]
$C_{41}H_{55}BrO_{26}$ 1043.774
Syrup. $[\alpha]_D$ -13.5 (c, 1.0 in $CHCl_3$).

Aspinall, G.O. *et al., J.C.S.*, 1958, 4408; 1961, 3461; 1965, 2685
Bailey, R.W. *et al., Oligosaccharides*, Pergamon Press, London, 1965, 50 (*occur*)
Aspinall, G.O. *et al., Carbohydr. Res.*, 1970, **12**, 143
Kubala, J. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 2809 (*isol*)
Srivastava, V.K. *et al., Carbohydr. Res.*, 1980, **86**, 203 (*Me gly, cmr*)
Asp, W.G. *et al., Food Chem.*, 1980, **5**, 147 (*synth*)
Bhattacharjee, A.K. *et al., Carbohydr. Res.*, 1981, **89**, 249 (*synth*)
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol*)
Kovac, P. *et al., Carbohydr. Res.*, 1985, **140**, 277; 1986, **153**, 237 (*Me gly, deriv, synth, pmr, cmr*)
Nashed, E.M. *et al., Carbohydr. Res.*, 1986, **158**, 125 (*allyl gly deriv, synth, pmr, cmr*)

α-D-Galactopyranosyl-(1→6)-α-D-galactopyranosyl-(1→6)-D-glucose G-13

[13382-86-0]
Manninotriose. Mnt



β-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441

Found free in cocoa beans, hazelnuts and in various plant mannans. Selectively utilised by bifidobacteria in the intestine but hardly utilised by other microorganisms. Increases faecal bifidobacteria and decreases Clostridia. $[\alpha]_D$ +167 (H_2O).

Phenylosazone:
Mp 122°.

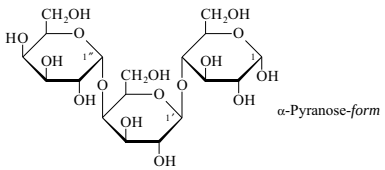
β-Pyranose-*form*

Undeca-Ac: [64544-38-3]
$C_{40}H_{54}O_{27}$ 966.85
Cryst. (EtOH). Mp 106-107.5°. $[\alpha]_D^{21}$ +132.7 (c, 0.98 in $CHCl_3$).

French, D. *et al., Adv. Carbohydr. Chem.*, 1954, **4**, 149 (*synth*)
Bailey, R.W. *et al., Biochem. J.*, 1963, **85**, 509 (*synth*)
Lombard, A. *et al., CA*, 1976, **85**, 59634t (*isol*)
Adachi, R. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 1901 (*β-Ac synth, pmr*)
Aamen, P. *et al., J. Sci. Food Agric.*, 1979, **30**, 869 (*isol*)
Wight, A.W. *et al., Food Chem.*, 1986, **21**, 167 (*hplc*)
Sugawara, S. *et al., Agric. Biol. Chem.*, 1990, **54**, 211 (*enzym synth, cmr*)
Wada, K. *et al., CA*, 1991, **115**, 204361w (*synth*)

α-D-Galactopyranosyl-(1→4)-β-D-galactopyranosyl-(1→4)-D-glucose, 9CI G-14

[66580-68-5]
Globotriose



α-Pyranose-*form*

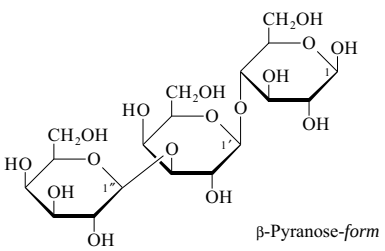
$C_{18}H_{32}O_{16}$ 504.441

Sweetener in bakery and confectionery. Amorph. $[\alpha]_D^{21}$ +101 (c, 0.5 in H_2O).

Jacquinet, J.C. *et al., Carbohydr. Res.*, 1985, **143**, 143 (*synth, pmr*)
Koike, K. *et al., Carbohydr. Res.*, 1987, **163**, 189 (*synth*)
Karlsson, H. *et al., HRC & CC, J. High Resolut. Chromatogr. Chromatogr. Commun.*, 1988, **11**, 820 (*glc, ms*)
Japan. Pat., 1989, 01 86 857; *CA*, **111**, 56168p (*use*)
Myers, R.L. *et al., Anal. Biochem.*, 1991, **192**, 156 (*hplc*)
Mueller, D. *et al., J.C.S. Perkin 1*, 1998, 2287-2294 (*synth, bibl*)

β-D-Galactopyranosyl-(1→3)-β-D-galactopyranosyl-(1→4)-D-glucose, 9CI G-15

[32694-82-9]
3′-Galactosyllactose



β-Pyranose-*form*

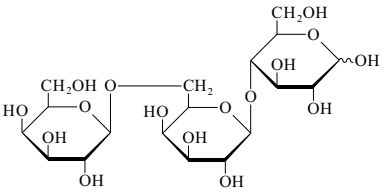
$C_{18}H_{32}O_{16}$ 504.441

Isol. from human milk. Solid (H_2O/EtOH/MeOH). Mp 200-202° dec. $[\alpha]_D^{23}$ +48 (c, 0.75 in H_2O) (+26.1).

Saito, T. *et al., Carbohydr. Res.*, 1987, **165**, 43 (*isol, cmr*)
Donald, A.S.R. *et al., Carbohydr. Res.*, 1988, **178**, 79 (*isol*)
Dumortier, V. *et al., Carbohydr. Res.*, 1990, **201**, 115 (*isol, enzymic synth, chromatog*)

β-D-Galactopyranosyl-(1→6)-β-D-galactopyranosyl-(1→4)-D-glucose G-16

[32581-31-0]
6′-Galactosyllactose



Pyranose-*form*

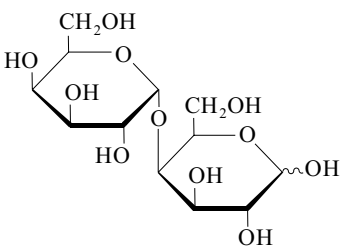
$C_{18}H_{32}O_{16}$ 504.441
Formed by the transferase action on lactose of the β-galactosidases from *Saccharomyces fragilis*, *Aspergillus flavus* and *Penicillium chrysogenum*. Isol. from human milk. Powder. Mp 187° (sinters at 167°). $[\alpha]_D^{22}$ +36 (c, 1.0 in H_2O).

Phenylosazone: [68067-46-9]
Yellow needles (EtOH aq.). Mp 229-231°.

Pazur, J.H. *et al., J. Biol. Chem.*, 1954, **208**, 439
Ballio, A. *et al., Tetrahedron*, 1960, **9**, 125 (*isol*)
Yamashita, K. *et al., Arch. Biochem. Biophys.*, 1974, **161**, 164 (*isol*)
Hallgren, P. *et al., J. Biol. Chem.*, 1977, **252**, 1014; 1034 (*isol*)
Chung, T.G. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2147 (*synth*)
Asp, N.G. *et al., Food Chem.*, 1980, **5**, 147 (*synth*)
Donald, A.S.R. *et al., Carbohydr. Res.*, 1988, **178**, 79 (*isol, struct*)
Urashima, T. *et al., Biochim. Biophys. Acta*, 1989, **992**, 375 (*cmr*)
Deya, E. *et al., CA*, 1991, **115**, 27841e (*enzymic synth*)

4-*O*-α-D-Galactopyranosyl-D-galactose, 9CI, 8CI G-17

[13117-26-5]
Galabiose. *Urobiose*



$C_{12}H_{22}O_{11}$ 342.299
Degradn. prod. of mucilage from common okra (*Hibiscus esculentus*). Cryst. (MeOH/1-butanol/H_2O). Mp 212-213°. $[\alpha]_D^{26}$ +170 (c, 1.0 in H_2O).

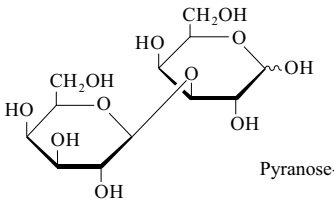
α-Pyranose-*form*

Octa-Ac:
$C_{28}H_{38}O_{19}$ 678.597
Cryst. (EtOH). Mp 153-154°. $[\alpha]_D^{24}$ +138 (c, 2.0 in $CHCl_3$).

Whistler, R.L. *et al., J.A.C.S.*, 1954, **76**, 1673 (*isol*)
Clancy, M.J. *et al., Arch. Biochem. Biophys.*, 1967, **118**, 724
Chacón-Fuertes, M.E. *et al., Carbohydr. Res.*, 1975, **43**, 51 (*synth*)
Dahmén, J. *et al., Carbohydr. Res.*, 1983, **113**, 219 (*synth*)
Svensson, G. *et al., Carbohydr. Res.*, 1986, **146**, 29 (*cryst struct*)
Frejd, T. *et al., Carbohydr. Res.*, 1988, **176**, 253; 271 (*pmr, cmr, conformn, derivs*)
Mueller, D. *et al., J.C.S. Perkin 1*, 1998, 2287-2294 (*synth*)

3-*O*-β-D-Galactopyranosyl-D-galactose, 9CI, 8CI G-18

[5188-48-7]



Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
Constit. of the hydrolysate of cashew nut shells. Mp 225° (198-200°, 159-170°). $[\alpha]_D^{18}$ +50 (c, 0.2 in H_2O). $[\alpha]_D^{26}$ +71 → +62 (c, 1.0 in H_2O).

β-Pyranose-*form*

Me glycoside:
$C_{13}H_{24}O_{11}$ 356.326
Mp 203-204°. $[\alpha]_D^{21}$ +25 (c, 0.9 in H_2O).

Me glycoside, hepta-Ac: [102854-37-5]
$C_{27}H_{38}O_{18}$ 650.586
Mp 189.5-190°. $[\alpha]_D$ -7.7 (c, 0.8 in $CHCl_3$).

Me glycoside, heptabenzoyl:
$C_{62}H_{52}O_{18}$ 1085.082
$[\alpha]_D$ +91 (c, 1.5 in $CHCl_3$).

2-Propenyl glycoside:
$C_{15}H_{26}O_{11}$ 382.364
Mp 213-215°. $[\alpha]_D^{21}$ +11 (c, 1.2 in H_2O).

Benzyl glycoside: [84553-71-9]
$C_{19}H_{28}O_{11}$ 432.424
Cryst. (MeOH). Mp 162-163°. $[\alpha]_D^{25}$ -4.2 (c, 1.8 in H_2O).

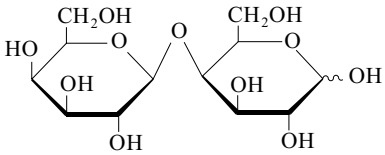
Benzyl glycoside, 4,6-O-benzylidene:
$C_{26}H_{32}O_{11}$ 520.532
Mp 263-264°. $[\alpha]_D^{25}$ +57 (c, 1.4 in DMF).

Benzyl glycoside, 4,6-O-benzylidene, penta-Ac:
$C_{36}H_{42}O_{16}$ 730.718
Cryst. (Et_2O/petrol). Mp 114-116°. $[\alpha]_D^{26}$ -13.4 (c, 1.5 in $CHCl_3$).

Hirst, E.L. *et al., J.C.S.*, 1954, 2622 (*isol*)
Rodén, L. *et al., J. Biol. Chem.*, 1966, **241**, 5949 (*isol*)
Aspinall, G.O. *et al., Carbohydr. Res.*, 1968, **7**, 421 (*isol*)
Sarkar, M. *et al., Indian J. Chem.*, 1974, **11**, 1129 (*isol*)
Chacón-Fuertes, M.E. *et al., Carbohydr. Res.*, 1975, **43**, 51 (*synth*)
Takeo, K. *et al., Carbohydr. Res.*, 1983, **112**, 158 (*benzyl gly*)
Nilsson, K.G.I. *et al., Carbohydr. Res.*, 1987, **167**, 95; 1988, **180**, 53 (*glycosides*)
Ziegler, T. *et al., J. Carbohydr. Chem.*, 1990, **9**, 135 (*Me gly*)

4-*O*-β-D-Galactopyranosyl-D-galactose, 9CI, 8CI G-19

[6206-28-6]



$C_{12}H_{22}O_{11}$ 342.299
Obt. by hydrol. of galactan from white lupin seeds (*Lupinus albus*) and of soya beans (*Glycine max*). Mp 204°. $[\alpha]_D^{20}$ +68 (c, 1.0 in H_2O).

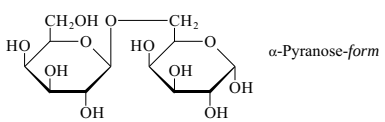
α-Pyranose-*form*

Octa-Ac:
$C_{28}H_{38}O_{19}$ 678.597
Mp 189-190°. $[\alpha]_D^{25}$ +54 (c, 1.8 in $CHCl_3$).

Curtis, E.J.C. *et al., Can. J. Chem.*, 1965, **43**, 2508 (*synth*)
Agrawal, G.D. *et al., Planta Med.*, 1972, **21**, 293; *CA*, **77**, 48734j (*isol*)
Chacon-Fuertes, M.E. *et al., Carbohydr. Res.*, 1975, **43**, 51 (*synth*)

6-*O*-β-D-Galactopyranosyl-D-galactose, 9CI, 8CI G-20

[5077-31-6]



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
Isol. from partial acid hydrolysates of the gums of *Spondias cytherea* (ambarella), *Opuntia ficus-indica* (Indian fig) and *Prunus persica*. $[\alpha]_D$ +39 (c, 0.53 in H_2O).

Phenylosazone:
Mp 180-182°.

α-Pyranose-*form*

1,2:3,4-Di-O-isopropylidene, tetra-Ac:
$C_{26}H_{38}O_{15}$ 590.577
Syrup. $[\alpha]_D$ -47 (c, 0.61 in $CHCl_3$).

β-Pyranose-*form*

Allyl glycoside:
$C_{15}H_{26}O_{11}$ 382.364
Cryst. + H_2O. Mp 134-135°. $[\alpha]_D^{21}$ -14.5 (c, 1.0 in H_2O).

Benzyl glycoside: Benzyl 6-O-β-D-galacto-pyranosyl-β-D-galactopyranoside
$C_{19}H_{28}O_{11}$ 432.424
$[\alpha]_D^{21}$ -27 (c, 0.7 in 50% MeOH aq.).

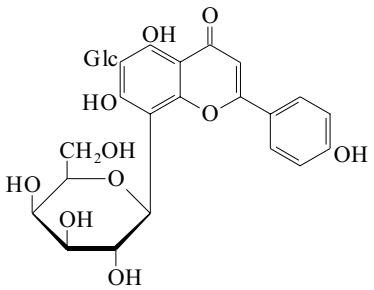
Pazur, J.H. *et al., J.A.C.S.*, 1958, **80**, 119 (*synth*)
Aspinall, G.O. *et al., J.C.S.*, 1961, 3461; 1958, 593 (*isol*)
Bailey, R.W. *et al., Oligosaccharides*, Pergamon, London, 1965, 50 (*occur*)
Kochetkov, N.K. *et al., Tetrahedron*, 1967, **23**, 693 (*α-deriv*)
Hellerqvist, C.G. *et al., Acta Chem. Scand.*, 1971, **25**, 743 (*pmr*)
Kamerling, J.P. *et al., Tetrahedron*, 1971, **27**, 4275 (*ms*)
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol*)
Lipkind, G.M. *et al., Carbohydr. Res.*, 1988, **175**, 59 (*cmr*)

Nilsson, K.G.I. *et al., Carbohydr. Res.*, 1988, **180**, 53 (*β-deriv*)

8-Galactopyranosyl-6-glucopyranosyl-4′,5,7-trihydroxyflavone G-21

[90898-93-4]

8-β-D-Galactopyranosyl-6-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 8-Galactopyranosyl-6-glucopyranosylapigenin. 8-Galactosyl-6-glucosylapigenin



$C_{27}H_{30}O_{15}$ 594.525

Yellow solid.

7-Me ether:8-Galactopyranosyl-6-glucopyranosyl-4′,5-dihydroxy-7-methoxyflavone. 8-Galactopyranosyl-6-glucopyranosylgenkwanin. 8-Galactosyl-6-glucosylgenkwanin

$C_{28}H_{32}O_{15}$ 608.552

Isol. from roots of *Glycine max* (soybean). Probable struct..

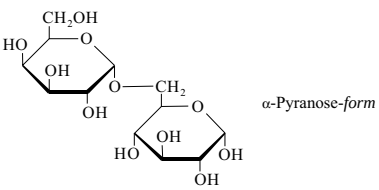
Dubois, M.A. *et al., Phytochemistry*, 1984, **23**, 706 (*isol*)

Jay, M. *et al., Phytochemistry*, 1984, **23**, 1153 (*deriv*)

6-*O*-α-D-Galactopyranosyl-D-glucose, 9CI G-22

[585-99-9]

Melibiose, 8CI



$C_{12}H_{22}O_{11}$ 342.299

Isol. from coffee beans, apple (*Pyrus malus*) and other plants. Sol. H_2O. Mp 85° dec. (dihydrate) Mp 179-181° (monohydrate). Approx. one-third as sweet as sucrose. Dihydrate reported to be β-anomer; monohydrate the α-anomer.

► LD_{50} (mus, ivn) 1000-3000 mg/kg.

Phenylosazone:

Mp 176-178°. $[\alpha]_D^{21}$ +43.2 (Py).

α-Pyranose-*form*

$[\alpha]_D^{20}$ +134 (c, 4 in H_2O).

[66009-10-7]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 309C (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 196C (*ir*)

Pictet, A. *et al., Helv. Chim. Acta*, 1926, **9**, 806 (*synth, dihydrate, β-pyr octa-Ac*)

Charlton, W. *et al., J.C.S.*, 1927, 1527 (*struct, β-Me pyr hepta-Me*)

Levene, P.A. *et al., J. Biol. Chem.*, 1930, **86**, 403 (*struct, β-pyr octa-Ac, β-Me pyr hepta-Ac, synth*)

Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 460 (*rev*)

Witonsky, P. *et al., J.O.C.*, 1959, **24**, 124 (*monohydrate, synth*)

Whistler, R.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 366 (*enzymic synth*)

Breitmaier, E. *et al., Chimia*, 1971, **25**, 362 (*cmr*)

de Bruyn, A. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 407 (*pmr*)

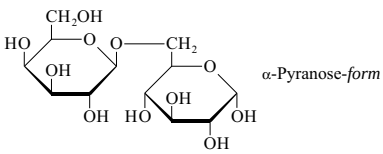
Kanters, J.A. *et al., Acta Cryst. B*, 1976, **32**, 2830 (*cryst struct*)

Bradbury, J.H. *et al., Carbohydr. Res.*, 1979, **71**, 15 (*pmr*)

6-*O*-β-D-Galactopyranosyl-D-glucose G-23

[28447-39-4]

Allolactose



$C_{12}H_{22}O_{11}$ 342.299

Reducing disaccharide. Isol. from human milk. Cryst. (EtOH). Mp 174-176° dec. $[\alpha]_D$ +30.7 (H_2O).

Phenylosazone:

Fine needles (H_2O). Mp 188-189° dec. $[\alpha]_D$ -51.6 (H_2O).

β-Pyranose-*form* [65207-30-9]

Octa-Ac: [41545-70-4]

$C_{28}H_{38}O_{19}$ 678.597

Mp 159-169°. $[\alpha]_D^{20}$ +1.8 (c, 1.9 in $CHCl_3$).

[645-03-4]

Polonowski, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1931, **192**, 1319 (*isol*)

Helferich, B. *et al., Ber.*, 1933, **66**, 806 (*synth*)

Zemplen, G. *et al., Acta Chim. Hung.*, 1951, **1**, 245; *CA*, **46**, 7053i

Kuhn, R. *et al., Chem. Ber.*, 1955, **88**, 1713 (*synth*)

Wallenfels, K. *et al., Adv. Carbohydr. Chem.*, 1961, **16**, 239 (*deriv*)

Pazur, J.H. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 303 (*enzymic synth*)

Ford, C.W. *et al., Aust. J. Chem.*, 1972, **25**, 889 (*isol*)

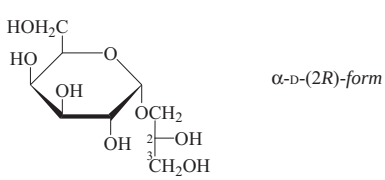
Suami, T. *et al., Carbohydr. Res.*, 1973, **26**, 234 (*synth*)

Kochetkov, N.K. *et al., Tet. Lett.*, 1977, **41**, 3681 (*deriv*)

1-*O*-Galactopyranosylglycerol G-24

[7420-23-7]

2,3-Dihydroxypropyl galactopyranoside, 9CI. Glyceryl galactopyranoside



$C_9H_{18}O_8$ 254.236

β-D-(2*R*)-*form* [16232-91-0]

Isol. from wheat flour lipids. Cryst. (MeOH). Mp 140.5-141.5°. $[\alpha]_D^{15}$ -9 (c, 0.6 in H_2O).

[42869-31-8]

Carter, H.E. *et al., J.A.C.S.*, 1956, **78**, 3735-3738 (*β-D-2R-form, isol*)

Wickberg, B. *et al., Acta Chem. Scand.*, 1958, **12**, 1187-1201 (*β-D-2R-form, β-D-2S-form, synth, ir*)

Silhavy, T.J. *et al., J. Biol. Chem.*, 1973, **248**, 6571 (*synth*)

Gent, P.A. *et al., J.C.S. Perkin 1*, 1975, 364-370 (*synth*)

Impellizzeri, G. *et al., Phytochemistry*, 1975, **14**, 1549-1557 (*isol*)

Beier, R.C. *et al., Can. J. Chem.*, 1980, **58**, 2800-2804 (*cmr*)

Beier, R.C. *et al., Carbohydr. Res.*, 1981, **93**, 141-143 (*synth*)

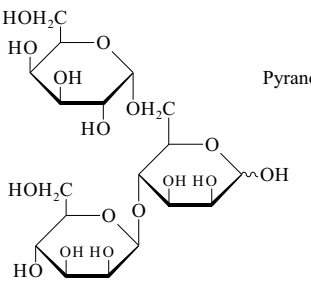
Boos, W. *et al., Methods Enzymol.*, 1982, **89D**, 59-64 (*synth*)

Michelsen, P. *et al., Chem. Scr.*, 1985, **25**, 217-218 (*ord, cd*)

Meng, J. *et al., Carbohydr. Res.*, 1987, **161**, 171-180 (*isol, pmr, cmr, abs config, bibl*)

α-D-Galactopyranosyl-(1 → 6)-[β-D-mannopyranosyl-(1 → 4)]-D-mannose, 9CI G-25

[61237-54-5]



$C_{18}H_{32}O_{16}$ 504.441

Isol. from partial acid hydrolysates of sickle senna *Cassia tora* and Lucerne (*Medicago sativa*) from enzymatic hydrolysates of guar (*Cyamopsis tetragonoloba*), carob (*Ceratonia siliqua*) galactomannans. Cryst. + 1½H_2O (MeOH). Mp 182-184°. $[\alpha]_D$ +119 (c, 1.2 in H_2O).

[82220-78-8]

Varshney, S.C. *et al., J.C.S. Perkin 1*, 1976, 1621

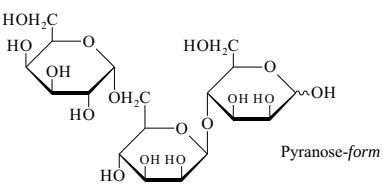
Shimizu, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 949

McCleary, B.V. *et al., Carbohydr. Res.*, 1983, **118**, 91; 1982, **104**, 285 (*occur, isol*)

α-D-Galactopyranosyl-(1 → 6)-β-D-mannopyranosyl-(1 → 4)-D-mannose G-26

[50728-36-4]

Galactosylmannobiose



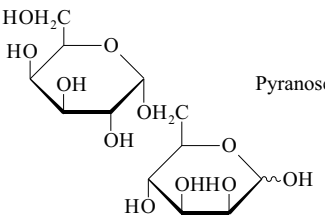
$C_{18}H_{32}O_{16}$ 504.441
Isol. from the partial acid hydrolysates of galactomannans from guar (*Cyamopsis tetragonoloba*). Cryst. + H_2O (EtOH). Mp 227-230°. $[\alpha]_D^{25}$ +93 (c, 1.0 in H_2O). $[\alpha]_D^{24}$ +31 (c, 0.4 in H_2O). $[\alpha]_D^{25}$ +93.3 → +98.4 (c, 1.2 in H_2O, 12 hr).

[58214-47-4]

Whistler, R.L. *et al., J.A.C.S.*, 1952, **74**, 5140 (*isol*)
Gupta, D.S. *et al., Indian J. Chem.*, 1975, **13**, 1152
Gupta, O.C.D. *et al., Carbohydr. Res.*, 1979, **73**, 145
McCleary, B.V. *et al., Carbohydr. Res.*, 1982, **104**, 285 (*isol*)
Singh, R.B. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1983, **57**, 1263 (*isol*)
Srivastava, C.H. *et al., CA*, 1988, **108**, 38236t (*isol*)

6-*O*-α-D-Galactopyranosyl-D-mannose, 9CI, 8CI G-27

[17296-19-4]
Epimelibiose



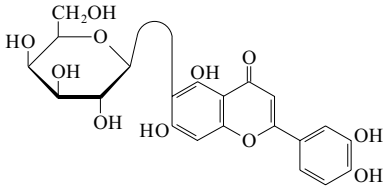
Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
Repeating unit in plant galactomannans. Isol. from partial acid hydrolysates of lucerne (*Medicago sativa*), fenugreek (*Trigonella foenum-graecum*), Palmyra palm nut (*Borassus flabellifer*), spruce-wood, seeds of *Anthyllis vulneraria*, *Sesbania aegyptiaca* and from the enzymic hydrolysate of guaran (*Cyamopsis tetragonoloba*). Cryst. (EtOH aq.). Mp 201-202°. $[\alpha]_D^{23}$ +120 (c, 1.0 in H_2O). $[\alpha]_D^{30}$ +124 (H_2O).

Whistler, R.L. *et al., J.A.C.S.*, 1951, **73**, 4189; 1952, **74**, 3795 (*isol*)
Jones, J.K.N. *et al., J.C.S.*, 1954, 295 (*synth*)
Courtois, J.E. *et al., Bull. Soc. Chim. Biol.*, 1957, **39**, 715 (*isol*)
Meier, H. *et al., Acta Chem. Scand.*, 1960, **14**, 749 (*isol*)
Mukherjee, A.K. *et al., Can. J. Chem.*, 1961, **39**, 1408 (*isol*)
Somme, R. *et al., Acta Chem. Scand.*, 1967, **21**, 685 (*isol*)
Helferich, B. *et al., Annalen*, 1974, 1514 (*synth*)
Voelter, W. *et al., Tet. Lett.*, 1974, 3597 (*synth*)
Bhattacharyya, S.B. *et al., Phytochemistry*, 1983, **22**, 161 (*isol*)

6-*C*-Galactopyranosyl-3′,4′,5,7-tetrahydroxyflavone G-28

[113349-18-1]
6-C-*Galactosylluteolin*

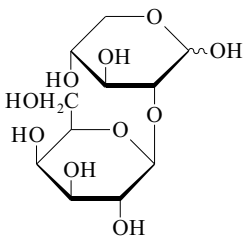


$C_{21}H_{20}O_{11}$ 448.382

6″-Deoxy: [132368-06-0] *6-C-(6-Deoxygalactopyranosyl)-3′,4′,5,7-tetrahydroxyflavone. 6*-C-*Fucopyranosylluteolin*
$C_{21}H_{20}O_{10}$ 432.383
Constit. of the juice of *Passiflora edulis* f. *flavicarpa* (yellow passion fruit).

Peterson, P.M. *et al., Biochem. Syst. Ecol.*, 1987, **15**, 647 (*isol*)
Herrara, Y. *et al., Biochem. Syst. Ecol.*, 1991, **19**, 665 (*isol*)

2-*O*-β-D-Galactopyranosyl-D-xylose G-29



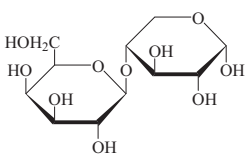
Pyranose-*form*

$C_{11}H_{20}O_{10}$ 312.273
Isol. from the partial acid hydrolysate of gum tragacanth. $[\alpha]_D$ +30 (H_2O).

Kooiman, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1961, **80**, 849
Aspinall, G.O. *et al., J.C.S.*, 1963, 1702 (*isol*)
Aragón, J.J. *et al., Carbohydr. Res.*, 1996, **290**, 209-216 (*synth, pmr, cmr*)

4-*O*-β-D-Galactopyranosyl-D-xylose, 9CI G-30

[14087-31-1]



α-Pyranose-*form*

$C_{11}H_{20}O_{10}$ 312.273
Isol. from partial acid hydrolysate of corn-hull hemicellulose and from bean cell wall. Constit. of the oligosaccharides from the linkage region of chondroitin 4-sulfate. Mp 201-211°. $[\alpha]_D^{22}$ +18 (c, 0.5 in H_2O) (+15).

α-Pyranose-*form*

Benzyl glycoside:Benzyl 4-O-*β-D-galactopyranosyl-α-D-xylopyranoside*
$C_{18}H_{26}O_{10}$ 402.397
Solid. $[\alpha]_D^{20}$ +63.7 (c, 1.0 in H_2O).

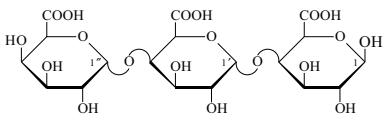
β-Pyranose-*form*

Benzyl glycoside: [67412-74-2] *Benzyl 4*-O-*β-D-galactopyranosyl-β-D-xylopyranoside*
$C_{18}H_{26}O_{10}$ 402.397
Mp 40-42°. $[\alpha]_D^{22}$ -38 (c, 0.5 in H_2O).

Montgomery, R. *et al., J.A.C.S.*, 1957, **79**, 698 (*isol*)
Aspinall, G.O. *et al., Adv. Carbohydr. Chem.*, 1959, **14**, 429
Lindberg, B. *et al., Carbohydr. Res.*, 1966, **2**, 413
Erbing, B. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 308
Gunnarsson, A. *et al., Carbohydr. Res.*, 1984, **133**, 75
Aragón, J.J. *et al., Carbohydr. Res.*, 1996, **290**, 209-216 (*synth, pmr, cmr*)
Fessner, W.D. *et al., Can. J. Chem.*, 2002, **80**, 739-742 (*synth*)

α-D-Galactopyranuronosyl-(1→4)-α-D-galactopyranuronosyl-(1→4)-D-galacturonic acid, 9CI, 8CI G-31

[6037-45-2]



β-Pyranose-*form*

$C_{18}H_{26}O_{19}$ 546.392
Isol. from enzymic hydrolysates (yeast or mould pectinases) of pectic acid. Also from partial acid hydrol. of *Medicago sativa* (lucerne) pectin. Mp 139-145° dec. $[\alpha]_D^{27}$ +185 (c, 0.12 in H_2O).

Pyranose-*form*

Ca salt:
Cryst. + 1 or 7H_2O. Mp 145-155° (monohydrate). $[\alpha]_D$ +154 (H_2O) (heptahydrate). Turns deep pink on melting.

β-Pyranose-*form*

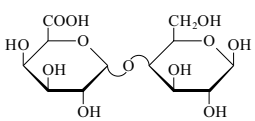
tert-*Butyldiphenylsilyl glycoside, 2,2′,2″,3,3′,3″,4″-heptabenzyl:* [129729-25-5]
Syrup + H_2O. $[\alpha]_D^{20}$ +93 (c, 0.3 in H_2O).

tert-*Butyldiphenylsilyl glycoside, 2,2′,2″,3,3′,3″,4″-heptabenzyl, tri-Me ester:* [129729-26-6]
Syrup + H_2O. $[\alpha]_D^{25}$ +66 (c, 0.8 in $CHCl_3$).

Phaff, H.J. *et al., Arch. Biochem. Biophys.*, 1954, **51**, 114; 1952, **36**, 231
McCready, R.M. *et al., J.A.C.S.*, 1954, **76**, 3035
Aspinall, G.O. *et al., J.C.S.*, 1961, 4215 (*isol*)
Jones, J.K.N. *et al., J.C.S.*, 1964, 1361
Banerji, N. *et al., Cellul. Chem. Technol.*, 1968, **2**, 655; *CA*, **71**, 82805h (*isol*)
Nakahara, Y. *et al., Carbohydr. Res.*, 1990, **200**, 1363 (*deriv, synth, pmr, cmr*)

4-*O*-α-D-Galactopyranuronosyl-D-galactose, 9CI G-32

[5887-86-5]



β-Pyranose-*form*

$C_{12}H_{20}O_{12}$ 356.283
Constit. of *Sterculia urens* (karaya gum).

β-Pyranose-*form*

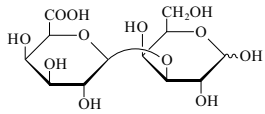
Me glycoside, 6′-Me ester, hexa-Ac:
Cryst. (EtOH). Mp 228.7-229.4°. $[\alpha]_D^{22.5}$ +95.9 (c, 0.73 in $CHCl_3$).

Bajpai, K.S. *et al., Indian J. Chem.*, 1970, **8**, 48

(*isol*)
Fujiwara, T. *et al., Carbohydr. Res.*, 1982, **101**, 305

3-*O*-β-D-Galactopyranuronosyl-D-galactose, 9CI G-33

[7268-75-9]

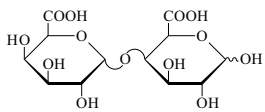


$C_{12}H_{20}O_{12}$ 356.283
Isol. from *Spondias dulcis* (ambarella) gum. $[\alpha]_D$ +56.2 (H_2O).

Parikh, V.M. *et al., Can. J. Chem.*, 1966, **44**, 327
Sarkar, M. *et al., Indian J. Chem.*, 1974, **11**, 1129 (*isol*)
Roy, A. *et al., Carbohydr. Res.*, 1975, **41**, 219
Basu, S. *et al., Carbohydr. Res.*, 1981, **94**, 215 (*isol*)

4-*O*-α-D-Galactopyranuronosyl-D-galacturonic acid G-34

[5894-59-7]



$C_{12}H_{18}O_{13}$ 370.266
Prepd. from pectin by enzymic hydrol. using yeast or mould pectinases or by acid hydrol.. Sole or major repeating unit of the pectin class of polysaccharides.

Ca salt:
Cryst. + $5H_2O$. Mp 130° (part. melt). $[\alpha]_D$ +119 (H_2O). Becomes dark pink at 130-140°.

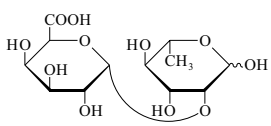
Pyranose-*form*

Me glycoside, 6,6′-di-Me ester:
$C_{15}H_{24}O_{13}$ 412.347
Mp 120-122°. $[\alpha]_D$ +162 (H_2O).

Phaff, H.J. *et al., Arch. Biochem. Biophys.*, 1952, **36**, 231; 1954, **51**, 102
Derungs, R. *et al., Helv. Chim. Acta*, 1954, **37**, 657 (*isol*)
Gee, M. *et al., J.O.C.*, 1958, **23**, 620 (*Me gly*)
Aspinall, G.O. *et al., J.C.S.*, 1961, 4215 (*isol*)
Jones, J.K.N. *et al., J.C.S.*, 1964, 1361

2-*O*-α-D-Galactopyranuronosyl-L-rhamnose G-35

[6118-79-2]
*Aldobiouronic acid B. 6-Deoxy-2-*O*-α-D-galactopyranuronosyl-L-mannose, 9CI*



$C_{12}H_{20}O_{11}$ 340.283
Reducing disaccharide. Isol. from partial acid hydrolysates of *Linum usitatissimum* (flax), *Plantago* seed, *Hibiscus esculentus* (okra). Amorph. $[\alpha]_D^{28}$ +50.8 (H_2O). $[\alpha]_D^{20}$ +96.1 (c, 0.4 in H_2O). $[\alpha]_D^{20}$ +105.5 (c, 1.06 in H_2O).

Ca salt:
$[\alpha]_D$ +92 (H_2O).

Ba salt: [69842-92-8]
Powder. $[\alpha]_D^{20}$ +75.3 (c, 0.24 in H_2O).

Pyranose-*form* [16749-72-7]

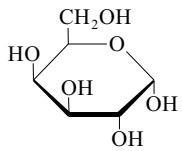
Me glycoside, penta-Me, Me ester:
$C_{19}H_{34}O_{11}$ 438.471
Mp 93-94°. $[\alpha]_D$ +129 ($CHCl_3$).

[65942-34-9]

Bailey, R.W. *et al., Oligosaccharides*, Pergamon Press, 1965, 132 (*occur*)
Bajpai, K.S. *et al., Indian J. Chem.*, 1969, **7**, 780 (*Me deriv*)
Sarkar, M. *et al., Indian J. Chem.*, 1973, **11**, 1129 (*isol*)
Tomoda, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2910; 1979, **27**, 1651 (*isol*)
Tomoda, M. *et al., Carbohydr. Res.*, 1986, **151**, 29; 1989, **190**, 323
Shigeru, E. *et al., Carbohydr. Res.*, 1986, **158**, 205

Galactose, 9CI, 8CI, USAN G-36

[26566-61-0]
Cerebrose



$C_6H_{12}O_6$ 180.157
An aq. soln. at 31° contains 30% α-pyr, 64% β-pyr, 2.5% α-fur, 3.5% β-fur and 0.02% aldehyde.

D-*form* [59-23-4]
The free sugar has been detected in some fruits. Polysaccharides agar, gum arabic, mesquite gum, western larch gum and many plant mucilages and gums contain galactose. Mp 118-120° (monohydrate). pK_{a1} 12.35 (25°). Sweet taste, sweetness = 0.33 × sucrose.
► Exp. reprod. and teratogenic effects (large doses). LW5490000

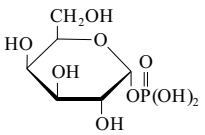
L-*form* [15572-79-9]
Occurs in agar-agar. Mp 163-165°. $[\alpha]_D^{22}$ -78 (H_2O).

[4198-47-4, 41846-88-2, 41846-89-3, 42789-83-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 192A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 298B; 298C (*nmr*)
Wolfrom, M.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 120 (*synth, D-form*)
Methods Carbohydr. Chem., 1962, **1**, 120; 122; 127 (*D-form, L-form*)
Araki, C. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 122 (*synth, L-form*)
Frush, H.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 127 (*synth, L-form*)
Stothers, J.B. *et al., Carbon-13 NMR Spectroscopy*, Academic Press, 1972,
Schaffer, R. *et al., The Carbohydrates*, 1972, **1A**, 69 (*occur*)
Dmietriev, B.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1975, 142
Ko, S.Y. *et al., Science (Washington, D.C.)*, 1983, **220**, 949 (*total synth, L-form*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib comp*)
Sturgeon, R.J. *et al., Carbohydr. Res.*, 1990, **200**, 499 (*occur, enantiomers*)
Vogt, D.C. *et al., Carbohydr. Res.*, 1990, **206**, 333 (*pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 774
Binch, H. *et al., Carbohydr. Res.*, 1998, **306**, 409-419 (*synth, L-form*)
Kroger, K. *et al., Eur. J. Ultrasound*, 1998, **8**, 17-24 (*use*)
Takeuchi, M. *et al., Synthesis*, 1999, 341-354 (*L-form, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GAV000

Galactose 1-dihydrogen phosphate, 8CI G-37

Galactose-1-phosphate



$C_6H_{13}O_9P$ 260.137
pK_{a1} 1; pK_{a2} 6.17.

α-D-Pyranose-*form* [2255-14-3]
Occurs in liver, milk, and yeasts. $[\alpha]_D^{25}$ +143 (H_2O). Yeast or bacterial preparations reversibly convert α-Galactose 1-phosphate into Glucose 6-phosphate *via* α-Glucose 1-phosphate.

Ba salt:
$[\alpha]_D$ +92 (H_2O).

Di-K salt: [19046-60-7]
$[\alpha]_D^{22}$ +100 (c, 1.57 in H_2O).

Dicyclohexylammonium salt:
Mp 147-153°. $[\alpha]_D^{26}$ +78.5 (H_2O).

β-D-Pyranose-*form* [2520-52-7]

Ba salt:
$[\alpha]_D$ +31.2 (H_2O).

Dicyclohexylammonium salt:
Mp 145-151°. $[\alpha]_D^{26}$ +21 (H_2O).

Biochem. Prep., 1955, **4**, 1 (*synth*)
Putman, E.W. *et al., J.A.C.S.*, 1957, **79**, 5057
MacDonald, D.L. *et al., The Carbohydrates*, 2nd Ed., Academic Press, 1972, **1A**, 253 (*rev*)
Lee, C. *et al., Biochemistry*, 1976, **15**, 697 (*conformn, pmr*)

β-Galactosidase G-38

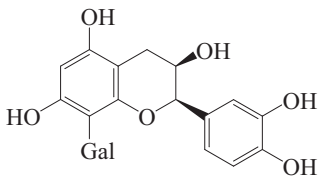
[9031-11-2]
Tilactase, INN. *Galactosidase, JAN. Galantase. Imulact. Lactase. Lactozyma. Lysolac. E.C. 3.2.1.23*

Enzyme; tetrameric with 4 identical subgroups; hydrolyses terminal, non-reducing β-D-galactose residues in β-D-galactosides. Enzyme used in the manuf. of candy and ice cream and for lactose reduction and flavour modification in dairy applications.
► LD_{50} (rat, ipr) 660 mg/kg. LW5840000

Wallenfels, K. *et al., Enzymes (3rd edn.)*, 1972, **7**, 617 (*rev*)
Shukla, T.P. *et al., CRC Crit. Rev. Food Technol.*, 1975, **5**, 325 (*rev*)
Wetlaufer, D.B. *et al., Adv. Protein Chem.*, 1981, **34**, 61 (*rev*)
Gey, M. *et al., Acta Biotechnol.*, 1989, **9**, 69 (*hplc*)
Rouwenhorst, R.J. *et al., Trends Biochem. Sci.*, 1989, **14**, 416 (*rev*)
Lin, M.-Y. *et al., Dig. Dis. Sci.*, 1993, **38**, 2022 (*use*)

Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1760
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 473-474
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GAV100

8-Galactosyl-3,3′,4′,5,7-pentahydroxyflavan G-39



$C_{21}H_{24}O_{11}$ 452.414

(2*R*,3*R*)-*form*

(-)-Epicatechin 8-C-galactoside. 8-Galactopyranosyl-(-)-epicatechin

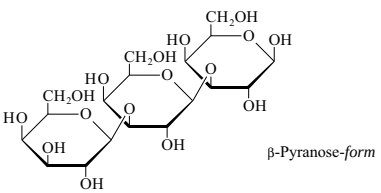
Constit. of cacao liquor (*Theobroma cacao*). Light brown amorph. powder. $[\alpha]_D$ -25.8 (c, 0.9 in MeOH). λ_{max} 280 (log ϵ 3.32) (MeOH).

Hatano, T. *et al., Phytochemistry*, 2002, **59**, 749-758 (*isol, cd, pmr, cmr*)

Galactotriose G-40

[5077-30-5]

O-*β*-D-*Galactopyranosyl-(1→3)*-O-*β*-D-*galactopyranosyl-(1→3)*-D-*galactose, 9CI*



β-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441

Constit. of the hydrolysate of a cashew-nut shell polysaccharide. Mp 240-245° (216°). $[\alpha]_D$ +58 (+51) (H_2O).

α-Pyranose-*form*

Allyl glycoside, 2,4,4′,4″,6,6′,6″-heptabenzyl, 2′,2″,3″-tribenzoyl: [106238-79-3]
$C_{91}H_{90}O_{19}$ 1487.701
Syrup. $[\alpha]_{436}$ +1.7 ($CHCl_3$).

Allyl glycoside, 2,2′,4,4′,4″,6,6′,6″-octabenzyl, 2″,3″-dibenzoyl: [106375-17-1]
$C_{91}H_{92}O_{18}$ 1473.717
Syrup. $[\alpha]_D$ +26 ($CHCl_3$).

β-Pyranose-*form*

Undecabenzoyl: [130651-32-0]
$C_{95}H_{76}O_{27}$ 1649.629
Syrup. $[\alpha]_D$ +68.8 (c, 0.5 in $CHCl_3$).

Me glycoside: [99606-03-8]
$C_{19}H_{34}O_{16}$ 518.468
Cryst. Mp 233-235°. $[\alpha]_D$ +31.4 (H_2O).

Me glycoside, 3″-benzyl, nonabenzoyl: [99605-99-9]
$C_{89}H_{76}O_{25}$ 1545.564
Syrup. $[\alpha]_D$ +58.3 ($CHCl_3$).

[71595-31-8]

Aspinall, G.O. *et al., J.C.S.*, 1958, 593
Bouveng, H.O. *et al., Acta Chem. Scand.*, 1959, **13**, 1884
Haq, S. *et al., Can. J. Chem.*, 1961, **39**, 1563
Bose, S. *et al., J. Indian Chem. Soc.*, 1972, **49**, 593
Honda, M.K. *et al., CA*, 1979, **91**, 153145e
Kovac, P. *et al., J.O.C.*, 1985, **50**, 5323 (*β-Me gly, synth, pmr, cmr*)
Chowdhary, M.S. *et al., Carbohydr. Res.*, 1986, **150**, 173 (*α-allyl gly, synth, pmr, cmr*)
Ziegler, T. *et al., J. Carbohydr. Chem.*, 1990, **9**, 135 (*undecabenzoyl synth, pmr, cmr*)
Soni, P.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 843 (*isol*)

Galacturonan, 8CI G-41

[9046-38-2]

Homogalacturonan

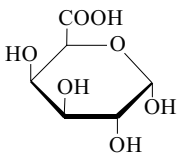
[→4)-α-D-GalA*p*-(1→4)-α-D-GalA*p*-(1→4)-α-D-GalA*p*-(1→]

A polysaccharide contg. linear chains of (1→4)-linked α-D-galacturonic acid residues. Occurs in pear juice (*Pyrus communis*), partly esterified.

Aspinall, G.O. *et al., The Carbohydrates*, 2nd edn. (Eds. Pigman W. *et al*), Academic Press, 1970, **2B**, 515 (*rev*)
Ovodov, Y.S. *et al., Khim. Prir. Soedin.*, 1975, **11**, 300; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 319 (*rev*)
Dick, A.J. *et al., Plant Physiol.*, 1989, **89**, 1394 (*occur*)

Galacturonic acid, 9CI, 8CI G-42

[14982-50-4]



α-D-Pyranose-*form*

$C_6H_{10}O_7$ 194.141

D-*form* [685-73-4]

Obt. from the hydrol. prods. of polymers of pectic substances. Monohydrate. Mp 156-159° dec. (sinters at 110°). $[\alpha]_D^{20}$ +98 → +50.9 (H_2O). Exists mostly in α-pyranose-form.

β-D-Pyranose-*form* [18968-14-4]

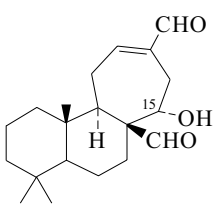
Mp 160° dec. $[\alpha]_D^{20}$ +27 → +55.6 (H_2O).

[17120-55-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 525C (*ir*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate*, 4th edn., J.A. Barth, Leipzig, 1935, 357 (*rev*)
Rees, D.A. *et al., J.C.S.(B)*, 1971, 1366 (*conformn, pmr*)
Merck Index, 12th edn., 1996, 735
Tang, H.R. *et al., Carbohydr. Res.*, 2001, **330**, 391-399 (*cmr, cryst struct*)

Galanal A G-43

[104086-74-0]



$C_{20}H_{30}O_3$ 318.455

Constit. of seeds of *Alpinia galanga* (greater galangal). Needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 167-169°. $[\alpha]_D$ -44 (c, 0.1 in $CHCl_3$). λ_{max} 232 (ϵ 7600) (EtOH) (Berdy).

15-Epimer: [104113-52-2] ***Galanal B***

$C_{20}H_{30}O_3$ 318.455

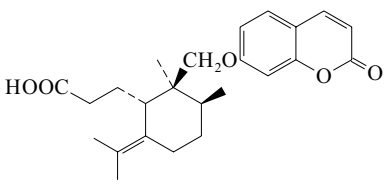
Constit. of seeds of *Alpinia galanga* (greater galangal). Needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 134-134.5°. $[\alpha]_D$ -48 (c, 0.1 in $CHCl_3$). λ_{max} 236 (ϵ 8000) (EtOH) (Berdy).

Morita, H. *et al., Planta Med.*, 1988, **54**, 117-120 (*isol, pmr, cmr*)
Abe, M. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2698-2700 (*isol, pmr, cmr, ms*)

Galbanic acid G-44

[3566-55-0]

*2,3-Dimethyl-6-(dimethylethylidene)-2-[[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-methyl]cyclohexanepropanoic acid. Asacoumarin B*



$C_{24}H_{30}O_5$ 398.498

Constit. of *Ferula gummosa* (galbanum) and other *Ferula* spp.. Cryst. Sol. MeOH, Et_2O; fairly sol. C_6H_6; poorly sol. hexane, H_2O. Mp 92-93°. $[\alpha]_D^{20}$ -35.2 (MeOH). Log P 5.98 (calc). Struct. of Asacoumarin B revised (1994).

▶ LD_{50} (mus, ipr) 227 mg/kg ; LD_{50} (mus, ipr) 2000 mg/kg. GW2580000

Me ester: ***Methyl galbanate***

$C_{25}H_{32}O_5$ 412.525

Oil. Bp 252°. $[\alpha]_D^{18}$ -25.8 (c, 1.16 in MeOH).

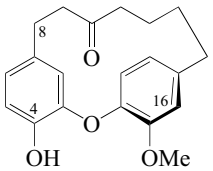
[122617-03-2]

Borisov, V.N. *et al., Khim. Prir. Soedin.*, 1973, **9**, 429; 1974, **10**, 516; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 400; 1974, **10**, 522 (*isol*)
Bagirov, V.Yu. *et al., Khim. Prir. Soedin.*, 1980, **16**, 620; *Chem. Nat. Compd. (Engl. Transl.)*, 1980, **16**, 438 (*struct*)
Martirosov, M.S. *et al., CA*, 1986, **104**, 122805 (*pharmacol*)
Mansurov, M.M. *et al., Farmakol. Toksikol. (Moscow)*, 1988, **51**, 47; 1990, **53(1)**, 51 (*pharmacol*)
Syrov, V.N. *et al., Farmakol. Toksikol. (Moscow)*, 1990, **53(2)**, 41 (*activity*)
Appendino, G. *et al., Phytochemistry*, 1994, **35**, 183 (*Asacoumarin B*)

Galeon G-45

[61576-08-7]

4-Hydroxy-17-methoxy-2-oxatricyclo[13.2.2.1^{3,7}]eicosa-3,5,7(20),15,17,18-hexaen-10-one, 9CI



(+)-*form*

$C_{20}H_{22}O_4$ 326.391

CAS numbering shown.

(+)-*form* [191999-64-1]

Constit. of *Myrica gale* (bog myrtle). Plates (hexane/EtOAc). Mp 178-180°. $[\alpha]_D$ +24.9 (c, 1.4 in $CHCl_3$).

9-(β-D-Glucopyranosyloxy): [207564-47-4]
$C_{26}H_{32}O_{10}$ 504.533
Powder. Mp 65-70°. $[\alpha]_D$ +6.5 (c, 0.6 in MeOH). λ_{max} 205 (log ε 4.49); 281 (log ε 3.53) (MeOH).

(-)-*form*

Constit. of *Myrica gale* (bog myrtle). Mp 178-181°. $[\alpha]_D^{20}$ -16 (c, 2.03 in $CHCl_3$).

*10*R-*Alcohol, 4-Me ether:* [206202-74-6] ***Platycarynol***
$C_{21}H_{26}O_4$ 342.434
Needles (hexane/EtOAc). Mp 137-138°. $[\alpha]_D^{20}$ -17.1 (c, 0.7 in $CHCl_3$).

16-Hydroxy: [191999-66-3] *Myricatomentogenin*
$C_{20}H_{22}O_5$ 342.391
Powder. $[\alpha]_D$ -50 (c, 0.1 in $CHCl_3$).

*16-Hydroxy, 10*R-*alcohol, 4-Me ether:* ***16-Hydroxyplatycarynol***
$C_{21}H_{26}O_5$ 358.433
Amorph. powder. $[\alpha]_D^{15}$ -58.5 (c, 0.3 in $CHCl_3$).

16-β-D-Glucopyranosyloxy: [191999-61-8] ***Myricatomentoside I***
$C_{26}H_{32}O_{10}$ 504.533
Constit. of *Myrica gale* var. *tomentosa*. Powder. $[\alpha]_D$ +8.6 (c, 0.5 in MeOH). λ_{max} 281 (log ε 3.58) (MeOH).

(ξ)-*form*

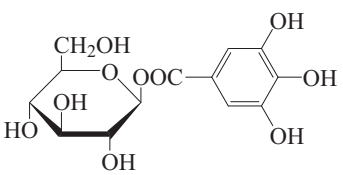
8ξ-Hydroxy: [61576-09-8] ***Hydroxygaleon***
$C_{20}H_{22}O_5$ 342.391
Constit. of *Myrica gale* (bog myrtle). Mp 183-184°.

Malterud, K.E. *et al., Tet. Lett.*, 1976, 3069 (*isol, ir, uv, pmr, ms, cryst struct*)
Morihara, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 820-823 (*abs config, derivs*)
Kim, S.-H. *et al., J. Nat. Prod.*, 1998, **61**, 643-645 (*isol, uv, pmr, cmr, ms*)
Tanaka, T. *et al., Phytochemistry*, 1998, **47**, 851-854 (*Platycarynol*)
Jiang, Z.-H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 737-740 (*16-Hydroxyplatycarynol*)

1-Galloylglucose G-46

[554-37-0]

3,4,5-Trihydroxybenzoyl glucoside. ***Glucogallin***



$C_{13}H_{16}O_{10}$ 332.263

β-D-Pyranose-*form* [13405-60-2]

1-O-Galloyl-β-D-glucopyranose. ***β-Glucogallin***

Isol. from various plants, e.g. *Rheum officinale* (Chinese rhubarb), *Eucalyptus* spp.. Needles (H_2O). Mp 205-206°. $[\alpha]_D^{18}$ -18.6 (c, 1 in H_2O).

6-O-(3,4,5-Trihydroxybenzoyl), 3′-O-[3,4,5-trihydroxybenzoyl-(→6)-β-D-glucopyranoside]: [146436-24-0] ***Cyclamenoside***
$C_{33}H_{34}O_{23}$ 798.618
Mp 144-145.5° (as tetradeca-Ac). $[\alpha]_D^{20}$ -58.3 (c, 0.87 in MeOH) (tetradeca-Ac).

6-O-(4-Hydroxy-3,5-dimethoxybenzoyl):1-O-Galloyl-6-O-syringoyl-β-D-glucopyranose
$C_{22}H_{24}O_{14}$ 512.423
Amorph. solid. $[\alpha]_D^{25}$ +4 (c, 0.18 in MeOH).

3′,5′-Di-Me ether: [112667-09-1] *1-O-Syringoyl-β-D-glucopyranose.* ***Erigeside C***
$C_{15}H_{20}O_{10}$ 360.317
Needles (MeOH/C_6H_6). Mp 122-126° Mp 159-161° Mp 199°. $[\alpha]_D$ -19.5 (c, 0.44 in Py). λ_{max} 218 (log ε 4.42); 281 (log ε 4.11) (no solvent reported).

Schmidt, O.T. *et al., Annalen*, 1961, **649**, 149-157 (*synth*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461-3470 (*isol, pmr*)
Klick, S. *et al., Phytochemistry*, 1988, **27**, 2177-2180 (*Erigeside C, synth, occur*)
Saijo, R. *et al., Phytochemistry*, 1990, **29**, 267-270 (*isol*)
Sakai, N. *et al., Chem. Lett.*, 1992, 2375-2378 (*Cyclamenoside*)
Yue, J. *et al., Phytochemistry*, 1994, **36**, 717-719 (*Erigeside C*)
Adnyana, I.K. *et al., Biol. Pharm. Bull.*, 2000, **23**, 1328-1332 (*1-Galloyl-6-syringoylglucose*)
Adnyana, I.K. *et al., Planta Med.*, 2001, **67**, 370-371 (*1-Galloyl-6-syringoylglucose*)

2-Galloylglucose G-47

[98917-85-2]

$C_{13}H_{16}O_{10}$ 332.263
Constit. of commercial rhubarb (*Rheum* spp.). Amorph. powder + $1\frac{1}{2}H_2O$. $[\alpha]_D^{25}$ +28.9 (c, 1.0 in H_2O).

Schmidt, O.T. *et al., Annalen*, 1961, **649**, 137 (*struct*)
Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1473 (*isol*)

4-Galloylglucose G-48

$C_{13}H_{16}O_{10}$ 332.263

β-D-Pyranose-*form* [84274-52-2]

4-Glucogallic acid
Isol. from commercial rhubarb (*Rheum* spp.). Grey prisms (Me_2CO) or needles + $\frac{1}{2}H_2O$. Sol. H_2O. Mp 233° (192-194°). $[\alpha]_D^{24}$ -13.7 (c, 1.31 in MeOH).

6-O-(3,4,5-Trihydroxybenzoyl): [87087-62-5] *Gallic acid 4-O-(6-galloylglucoside)*
$C_{20}H_{20}O_{14}$ 484.37
Isol. from commercial rhubarb (*Rheum* spp.). Prisms + $\frac{1}{2}H_2O$ (H_2O). Mp 192-194°. $[\alpha]_D^{20}$ -65.2 (c, 0.81 in Me_2CO).

*1-O-(3,4-Dihydroxy-*E*-cinnamoyl):* [306306-45-6] ***1-O-Caffeoyl-4-O-galloyl-β-D-glucopyranose***
$C_{22}H_{22}O_{13}$ 494.408

*3-O-(3,4-Dihydroxy-*E*-cinnamoyl):* ***3-O-Caffeoyl-4-O-galloyl-β-D-glucopyranose***
$C_{22}H_{22}O_{13}$ 494.408
Amorph. yellow powder. $[\alpha]_D^{15}$ -144.2 (c, 0.7 in MeOH).

Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1652; 1989, **37**, 2030 (*galloylglucosides*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 117 (*galloylglucosides*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3237 (*Glucogallic acid*)
Jiang, Z.-H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 887-892

6-Galloylglucose G-49

[34781-46-9]

β-D-Glucopyranose 6-(3,4,5-trihydroxybenzoate), 9CI

$C_{13}H_{16}O_{10}$ 332.263
Isol. from coml. rhubarb. Cryst. + $2H_2O$ (H_2O). Mp 166° (sinters from 110°). $[\alpha]_D$ +54.5 → +36.8 (12h) (c, 1.9 in H_2O). $[\alpha]_D^{22}$ +21.3 (c, 0.4 in H_2O).

β-D-Pyranose-*form*

Me glycoside: [88647-06-7] *Methyl 6-O-galloyl-β-D-glucopyranoside*
$C_{14}H_{18}O_{10}$ 346.29
Tannin constit. of burnet bloodwort (*Sanguisorba officinalis*). Pale yellow amorph. powder. $[\alpha]_D^{22}$ -18.6 (c, 1.3 in H_2O).

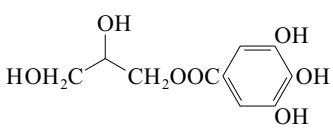
Me glycoside, O-*(3,4-dihydroxybenzoyl):* [88847-09-0] *Methyl 6-O-digalloyl-β-D-glucopyranoside*
$C_{21}H_{22}O_{14}$ 498.396
Isol. from the underground part of burnet bloodwort (*Sanguisorba officinalis*). Off-white amorph. powder + $\frac{1}{2}$ H_2O. $[\alpha]_D^{25}$ -16 (c, 0.72 in Me_2CO). Conts. an equilibrating galloylgalloyl residue.

[13186-19-1, 33040-89-0]

Schmidt, O.T. *et al., Annalen*, 1951, **571**, 29 (*synth*)
Gstirner, F. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1962, **295**, 23; 1966, **299**, 640 (*isol*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1652; 1989, **37**, 2030 (*pmr, cmr, deriv*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 117 (*struct, pmr, cmr*)
Saijo, R. *et al., Phytochemistry*, 1990, **29**, 267 (*pmr*)
Hsu, F.-L. *et al., J. Nat. Prod.*, 1994, **57**, 308 (*isol, props*)

1-*O*-Galloylglycerol G-50

[87087-60-3]

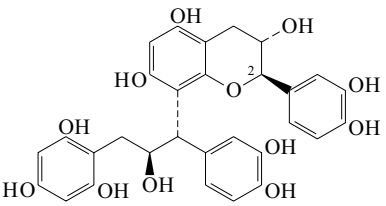


$C_{10}H_{12}O_7$ 244.201
Isol. from commercial rhubarb. Prisms (H_2O). Mp 188-190°. $[\alpha]_D^{20}$ +3.1 (c, 0.45 in MeOH).

Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1652 (*pmr, cmr*)
Saijo, R. *et al., Phytochemistry*, 1990, **29**, 267 (*pmr*)

Gambiriin A_1 G-51

[76250-49-2]



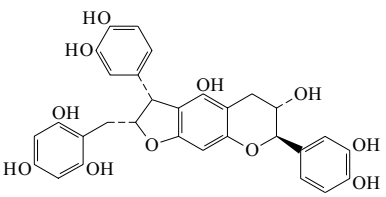
$C_{30}H_{28}O_{12}$ 580.544
Isol. from *Sanguisorba officinalis* (burnet bloodwort). Powder. $[\alpha]_D$ -14.2 (Me_2CO).

2-Epimer: [76250-48-1] ***Gambiriin A_2***
$C_{30}H_{28}O_{12}$ 580.544
Light-tan powder. $[\alpha]_D$ +66.8 (Me_2CO).

Nonaka, G. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3145 (*isol*)
Tanaka, T. *et al., Phytochemistry*, 1983, **22**, 2575 (*isol*)

Gambiriin B_3 G-52

[76236-90-3]

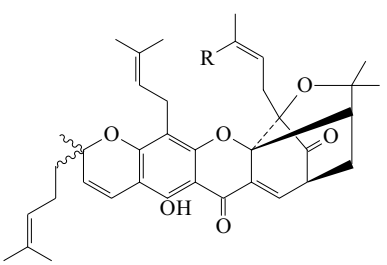


$C_{30}H_{26}O_{11}$ 562.529
Isol. from *Sanguisorba officinalis* (burnet bloodwort). Needles + $3H_2O$. Mp 271-274° dec. $[\alpha]_D$ -20 (MeOH).

Nonaka, G. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3145 (*isol*)
Tanaka, T. *et al., Phytochemistry*, 1983, **22**, 2575 (*isol*)

Gambogic acid G-53

[2752-65-0]
Guttic acid. Guttatic acid. β-Guttilactone. α-Gambogic acid. β-Guttiferin



R = COOH

$C_{38}H_{44}O_8$ 628.761
The name Guttic (Guttatic) acid is a transliteration of the French/Italian names for the substance. The English equiv. is stated to be Gambogic acid. Gamboge is also known as Gummi Gutta. Isol. from Gamboge resin (exudate of *Garcinia morella*). Cryst. or amorph. mass. Mp 86-91°. $[\alpha]_D^{24}$ -698 ($CHCl_3$). Closely related to Morellin, M-759.

▶ LD_{50} (rat, ipr) 88 mg/kg. PB9268200

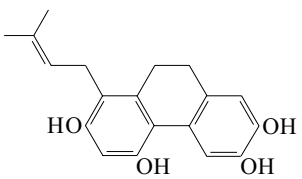
Py salt:
Golden yellow needles. Mp 138° Mp 150-151° (dimorph.). $[\alpha]_D$ -550 (c, 1.0 in $CHCl_3$).

(E)-Isomer: [149655-52-7] ***Isogambogic acid***
$C_{38}H_{44}O_8$ 628.761
$[\alpha]_D^{20}$ -408 (c, 0.1 in $CHCl_3$).

Amorosa, M. *et al., Ann. Chim. (Rome)*, 1966, **56**, 232
Ahmad, A.S. *et al., J.C.S.(C)*, 1966, 772 (*struct*)
Arnone, A. *et al., Tet. Lett.*, 1967, 4201 (*pmr, struct*)
Lin, L.-J. *et al., Magn. Reson. Chem.*, 1993, **31**, 340 (*Isogambogic acid*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBA125

Gancaonin V G-54

[134958-57-9]

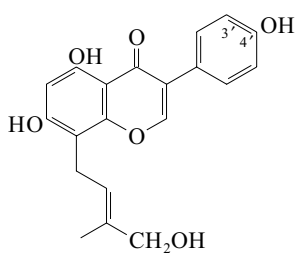


$C_{19}H_{20}O_4$ 312.365
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Cryst. (Me_2CO/hexane). Mp 170-173°.

Fukai, T. *et al., Phytochemistry*, 1991, **30**, 1245 (*isol, pmr, cmr*)

Gancaonin C G-55

[124596-87-8]
5,7-Dihydroxy-8-(4-hydroxy-3-methyl-2-butenyl)-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. 4′,5,7-Trihydroxy-8-(4-hydroxyprenyl)isoflavone



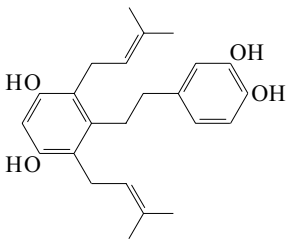
$C_{20}H_{18}O_6$ 354.359
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow prisms (C_6H_6/Me_2CO). Mp 213°.

3′-Hydroxy, 4′-Me ether: [124596-88-9] ***Gancaonin D****. 3′,5,7-Trihydroxy-4′-methoxy-8-(4-hydroxyprenyl)isoflavone*
$C_{21}H_{20}O_7$ 384.385
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow cryst. (C_6H_6/Me_2CO). Mp 234-236°.

Fukai, T. *et al., Heterocycles*, 1989, **29**, 1369; 1990, **31**, 373 (*isol, pmr, cmr*)

Gancaonin R G-56

[134958-53-5]
3,3′,4′,5-Tetrahydroxy-2,6-diprenylbibenzyl

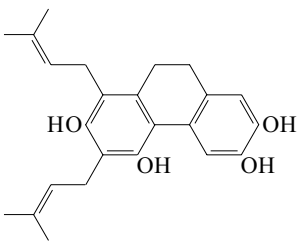


$C_{24}H_{30}O_4$ 382.499
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Cryst. (Me_2CO/hexane). Mp 142-144°.

Fukai, T. *et al., Phytochemistry*, 1991, **30**, 1245 (*isol, pmr, cmr*)

Gancaonin U G-57

[134958-56-8]

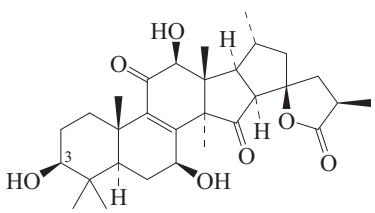


$C_{24}H_{28}O_4$ 380.483
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Cryst. (Et_2O/hexane). Mp 72-74°.

Fukai, T. *et al., Phytochemistry*, 1991, **30**, 1245 (*isol, pmr, cmr*)

Ganosporelactone B G-58

[138008-05-6]



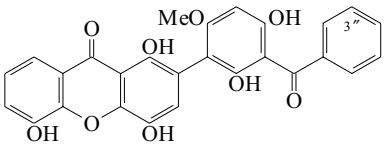
$C_{30}H_{42}O_7$ 514.658
Isol. from the spores of *Ganoderma lucidum* (reishi). Cryst. Mp 235-237°. $[\alpha]_D^{12}$ +68.8 (c, 0.08 in $CHCl_3$).

3-Ketone: [138008-04-5] ***Ganosporelactone A***
$C_{30}H_{40}O_7$ 512.642
Isol. from the spores of *Ganoderma lucidum* (reishi). Cryst. Mp 238-240°. $[\alpha]_D^{13}$ +74.5 (c, 0.06 in $CHCl_3$).

Chen, R. *et al., Yaoxue Xuebao*, 1991, **26**, 430-436

Garciduol A G-59

[176257-85-5]



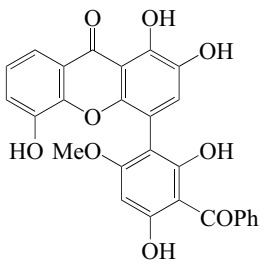
$C_{27}H_{18}O_9$ 486.434
Constit. of the roots of *Garcinia dulcis* (mundu). Yellow powder. λ_{max} 212 ; 230 (sh) ; 250 ; 265 (sh) ; 311 ; 400 (MeOH).

3″-Hydroxy: [176257-86-6] ***Garciduol B***
$C_{27}H_{18}O_{10}$ 502.433
Constit. of *Garcinia dulcis* (mundu). Yellow powder. λ_{max} 207 ; 250 ; 268 (sh) ; 314 ; 400 (sh) (MeOH).

Iinuma, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1744 (*isol, uv, pmr, cmr, ms*)

Garciduol C G-60

[182127-82-8]

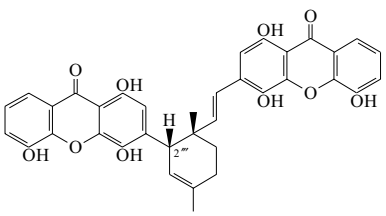


$C_{27}H_{18}O_9$ 486.434
Constit. of the root of *Garcinia dulcis* (mundu). Amorph. yellow solid. λ_{max} 212 ; 228 (sh) ; 250 ; 275 (sh) ; 312 ; 401 (MeOH).

Iinuma, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1744-1747 (*isol, uv, pmr, cmr, ms, ir*)

Garcilivin A G-61

[136364-57-3]

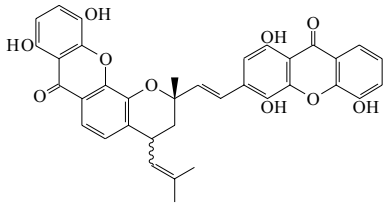


$C_{36}H_{28}O_{10}$ 620.611
Constit. of *Garcinia livingstonei* (imbe). Yellow needles (MeOH). Mp 143-144°.

2‴-Epimer: [145107-56-8] ***Garcilivin C***
$C_{36}H_{28}O_{10}$ 620.611
Constit. of *Garcinia livingstonei* (imbe). Yellow amorph. powder. Mp 162-163°.

Sordat-Diserens, I. *et al., Phytochemistry*, 1991, **31**, 3589 (*isol, pmr, cmr*)

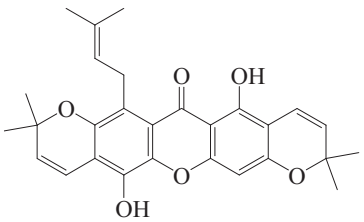
Garcilivin B G-62



$C_{36}H_{28}O_{10}$ 620.611
Constit. of *Garcinia livingstonei* (imbe). Yellow amorph. powder. Mp 195-197°.

Sordat-Diserens, I. *et al., Phytochemistry*, 1991, **31**, 3589 (*isol, pmr, cmr*)

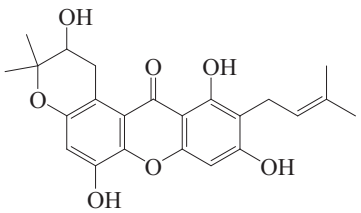
Garcimangosone A G-63



$C_{28}H_{28}O_6$ 460.526
Constit. of the dried fruit hulls of *Garcinia mangostana* (mangosteen). Yellow powder. Mp 143-145°. λ_{max} 285 (log ϵ 4.69); 342 (log ϵ 4.25) (MeOH).

Huang, Y.-L. *et al., J. Nat. Prod.*, 2001, **64**, 903-906

Garcimangosone C G-64

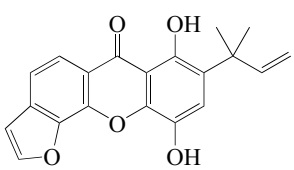


$C_{23}H_{24}O_7$ 412.438
Constit. of the dried fruit hulls of *Garcinia mangostana* (mangosteen). Yellow powder. Mp 260-262°. λ_{max} 242 (log ϵ 4.18); 261 (log ϵ 4.03); 442 (log ϵ 4.11) (MeOH).

Huang, Y.-L. *et al., J. Nat. Prod.*, 2001, **64**, 903-906

Garciniaxanthone G G-65

[175617-26-2]
Dulciol D

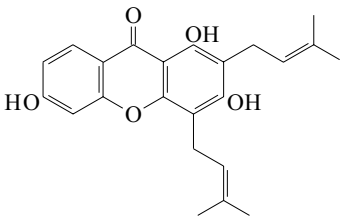


$C_{20}H_{16}O_5$ 336.343
Constit. of *Garcinia dulcis* (mundu). Yellow needles. Mp 194-196°. λ_{max} 232 (ϵ 13100); 245 (ϵ 11500); 267 (ϵ 7890); 288 (ϵ 14600); 404 (ϵ 2400) (EtOH).

Minami, H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2103 (*isol, uv, ir, pmr, cmr, ms*)
Iinuma, M. *et al., J. Nat. Prod.*, 1996, **59**, 472 (*isol, uv, ir, pmr, cmr, ms*)

Garcinone A G-66

[76996-29-7]

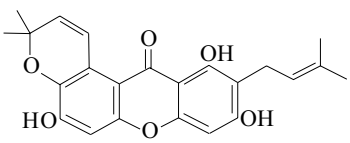


$C_{23}H_{24}O_5$ 380.44
The assigned struct. (illus.) has been synthesised and is incorrect. Constit. of *Garcinia mangostana* (mangosteen). Yellow cryst. ($CHCl_3$/MeOH). Mp 224-225°.

Sen, A.K. *et al., Phytochemistry*, 1982, **21**, 1747
Ahluwalia, V.K. *et al., Tetrahedron*, 1984, **40**, 3303

Garcinone B G-67

[76996-28-6]
5,9,11-Trihydroxy-3,3-dimethyl-10-(3-methyl-2-butenyl)pyrano[3,2-a]xanthen-12(3H)-one, 9CI

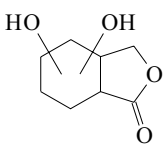


$C_{23}H_{22}O_6$ 394.423
Constit. of *Garcinia mangostana* (mangosteen). Dull-yellow solid (C_6H_6/MeOH). Mp 190-192°.

Sen, A.K. *et al., Phytochemistry*, 1982, **21**, 1747
Ishiguro, K. *et al., Phytochemistry*, 1995, **38**, 867 (*isol, pmr*)

Garlicin G-68

[126526-79-2]
Hexahydrodihydroxy-1(3H)-isobenzofuranone



$C_8H_{12}O_4$ 172.18
Exact struct. not known. Various analogues have been synthesised. Isol. from garlic (*Allium sativa*). Sol. $CHCl_3$; fairly sol. H_2O.

Nour, R.A. *et al., Annalen*, 1992, 383

Gassericins G-69

Peptides. Prod. by *Lactobacillus gasseri*. Bacteriocins with potential food uses.

Gassericin A [157480-86-9]

[221902-06-3]

Prod. by *Lactobacillus gasseri* La39.

Gassericin B1 [188596-37-4]
Prod. by *Lactobacillus gasseri* JCM 2124.

Gassericin B2 [188596-38-5]
Prod. by *Lactobacillus gasseri* JCM 2124.

Gassericin B3 [188596-39-6]
Prod. by *Lactobacillus gasseri* JCM 2124.

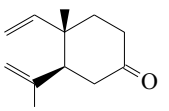
Gassericin B4 [188596-40-9]
Prod. by *Lactobacillus gasseri* JCM 2124.

Gassericin KT7 [289718-37-2]
Prod. by *Lactobacillus gasseri* KT7 isol. from infant faeces.

Kawai, Y. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1218-1221; 1998, **62**, 887-892; 2438-2440 (*Gassericin A, isol, struct*)
Tahara, T. *et al., FEMS Microbiol. Lett.*, 1997, **148**, 97-100 (*Gassericins B, isol*)

Geijerone G-70

[41411-01-2]
4-Ethenyl-4-methyl-3-(1-methylethenyl)cyclohexanone, 9CI. 3-Isopropenyl-4-methyl-4-vinylcyclohexanone



Absolute configuration

$C_{12}H_{18}O$ 178.274
Constit. of *Juniperus communis* (juniper). $Bp_{0.1}$ 81-86°. $[\alpha]_D^{20}$ -27.8 (CCl_4).

Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 564
Kato, M. *et al., J.C.S. Perkin 1*, 1979, 2740 (*synth*)
Kim, D. *et al., J.O.C.*, 1987, **52**, 4633 (*synth*)
Wakamatsu, T. *et al., Heterocycles*, 1987, **26**, 1203 (*synth*)

Gelatin, BAN, JAN, USAN G-71

[9000-70-8]
Gelfoam. Puragel. Emagel. Gelafusal. Gelatine bloom 250. Gelrite. Nikkol CCP4. Pharmagel A. Rousselot 3046. Spongiofort
Used in foods as stabiliser, surface-finishing agent and thickener. Derived from collagen. Sl. yellow sheets, flakes or coarse powder. Sol. hot H_2O, glycerol, AcOH; insol. org. solvs. Polymerised denatured gelatin also used as a plasma volume expander (Polygeline, BAN, INN).

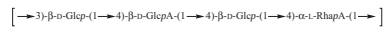
► LX8580000

[9015-56-9]

Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1948, **4**, 297
Veis, A. *et al., The Macromolecular Chemistry of Gelatin*, Academic Press, New York, 1964,
Labrude, P. *et al., J. Pharm. Belg.*, 1976, **31**, 191 (*Polygeline*)
Ward, A.G. *et al., The Science and Technology of Gelatin*, Academic Press, London, 1977,
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **12**, 406 (*rev*)
Poppe, J. *et al., Thickening and Gelling Agents for Food*, (Ed. Imeson, A.), Blackie, 1992, 98 (*use, rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 199-201
Videm, V. *et al., Scand. J. Immunol.*, 1994, **39**, 314 (*Polygeline*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 766
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1165-1169 (*props, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PCU360

Gellan gum G-72

[71010-52-1]
PS60. Gel-Gro. Gelrite. Kelcogel. Phytagel. E418

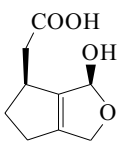


Polysaccharide. Struct. of backbone shown: also contains *ca.* 1Ac per repeating unit as well as some L-glycerate and poly(β-hydroxybutyrate) repeating units. Thickener and stabiliser for foods, chewing gum base. Samples contain variable amounts of cations, props. vary with degree of salt formn..

O'Neill, M.A. *et al., Carbohydr. Res.*, 1983, **124**, 123
Jansson, P.E. *et al., Carbohydr. Res.*, 1983, **124**, 135
Talashek, T.A. *et al., Carbohydr. Res.*, 1987, **160**, 303 (*props*)
Chandrasekaran, R. *et al., Carbohydr. Res.*, 1988, **175**, 1; **181**, 23 (*cryst struct*)
Doner, L.W. *et al., Carbohydr. Res.*, 1995, **273**, 225-233 (*purifn, props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1169-1170 (*props*)

Genipic acid, 9CI G-73

[6902-76-7]
2-Hydroxy-3-oxabicyclo[3.3.0]oct-1(5)-eneacetic acid



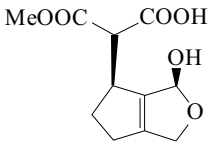
$C_9H_{12}O_4$ 184.191
Isol. from the jagua fruit *Genipa americana*. Amorph. hygroscopic powder. $[\alpha]_D^{27}$ -105 (c, 1 in EtOH).

NH_4 salt:
Cryst. Mp 125-130° dec.

Me ester:
Oil.

Tallent, W.H. *et al., Tetrahedron*, 1964, **20**, 1781 (*isol, ir, uv, nmr, struct*)
Whitesell, J.K. *et al., J.O.C.*, 1978, **43**, 1650 (*synth*)

Genipinic acid G-74

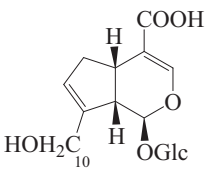


$C_{11}H_{14}O_6$ 242.228
Isol. from the jagua fruit *Genipa americana*. Amorph. powder. $[\alpha]_D^{27}$ -126 (c, 1 in EtOH). λ_{max} 203 (ε 3200) (EtOH) (Berdy). λ_{max} 274 (ε 15800) (EtOH-NaOH) (Berdy).

Tallent, W.H. *et al., Tetrahedron*, 1964, **20**, 1781 (*isol, ir, uv, nmr, struct*)

Geniposidic acid G-75

[27741-01-1]



$C_{16}H_{22}O_{10}$ 374.344
Constit. of *Genipa americana* (genipap). $[\alpha]_D^{24}$ +19.3 (c, 1 in MeOH).

Me ester: [24512-63-8] ***Geniposide**. Genipin 1-glucoside. Jasminoidin*
$C_{17}H_{24}O_{10}$ 388.371
Cryst. (Me_2CO). Sol. H_2O; poorly sol. hexane. Mp 163-164°. $[\alpha]_D$ +7.5. λ_{max} 235 (ε 15500) (H_2O) (Berdy).

β-D-Glucopyranosyl ester: [126005-84-3] ***Asystasioside D***
$C_{22}H_{32}O_{15}$ 536.486
Cryst. (as nona-Ac). Mp 177-179° (nona-Ac). $[\alpha]_D^{28}$ -7 (c, 0.4 in $CHCl_3$) (nona-Ac).

6′-O-β-D-Glucopyranosyl, Me ester: [29307-60-6] *Genipin 1-gentiobioside*
$C_{23}H_{34}O_{15}$ 550.513
Cryst. (EtOH). Mp 193-195°. λ_{max} 238 (log ε 4.11) (EtOH).

6′-O-[4-Hydroxy-Z-cinnamoyl-(→6)-β-D-glucopyranosyl], Me ester:6′′-O-p-cis-Coumaroylgenipin gentiobioside
$C_{32}H_{40}O_{17}$ 696.658
Amorph. powder. $[\alpha]_D$ +7.05 (c, 0.15 in MeOH). λ_{max} 230 (log ε 4.14); 308 (log ε 4.09) (MeOH).

10-Ac:10-O-Acetylgeniposidic acid
$C_{18}H_{24}O_{11}$ 416.381
Foam. $[\alpha]_D^{20}$ +7 (c, 0.6 in MeOH).

10-Ac, Me ester: [62218-50-2]
$C_{19}H_{26}O_{11}$ 430.408
Cryst. (EtOH). Mp 173-175°. $[\alpha]_D^{30}$ +22.1 (c, 2.7 in MeOH).

Penta-Ac, Me ester: [49776-64-9] *Penta-O-acetylgeniposide*
$C_{27}H_{34}O_{15}$ 598.557
Needles. Mp 137.5-138°. $[\alpha]_D^{20}$ +11 (c, 0.5 in EtOH). λ_{max} 235 (log ε 4.19) (EtOH).

10-(5-Phenyl-2E,4E-pentadienoyl):

[97868-32-1] ***10-(5-Phenyl-2,4-pentadie-***

noyl)geniposidic acid
$C_{27}H_{30}O_{11}$ 530.527Isol. as Me ester
λ_{max} 308 (log ϵ 4.47) (MeOH) (Me ester).

10-(4-Hydroxybenzoyl): [222527-90-4]
$C_{23}H_{26}O_{12}$ 494.451
Amorph. powder. $[\alpha]_D^{25}$ -18.7 (c, 0.31 in MeOH). λ_{max} 236 (log ϵ 3.64); 284 (log ϵ 1.82); 320 (log ϵ 1.89) (MeOH).

*10-*O-E-*Cinnamoyl:* [405283-36-5]
$C_{25}H_{28}O_{11}$ 504.49

*10-*O-*(4-Hydroxy-*E*-cinnamoyl):* [405283-37-6]
$C_{25}H_{28}O_{12}$ 520.489

*10-(3,4-Dihydroxy-*E*-cinnamoyl):* [367513-00-6]
$C_{25}H_{28}O_{13}$ 536.488

*10-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* [367512-99-0]
$C_{26}H_{30}O_{13}$ 550.515

*10-(3,4-Dimethoxy-*E*-cinnamoyl):* [222527-89-1]
$C_{27}H_{32}O_{13}$ 564.542
Powder. $[\alpha]_D^{25}$ -29.4 (c, 0.19 in MeOH). λ_{max} 236 (log ϵ 4.08); 288 (log ϵ 2.45); 320 (log ϵ 2.61) (MeOH).

*10-(3,4-Dimethoxy-*Z*-cinnamoyl):* [367512-98-9]
$C_{27}H_{32}O_{13}$ 564.542

Aglycone, Me ester: [6902-77-8] ***Genipin***
$C_{11}H_{14}O_5$ 226.229
Constit. of *Genipa americana* (genipap). Cryst. (MeOH). Mp 120-121°. $[\alpha]_D$ +135 (MeOH).

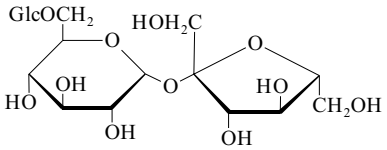
▶GY5828000

Aglycone, 10-Ac, Me ester: [62218-51-3] *Genipin acetate*
$C_{13}H_{16}O_6$ 268.266
Oil. $[\alpha]_D^{20}$ +22.6 (c, 0.06 in $CDCl_3$).

Bentley, T.W. *et al., J.C.S.(C)*, 1967, 2234 (*ms*)
Endo, T. *et al., Chem. Pharm. Bull.*, 1970, **18**, 1066-1067 (*Genipin 1-gentiobioside*)
Inouye, H. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1287 (*biosynth*)
Endo, T. *et al., Chem. Pharm. Bull.*, 1973, **21**, 2684 (*biosynth*)
Takeda, Y. *et al., Phytochemistry*, 1975, **14**, 2647 (*biosynth*)
Takeda, Y. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2644 (*deriv*)
Buyuk, G. *et al., Tet. Lett.*, 1978, 3803 (*synth, bibl*)
Koenig, G. *et al., Phytochemistry*, 1985, **24**, 1245-1248 (*Phenylpentadienoylgeniposide*)
Uesato, S. *et al., Phytochemistry*, 1986, **25**, 2515 (*biosynth*)
Demuth, H. *et al., Phytochemistry*, 1989, **28**, 3361 (*Asystasioside D*)
Wang, C.J. *et al., Anticancer Res.*, 1992, **12**, 911-915 (*Pentaacetylgeniposide*)
Drewes, S.E. *et al., J. Nat. Prod.*, 1996, **59**, 1169-1170 (*Genipin acetate*)
Jensen, S.R. *et al., Phytochemistry*, 1996, **42**, 1633-1636 (*10-Ac*)
Machida, K. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1295-1300 (*cis-Coumaroylgenipin gentiobioside*)
Takeda, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 284-286 (*Leonotis nepetaefolia esters*)
Narukawa, Y. *et al., Nat. Med. (Tokyo)*, 2001, **55**, 79-82; *CA*, **135**, 341514a (*Leonotis nepetaefolia esters*)
Shaker, K.H. *et al., Z. Naturforsch., C*, 2001, **56**, 965-968 (*Avicennia marina constits*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GCM300

Gentianose G-76

[25954-44-3]
β-D-Fructofuranosyl O-*β-D-glucopyranosyl-(1→6)-α-D-glucopyranoside, 9CI, 8CI. β-D-Glucopyranosyl-(1→6)-α-D-glucopyranosyl-(1→2)-β-D-fructofuranoside*



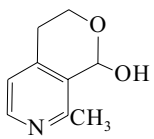
$C_{18}H_{32}O_{16}$ 504.441
Occurs in roots of *Gentiana lutea* (yellow gentian). Mp 212°. $[\alpha]_D^{25}$ +30.8 (c, 0.5 in H_2O).

Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Mp 80-93°. $[\alpha]_D^{20}$ +32.2 (c, 0.85 in $CHCl_3$).

Haworth, W.N. *et al., J.C.S.*, 1923, 3120
Suami, T. *et al., Carbohydr. Res.*, 1972, **21**, 451 (*synth, pmr*)
Samuelson, O. *et al., Methods Carbohydr. Chem.*, 1972, **6**, 66 (*chromatog*)

Gentiatibetine G-77

[26005-36-7]
Gentiotibetine

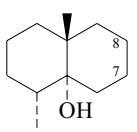


$C_9H_{11}NO_2$ 165.191
Alkaloid from *Gentiana lutea* (yellow gentian). Mp 161.5°.

Rulko, F. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1967, **41**, 567 (*uv, ir, pmr, ms, struct*)

Geosmin G-78

[19700-21-1]
*Octahydro-4,8*a*-dimethyl-4*a*(2*H*)-naphthalenol, 9CI. 1,10-Dimethyl-9-decalol. 11,12,13-Trinor-5-eudesmanol*



Absolute configuration

$C_{12}H_{22}O$ 182.305
Noreudesmane numbering shown. Implicated in off-flavour of shellfish, freshwater fish, drinking water and some vegetables. Oil with characteristic penetrating earthy odour. $[\alpha]_D^{25}$ -140 (MeOH). $[\alpha]_D$ -16.5 ($CHCl_3$). Stereoisomers known synthetically.

▶QK4249000

*7,8-Didehydro:1,2,3,4,4*a*,5,8,8*a*-Octahydro-4,8*a*-dimethylnaphthalen-4*a*-ol. 11,12,13-Trinor-7-eudesmen-5-ol.* ***Dehydrogeosmin***
$C_{12}H_{20}O$ 180.289
Oil.

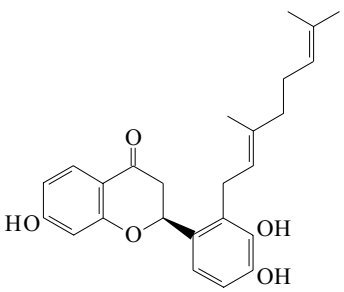
(±)-form [16423-19-1]
Oil, cryst. on standing. Mp 78-82°.

[5173-69-3, 5173-70-6, 16452-32-7, 23333-91-7, 62823-65-8, 73428-92-9]

Marshall, J.A. *et al., J.O.C.*, 1966, **31**, 1020; 1968, **33**, 2593 (*synth*)
Gerber, N.N. *et al., Tet. Lett.*, 1968, 2971 (*isol, struct*)
Ayer, W.A. *et al., Can. J. Chem.*, 1976, **54**, 3276 (*isol, struct, synth, abs config*)
Gerber, N.N. *et al., J. Chem. Ecol.*, 1977, **3**, 475 (*isol*)
Gerber, N.N. *et al., Phytochemistry*, 1977, **16**, 2025 (*cmr*)
Gerber, N.N. *et al., Dev. Ind. Microbiol.*, 1978, **20**, 225 (*rev*)
Maga, J.A. *et al., Food Res. Int.*, 1987, **3**, 269-284 (*occur, rev*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1990, **73**, 133 (*isol, synth, ms, pmr, cmr*)
Hansson, L. *et al., Acta Chem. Scand.*, 1992, **46**, 103 (*synth*)
Swarts, H.J. *et al., Tetrahedron*, 1992, **48**, 5497 (*synth*)
Huber, U. *et al., Helv. Chim. Acta*, 1993, **76**, 1949 (*synth, abs config*)
Feng, Z. *et al., Helv. Chim. Acta*, 1993, **76**, 2547 (*biosynth*)
Conte, E.D. *et al., J. Agric. Food Chem.*, 1996, **44**, 829-835 (*anal, occur*)
Saito, A. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 2923 (*synth*)
Fuhshuku, K. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2267-2272 (*synth*)

2′-Geranyl-3′,4′,7-trihydroxyflavanone G-79

[121001-59-0]



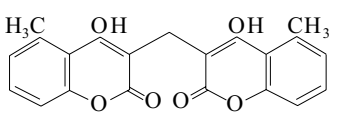
$C_{25}H_{28}O_5$ 408.493

(E)-form [113866-90-3]
Constit. of *Artocarpus communis* (breadfruit).

Fujimoto, Y. *et al., CA*, 1988, **108**, 164664 (*isol*)

Gerberinol 1 G-80

[84153-78-6]
*3,3′-Methylenebis[4-hydroxy-5-methyl-2*H*-1-benzopyran-2-one], 9CI. Gerberinol*

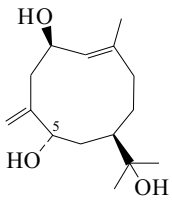


$C_{21}H_{16}O_6$ 364.354
Constit. of *Diospyros kaki* (Japanese persimmon). Cryst. (EtOAc). Mp 267-269°. λ_{max} 292 (MeOH) (Berdy).

Sengupta, P. *et al., J. Indian Chem. Soc.*, 1985, **62**, 916 (*isol*)
Chatterjea, J.N. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 796 (*synth*)

Paknikar, S.K. *et al., Phytochemistry*, 1996, **41**, 931 (*isol, uv, ir, pmr*)

1(10),4(15)-Germacradiene-2,5,11-triol G-81



$C_{15}H_{26}O_3$ 254.369

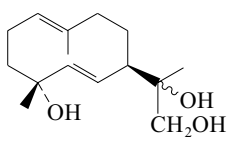
(1(10)*E*,2β,5β)-*form*

1-Ac: [86787-28-2] ***Tanacetol B***
$C_{17}H_{28}O_4$ 296.406
Constit. of *Tanacetum vulgare* (tansy). Cryst. (Et_2O). Mp 163°. $[\alpha]_D^{25}$ -65.4 (c, 1.5 in MeOH).

5-Ketone, 2-Ac: [86778-06-5] *2-Acetoxy-11-hydroxy-1(10),4(15)-germacradien-5-one.* ***Tanacetol A***
$C_{17}H_{26}O_4$ 294.39
Constit. of *Tanacetum vulgare* (tansy). Cryst. ($EtOAc/C_6H_6$). Mp 98°. $[\alpha]_D^{25}$ -99 (c, 1 in $CHCl_3$).

Appendino, G. *et al., Phytochemistry*, 1983, **22**, 509

1(10),5-Germacradiene-4,11,12-triol G-82



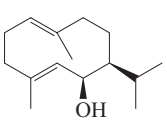
$C_{15}H_{26}O_3$ 254.369

(1(10)*E*,4α,5*E*)-*form*

12-Ac: [143305-08-2]
$C_{17}H_{28}O_4$ 296.406
Constit. of *Laurus nobilis* (bay laurel). Oil. $[\alpha]_D^{25}$ -73 (c, 1.9 in CH_2Cl_2).

Appendino, G. *et al., Phytochemistry*, 1992, **31**, 2537 (*isol, pmr, cmr*)

1(10),4-Germacradien-6-ol G-83



(1(10)*E*,4*E*,6β)-*form*

$C_{15}H_{26}O$ 222.37

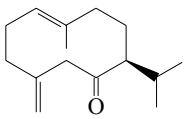
(1(10)*E*,4*E*,6β)-*form* [64395-16-0]
Syrup. $[\alpha]_D^{20}$ -14.8 (c, 1 in $CHCl_3$).

Ketone: [50281-45-3] *1(10),4-Germacradien-6-one.* ***Acoragermacrone****. Bacchascandone*
$C_{15}H_{24}O$ 220.354
Constit. of *Acorus calamus* (sweet flag). Liq. $Bp_{0.01}$ 130°. $[\alpha]_D^{24}$ +28.5 (c, 0.95 in $CHCl_3$).

[74559-99-2]

Niwa, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2930; 1976, **49**, 3148 (*isol, synth*)
Still, W.C. *et al., J.A.C.S.*, 1977, **99**, 4186 (*synth*)
Takahashi, T. *et al., Tet. Lett.*, 1983, **24**, 3485 (*synth*)
Dominguez, X.A. *et al., Rev. Latinoam. Quim.*, 1986, **17**, 207

1(10),4(15)-Germacradien-6-one G-84



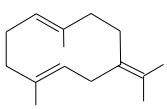
$C_{15}H_{24}O$ 220.354

(*E*)-*form* [25645-19-6]
Preisocalamendiol
Constit. of *Acorus calamus* (sweet flag). Oil.

Yamamura, S. *et al., Tetrahedron*, 1971, **27**, 5419 (*isol*)
Kato, K. *et al., Tetrahedron*, 1971, **27**, 5987 (*synth*)
Horibe, I. *et al., Tet. Lett.*, 1975, 2849 (*pmr*)
Still, W.C. *et al., J.A.C.S.*, 1977, **99**, 4186 (*synth*)
Zdero, C. *et al., Phytochemistry*, 1989, **28**, 531 (*isol*)

1(10),4,7(11)-Germacratriene G-85

8-Isopropylidene-1,5-dimethylcyclodeca-1,5-diene

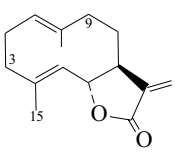


$C_{15}H_{24}$ 204.355

(1(10)*E*,4*E*)-*form* [15423-57-1]
Germacrene B*. Germacratriene*
Constit. of the peel oil of yuzu *Citrus junos*. Oil.

Ognyanov, I. *et al., Coll. Czech. Chem. Comm.*, 1958, **23**, 2033 (*synth*)
Allen, F.H. *et al., Chem. Comm.*, 1967, 588 (*cryst struct*)
Nishimura, K. *et al., Tet. Lett.*, 1969, 3097 (*isol*)
Minnaard, A.J. *et al., J.O.C.*, 1997, **62**, 7366-7345 (*synth*)

1(10),4,11(13)-Germacratrien-12,6-olide G-86



(1(10)*E*,4*E*,6α)-*form*

$C_{15}H_{20}O_2$ 232.322Log P 3.59 (calc).

(1(10)*E*,4*E*,6α)-*form* [553-21-9]
Costunolide
Constit. of costus root (*Saussurea lappa*). Cryst. (MeOH). Mp 106-107°. $[\alpha]_D$ +128 (c, 0.45 in $CHCl_3$). Pharmacol. active isomer λ_{max} 210 (ε 10800) (MeOH) (Berdy). λ_{max} 204 (ε 18800) (EtOH) (Berdy).

► LY4270000

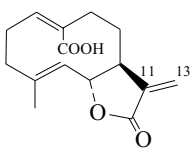
11β,13-Dihydro: See 1(10),4-Germacradien-12,6-olide in *The Combined Chemical Dictionary.*

(1(10)*E*,4*E*,6β)-*form*
Oil. $[\alpha]_D^{24}$ -164 (c, 0.91 in $CHCl_3$).

(1(10)*Z*,4*E*,6α)-*form* [125514-73-0]
Melampolide
Plates (Et_2O). Mp 144-145°. $[\alpha]_D^{20}$ +1.4 (c, 0.84 in $CHCl_3$).

Rao, A.S. *et al., Tetrahedron*, 1960, **9**, 275 (*isol*)
Bouill, M.J. *et al., Acta Cryst. B*, 1976, **32**, 3203 (*cryst struct*)
Kanasaki, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 1239
Grieco, P.A. *et al., J.O.C.*, 1977, **42**, 1717 (*synth*)
Shibuya, H. *et al., Chem. Lett.*, 1986, 85 (*synth*)
Takahashi, T. *et al., Tetrahedron*, 1987, **43**, 5499 (*synth*)
Ming, C.W. *et al., Phytochemistry*, 1989, **28**, 3233 (*isol, pmr, cmr, ir, cryst struct, Melampolide*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)
Taniguchi, M. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2064-2067 (*activity*)
Jacobsson, U. *et al., Phytochemistry*, 1995, **39**, 839 (*Costunolide, pmr, cmr*)
Park, H.-J. *et al., J. Nat. Prod.*, 1996, **59**, 1128 (*Costunolide, pmr, cmr*)
Fischer, N.H. *et al., Phytochemistry*, 1998, **49**, 559-564 (*activity*)
Jang, D.S. *et al., Saengyak Hakhoechi*, 1998, **29**, 67-70 (*activity*)

1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid G-87



(1(10)*E*,4*E*,6α)-*form*

$C_{15}H_{18}O_4$ 262.305

(1(10)*Z*,4*E*,6α)-*form*
Taraxinic acid*. Taraxin acid*
Cryst. Mp 156-157°. $[\alpha]_D^{21}$ -34.5 (c, 1 in MeOH).

β-D-Glucopyranosyl ester: [75911-14-7]
$C_{21}H_{28}O_9$ 424.447
Constit. of *Taraxacum officinale* (dandelion). Cryst. (CH_2Cl_2/MeOH). Mp 84-86°.

11,13-Dihydro, β-D-glucopyranosyl ester: [75911-16-9]
$C_{21}H_{30}O_9$ 426.463
Constit. of *Taraxacum officinale* (dandelion). Cryst. Mp 84-86°.

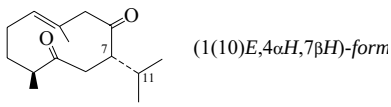
(1(10)*E*,4*E*,6α)-*form* [106794-14-3]
Perydiscolic acid
Yellow gum.

β-D-Glucopyranosyl ester: [93303-17-4]
Ainsliaside B
$C_{21}H_{28}O_9$ 424.447
Needles (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 157-161°. $[\alpha]_D^{19}$ +83.4 (c, 0.51 in MeOH).

Hansel, R. *et al., Phytochemistry*, 1980, **19**, 857
Jin, H. *et al., Yakugaku Zasshi*, 1982, **102**, 911 (*Taraxinic acid*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3043 (*Ainsliaside B*)
Maldonado, E. *et al., Phytochemistry*, 1987, **26**, 205 (*Perydiscolic acid*)
Kashiwada, Y. *et al., J. Asian Nat. Prod. Res.*, 2001, **3**, 191-197; *CA*, **135**, 322608t (*glucosides*)

1(10)-Germacrene-5,8-dione G-88

3-Isopropyl-6,10-dimethyl-6-cyclodecene-1,4-dione



(1(10)*E*,4α*H*,7β*H*)-*form*

$C_{15}H_{24}O_2$ 236.353Log P 3.16 (calc).

(1(10)*E*,4α*H*,7β*H*)-*form* [13657-68-6]
Curdione
Constit. of *Curcuma zedoaria* (zedoary). Cryst. Poorly sol. hexane. Mp 61-62°. $[\alpha]_D^{25}$ +26 (c, 1.00 in $CHCl_3$). Log P 3.16 (calc). Pharmacol. active isomer.
► LD_{50} (mus, ipr) 414 mg/kg. LY3960000

7,11-Didehydro: [38230-32-9] *1(10),7(11)-Germacradiene-5,8-dione.* ***Dehydrocurdione***
$C_{15}H_{22}O_2$ 234.338
From *Curcuma zedoaria* (zedoary). Oil. $[\alpha]_D$ +67.9 (c, 0.5 in $CHCl_3$).

(1(10)*E*,4α*H*,7α*H*)-*form*
Neocurdione
Cryst. (pentane). Mp 45-47°. $[\alpha]_D^{22}$ -65.8 (c, 1.2 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1390; 1972, **20**, 987-989 (*isol, struct*)
Inayama, S. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1323-1326; 2179-2182 (*abs config, cryst struct*)
Shibuya, H. *et al., Yakugaku Zasshi*, 1986, **106**, 212-216 (*isol, Dehydrocurdione*)
Harimaya, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 843 (*isol, cryst struct, Neocurdione*)
Panddji, C. *et al., Phytochemistry*, 1993, **34**, 415 (*isol*)
Jiang, T. *et al., Zhonghua Pifuke Zazhi*, 1999, **32**, 316-318; *CA*, **133**, 101863d (*activity*)
Phan, M.G. *et al., Tap Chi Hoa Hoc*, 2000, **38**, 91-94 (*activity*)

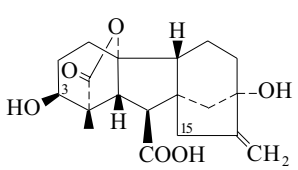
Ghatti gum G-89

[9000-28-6]
Gum ghatti. Indian gum. FEMA 2519
A water-sol. polysaccharide made up of Ca and Mg salts of L-arabinose, D-galactose, D-mannose, D-xylose and D-glucuronic acids. Emulsifier.

Merck Index, 12th edn., 1996, 4424
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1199-1201

Gibberellin A_1 G-90

[545-97-1]
Gibberellin A. Bean factor I



$C_{19}H_{24}O_6$ 348.395
Cryst. (EtOAc or EtOAc/petrol). Mp 255-258° dec Mp 285° dec. (dimorph). $[\alpha]_D^{25}$ +36 (EtOH).

β-D-Glucopyranosyl ester: [54788-51-1]
$C_{25}H_{34}O_{11}$ 510.537
Constit. of the seeds of *Phaseolus vulgaris* (kidney bean).

3-Epimer: [1166-98-9] ***3-Epigibberellin A_1.*** *Pseudogibberellin A_1*
$C_{19}H_{24}O_6$ 348.395
Constit. of *Lactuca sativa* (lettuce).

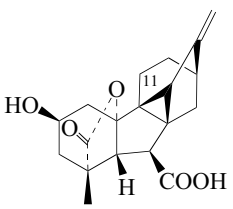
15β-Hydroxy: [105593-21-3] ***Gibberellin A_{72}***
$C_{19}H_{24}O_7$ 364.394
Isol. from seeds of *Helianthus annuus* (sunflower).

15β-Hydroxy, 3-epimer: [128712-79-8] ***3-Epigibberellin A_{72}.*** *3*-epi-*Gibberellin A_{72}*
$C_{19}H_{24}O_7$ 364.394
Isol. from *Helianthus annuus* (sunflower).

MacMillan, J. *et al., Tetrahedron*, 1960, **11**, 60 (*struct*)
Durley, R.C. *et al., Planta Med.*, 1973, **109**, 357 (*biosynth*)
Hiraga, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 2511; 2521 (*glucosyl ester*)
Lombardo, L. *et al., J.A.C.S.*, 1980, **102**, 6626 (*synth*)
Voigt, B. *et al., Tetrahedron*, 1983, **39**, 449 (*synth*)
MacMillan, J. *et al., J.C.S. Perkin 1*, 1986, 309 (*synth*)
Hutchison, M. *et al., Phytochemistry*, 1988, **27**, 2695 (*Gibberellin A_{72}*)
Shimano, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 276 (*synth*)
Castellaro, S.J. *et al., J.C.S. Perkin 1*, 1990, 145 (*3-Epigibberellin A_{72}*)
Gaskin, P. *et al., Phytochemistry*, 1995, **38**, 1 (*3-Epigibberellin A_1*)
Kobayashi, M. *et al., Phytochemistry*, 2000, **55**, 317-321 (*biosynth*)

Gibberellin A_{105} G-91

[114596-77-9]



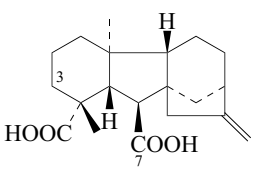
$C_{19}H_{22}O_5$ 330.38
Constit. of apple seeds (*Malus domestica*).

2-Deoxy, 11β-hydroxy: ***Gibberellin A_{108}***
$C_{19}H_{22}O_5$ 330.38
Constit. of apple seeds (*Malus domestica*).

Pour, M. *et al., Aust. J. Chem.*, 1997, **50**, 289-299 (*synth*)

Gibberellin A_{12} G-92

[1164-45-0]
1,4a-Dimethyl-8-methylenegibbane-1,10-dicarboxylic acid, 9CI



$C_{20}H_{28}O_4$ 332.439
Cryst. (EtOH/petrol). Mp 245-248°.

7-Aldehyde: [19436-07-8] ***Gibberellin A_{12} 7-aldehyde***
$C_{20}H_{28}O_3$ 316.439
Constit. of *Phaseolus* spp., *Pisum sativum* (peas) and other plant spp..

2β-Hydroxy: ***Gibberellin A_{110}***
$C_{20}H_{28}O_5$ 348.438
Constit. of *Spinacia oleracea* (spinach) and *Elaeis guineensis* (African palm oil).

3β-Hydroxy: [4955-22-0] ***Gibberellin A_{14}***
$C_{20}H_{28}O_5$ 348.438
Cryst. (EtOAc/petrol). Mp 242-243°. $[\alpha]_D^{17}$ -73 (c, 0.4 in EtOH).

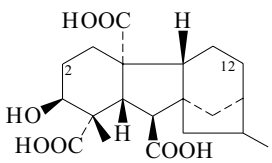
12α-Hydroxy: [75803-47-3] ***Gibberellin A_{111}***
$C_{20}H_{28}O_5$ 348.438
Constit. of *Raphanus sativus* (radish).

12β-Hydroxy: [90806-15-8] ***Gibberellin A_{112}***
$C_{20}H_{28}O_5$ 348.438
Constit. of *Matthiola incana* and *Raphanus sativus* (radish).

Jones, K.C. *et al., Phytochemistry*, 1968, **7**, 283-291 (*GA_{14}, struct*)
Bearder, J.R. *et al., Phytochemistry*, 1973, **12**, 2173-2179 (*biosynth*)
Graebe, J.E. *et al., Phytochemistry*, 1974, **13**, 1433-1440 (*biosynth*)
Nakata, T. *et al., Tet. Lett.*, 1976, 1515-1518 (*GA_{12}, synth*)
Mori, K. *et al., Tetrahedron*, 1976, **32**, 1497-1502 (*GA_{12}, synth*)
Turnbull, C.G.N. *et al., Phytochemistry*, 1986, **25**, 97-101 (*biosynth*)
Zhu, Y.-X. *et al., Phytochemistry*, 1988, **27**, 2549-2552 (*biosynth*)
Hao, X.-J. *et al., Chin. Chem. Lett.*, 1997, **8**, 951-952 (*GA_{12}, synth*)
Hisamatsu, T. *et al., Phytochemistry*, 1998, **47**, 3-6 (*GA_{112}*)
Owen, D.J. *et al., Phytochemistry*, 1998, **47**, 331-337 (*GA_{110}, synth*)
Nakayama, M. *et al., Phytochemistry*, 1998, **48**, 587-593 (*GA_{111}, GA_{112}*)
Toyota, M. *et al., J.A.C.S.*, 2000, **122**, 9036-9037; 2001, **123**, 1856-1861 (*synth, GA_{12}, GA_{111}, GA_{112}*)
Urrutia, O. *et al., Phytochemistry*, 2001, **56**, 505-511 (*biosynth*)

Gibberellin A_{13} G-93

[2922-24-9]
Fujic acid



$C_{20}H_{26}O_7$ 378.421
Identity with Fujic acid not certain.Cryst. (EtOAc/petrol). Mp 194-196° dec. $[\alpha]_D^{17}$ -48 (c, 0.25 in EtOH).

2β-Hydroxy: [54605-43-5] ***Gibberellin A_{43}***
$C_{20}H_{26}O_8$ 394.421
From *Cucurbita maxima*.

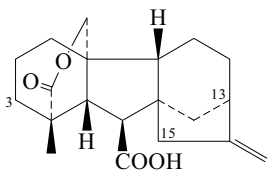
12α-Hydroxy: [57672-81-8] ***Gibberellin A_{39}***
$C_{20}H_{26}O_8$ 394.421
Constit. of the seeds of *Cucurbita pepo* and *Cucurbita maxima*. Gum. $[\alpha]_D^{19}$ -18 (c, 1.3 in EtOH).

Galt, R.H.B. *et al., J.C.S.*, 1965, 3143 (*isol*)

Graebe, J.E. *et al., Planta*, 1974, **120**, 307 (*biosynth*)
Beeley, L.J. *et al., Phytochemistry*, 1975, **14**, 779 (*deriv*)
Fukui, H. *et al., Agric. Biol. Chem.*, 1977, **41**, 181 (*deriv*)
Dockerell, B. *et al., Chem. Comm.*, 1977, 919 (*biosynth*)
Ellames, G. *et al., J.C.S. Perkin 1*, 1979, 1922 (*cryst struct*)
MacMillan, J. *et al., Phytochemistry*, 1984, **23**, 553 (*isol*)

Gibberellin A_{15} G-94

[13744-18-8]



$C_{20}H_{26}O_4$ 330.423
Cryst. (Me_2CO/petrol). Mp 274-276°. $[\alpha]_D$ +5.

3β-Hydroxy: [38231-54-8] ***Gibberellin A_{37}***
$C_{20}H_{26}O_5$ 346.422
Constit. of *Cucurbita maxima*. Cryst. (EtOAc/petrol). Mp 228-230°.

3β-Hydroxy, β-D-glucopyranosyl ester: [36702-72-4] ***Gibberellin A_{37} glucosyl ester***
$C_{26}H_{36}O_{10}$ 508.564
Constit. of the seeds of *Phaseolus vulgaris* (kidney beans).

12α-Hydroxy: [90806-31-8] ***Gibberellin A_{113}***
$C_{20}H_{26}O_5$ 346.422
Constit. of *Raphanus sativus* (radish).

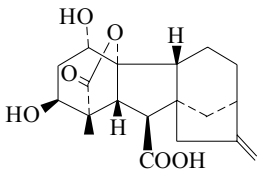
12β-Hydroxy: ***Gibberellin A_{114}***
$C_{20}H_{26}O_5$ 346.422
Constit. of *Raphanus sativus* (radish).

15β-Hydroxy: [73208-09-0] ***Gibberellin A_{64}***
$C_{20}H_{26}O_5$ 346.422
Isol. from seeds of *Helianthus annuus* (sunflower).

Cross, B.E. *et al., J.C.S.(C)*, 1971, 1539 (*synth*)
Bearder, J.R. *et al., J.C.S. Perkin 1*, 1973, 2824 (*Gibberellin A_{37}*)
Hiraga, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 2511
Graebe, J.E. *et al., Phytochemistry*, 1974, **13**, 1433 (*biosynth*)
Fujita, E. *et al., J.C.S. Perkin 1*, 1977, 611 (*synth*)
Yamane, H. *et al., Phytochemistry*, 1977, **16**, 831 (*isol*)
Lombardo, L. *et al., J.O.C.*, 1983, **48**, 2298 (*synth*)
Hutchison, M. *et al., Phytochemistry*, 1988, **27**, 2695 (*Gibberellin A_{64}*)
Nakayama, M. *et al., Phytochemistry*, 1998, **48**, 587-593 (*GA_{113}, GA_{114}*)

Gibberellin A_{16} G-95

[25509-93-7]



$C_{19}H_{24}O_6$ 348.395
Cryst. (MeOH aq.). Mp 157-165°.

1-Epimer: [72533-75-6] ***Gibberellin A_{54}***
$C_{19}H_{24}O_6$ 348.395
From *Triticum aestivum* (wheat). Cryst. (Me_2CO/hexane). Mp 243-246°.

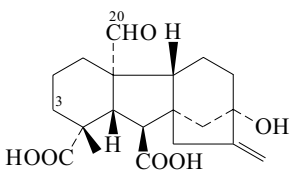
13-Hydroxy: [75082-54-1] ***Gibberellin A_{57}***
$C_{19}H_{24}O_7$ 364.394
Amorph.

1-Epimer, 2β-hydroxy: [132043-65-3] ***Gibberellin A_{79}***
$C_{19}H_{24}O_7$ 364.394
Constit. of *Triticum aestivum* (wheat).

McInnes, A.G. *et al., Can. J. Biochem.*, 1973, **51**, 1470 (*biosynth*)
Bearder, J.R. *et al., J.C.S. Perkin 1*, 1973, 2824 (*isol*)
Murofushi, N. *et al., Agric. Biol. Chem.*, 1979, **43**, 2179; 1980, **44**, 1583 (*derivs*)
Gaskin, P. *et al., Agric. Biol. Chem.*, 1980, **44**, 1589 (*deriv*)
Voigt, B. *et al., Tetrahedron*, 1983, **39**, 449 (*synth*)
Penny, M. *et al., Phytochemistry*, 1993, **33**, 951 (*GA_{79}*)

Gibberellin A_{19} G-96

[6980-44-5]
Bamboo gibberellin



$C_{20}H_{26}O_6$ 362.422
Constit. of moso bamboo shoots (*Phyllostachys edulis*). Cryst. (EtOAc/EtOH/hexane). Mp 236-237°.

20-Carboxylic acid: [18411-79-5] ***Gibberellin A_{17}***
$C_{20}H_{26}O_7$ 378.421
Isol. from seeds of *Phaseolus vulgaris* (kidney bean). Amorph. Mp 140-150°.

2β-Hydroxy: [174693-32-4] ***Gibberellin A_{99}***
$C_{20}H_{26}O_7$ 378.421
Constit. of *Spinacia oleracea* (spinach).

3β-Hydroxy: [20134-29-6] ***Gibberellin A_{23}***. *Lupinus gibberellin II*
$C_{20}H_{26}O_7$ 378.421
Cryst. (H_2O). Mp 179-181°.

3β-Hydroxy, 20-carboxylic acid: [32780-05-5] ***Gibberellin A_{28}***
$C_{20}H_{26}O_8$ 394.421
Cryst. (EtOAc/MeOH). Mp 224-225° dec. $[\alpha]_D^{12}$ -6.8 (c, 1.2 in EtOH).

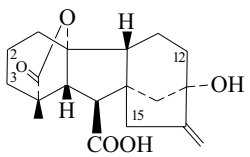
12α-Hydroxy: [328058-47-5] ***Gibberellin A_{125}***
$C_{20}H_{26}O_7$ 378.421
Constit. of strawberry (*Fragaria* x *ananassa*).

15β-Hydroxy: ***Gibberellin A_{102}***
$C_{20}H_{26}O_7$ 378.421
Constit. of seeds of *Helianthus annuus* (sunflower).

Murofushi, N. *et al., Agric. Biol. Chem.*, 1966, **30**, 917; 1979, **43**, 1159 (*isol, biosynth*)
Pryce, R.J. *et al., Tet. Lett.*, 1967, 4173 (*Gibberellin A_{17}*)
Fukui, H. *et al., Phytochemistry*, 1971, **10**, 671 (*GA_{28}*)
Fukui, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 1063 (*Gibberellin A_{23}*)
Dawe, R.D. *et al., Tet. Lett.*, 1985, **26**, 363 (*synth*)
Kurogochi, S. *et al., Phytochemistry*, 1987, **26**, 2895-2900 (*GA_{19}*)
Owen, D.J. *et al., Phytochemistry*, 1996, **42**, 921-925 (*GA_{102}*)
Mander, L.N. *et al., Phytochemistry*, 1996, **43**, 23-28 (*GA_{99}*)
Mander, L.N. *et al., Tet. Lett.*, 1996, **37**, 723-726 (*GA_{99}*)
Kobayashi, M. *et al., Phytochemistry*, 2000, **55**, 317-321 (*biosynth*)
Blake, P.S. *et al., Phytochemistry*, 2000, **55**, 887-890 (*GA_{125}*)

Gibberellin A_{20} G-97

[19143-87-4]
Pharbitis gibberellin



$C_{19}H_{24}O_5$ 332.396
Cryst. Mp 232-233°.

13-O-β-D-Glucopyranoside: [73607-09-7]
$C_{25}H_{34}O_{10}$ 494.538
Constit. of barley *Hordeum vulgare*.

1,2-Didehydro: [78259-50-4] ***Gibberellin A_{95}***
$C_{19}H_{22}O_5$ 330.38
Constit. of *Prunus cerasus* (cherry) seeds. Foam.

1α-Hydroxy: [83455-35-0] ***Gibberellin A_{118}***
$C_{19}H_{24}O_6$ 348.395
Constit. of immature *Prunus persica* (peach) seeds.

1β-Hydroxy, 2β,3β-epoxide: [188895-39-8] ***Gibberellin A_{93}***
$C_{19}H_{22}O_7$ 362.379
Constit. of *Triticum aestivum* (wheat). Powder (EtOAc/petrol). Mp 145-146°.

2α-Hydroxy: [103462-00-6] ***Gibberellin A_{81}***. *2*-epi-*Gibberellin A_{29}*
$C_{19}H_{24}O_6$ 348.395
Constit. of garden pea (*Pisum sativum*) and oranges (*Citrus sinensis*). Gum.

2β-Hydroxy: [29774-53-6] ***Gibberellin A_{29}***
$C_{19}H_{24}O_6$ 348.395
Cryst. (as 2-Me ether). Mp 197-200° (2-Me ether).

2β-Hydroxy, 2-O-β-D-glucopyranoside: [30046-29-8] ***2-O-Glucosylgibberellin A_{29}***
$C_{25}H_{34}O_{11}$ 510.537
Mp 269-272° (as penta-Ac).

12α-Hydroxy: [128230-24-0] ***Gibberellin***

A_{77}
$C_{19}H_{24}O_6$ 348.395
Constit. of *Raphanus sativus* (radish).

12α-Hydroxy, 1,2-didehydro: [357401-45-7] ***Gibberellin GA_{126}***
$C_{19}H_{22}O_6$ 346.379
Constit. of immature *Prunus persica* (peach) seeds.

15β-Hydroxy: [105593-16-6] ***Gibberellin A_{67}***
$C_{19}H_{24}O_6$ 348.395
Constit. of seeds of sunflower (*Helianthus annuus*). Cryst. (Me_2CO/petrol). Mp 135-137°.

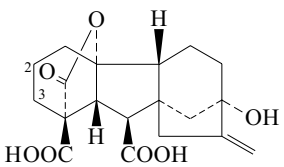
2,3-Dihydroxy: Gibberellin A_8,

2β,15β-Dihydroxy: [128712-78-7] ***Gibberellin A_{76}***. *15β-Hydroxygibberellin A_{29}*
$C_{19}H_{24}O_7$ 364.394
Constit. of sunflower seeds *Helianthus annuus*.

Murofushi, N. *et al., Agric. Biol. Chem.*, 1968, **32**, 1239 (*struct*)
MacMillan, J. *et al., Tet. Lett.*, 1968, 1357 (*struct*)
Yokota, T. *et al., Agric. Biol. Chem.*, 1971, **35**, 583 (*deriv*)
Railton, I.D. *et al., Phytochemistry*, 1974, **13**, 793 (*biosynth*)
Bearder, J.R. *et al., Phytochemistry*, 1975, **14**, 1741 (*biosynth*)
Durley, R.C. *et al., Plant Physiol.*, 1979, **64**, 214 (*biosynth*)
Duri, Z.J. *et al., J.C.S. Perkin 1*, 1981, 161 (*synth*)
Kirkwood, P.S. *et al., J.C.S. Perkin 1*, 1982, 699 (*synth*)
Kamiya, Y. *et al., Phytochemistry*, 1983, **22**, 681 (*biosynth*)
Arigayo, S. *et al., Plant Cell Physiol.*, 1984, **25**, 1395 (GA_{29})
Dolan, S.C. *et al., J.C.S. Perkin 1*, 1986, 2741 (GA_{67})
Nakayama, M. *et al., Agric. Biol. Chem.*, 1990, **54**, 837 (GA_{77})
Castellaro, S.J. *et al., J.C.S. Perkin 1*, 1990, 145 (GA_{76})
Beale, M.H. *et al., J.C.S. Perkin 1*, 1991, 1191 (GA_{81}, *bibl, synth*)
Nakayama, M. *et al., Phytochemistry*, 1996, **42**, 913 (GA_{95})
Findlow, S. *et al., J.C.S. Perkin 1*, 1997, 751-757 (GA_{93})
Senns, B. *et al., Phytochemistry*, 1998, **48**, 1275-1280 (*13-glucoside*)
Kobayashi, M. *et al., Phytochemistry*, 2000, **55**, 317-321 (*biosynth*)
Nakayama, M. *et al., Phytochemistry*, 2001, **57**, 749-758 (GA_{118}, GA_{126})

Gibberellin A_{21} G-98

[18450-93-6]
Canavalia gibberellin I



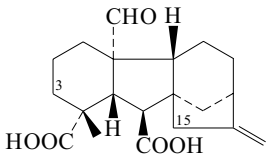
$C_{19}H_{22}O_7$ 362.379
Constit. of the immature seeds of *Canavalia gladiata* (sword bean). Cryst. Mp 244-246°.

2,3-Didehydro: [78333-20-7] ***Gibberellin A_{59}***
$C_{19}H_{20}O_7$ 360.363
Constit. of *Canavalia gladiata* (sword bean). Cryst. Mp 248° dec.

Murofushi, N. *et al., Agric. Biol. Chem.*, 1969, **33**, 598 (*isol*)
Yokota, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 1251 (*deriv*)

Gibberellin A_{24} G-99

[19427-32-8]



$C_{20}H_{26}O_5$ 346.422
Cryst. (Me_2CO/petrol). Mp 199-203°. $[\alpha]_D^{23}$ -88 (c, 0.6 in EtOH).

3β-Hydroxy: [38076-57-2] ***Gibberellin A_{36}***
$C_{20}H_{26}O_6$ 362.422
Cryst. (EtOAc/petrol). Mp 205-208°.

12α-Hydroxy: [137694-17-8] ***Gibberellin Ga_{115}***
$C_{20}H_{26}O_6$ 362.422
Constit. of *Raphanus sativus* (radish).

12β-Hydroxy: [90806-27-2] ***Gibberlin GA_{116}***
$C_{20}H_{26}O_6$ 362.422
Constit. of *Raphanus sativus* (radish).

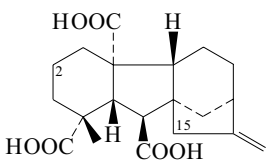
15β-Hydroxy: [79515-13-2] ***Gibberellin A_{65}***
$C_{20}H_{26}O_6$ 362.422
Isol. from seeds of *Helianthus annuus* (sunflower).

20-Carboxylic acid: Gibberellin A_{25},

Harrison, D.M. *et al., J.C.S.(C)*, 1971, 631 (*isol*)
Bearder, J.R. *et al., J.C.S. Perkin 1*, 1973, 2824 (*Gibberellin A_{36}*)
Graebe, J.E. *et al., Phytochemistry*, 1974, **13**, 1433 (*biosynth*)
Kurogochi, S. *et al., Phytochemistry*, 1987, **26**, 2895 (*isol*)
Hutchison, M. *et al., Phytochemistry*, 1988, **27**, 2695 (*Gibberellin A_{65}*)
Nakayama, M. *et al., Phytochemistry*, 1998, **48**, 587-593 (Ga_{115}, GA_{116})

Gibberellin A_{25} G-100

[28535-69-5]



$C_{20}H_{26}O_6$ 362.422
Cryst. Mp 154-157° Mp 248-252° (double Mp). $[\alpha]_D^{27}$ -69 (c, 0.7 in EtOH).

2β-Hydroxy: [60346-28-3] ***Gibberellin A_{46}***
$C_{20}H_{26}O_7$ 378.421
Cryst. (Me_2CO/petrol) (as tri-Me ester). Mp 138-140° (tri-Me ester).

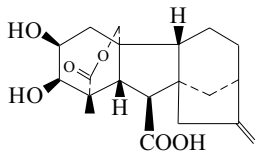
15β-Hydroxy: [70980-48-2] ***Gibberellin A_{66}***
$C_{20}H_{26}O_7$ 378.421
Isol. from seeds of *Helianthus annuus* (sunflower).

3-Hydroxy: Gibberellin A_{13},

Crozier, A. *et al., Can. J. Bot.*, 1970, **48**, 867
Harrison, D.M. *et al., J.C.S.(C)*, 1971, 631
Beeley, L.J. *et al., J.C.S. Perkin 1*, 1976, 1022 (*Gibberellin A_{46}*)
Hutchison, M. *et al., Phytochemistry*, 1988, **27**, 2695 (*Gibberellin A_{66}*)

Gibberellin A_{27} G-101

[23365-01-7]



$C_{20}H_{26}O_6$ 362.422
Cryst. Mp 163-165°.

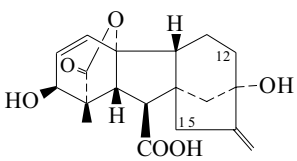
3-O-β-D-Glucopyranoside: [24568-47-6]
$C_{26}H_{36}O_{11}$ 524.564
Mp 234-236° (as penta-Ac).

11β-Hydroxy: [68062-24-8] ***Gibberellin A_{52}***
$C_{20}H_{26}O_7$ 378.421
Constit. of immature seeds of *Lagenaria leucantha* (bottle gourd). Cryst. (EtOAc/hexane). Mp 273-274°. $[\alpha]_D^{24}$ -10 (c, 0.6 in MeOH). Struct. revised in 1992.

Yokota, T. *et al., Agric. Biol. Chem.*, 1971, **35**, 573; 583
Fukui, H. *et al., Agric. Biol. Chem.*, 1978, **42**, 1571 (*deriv*)
Bhaskar, K.V. *et al., Phytochemistry*, 1992, **31**, 1455 (GA_{52})

Gibberellin A_3 G-102

[77-06-5]
Gibberellic acid, BSI. Gibberellin X. Berelex. Gibrescol. Gibrofit. GA_3. Activol



$C_{19}H_{22}O_6$ 346.379
Cryst. (EtOAc/petrol). Mp 235° dec. $[\alpha]_D^{26}$ +92 (EtOH).

▶ LD_{50} (rat, orl) 6300 mg/kg. LY8990000

Me ester: [510-50-9]
Needles (C_6H_6/MeOH). Mp 209-210°. $[\alpha]_D$ +75 (c, 0.5 in EtOH).

3-O-β-D-Glucopyranoside:
$C_{25}H_{32}O_{11}$ 508.521
Cryst. Mp 173-177°.

3-Ac: [7648-02-4]
$C_{21}H_{24}O_7$ 388.416
Cryst. (EtOAc/petrol). Mp 226° dec. $[\alpha]_D^{20}$ +150 (c, 0.2 in $CHCl_3$).

12α-Hydroxy: ***Gibberellin A_{87}***
$C_{19}H_{22}O_7$ 362.379
Constit. of *Prunus avium* (wild cherry).

12α-Hydroxy, 1,2-dihydro: [138693-60-4] ***Gibberellin A_{85}***
$C_{19}H_{24}O_7$ 364.394

12α,15β-Dihydroxy: [32165-30-3] ***Gibberellin A_{32}***
$C_{19}H_{22}O_8$ 378.378
Obt. from immature seeds of *Prunus*

persica (peaches). Mp 190-193° (as Me ester).

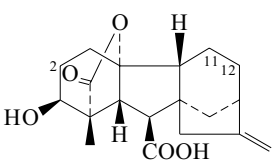
12α,15β-Dihydroxy, 1,2-dihydro: [138703-93-2] ***Gibberellin A_{86}***
$C_{19}H_{24}O_8$ 380.394
Constit. of *Prunus persica* (peaches).

[125-67-7]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1145B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 703A (*ir*)
Cross, B.E. *et al., Chem. Comm.*, 1965, 535 (*biosynth*)
McCapra, F. *et al., J.C.S.(C)*, 1966, 1577 (*cryst struct*)
Schreiber, K. *et al., Phytochemistry*, 1966, **5**, 1221 (*isol*)
Verbiscar, A.J. *et al., Phytochemistry*, 1967, **7**, 807 (*biosynth*)
Yamaguchi, I. *et al., Agric. Biol. Chem.*, 1970, **34**, 1439 (*deriv*)
Yokota, T. *et al., Agric. Biol. Chem.*, 1971, **35**, 583 (*isol*)
Dawson, R.M. *et al., Phytochemistry*, 1975, **14**, 2593 (*biosynth*)
Hook, J.M. *et al., J.A.C.S.*, 1980, **102**, 6628 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1982, **104**, 6129 (*synth*)
Kutschabsky, L. *et al., J.C.S. Perkin 1*, 1983, 1653 (*cryst struct*)
Schwartz, E. *et al., Pharmazie*, 1983, **38**, 716 (*pharmacol*)
Al-Ekabi, H.K. *et al., Can. J. Chem.*, 1984, **62**, 1996 (*ms*)
Hook, J.N. *et al., J.O.C.*, 1984, **49**, 3250 (*synth*)
Lewer, P. *et al., Phytochemistry*, 1984, **23**, 2803 (*biosynth*)
Danheiser, R.L. *et al., Strategies Tactics Org. Synth.*, 1984, 21; *CA*, **102**, 6856 (*book*)
Synform, 1984, **2**, 197 (*rev*)
Hossain, M.B. *et al., Acta Cryst. C*, 1988, **44**, 1022 (*cryst struct*)
Pesticide Manual, 9th edn., 1991, No. 6910
Bhaskar, K.V. *et al., Tet. Lett.*, 1991, **32**, 6203 (GA_{85}, GA_{86})
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A797
Sheng, C. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 564 (*isol*, GA_{85})
Blake, P.S. *et al., Phytochemistry*, 1993, **32**, 781 (GA_{87})
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GEM000

Gibberellin A_4 G-103

[468-44-0]



$C_{19}H_{24}O_5$ 332.396
Cryst. in two forms. Mp 222° dec Mp 255° dec. (dimorph.). $[\alpha]_D^{20}$ -3 (c, 0.34 in MeOH). Gibberellin D was a mixt. of Gibberellins A_4 and Gibberellin A_7, .

β-D-Glucopyranosyl ester: [54788-52-2]
$C_{25}H_{34}O_{10}$ 494.538
Constit. of seeds of French bean (*Phaseolus vulgaris*).

2α-Hydroxy: [60491-91-0] ***Gibberellin A_{47}***
$C_{19}H_{24}O_6$ 348.395

2α-Hydroxy, Me ester:
Cryst. (MeOH). Mp 242-245°.

2β-Hydroxy: [32630-92-5] ***Gibberellin A_{34}***
$C_{19}H_{24}O_6$ 348.395
Cryst. Mp 218-219°.

11β-Hydroxy: [35214-68-7] ***Gibberellin A_{35}***
$C_{19}H_{24}O_6$ 348.395
Cryst. Mp 252-254°.

11-O-β-D-Glucopyranosyloxy: [35214-69-8] *Gibberellin A_{35} glucoside*
$C_{25}H_{34}O_{11}$ 510.537
Needles (as penta-Ac). Mp 175-177° (penta-Ac).

2β,11β-Dihydroxy: [68062-25-9] ***Gibberellin A_{50}***
$C_{19}H_{24}O_7$ 364.394
Constit. of immature seeds of bottle gourd (*Lagenaria leucantha*). Glass. $[\alpha]_D^{18}$ -7 (c, 0.16 in MeOH).

9,11-Didehydro: [146959-87-7] ***Gibberellin A_{88}***
$C_{19}H_{22}O_5$ 330.38
Constit. of apple seeds (*Malus domestica*).

16,17-Dihydro, 17-hydroxy: [135546-07-5] ***16,17-Dihydro-17-hydroxygibberellin A_4***
$C_{19}H_{26}O_6$ 350.411

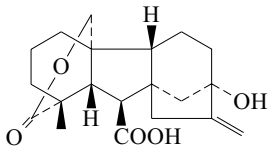
16,17-Dihydro, 16α,17-dihydroxy, 17-O-β-D-glucopyranoside: [159858-83-0]
$C_{25}H_{36}O_{12}$ 528.552
Constit. of rice (*Oryza sativa*) flower anthers.

[8030-53-3, 53663-71-1]

Aldridge, D.C. *et al., J.C.S.*, 1965, 3539 (*struct*)
Mori, K. *et al., Tetrahedron*, 1969, **25**, 1293 (*synth*)
Murofushi, N. *et al., Agric. Biol. Chem.*, 1971, **35**, 441 ($Gibberellin\ A_{34}$)
Yamane, H. *et al., Agric. Biol. Chem.*, 1974, **38**, 649 ($Gibberellin\ A_{35}$)
Hiraga, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 2511; 2521 (*glucosyl ester*)
Beeley, L.J. *et al., J.C.S. Perkin 1*, 1976, 1022 (*synth*)
Kamienska, A. *et al., Plant Physiol.*, 1976, **58**, 76 (*biosynth*)
McInnes, A.G. *et al., Can. J. Biochem.*, 1977, **55**, 728 (*biosynth*)
Fukui, H. *et al., Agric. Biol. Chem.*, 1978, **42**, 1571 ($Gibberellin\ A_{50}$)
Ellames, G. *et al., J.C.S. Perkin 1*, 1979, 1922 (*cryst struct*)
Cossey, A.L. *et al., Tet. Lett.*, 1980, 4383 (*synth*)
MacMillan, J. *et al., J.C.S. Perkin 1*, 1984, 351 (*pmr*)
Beale, M.H. *et al., Phytochemistry*, 1984, **23**, 565 (*cmr*)
Turnbull, C.G.N. *et al., Phytochemistry*, 1986, **25**, 1823 (*biosynth*)
Sassa, T. *et al., Agric. Biol. Chem.*, 1989, **53**, 303 (*isol*)
Mander, L.N. *et al., Tet. Lett.*, 1990, **31**, 423 (*synth*)
Picciarelli, P. *et al., Phytochemistry*, 1991, **30**, 1789 ($Dihydrohydroxygibberellin\ A_4$)
Hedden, P. *et al., Phytochemistry*, 1993, **32**, 231 ($Gibberellin\ A_{88}$)
Hasegawa, M. *et al., Phytochemistry*, 1994, **37**, 629 ($Dihydrodihydroxygibberellin\ A_4$ *glucoside*)
Pesticide Manual, 12th edn., 2000, No. 404

Gibberellin A_{44} G-104

[36434-15-8]
13-Hydroxygibberellin A_{15}



$C_{20}H_{26}O_5$ 346.422
Found in *Pisum sativum* (pea), *Spinacea oleracea* (spinach), *Triticum aestivum* (wheat), *Vicia faba* and other plants. Cryst. (Me_2CO/EtOAc). Mp 230-233°. $[\alpha]_D$ +5.85 (c, 0.513 in EtOH).

2β-Hydroxy: ***Gibberellin A_{98}***
$C_{20}H_{26}O_6$ 362.422
Constit. of *Spinacia oleracea* (spinach).

3β-Hydroxy: [36434-14-7] ***Gibberellin A_{38}***. *3,13-Dihydroxygibberellin A_{15}*
$C_{20}H_{26}O_6$ 362.422
Isol. from immature seeds of *Phaseolus vulgaris* (French bean). Gum (as Me ester).

3β-Hydroxy, β-D-glucopyranosyl ester: [36702-73-5]
$C_{26}H_{36}O_{11}$ 524.564
Isol. from *Phaseolus vulgaris* (French bean). Cryst. (Me_2CO/EtOAc/hexane). Mp 259-261°. $[\alpha]_D^{20}$ +29.5.

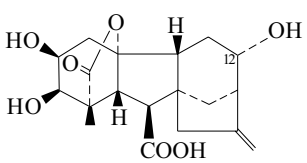
12α-Hydroxy: [328058-46-4] ***Gibberellin A_{24}***
$C_{20}H_{26}O_6$ 362.422
Constit. of strawberry (*Fragaria* x *ananassa*).

15β-Hydroxy: ***Gibberellin A_{101}***
$C_{20}H_{26}O_6$ 362.422
Constit. of seeds of *Helianthus annuus* (sunflower).

Hiraga, K. *et al., Agric. Biol. Chem.*, 1972, **36**, 345-347; 1974, **38**, 2521-2527 ($Gibberellin\ A_{38}$)
Fukui, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 1003-1012 (*isol, struct*)
Gaskin, P. *et al., Agric. Biol. Chem.*, 1980, **44**, 1589-1593 (*isol*)
Owen, D.J. *et al., Phytochemistry*, 1996, **42**, 921-925 (GA_{101})
Mander, L.N. *et al., Phytochemistry*, 1996, **43**, 23-28 (GA_{98})
Kobayashi, M. *et al., Phytochemistry*, 2000, **55**, 317-321 (*biosynth*)
Blake, P.S. *et al., Phytochemistry*, 2000, **55**, 887-890 (GA_{124})

Gibberellin A_{49} G-105

[62071-02-7]



$C_{19}H_{24}O_7$ 364.394
Isol. from seeds of *Cucurbita pepo*. Gum. $[\alpha]_D^{20}$ +11 (c, 0.19 in MeOH).

12-Ketone: [23365-02-8] ***Gibberellin A_{26}***
$C_{19}H_{22}O_7$ 362.379
Cryst. Mp 254-257°.

12-Ketone, 3-O-β-D-glucopyranoside: [24502-82-7]
$C_{25}H_{32}O_{12}$ 524.521

12-Epimer: [62071-05-0] ***Gibberellin A_{48}***
$C_{19}H_{24}O_7$ 364.394

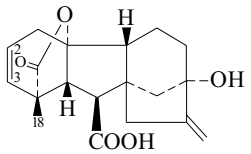
From seeds of *Cucurbita pepo*. Gum. $[\alpha]_D^{28}$ -17 (c, 0.3 in MeOH).

Yokota, T. *et al., Agric. Biol. Chem.*, 1971, **35**, 573; 583

Fukui, H. *et al., Agric. Biol. Chem.*, 1977, **41**, 181 (*Gibberellin A_{48}, Gibberellin A_{49}*)

Gibberellin A_5 G-106

[561-56-8]
Bean factor II



$C_{19}H_{22}O_5$ 330.38
Cryst. (Me_2CO/petrol or Et_2O). Mp 260-261°. $[\alpha]_D$ -77 (c, 0.5 in EtOH). pK_{a1} 4.09 (25°).

2β,3β-Epoxide: [19147-78-5] ***Gibberellin A_6***
$C_{19}H_{22}O_6$ 346.379
Cryst. (Me_2CO/petrol). Mp 206-209°. $[\alpha]_D$ -28 (EtOH).

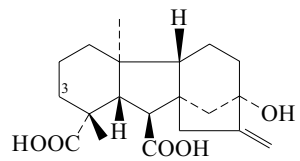
18-Hydroxy: [18450-94-7] ***Gibberellin A_{22}***. *Canavalia gibberellin II*
$C_{19}H_{22}O_6$ 346.379
Isol. from immature seeds of *Canavalia gladiata* (sword bean). Cryst. Mp 213-214°.

1β-Hydroxy: ***Gibberellin A_{92}***
$C_{19}H_{22}O_6$ 346.379
Constit. of *Triticum aestivum* (wheat).

MacMillan, J. *et al., Tetrahedron*, 1960, **11**, 60; 1962, **18**, 349
Murofushi, N. *et al., Agric. Biol. Chem.*, 1969, **33**, 598 (*Gibberellin A_{22}*)
Schneider, G. *et al., Tetrahedron*, 1977, **33**, 1391 (*pmr*)
Bearder, J.R. *et al., J.C.S. Perkin 1*, 1981, 672 (*synth*)
Shimano, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 276 (*synth*)
Penny, M. *et al., Phytochemistry*, 1994, **37**, 1063 (*Gibberellin A_{92}*)

Gibberellin A_{53} G-107

[51576-08-0]



$C_{20}H_{28}O_5$ 348.438
Isol. from *Vicia faba* and spinach (*Spinacia oleracea*). Cryst. (Me_2CO/petrol). Mp 261-274°.

2β-Hydroxy: [128533-05-1] ***Gibberellin A_{97}***
$C_{20}H_{28}O_6$ 364.438
Constit. of spinach (*Spinacia oleracea*).

3β-Hydroxy: [23313-48-6] ***Gibberellin A_{18}***. *Lupinus gibberellin I*
$C_{20}H_{28}O_6$ 364.438
Cryst. (Me_2CO). Mp 240-242°. $[\alpha]_D$ -28 (c, 1 in EtOH).

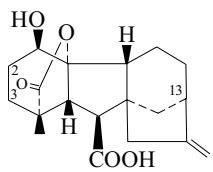
12α-Hydroxy: [171204-47-0] ***Gibberellin A_{123}***
$C_{20}H_{28}O_6$ 364.438
Constit. of strawberry (*Fragaria* x *ananassa*).

15β-Hydroxy: ***Gibberellin A_{100}***
$C_{20}H_{28}O_6$ 364.438
Constit. of sunflower (*Helianthus annuus*) seeds.

Koshimizu, K. *et al., Agric. Biol. Chem.*, 1968, **32**, 1135 (*struct*)
Bearder, J.R. *et al., Phytochemistry*, 1975, **14**, 1741 (*biosynth*)
Sponsel, V.M. *et al., Planta*, 1979, **146**, 101
Mander, L.M. *et al., Aust. J. Chem.*, 1996, **49**, 249 (*synth*)
Owen, D.J. *et al., Phytochemistry*, 1996, **42**, 921 (*GA_{100}*)
Mander, L.N. *et al., Phytochemistry*, 1996, **43**, 23 (*GA_{97}*)
Blake, P.S. *et al., Phytochemistry*, 2000, **55**, 887-890 (*GA_{123}*)

Gibberellin A_{61} G-108

[81826-98-4]



$C_{19}H_{24}O_5$ 332.396
Constit. of *Triticum aestivum* (wheat). Cryst. (Me_2CO/petrol). Mp 257-259°.

13-Hydroxy: [81826-97-3] ***Gibberellin A_{60}***
$C_{19}H_{24}O_6$ 348.395
Constit. of *Triticum aestivum* (wheat). Cryst. (Me_2CO/petrol). Mp 245-247°.

2,3-Didehydro: [81826-99-5] ***Gibberellin A_{62}***
$C_{19}H_{22}O_5$ 330.38
Constit. of *Pyrus malus* (apple). Gum.

2β-Hydroxy: [152110-34-4] ***Gibberellin A_{90}***
$C_{19}H_{24}O_6$ 348.395
Constit. of *Triticum aestivum* (wheat).

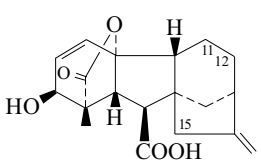
2β,13-Dihydroxy: [160965-01-5] ***Gibberellin A_{91}***
$C_{19}H_{24}O_7$ 364.394
Constit. of *Triticum aestivum* (wheat).

Kirkwood, P.S. *et al., J.C.S. Perkin 1*, 1982, 689 (*isol, struct, synth*)
Shimano, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 276 (*synth*)
Penny, M. *et al., Phytochemistry*, 1993, **33**, 951 (*GA_{90}*)
Penny, M. *et al., Phytochemistry*, 1994, **37**, 1063 (*GA_{91}*)

Gibberellin A_7 G-109

[510-75-8]

[8065-43-8]
13-Deoxygibberellin A_3



$C_{19}H_{22}O_5$ 330.38
Cryst. (Me_2CO/petrol). Mp 202°. $[\alpha]_D^{21}$ +20 (c, 0.5 in EtOH). pK_{a1} 4.11 (25°).

16,17-Dihydro, 16α,17-dihydroxy, 17-O-β-D-glucopyranoside: [159858-84-1]
$C_{25}H_{34}O_{12}$ 526.536
Constit. of rice (*Oryza sativa*) flower anthers.

11β-Hydroxy: [128053-62-3] ***11β-Hydroxygibberellin A_7***
$C_{19}H_{22}O_6$ 346.379
Constit. of *Eriobotrya japonica* (loquat).

12α-Hydroxy: [32450-00-3] ***Gibberellin A_{30}***
$C_{19}H_{22}O_6$ 346.379
Cryst. Mp 188-191°.

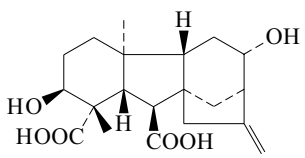
15β-Hydroxy: [71177-41-8] ***Gibberellin A_{68}***
$C_{19}H_{22}O_6$ 346.379
Constit. of apple and pear seeds.

[53663-71-1]

Cross, B.E. *et al., Tetrahedron*, 1962, **18**, 451 (*struct*)
Aldridge, D.C. *et al., J.C.S.*, 1965, 3539 (*struct*)
Murofushi, N. *et al., Agric. Biol. Chem.*, 1970, **34**, 1436 (*deriv*)
Dolan, S.C. *et al., J.C.S. Perkin 1*, 1985, 2741 (*deriv*)
Mander, L.N. *et al., Tet. Lett.*, 1990, **31**, 423 (*synth*)
Hasegawa, M. *et al., Phytochemistry*, 1994, **37**, 629 (*deriv*)
Pesticide Manual, 12th edn., 2000, 404

Gibberellin A_{74} G-110

[90806-14-7]

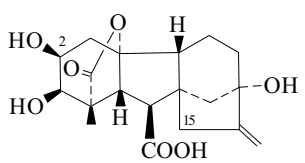


$C_{20}H_{28}O_6$ 364.438
Constit. of *Cucurbita maxima*.

Murofushi, N. *et al., Agric. Biol. Chem.*, 1988, **52**, 1825 (*isol, pmr*)

Gibberellin A_8 G-111

[7044-72-6]



$C_{19}H_{24}O_7$ 364.394
Cryst. (EtOAc). Mp 210-215° dec. $[\alpha]_D^{23}$ +30 (c, 2 in EtOH).

2-O-β-D-Glucopyranoside: [18894-12-7] *Gibberellin A_8 2-glucoside.* ***Phaseolus ε.*** *Gibberellin A_8 3-glucopyranoside (incorr.)*
$C_{25}H_{34}O_{12}$ 526.536
Isol. from *Hordeum vulgare* (barley) and *Phaseolus coccineus* (scarlet runner bean). Amorph. $[\alpha]_D^{17}$ +6.7 (c, 0.6 in MeOH).

2-O-β-D-Glucopyranoside, hexa-Ac:
Cryst. (EtOAc/petrol). Mp 247°. $[\alpha]_D^{13}$ +14.6 (MeOH).

2-Epimer: [72533-76-7] ***Gibberellin A_{56}***
$C_{19}H_{24}O_7$ 364.394
Amorph. Mp 217-219° (as Me ester).

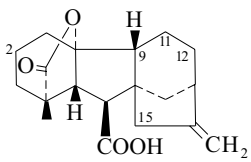
12α-Hydroxy: [147526-81-6] ***Gibberellin A_{89}***
$C_{19}H_{24}O_8$ 380.394

15β-Hydroxy: ***Gibberellin A_{75}***
$C_{19}H_{24}O_8$ 380.394
Constit. of seeds of *Helianthus annuus* (sunflower).

MacMillan, J. *et al., Tetrahedron*, 1962, **18**, 349 (*struct*)
Crozier, A. *et al., Can. J. Bot.*, 1970, **48**, 867 (*biochem*)
Schreiber, K. *et al., Phytochemistry*, 1970, **9**, 189-198 (*2-glucoside*)
Yokota, T. *et al., Agric. Biol. Chem.*, 1971, **35**, 583 (*struct*)
Murofushi, N. *et al., Agric. Biol. Chem.*, 1979, **43**, 2179 (*deriv*)
Castellaro, S.J. *et al., J.C.S. Perkin 1*, 1990, 145 (GA_{75})
Sheng, C. *et al., Phytochemistry*, 1992, **31**, 4055-4057 (GA_{89})
Pankrushina, N.A. *et al., Khim. Prir. Soedin.*, 1994, **30**, 663; *Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 613 (*synth*)
Senns, B. *et al., Phytochemistry*, 1998, **48**, 1275-1280 (*2-glucoside*)

Gibberellin A_9 G-112

[427-77-0]



$C_{19}H_{24}O_4$ 316.396
Cryst. (Me_2CO/petrol), gum. Mp 208-211°. $[\alpha]_D^{17}$ -22 (c, 0.25 in EtOH).

1,2-Didehydro: [59102-35-1] ***Gibberellin A_{120}***
$C_{19}H_{22}O_4$ 314.38
Constit. of immature *Prunus persica* (peach) seeds.

9,11-Didehydro: [121688-19-5] ***Gibberellin A_{73}***
$C_{19}H_{22}O_4$ 314.38

1α-Hydroxy: [328058-45-3] ***Gibberellin A_{119}***
$C_{19}H_{24}O_5$ 332.396
Constit. of immature *Prunus persica* (peach) seeds.

1β-Hydroxy, 2β,3β-epoxide: [188895-37-6] ***Gibberellin A_{94}***
$C_{19}H_{22}O_6$ 346.379
Constit. of *Triticum aestivum* (wheat). Solid (EtOAc/petrol). Mp 142-144°.

2α-Hydroxy: [51787-36-1] ***Gibberellin A_{40}***
$C_{19}H_{24}O_5$ 332.396
Cryst. Mp 212-213°.

2β-Hydroxy: [56978-14-4] ***Gibberellin A_{51}***
$C_{19}H_{24}O_5$ 332.396
Found in immature seeds of *Pisum sativum* (pea). Cryst. (EtOAc/hexane). Mp 190-193°.

12α-Hydroxy: [52846-39-6] ***Gibberellin A_{70}***
$C_{19}H_{24}O_5$ 332.396
Constit. of immature *Prunus persica* (peach) seeds.

12α-Hydroxy, 1,2-didehydro: [357401-43-5] ***Gibberellin A_{121}***
$C_{19}H_{22}O_5$ 330.38
Constit. of immature *Prunus persica* (peach) seeds.

12α-Hydroxy, 9,11-didehydro, Me ester: [220786-72-1] ***Gibberellin A_{117}***
$C_{20}H_{24}O_5$ 344.407

12β-Hydroxy: [90364-70-8] ***Gibberellin A_{69}***
$C_{19}H_{24}O_5$ 332.396
Constit. of immature *Prunus persica* (peach) seeds.

12β-Hydroxy, 1,2-didehydro: [357401-44-6] ***Gibberellin A_{122}***
$C_{19}H_{22}O_5$ 330.38
Constit. of immature *Prunus persica* (peach) seeds.

13α-Hydroxy, 9,11-didehydro: [132842-67-2] ***Gibberellin A_{109}***
$C_{19}H_{22}O_5$ 330.38

15β-Hydroxy: [55812-47-0] ***Gibberellin A_{45}***
$C_{19}H_{24}O_5$ 332.396
Constit. of *Pyrus communis* (pear).

3β,12α-Dihydroxy: [77288-90-5] ***Gibberellin A_{58}***
$C_{19}H_{24}O_6$ 348.395
Obt. from *Cucurbita maxima*. Gum.

3α,15β-Dihydroxy: [164932-63-2] ***3-Epigibberellin A_{63}***
$C_{19}H_{24}O_6$ 348.395

3β,15β-Dihydroxy: [63351-80-4] ***Gibberellin A_{63}***
$C_{19}H_{24}O_6$ 348.395
From *Pyrus communis* (pear).

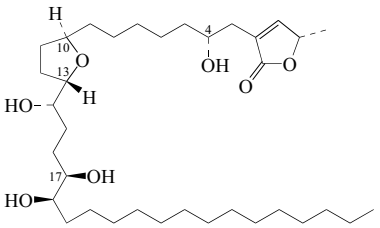
1β,3β,12α-Trihydroxy: [55035-85-3] ***Gibberellin A_{55}***
$C_{19}H_{24}O_7$ 364.394
Constit. of *Curcurbita maxima*. Gum.

Hanson, J.R. *et al., J.C.S.*, 1965, 3550 (*struct*)
Mori, K. *et al., Tetrahedron*, 1969, **25**, 1293 (*synth*)
Yamagushi, I. *et al., J.C.S. Perkin 1*, 1975, 996 (*derivs*)
Bearder, J.R. *et al., Tet. Lett.*, 1975, 669 (*deriv*)
Beeley, L.J. *et al., J.C.S. Perkin 1*, 1976, 1022 (*synth*)
Sponsel, V.M. *et al., Planta*, 1977, **135**, 129 (*deriv*)
Duri, Z.J. *et al., J.C.S. Perkin 1*, 1981, 161 (GA_9, *synth*)
Kamiya, Y. *et al., Phytochemistry*, 1983, **22**, 681-689 (*biosynth*)
Beale, M.H. *et al., Phytochemistry*, 1984, **23**, 565-567 (GA_{58})
Dolan, S.C. *et al., J.C.S. Perkin 1*, 1985, 651-654 (GA_{45}, GA_{63})
Abouamer, K.M. *et al., J.C.S. Perkin 1*, 1987, 1991-1994 (GA_9, *cryst struct*)
Yamane, H. *et al., Tet. Lett.*, 1988, **29**, 3959-3962 (GA_{73})
Sassa, T. *et al., Agric. Biol. Chem.*, 1989, **37**, 303-304 (GA_9)
Shimano, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 276-278 (GA_{55}, *synth*)
Kraft-Klaunzer, P. *et al., Tet. Lett.*, 1990, **31**, 6235-6238 (*synth*)
Yamauchi, T. *et al., Phytochemistry*, 1995, **38**, 1345-1348 (*3-Epi-GA_{63}*)
Findlow, S. *et al., J.C.S. Perkin 1*, 1997, 751-757 (GA_{94})
Wynne, G.M. *et al., Phytochemistry*, 1998, **47**, 1177; **49**, 1837-1840 (GA_{109}, GA_{117})
Nakayama, M. *et al., Phytochemistry*, 2001, **57**, 749-758 (GA_{69}, GA_{70}, GA_{119}, GA_{120}, GA_{121}, GA_{122})

Gigantetrocin A G-113

[134955-48-9]

[163253-85-8]
Howiicin F



$C_{35}H_{64}O_7$ 596.886
Acetogenin. Constit. of *Annona muricata* (soursop). Amorph. solid. Mp 80-81°. $[\alpha]_D^{25}$ +10.3 ($CHCl_3$).

4-Ac: [181815-43-0] ***4-Acetylgigantetrocin A***
$C_{37}H_{66}O_8$ 638.924
Oil. $[\alpha]_D$ +13.5 (c, 0.11 in MeOH). λ_{max} 208 (log ε 3.2) (EtOH).

4-Deoxy: [134955-49-0]

[163253-83-6] ***Gigantriocin***. *Howiicin D*
$C_{35}H_{64}O_6$ 580.887
Cryst. Mp 69-71°. $[\alpha]_D$ +18 ($CHCl_3$).

17,18-Diepimer: [153220-49-6]

[163253-86-9] ***Gigantetrocin B***. *Howiicin G*
$C_{35}H_{64}O_7$ 596.886
Constit. of *Annona muricata* (soursop). Mp 91-92°. $[\alpha]_D^{25}$ +4.1 (c, 0.41 in $CHCl_3$). Identity of Howiicin G stereochem. with Gigantetrocin B not confirmed.

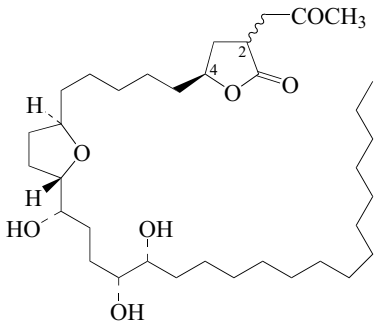
Stereoisomer(?):

[144239-83-8, 144239-84-9] *Densicomacin*
$C_{35}H_{64}O_7$ 596.886
Cryst. Mp 83-84°. $[\alpha]_D$ +26 (c, 0.05 in MeOH). Isol. as a mixture of the C-14 epimers of Gigantetrocin A and are known as Densiomacin 1 and 2. λ_{max} 209 (ε 7080) (MeOH) (Berdy).

Fang, X.-P. *et al., Heterocycles*, 1991, **32**, 11 (*isol, pmr, cmr*)
Yu, J.G. *et al., J.O.C.*, 1992, **57**, 6198 (*Densicomacin*)
Rieser, M.J. *et al., Helv. Chim. Acta*, 1993, **76**, 2433 (*Gigantetrocin B*)
Yu, J.G. *et al., J.O.C.*, 1993, **58**, 3222
Yang, R.-Z. *et al., Zhiwu Xuebao*, 1994, **36**, 561-567; *CA*, **122**, 310664b (*Howiicins*)
Zeng, L. *et al., Bioorg. Med. Chem.*, 1996, **4**, 1271-1279 (*4-Ac*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)
Wang, Z.-M. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 667-670 (*synth*)

Gigantetrocinone G-114

[152686-53-8, 152784-20-8]

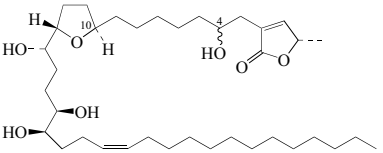


$C_{35}H_{64}O_7$ 596.886
Constit. of *Asimina triloba* (pawpaw). Mp 91-92°. $[\alpha]_D$ +10 (c, 0.2 in $CHCl_3$). A mixt. of 2,4-*cis* and 2,4-*trans*-isomers. CA name is incorrect λ_{max} 205 (MeOH) (Berdy).

Zhao, G.-X. *et al., Phytochemistry*, 1993, **33**, 1065-1073 (*isol, struct*)
Ye, Q. *et al., J. Nat. Prod.*, 1995, **58**, 1398-1406 (*isol*)

Gigantetronenin G-115

[145403-31-2]



$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona muricata* (soursop). Wax. Mp 57-59°. $[\alpha]_D^{20}$ +10 (c, 0.2 in $CHCl_3$). λ_{max} 208 (ε 6000) (MeOH) (Berdy).

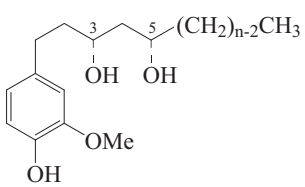
4-Deoxy: [145403-35-6] ***Gigantrionenin***
$C_{37}H_{66}O_6$ 606.925
Wax. Mp 55-57°. $[\alpha]_D$ +17 (c, 0.2 in $CHCl_3$).

4-Deoxy, 10-epimer: [182073-16-1] **cis-*Gigantrionenin***
$C_{37}H_{66}O_6$ 606.925
Oil. $[\alpha]_D$ +8.5 (c, 0.2 in MeOH). λ_{max} 207 (log ε 3.1) (EtOH).

Fang, X.-P. *et al., J. Nat. Prod.*, 1992, **55**, 1655 (*isol, pmr, cmr, ms*)
Zeng, L. *et al., Bioorg. Med. Chem.*, 1996, **4**, 1271 (*cis-Gigantrionenin*)

Gingerdiols G-116

Gingediols



Minor constits. of ginger (*Zingiber officinale*).

[4]-Gingerdiol [53254-75-4]
1-(4-Hydroxy-3-methoxyphenyl)-3,5-octanediol, 9CI
$C_{15}H_{24}O_4$ 268.352

3,5-Di-Ac: [53254-50-5]
$C_{19}H_{28}O_6$ 352.427
Constit. of ginger (*Zingiber officinale*).

[6]-Gingerdiol [53318-09-5]
1-(4-Hydroxy-3-methoxyphenyl)-3,5-decanediol, 9CI
$C_{17}H_{28}O_4$ 296.406
Oil. $[\alpha]_D^{25}$ +7.5 (c, 1.5 in $CHCl_3$).

5-O-β-D-Glucopyranoside:
$C_{23}H_{38}O_9$ 458.548
Constit. of ginger (*Zingiber officinale*) rhizomes. Oil. $[\alpha]_D^{24}$ -13.3 (c, 0.72 in MeOH).

4′-O-β-D-Glucopyranoside:
$C_{23}H_{38}O_9$ 458.548
Constit. of ginger (*Zingiber officinale*) rhizomes. Amorph. powder. $[\alpha]_D^{24}$ -29.3 (c, 0.69 in MeOH).

3-Ac: [143519-17-9]
$C_{19}H_{30}O_5$ 338.443
Constit. of ginger (*Zingiber officinale*) rhizomes. Oil.

5-Ac: [143519-16-8]
$C_{19}H_{30}O_5$ 338.443
Constit. of ginger (*Zingiber officinale*) rhizomes. Oil.

3,5-Di-Ac: [143615-75-2]
$C_{21}H_{32}O_6$ 380.48
Constit. of ginger (*Zingiber officinale*) rhizomes. Oil. $[\alpha]_D^{20}$ -3.8 (c, 0.5 in $CHCl_3$).

Tri-Ac: [39886-90-3] *Dihydrogingerol*
$[\alpha]_D^{23}$ -0.8.

3′-Me ether, 3,5-di-Ac: [143519-18-0]
$C_{22}H_{34}O_6$ 394.507
Constit. of ginger (*Zingiber officinale*) rhizomes. Oil. $[\alpha]_D^{24}$ -1.4 (c, 0.7 in $CHCl_3$).

3-Epimer, 3-Ac:
$C_{19}H_{30}O_5$ 338.443

3-Epimer, 5-Ac:
$C_{19}H_{30}O_5$ 338.443

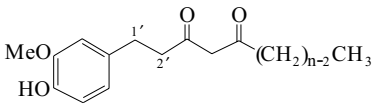
[8]-Gingerdiol [53254-76-5]
1-(4-Hydroxy-3-methoxyphenyl)-3,5-dodecanediol, 9CI
$C_{19}H_{32}O_4$ 324.459

[10]-Gingerdiol [53254-77-6]
1-(4-Hydroxy-3-methoxyphenyl)-3,5-tetradecanediol, 9CI
$C_{21}H_{36}O_4$ 352.513

[39886-85-6, 99827-31-3]

Murata, T. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2291 (*isol, struct, ir, pmr*)
Masada, Y. *et al., Yakugaku Zasshi*, 1974, **94**, 735; *CA*, **81**, 166345p (*isol*)
Kimura, I. *et al., Jpn. J. Pharmacol.*, 1988, **48**, 257 (*pharmacol*)
Kikuzaki, H. *et al., Phytochemistry*, 1992, **31**, 1783 (*isol, struct*)
Juch, M. *et al., Helv. Chim. Acta*, 1997, **80**, 436-448 (*Plectranthus acetates*)
Sekiwa, Y. *et al., J. Agric. Food Chem.*, 2000, **48**, 373-377 (*6-Gingerdiol glucosides*)

Gingerdiones G-117



A series of homologous compds. from ginger (*Zingiber officinale*). Enolised β-diketones.

[6]Gingerdione [61871-71-4]
1-(4-Hydroxy-3-methoxyphenyl)-3,5-decanedione
$C_{17}H_{24}O_4$ 292.374
Constit. of *Zingiber officinale* (ginger). Oil.

1′,2′-Didehydro: [76060-35-0] ***[6]-Dehydrogingerdione***
$C_{17}H_{22}O_4$ 290.358
Isol. from *Zingiber officinale* (ginger). Yellow needles. Mp 83.5-84.5°. Enolised.

[8]Gingerdione [77334-06-6]
1-(4-Hydroxy-3-methoxyphenyl)-3,5-dodecanedione, 9CI
$C_{19}H_{28}O_4$ 320.428
Constit. of *Zingiber officinale* (ginger).

1,2-Didehydro: [77334-08-8] ***[8]-Dehydrogingerdione***
$C_{19}H_{26}O_4$ 318.412
From *Zingiber officinale* (ginger). Mp 48-49°.

[10]Gingerdione
1-(4-Hydroxy-3-methoxyphenyl)-3,5-tetradecanedione
$C_{21}H_{32}O_4$ 348.481
Isol. from *Zingiber officinale* (ginger). Solid.

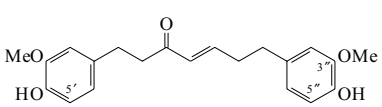
1′,2′-Didehydro: [82206-04-0] ***[10]-Dehydrogingerdione***
$C_{21}H_{30}O_4$ 346.466
From *Zingiber officinale* (ginger). Yellow needles. Mp 65-69.5°.

[12]Gingerdione [91815-31-5]
1-(4-Hydroxy-3-methoxyphenyl)-3,5-hexadecanedione, 9CI
$C_{23}H_{36}O_4$ 376.535
From *Zingiber officinale* (ginger). Mp 44-45°.

Denniff, P. *et al., J.C.S. Perkin 1*, 1981, 82 (*synth*)
Harvey, D.J. *et al., J. Chromatogr.*, 1981, **212**, 75
Kiuchi, F. *et al., Chem. Pharm. Bull.*, 1982, **30**, 754

Gingerenone A G-118

[128700-97-0]
1,7-Bis(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one, 9CI



$C_{21}H_{24}O_5$ 356.418
Constit. of *Zingiber officinale* (ginger). Oil.

Di-O-de-Me: [41137-87-5] *1,7-Bis(3,4-dihydroxyphenyl)-4-hepten-3-one, 9CI.* ***Hirsutenone.*** *Hirsutanone (incorr.)*
$C_{19}H_{20}O_5$ 328.364The name Hirsuta-

none, used in CA, is apparently incorrect.

5′-Methoxy: [128700-99-2] *1-(4-Hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one.* ***Isogingerenone B***
$C_{22}H_{26}O_6$ 386.444
Constit. of *Zingiber officinale* (ginger).

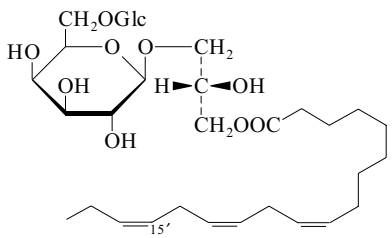
5′′-Methoxy: [128700-98-1] *7-(4-Hydroxy-3,5-dimethoxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one.* ***Gingerenone B***
$C_{22}H_{26}O_6$ 386.444
Constit. of *Zingiber officinale* (ginger).

3′′-Demethoxy: [128701-01-9] *1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-4-hepten-3-one.* ***Gingerenone C***
$C_{20}H_{22}O_4$ 326.391
Constit. of *Zingiber officinale* (ginger).
Oil.

Endo, K. *et al., Phytochemistry*, 1990, **29**, 797-799 (*isol, pmr, cmr*)
Martin-Cordero, C. *et al., Phytochemistry*, 2001, **58**, 567-569 (*Hirsutenone*)

Gingerglycolipid A G-119

[145937-22-0]



$C_{33}H_{56}O_{14}$ 676.797
Constit. of *Zingiber officinale* (ginger).
Powder. $[\alpha]_D^{20}$ +37.7 (c, 10 in MeOH).

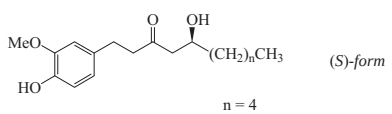
15′,16′-Dihydro: [88168-90-5] ***Gingerglycolipid B***
$C_{33}H_{58}O_{14}$ 678.813
From *Zingiber officinale* (ginger). Powder. $[\alpha]_D^{20}$ +50.9 (c, 7.5 in MeOH).

12′,13′,15′,16′-Tetrahydro: [35949-86-1] ***Gingerglycolipid C***
$C_{33}H_{60}O_{14}$ 680.829
From *Zingiber officinale* (ginger). Powder. $[\alpha]_D^{20}$ +26.9 (c, 10 in MeOH).

Baruah, P. *et al., Phytochemistry*, 1983, **22**, 1741 (*isol, pmr*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1226 (*isol, pmr, cmr*)

[6]-Gingerol G-120

5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-decanone, 9CI



(*S*)-*form*

$C_{17}H_{26}O_4$ 294.39
The major member of a series of compounds present in ginger. The name derives from its retroaldol cleavage to hexanal. [3], [4], [5], [8] and [10]Gingerols have also been isol..

(R)-form
Yellow oil. $[\alpha]_D$ -25.1 (c, 1 in $CHCl_3$).

(S)-form [23513-14-6]
Constit. of ginger *Zingiber officinale*. Pungent yellow oil. $[\alpha]_D$ +26.5 (c, 1 in $CHCl_3$). λ_{max} 282 (ϵ 2560) (MeOH) (Berdy). λ_{max} 211 ; 282 (EtOH) (Berdy).

▶ HE0757000

Me ether: ***Methylgingerol***
$C_{18}H_{28}O_4$ 308.417
Present in ginger. Cryst. (hexane/C_6H_6). Mp 65.5-66°. $[\alpha]_D^{23}$ +28.4 (c, 2 in $CHCl_3$).

[23513-08-8, 23513-15-7, 41743-67-3, 41743-68-4, 41743-69-5, 99742-03-7]

Connell, D.W. *et al., Aust. J. Chem.*, 1969, **22**, 1033 (*isol, struct*)
Enders, D. *et al., Chem. Ber.*, 1979, **112**, 3703 (*synth*)
Denniff, P. *et al., J.C.S. Perkin 1*, 1980, 2637 (*biosynth*)
Giovanni, B.P. *et al., J.C.S. Perkin 1*, 1982, 2983 (*synth*)
Kato, N. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1679 (*synth*)
Solladie, G. *et al., J.O.C.*, 1993, **58**, 2181 (*synth, bibl*)
Fleming, S.A. *et al., Synth. Commun.*, 1999, **29**, 1933-1939 (*synth, pmr, cmr*)

[8]-Gingerol G-121

[107257-17-0]
5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-dodecanone, 9CI
As [6]-Gingerol, G-120 with
n = 6
$C_{19}H_{30}O_4$ 322.444

(R)-form [135272-33-2]
Mp 35°. $[\alpha]_D^{25}$ -25.9 (c, 0.5 in $CHCl_3$).

(S)-form [23513-08-8]
Constit. of ginger, the rhizome of *Zingiber officinale*. Mp 29-30°. $[\alpha]_D$ +26 (c, 0.9 in $CHCl_3$).

(±)-form [77398-92-6]
Mp 32-34°.

Cornell, D.W. *et al., Aust. J. Chem.*, 1969, **22**, 1033-1043 (*isol, struct*)
Shogi, N. *et al., J. Pharm. Sci.*, 1982, **71**, 1174-1175 (*isol, uv, pmr, cmr*)
Kato, N. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1679-1682 (*synth*)
Martin, M. *et al., Chirality*, 1991, **3**, 151-155 (*enantiomers, synth, ir, pmr*)
Solladie, G. *et al., J.O.C.*, 1993, **58**, 2181-2185 (*synth, pmr, cmr*)
Fleming, S.A. *et al., Synth. Commun.*, 1999, **29**, 1933-1939 (*synth, pmr, cmr*)

[10]-Gingerol G-122

[107257-18-1]
5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-tetradecanone, 9CI
As [6]-Gingerol, G-120 with
n = 8
$C_{21}H_{34}O_4$ 350.497

(S)-form [23513-15-7]
Constit. of ginger, the rhizome of *Zingiber officinale*. Mp 45-46°. $[\alpha]_D$ +22.7 (c, 1.02 in $CHCl_3$).

(±)-form [77398-93-7]
Solid (petrol). Mp 44-45° (40°).

Cornell, D.W. *et al., Aust. J. Chem.*, 1969, **22**, 1033-1043 (*isol, struct*)
Shogi, N. *et al., J. Pharm. Sci.*, 1982, **71**, 1174-1175 (*isol, uv, pmr, cmr*)
Kato, N. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1679-1682 (*synth*)
Solladie, G. *et al., J.O.C.*, 1993, **58**, 2181-2185 (*synth, pmr, cmr*)
Fleming, S.A. *et al., Synth. Commun.*, 1999, **29**, 1933-1939 (*synth, pmr, cmr*)

[12]-Gingerol G-123

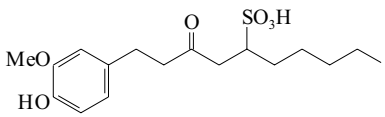
[104264-55-3]

[77333-95-0, 107257-19-2]
5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-hexadecanone, 9CI
As [6]-Gingerol, G-120 with
n = 10
$C_{23}H_{38}O_4$ 378.551
Constit. of *Zingiber officinale* (ginger).

Kato, N. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1679-1682 (*synth*)
Chen, C.C. *et al., J. Chromatogr.*, 1986, **360**, 163-173 (*isol*)

6-Gingesulfonic acid G-124

[145937-21-9]

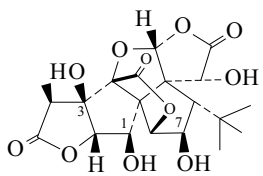


$C_{17}H_{26}O_6S$ 358.455
Isol. from the rhizome of *Zingiber officinale* (ginger). Powder. $[\alpha]_D$ -1 (MeOH).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1226

Ginkgolide C G-125

[15291-76-6]



$C_{20}H_{24}O_{11}$ 440.403
Bitter principle from *Ginkgo biloba* (ginkgo). Cryst. (EtOH). Mp 280° dec. $[\alpha]_D$ -19 (c, 1 in dioxan). Ginkgolides A, B and C are components of commercially available *Ginkgo biloba* extract (GBE).

1-Deoxy: [107438-79-9] ***Ginkgolide J***
$C_{20}H_{24}O_{10}$ 424.404
Isol. from *Ginkgo biloba* (ginkgo). Prisms. Mp 320°. $[\alpha]_D^{20}$ -2.5 (c, 1 in dioxan). Dec. at 295°.

3-Deoxy: [15291-78-8] ***Ginkgolide M***
$C_{20}H_{24}O_{10}$ 424.404
Isol. from *Ginkgo biloba* (ginkgo). Cryst. (EtOH). Mp 280° dec. $[\alpha]_D$ -39 (c, 1 in dioxan).

7-Deoxy: [15291-77-7] ***Ginkgolide B. BN52021***
$C_{20}H_{24}O_{10}$ 424.404
Isol. from *Ginkgo biloba* (ginkgo). Cryst. (EtOH). Mp 280° dec. $[\alpha]_D$ -63 (c, 1 in dioxan). Log P -2.73 (uncertain value) (calc).

1,7-Dideoxy: [15291-75-5] ***Ginkgolide A***

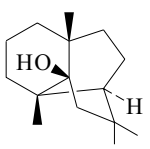
$C_{20}H_{24}O_9$ 408.404
Bitter principle from *Ginkgo biloba* (ginkgo). Cryst. (EtOH). Mp 280° dec. $[\alpha]_D$ -39 (c, 1 in dioxan). Log P -1.57 (uncertain value) (calc).

[99796-69-7]

Sakabe, N. *et al., Chem. Comm.*, 1967, 259-261 (*Ginkgolide A, cryst struct*)
Maruyama, M. *et al., Tet. Lett.*, 1967, 299-302; 303-308; 309-313; 315-319; 321-326 (*isol, struct, pmr*)
Nakanishi, K. *et al., J.A.C.S.*, 1971, **93**, 3546-3547 (*Ginkgolide B, biosynth*)
Braquet, P. *et al., Adv. Prostaglandin, Thromboxane, Leukotriene Res.*, 1986, **16**, 179-198 (*rev*)
Weinges, K. *et al., Annalen*, 1986, 1057-1066; 1991, 81-83 (*cryst struct, synth, Ginkgolide B, Ginkgolide C*)
Weinges, K. *et al., Annalen*, 1987, 521-526 (*Ginkgolide J*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1140
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 451 (*bibl, synth*)
Van Beek, T.A. *et al., Tetrahedron*, 1996, **52**, 4505-4514 (*cmr*)
Crimmins, M.T. *et al., J.A.C.S.*, 2000, **122**, 8453-8463 (*Ginkgolide B, synth*)
Zhao, J.-P. *et al., Acta Cryst. C*, 2002, **58**, o195-o198 (*cryst struct*)

Ginsenol G-126

[117591-80-7]
*Octahydro-2,2,4,7*a*-tetramethyl-1,4-ethano-3a*H*-inden-3*a*-ol, 9CI*

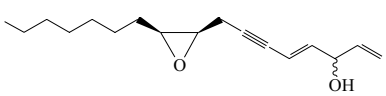


$C_{15}H_{26}O$ 222.37
Isol. from ginseng plant rootlets. Oil. $[\alpha]_D$ -18.3 (c, 1.1 in $CHCl_3$).

Iwabuchi, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2447 (*isol, pmr, cmr, struct*)

Ginsenoyne I G-127

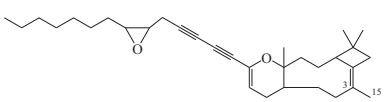
[141947-40-2]
9,10-Epoxy-1,4-heptadecadien-6-yn-3-ol



$C_{17}H_{26}O_2$ 262.391
Found in ginseng roots. Oil. $[\alpha]_D$ -81.1 (c, 4.35 in $CHCl_3$). λ_{max} 229 (ϵ 14500) (EtOH) (Berdy).

Hirakura, K. *et al., Phytochemistry*, 1992, **31**, 899 (*isol, pmr, cmr, struct*)

Ginsenoyne M G-128

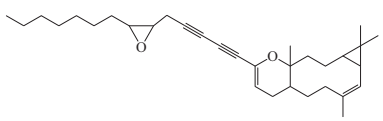


$C_{32}H_{46}O_2$ 462.714
Constit. of the roots of *Panax ginseng* (ginseng). Oil. $[\alpha]_D$ -58.6 (c, 2.1 in $CHCl_3$). λ_{max} 212 (log ϵ 4.35); 241 (log ϵ 3.79); 253 (log ϵ 4.01); 267 (log ϵ 4.22); 283 (log ϵ 4.17) (EtOH).

$\Delta^{3,15}$-Isomer: ***Ginsenoyne L***
$C_{32}H_{46}O_2$ 462.714
Constit. of the roots of *Panax ginseng*. Oil. $[\alpha]_D$ -37.3 (c, 3.3 in $CHCl_3$). λ_{max} 212 (log ϵ 4.25); 240 (log ϵ 3.72); 253 (log ϵ 3.95); 267 (log ϵ 4.15); 283 (log ϵ 4.1) (EtOH).

Hirakura, K. *et al., Heterocycles*, 2000, **53**, 2451-2457

Ginsenoyne N G-129

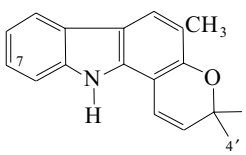


$C_{32}H_{46}O_2$ 462.714
Constit. of the roots of *Panax ginseng* (ginseng). Oil. $[\alpha]_D$ +10.3 (c, 1.7 in $CHCl_3$). λ_{max} 212 (log ϵ 4.33); 240 (log ϵ 3.77); 253 (log ϵ 3.95); 267 (log ϵ 4.15); 283 (log ϵ 4.11) (EtOH).

Hirakura, K. *et al., Heterocycles*, 2000, **53**, 2451-2457

Girinimbine G-130

[23095-44-5]
*3,11-Dihydro-3,3,5-trimethylpyrano[3,2-*a*]carbazole, 9CI*



$C_{18}H_{17}NO$ 263.338
Alkaloid from the roots of *Murraya koenigii* (curry leaf tree). Cryst. (cyclohexane, hexane or CH_2Cl_2/hexane). Mp 175°.

N-*Me:*
Cryst. (EtOH). Mp 150°.

7-Hydroxy: [134779-17-2] ***Murrayamine A***. *Mukoenine C*
$C_{18}H_{17}NO_2$ 279.338
Alkaloid from the roots of *Murraya koenigii* (curryleaf tree). Needles (Me_2CO). Mp 162-163°. Mukoenine C from *M. koenigii* descr. as an oil λ_{max} 221 (ϵ 10450); 240 (ϵ 11750); 294 (ϵ 9100); 342 (ϵ 2240); 349 (ϵ 1600); 360 (ϵ 1620) (MeOH) (Berdy).

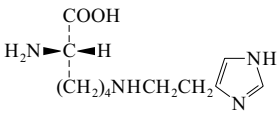
4′-Acetoxy: [175669-19-9] ***Murrayamine K***
$C_{20}H_{19}NO_3$ 321.375
Needles (Me_2CO). Mp 127-128°.

7-Hydroxy, 4′-acetoxy: [175669-18-8] ***Murrayamine I***
$C_{20}H_{19}NO_4$ 337.374
Oil.

Dutta, N.L. *et al., Indian J. Chem.*, 1969, **7**, 307 (*uv, pmr, struct*)
Kureel, S.P. *et al., Chem. Ind. (London)*, 1970, 1262 (*synth*)
Joshi, B.S. *et al., Tetrahedron*, 1970, **26**, 1475 (*isol, uv, ir, pmr*)
Joshi, B.S. *et al., Phytochemistry*, 1972, **11**, 2065 (*isol, uv, ir, pmr*)
Oikawa, Y. *et al., Heterocycles*, 1976, **5**, 233 (*synth, ms*)
Narasimhan, N.S. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 329 (*synth*)
Roy, S. *et al., J. Indian Chem. Soc.*, 1981, **58**, 1212 (*isol*)
Wu, T.-S. *et al., Phytochemistry*, 1991, **30**, 1048; 1052; 1996, **41**, 1433 (*Murrayamine A, Murrayamine I, Murrayamine K*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*Mukoenine C*)
Knölker, H.J. *et al., Tet. Lett.*, 1996, **37**, 7947 (*synth*)

Gizzerosine G-131

N^6-*[2-(1*H*-Imidazol-4-yl)ethyl]lysine, 9CI. 2-Amino-9-(4-imidazolyl)-7-azanonanoic acid*



(*S*)-*form*

$C_{11}H_{20}N_4O_2$ 240.305

(R)-form [103548-50-1]
D-form
Cryst. (MeOH) (as dihydrochloride). Mp 252-254° dec. (dihydrochloride). $[\alpha]_D^{22}$ -9.1 (c, 1.26 in H_2O). CAS no. refers to hydrochloride.

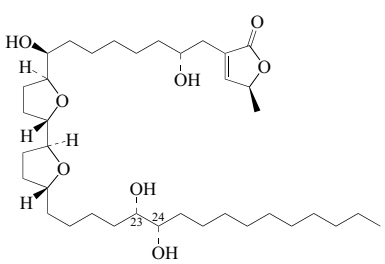
(S)-form [89238-78-8]
L-form
Isol. from mackerel meal. Prod. as a contaminant during fish meal manufacturing by reaction between histidine and protein in the fish meat. Causes gizzard erosion ("black vomit") in chicks. Cryst. (MeOH aq.) (as dihydrochloride). Mp 251-252° dec. (dihydrochloride). $[\alpha]_D^{22}$ +10.3 (c, 1.28 in H_2O).

(±)-form [88252-77-1]

[88238-60-2]
Fine prisms (MeOH aq.)(as dihydrochloride). Mp 253-256° dec. (as dihydrochloride).

Okazaki, T. *et al., Agric. Biol. Chem.*, 1983, **47**, 2949 (*isol*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 5307 (*synth*)
Murakita, H. *et al., J. Chromatogr.*, 1990, **515**, 527-530 (*hplc*)
Rosselot, G. *et al., Poultry Sci.*, 1996, **75**, 873-880

Glabracin A G-132



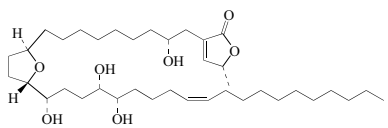
$C_{37}H_{66}O_8$ 638.924

Constit. of the leaves of *Annona glabra* (pond apple). Wax. $[\alpha]_D^{25}$ -11.6 (c, 0.01 in $CHCl_3$). C-23/C-24 possesses *erythro*-config. λ_{max} 220 (log ϵ 3.89) (MeOH).

Diastereoisomer: ***Glabracin B***
$C_{37}H_{66}O_8$ 638.924
Constit. of the leaves of *Annona glabra* (pond apple). Wax. $[\alpha]_D^{25}$ +16.9 (c, 0.05 in $CHCl_3$). C-23/C-24 possesses *threo*-config. λ_{max} 223 (log ϵ 3.58) (MeOH). λ_{max} 221 (ϵ 4466); 223 (ϵ 3800) (MeOH) (Berdy).

Liu, X.-X *et al., Bioorg. Med. Chem.*, 1998, **6**, 959-965 (*isol, uv, ir, pmr, cmr, ms*)

Glabranin G-133

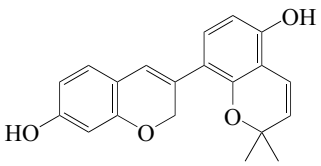


$C_{37}H_{66}O_7$ 622.924
Constit. of the seeds of *Annona glabra* (pond apple). Amorph.

Gallardo, T. *et al., Phytochemistry*, 1998, **47**, 811-816 (*isol, pmr, cmr, ms*)

Glabrene G-134

[60008-03-9]
*2′,2′-Dimethyl[3,8′-bi-2*H*-1-benzopyran]-5′,7-diol, 9CI*



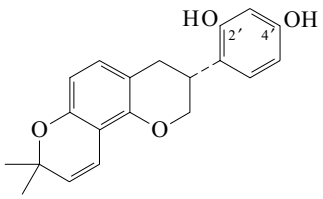
$C_{20}H_{18}O_4$ 322.36
Struct. revised in 1996. Constit. of root of *Glycyrrhiza glabra* (licorice). Pale brown plates (C_6H_6/Me_2CO); plates (MeOH aq.). Mp 200-203° dec. λ_{max} 245 ; 283 ; 293 ; 321 (MeOH) (Berdy). λ_{max} 248 (ϵ 7400); 281 (ϵ 18000); 297 (ϵ 19600); 324 (ϵ 20900) (EtOH) (Berdy).

Di-Ac:
$C_{24}H_{22}O_6$ 406.434
Needles (EtOH). Mp 148-150°.

Kinoshita, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 991-994 (*isol, pmr, ir, uv*)
Mitscher, L.A. *et al., Heterocycles*, 1978, **9**, 1533 (*uv, pmr, ms*)
Fukai, T. *et al., Phytochemistry*, 1996, **43**, 1119-1124 (*pmr, cmr, ms, struct*)
Kinoshita, T. *et al., Nat. Prod. Lett.*, 1997, **9**, 289-296 (*isol, cmr, struct*)

Glabridin G-135

*4-[3,4-Dihydro-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b′*]dipyran-3-yl]-1,3-benzenediol*



$C_{20}H_{20}O_4$ 324.376

(R)-form [59870-68-7]
Isol. from *Glycyrrhiza glabra* (licorice). Plates (C_6H_6). Mp 154-155°. $[\alpha]_D^{20}$ +8.2 (c, 2.07 in $CHCl_3$). λ_{max} 228 ; 281 (ϵ 12500); 282 ; 287 (ϵ 11300); 312 (MeOH) (Berdy). λ_{max} 281 (ϵ 15200); 288 ; 312 (EtOH) (Berdy).

2′-Me ether: ***2′-O-Methylglabridin***
$C_{21}H_{22}O_4$ 338.402
Isol. from *Glycyrrhiza glabra* (licorice). Needles (EtOH). Mp 124-126°.

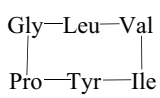
4′-Me ether: [68978-09-6] ***4′-O-Methylglabridin***
$C_{21}H_{22}O_4$ 338.402
Isol. from *Glycyrrhiza glabra* (licorice). Needles (cyclohexane). Mp 120-121°. $[\alpha]_D^{28}$ +10.2 (c, 1.04 in $CHCl_3$).

3′-Hydroxy, 4′-Me ether: [74046-05-2] ***3′-Hydroxy-4′-methoxyglabridin***
$C_{21}H_{22}O_5$ 354.402
Isol. from *Glycyrrhiza glabra* (licorice). Cryst. (cyclohexane). Mp 104-105°. $[\alpha]_D^{25}$ +10.28 (c, 1.41 in $CHCl_3$). Struct. revised in 1996. Prev. assigned as 3′-Methoxyglabridin λ_{max} 280 (ϵ 9600); 311 (ϵ 2300) (MeOH) (Berdy). λ_{max} 279 ; 288 (EtOH) (Berdy).

Saitoh, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 752 (*isol, struct*)
Mitscher, L.A. *et al., J. Nat. Prod.*, 1980, **43**, 259 (*isol, derivs*)
Vermes, B. *et al., Annalen*, 1983, 2034 (*synth*)
Castro, O. *et al., J. Nat. Prod.*, 1986, **49**, 680 (*deriv*)
Seifert, K. *et al., Z. Naturforsch., C*, 1993, **48**, 550 (*isol, pmr, cmr*)
Kinoshita, T. *et al., Heterocycles*, 1996, **43**, 581 (*3′-Hydroxy-4′-methoxyglabridin*)

Glabrin A G-136

[162157-00-8]
Cyclo(glycylleucylvalylisoleucyltyrosylprolyl)

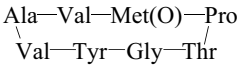


$C_{33}H_{50}N_6O_7$ 642.794
Cyclic peptide. Constit. of the seeds of *Annona glabra* (pond apple). Needles ($CHCl_3$/MeOH). Mp 300-303°. $[\alpha]_D^{28}$ -195.9 (c, 0.8 in MeOH). λ_{max} 204 (log ϵ 4.27); 225 (log ϵ 4.06); 279 (log ϵ 3.19) (MeOH).

Li, C.-M. *et al., Chin. Chem. Lett.*, 1995, **6**, 39 (*isol, pmr, cmr, ms*)

Li, C.-M. *et al., Phytochemistry*, 1998, **47**, 1293-1296 (*isol, uv, pmr, cmr, ms*)

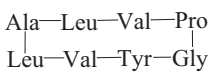
Glabrin B G-137



$C_{38}H_{58}N_8O_{11}S$ 834.989
Constit. of the seeds of *Annona glabra* (pond apple). Needles (MeOH). Mp 205°. $[\alpha]_D^{29}$ -76.7 (c, 0.4 in MeOH). λ_{max} 202 (log ϵ 2.94); 225 (log ϵ 3.01); 279 (log ϵ 2.11) (MeOH).

Li, C.-M. *et al., Phytochemistry*, 1998, **47**, 1293-1296 (*isol, uv, pmr, cmr, ms*)

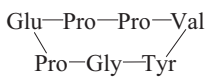
Glabrin C G-138



$C_{41}H_{64}N_8O_9$ 813.005
Cyclic peptide. Constit. of the seeds of *Annona glabra* (pond apple). Amorph. powder. Mp 153°. $[\alpha]_D^{29}$ -35.1 (c, 0.23 in MeOH). λ_{max} 202 (log ϵ 4.49); 221 (log ϵ 3.99); 279 (log ϵ 2.86) (MeOH).

Li, C.M. *et al., Phytochemistry*, 1999, **50**, 1047-1052 (*isol, uv, ir, pmr, cmr, ms*)

Glabrin D G-139

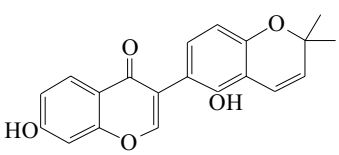


$C_{36}H_{49}N_7O_{10}$ 739.824
Cyclic peptide. Constit. of the seeds of *Annona glabra* (pond apple). Amorph. powder. Mp 219°. $[\alpha]_D^{29}$ -53.5 (c, 0.55 in MeOH). λ_{max} 203 (log ϵ 4.54); 220 (log ϵ 4.14); 279 (log ϵ 3.17) (MeOH).

Li, C.M. *et al., Phytochemistry*, 1999, **50**, 1047-1052 (*isol, uv, ir, pmr, cmr, ms*)

Glabrone G-140

[60008-02-8]
*7-Hydroxy-3-(5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-4*H*-1-benzopyran-4-one, 9CI. Eurycarpin B*



$C_{20}H_{16}O_5$ 336.343
Constit. of root of *Glycyrrhiza glabra* (licorice). Needles (Me_2CO). Mp 224-226°.

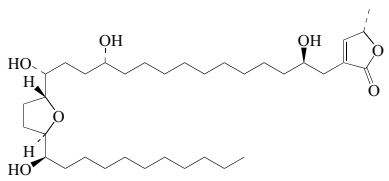
Di-Ac: [60008-04-0]
$C_{24}H_{24}O_7$ 424.449
Prisms (EtOH). Mp 218-220°.

Di-Me ether: [60008-05-1]
$C_{22}H_{20}O_5$ 364.397
Plates (EtOH aq.). Mp 124-125.5°.

Kinoshita, T. *et al., Chem. Pharm. Bull.*, 1976,

24, 991-994 (*isol, ms, pmr, uv*)
Mohamed, S.E.N. *et al., J.C.S. Perkin 1*, 1987, 431 (*synth*)
Kinoshita, T. *et al., Nat. Prod. Lett.*, 1997, **9**, 289-296 (*isol, cmr*)
Zhang, Y. *et al., Yaoxue Xuebao*, 1997, **32**, 301-304 (*Eurycarpin B*)

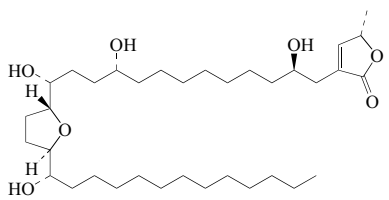
Glacin A G-141



$C_{35}H_{64}O_7$ 596.886
Constit. of the leaves of *Annona glabra* (pond apple). Waxy solid. $[\alpha]_D^{25}$ +6 ($CHCl_3$). λ_{max} 218 (log ϵ 3.83) (MeOH).

Liu, X.-X. *et al., J. Nat. Prod.*, 1998, **61**, 620-624 (*isol*)

Glacin B G-142

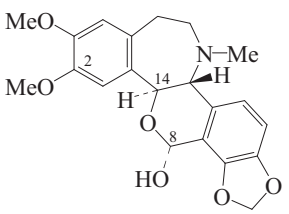


$C_{35}H_{64}O_7$ 596.886
Constit. of the leaves of *Annona glabra* (pond apple). Waxy solid. $[\alpha]_D$ +4.8 ($CHCl_3$). λ_{max} 221 (log ϵ 3.65) (MeOH).

Liu, X.-X. *et al., J. Nat. Prod.*, 1998, **61**, 620-624 (*isol, uv, ir, pmr, cmr, ms*)

Glaucamine G-143

[2255-44-9]
2,3-Dimethoxy-16-methyl-10,11-[methylenebis(oxy)]rheadan-8-ol, 9CI. Alkaloid R-L



$C_{21}H_{23}NO_6$ 385.416
Various numbering schemes in use. Alkaloid from *Papaver rhoeas* (corn poppy). Plates ($CHCl_3$/EtOH). Mp 222-223°. $[\alpha]_D^{22}$ +298 (c, 0.25 in $CHCl_3$). λ_{max} 238 (log ϵ 4); 286 (log ϵ 3.8) (no solvent reported).

Hydrochloride:
Mp 201-203°.

Me ether: [18104-26-2] ***Epiglaudine***. O-*Methylglaucamine. Glaupavine*
$C_{22}H_{25}NO_6$ 399.443
Identity of Glaupavine with Epiglaudine not certain.$[\alpha]_D^{22}$ +293 (c, 0.1 in $CHCl_3$).

Me ether, N-*de-Me:* [25651-16-5] ***Papaverrubine H***. *14-Epipapaverrubine B.* O-*Methylpapaverrubine C*
$C_{21}H_{23}NO_6$ 385.416
Amorph. Mp 70-71°. $[\alpha]_D$ +308 ($CHCl_3$).

Et ether: [77658-93-6] O-*Ethylglaucamine*
$C_{23}H_{27}NO_6$ 413.469Prob. an artifact.

O^2-*De-Me:* [18361-67-6] **N-*Methyl-14-O-demethylepiporphyroxine***. *Alkaloid A4*
$C_{20}H_{21}NO_6$ 371.389
Alkaloid from *Papaver somniferum* (opium poppy). Prisms (MeOH). Mp 217-218°. $[\alpha]_D^{20}$ +340 (c, 0.2 in MeOH).

O^2-*De-Me,* O^8-*Me,* N-*de-Me:* [22584-46-9] ***Papaverrubine C***. *Epiporphyroxine. 14-Epipapaverrubine D*
$C_{20}H_{21}NO_6$ 371.389
Prisms (C_6H_6/petrol). Mp 190-191.5°. $[\alpha]_D$ +283 ($CHCl_3$).

8-Epimer, Me ether: [5140-40-9] ***Glaudine***. O,N-*Dimethylporphyroxine.* O,N-*Dimethylpapaverrubine D.* N-*Methylpapaverrubine B*
$C_{22}H_{25}NO_6$ 399.443
Alkaloid from *Papaver rhoeas* (corn poppy) and *Papaver somniferum* (opium poppy). Cryst. (heptane). Mp 103-105°. $[\alpha]_D^{24}$ +455 (c, 0.5 in $CHCl_3$). λ_{max} 237 (log ϵ 4.03); 287 (log ϵ 3.92) (MeOH).

8-Epimer, Me ether, hydrochloride:
Mp 185-187°.

8-Epimer, Me ether, N-*de-Me:* [5140-39-6] ***Papaverrubine B***. O-*Methylporphyroxine.* O-*Methylpapaverrubine D.* N-*Demethylglaudine*
$C_{21}H_{23}NO_6$ 385.416
Alkaloid from *Papaver rhoeas* (corn poppy). Cryst. (MeOH). Mp 201-203°. $[\alpha]_D$ +398 ($CHCl_3$). λ_{max} 236 (log ϵ 4.06); 286 (log ϵ 3.86) (MeOH).

8-Epimer: [35321-05-2] *Epiglaucamine*
Amorph. $[\alpha]_D^{21}$ +126 (c, 0.27 in $CHCl_3$).

8-Epimer, O^2-*de-Me,* O^8-*Me:* [18211-29-5] **N-*Methylporphyroxine***. N-*Methylpapaverrubine D*
$C_{21}H_{23}NO_6$ 385.416
Alkaloid from *Papaver somniferum* (opium poppy).

8-Epimer, O^2-*de-Me,* O^8-*Me,* N-*de-Me:* [18104-24-0] ***Papaverrubine D***. *Porphyroxine*
$C_{20}H_{21}NO_6$ 371.389
Needles (MeOH). Mp 237-239° (234-236°). $[\alpha]_D$ +391 ($CHCl_3$).

8,14-Diepimer: [6598-99-8] ***Oreogenine***
$C_{21}H_{23}NO_6$ 385.416
Mp 173-175° (as methiodide). Indefinite Mp.

8,14-Diepimer, Me ether: [6516-48-9] ***Oreodine***. N-*Methylpapaverrubine F*
$C_{22}H_{25}NO_6$ 399.443
Cryst. (Et_2O). Mp 184-186°. $[\alpha]_D^{22}$ +224 (c, 0.1 in $CHCl_3$). λ_{max} 237 (log ϵ 3.96); 289 (log ϵ 3.72) (no solvent reported).

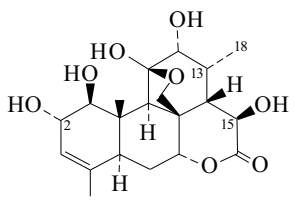
8,14-Diepimer, Me ether, N-*de-Me:* [19914-48-8] ***Papaverrubine F***. N-*Demethyloreodine*
$C_{21}H_{23}NO_6$ 385.416
Needles (Me_2CO). Mp 223-225°.

8,14-Diepimer, Et ether: O-*Ethyloreogenine*
$C_{23}H_{27}NO_6$ 413.469Prob. an artifact.

Pfeifer, S. *et al., Pharmazie*, 1964, **19**, 678; 724; 1968, **23**, 82; 267; 1972, **27**, 48 (*Papaverrubines, Glaudine*)
Pfeifer, S. *et al., Pharmazie*, 1964, **19**, 786; 1965, **20**, 585 (*Oreogenine*)
Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 3687-3696 (*Epiglaudine, Glaudine, Glaupavine, isol, synth, uv*)
Pfeifer, S. *et al., J. Pharm. Pharmacol.*, 1966, **18**, 133-134 (*Papaverrubine D, struct*)
Cross, A.D. *et al., Pharmazie*, 1966, **21**, 181 (*Oreogenine, Oreodine, stereochem*)
Mann, I. *et al., Pharmazie*, 1966, **21**, 700 (*Papaverrubine F, isol, uv, ir, struct*)
Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1967, **56**, 1658 (*Papaverrubine D, Oreodine, isol, ord, cd, pmr, struct, config*)
Dolejš, L. *et al., Tetrahedron*, 1967, **23**, 2997-3005 (*Oreodine, Papaverrubines B,D, Glaudine, ms*)
Shamma, M. *et al., Chem. Comm.*, 1968, 212-214 (*Papaverrubines B,C,D, Epiglaudine, Glaudine, stereochem*)
Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1968, **57**, 30-35 (*N-Methyl-14-O-demethylepiporphyroxine, Epiglaudine, Papaverrubine D, Glaudine, isol, uv, ir, pmr, struct*)
Slavíková, L. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 761-763 (*Papaverrubines*)
Sariyar, G. *et al., Phytochemistry*, 1980, **19**, 2189-2192 (*Oreogenine, Oreodine, Ethyloreogenine, Epiglaudine, Glaudine, isol, pmr, ms*)
Phillipson, J.D. *et al., Planta Med.*, 1981, **41**, 105 (*Glaudine, Oreogenine, isol*)
Preininger, V. *et al., Planta Med.*, 1981, **41**, 119 (*Glaudine, isol*)
Sariyar, G. *et al., Planta Med.*, 1983, **49**, 43 (*Oreogenine, isol*)

Glaucarubol G-144

[1448-22-2]



$C_{20}H_{28}O_8$ 396.436
Cryst. Mp 290-292°. $[\alpha]_D^{25}$ +38 (c, 0.8 in Py).

2-O-*β*-D-*Glucopyranoside:* [145940-75-6] ***Casteloside B***
$C_{26}H_{38}O_{13}$ 558.578
Amorph. powder (2-propanol). Mp 212-214°.

15-O-*β*-D-*Glucopyranoside:* [89202-77-7] ***Glaucarubol 15-O-β-D-glucopyranoside***
$C_{26}H_{38}O_{13}$ 558.578
Constit. of *Simarouba glauca* (aceituno). Cryst. (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 263-264°. $[\alpha]_D^{22}$ +12.1 (c, 0.99 in Py).
▶ Toxic.

15-Ac: [222609-91-8] ***15-Acetylglaucarubol***
$C_{22}H_{30}O_9$ 438.474
Cryst. (MeOH). Mp 254-256°. $[\alpha]_D^{25}$ +34.6 (c, 1 in Py).

15-(2-Methylbutanoyl): [74148-51-9] ***Excelsin***†
$C_{25}H_{36}O_9$ 480.554

Cryst. (MeOH). Mp 268-270°.

15-(2-Hydroxy-2-methylbutanoyl): [1448-23-3] ***Glaucarubin***. *β-Kirondrin*
$C_{25}H_{36}O_{10}$ 496.553
Isol. from *Simarouba glauca* (aceituno). Cryst. Mp 250-255° dec. $[\alpha]_D^{25}$ +69 (c, 0.6 in MeOH). Log P -2.3 (uncertain value) (calc).

▶ LD_{50} (rat, orl) 800 mg/kg , LD_{50} (mus, scu) 28 mg/kg. ET4730500

15-(2-Acetoxy-2-methylbutanoyl): [68703-93-5] ***2′-Acetylglaucarubin***
$C_{27}H_{38}O_{11}$ 538.591
Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 243-246°. $[\alpha]_D$ +29.5 (c, 1.1 in Py). λ_{max} 240 (ϵ 10700) (EtOH) (Berdy).

2-Ketone: [1990-01-8] ***Glaucarubolone***
$C_{20}H_{26}O_8$ 394.421
Cryst. (Me_2CO). Mp 255-258°. $[\alpha]_D$ -34 (c, 1.5 in Py). λ_{max} 240 (ϵ 9000) (EtOH) (Berdy).

*2-Ketone, 15-*O*-β-D-glucopyranoside:* [89202-76-6] ***Glaucarubolone 15-O-β-D-glucopyranoside***
$C_{26}H_{36}O_{13}$ 556.563
Constit. of *Simarouba glauca* (aceituno). Cryst. (MeOH). Mp 252-254°. $[\alpha]_D^{22}$ -25.7 (c, 1.01 in Py).

▶ Toxic.

2-Ketone, 15-Ac: [84062-60-2] ***Holacanthone***
$C_{22}H_{28}O_9$ 436.458
Cryst. Mp 253-254°. Log P -2.63 (uncertain value) (calc). λ_{max} 240 (ϵ 8720) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 25 mg/kg. KD0240000

2-Ketone, 15-(2-methylbutanoyl): [53683-73-1] ***Ailanthinone***
$C_{25}H_{34}O_9$ 478.538
Cryst. (Me_2CO/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 227-230°. $[\alpha]_D^{27}$ +90 (c, 0.1 in $CHCl_3$). Log P -1.27 (uncertain value) (calc). λ_{max} 239 (ϵ 11000) (EtOH) (Derep).

2-Ketone, 15-(3-methylbutanoyl): [70424-54-3] ***Castelanone***
$C_{25}H_{34}O_9$ 478.538
Cryst. Mp 237-239°. $[\alpha]_D$ +46.6 (c, 0.15 in $CHCl_3$). λ_{max} 239 (ϵ 12000) (EtOH) (Berdy).

2-Ketone, 15-(2-hydroxy-2-methylbutanoyl): [1259-86-5] ***Glaucarubinone***. *α-Kirondrin*
$C_{25}H_{34}O_{10}$ 494.538
Cryst. (Me_2CO). Mp 228-230°. $[\alpha]_D$ +50 (c, 0.34 in MeOH). Log P -2.18 (uncertain value) (calc). λ_{max} 239 (ϵ 11000) (EtOH) (Derep).

2-Ketone, 15-(3-hydroxy-3-methylbutanoyl): [74156-49-3] ***Soularubinone***
$C_{25}H_{34}O_{10}$ 494.538
Cryst. Mp 236-238°. $[\alpha]_D$ +47.6 (c, 0.7 in MeOH).

2-Ketone, 15-(2-acetoxy-2-methylbutanoyl): [33957-83-4] *2′-Acetylglaucarubinone*
$C_{27}H_{36}O_{11}$ 536.575
Cryst. (Me_2CO/hexane). Mp 170-172°. $[\alpha]_D^{23}$ +77 (c, 0.1 in $CHCl_3$). λ_{max} 240 (ϵ 10700) (EtOH).

*2-Ketone, 15-*O*-(3-ethyl-3*S*-hydroxy-4-methylpentanoyl):* [160791-11-7] ***Peninsularinone***
$C_{28}H_{40}O_{10}$ 536.618
Cryst. (EtOAc). Mp 221-223°. $[\alpha]_D^{25}$ -22.6 (c, 0.19 in Py).

13,18-Didehydro, 15-(3-methylbutanoyl): [65995-66-6] ***13,18-Dehydroglaucarubol 15-isovalerate***
$C_{25}H_{34}O_9$ 478.538

13,18-Didehydro, 2-ketone, 15-(2-methylbutanoyl): [53683-70-8] ***Dehydroailanthinone***
$C_{25}H_{32}O_9$ 476.522
Glass. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{23}$ +39.6 (c, 0.24 in $CHCl_3$). λ_{max} 238 (ϵ 10900) (EtOH) (Berdy).

13,18-Didehydro, 2-ketone, 15-(2-hydroxy-2-methylbutanoyl): [68703-94-6] ***13,18-Dehydroglaucarubinone***
$C_{25}H_{32}O_{10}$ 492.522
Mp 215-218°. $[\alpha]_D$ +34.7 (c, 0.95 in MeOH). λ_{max} 252 (MeOH) (Berdy).

Δ^4-Isomer: ***Δ^4-Glaucarubol***
$C_{20}H_{28}O_8$ 396.436
Cryst. (EtOAc). Mp 177-180°. $[\alpha]_D^{25}$ +86.9 (c, 0.88 in Py).

Δ^4-Isomer, 15-Ac: [222609-92-9] ***15-Acetyl-Δ^4-glaucarubol***
$C_{22}H_{30}O_9$ 438.474
Cryst. (EtOAc). Mp 184-186°. $[\alpha]_D^{25}$ +114.7 (c, 0.6 in MeOH).

15-Deoxy: See Chaparrin in *The Combined Chemical Dictionary.*

*18-Hydroxy, 2-ketone, 15-*O*-β-D-glucopyranoside:* [99877-89-1]
$C_{26}H_{36}O_{14}$ 572.562
Amorph. λ_{max} 240 (MeOH).

*18-Hydroxy, 2-ketone, 15-*O*-[α-D-xylofuranosyl-(1→6)-β-D-glucopyranoside]:* [99877-92-6]
$C_{31}H_{44}O_{18}$ 704.678
Amorph. λ_{max} 240 (MeOH).

1-Epimer, 2-ketone: [222609-94-1] ***1-Epiglaucarubolone***
$C_{20}H_{26}O_8$ 394.421
Cryst. (EtOH/EtOAc). Mp 276-278°. $[\alpha]_D^{25}$ +34.5 (c, 0.4 in Py).

1-Epimer, 2-ketone, 15-Ac: [222609-90-7] ***1-Epiholocanthone***
$C_{22}H_{28}O_9$ 436.458
Cryst. (CH_2Cl_2). Mp 243-245°. $[\alpha]_D^{25}$ +23.2 (c, 0.41 in Py).

*15-Epimer, 2-*O*-β-D-glucopyranoside:* [366497-87-2] ***Iandonoside A***
$C_{26}H_{38}O_{13}$ 558.578
Amorph. powder. $[\alpha]_D^{20}$ +19.1 (c, 0.3 in MeOH).

1,5-Diepimer, 2-ketone: [222609-93-0] ***1-Epi-5-isoglaucarubolone***
$C_{20}H_{26}O_8$ 394.421
Cryst. ($EtOAc/CH_2Cl_2$). Mp 251-252°. $[\alpha]_D^{25}$ -28.3 (c, 2.76 in Py).

Ham, A. *et al., J.A.C.S.*, 1954, **76**, 6066 (*isol, ir, Glaucarubin*)
Polonsky, J. *et al., Bull. Soc. Chim. Fr.*, 1964, 1827; 1965, 2793 (*pmr, struct*)
Kartha, G. *et al., J.A.C.S.*, 1964, **86**, 3630 (*cryst struct, Glaucarubin*)
Nyburg, S.C. *et al., Chem. Comm.*, 1965, 203 (*abs config*)
Gaudemer, A. *et al., Phytochemistry*, 1965, **4**, 149 (*Glaucarubinone*)
Stöcklin, W. *et al., Phytochemistry*, 1969, **8**, 1565 (*struct*)
Moron, J. *et al., Phytochemistry*, 1971, **10**, 585 (*biosynth*)
Kupchan, S.M. *et al., J.O.C.*, 1975, **40**, 654-656 (*Ailanthinone, Dehydroailanthinone, 2′-Acetylglaucarubinone*)
Gottlieb, H.E. *et al., J.O.C.*, 1975, **40**, 2499 (*cmr*)
Ogura, M. *et al., J. Nat. Prod.*, 1977, **40**, 579 (*deriv*)
Polonsky, J. *et al., Experientia*, 1978, **34**, 1172 (*isol*)
Polonsky, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1979, **288**, 269 (*Castelanone*)
Khan, S.A. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 183 (*Excelsin*)
Tri, M.V. *et al., J. Nat. Prod.*, 1981, **44**, 279 (*Soularubinone*)
Handa, S.S. *et al., J. Nat. Prod.*, 1983, **46**, 359 (*Holacanthone*)
Bhatnagar, S. *et al., Tet. Lett.*, 1984, **25**, 299 (*cryst struct*)
Bhatia, N. *et al., J. Indian Chem. Soc.*, 1985, **62**, 75 (*cmr*)
Lumonadio, L. *et al., Phytochemistry*, 1985, **24**, 2387-2389 (*2-ketone 18-hydroxy derivs*)
Chaudhuri, S.K. *et al., Phytochemistry*, 1992, **31**, 3961 (*Casteloside B*)
Fleck, T.J. *et al., Tet. Lett.*, 1992, **33**, 1813 (*synth*)
Grieco, P.A. *et al., J.A.C.S.*, 1993, **115**, 6078 (*synth*)
Grieco, P.A. *et al., Phytochemistry*, 1994, **37**, 1451 (*Peninsularinone*)
Rodriguez Fo, E. *et al., Phytochemistry*, 1996, **43**, 857 (*Glaucarubolone, pmr, cmr*)
Vieira, I.J.C. *et al., Fitoterapia*, 1998, **69**, 88-90 (*Glaucarubol, Glaucarubolone, pmr, cmr*)
Ozeki, A. *et al., J. Nat. Prod.*, 1998, **61**, 776-780 (*activity*)
Dayan, F.E. *et al., Pestic. Biochem. Physiol.*, 1999, **65**, 15 (*activity*)
Grieco, P.A. *et al., Phytochemistry*, 1999, **50**, 637-645 (*Castela polyandra constits, cryst struct*)
Kanchanapoom, T. *et al., Phytochemistry*, 2001, **57**, 1205-1208 (*Iandonoside A*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GEW700

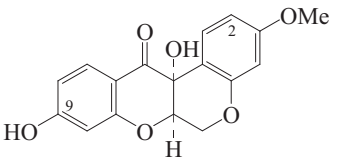
Gliadin G-145

Alkali-soluble protein components of wheat. Rich in glutamine (*ca.* 37%) and proline (*ca*. 17%). A complex mixt. with over 100 components which can be classified by their primary structure into 4 different protein types: ω5-, ω1,2-, α- and γ-gliadins. Isol. from wheat flour or wheat gluten. Sol. bases, MeOH aq.; poorly sol. H_2O, MeOH.

Kasarda, D.D. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1984, **81**, 4712-4716 (*α-Gliadin, struct*)
Rafalski, J.A. *et al., Gene*, 1986, **43**, 221-229 (*γ-Gliadin, struct*)
Shewry, P.R. *et al., J. Cereal Sci.*, 1986, **4**, 97-106 (*rev*)

Gliricidol G-146

[220386-00-5]
*6*a*,12*a*-Dihydro-9,12*a*-dihydroxy-3-methoxy[1]benzopyrano[3,4-*b*][1]benzopyran-12(6*H*)-one*



$C_{17}H_{14}O_6$ 314.294
Amorph. yellow solid. Mp 118-121°. $[\alpha]_D^{25}$ +230 (c, 1 in MeOH). λ_{max} 292 (log ϵ 4.56) (MeOH).

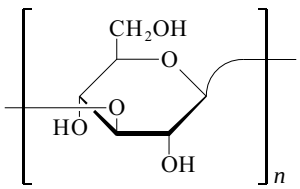
2-Methoxy: [220386-02-7] ***2-Methoxygliricidol***
$C_{18}H_{16}O_7$ 344.32
Amorph. yellow solid. Mp 125-128°. $[\alpha]_D^{25}$ +228 (c, 1 in MeOH). λ_{max} 292 (log ϵ 4.56) (MeOH).

2-Methoxy, 9-Me ether: [66280-24-8] ***12a-Hydroxymunduserone***
$C_{19}H_{18}O_7$ 358.347
Constit. of *Pachyrrhizus erosus* (yam bean). Light yellow needles (MeOH/$CHCl_3$). Mp 300°. $[\alpha]_D$ +33.3 ($CHCl_3$).

Kalra, A.J. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 1084 (*12a-Hydroxymunduserone*)
Rastrelli, L. *et al., J. Nat. Prod.*, 1999, **62**, 188-190 (*Gliricidol, 2-Methoxygliricidol*)

β-D-(1→3)-Glucan G-147

[51052-65-4]
Pachyman. Callose. Paramylon



Sol. H_2O. Curdlan below is a well-studied variant having n = 540. Also closely related is Laminarin which has a limited amount of chain branching.

Curdlan [54724-00-4]
Cerdlan. Kerdlan. TAK-N
Gelling agent for foods. Insol. H_2O but absorbs H_2O. Suspensions heated >54° form a firm gel. Phase 1 clinical trials (1995)

Sulfate: [115743-28-7] ***Curdlan sulfate***

Wheelan, W.J. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 330 (*isol, bibl*)
Harada, T. *et al., ACS Symp. Ser.*, 1977, **45**, 265 (*rev, synth, props, use*)
Marchenault, R.H. *et al., Carbohydr. Res.*, 1979, **75**, 231-242 (*struct*)
Deslandes, Y. *et al., Macromolecules*, 1980, **13**, 1466 (*cryst struct, bibl*)
Saito, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2093; 1987, **60**, 4259; 1989, **62**, 392 (*conformn, cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **16**, 595
Demleitner, S. *et al., Carbohydr. Res.*, 1992, **226**, 239; 247 (*synth, pharmacol*)
Kai, A. *et al., Carbohydr. Res.*, 1993, **240**, 153 (*bibl, biosynth*)
Gordon, M. *et al., J. Med. (Westbury, N.Y.)*, 1994, **25**, 163-180; 1995, **26**, 97-131 (*pharmacol, curdlan sulfate*)
Yoshida, T. *et al., Carbohydr. Res.*, 1995, **276**, 425 (*curdlan sulfate*)
Alban, S. *et al., Thromb. Res.*, 1995, **78**, 201 (*curdlan sulfate*)
Kulicke, W.M. *et al., Carbohydr. Res.*, 1997, **297**, 135-143 (*struct, props*)
Müller, A. *et al., Carbohydr. Res.*, 1997, **299**, 203-208 (*isol, purifn*)
Masihi, K.N. *et al., Int. J. Immunopharmacol.*, 1997, **19**, 463-468 (*curdlan sulfate*)
Tylianakis, M. *et al., Carbohydr. Res.*, 1999, **315**, 16-34 (*cmr*)
Shimizu, J. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 466-469 (*curdlan*)
Naito, T. *et al., J. Acquir. Immune Defic. Syndr.*, 2001, **26**, 512-513 (*curdlan sulfate*)

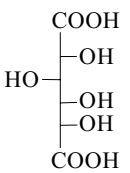
endo-1,3(4)-β-Glucanase, 9CI G-148

[62213-14-3]
Laminarinase. β-1,3-Glucanase. Endoglucanase. E.C. 3.2.1.6
Enzyme. Used in the manuf. of starch syrups, wine and fruit juices; in brewing increases extract yield and brewing capacity. Hydrolyses laminarin, lichenan and cereal β-glycans to oligosaccharides (3-5 glucose units) and minor amounts of disaccharides.

Reese, E.T. *et al., Can. J. Microbiol.*, 1959, **5**, 173-185 (*isol*)
Muller, J.J. *et al., J. Biol. Chem.*, 1998, **273**, 3438-3446 (*cryst struct*)

Glucaric acid, 9CI, 8CI G-149

[25525-21-7]
Saccharic acid. Glucosaccharic acid. Hydroxalic acid. Metatartaric acid†. Gularic acid



$C_6H_{10}O_8$ 210.14
For stereoisomers see Galactaric acid, G-1, Allaric acid, Idaric acid and Mannaric acid.

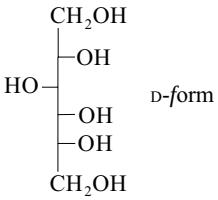
D-*form* [87-73-0]
D-Glucaric acid. L-Gularic acid
Present in apples and grapefruit. V. sol. H_2O. Mp 125-126°. $[\alpha]_D^{19}$ +6.9 → +20.6 (18 d) (H_2O). pK_a 5. Delequescent, free acid difficult to crystallise.

[5793-88-4]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 460A (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 554B (*ir*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate*, Edwards Bros. Inc., Ann Arbor, 1943, 288
Mehltretter, C.L. *et al., Methods Carbohydr. Chem.*, 1963, **2**, 46 (*D-form, synth*)
Matsunaga, I. *et al., Chem. Pharm. Bull.*, 1969, **17**, 1383; 1972, **20**, 284 (*D-form, D-di-Me ester benzylidene, glc*)
Horton, D. *et al., Carbohydr. Res.*, 1982, **105**, 95 (*pmr, cmr, conformn*)
Marsh, C.A. *et al., Carbohydr. Res.*, 1986, **153**, 119 (*biosynth*)
Merbouh, N. *et al., Carbohydr. Res.*, 2001, **336**, 75-78 (***synth***)

Glucitol, 9CI, 8CI G-150

[26566-34-7]
Sorbitol. Gulitol. gulo-*Hexitol.* gluco-*Hexitol. E420*



$C_6H_{14}O_6$ 182.173
For stereoisomers see Allitol, Galactitol, Iditol, D-Mannitol, and Talitol. Sorbitol is a common trivial name for glucitol but is imprecise and should be discouraged. Reduction of sorbose can produce either glucitol or iditol. Furthermore, D-glucitol is usually referred to as D-sorbitol whereas reduction of D-sorbose gives L-glucitol.

D-*form* [50-70-4]
D-Glucitol. L-Gulitol. FEMA 3029. Many other names
Occurs widely in plants ranging from algae to the higher orders. Fruits of the plant family Rosaceae, which include apples, pears, cherries, apricots, contain appreciable amounts. Rich sources are the fruits of the *Sorbus* and *Crataegus* spp. Sweetening agent and humectant and many other food uses. Needles + ½ or $1H_2O$ (EtOH) with sweet taste (60% of sucrose). Freely sol. H_2O; fairly sol. hot EtOH; spar. sol. cold EtOH. Mp 92° (labile form) Mp 97° (stable form) Mp 110-112° (anhyd.). $[\alpha]_D$ +7 (borax). $[\alpha]_D$ +31 (molybdate). pK_a 13 (60°). The name D-Sorbitol has been used for this compound but should not be employed (see above). Several polymorphs known.
▶ Gastrointestinal effects by ingestion, LD_{50} (rat, orl) 15900 mg/kg. LZ4290000

[45007-61-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 186A; 624C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 289B; 1054B (*nmr*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 275
Park, Y.J. *et al., Acta Cryst. B*, 1971, **27**, 2393 (*cryst struct*)
Brimacombe, J.S. *et al., The Carbohydrates*, Academic Press, 1972, **1A**, 479 (*rev*)
Colson, P. *et al., Can. J. Chem.*, 1975, **53**, 1030 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **1**, 754 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, GEY000
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 477-480
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1314; 1369; 1375
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2624-2628 (*use, occur*)
Schouten, A. *et al., Carbohydr. Res.*, 1998, **312**, 131-137 (*cryst struct, polymorphism*)

Newman, A.W. *et al., Anal. Profiles Drug Subst.*, 1999, **26**, 459-502 (*rev*)

Glucoamylase, 9CI G-151

[9032-08-0]

Glucan 1,4-α-glucosidase. 1,4-α-D-Glucan glucohydrolase. Amyloglucosidase. γ-Amylase. exo-*1,4-α-Glucosidase. E.C. 3.2.1.3*

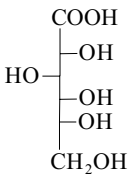
Enzyme. Used in the manuf. of glucose and fructose syrups, in brewing low calorie beers, and in increasing fruit juice yields. Hydrolyses terminal 1,4-linked α-D-glucose residues successively from non-reducing ends of polysaccharide chains with release of β-D-glucose; acts on amylose and amylopectin.

Vihinen, M. *et al., Crit. Rev. Biochem. Mol. Biol.*, 1989, **24**, 329-418 (*rev*)
Sauer, J. *et al., Biochim. Biophys. Acta*, 2000, **1543**, 275-293 (*rev*)
Pandey, A. *et al., Biotechnol. Appl. Biochem.*, 2000, **31**, 135-152 (*rev*)

Gluconic acid, 9CI, 8CI G-152

[133-42-6]

gluco-*Hexonic acid. E574*



$C_6H_{12}O_7$ 196.157

D-***form*** [526-95-4]

Dietary supplement, acidity regulator approved in Japan. Component of bottle rinsing formulations. Needles. Sol. H_2O. Mp 130-132°. $[\alpha]_D^{20}$ -6.7 → +11.7 (H_2O, 5 d). pK_a 3.76 (17°).

► LZ5057100

Na salt: [14906-97-9]

[527-07-1] *Sodium gluconate. E576*

Flavouring ingredient, sequestrant. Mp 206° dec. $[\alpha]_D^{23}$ +12.1 (c, 1.75 in H_2O).

► LZ5235000

K salt: [299-27-4] *Potassium gluconate. E577*

Dietary supplement (potassium), sequestrant. Mp 183° dec. $[\alpha]_D^{20}$ +11.7 (c, 1.2 in H_2O).

► LZ5230000

NH_4 salt: [2554-04-3]

Sequestrant used in foods. Deliquescent needles.

Mg salt: [3632-91-5] *Magnesium gluconate. Almora. Ultra-Mg*

Firming agent, flavour enhancer. Hydrate. Mp 200° dec. $[\alpha]_D^{20}$ +11 (c, 1.8 in H_2O).

Ca salt: [299-28-5]

[66905-23-5] *Calcium gluconate, USAN. Calcicol. Calglucon. E578*

Food additive: firming agent, sequestrant, stabiliser, texturiser. Anticaking agent in powdered coffee. $[\alpha]_D^{20}$ +8.5 (c, 3.0 in H_2O). Component of Calcet.

► Human (infant) adverse systemic effects when used therapeutically. LD_{50} (mus, ipr) 2200 mg/kg. EW2100000

*Zn(*II*) salt:* [4468-02-4] *Bis(*D*-gluconato-O^1,O^2)zinc, 9CI. Zinc(*II*) gluconate*

$C_{12}H_{22}O_{14}Zn$ 455.687

Dietary zinc supplement. Powder.

*Fe(*II*) salt:* [299-29-6]

[6047-12-7, 12389-15-0, 18829-42-0, 22830-45-1, 25126-39-0, 38658-53-6, 101197-68-6] *Ferrous gluconate, USAN. Bis(*D*-gluconato-O^1,O^2)iron. Iron(*II*) gluconate. Acroferon. Enteron. Fergon. Ferrose. Glucoferron. Haemex-G. Ironate. Neoferron. E579. Many other names*

$C_{12}H_{22}FeO_{14}$ 446.144

Dietary supplement, food colour for ripe olives. Yellow-grey powder + $2H_2O$. Sol. H_2O, insol. EtOH.

► LD_{50} (rat, orl) 2237 mg/kg. LZ5150000

*Fe(*III*)-Na salt:* [34089-81-1] *Ferrlecit*

Dietary supplement.

*Cu(*II*) salt:* [527-09-3]

[13005-35-1] *Bis(*D*-gluconato)copper. Copper(*II*) gluconate*

Mp 155-157°. $[\alpha]_D^{26}$ +15 (c, 1 in H_2O).

Mn(II) *salt:* [6485-39-8]

Dietary supplement. Slightly pink-coloured powder.

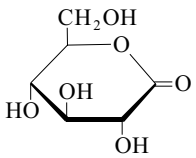
Polymer with D*-glucitol, Fe(*III*) salt:* [56959-18-3] ***Glusoferron, INN***

[921-62-0, 18016-24-5, 57775-17-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 553D; 554A; **2**, 1287B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 856B; 856C (*nmr*)
Robison, R. *et al., Biochem. J.*, 1931, **25**, 323 (*6-phosphate*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate*, Edwards Bros. Inc., Ann Arbor, 1943, 285
Green, J.W. *et al., Adv. Carbohydr. Chem.*, 1948, **3**, 153 (*rev*)
Seegmüller, J.E. *et al., J. Biol. Chem.*, 1951, **192**, 175-180 (*6-phosphate salts, !synth*)
Scott, D.B.M. *et al., Biochem. J.*, 1957, **65**, 686 (*6-phosphate*)
Tanabe, H. *et al., CA*, 1962, **58**, 8617ef (*Fe complexes*)
Frush, H.L. *et al., Methods Carbohydr. Chem.*, 1963, **2**, 14 (*synth, Ca salt*)
Fisch, D.C. *et al., Methods Enzymol.*, 1966, **9**, 53 (*cyclohexylammonium salt*)
Zhadanov, Y.A. *et al., Zh. Obshch. Khim.*, 1969, **39**, 1128
Schmitz, H. *et al., Arzneim.-Forsch.*, 1971, **21**, 509 (*Fe salt, pharmacol*)
Samochowiec, L. *et al., Clin. Ter. (Rome)*, 1971, **56**, 341; *CA*, **75**, 61780z (*metab*)
Bermejo Martinez, F. *et al., Mikrochim. Acta*, 1971, **1**, 489 (*detn, Mn*)
U.K. Pat., 1972, 1 269 023, (*Joh Benckiser*); *CA*, **77**, 34855n (*Fe salt, synth*)
Harvey, D.J. *et al., J. Chromatogr.*, 1973, **76**, 51 (*6-phosphate Na salt, ms, gc*)
Smith, G.D. *et al., Acta Cryst. B*, 1974, **30**, 1760-1766 (*6-phosphate, cryst struct*)
Lembeck, F. *et al., Arzneim.-Forsch.*, 1975, **25**, 1570 (*pharmacol*)
London, R.E. *et al., J. Magn. Reson.*, 1975, **18**, 557 (*6-phosphate, cmr*)
Horton, D. *et al., Carbohydr. Res.*, 1983, **119**, 263 (*pmr, cmr, conformn*)
Lis, T. *et al., Carbohydr. Res.*, 1983, **122**, 23 (*cryst struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CAS750
Olafsdottir, E.S. *et al., Phytochemistry*, 1992, **31**, 4129 (*biosynth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, (*Fe salt, synonyms*)
Coldwell, S.E. *et al., Am. J. Physiol.*, 1996, **271**, R1-R10 (*Ferrlecit*)
Food Chemicals Codex, 4th. Ed., 1996, 443-445 (*Zn complex*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 137; 386-388; 1110-1111; 1204-1205; 1623-1624; 1654-1655; 2297-2298; 2559-2560 (*salts, use*)
Nissenson, A.R. *et al., Am. J. Kidney Dis.*, 1999, **33**, 464-470; 471-482 (*Ferrlecit*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 578
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLG800; SHK800

1,5-Gluconolactone G-153

Gluconic acid δ-lactone, 9CI. E575



$C_6H_{10}O_6$ 178.141

D-***form*** [90-80-2]

Fujiglucon

Food additive; uses include acidifier, pH control agent, sequestrant. Mp 150-152°. $[\alpha]_D^{20}$ +66 → +9 (1 d) (c, 5.0 in H_2O).

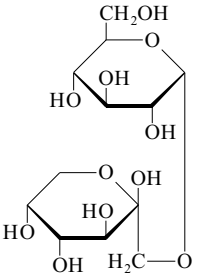
► LZ5184000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1153C (*nmr*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 411H (*ir*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate*, Edwards Bros., Ann Arbor, 1943, 279 (*rev, derivs*)
Isbell, H.S. *et al., Methods Carbohydr. Chem.*, 1963, **2**, 16 (*D-form, synth*)
Hackert, M.L. *et al., Acta Cryst. B*, 1971, **27**, 203 (*cryst struct*)
Walaszek, Z. *et al., Carbohydr. Res.*, 1982, **106**, 193 (*pmr, cmr, conformn*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1205-1207 (*props, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GFA200

1-*O*-α-D-Glucopyranosyl-D-fructose, 9CI G-154

[51411-23-5]

Trehalulose



β-Pyranose-*form*

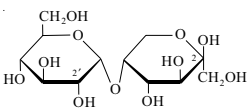
$C_{12}H_{22}O_{11}$ 342.299
Anticaries sweetening agent. Amorph. powder. Mp 90-95°. $[\alpha]_D^{20}$ +50 (c, 1.0 in H_2O).

β-Pyranose-*form* [90689-37-5]

*2′,3′,4′,6′-Tetrabenzyl, 2,3:4,5-di-*O*-isopropylidene:* [74024-22-9]
$C_{46}H_{54}O_{11}$ 782.926
$[\alpha]_D^{22}$ +22.5 (c, 1.3 in $CHCl_3$).
Avigad, G. *et al., Biochem. J.*, 1959, **73**, 587 (*synth*)
Pavia, A.A. *et al., Carbohydr. Res.*, 1980, **79**, 79 (*deriv*)
Munir, M. *et al., Carbohydr. Res.*, 1987, **164**, 477 (*synth*)
Bates, R.B. *et al., Carbohydr. Res.*, 1990, **201**, 342 (*isol, cmr, pmr*)

5-*O*-α-D-Glucopyranosyl-D-fructose, 9CI, 8CI G-155

[7158-70-5]
Leucrose



β-D-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
An aq. soln. at 20° conts. 1.9% α-pyr. and 98.1% β-pyr. forms. Non-cariogenic sweetening agent with approx. 40-50% of the sweetening power of sucrose. Found in honey. Mp 161-163° (156°). $[\alpha]_D^{25}$ -8.2 → +7.6 (c, 4 in H_2O).

Phenylosazone:
Mp 186-188°.

Phenylosotriazole:
Mp 108-109°.

Phenylosotriazole, hepta-Ac:
Mp 150-151°.

β-Pyranose-*form*

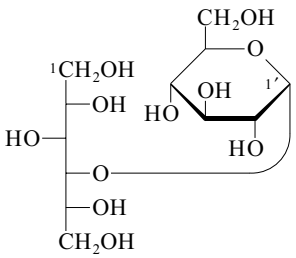
*Benzyl glycoside, 2′,3′,4′,6′-tetrabenzyl:-Benzyl 5-*O*-(2,3,4,6-tetra-*O*-benzyl-α-D-glucopyranosyl)-β-D-fructopyranoside*
$C_{47}H_{52}O_{11}$ 792.921
Syrup. $[\alpha]_D^{20}$ -8.5 (c, 0.7 in $CHCl_3$).

*Benzyl glycoside, 1,3,4-tribenzoyl, 2′,3′,4′,6′-tetrabenzyl:Benzyl 1,3,4-tri-*O*-benzoyl-5-*O*-(2,3,4,6-tetra-*O*-benzyl-α-D-glucopyranosyl)-β-D-fructopyranoside*
$C_{68}H_{64}O_{14}$ 1105.245
Mp 45°. $[\alpha]_D^{20}$ -56.5 (c, 1.0 in $CHCl_3$).

Stodola, F.H. *et al., J.A.C.S.*, 1952, **74**, 3202; 1956, **78**, 2514 (*isol, struct, synth*)
Watanabe, T. *et al., CA*, 1962, **56**, 5228 (*isol*)
Chiba, S. *et al., Agric. Biol. Chem.*, 1971, **35**, 1292 (*enzymatic synth*)
de Bruyn, A. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 799 (*pmr*)
Thiem, J. *et al., Carbohydr. Res.*, 1989, **189**, 65; 1990, **205**, 333 (*synth, cmr, cryst struct*)
Lichtenthaler, F.W. *et al., J.C.S. Perkin 2*, 1990, 1489 (*equilib*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1569-1570

4-*O*-α-D-Glucopyranosyl-D-glucitol, 9CI G-156

[585-88-6]
Maltitol. E965



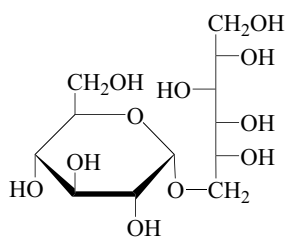
$C_{12}H_{24}O_{11}$ 344.315
Permitted bulk sweetener for foods. Mp 149-152°. $[\alpha]_D^{21}$ +107 (c, 10 in H_2O). Use as bulk sweetener currently (1997) not permitted in USA.

► LZ4394000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 308A (*nmr*)
Aldrich Library of NMR Spectra, **1**, 308A (*pmr*)
Karrer, P. *et al., Helv. Chim. Acta*, 1937, **20**, 88 (*synth*)
Hoffman, R.E. *et al., Magn. Reson. Chem.*, 1988, **26**, 425 (*pmr, cmr*)
Shinohara, Y. *et al., Yakugaku Zasshi*, 1988, **108**, 1046 (*synth, deriv*)
Japan. Pat., 1990, 0 242 997; *CA*, **113**, 4712h (*enzym synth*)
Paskach, T.J. *et al., Carbohydr. Res.*, 1991, **215**, 1 (*hplc*)
Hedin, P.A. *et al., J. Agric. Food Chem.*, 1991, **39**, 1106 (*ms*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 287-288
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1371
Schouten, A.. *et al., Carbohydr. Res.*, 1999, **322**, 298-302 (*cryst struct*)

6-*O*-α-D-Glucopyranosyl-D-glucitol, 9CI, 8CI G-157

[534-73-6]
*6-*O*-α-D-Glucopyranosyl-D-sorbitol. Isomaltitol. E953*



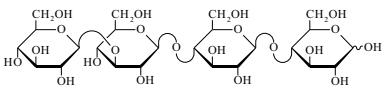
$C_{12}H_{24}O_{11}$ 344.315
Low calorie sweetener with half the sweetness of sucrose. Widely approved for food usage as a component of isomalt. Mixts. with the epimer, are known as Palatinit or Isomalt and used as reduced-calorie sugar substitutes. Cryst. (MeOH) or needles. Mp 165.5-167°. $[\alpha]_D^{28}$ +89 (c, 4 in H_2O).

Nona-Ac: [41897-25-0]
$C_{30}H_{42}O_{20}$ 722.65
Cryst. (EtOH). Mp 114-115°. $[\alpha]_D^{29}$ +70 (c, 1 in $CHCl_3$).

Wolfrom, M.L. *et al., J.A.C.S.*, 1952, **74**, 1062-1064 (*nona-O-Ac, synth*)
Manners, D.J. *et al., Carbohydr. Res.*, 1968, **7**, 291-298 (*synth*)
Hellerquist, C.G. *et al., Acta Chem. Scand.*, 1971, **25**, 243-244 (*synth, pmr*)
Govorchenko, V.I. *et al., Carbohydr. Res.*, 1973, **29**, 421-425 (*synth*)
Lichtenthaler, F.W. *et al., Annalen*, 1981, 2372-2383 (*cryst struct*)
Shimamura, A. *et al., Carbohydr. Res.*, 1991, **220**, 243-248 (*synth, cmr*)
Willibald-Ettle, I. *et al., Advances in Sweeteners*, (ed. Grenby, T.H.), Blackie, 1996, 134-149 (*rev, isomalt, use, props*)
Cataldi, T.R.I. *et al., J. Agric. Food Chem.*, 1999, **47**, 157-163

β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-D-glucose G-158

[58484-04-1]
3-β-Glucosylcellotriose. 4-β-Laminaribiosylcellobiose



Pyranose-*form*

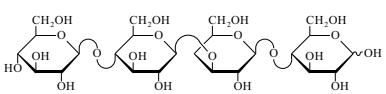
$C_{24}H_{42}O_{21}$ 666.583
Isol. from cellulase hydrolysates of oat β-glucan. Mp 221-224°. $[\alpha]_D$ +10.6 (in H_2O).

Dihydrate:
Mp 187-188°.

Parrish, F.W. *et al., Can. J. Chem.*, 1960, **38**, 2094 (*isol*)
Perlin, A.S. *et al., Can. J. Chem.*, 1962, **40**, 50 (*isol*)
Luchsinger, W.W. *et al., Carbohydr. Res.*, 1976, **46**, 1
Takeo, K. *et al., Carbohydr. Res.*, 1986, **147**, 265 (*synth, pmr, cmr*)

β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-D-glucose G-159

[103762-93-2]
3-β-Cellobiosylcellobiose



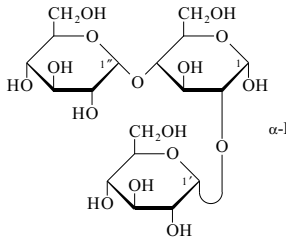
Pyranose-*form*

$C_{24}H_{42}O_{21}$ 666.583
Isol. from cellulase hydrolysates of oat β-glucan. Mp 223-226°. $[\alpha]_D$ +19.8 (H_2O).

Parrish, F.W. *et al., Can. J. Chem.*, 1960, **38**, 2094 (*isol*)
Perlin, A.S. *et al., Can. J. Chem.*, 1962, **40**, 50 (*isol*)
Takeo, K. *et al., Carbohydr. Res.*, 1986, **147**, 265 (*synth, pmr, cmr*)

α-D-Glucopyranosyl-(1 → 2)-[α-D-glucopyranosyl-(1 → 4)]-D-glucose, 9CI G-160

[34174-65-7]
Centose



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Constit. of honey. Patented for food use. $[\alpha]_D^{15}$ +142.3 (c, 0.59 in H_2O).

β-Pyranose-*form* [29581-60-0]

Undeca-Ac: [29581-59-7]
$C_{40}H_{54}O_{27}$ 966.85
$[\alpha]_D^{15}$ +103 (c, 2.5 in $CHCl_3$).

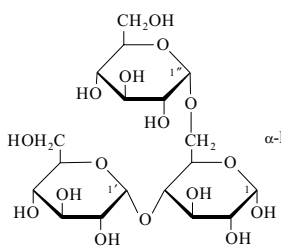
Undeca-Me:
$C_{29}H_{54}O_{16}$ 658.736
$[\alpha]_D^{25}$ +113 (c, 1.5 in $CHCl_3$).

[19774-14-2]

Siddiqui, I.R. *et al., Carbohydr. Res.*, 1968, **6**, 250 (*isol*)
Koeppen, B.H. *et al., Carbohydr. Res.*, 1970, **13**, 417 (*synth*)
Nishi, K. *et al., Agric. Biol. Chem.*, 1975, **39**, 737 (*synth*)
Japan. Pat., 1988, 63 240 756; 63 240 757; 63 261 492; *CA*, **110**, 74132f; 74133g; 152832a (*use, enzymic manuf*)

α-D-Glucopyranosyl-(1 → 4)-[α-D-glucopyranosyl-(1 → 6)]-D-glucose, 9CI G-161

[25218-29-5]
4,6-Di-O-*(α-D-glucopyranosyl)-D-glucose.*
6-O-*Glucosylmaltose*



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Isol. from the partial acid hydrolysate of amylopectin (waxy rice starch). Syrup. $[\alpha]_D^{22}$ +139 (c, 0.3 in H_2O) (+125).

α-Pyranose-*form*

Benzyl glycoside, decabenzyl: [82807-87-2]
$C_{95}H_{98}O_{16}$ 1495.81
Syrup. $[\alpha]_D^{20}$ +82 (c, 1.7 in $CHCl_3$).

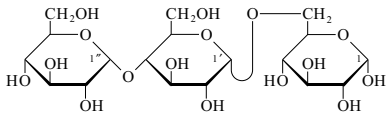
β-Pyranose-*form*

Me glycoside: [97672-52-1]
$C_{19}H_{34}O_{16}$ 518.468
Syrup. $[\alpha]_D$ +85.4 (H_2O).

de Souza, R. *et al., Tet. Lett.*, 1964, 1215 (*synth, struct*)
Ogawa, K. *et al., CA*, 1970, **72**, 117 680z (*isol*)
Eby, R. *et al., Carbohydr. Res.*, 1980, **79**, 53 (*synth*)
Morishima, N. *et al., Chem. Lett.*, 1982, 1039 (*benzyl gly deriv, cmr*)
Koto, S. *et al., Carbohydr. Res.*, 1984, **130**, 73 (*synth, cmr*)
Bock, K. *et al., J. Carbohydr. Chem.*, 1984, **3**, 581 (*Me gly, cmr*)

α-D-Glucopyranosyl-(1 → 4)-α-D-glucopyranosyl-(1 → 6)-D-glucose G-162

[32581-33-2]
6-α-Maltosylglucose. Isopanose



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Present in honey and beer. $[\alpha]_D$ +128 (H_2O).

α-Pyranose-*form*

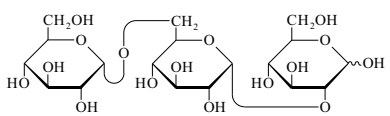
Benzyl glycoside, decabenzyl: [83921-71-5]
$C_{95}H_{98}O_{16}$ 1495.81
Syrup. $[\alpha]_D^{20}$ +74 (c, 1.0 in $CHCl_3$).

[3810-66-0]

Peat, S. *et al., J.C.S.*, 1959, 3223 (*isol*)
Pazur, J.H. *et al., J. Biol. Stand.*, 1960, **235**, 297 (*synth*)
Siddiqui, I.R. *et al., CA*, 1968, **69**, 95213h (*isol*)
Bethgate, G.N. *et al., Chem. Ind. (London)*, 1969, 520 (*isol*)
Ogawa, K. *et al., CA*, 1970, **72**, 117680z
Sakano, Y. *et al., Carbohydr. Res.*, 1978, **61**, 175
Morishima, N. *et al., Chem. Lett.*, 1982, 1383 (*benzyl gly deriv*)

α-D-Glucopyranosyl-(1 → 6)-α-D-glucopyranosyl-(1 → 2)-D-glucose, 9CI G-163

[40983-70-8]
2-α-Isomaltosylglucose



Pyranose-*form*

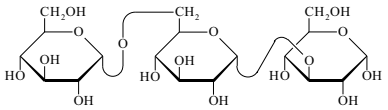
$C_{18}H_{32}O_{16}$ 504.441
Isol. from sake. $[\alpha]_D^{12}$ +148 (c, 1.8 in H_2O).

[25242-83-5, 55177-32-7]

Yamauchi, F. *et al., Agric. Biol. Chem.*, 1969, **33**, 1295 (*synth*)
Sakakibara, K. *et al., Carbohydr. Res.*, 1972, **25**, 443 (*synth*)
Baba, S. *et al., CA*, 1975, **82**, 153725h (*isol*)
Watanabe, T. *et al., Carbohydr. Res.*, 1980, **83**, 119

α-D-Glucopyranosyl-(1 → 6)-α-D-glucopyranosyl-(1 → 3)-D-glucose, 8CI G-164

[23393-10-4]
3-α-Isomaltosylglucose



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Constit. of honey. $[\alpha]_D^{12}$ +155 (c, 0.7 in H_2O).

α-Pyranose-*form*

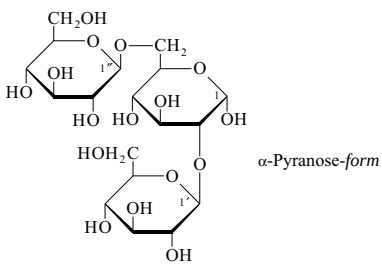
Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Cryst. (EtOH). Mp 120°. $[\alpha]_D^{22}$ +111 (c, 2.3 in $CHCl_3$).

[21291-02-1]

Abdullah, M. *et al., J.C.S.*, 1962, 176 (*synth*)
Siddiqui, I.R. *et al., CA*, 1968, **69**, 95213h (*isol*)
Yamauchi, F. *et al., Agric. Biol. Chem.*, 1969, **33**, 103; 1295 (*isol*)

β-D-Glucopyranosyl-(1 → 2)-[β-D-glucopyranosyl-(1 → 6)]-D-glucose, 9CI G-165

[90366-13-5]
Neopolitanose



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441

1-O-*Octanoyl:* [255904-23-5]
$C_{26}H_{46}O_{17}$ 630.639
Constit. of the fruit of Indian mulberry (*Morinda citrifolia*), a plant eaten as a famine food and occasionally as a staple in the Pacific region. Powder.

α-Pyranose-*form*

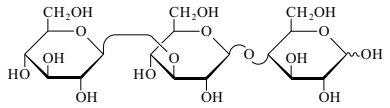
Undeca-Ac: [90332-61-9]
$C_{40}H_{54}O_{27}$ 966.85
Cryst. (EtOH). Mp 188-190°.

Me glycoside: [88988-42-5]
$C_{19}H_{34}O_{16}$ 518.468
Cryst. Mp 262-265°. $[\alpha]_D$ +28.4 (H_2O).

Temeriusz, A. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1982, **56**, 141 (*α-Me gly synth*)
Pychener, M. *et al., Helv. Chim. Acta*, 1984, **67**, 386 (*isol, pmr, ms*)
Wang, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 4880-4882 (*1-octanoyl*)

β-D-Glucopyranosyl-(1 → 3)-β-D-glucopyranosyl-(1 → 4)-D-glucose, 9CI G-166

[32581-38-7]
4-β-Laminaribiosylglucose



Pyranose-*form*

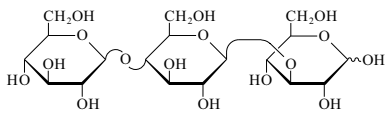
$C_{18}H_{32}O_{16}$ 504.441
Present in the partial acid hydrolysates of oat β-glucan. Cryst. (EtOH aq.). Mp 229-231°. $[\alpha]_D^{25}$ +13 (c, 1.4 in H_2O).

Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Cryst. (EtOH). Mp 120-122°. $[\alpha]_D$ -20 ($CHCl_3$).

Peat, S. *et al., J.C.S.*, 1957, 3916
Parrish, F.W. *et al., Can. J. Chem.*, 1960, **38**, 2094 (*isol*)
Perlin, A.S. *et al., Can. J. Chem.*, 1962, **40**, 50 (*isol*)
Takeo, K. *et al., Carbohydr. Res.*, 1986, **147**, 265 (*synth*)

β-D-Glucopyranosyl-(1 → 4)-β-D-glucopyranosyl-(1 → 3)-D-glucose, 9CI, 8CI G-167

[32581-36-5]
3-β-Cellobiosylglucose



Pyranose-*form*

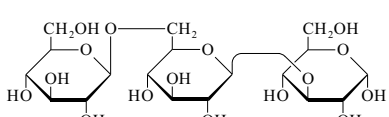
$C_{18}H_{32}O_{16}$ 504.441
Obt. from partial acid and enzymic hydrol. of oat β-glucan and barley β-glucan. Cryst. (EtOH aq.). Mp 236-239°. $[\alpha]_D^{25}$ +11.7 (c, 1.5 in H_2O).

Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Cryst. Mp 108-110°. $[\alpha]_D$ -8.3 ($CHCl_3$).

Peat, S. *et al., J.C.S.*, 1957, 3916 (*isol*)
Moscatelli, E.A. *et al., J. Biol. Chem.*, 1961, **236**, 2858
Perlin, A.S. *et al., Can. J. Chem.*, 1962, **40**, 50 (*isol*)
Yamamoto, R. *et al., Carbohydr. Res.*, 1978, **67**, 275
Kato, Y. *et al., Carbohydr. Res.*, 1982, **109**, 233
Takeo, K. *et al., Carbohydr. Res.*, 1986, **147**, 265 (*synth*)

β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 3)-D-glucose, 9CI G-168

[32581-32-1]
3-β-Gentiobiosylglucose



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Repeating unit of the extracellular β-D-glucan from the fungus *Botrytis cinerea* responsible for clarification difficulties in wine technology. Prisms + $2H_2O$. Mp 223-223° dec. $[\alpha]_D^{15}$ -4.35 → +1.58 (c, 1.0 in H_2O).

α-Pyranose-*form*

Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Cryst. (EtOH). Mp 179-180°. $[\alpha]_D^{15}$ -11 ($CHCl_3$).

β-Pyranose-*form* [47751-20-2]

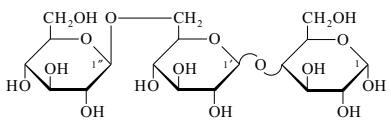
Undeca-Ac:
Prisms (EtOH). Mp 169-170°. $[\alpha]_D^{15}$ -27.9 ($CHCl_3$).

[34213-21-3]

Peat, S. *et al., J.C.S.*, 1960, 175; 1958, 3862 (*isol, synth*)
Turvey, J.R. *et al., J.C.S.*, 1960, 2366 (*synth*)
Handa, N. *et al., Nature (London)*, 1961, **192**, 1078 (*isol*)
Gestetner, B. *et al., Phytochemistry*, 1971, **10**, 2221 (*isol*)
Ueno, Y. *et al., Carbohydr. Res.*, 1973, **28**, 140 (*isol*)
Dubourdieu, D. *et al., Carbohydr. Res.*, 1981, **93**, 294 (*isol*)

β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 4)-D-glucose G-169

[100676-05-9]
4-β-Gentiobiosylglucose



α-Pyranose-*form*

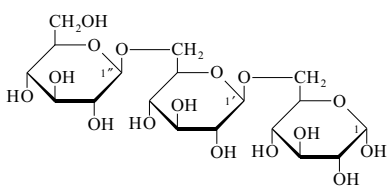
$C_{18}H_{32}O_{16}$ 504.441
Prod. by transferase action on cellobiose of β-glucosides of barley (*Hordeum vulgare*). Claimed use as low-calorie flavouring agent in food, beverages, medicines. Promotes growth of beneficial intestinal flora. $[\alpha]_D$ +10.2 (H_2O).

Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Cryst. Mp 205°. $[\alpha]_D$ -13 ($CHCl_3$).

Crook, E.M. *et al., Biochem. J.*, 1957, **65**, 1 (*isol*)
Anderson, F.B. *et al., Biochem. J.*, 1959, **71**, 407 (*isol*)
Berger, L.S. *et al., Biochem. Biophys. Res. Commun.*, 1961, **6**, 62 (*isol*)
Djordjevic, S.P. *et al., Carbohydr. Res.*, 1986, **148**, 87 (*isol, cmr*)
Eur. Pat., 1991, 415 720; *CA*, **115**, 181869b (*use*)

β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 6)-D-glucose, 9CI G-170

[32590-17-3]
Gentiotriose, 8CI



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441
Low-calorie flavouring agent in food, beverages and medicines. Promotes growth of beneficial intestinal flora. $[\alpha]_D$ -6.5 (c, 2.0 in H_2O).

β-Pyranose-*form*

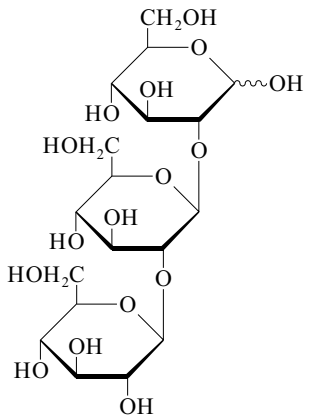
Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Mp 220-221°. $[\alpha]_D^{20}$ -7 (c, 1.0 in $CHCl_3$).

6‴-Trichloroacetyl, deca-Ac:
$C_{40}H_{51}Cl_3O_{27}$ 1070.185
Mp 200°. $[\alpha]_D^{20}$ -3 (c, 1.96 in $CHCl_3$).

Lindberg, B. *et al., Acta Chem. Scand.*, 1954, **8**, 985
McGrath, D. *et al., Carbohydr. Res.*, 1969, **11**, 453
Excoffier, G. *et al., Carbohydr. Res.*, 1976, **46**, 201 (*synth, pmr*)
Daniel, P.F. *et al., Methods Enzymol.*, 1987, **138**, 94 (*anal, hplc*)
Japan. Pat., 1989, 01 222 779; *CA*, **112**, 117369z (*manuf*)
Eur. Pat., 1991, 415 720; *CA*, **115**, 181869b (*use*)
Zhu, Y. *et al., Carbohydr. Res.*, 2001, **332**, 1-21 (*synth*)

β-D-Glucopyranosyl-(1 → 2)-β-D-glucopyranosyl-(1 → 2)-β-D-glucose, 9CI G-171

[32581-40-1]
Sophorotriose



$C_{18}H_{32}O_{16}$ 504.441
Present in potato and pea plants. Cryst. (MeOH aq.). Mp 218-223°. $[\alpha]_D$ +16 → +11 (c, 1.0 in H_2O, 18h).

β-Pyranose-*form*

1-O-(3,4-Dihydroxycinnamoyl):1-O-Caffeoyl-β-sophorotriose
$C_{27}H_{38}O_{19}$ 666.586

Allyl glycoside, 2″-Ac, nonabenzyl: [88988-49-2]
$C_{86}H_{92}O_{17}$ 1397.663
Syrup. $[\alpha]_D^{25}$ -0.56 (c, 1.0 in $CHCl_3$).

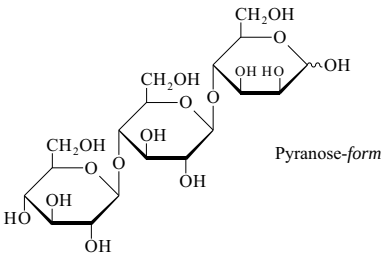
[50906-47-3]

Gorin, P.A.T. *et al., Can. J. Chem.*, 1961, **39**, 1067 (*constit*)
Furuya, M. *et al., Nature (London)*, 1962, **193**, 456 (*constit*)
Karkkainen, J. *et al., Carbohydr. Res.*, 1971, **17**, 11 (*glc, ms*)
Schmid, R.D. *et al., Phytochemistry*, 1973, **12**, 2269 (*isol, ms*)
Ogawa, T. *et al., Carbohydr. Res.*, 1983, **123**, C16 (*β-allyl gly*)

Al-Samarrai, T.H. *et al., Infect. Immun.*, 1983, **40**, 629 (*constit*)
Allen, P.Z. *et al., Mol. Immunol.*, 1988, **25**, 1011 (*immunol*)
Brinkmeier, E. *et al., Phytochemistry*, 1999, **52**, 297-302 (*Caffeoylsophorotriose*)

β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-D-mannose, 9CI G-172

[28072-83-5]

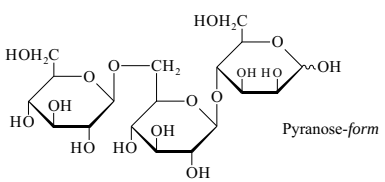


$C_{18}H_{32}O_{16}$ 504.441
Present in asparagus seeds. Isol. from the hydrolysates of konjac glucomannan (*Amorphophallus konjac*). Mp 249-251° (257°). $[\alpha]_D$ +8.5 → -4.3 (c, 1.4 in H_2O).

Kato, K. *et al., Agric. Biol. Chem.*, 1969, **33**, 1446 (*isol*)
Takahashi, R. *et al., Agric. Biol. Chem.*, 1984, **48**, 2943 (*isol*)
Koleva, M. *et al., CA*, 1984, **100**, 20436h
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1988, **52**, 519 (*synth*)
Goldberg, R. *et al., Carbohydr. Res.*, 1991, **210**, 263 (*isol, pmr, hplc*)

β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→4)-D-mannose, 9CI G-173

[61237-56-7]

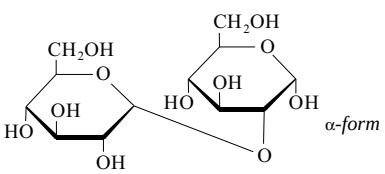


$C_{18}H_{32}O_{16}$ 504.441
Isol. from partial acid hydrolysates of *Cassia tora* (charota). Mp 176-180°. $[\alpha]_D$ -11.8 (c, 0.57 in H_2O).

Varshney, S.C. *et al., J.C.S. Perkin 1*, 1976, 1621

2-*O*-α-D-Glucopyranosyl-D-glucose, 9CI, 8CI G-174

[2140-29-6]
Kojibiose



$C_{12}H_{22}O_{11}$ 342.299
Occurs in saké and honey. Prisms. Mp 187-188°. $[\alpha]_D^{18}$ +162 → +137 (c, 2.1 in H_2O).

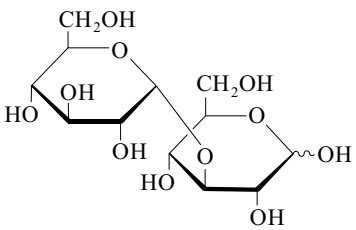
α-Pyranose-*form* [37169-66-7]
Octa-Ac:
[20970-96-1]
$C_{28}H_{38}O_{19}$ 678.597
Mp 167-168°. $[\alpha]_D^{17}$ +152 (c, 1.5 in $CHCl_3$).

β-Pyranose-*form* [37169-67-8]
Octa-Ac: [31873-02-6]
Mp 118°. $[\alpha]_D$ +112 ($CHCl_3$).

Yamauchi, F. *et al., Nature (London)*, 1961, **189**, 753 (*isol*)
Usui, T. *et al., J.C.S. Perkin 1*, 1973, 2425-2432 (*cmr*)
Usui, T. *et al., Carbohydr. Res.*, 1974, **33**, 105-116 (*pmr*)
Dick, W.E. *et al., Carbohydr. Res.*, 1974, **36**, 319-329 (*synth, octa-Ac*)
Ganfield, M.-C. *et al., J. Biol. Chem.*, 1975, **250**, 702-709 (*isol*)
Bradbury, J.H. *et al., Carbohydr. Res.*, 1979, **71**, 15-24 (*pmr*)
Watanabe, T. *et al., Carbohydr. Res.*, 1982, **110**, 170-175 (*isol*)
Takeo, K. *et al., Carbohydr. Res.*, 1987, **162**, 95-109 (*α-octa-Ac*)

3-*O*-α-D-Glucopyranosyl-D-glucose, 9CI, 8CI G-175

[497-48-3]
Nigerose. Sakebiose



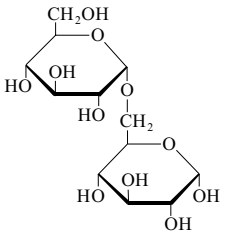
$C_{12}H_{22}O_{11}$ 342.299
Detected in saké. Can be obt. preparatively by hydrol. of the D-glucan from fruiting bodies of the bracket fungus *Laetiporus sulphureus* (sulphur polypore) (Takeo *et al*). Mp 156°. $[\alpha]_D^{20}$ +125 → +138 (c, 2 in H_2O).

β-Pyranose-*form*
Octa-Ac: [22352-62-1]
$C_{28}H_{38}O_{19}$ 678.597
Needles (Et_2O). Mp 152-153°. $[\alpha]_D^{12}$ +83 (c, 2.1 in $CHCl_3$).

Stacey, M. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 339 (*isol*)
Yamanchi, F. *et al., Nature (London)*, 1964, **204**, 1088 (*isol*)
Lemieux, R.U. *et al., Can. J. Chem.*, 1973, **51**, 42 (*α-D-pyr, synth*)
Usui, T. *et al., J.C.S. Perkin 1*, 1973, 2425 (*cmr*)
de Bruyn, A. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 721 (*pmr*)
Igarashi, K. *et al., Carbohydr. Res.*, 1975, **39**, 341 (*β-D-pyr octa-Ac*)
Excoffier, G. *et al., Carbohydr. Res.*, 1976, **51**, 280 (*β-D-pyr octa-Ac, pmr*)
Neuman, A. *et al., Carbohydr. Res.*, 1980, **80**, 15 (*Me gly, cryst struct*)
Takeo, K. *et al., Carbohydr. Res.*, 1983, **113**, 281 (*isol*)

6-*O*-α-D-Glucopyranosyl-D-glucose, 9CI G-176

[499-40-1]
Isomaltose. Brachiose



$C_{12}H_{22}O_{11}$ 342.299
Isolated from partial hydrolysates of amylopectin and dextrans. Sol. H_2O; poorly sol. MeOH, C_6H_6, butanol. Mp 120°. $[\alpha]_D$ +120 (H_2O).

α-Pyranose-*form*
Me glycoside: Methyl α-maltoside
$C_{13}H_{24}O_{11}$ 356.326
Amorph. solid. $[\alpha]_D^{20}$ +107 (c, 0.18 in EtOH).

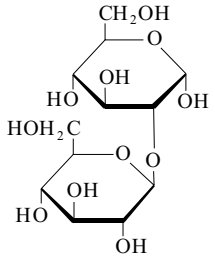
β-Pyranose-*form*
Octa-Ac: [22352-61-0]
$C_{28}H_{38}O_{19}$ 678.597
Prisms (EtOH). Mp 143-144°. $[\alpha]_D^{25}$ +97 (c, 2.7 in $CHCl_3$).
Octakis(4-nitrobenzoyl):
Mp 188°. $[\alpha]_D$ +22 (2,5-hexanedione).
Me glycoside: Methyl β-isomaltoside
$C_{13}H_{24}O_{11}$ 356.326
$[\alpha]_D^{20}$ +53.2 (+50) (H_2O).

[24822-33-1]

Georges, L.W. *et al., J.A.C.S.*, 1947, **69**, 473 (*β-D-pyr-octa-Ac*)
Lindberg, B. *et al., Acta Chem. Scand.*, 1949, **3**, 1355 (*β-D-pyr-octa-Ac*)
Montgomery, E.M. *et al., J.A.C.S.*, 1949, **71**, 1682 (*isol*)
Jeanes, A. *et al., J.A.C.S.*, 1953, **75**, 5911 (*isol*)
Takasawa, A. *et al., J. Antibiot., Ser. A*, 1954, **7**, 51 (*isol*)
Turvey, J.R. *et al., Biochem. J.*, 1957, **67**, 49 (*isol, β-octa-Ac*)
Wolfrom, M.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 316; 1963, **2**, 341 (*synth*)
Pazur, J.H. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 319 (*synth*)
Ninomiya, E. *et al., CA*, 1971, **74**, 86374 (*isol*)
Takiura, K. *et al., Chem. Pharm. Bull.*, 1973, **21**, 523 (*synth*)
Helferich, B. *et al., Annalen*, 1974, 1514 (*synth*)
Berry, J.M. *et al., Carbohydr. Res.*, 1974, **38**, 339 (*synth*)
Colson, P. *et al., J.A.C.S.*, 1974, **96**, 8081 (*conformn, cmr*)
Bradbury, J.H. *et al., Carbohydr. Res.*, 1979, **71**, 15 (*pmr*)
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2995 (*cmr*)
Hamann, C.H. *et al., Carbohydr. Res.*, 1994, **265**, 1 (*Me glycosides*)

2-*O*-β-D-Glucopyranosyl-D-glucose, 9CI G-177

[534-46-3]
Sophorose



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
Needles (MeOH aq.). Mp 196-198°. $[\alpha]_D^{20}$ +33 → +19.1 (c, 1.2 in H_2O).

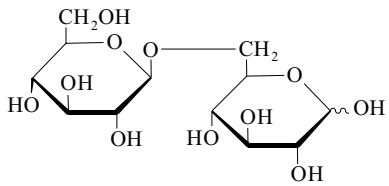
β-Pyranose-*form* [26887-94-5]

Benzyl glycoside: [76819-28-8] *Benzyl 2-O-β-D-glucopyranosyl-β-D-glucopyranoside. Benzyl β-sophoropyranoside.* ***Zizybeoside I***
$C_{19}H_{28}O_{11}$ 432.424
Isol. from *Zizyphus jujuba* (Chinese date). Needles (MeOH aq.). Mp 192-193°. $[\alpha]_D^{23}$ -32.6 (c, 1.03 in H_2O).

Okamura, N. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3507 (*Zizybeoside I*)

6-*O*-β-D-Glucopyranosyl-D-glucose, 9CI G-178

[554-91-6]
Gentiobiose, 8CI. *Amygdalose*



$C_{12}H_{22}O_{11}$ 342.299

β-Pyranose-*form* [5996-00-9]
Mp 190-195°. $[\alpha]_D^{22}$ -0.8 → +10 (c, 3.0 in H_2O).

*1,2-Bis-*O*-(4-hydroxy-3,5-dimethoxycinnamoyl):* ***1,2-Disinapoylgentiobiose***
$C_{34}H_{42}O_{19}$ 754.694
Constit. of broccoli florets (*Brassica oleracea* var. *italica*). Oil. λ_{max} 227 ; 240 ; 262 ; 330 (No solvent reported).

1-O-(4-Hydroxy-3,5-dimethoxycinnamoyl), 2-O-(4-hydroxy-3-methoxycinnamoyl): ***2-Feruloyl-1-sinapoylgentiobiose***
$C_{33}H_{40}O_{18}$ 724.668
Constit. of broccoli florets (*Brassica oleracea* var. *italica*). Oil. λ_{max} 223 ; 241 ; 330 (no solvent reported).

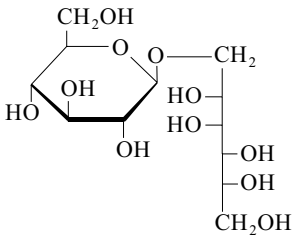
*1,2′-Bis-*O*-(4-hydroxy-3,5-dimethoxycinnamoyl), 2-O-(4-hydroxy-3-methoxycinnamoyl):* ***2-Feruloyl-1,2′-disinapoylgentiobiose***
$C_{44}H_{50}O_{22}$ 930.866
Constit. of broccoli florets (*Brassica oleracea* var. *italica*). Oil. λ_{max} 256 ; 268 ; 355 (No solvent reported).

*1,2,2′-Tris-*O*-(4-hydroxy-3,5-dimethoxycinnamoyl):* [155380-01-1] ***1,2,2′-Trisinapoylgentiobioside***
$C_{45}H_{52}O_{23}$ 960.892
Constit. of broccoli florets. Pale yellow powder. Mp 155-158°.

Sakushima, A. *et al., Phytochemistry*, 1994, **35**, 1481 (*Trisinapoylgentiobioside*)
Price, K.R. *et al., Phytochemistry*, 1997, **45**, 1683 (*cinnamoylgentiobioses*)

1-*O*-D-Glucopyranosyl-D-mannitol, 8CI G-179

[28971-30-4]



$C_{12}H_{24}O_{11}$ 344.315

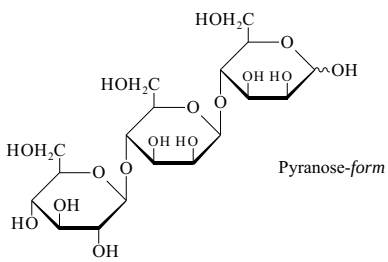
α-form [20942-99-8]
E953
Low nutritive sweetener with half sweetness of sucrose. Component of Isomalt. Mp 122-125°. $[\alpha]_D^{20}$ +87.3 (c, 0.2 in H_2O).

[64519-82-0]

Manners, D.J. *et al., Carbohydr. Res.*, 1968, **7**, 291-298 (*α-form, synth*)
Helferich, B. *et al., Chem. Ber.*, 1973, **106**, 2508-2512 (*α-form, synth*)
Lindner, H.J. *et al., Carbohydr. Res.*, 1981, **93**, 1315 (*cryst struct*)

β-D-Glucopyranosyl-(1→4)-β-D-mannopyranosyl-(1→4)-D-mannose, 9CI, 8CI G-180

[28072-82-4]



Pyranose-*form*

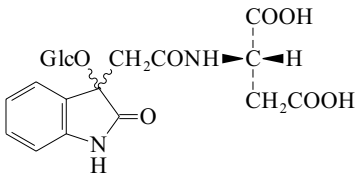
$C_{18}H_{32}O_{16}$ 504.441
Isol. from the hydrolysates of konjac glucomannan (*Amorphophallus konjac*). Cryst. (MeOH). Mp 174-176° (160-162°). $[\alpha]_D^{25}$ -16 (c, 0.5 in H_2O). $[\alpha]_D^{24}$ -7.8 (H_2O).

[94799-30-1]

Perila, O. *et al., Can. J. Chem.*, 1961, **39**, 815
Aspinall, G.O. *et al., J.C.S.*, 1962, 214
Kato, K. *et al., Carbohydr. Res.*, 1973, **29**, 469 (*struct*)
Tomoda, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1807 (*isol*)
Shimizu, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 949 (*isol*)
Takahashi, R. *et al., Agric. Biol. Chem.*, 1984, **48**, 2943
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1988, **52**, 519 (*synth*)
Singh, R.B. *et al., J. Indian Chem. Soc.*, 1989, **66**, 258 (*isol, struct*)

N-[[3-(β-D-Glucopyranosyloxy)-2,3-dihydro-2-oxo-1*H*-indol-3-yl]acetyl]aspartic acid, 9CI G-181

[99694-85-6]

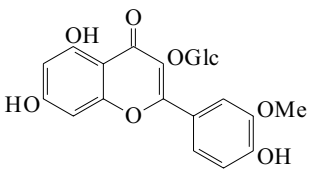


$C_{20}H_{24}N_2O_{12}$ 484.416
Constit. of the seedlings of *Vicia faba*. Powder.

Tsurumi, S. *et al., Plant Physiol.*, 1985, **79**, 667 (*isol*)

3-Glucopyranosyloxy-4′,5,7-trihydroxy-3′-methoxyflavone G-182

[5041-82-7]
Isorhamnetin 3-glucoside. 3-Glucosylisorhamnetin



$C_{22}H_{22}O_{12}$ 478.409
Mp 215-218° (177-179°). $[\alpha]_D$ -21.7 (c, 0.06 in MeOH). λ_{max} 209 ; 259 ; 359 (MeOH) (Berdy).

2″-O-β-D-Apiofuranosyl, 6″-O-α-L-rhamnopyranosyl: [165605-18-5]
$C_{33}H_{40}O_{20}$ 756.667
Constit. of the pseudocereal *Chenopodium pallidicaule* (canihua).

6″-O-β-D-Xylopyranosyl: [142905-19-9]
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Cistus ladanifer* (labdanum) bee pollen.

2″-O-α-L-Rhamnopyranosyl: [55033-90-4] *Isorhamnetin 3-neohesperidoside.* ***Calendoflavoside***
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Zea mays* (sweet corn). Mp 194-197°. $[\alpha]_D^{23}$ -104 (c, 0.1 in MeOH).

4′-O-α-L-Rhamnopyranoside, 6″-O-α-L-rhamnopyranosyl: [81053-13-6]
$C_{34}H_{42}O_{20}$ 770.694
Isol. from *Cucurbita pepo*. Cryst. (MeOH). Mp 190.5-192°. $[\alpha]_D^{35}$ +64.4 (c, 0.3 in MeOH).

6″-O-β-L-Rhamnofuranosyl: [37138-79-7]
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Calendula officinalis* (pot marigold).

*2″,6″-Di-*O*-α-L-rhamnopyranosyl:* [104472-68-6] ***Typhaneoside***
$C_{34}H_{42}O_{20}$ 770.694
Isol. from *Calendula officinalis* (pot marigold). Amorph. yellow powder. Mp 148-150°. $[\alpha]_D^{20}$ -58 (c, 1.3 in MeOH).

2″-O-β-D-Glucopyranosyl, 7-O-β-D-glucopyranoside: [17331-29-2] ***Brassicoside***
$C_{34}H_{42}O_{22}$ 802.693

From *Brassica napus*. Cryst. + $3H_2O$. Mp 209-212°.

3″-O-*β-D-Glucopyranosyl:* [171828-59-4]
Isorhamnetin 3-β-laminaribioside
$C_{28}H_{32}O_{17}$ 640.551
Constit. of the bracken fern *Pteridium aquilinum*. λ_{max} 256 ; 265 (sh) ; 354 (MeOH).

4′-O-*β-D-Glucopyranoside:* [28288-98-4]
Dactylin. *Astragalegoside. Dactilin. Isorhamnetin 3,4′-diglucoside*
$C_{28}H_{32}O_{17}$ 640.551
Isol. from *Zea mays* (sweet corn) and other plants. Yellow cryst. (EtOH). Mp 187-189°. $[\alpha]_D^{20}$ -85 (0.1*M* NaOH aq.).

6″-O-*[α-L-Rhamnopyranosyl-(1→3)-α-L-rhamnopyranosyl]:* [122342-15-8]
$C_{34}H_{42}O_{20}$ 770.694
Constit. of *Calendula officinalis* (pot marigold).

?″-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranosyl]:* [169627-64-9] *Isorhamnetin 3-(rutinosylglucoside)*
$C_{34}H_{42}O_{21}$ 786.693
Isol. from *Aspidosperma quebracho-blanco* (quebracho).

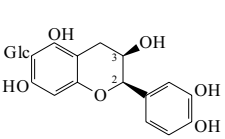
6″-O-*Malonyl:* [86555-37-5]
$C_{25}H_{24}O_{15}$ 564.456
Isol. from *Pyrus communis* (pear).

[11020-74-9, 28878-65-1, 38907-36-7, 39040-06-7, 50867-22-6, 74365-54-1, 94799-73-2]

Inglett, G.E. *et al., Nature (London)*, 1956, **178**, 1346 (*Dactylin*)
Hörhammer, L. *et al., Tet. Lett.*, 1966, 567-571 (*Brassicoside, synth*)
Biryuk, V.A. *et al., Farm. Zh. (Kiev)*, 1972, **27**, 44 (*6″-rhamnosyl*)
Bacon, J.D. *et al., Phytochemistry*, 1975, **14**, 295-296 (*2″-L-rhamnosyl*)
Parker, W.H. *et al., Phytochemistry*, 1975, **14**, 553-555 (*6″-rhamnosylrhamnosyl*)
Wong, E. *et al., N.Z. J. Sci.*, 1980, **23**, 39 (*6″-xylosyl*)
Itokawa, H. *et al., Phytochemistry*, 1981, **20**, 2421-2422 (*4′,6″-dirhamnoside*)
Ceska, O. *et al., Phytochemistry*, 1984, **23**, 1822-1823 (*Dactylin, Calendoflavoside*)
Wald, B. *et al., Phytochemistry*, 1989, **28**, 663-664 (*6″-malonyl*)
Webby, R.F. *et al., Phytochemistry*, 1990, **29**, 289-292 (*6″-dirhamnosyl*)
Tomas-Lorente, F. *et al., Phytochemistry*, 1992, **31**, 2027-2029 (*6″-xylosyl*)
Rastrelli, L. *et al., J. Agric. Food Chem.*, 1995, **43**, 2020 (*2″-apiosyl-6″-rhamnosyl*)
Elgamal, M.H.A. *et al., Fitoterapia*, 1998, **69**, 549-550 (*Isorhamnetin 3-glucoside, pmr, cmr*)
Beck, M.-A. *et al., Phytochemistry*, 1999, **50**, 329-332 (*rhamnosylrhamnosyl*)

6-Glucopyranosyl-3,3′,4′,5,7-pentahydroxyflavan G-183

6-Glucopyranosyl-3′,4′,5,7-tetrahydroxy-3-flavanol



(2*R*,3*R*)-*form*

$C_{21}H_{24}O_{11}$ 452.414

(2*R*,3*R*)-*form* [103215-49-2]
(-)-Epicatechin 6-C-glucoside. 6-Glucopyranosyl-(-)-epicatechin. 6-Glucosyl-(-)-epicatechin
Isol. from bark of Chinese cinnamon *Cinnamomum cassia*. Off-white powder + $1H_2O$. $[\alpha]_D^{19}$ +8.85 (c, 1.1 in MeOH).

(2*R*,3*S*)-*form* [105371-27-5]
(+)-Catechin 6-C-glucoside. 6-Glucopyranosyl-(+)-catechin. 6-Glucosyl-(+)-catechin
Isol. from *Rheum* sp. (rhubarb). Powder $+2H_2O$. $[\alpha]_D^{23}$ +34.8 (c, 0.61 in MeOH).

Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3201 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 623; 643 (*isol*)

8-Glucopyranosyl-3,3′,4′,5,7-pentahydroxyflavan G-184

8-β-D-Glucopyranosyl-3,3′,4′,5,7-tetrahydroxy-3-flavanol

$C_{21}H_{24}O_{11}$ 452.414

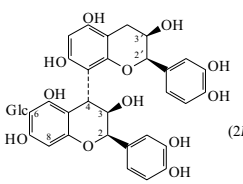
(2*R*,3*R*)-*form* [103215-48-1]
(-)-Epicatechin 8-C-glucoside. 8-Glucopyranosyl-(-)-epicatechin. 8-Glucosyl-(-)-epicatechin
Isol. from bark of Chinese cinnamon *Cinnamomum cassia*. Off-white powder + $1H_2O$. $[\alpha]_D^{19}$ -37.5 (c, 0.9 in Me_2CO).

(2*R*,3*S*)-*form* [105371-26-4]
(+)-Catechin 8-C-glucoside. 8-Glucopyranosyl-(+)-catechin. 8-Glucosyl-(+)-catechin
Isol. from *Rheum* sp. (rhubarb). Powder + $1H_2O$. $[\alpha]_D^{23}$ -60.2 (c, 0.64 in MeOH).

Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3201 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 633; 643 (*isol*)

6-Glucopyranosylprocyanidin B G-185

2,2′-Bis(3,4-dihydroxyphenyl)-6-β-D-glucopyranosyl-3,3′,4,4′-tetrahydro-[4,8′-bi-2H-1-benzopyran]-3,3′,5,5′,7,7′-hexol, 9CI. 6-Glucosylprocyanidin B



(2*R*,2′*R*,3*R*,3′*R*,4*R*)-*form*

$C_{36}H_{36}O_{17}$ 740.67

(2*R*,2′*R*,3*R*,3′*R*,4*R*)-*form* [103215-59-4]
6-Glucopyranosylprocyanidin B$_2$
Isol. from Chinese cinnamon bark (*Cinnamomum cassia*) and *Rheum* sp. (rhubarb). Off-white powder $+2H_2O$. $[\alpha]_D^{21}$ +12.5 (c, 1.1 in Me_2CO).

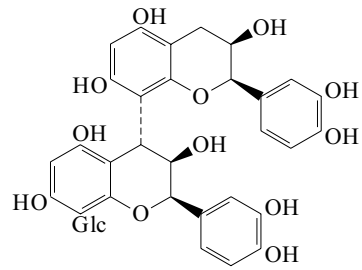
(2*R*,2′*R*,3*R*,3′*S*,4*R*)-*form* [105371-29-7]
6-Glucopyranosylprocyanidin B$_1$. *Procyanidin B, 6-C-glucoside*
Isol. from rhubarb *Rheum* sp.. Tan powder + $1H_2O$. $[\alpha]_D^{19}$ +45.1 (c, 0.79 in MeOH).

[105330-50-5]

Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 643 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3208 (*isol*)

8-Glucopyranosylprocyanidin B G-186

2,2′-Bis(3,4-dihydroxyphenyl)-8-β-D-glucopyranosyl-3,3′,4,4′-tetrahydro-[4,8′-bi-2H-1-benzopyran]-3,3′,5,5′,7,7′-hexol, 9CI. 8-Glucosylprocyanidin B



$C_{36}H_{36}O_{17}$ 740.67

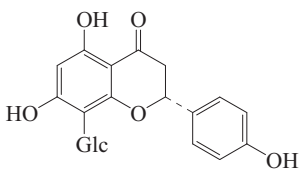
(2*R*,2′*R*,3*R*,3′*R*,4*R*)-*form* [103215-58-3]
8-Glucopyranosylprocyanidin B$_2$
Isol. from Chinese cinnamon bark (*Cinnamomum cassia*) and *Rheum* sp. (rhubarb). Off-white powder + $2H_2O$. $[\alpha]_D^{21}$ +18.2 (c, 1 in Me_2CO).

(2*R*,2′*R*,3*R*,3′*S*,4*R*)-*form* [105371-28-6]
8-Glucopyranosylprocyanidin B$_1$
Isol. from rhubarb *Rheum* sp.. Tan powder + $1\frac{1}{2}H_2O$. $[\alpha]_D^{19}$ +33.7 (c, 0.88 in MeOH).

Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 643 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3208 (*isol*)

8-Glucopyranosyl-4′,5,7-trihydroxyflavanone G-187

8-β-D-Glucopyranosyl-2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Isohemiphloin***



(*R*)-*form*

$C_{21}H_{22}O_{10}$ 434.399

(R)-form

2″-O-*α-L-Rhamnopyranosyl:*
$C_{27}H_{32}O_{14}$ 580.541
Constit. of *Eriobotrya japonica* (loquat). Pale yellow powder. $[\alpha]_D$ +5.3 (c, 1 in MeOH). λ_{max} 218 (log ε 4.43); 290 (log ε 4.2); 328 (sh) (log ε 3.63) (MeOH).

(S)-form [3682-02-8]
Non cryst. $[\alpha]_D^{20}$ -12.1 (c, 0.62 in Me_2CO aq.).

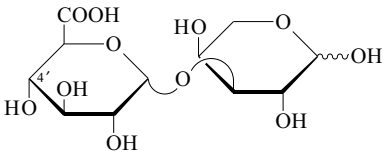
Hepta-Ac:
Mp 223-224°.

2″-O-*α-L-Rhamnopyranosyl:*
Constit. of *Eriobotrya japonica* (loquat). Pale yellow powder. $[\alpha]_D$ +25.3 (c, 1 in MeOH). λ_{max} 214 (log ε 4.39); 225 (sh) (log ε 4.36); 290 (log ε 4.12); 325 (sh) (log ε 3.64) (MeOH).

Hillis, W.E. *et al., Aust. J. Chem.*, 1963, **16**, 147; 1965, **18**, 531 (*isol, pmr*)
Lorente, F.T. *et al., An. Quim., Ser. C*, 1983, **79**, 456 (*isol*)

Ito, H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 687-693 (*2′′-rhamnosyl derivs*)

3-*O*-α-D-Glucopyranuronosyl-L-arabinose G-188

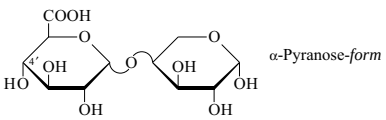


$C_{11}H_{18}O_{11}$ 326.257

O$^{4'}$*-Me:3-O-(4-O-Methyl-α-D-glucopyranuronosyl)-L-arabinose*
$C_{12}H_{20}O_{11}$ 340.283
Isol. from the autohydrolysate of golden apple (*Spondias cytherea*) gum. $[\alpha]_D$ +123 (H_2O).

Lindgren, B.O. *et al., Acta Chem. Scand.*, 1957, **11**, 1365 (*isol*)

4-*O*-α-D-Glucopyranuronosyl-L-arabinose G-189



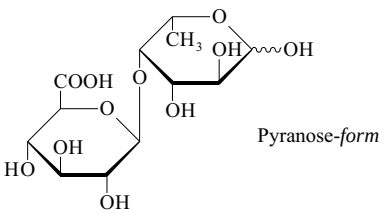
$C_{11}H_{18}O_{11}$ 326.257

4′-Me:4-O-(4-O-Methyl-α-D-glucopyranuronosyl)-L-arabinose
$C_{12}H_{20}O_{11}$ 340.283
Isol. from the partial hydrolysates of lemon gum. $[\alpha]_D$ +134 (H_2O).

Andrews, P. *et al., J.C.S.*, 1954, 1724 (*isol*)
Guzman, E. *et al., Rev. Esp. Fisiol.*, 1960, **16**, 331

4-*O*-β-D-Glucopyranuronosyl-L-fucose G-190

[16749-74-9]

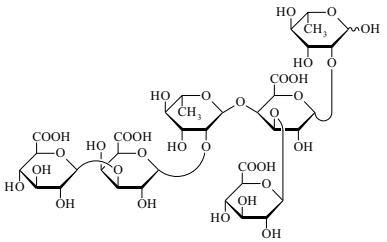


$C_{12}H_{20}O_{11}$ 340.283
Reducing disaccharide. Isol. from the partial acid hydrolysate of tragacanthic acid, the major polysaccharide component of tragacanth gum. $[\alpha]_D$ -18 (c, 1.5 in H_2O).

Aspinall, G.O. *et al., J.C.S.(C)*, 1967, 1086 (*isol*)

β-D-Glucopyranuronosyl-(1 → 3)-α-D-galactopyranuronosyl-(1 → 2)-α-L-rhamnopyranosyl-(1 → 4)-[β-D-glucopyranuronosyl-(1 → 3)]-α-D-galactopyranuronosyl-(1 → 2)-L-rhamnopyranose G-191

[71562-84-0]

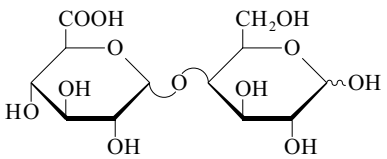


$C_{36}H_{54}O_{33}$ 1014.803
Isol. from the hydrolysate of the mucilage in the roots of *Abelmoschus manihot* (aibika) and *Althaea officinalis* (marsh mallow). Powder. Mp 172-176° dec. $[\alpha]_D^{20}$ +81.4 (c, 1.4 in H_2O).

Tomoda, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1357; 2910; 1979, **27**, 1651; 1980, **28**, 824

4-*O*-α-D-Glucopyranuronosyl-D-galactose G-192

[14402-41-6]



$C_{12}H_{20}O_{12}$ 356.283
Isol. from partial acid hydrolysates of tragacanthic acid, the major polysaccharide component of gum tragacanth. $[\alpha]_D$ +87 (c, 1.4 in H_2O). $[\alpha]_D^{20}$ +58 (c, 1.2 in H_2O).

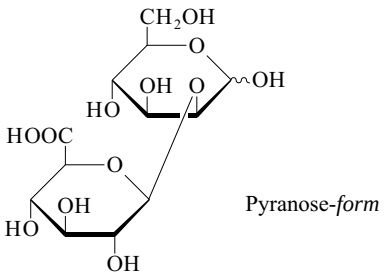
Ba salt:
$[\alpha]_D$ +110 (+67) (H_2O).

Me glycoside, hexa-Me, Me ester:
$C_{20}H_{36}O_{12}$ 468.497
$Bp_{0.75}$ 195-225° (bath) (lit. gives a pressure range).

Mukherjee, S.H. *et al., J.A.C.S.*, 1955, **77**, 422
Charlson, A.J. *et al., J.C.S.*, 1955, 1428 (*isol*)
Aspinall, G.O. *et al., J.C.S.(C)*, 1967, 1086 (*isol*)
Audichya, J.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 601 (*isol*)

2-*O*-β-D-Glucopyranuronosyl-D-mannose, 8CI G-193

[4539-91-7]



$C_{12}H_{20}O_{12}$ 356.283
Present as a structural unit in plant gums, e.g. damson (*Prunus insitia*), cherry (*Prunus cerasus*), *Anogeissus lattifolia* (gum ghatti). $[\alpha]_D$ -32 (H_2O).

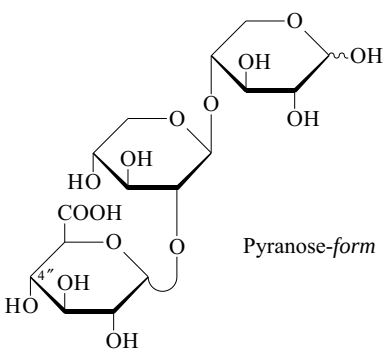
Ba salt:
$[\alpha]_D$ -30 (H_2O).

Me glycoside, hexa-Me, 6′-Me ester:
[70051-79-5]
$C_{20}H_{36}O_{12}$ 468.497
Mp 141°. $[\alpha]_D$ -22 ($CHCl_3$).

[52554-63-9, 52554-64-0]

Stephen, A.M. *et al., J.C.S.*, 1956, 4487
Drummond, D.W. *et al., J.C.S.*, 1961, 3908 (*isol*)
Smith, F. *et al., J.C.S.*, 1961, 4892 (*isol, Me gly*)
Sloneker, J.H. *et al., Can. J. Chem.*, 1962, **40**, 2066 (*isol*)
Misaki, A. *et al., Can. J. Chem.*, 1962, **40**, 2204 (*isol*)

α-D-Glucopyranuronosyl-(1 → 2)-β-D-xylopyranosyl-(1 → 4)-D-xylose G-194



$C_{16}H_{26}O_{15}$ 458.372

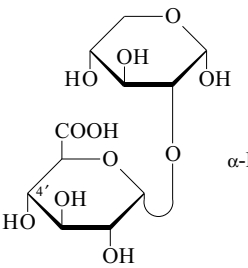
O$^{4''}$*-Me:* [10365-86-3] *4-O-Methyl-α-D-glucopyranosyl-(1 → 2)-β-D-xylopyranosyl-(1 → 4)-D-xylose*
$C_{17}H_{28}O_{15}$ 472.399
From oat hull hemicelluloses. Cryst. + 3H_2O. Mp 180-187°. $[\alpha]_D$ +59 (H_2O).

Hamilton, J.K. *et al., J.A.C.S.*, 1957, **79**, 6464 (*isol*)
Roudier, A.J. *et al., Bull. Soc. Chim. Fr.*, 1960, **28**, 2074 (*isol*)
Srivastava, H.C. *et al., J.O.C.*, 1961, **26**, 3958 (*isol*)
Timell, T.E. *et al., J.O.C.*, 1962, **27**, 1804

2-*O*-α-D-Glucopyranuronosyl-D-xylose, 9CI, 8CI G-195

[17676-51-6]

Aldobiouronic acid D_3



α-Pyranose-*form*

$C_{11}H_{18}O_{11}$ 326.257

Isol. from partial acid hydrolysates of gum chagual (*Puya* spp.) and the hemicelluloses from corn hulls and wheat bran. Amorph. $[\alpha]_D^{20}$ +101 (88) (H_2O).

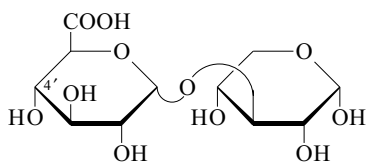
4′-Me: [7382-52-7] *2-O-(4-O-Methyl-α-D-glucopyranuronosyl)-D-xylose, 9CI, 8CI*
Important aldobiouronic acid that occurs as a structural unit of polysaccharides. Widely distributed in plants. Amorph. powder. $[\alpha]_D^{20}$ +108 (c, 1.0 in H_2O). Opt. rotns. reported vary between +70 and +110.

[1693-81-8, 29412-02-0]

Jones, J.K.N. *et al., J.C.S.*, 1952, 2750; 3389; 1957, 669; 1958, 1059 (*isol, 4′-Me*)
Dutton, G.G.S. *et al., J.A.C.S.*, 1956, **78**, 2505; 1958, **80**, 4420 (*isol*)
Adams, G.A. *et al., J.A.C.S.*, 1956, **78**, 2842 (*isol*)
Roudier, A.J. *et al., Bull. Soc. Chim. Fr.*, 1960, **28**, 2074 (*isol*)
Pazur, J.H. *et al., The Carbohydrates*, 1970, 120 (*4′-Me, rev*)
Maekawa, E. *et al., Agric. Biol. Chem.*, 1973, **37**, 2073 (*isol*)
Kováč, P. *et al., Carbohydr. Res.*, 1981, **93**, 144 (*4′-Me, 4′-Me Me ester, cmr*)

3-*O*-α-D-Glucopyranuronosyl-D-xylose, 9CI G-196

[85269-45-0]



α-Pyranose-*form*

$C_{11}H_{18}O_{11}$ 326.257

Isol. from hemicellulose hydrolysates, from pear cell-wall xylan, from various wheat-straw preparations and from corn hulls. $[\alpha]_D$ +18 (H_2O).

Pyranose-*form*

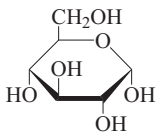
4′-Me: [66634-88-6] *3-O-(4-O-Methyl-α-D-glucopyranuronosyl)-D-xylose, 9CI*
$C_{12}H_{20}O_{11}$ 340.283
$[\alpha]_D$ +65 (H_2O).

Hexa-Me:
$C_{17}H_{30}O_{11}$ 410.417
$[\alpha]_D$ +12.4 (H_2O).

Chanda, S.K. *et al., J.C.S.*, 1951, 1240
Adams, G.A. *et al., Can. J. Chem.*, 1952, **30**, 698; 1953, **31**, 134 (*isol*)
Bishop, C.T. *et al., Can. J. Chem.*, 1953, **31**, 134; 1955, **33**, 1521 (*isol*)
Aspinall, G.O. *et al., J.C.S.*, 1954, 1731 (*isol*)
Brasch, D.J. *et al., Tappi*, 1956, **39**, 581; 768 (*isol, deriv*)
Bailey, R.W. *et al., Oligosaccharides*, Pergamon, 1965, **4**, 137 (*occur, deriv*)
Yoshida, S. *et al., Agric. Biol. Chem.*, 1990, **54**, 1319 (*isol*)

Glucose, 9CI, 8CI G-197

Dextrose. Grape sugar. Blood sugar. Corn sugar. Cerelose



α-D-Pyranose-*form*

$C_6H_{12}O_6$ 180.157

An aq. soln. contains 37.3% α-pyr, 62.6% β-pyr, 0.1% β-fur and 0.002% aldehyde.

D-*form* [50-99-7]

[5996-10-1]

Occurs free in fruits, honey and plant juices. Major component of many oligosaccharides and polysaccharides. Occurs in sucrose combined with fructose. Comly. available by the acid hydrol. of potato starch (Europe) and cornstarch (USA). Food additive: nutritive sweetener, humectant. pK_{a1} 12.34 (25°). Sweet taste, sweetness = 0.46 x sucrose.

▶ Reacts violently with Na_2O_2 plus KNO_3, and other strong oxidants. LD_{50} (rat, orl) 25800 mg/kg. Human and exp. reprod. and teratogenic effects (large doses). LZ6600000

Penta-Ac: [3891-59-6] *2,3,4,5,6-Penta-O-acetyl-D-glucose. FEMA 2524*
$C_{16}H_{22}O_{11}$ 390.343
Commercial product usually a mixture of 90% β-D and 10% α-D. Flavouring agent. Bitter flavour. Mp 114° (α-anomer) Mp 135° (β-anomer). $[\alpha]_D^{20}$ +102 (c, 1 in $CHCl_3$) (α-anomer). $[\alpha]_D^{20}$ +4.4 (c, 1 in $CHCl_3$) (β-anomer).

D-Pyranose-*form*

α-D-Pyranose-*form* [492-62-6]

[26655-34-5, 31178-74-2]

Cryst. (hot EtOH or H_2O). Mp 146° (anhyd.) Mp 83° (monohyd.). $[\alpha]_D^{20}$ +111.2 → +52.5 (c, 10 in H_2O).

β-D-Pyranose-*form* [492-61-5]

[28905-12-6, 31258-47-6]

Cryst. (EtOH aq., Py at 0° or hot AcOH aq.). Mp 148-150° (anhyd.). $[\alpha]_D^{20}$ +17.5 → +52.5 (c, 10 in H_2O).

D-Furanose-*form*

β-D-Furanose-*form* [30412-16-9]

[815-92-9, 8013-17-0, 39281-65-7, 41846-85-9, 41846-86-0, 53691-70-6, 53691-71-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 190B-625A; 625A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 300A; 1056A; 301A; **2**, 1284C (*nmr*)

Saha, H. *et al., J.C.S.*, 1922, **121**, 1044-1046 (*isol, DL-form*)
Wolfrom, M.L. *et al., J.A.C.S.*, 1929, **51**, 2188-2193 (*pentaacetyl*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate*, Edwards Bros. Inc., Ann Arbor, 1943, 208; 211
Dean, G.R. *et al., Adv. Carbohydr. Chem.*, 1950, **5**, 127-143 (*manuf*)
Percival, E. *et al., Structural Carbohydr. Chem.*, (Miller, J.G., Ed.), 1962, 51 (*rev*)
Hough, L. *et al., Rodd's Chem. Carbon Compd. (2nd edn.)*, 1967, **1F**, 237 (*occur, isol*)
Schaffer, R. *et al., The Carbohydrates*, (Pigman, W. et al, Ed.), Academic Press, 2nd Ed., 1972, **1A**, 86 (*occur*)
Jeffrey, G.A. *et al., Carbohydr. Res.*, 1973, **28**, 233-241 (*cryst struct, α-D-form*)
Wander, J.D. *et al., Adv. Carbohydr. Chem. Biochem.*, 1976, **32**, 15-123 (*dithioacetals, rev*)
Vignon, M.R. *et al., Tet. Lett.*, 1976, 2445-2448 (*cmr*)
Mathlouthi, M. *et al., Carbohydr. Res.*, 1980, **81**, 203-212; 213-223 (*Raman*)
Bock, K. *et al., Annu. Rep. NMR Spectrosc.*, (Webb, G.A., ed.), Acad Press, London and New York, 1982, **13**, 37; 41 (*pmr, cmr*)
Curatolo, W. *et al., Carbohydr. Res.*, 1983, **112**, 297-300 (*pmr*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15-68 (*equilib, rev*)
Dziedzic, S.Z. *et al., Glucose Syrups: Sci. Technol.*, Elsevier, 1984, (*rev*)
Kieboom, A.P.G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1984, **103**, 1-12 (*rev, use*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 541 (*synonyms*)
Mikamo, M. *et al., Carbohydr. Res.*, 1989, **191**, 150-153 (*synth, bibl, 2,3,4,6-tetra-Ac*)
Mostad, A. *et al., Acta Chem. Scand.*, 1994, **48**, 276-278 (*cryst struct, α-form*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 154-157
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1363
Merck Index, 12th edn., 1996, 4467
Okuyama, E. *et al., Chem. Pharm. Bull.*, 1998, **46**, 655-662 (*Vitex rotundifolia constit, isol, uv, pmr, cmr*)
Takeuchi, M. *et al., Synthesis*, 1999, 351-354 (*D-form, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GFG000

Glucose oxidase, 9CI G-198

[9001-37-0]

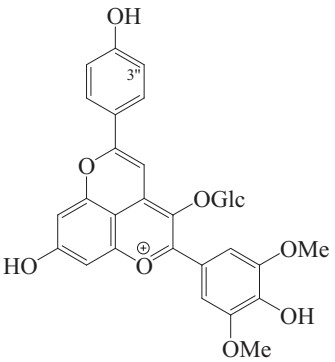
Glucose oxyhydrase. β-D-Glucose: oxygen 1-oxidoreductase. Glucose aerodehydrogenase. Corylophyline. E.C. 1.1.3.4. GOD

A flavoprotein, MW 160 kDa, consisting of 2 identical subunits each containing one FAD unit as cofactor; glycosylated with a carbohydrate content of 16% (w/w). Catalyses the oxidn. of β-D-glucose to D-glucono-1,5-lactone and H_2O_2 using O_2 as the electron acceptor. Used in the food industry as a non toxic preservative to remove residual glucose and oxygen from food and beverages. Amorph. powder or cryst. Sol. H_2O; prac. insol. EtOH, $CHCl_3$, Et_2O.

Swoboda, B.E.P. *et al., J. Biol. Chem.*, 1965, **240**, 2209-2215 (*isol*)
Bentley, R. *et al., Methods Enzymol.*, 1966, **9**, 86 (*isol*)

Bright, H. *et al., The Enzymes*, (Boyer, P., Ed.), 3rd Ed., Academic Press, N,Y., 1975, **12B**, 421 (*rev*)
Raba, J. *et al., Crit. Rev. Anal. Chem.*, 1995, **25**, 1-42 (*rev, use*)
Merck Index, 12th edn., 1996, 4468
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1209-1210 (*use*)

3-Glucosyloxy-8-hydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-5-(4-hydroxyphenyl)pyrano[4,3,2-*de*]-1-benzopyrylium(1+) G-199



$C_{31}H_{29}O_{13}^{\oplus}$ 609.562
Pigment isol. from red wine made from grapes (*Vitis vinifera*). λ_{max} 507 (no solvent reported).

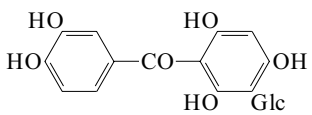
6‴-O-(4-Hydroxy-E-cinnamoyl):
$C_{40}H_{35}O_{15}^{\oplus}$ 755.708
Pigment isol. from red wine made from grapes (*Vitis vinifera*).

3″-Methoxy:
$C_{32}H_{31}O_{14}^{\oplus}$ 639.589
Pigment isol. from Australian wine.

Fulcrand, H. *et al., J.C.S. Perkin 1*, 1996, 735-739 (*isol, uv, pmr, ms*)
Asenstorfer, R.E. *et al., J. Agric. Food Chem.*, 2001, **48**, 5957-5963 (*3″-methoxy*)

3-Glucosyl-2,3′,4,4′,6-pentahydroxybenzophenone G-200

[92631-83-9]
3-Glucosylmaclurin



$C_{19}H_{20}O_{11}$ 424.36
Constit. of leaves of *Mangifera indica* (mango). Yellow amorph. powder. $[\alpha]_D^{25}$ +33.2 (c, 0.9 in MeOH).

6″-(4-Hydroxybenzoyl): [92665-82-2]
$C_{26}H_{24}O_{13}$ 544.468
Constit. of leaves of *Mangifera indica* (mango). Yellow amorph. powder. $[\alpha]_D^{31}$ -50 (c, 0.80 in MeOH).

2″-(3,4,5-Trihydroxybenzoyl), 6″-(4-hydroxybenzoyl): [92631-84-0]
$C_{33}H_{28}O_{17}$ 696.574
Constit. of leaves of *Mangifera indica* (mango). Yellow amorph. powder. $[\alpha]_D^{24}$ -181.3 (c, 0.4 in MeOH).

6″-(3,4,5-Trihydroxybenzoyl), 2″-(p-hydroxybenzoyl): [92631-85-1]
$C_{33}H_{28}O_{17}$ 696.574
Constit. of leaves of *Mangifera indica* (mango). Pale yellow needles (H_2O). Mp 193-194°. $[\alpha]_D^{24}$ -143.8 (c, 0.4 in MeOH).

2″,3″,6″-Tris(3,4,5-trihydroxybenzoyl): [92631-86-2]
$C_{40}H_{32}O_{23}$ 880.679
Constit. of leaves of *Mangifera indica* (mango). Yellow amorph. powder + $1H_2O$. $[\alpha]_D^{30}$ -48.8 (c, 0.4 in MeOH).

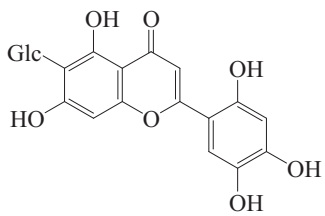
3′-Me ether: ***Telephenone A***
$C_{20}H_{22}O_{11}$ 438.387
Pale yellow powder. $[\alpha]_D$ -10.4 (c, 0.35 in Py). λ_{max} 211 ; 313 (MeOH).

3′,4′-Di-Me ether: ***Telephenone B***
$C_{21}H_{24}O_{11}$ 452.414
Pale yellow powder. $[\alpha]_D$ -14.5 (c, 0.3 in Py). λ_{max} 210 ; 313 (MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2676
Li, J.-C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1354-1355 (*Telephenones*)

6-Glucosyl-2′,4′,5,5′,7-pentahydroxyflavone G-201

2′-Hydroxyisoorientin

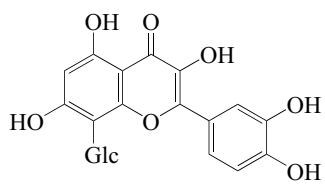


$C_{21}H_{20}O_{12}$ 464.382
Constit. of the leaves of barley, *Hordeum vulgare*. λ_{max} 262 ; 378 (MeOH).

Norbaek, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 1703-1707

8-Glucosyl-3,3′,4′,5,7-pentahydroxyflavone G-202

Quercetin 8-C-glucoside. 8-Glucopyranosylquercetin



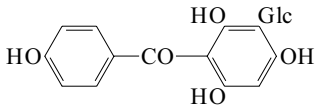
$C_{21}H_{20}O_{12}$ 464.382

2″-O-α-L-Rhamnopyranoside: [182062-20-0]
$C_{27}H_{30}O_{16}$ 610.524
Constit. of the leaves of *Eucalyptus globulus* (Tasmanian blue gum). Yellow powder. λ_{max} 256 ; 302 ; 374 (MeOH).

Manguro, L.O.A. *et al., Nat. Prod. Lett.*, 1995, **7**, 163 (*isol, uv, ir, pmr, cmr, ms*)

3-Glucosyl-2,4,4′,6-tetrahydroxybenzophenone G-203

Iriflophenone 3-C-β-D-glucopyranoside. 3-Glucosyliriflophenone



$C_{19}H_{20}O_{10}$ 408.361
Amorph. $[\alpha]_D$ +41. First benzophenone isol. from ferns.

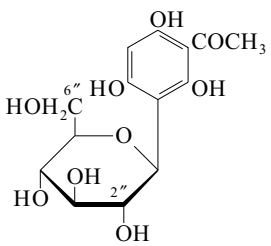
2″,6″-Di-O-galloyl: [92631-87-3]
$C_{33}H_{28}O_{18}$ 712.573
Isol. from leaves of *Mangifera indica* (mango). $[\alpha]_D$ -135 (c, 1.0 in MeOH).

2″,3″,6″-Tri-O-galloyl: [92631-88-4]
$C_{40}H_{32}O_{22}$ 864.68
Isol. from leaves of *Mangifera indica* (mango). Yellow amorph. powder. $[\alpha]_D$ -47.4 (c, 0.7 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2676
Murakami, T. *et al., Yakugaku Zasshi*, 1986, **106**, 378

3′-Glucosyl-2′,4′,6′-trihydroxyacetophenone G-204

[88885-07-8]
1-(3-Glucopyranosyl-2,4,6-trihydroxyphenyl)ethanone, 9CI. 2-Acetyl-4-β-D-glucopyranosyl-1,3,5-benzenetriol



$C_{14}H_{18}O_9$ 330.291
Constit. of the leaves of *Syzygium aromaticum* (clove). Amorph. powder + $^1/_2H_2O$. Mp 167-169°. $[\alpha]_D^{21}$ +49.3 (c, 0.8 in MeOH).

2″-O-(3,4,5-Trihydroxybenzoyl): [152041-18-4]
$C_{21}H_{22}O_{13}$ 482.397
Constit. of *Syzygium aromaticum* (clove). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ -98.6 (c, 0.9 in MeOH).

6″-O-(3,4,5-Trihydroxybenzoyl): [152041-19-5]
$C_{21}H_{22}O_{13}$ 482.397
Constit. of *Syzygium aromaticum* (clove). Amorph. powder. $[\alpha]_D^{28}$ -49 (c, 1.4 in MeOH).

2″,3″-Di-O-(3,4,5-trihydroxybenzoyl): [152041-20-8]
$C_{28}H_{26}O_{17}$ 634.503
Constit. of *Syzygium aromaticum* (clove). Amorph. powder. $[\alpha]_D^{28}$ +30.2 (c, 1.7 in MeOH).

2″,6″-Di-O-(3,4,5-trihydroxybenzoyl): [152041-21-9]
$C_{28}H_{26}O_{17}$ 634.503
Constit. of *Syzygium aromaticum*

(clove). Amorph. powder + ½H_2O. $[\alpha]_D^{28}$ -140.4 (c, 1.3 in MeOH).

*2″,3″,6″-Tris-*O*-(3,4,5-trihydroxybenzoyl):* [152041-22-0]
$C_{35}H_{30}O_{21}$ 786.609
Constit. of *Syzygium aromaticum* (clove). Amorph. powder. $[\alpha]_D^{28}$ -13 (c, 1.4 in MeOH).

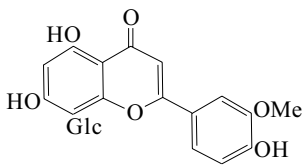
*2″,3″,4″,6″-Tetrakis-*O*-(3,4,5-trihydroxybenzoyl):* [152041-23-1]
$C_{42}H_{34}O_{25}$ 938.716
Constit. of *Syzygium aromaticum* (clove). Amorph. powder + 2H_2O. $[\alpha]_D^{21}$ -16.3 (c, 1 in MeOH).

*2″,3″-Bis-*O*-(3,4,5-trihydroxybenzoyl) 4″,6″-*O*-(*S*)-hexahydroxydiphenoyl:* [152041-24-2]
$C_{42}H_{32}O_{25}$ 936.7
Constit. of *Syzygium aromaticum* (clove). Tan powder + 2H_2O. $[\alpha]_D^{21}$ +59.3 (c, 1 in MeOH).

Onodera, J. *et al., Chem. Lett.*, 1983, 1487 (*synth*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1232 (*isol, pmr, cmr*)

8-Glucosyl-4′,5,7-trihydroxy-3′-methoxyflavone G-205

[301-16-6]
*8-Glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*



$C_{22}H_{22}O_{11}$ 462.409

β-D-Pyranose-*form*
***Scoparin*†.** *Scoparoside*
Light-yellow needles (MeOH aq.). Sol. hot H_2O. Mp 253° dec. Log P -2.34 (calc).

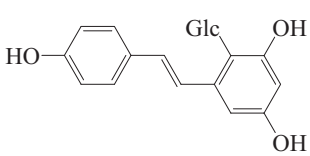
*2″-*O*-β-D-Glucopyranoside:* [124902-15-4]
Scoparin 2″-glucoside
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Setaria italica* (foxtail millet).

*2″-*O*-β-D-Xylopyranoside:* [124934-30-1]
Scoparin 2″-xyloside
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Setaria italica* (foxtail millet).

Gluchoff-Fiasson, K. *et al., Phytochemistry*, 1989, **28**, 2471 (*2″-glucoside, 2″-xyloside*)

2-Glucosyl-3,4′,5-trihydroxystilbene G-206

*2-*C*-β-D-Glucopyranosylresveratrol. Resveratrol 2-*C*-glucoside*



$C_{20}H_{22}O_8$ 390.389

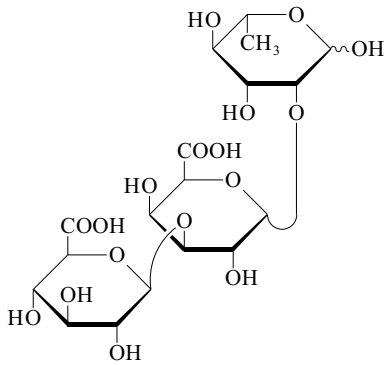
(E)-form
Isol. from riesling wine. Amorph. powder. $[\alpha]_D^{24}$ +23 (c, 0.1 in MeOH). λ_{max} 212 ; 293 (MeOH).

(Z)-form
Isol. from Riesling wine.

Baderschneider, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 2681-2686
Tanaka, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 785-787 (*isol, pmr, cmr*)

β-D-Glucuronopyranosyl-(1→3)-α-D-galacturonopyranosyl-(1→2)-L-rhamnose G-207

[122620-32-0]
β-D-Glucopyranuronosyl-(1→3)-α-D-galactopyranuronosyl-(1→2)-6-deoxy-L-mannose, 9CI



$C_{18}H_{28}O_{17}$ 516.409
Isol. from the partial acid hydrolsates of the mucilage of *Abelmoschus manihot* (aibika) and Okra mucilage R in fruits and roots of *Abelmoschus esculentus*. $[\alpha]_D$ +85.4 (H_2O).

Aspinall, G.O. *et al., J.C.S.*, 1965, 4325
Tomoda, M. *et al., Chem. Pharm. Bull.*, 1979, **27**, 1651 (*isol*)
Tomoda, M. *et al., Carbohydr. Res.*, 1986, **151**, 29; 1989, **190**, 323 (*isol*)
Raju, T.S. *et al., Carbohydr. Res.*, 1989, **191**, 321 (*isol*)

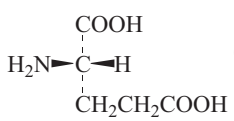
Glutacin G-208

[91105-05-4]
Struct. unknown. Bacteriocin prod. by *Corynebacterium glutamicum*.

Karabekov, B.P. *et al., Mikrobiologiya*, 1984, **53**, 261-265; *CA*, **101**, 51370g (*isol*)

Glutamic acid G-209

[6899-05-4]
2-Aminopentanedioic acid, 9CI. 2-Aminoglutaric acid. Glutaminic acid. Glu. E620. FEMA 3285



(*S*)-*form*

$C_5H_9NO_4$ 147.13

(S)-form [56-86-0]
L-form
Obt. from acid hydrol. of proteins. Since 1965 the industrial source of glutamic acid for MSG production has been bacterial fermentation of carbohydrate sources such as molasses and corn starch hydrolysate in the presence of a nitrogen source such as ammonium salts or urea. Annual production approx. 350000t worldwide in 1988. Seasoning additive in food manuf. (as Na, K and NH_4 salts). Dietary supplement, nutrient. Rhombic cryst. (EtOH aq.). Spar. sol. EtOH, H_2O (0.84 g/100g at 25°). Mp 224-225° (211-213°, 247-249°) dec. $[\alpha]_D^{25}$ +17 (c, 2 in H_2O). $[\alpha]_D^{25}$ +46.8 (c, 2 in 5*M* HCl). pK_{a3} 9.6 (25°,NH_2). Isoelectric point 3.24. Appetising taste.
▶ Human systemic effects by ingestion and intravenous routes. LZ9700000

Hydrochloride: [138-15-8]
Dietary supplement, nutrient, flavouring agent and enhancer. Mp 202° dec Mp 213° (rapid heating).

Na salt: [142-47-2]

[6106-04-3, 16177-21-2] ***Monosodium glutamate. MSG. Chinese seasoning. Accent. Ajinomoto. Glutacyl. Glutavene. RL-50. E621***
$C_5H_8NNaO_4$ 169.112
Food flavour enhancer. Rhombic prisms + 1H_2O (H_2O) with characteristic meaty taste ("umami"). $[\alpha]_D^{20}$ +25.16 (c, 10 in 2*M* HCl). $[\alpha]_D^{20}$ -4 (c, 1.2 in H_2O). Monohydrate loses water of crystallisation at 120°, undergoes intramolecular dehydration at 155° and dec. at 225°. Taste threshold 0.3% in H_2O.

K salt: [19473-49-5] *Monopotassium glutamate. E622*
$C_5H_8KNO_4$ 185.221
Flavour enhancer; salt substitute.

Ca salt (2:1): [5996-22-5] *Calcium diglutamate. E623*
$C_{10}H_{16}CaN_2O_8$ 332.323
Flavour enhancer; salt substitute.

NH_4 salt: [7558-63-6] *Monoammonium glutamate. E624*
$C_5H_{12}N_2O_4$ 164.161
Flavour enhancer.

[997-42-2, 5996-22-5, 7558-63-6, 11070-68-1, 19285-83-7, 21752-29-4, 24938-00-9, 25513-46-6, 25683-11-8, 63663-21-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 589D; 590A; 590C; 678B; 781D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1077C; 1120A; 1277B (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 286 (*synth*)
Archibald, R.M. *et al., Chem. Rev.*, 1945, **37**, 161 (*biochem*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 25), Wiley, N.Y., 1961, 1929 (*isol, synth, rev*)
U.S. Pat., 1961, 3002889; *CA*, **55**, 12766i (*manuf*)
Huffman, C.W. *et al., Chem. Rev.*, 1963, **63**, 625 (*synth*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Zintel, J.A. *et al., Can. J. Chem.*, 1969, **47**, 411 (*enz synth*)
Vinogradov, I.P. *et al., Opt. Spektrosk.*, 1971, **30**, 27 (*uv*)
Sequieira, A. *et al., Acta Cryst. B*, 1972, **28**, 2514 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2371 (*occur*)
Voelter, W. *et al., Monatsh. Chem.*, 1974, **105**, 1110-1135 (*cmr*)

Synth. Prod. Util. Amino Acids, (Kaneko, T. *et al*, Ed.), Halsted Press, 1974, 101 (*synth*)
Traldi, P. *et al., Org. Mass Spectrom.*, 1982, **17**, 245 (*ms*)
Sano, C. *et al., Anal. Sci.*, 1989, **5**, 121-122 (*cryst struct, monosodium glutamate hydrate*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, GFO000; GFO025
Araki, K *et al., Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley*, 1991, **2**, 571-579 (*monosodium glutamate, rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 586; 587
Takano, S. *et al., Synthesis*, 1994, 601 (*S-form, synth*)
Dunitz, J.D. *et al., Acta Cryst. C*, 1995, **51**, 1377 (*cryst struct*)
Merck Index, 12th edn., 1996, 1070 (*monosodium glutamate, rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1211-1214; 1895-1896; 1907-1912
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, No. 1351 (*monosodium glutamate*)
Halpern, B.P. *et al., J. Nutr.*, Suppl. 4S, 2000, **130**, 910S-914S (*use, rev*)
Kawakita, T. *et al., Ullmann's Encycl. Ind. Chem.*, 5th. Ed., **A16**, 711-718 (*monosodium glutamate, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GFO000; GFO025

Glutaminase G-210

[9001-47-2]

L-Glutamine aminohydrolase. E.C. 3.5.1.2

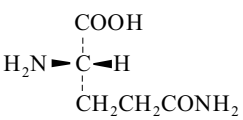
Enzyme. Used to hydrolyse defatted soy beans in soy sauce manuf..

Hartman, S.C. *et al., Methods Enzymol.*, 1970, **17**, 941 (*isol*)
Svenneby, G. *et al., Biochem. Soc. Trans.*, 1987, **15**, 213-215 (*rev*)
Hamada, J.S. *et al., CRC Crit. Rev. Food Sci. Nutri.*, 1994, **34**, 283-292 (*use*)

Glutamine, 9CI G-211

[6899-04-3]

2,5-Diamino-5-oxopentanoic acid. Glutamic acid 5-amide. γ-Glutamine. NSC 97925. Gln



(*S*)-*form*

$C_5H_{10}N_2O_3$ 146.146Log P -3.46 (calc).

(*S*)-*form* [56-85-9]

L-form. ***Levoglutamide, INN***. *Energlut. Glutaven. Iperphos. Memoril. FEMA 3684. Many other names*

Widely distributed in plants, e.g. beetroot. Flavouring ingredient. Dietary supplement. Needles (EtOH aq.). Spar. sol. H_2O (3.6 g/100 g at 25°), EtOH. Mp 184-185° dec. $[\alpha]_D^{19}$ +9.2 (H_2O). $[\alpha]_D$ +46.5 (5*M* HCl). pK_{a2} 9.01 (25°, 0.1*M* KNO_3). Isoelectric point 5.65. Sweet taste.

► LD_{50} (rat, orl) 7500 mg/kg. Exp. reprod. effects (very large dose). MA2275100

N^5-*(2-Hydroxyethyl):* [2650-74-0] N-*(γ-Glutamyl)ethanolamine, 8CI*

$C_7H_{14}N_2O_4$ 190.199

Constit. of the fruiting body of *Agaricus bisporus* (button mushroom). Cryst. (EtOH aq.). Mp 188.5-191°. $[\alpha]_D^{19}$ +5.8 (c, 1.8 in H_2O).

N^5-*(4-Hydroxyphenyl):* [30382-24-2] ***γ-Glutaminyl-4-hydroxybenzene***

$C_{11}H_{14}N_2O_4$ 238.243

Isol. from the gill tissue of the edible mushrooms *Agaricus bisporus* (button mushroom) and *Agaricus hortensis*. Sol. H_2O; fairly sol. MeOH. Mp 231.5° (225-226°). $[\alpha]_D$ +30 (1*M* HCl). λ_{max} 246 (H_2O) (Berdy). λ_{max} 246 (HCl) (Berdy). λ_{max} 260 (NaOH) (Berdy).

► LD_{50} (mus, ipr) 5000 mg/kg. MA2276400

N^5-*(4-Methoxybenzyl):* **N^5-*(4-Methoxybenzyl)glutamine***

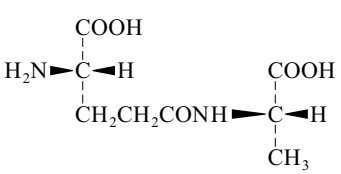
$C_{13}H_{18}N_2O_4$ 266.296

Constit. of the xylem sap of the roots of *Cucurbita maxima* x *Cucurbita moschata*. Amorph. solid. Mp 214-215° dec. $[\alpha]_D^{22}$ +23 (c, 0.1 in 1*M* HCl). λ_{max} 224 (log ϵ 4.1); 273 (log ϵ 3.2) (H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 782D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1278B (*nmr*)
Archibald, R.M. *et al., Chem. Rev.*, 1945, **37**, 161 (*rev, props*)
Lepp, A. *et al., Biochem. Prep.*, 1957, **5**, 79 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 25), Wiley, N.Y., 1961, 1929 (*isol, synth*)
Kline, G.B. *et al., J.O.C.*, 1961, **26**, 1854 (*synth*)
Olesen Larsen, P. *et al., Acta Chem. Scand.*, 1967, **21**, 1592-1604 (*N^5-2-hydroxyethyl, isol, synth*)
Bak, B. *et al., J. Mol. Spectrosc.*, 1968, **26**, 78 (*pmr*)
Weaver, R.F. *et al., J. Biol. Chem.*, 1971, **246**, 2010 (*γ-Glutaminyl-4-hydroxybenzene*)
Koetzle, T.F. *et al., Acta Cryst. B*, 1973, **29**, 2571 (*cryst struct*)
Voelter, W. *et al., Monatsh. Chem.*, 1974, **105**, 1110 (*cmr*)
Synth. Prod. Util. Amino Acids, (Kaneko, T. *et al*, Ed.), Halsted Press, 1974, 109 (*synth*)
London, R.E. *et al., J.A.C.S.*, 1978, **100**, 3723 (*cmr*)
Jaeger, P. *et al., N. Engl. J. Med.*, 1986, **315**, 1120 (*rev*)
Tachiki, T. *et al., Prog. Ind. Microbiol.*, 1986, **24**, 121 (*rev, synth*)
Yoshifuji, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2994 (*synth*)
Van Oycke, S. *et al., Bull. Soc. Chim. Belg.*, 1988, **97**, 297-311 (*N^5-2-hydroxyethyl, isol, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, GFO050
Suresh, S. *et al., Acta Cryst. C*, 1996, **52**, 1313 (*cryst struct, DL-form*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GFO050

N-γ-Glutamylalanine G-212

N-*γ-Glutaminylalanine*



$C_8H_{14}N_2O_5$ 218.209

L-L-*form* [5875-41-2]

Cryst. (EtOH aq.). Mp 185-187° Mp 194-195° dec. $[\alpha]_D$ -28 (c, 2 in H_2O).

N-*Benzyloxycarbonyl:*

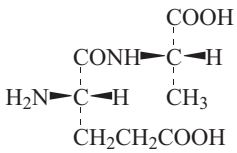
Cryst. (Me_2CO/Et_2O). Mp 150-154°.

L-D-*form*

Isol. from young pea shoots *Pisum sativum*. Mp 210-211° dec. $[\alpha]_D^{29}$ +44 (c, 1 in H_2O).

Rowlands, D.A. *et al., J.C.S.*, 1952, 3937-3940 (*L-L-form, synth*)
Morris, C.J. *et al., J. Biol. Chem.*, 1964, **239**, 1833-1835 (*L,L-form, isol*)
Kristensen, I. *et al., Acta Chem. Scand.*, 1973, **27**, 3123-3125 (*pmr*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 2155-2157 (*pmr*)
Fukuda, M. *et al., Biochim. Biophys. Acta*, 1973, **304**, 363-366 (*L,D-form, L,L-form, isol, synth*)

α-Glutamylalanine G-213



L-L-*form*

$C_8H_{14}N_2O_5$ 218.209

L-D-*form* [76186-47-5]

Isol. from seedlings of *Pisum sativum* (pea). Mp 210-211° dec. $[\alpha]_D^{29}$ +41 (c, 1.0 in H_2O).

L-L-*form*

N-*Benzyloxycarbonyl, amide:* [150171-38-3]

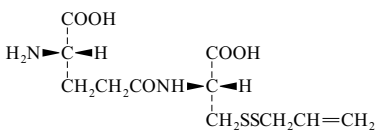
$C_{16}H_{21}N_3O_6$ 351.358

$[\alpha]_D^{25}$ -16.7 (c, 0.76 in MeOH).

[56416-96-7, 56416-97-8]

Kasai, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 2155 (*pmr*)
Fukuda, M. *et al., Biochim. Biophys. Acta*, 1973, **304**, 363 (*isol, struct, synth*)
Fukuda, M. *et al., Phytochemistry*, 1973, **12**, 2593 (*isol*)
Szewczuk, A. *et al., Can. J. Biochem.*, 1975, **53**, 706
Kawasaki, Y. *et al., Biochim. Biophys. Acta*, 1982, **716**, 194
Khumtaveeporn, K. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 2563-2572 (*L-L-form, N-Boc amide*)

γ-Glutamyl-*S*-allylthiocysteine G-214



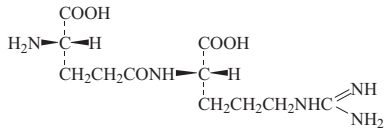
$C_{11}H_{18}N_2O_5S_2$ 322.406

L-L-*form*

Constit. of garlic (*Allium sativum*). Fine needles (Me_2CO aq.). Mp 148-149°. $[\alpha]_D^{23.5}$ -55.1 (c, 0.39 in 6*M* HCl).

Sugii, M. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1114 (*isol*)

N^2-γ-Glutamylarginine G-215



$C_{11}H_{21}N_5O_5$ 303.317

L,L-*form* [31106-03-3]
Constit. of *Allium cepa* (onion), *Panax ginseng* (ginseng). $[\alpha]_D^{23}$ +9.9 (c, 1 in 1*M* HCl).

Matsutani, H. *et al., Phytochemistry*, 1988, **27**, 931-932 (*isol, synth*)
Chen, Z.-K. *et al., J. Pept. Res.*, 1998, **52**, 137-142 (*isol*)

N^{α}-Glutamylaspartic acid G-216

$HOOCCH_2CH_2CH(NH_2)CONHCH(COOH)CH_2COOH$

$C_9H_{14}N_2O_7$ 262.219

L-L-*form* [3918-84-1]
Found in soybean. Monohydrate. Mp 138-141°. $[\alpha]_D^{15}$ +29.4 (H_2O).

Tri-tert-*butyl ester:*
$C_{21}H_{38}N_2O_7$ 430.54
Mp 57-61° (as hydrochloride).

N-*Benzyloxycarbonyl,* Asp-*di-Et ester:*
$C_{21}H_{28}N_2O_9$ 452.46
Cryst. (EtOAc/petrol). Mp 119-120°. $[\alpha]_D^{25}$ -3.2 (c, 1.4 in AcOH).

LeQuesne, W.J. *et al., J.C.S.*, 1950, 1954; 1959 (*synth*)
Taschner, E. *et al., Annalen*, 1961, **646**, 127 (*synth*)
Klieger, E. *et al., Annalen*, 1963, **661**, 193 (*synth*)
Ishikawa, Y. *et al., Agric. Biol. Chem.*, 1967, **31**, 490 (*synth*)
Meguro, H. *et al., Agric. Biol. Chem.*, 1968, **32**, 518 (*ord*)

N^{γ}-Glutamylaspartic acid G-217

$HOOCCH(NH_2)CH_2CH_2CONHCH(COOH)CH_2COOH$

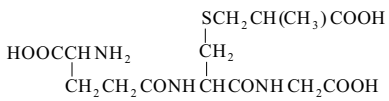
$C_9H_{14}N_2O_7$ 262.219

L-L-*form* [16804-55-0]
Constit. of seeds of *Vigna radiata* (mung bean) and *Vicia faba*. Mp 192-195° dec. $[\alpha]_D^{18}$ +19.5 (c, 2 in *M* HCl).

Le Quesne, W.J. *et al., J.C.S.*, 1950, 1954 (*synth*)
Taschner, E. *et al., Annalen*, 1961, **646**, 127 (*synth*)
Klieger, E. *et al., Annalen*, 1963, **661**, 193 (*synth*)
Ishikawa, Y. *et al., Agric. Biol. Chem.*, 1967, **31**, 490 (*synth*)
Meguro, H. *et al., Agric. Biol. Chem.*, 1968, **32**, 518 (*ord*)
Ito, K. *et al., Phytochemistry*, 1972, **11**, 2541 (*occur*)
Kasai, T. *et al., Phytochemistry*, 1986, **25**, 679 (*occur*)

γ-L-Glutamyl-*S*-(2-carboxy-1-propyl)cysteinylglycine G-218

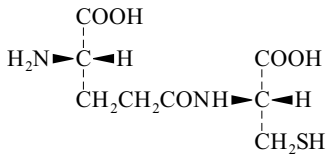
[6710-22-1]



$C_{14}H_{23}N_3O_8S$ 393.417
Constit. of onion (*Allium cepa*) and garlic (*Allium sativum*). Needles. $[\alpha]_D^{22}$ -38.1 (H_2O).

Virtanen, A.J. *et al., Z. Physiol. Chem.*, 1960, **322**, 8 (*isol*)
Suzuki, T. *et al., Chem. Pharm. Bull.*, 1961, **9**, 77 (*isol*)
Tsuboi, S. *et al., J. Agric. Food Chem.*, 1989, **37**, 611 (*hplc*)

N-γ-Glutamylcysteine G-219



$C_8H_{14}N_2O_5S$ 250.275

L-L-*form* [636-58-8]
Prisms (EtOH). Mp 164-166°. $[\alpha]_D^{28}$ +12.4 (c, 1.69 in H_2O).

S-*Me:* ***γ-Glutamyl-S-methylcysteine***
$C_9H_{16}N_2O_5S$ 264.302
Constit. of many edible vegetable species. Cryst. Mp 107-109°. $[\alpha]_D^{23}$ -20.5 (c, 2.22 in H_2O).

S-*Me,* S-*oxide:* ***γ-Glutamyl-S-methylcysteine sulfoxide***
$C_9H_{16}N_2O_6S$ 280.301
Present in garlic (*Allium sativum*).

S-*Vinyl:γ-Glutamyl*-S-*ethenylcysteine. γ-Glutamyl*-S-*vinylcysteine*
$C_{10}H_{16}N_2O_5S$ 276.313
$[\alpha]_D^{23}$ -5 (c, 2 in H_2O). λ_{max} 222 (log ε 3.74) (H_2O).

S-*Propyl:* [91212-00-9] **N-*γ-Glutamyl*-S-*propylcysteine***
$C_{11}H_{20}N_2O_5S$ 292.355
Isol. from garlic (*Allium sativum*) and chives (*Allium schoenoprasum*).

S-*(E)-1-Propenyl:* [134677-41-1]
$C_{11}H_{18}N_2O_5S$ 290.34
Constit. of garlic (*Allium sativum*). $[\alpha]_D^{20}$ -12.3 (c, 0.39 in H_2O).

S-*(Z)-1-Propenyl:* [91216-96-5] **N-*γ-Glutamyl*-S-*(1-propenyl)cysteine***
$C_{11}H_{18}N_2O_5S$ 290.34
Constit. of *Allium* spp..

S-*(1-Propenyl),* S-*oxide:* ***γ-Glutamyl-S-(1-propenyl)cysteine sulfoxide***
$C_{11}H_{18}N_2O_6S$ 306.339
Constit. of onion (*Allium cepa*). Poss. artifact.

S-*(2-Propenyl):* **N-*γ-Glutamyl*-S-*allylcysteine***
$C_{11}H_{18}N_2O_5S$ 290.34
Isol. from garlic (*Allium sativum*)and chives (*Allium schoenoprasum*). Mp 156-158.5° dec. $[\alpha]_D^{23}$ -17.1 (H_2O).

S-*(2-Propenylthio):* [94504-37-7] N-*γ-Glutamyl*-S-*(allylthio)cysteine*
$C_{11}H_{18}N_2O_5S_2$ 322.406
Constit. of garlic (*Allium sativum*). $[\alpha]_D^{20}$ -64.8 (c, 0.26 in H_2O).

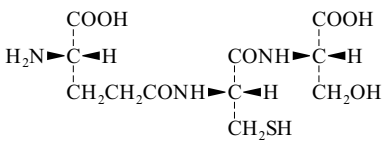
Disulfide: [23052-19-9] *γ-Glutamylcysteine (2→2′)disulfide, 9CI.* **N,N′-*Bis(γ-glutamyl)cystine***. N-*γ-Glutamylcystine*
$C_{16}H_{26}N_4O_{10}S_2$ 498.534
Isol. from chives (*Allium schoenoprasum*) and from shiitake mushrooms (*Lentinus edodes*). Cryst. (Me_2CO aq.) or amorph. powder. $[\alpha]_D$ -120. Dec. at *ca.* 187°.

[33514-37-3, 56328-22-4]

Zacharius, R.M. *et al., Arch. Biochem. Biophys.*, 1958, **73**, 281-283; 1959, **80**, 199-209 (*isol, synth, deriv*)
Rinderknecht, H. *et al., Helv. Chim. Acta*, 1958, **41**, 1-11 (*isol, S-Me*)
Sheehan, J.C. *et al., J.A.C.S.*, 1958, **80**, 1158-1164 (*synth*)
Taschner, E. *et al., Annalen*, 1961, **646**, 127-133; 1963, **663**, 188-193 (*derivs*)
Suzuki, T. *et al., Chem. Pharm. Bull.*, 1961, **9**, 77-78 (*S-methyl sulfoxide, occur*)
Virtaten, A.I. *et al., Suom. Kemistil. B*, 1961, **34**, 44; 144; 1962, **35**, 52; 245; *CA*, **56**, 10586; **57**, 6323a; **58**, 7135 (*isol, derivs*)
Ettala, T. *et al., Acta Chem. Scand.*, 1962, **16**, 2061-2063 (*biosynth*)
Matikkala, E.J. *et al., Acta Chem. Scand.*, 1962, **16**, 2461-2462; 1963, **17**, 1799-1801 (*S-propenyl, S-propyl, isol*)
Obata, Y. *et al., Agric. Biol. Chem.*, 1964, **28**, 624-626 (*synth, L-L-S-Me*)
Thompson, G.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1975, **72**, 1985-1988 (*disulfide*)
Aoyagi, Y. *et al., Nippon Nogei Kagaku Kaishi*, 1980, **54**, 283; *CA*, **93**, 68939p (*disulfide*)
Wu, S.-H. *et al., J. Chromatogr.*, 1982, **245**, 268-270 (*S-Me, isol, hplc*)
Gushima, H. *et al., Agric. Biol. Chem.*, 1983, **47**, 1927-1928 (*cloning*)
Lawson, L.D. *et al., J. Nat. Prod.*, 1991, **54**, 436-444 (*derivs*)
Muetsch-Eckner, M. *et al., Phytochemistry*, 1992, **31**, 2389-2391 (*isol, derivs*)
Enneking, D. *et al., Phytochemistry*, 1998, **48**, 643-645 (*S-vinyl, isol*)

γ-Glutamylcysteinylserine G-220

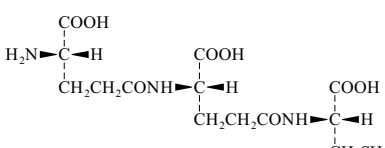
[144331-30-6]



$C_{11}H_{19}N_3O_7S$ 337.353
Constit. of many grasses incl. *Triticum aestivum* (wheat).

Klapheck, S. *et al., Bot. Acta*, 1992, **105**, 174 (*isol*)

γ-Glutamyl-γ-glutamylcysteine G-221



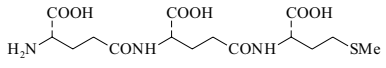
$C_{13}H_{21}N_3O_8S$ 379.39

L-L-L-*form*

S-*Me:* [102148-93-6] *(γ-Glutamyl-γ-glutamyl)*-S-*methylcysteine*
$C_{14}H_{23}N_3O_8S$ 393.417
Constit. of the seeds of *Vigna radiata* (mung bean).

Kasai, T. *et al., Phytochemistry*, 1986, **25**, 679

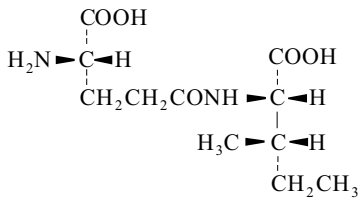
γ-Glutamyl-γ-glutamylmethionine G-222



$C_{15}H_{25}N_3O_8S$ 407.444

(all-L)-*form* [41515-84-8]
Isol. from the seeds of *Phaseolus radiatus* var. *typicus*. No phys. props. reported.
Kasai, T. *et al., Agric. Biol. Chem.*, 1972, **36**, 2621 (*isol, synth*)

N-γ-Glutamylisoleucine G-223



$C_{11}H_{20}N_2O_5$ 260.289

L-L-*form* [23632-83-9]
Constit. of onion *Allium cepa* and mung bean (*Vigna radiata*). Needles.
Virtanen, A.I. *et al., Suom. Kemistil. B*, 1961, **34**, 53; *CA*, **56**, 716 (*isol*)
Kasai, T. *et al., Phytochemistry*, 1986, **25**, 679-682 (*occur*)
Anderson, M.E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1986, **83**, 5029 (*biochem*)

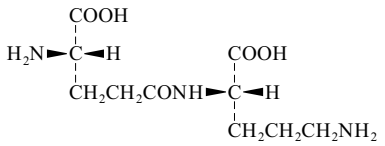
N-γ-Glutamylmethionine G-224

[4381-82-2]
N-*[1-Carboxy-3-(methylthio)propyl]glutamine, 9CI*
$HOOCCH(NH_2)CH_2CH_2CONHCH(COOH)CH_2CH_2SMe$
$C_{10}H_{18}N_2O_5S$ 278.329

L-L-*form* [17663-87-5]
Isol. from the seeds of onion (*Allium cepa*), kidney bean (*Phaseolus vulgaris*), mung bean (*Vigna radiata*), garlic (*Allium sativum*) and black gram (*Vigna mungo*). Mp 203-205° Mp 228-231°. $[\alpha]_D^{20}$ -9 (c, 1.4 in H_2O).
N-*Trityl:*
Mp 140° approx.
S-*Oxide:* [39015-69-5] ***γ-L-Glutamyl-L-methionine sulfoxide***
$C_{10}H_{18}N_2O_6S$ 294.328
Isol. from the seeds of mung bean (*Vigna radiata*) and black gram (*Vigna mungo*).

(L-DL)-*form*
S-*Oxide:* [54836-99-6] ***γ-Glutamyl-DL-methionine sulfoxide***
$C_{10}H_{18}N_2O_6S$ 294.328
Isol. from the seeds of *Fagus silvatica* (beechnuts). Cryst.
[66512-52-5]
Amiard, G. *et al., CA*, 1961, **55**, 4380 (*synth*)
Virtanen, A.I. *et al., Suom. Kemistil. B*, 1961, **34**, 53; *CA*, **56**, 716 (*isol*)
Morris, C.J. *et al., J. Biol. Chem.*, 1963, **238**, 650 (*isol, synth*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1971, **35**, 1603; 1972, **36**, 967 (*isol*)
Nishimura, H. *et al., Tetrahedron*, 1972, **28**, 4503 (*ms*)
Orlowski, M. *et al., J. Biol. Chem.*, 1973, **248**, 2836 (*synth*)
Carson, J.F. *et al., J.C.S. Perkin 1*, 1974, 685 (*synth*)
Kristensen, I. *et al., Phytochemistry*, 1974, **13**, 2803 (*isol*)
Otoul, E. *et al., Phytochemistry*, 1975, **14**, 173 (*isol*)
Wu, S.H. *et al., J. Chromatogr.*, 1982, **245**, 268 (*isol, hplc*)
Anderson, M.E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1986, **83**, 5029 (*biochem*)

N^2-γ-Glutamylornithine G-225



$C_{10}H_{19}N_3O_5$ 261.277

L-L-*form* [56523-61-6]
Constit. of the edible shiitake mushroom (*Lentinus edodes*). Cryst. + $1H_2O$. Mp 209°. $[\alpha]_D^{25}$ +5.2 (c, 1 in 1*M* HCl).
N^5-*Ac:* [102148-92-5] N^5-*Acetyl*-N^2-*γ-glutamylornithine, 9CI*
$C_{12}H_{21}N_3O_6$ 303.314
Constit. of the seeds of green gram (*Vigna radiata*). $[\alpha]_D^{22}$ -6.7 (c, 2.3 in H_2O).
Losse, G. *et al., Annalen*, 1964, **676**, 232 (*synth*)
Lou, M.F. *et al., Biochemistry*, 1975, **14**, 3503 (*isol*)
Aoyagi, Y. *et al., Agric. Biol. Chem.*, 1982, **46**, 1939 (*isol*)
Roesel, R.A. *et al., Clin. Chim. Acta*, 1984, **140**, 133 (*occur*)
Kasai, T. *et al., Phytochemistry*, 1986, **25**, 679 (*N^5-Acetyl-N^2-glutamylornithine*)

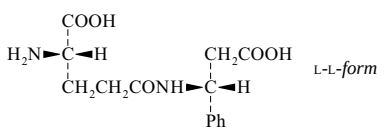
N-γ-Glutamylphenylalanine G-226

N-*(1-Carboxy-2-phenylethyl)glutamine, 9CI*
$HOOCCH(NH_2)CH_2CH_2$-$CONHCH(CH_2Ph)COOH$
$C_{14}H_{18}N_2O_5$ 294.307

L-L-*form* [6810-81-7]
Present in onion (*Allium cepa*), garlic (*Allium sativum*) and soybeans. Mp 164-174° dec. $[\alpha]_D$ +17.3 (H_2O).
Virtanen, A.I. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1960, **322**, 8 (*isol*)
Virtanen, A.I. *et al., Suom. Kemistil. B*, 1960, **33**, 83; **34**, 44; 53 (*isol*)
Morris, C.J. *et al., Biochemistry*, 1962, **1**, 706 (*isol*)

γ-Glutamyl-β-phenyl-β-alanine G-227

N-*[(α-Carboxymethyl)benzyl]glutamine. γ-Glutamyl-β-aminophenylpropanoic acid*



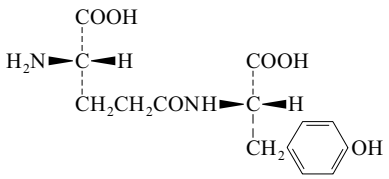
$C_{14}H_{18}N_2O_5$ 294.307

L-L-*form* [10275-84-0]
Isol. from *Phaseolus angularis* (Azuki bean). Cryst. (EtOH aq.). Mp 213-214°. $[\alpha]_D^{17}$ +65.3 (c, 0.68 in H_2O).

L_{Glu}-D-*form*
Off-white needles (H_2O). Mp 217-219°.
Koyama, M. *et al., Agric. Biol. Chem.*, 1966, **30**, 472; 1967, **31**, 738 (*isol, struct, ir, synth*)
Corbin, J.L. *et al., Phytochemistry*, 1986, **25**, 527 (*isol, struct*)

N-γ-Glutamyltyrosine, 9CI G-228

[6720-09-8]
N-*[1-Carboxy-2-(4-hydroxyphenyl)ethyl]glutamine, 9CI*



$C_{14}H_{18}N_2O_6$ 310.306

L-L-*form* [7432-23-7]
Isol. from the seeds of *Glycine max* (soybean). Cryst. Mp 221-222° dec. $[\alpha]_D^{31}$ +26.6 (c, 4).
Morris, C.J. *et al., Biochemistry*, 1962, **1**, 706 (*isol, synth*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1966, **30**, 979; *CA*, **81**, 14851; **85**, 16729 (*isol, pmr, ir*)
Larsen, P.O. *et al., Acta Chem. Scand.*, 1967, **21**, 2908 (*isol*)
Przybylska, J. *et al., CA*, 1970, **73**, 106269; 1972, **76**, 138129 (*isol*)
Kristensen, I. *et al., Acta Chem. Scand.*, 1973, **27**, 3123
Kristensen, I. *et al., Phytochemistry*, 1974, **13**, 2803 (*isol, nmr*)

N-γ-Glutamylvaline G-229

$HOOCCH(NH_2)CH_2CH_2CONHCH(COOH)CH(CH_3)_2$
$C_{10}H_{18}N_2O_5$ 246.263

L-L-*form* [2746-34-1]
From onion (*Allium cepa*). Cryst. (Me_2CO aq.). Mp 207°. $[\alpha]_D$ 0 (c, 2.4 in H_2O).
N-*Benzyloxycarbonyl:*
$C_{18}H_{24}N_2O_7$ 380.397
Mp 153-156°.
Rowlands, D.A. *et al., J.C.S.*, 1952, 3937 (*synth*)
Virtanen, A.I. *et al., Suom. Kemistil. B*, 1961, **34**, 53; *CA*, **56**, 716f (*isol*)
Morris, C.J. *et al., J. Biol. Chem.*, 1964, **239**, 1833 (*isol*)
Sano, I. *et al., J. Neurochem.*, 1966, **13**, 711 (*isol*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 2155; 1974, **38**, 1257 (*nmr*)
Hasegawa, M. *et al., Agric. Biol. Chem.*, 1978, **42**, 371; 383 (*synth*)
Anderson, M.E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1986, **83**, 5029 (*biochem*)

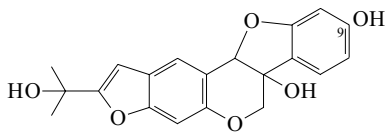
Gluten allergenic peptide G-230

H-Ser-[Gln]$_4$-Pro-Pro-Phe-Ser-[Gln]$_3$-Pro-Pro-Phe-Ser-[Gln]$_4$-Pro-Pro-Phe-Ser-[Gln]$_3$-Pro-Pro-Pro-Phe-OH
Isol. from the chymotryptic hydrolysate of gluten.
Watanabe, M. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1596

Glyceofuran G-231

[78873-52-6]

*2-(1-Hydroxy-1-methylethyl)-6*H*-benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-6*a*,9(11*a*H)-diol, 9CI*



$C_{20}H_{18}O_6$ 354.359

Isol. from cotyledons and hypocotyls of *Glycine max* after treatment with *Pseudomonas pisi* or sodium iodoacetate. Needles (Me_2CO/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 181° dec. $[\alpha]_D$ -242 (c, 0.03 in MeOH). λ_{max} 250 (ϵ 12000); 257 (ϵ 13300); 293 (ϵ 10000) (MeOH) (Berdy). λ_{max} 214 ; 250 ; 298 (MeOH-NaOH) (Berdy). λ_{max} 253 ; 275 ; 294 ; 305 ; 346 ; 362 (HCl) (Berdy).

9-Me ether: [78876-29-6] ***9*-O-*Methylglyceofuran***

$C_{21}H_{20}O_6$ 368.385

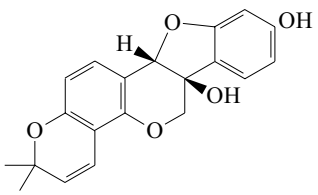
From *Glycine max* (soy bean). $[\alpha]_D$ -247 (c, 0.02 in MeOH).

Ingham, J.L. *et al., Phytochemistry*, 1981, **20**, 795 (*struct, uv, nmr, ms*)

Glyceollin I G-232

[57103-57-8]

*2,2-Dimethyl-2*H*,6*H*-benzofuro[3,2-*c*]pyrano[2,3-*h*][1]benzopyran-6*a*,9(11*a*H)-diol, 9CI*



$C_{20}H_{18}O_5$ 338.359

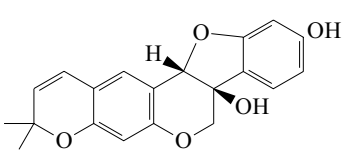
Formerly considered to be 6*a*-Hydroxyphaseollin, H-711. Phytoalexin from soybean seedlings.

Burden, R.S. *et al., Phytochemistry*, 1975, **14**, 1389 (*struct*)
Lyne, R.L. *et al., Chem. Comm.*, 1976, 497 (*isol, pmr*)
Banks, S.W. *et al., Phytochemistry*, 1983, **22**, 2729 (*biosynth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*occur*)

Glyceollin II G-233

[67314-98-1]

*3,3-Dimethyl-3*H*,7*H*-benzofuro[3,2-*c*]pyrano[3,2-*g*][1]benzopyran-7*a*,10(12*a*H)-diol, 9CI*



$C_{20}H_{18}O_5$ 338.359

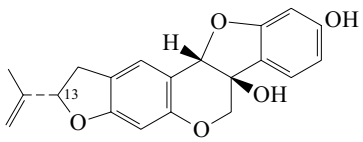
Phytoalexin from *Glycine max* (soybean). Cryst. (toluene). Mp 89-93°. λ_{max} 227 (ϵ 38500); 285 (ϵ 8760); 307 (ϵ 6200); 318 (ϵ 5800) (EtOH) (Berdy).

Lyne, R.L. *et al., Chem. Comm.*, 1976, 497 (*isol*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*occur*)
Banks, S.W. *et al., Phytochemistry*, 1983, **22**, 2729 (*biosynth*)

Glyceollin III G-234

[61080-23-7]

*1,2-Dihydro-2-(1-methylethenyl)-6*H*-benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-6*a*,9(11*a*H)-diol, 9CI*



$C_{20}H_{18}O_5$ 338.359

Phytoalexin from *Glycine max* (soybean). Cryst. (EtOH aq.). Mp 149-153°. λ_{max} 287 (ϵ 9400); 292 (ϵ 9600) (EtOH) (Berdy).

13-Epimer: [79082-46-5] ***Canescacarpin***. *Glyceollin V*

$C_{20}H_{18}O_5$ 338.359

Cryst. (EtOH). Mp 164-167°. λ_{max} 287 (ϵ 8960); 292 (ϵ 9210) (EtOH) (Berdy).

Lyne, R.L. *et al., Chem. Comm.*, 1976, 497 (*isol*)
Lyne, R.L. *et al., Tet. Lett.*, 1981, 2483 (*Canescacarpin*)
Banks, S.W. *et al., Phytochemistry*, 1983, **22**, 2729 (*biosynth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*occur*)
Kraus, C. *et al., Phytochemistry*, 1995, **40**, 739 (*occur, pmr*)

Glycerol, INN G-235

[56-81-5]

1,2,3-Propanetriol, 9CI. Glycerin, JAN, USAN. Glyceritol. Amylac. Babylax. Bulboid. Cristal. Dagralax. Glyrol. Luxoral. Meprolax. Osmoglyn. E422. FEMA 2525. Many other names

$HOCH_2CH(OH)CH_2OH$

$C_3H_8O_3$ 92.094

Many acyl derivs. (glycerides) have separate entries. Found extensively in esterified form in animal and plant glycerides. Humectant, emollient and solvent in foods. Syrup with sweet taste. Misc. H_2O, EtOH; insol. C_6H_6, $CHCl_3$, CCl_4. d_{15}^{15} 1.27. Mp 17.8°. Bp 290° part. dec. Bp_{20} 182°. n_D^{20} 1.4720. pK_{a1} 14.4. V. hygroscopic. Steam-volatile.

▶ Fl. p. 160°, autoignition temp. 370/393°. Reacts violently or explosively with many oxid. agents. OES: long-term 10 mg m^{-3} (mist). Skin and eye irritant. Ingestion can cause headache and vomiting. Exp. reprod. effects. MA8050000

Tribenzoyl: [614-33-5] *Glycerol tribenzoate. FEMA 3398*

$C_{24}H_{20}O_6$ 404.418

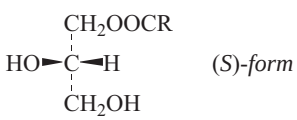
Flavouring ingredient. Mp 76° (72°).

[6990-26-7, 18673-08-0, 28959-04-8, 36887-04-4, 51432-61-2, 69790-27-8, 117591-83-0, 117591-84-1]

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Glycerol 1-alkanoates G-236

1-O-*Acylglycerols*



(S)-form

Chiral compds. The (*S*)-enantiomers correspond to 1-*O*-acyl-*sn*-glycerol. The diacetates are components of Acetolein, glycerol esterified with long-chain fatty acids and acetic acid, which is presumably used in foods such as ice-cream. Acyl migrations, particularly under the influence of heat, acidic or alkaline conditions, can result in the interconversion of 1(3)-acyl- and 2-acylglycerols.

Glycerol 1-propanoate [624-47-5]

1-Monopropionin, 8CI. 1,2,3-Propanetriol 1-propanoate. Propionin

$C_6H_{12}O_4$ 148.158

Bp_3 132-134° (± -form). Coml. samples are likely to contain some 2-isomer.

Di-Ac: [36600-62-1]
$C_{10}H_{16}O_6$ 232.233
Bp_{12} 150°.

Glycerol 1-hexanoate
$C_9H_{18}O_4$ 190.239

2-Phosphate:
$C_9H_{19}O_7P$ 270.219
Mp 261-263° (Ba salt).

Glycerol 1-octanoate [502-54-5]

[19670-49-6, 26402-26-6] *Octanoic acid 2,3-dihydroxypropyl ester. 1-Monooctanoin. α-Monocaprylin. 1-O-Octanoylglycerol*
$C_{11}H_{22}O_4$ 218.292
Mp 28-30° (*S*-form) Mp 39.5-40.5° (±-form). $[\alpha]_D$ -6.6 (c, 10.2 in Py) (*S*-form).

Glycerol 1-decanoate [2277-23-8]

[19670-50-9, 26402-22-2] *Decanoic acid 2,3-dihydroxypropyl ester. 1-Monodecanoin. α-Monocaprin*
$C_{13}H_{26}O_4$ 246.346
Mp 44° (*S*-form) Mp 53° (27°)(±-form). $[\alpha]_D$ -5.5 (c, 10 in Py) (*S*-form). Racemate shows polymorphism.

Glycerol 1-dodecanoate [142-18-7]

[27215-38-9, 40738-26-9, 104266-02-6] *2,3-Dihydroxypropyl dodecanoate. 1-Monolaurin. α-Monolaurin. Glycerol 1-laurate. Lauricidin*
$C_{15}H_{30}O_4$ 274.4
Sol. MeOH, bases, hexane; poorly sol. H_2O. Mp 54-55° (*S*-form) Mp 63° (± -form). Bp_1 186°. $[\alpha]_D$ -4.9 (Py) (*S*-form).

► LD_{50} (rat, orl) 53000 mg/kg. OF1600000

2-Phosphate:
$C_{15}H_{31}O_7P$ 354.379
Needles (as Ba salt). Mp 245-255° (Ba salt).

Glycerol 1-(5-hydroxydodecanoate) [26446-32-2]
$C_{15}H_{30}O_5$ 290.399
Butter-like flavouring ingredient. No phys. props. reported.

Glycerol 1-tetradecanoate [589-68-4]

[27214-38-6] *1-O-Tetradecanoylglycerol. 1-Monomyristin. α-Monomyristin. Glycerol 1-myristate. 1-Myristoylglycerol. 2,3-Dihydroxypropyl tetradecanoate*
$C_{17}H_{34}O_4$ 302.453
Mp 63-64° (*R*-form) Mp 70-71° (± -form). $[\alpha]_D$ -4 (c, 2.8 in Py) (*R*-form).

Glycerol 1-(13-hydroxy-2*E*,4*E*,8*E*-tetradecatrienoate)

[162110-39-6, 162110-40-9] *3-(13-Hydroxy-2,4,8-tetradecatrienoyloxy)-1,2-propanediol. 1-(13-Hydroxy-2,4,8-tetradecatrienoyl)glycerol*
$C_{17}H_{28}O_5$ 312.405*R*- and *S*- diastereomers isol., both having 13′*S*- side-chain config..

Glycerol 12*S*-methyltetradecanoate [19207-26-2] *1-O-(12-Methyltetradecanoyl)glycerol.* ***Aggreceride A***
$C_{18}H_{36}O_4$ 316.48
Sol. MeOH, C_6H_6, H_2O. Mp 29-30°. $[\alpha]_D^{21}$ +9.7 (c, 0.33 in $CHCl_3$) (+7.2). Assigned *R*-config. at glycerol.

► XB8604000

Glycerol 1-hexadecanoate [542-44-9]

[5309-46-6, 19670-51-0, 26657-96-5, 32899-41-5] *1-O-Hexadecanoylglycerol. α-Monopalmitin. Glycerol 1-palmitate. 1-Palmitoylglycerol. Hexadexanoic acid 2,3-dihydroxypropyl ester*
$C_{19}H_{38}O_4$ 330.507
Minor component of olive oil and other vegetable oils. Mp 71-72° *R*-form Mp 77° (± -form). $[\alpha]_D$ -4.3 (c, 10 in Py) (±-form).

3-O-β-D-Galactopyranoside: [35949-84-9] *1-O-β-D-Galactopyranosyl-3-O-hexadecanoylglycerol*
$C_{25}H_{48}O_9$ 492.649
Amorph. powder. Mp 119-121°. $[\alpha]_D^{31}$ +9.2 (c, 0.8 in MeOH). C-2 shows (*S*)-config..

Glycerol 1-(9-hexadecenoate)
$C_{19}H_{36}O_4$ 328.491

3-O-β-D-Galactopyranoside: [157807-76-6]
$C_{25}H_{46}O_9$ 490.633
Amorph. powder. $[\alpha]_D^{31}$ +8.6 (c, 0.7 in MeOH).

Glycerol 1-(7*Z*,10*Z*,13*Z*-hexadecatrienoate)
$C_{19}H_{32}O_4$ 324.459

3-O-β-D-Galactopyranoside: [209003-77-0]
$C_{25}H_{42}O_9$ 486.601
Oil. $[\alpha]_D^{23}$ -24 (c, 0.6 in MeOH).

Glycerol 1-(4,7,10,13-hexadecatetraenoate)
$C_{19}H_{30}O_4$ 322.444

3-O-β-D-Galactopyranoside: [189373-34-0]
$C_{25}H_{40}O_9$ 484.586
Amorph. powder. $[\alpha]_D^{23}$ -18.7 (c, 1.6 in MeOH).

Glycerol 1-(14-methylpentadecanoate)
[104700-85-8] *1-O-(14-Methylpentadecanoyl)glycerol.* ***Aggreceride B***
$C_{19}H_{38}O_4$ 330.507
Sol. MeOH, C_6H_6, H_2O. Tentatively assigned *R*-config..

Glycerol 1-(15-methylhexadecanoate)
[104700-86-9] *1-O-(15-Methylhexadecanoyl)glycerol.* ***Aggreceride C***
$C_{20}H_{40}O_4$ 344.534
Sol. MeOH, C_6H_6, H_2O. *R*-config. tentatively asigned.

Glycerol 1-octadecanoate [123-94-4]

[1319-95-5, 11099-07-3, 14811-92-8, 22610-63-5, 31566-31-1] *1-O-Octadecanoylglycerol. α-Monostearin. Glycerol 1-stearate. 1-O-Stearoylglycerol. Octadecanoic acid 2,3-dihydroxypropyl ester. FEMA 2527. E471*
$C_{21}H_{42}O_4$ 358.56
Coating agent, emulsifier, lubricant, texturiser in food processing. Used in grain products and pastas. Mp 74-75° (*R*-form) Mp 77-79° (± -form). $[\alpha]_{Hg}^{27}$ -34.1 (EtOH) (*R*-form). Racemate exhibits polymorphism.

Glycerol 1-(9*E*-octadecenoate) [2716-53-2] *1-O-(9E-Octadecenoyl)glycerol. α-Monoelaidin*
$C_{21}H_{40}O_4$ 356.545
Cryst. Mp 58.5° (± -form). Exhibits polymorphism.

Glycerol 1-(9*Z*-octadecenoate) [30836-40-9]

[111-03-5, 25496-72-4, 34487-30-4, 37220-82-9] *1-O-(9Z-Octadecenoyl)glycerol. α-Monoolein. 1-Oleoylglycerol*
Cryst. Mp 35° (± -form). $[\alpha]_D$ -3.6 (c, 10 in Py) (*R*-form). Exhibits polymorphism.

2-Ac: [92282-11-6]

[84746-00-9, 86390-77-4] *2-Acetyl-1-oleoyl-glycerol. OAG*
$C_{23}H_{42}O_5$ 398.582

Glycerol 1-(9*Z*,12*Z*-octadecadienoate)

[2258-92-6, 2277-28-3, 26545-74-4, 67968-46-1] *1-O-(9,12-Octadecadienoyl)glycerol. 1-Monolinolein. α-Monolinolein*
$C_{21}H_{38}O_4$ 354.529
Mp 14-15° (± -form). $[\alpha]_D$ -5.2 (c, 1.56 in MeOH) (*R*-form).

3-O-β-D-Galactopyranoside: [88110-55-8]
$C_{27}H_{48}O_9$ 516.671
Oil. $[\alpha]_D^{23}$ -24 (c, 0.1 in MeOH).

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate)
1-O-(9,12,15-Octadecatrienoyl)glycerol. α-Monolinolenin. 1-Monolinolenin
$C_{21}H_{36}O_4$ 352.513
Cryst. in two forms (EtOH/C_6H_6 at -20°). Mp -15.7–13.5°.

Glycerol 1-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{21}H_{34}O_4$ 350.497

3-O-β-D-Galactopyranoside: [119105-25-8] ***Hemolysin 1***
$C_{27}H_{44}O_9$ 512.639

Glycerol 1-(7*Z*,9*Z*,12*Z*-octadecatrien-5-ynoate) [76152-36-8] *1-O-(7,9,11-Octadecatrien-5-ynoyl)glycerol*
$C_{21}H_{32}O_4$ 348.481
$[\alpha]_D$ -1.5 (c, 0.5 in $CHCl_3$).

Glycerol 1-(9,12,15-octadecatrien-6-ynoate)
[93633-56-8]
$C_{21}H_{32}O_4$ 348.481
Sol. $CHCl_3$, Et_2O; poorly sol. H_2O.

Glycerol 1-(10-methyl-9*Z*-octadecenoate)
[177602-94-7] *1-O-(10-Methyl-9-octadecenoyl)glycerol*
$C_{22}H_{42}O_4$ 370.571
Oil. λ_{max} 210 (MeOH).

Glycerol 1-docosanoate [6916-74-1]

[30233-64-8, 93922-54-4, 111467-65-3] *Glycerol 1-behenate. 1-Behenoylglycerol*
$C_{25}H_{50}O_4$ 414.668
Mp 85.5° (*R*-form or *S*-form). $[\alpha]_D^{22}$ +2.4 (c, 5 in Py) (*S*-form).

Glycerol 1-(22-hydroxydocosanoate) *1-(22-Hydroxydocosanoyl)glycerol*
$C_{25}H_{50}O_5$ 430.667

22′-O-(3,4-Dihydroxycinnamoyl): [158957-68-7]
$C_{34}H_{56}O_8$ 592.812Config. not determined.

Glycerol 1-tetracosanoate [177794-18-2]

[93894-92-9, 118605-21-3] *Tetracosanoic acid 2,3-dihydroxypropyl ester, 9CI. 1-O-Lignoceroylglycerol. 1-O-Tetracosanoylglycerol*
$C_{27}H_{54}O_4$ 442.721

Glycerol 1-(24-hydroxytetracosanoate)
[162522-33-0] *1-O-(24-Hydroxytetracosanoyl)glycerol*
$C_{27}H_{54}O_5$ 458.721Config. not determined.

Glycerol 1-(26-hydroxyhexacosanoate)
[177602-14-1] *1-(26-Hydroxyhexacosanoyl)glycerol*
$C_{29}H_{58}O_5$ 486.774
Gum. Racemic.

26′-O-(4-Hydroxy-3-methoxycinnamoyl)(E-): [109031-30-3] *1-[(26-Feruloyloxy)hexacosanoyl]glycerol*
$C_{39}H_{66}O_8$ 662.946
Mp 72-75°.

26′-O-*(4-Hydroxy-3-methoxycinnamoyl)(Z-):* [109031-38-1]
$C_{39}H_{66}O_8$ 662.946

Glycerol 1-(29-hydroxynonacosanoate) [233685-19-3] ***1*-O-*(29-Hydroxynonacosanoyl)glycerol***
$C_{32}H_{64}O_5$ 528.855Config. not determined.

[28060-90-4]

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Mattson, F.H. *et al., J. Lipid Res.*, 1962, **3**, 281-296 (*rev, acyl migration*)
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Mukherjee, R.K. *et al., Phytochemistry*, 1994, **37**, 1641-1643 (*Glycerol 1-(24-hydroxytetracosanoate)*)
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Rho, M.C. *et al., J. Nat. Prod.*, 1996, **59**, 308 (*hexadecanoyl galactoside*)
Rho, M.C. *et al., Planta Med.*, 1996, **62**, 473 (*9-hexadecenoyl galactoside*)
Kong, L. *et al., Zhiwu Xuebao*, 1996, **38**, 161-166 (*Glycerol 1-tetracosanoate*)
Barton, R.H. *et al., Aust. J. Chem.*, 1997, **50**, 355-361 (*acyl migration*)
Pettit, G.R. *et al., Can. J. Chem.*, 1997, **75**, 920 (*1-hexadecanoyl glycoside*)
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Rho, M.C. *et al., Phytochemistry*, 1997, **44**, 1507 (*hexadecatetraenoyl galactoside*)
Zou, K. *et al., CA*, 1999, **131**, 127577x (*isol*)
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Glycerol 2-alkanoates G-237

2-O-*Acylglycerols*
$RCOOCH(CH_2OH)_2$
Achiral compds. (cf. Glycerol 1-alkanoates, G-236).Acyl migration, particularly under the influences of heat, acidic or alkaline conditions, can result in the interconversion of 1(3)-acyl- and 2-acylglycerols.

Glycerol 2-octanoate [4228-48-2]

[26402-26-6]
2-Hydroxy-1-(hydroxymethyl)ethyl octanoate. 2-Monooctanoin. β-Monocaprylin. 2-O-*Octanoylglycerol*

$C_{11}H_{22}O_4$ 218.292
Cryst. (Et_2O/petrol). Mp 29.8°.

Glycerol 2-decanoate [3376-48-5]

[26402-22-2]
2-Hydroxy-1-(hydroxymethyl)ethyl decanoate. 2-Monodecanoin. β-Monocaprin. 2-O-*Decanoylglycerol*

$C_{13}H_{26}O_4$ 246.346
Mp 40.4°.

Glycerol 2-dodecanoate [1678-45-1]

[27215-38-9]
2-Hydroxy-1-(hydroxymethyl)ethyl dodecanoate. 2-O-*Dodecanoylglycerol. Glycerol 2-laurate. β-Monolaurin*

$C_{15}H_{30}O_4$ 274.4
Mp 51°.

Glycerol 2-tetradecanoate

[27214-38-6]
2-O-*Tetradecanoylglycerol. Glycerol 2-myristate. β-Monomyristin*

$C_{17}H_{34}O_4$ 302.453
Cryst. (petrol). Mp 60-61°.

Glycerol 2-hexadecanoate [23470-00-0]

[26657-96-5, 75656-12-1]
Hexadecanoic acid 2-hydroxy-1-(hydroxymethyl)ethyl ester, 9CI. 2-O-*Hexadecanoylglycerol. Glycerol 2-palmitate. β-Monopalmitin*

$C_{19}H_{38}O_4$ 330.507
Minor component of olive oil and other vegetable oils. Cryst. (petrol). Mp 69°.

Glycerol 2-octadecanoate [621-61-4]

[1319-95-5, 11099-07-3, 31566-31-1]
2-Hydroxy-1-(hydroxymethyl)ethyl octadecanoate. 2-O-*Octadecanoylglycerol. Glycerol 2-stearate. β-Monostearin*

$C_{21}H_{42}O_4$ 358.56
Cryst. (petrol). Mp 74°.

Glycerol 2-(9*E*-octadecenoate)
2-O-*(9E-Octadecenoyl)glycerol. β-Monoelaidin*
$C_{21}H_{40}O_4$ 356.545
Mp 53.7°.

Glycerol 2-(9*Z*-octadecenoate) [3443-84-3]
2-O-*(9Z-Octadecenoyl)glycerol. β-Monoolein*
$C_{21}H_{40}O_4$ 356.545
Mp 26°.

Glycerol 2-(9*Z*,12*Z*-octadecadienoate) [3443-82-1]
2-O-*(9Z,12Z-octadecadienoyl)glycerol. β-Monolinolein*
$C_{21}H_{38}O_4$ 354.529
Oil; cryst. (petrol at -35°). Mp 8.9°.

Glycerol 2-(9*Z*-eicosenoate)
2-(9Z-Eicosenoyl)glycerol. 2-O-*Gadoleoylglycerol*
$C_{23}H_{44}O_4$ 384.598

1-O-*β-D-Glucopyranoside:* [239082-53-2]
$C_{29}H_{54}O_9$ 546.74C-2 is a chiral centre but the abs. config. is unknown.

Glycerol 2-(5*Z*,8*Z*,11*Z*,14*Z*-eicosatetraenoate) [53847-30-6]
2-O-*(5Z,8Z,11Z,14Z-Eicosatetraenoyl)glycerol. Glycerol 2-arachidonate. 2-Arachidonylglycerol*
$C_{23}H_{38}O_4$ 378.551

Glycerol 2-tetracosanoate [118605-19-9] ***2*-O-*Tetracosanoylglycerol***
$C_{27}H_{54}O_4$ 442.721

Crossley, A. *et al., J.C.S.*, 1959, 760-764 (*acyl migration*)
Mattson, F.H. *et al., J. Lipid Res.*, 1962, **3**, 281-296 (*rev, acyl migration*)
Cook, P.F.E. *et al., J.C.S.*, 1965, 4594 (*Glycerol 2-tetradecanoate*)
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Millqvist, A. *et al., Enzyme Microb. Technol.*, 1994, **16**, 1042-1047 (*synth*)
Boswinkel, G. *et al., J. Am. Oil Chem. Soc.*, 1996, **73**, 707-711 (*acyl migration*)
Kong, L. *et al., Zhiwu Xuebao*, 1996, **38**, 161-166 (*Glycerol 2-tetracosanoate*)
Barton, R.H. *et al., Aust. J. Chem.*, 1997, **50**, 355-361 (*acyl migration*)
Zou, K. *et al., CA*, 1999, **131**, 127577x (*isol*)
Han, L. *et al., Tet. Lett.*, 1999, **40**, 1631-1634 (*synth*)
Fat Digestion and Absorption, (eds. Christophe, A.B *et al*), AOCS Press, 2000, (*book*)
Lyubachevskaya, G. *et al., Lipids*, 2000, **35**, 1353-1358 (*acyl migration, metab*)
Intestinal Lipid Metabolism, (eds. Mansbach, C.M. *et al*), Kluwer, 2001, (*book*)

Glycerol 1,2-diacetate G-238

[102-62-5]

[25395-31-7]
1,2-Diacetylglycerol. 1,2,3-Propanetriol 1,2-diacetate. 1,2-Diacetin

$AcOCH_2CH(OAc)CH_2OH$

$C_7H_{12}O_5$ 176.169

▶AK3500000

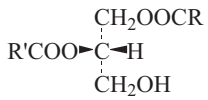
(±)-*form* [101364-64-1]
Solv.; used for decaffeinating coffee. Hygroscopic liq. Sol. H_2O. d_4^{15} 1.12. Bp_{12} 140-142°. Component of coml. Diacetin (Diacetylglycerol), a mixt. with Glycerol 1,3-diacetate.

Wegscheider, R. *et al., Monatsh. Chem.*, 1913, **34**, 1067; 1081 (*synth*)
Wahl, A. *et al., Bull. Soc. Chim. Fr.*, 1925, **37**, 713 (*bibl*)
Golendeev, V.P. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1936, **6**, 1841 (*synth*)

Japan. Pat., 1977, 78 98 920; *CA*, **90**, 22339c (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DBF600

Glycerol 1,2-dialkanoates G-239

1,2-Di-O-*acylglycerols*



(*S*)-*form*

Chiral molecules, whether R and R′ are the same or different. The biol. important S-enantiomer corresponds to 1,2-diacyl-*sn*-glycerol. 3-Phosphates have the *R*-config. Props. of individual compds. refer to this enantiomer unless otherwise stated. Surfactants, used as food emulsifiers. Other food-processing uses for mixts. of mono- and diglycerides include dough strengthener, formulation aid, flavouring agent, lubricant, stabiliser, surface active agent, and texturiser. Acyl migration, particularly under the influence of heat, acidic or alkaline conditions, can result in the interconversion of 1,2-di-*O*-acyl- and 1,3-di-*O*-acylglycerols. Commercial preps., prepared by chemical glycerolysis of triacylglycerols, contain mixts. of mono- and diacylglycerols. The diacylglycerol component forms an equilib. mixt. with a mole ratio of approx. 1.5:1 of the 1,3- and 1,2(2,3)-regioisomers.

Glycerol 1,2-dioctanoate [1069-87-0]

[60514-48-9, 104195-35-9, 113973-38-9] *Octanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di*-O-*octanoylglycerol. α,β-Dicaprylin. Glycerol 1,2-dicaprylate. 1,2-Dioctanoin*

$C_{19}H_{36}O_5$ 344.49
Liq. d 0.98. $[\alpha]_D^{22}$ +3.5 (neat). $[\alpha]_D^{22}$ -3.4 (c, 10 in $CHCl_3$). n_D^{23} 1.4745.

Glycerol 1-dodecanoate 2-(3*Z*-hexenoate)

$C_{21}H_{38}O_5$ 370.528

3-O-*[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranoside]:* ***Capsoside A***
$C_{33}H_{58}O_{15}$ 694.812
Constit. of the fruit of *Capsicum annuum* var. *acuminatum*. $[\alpha]_D^{25}$ +30 (c, 0.2 in H_2O).

Glycerol 1,2-didodecanoate [17598-94-6]

[59540-17-9, 60562-15-4] *Dodecanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di*-O-*dodecanoylglycerol. 1,2-Dilauroylglycerol. α,β-Dilaurin*

$C_{27}H_{52}O_5$ 456.705
Cryst. Mp 45-47° (*S*-form) Mp 20° (racemate) Mp 39° (racemate). $[\alpha]_D^{23}$ +6.9 (c, 7.33 in $CHCl_3$). Exhibits polymorphism.

Glycerol 1,2-ditetradecanoate [20255-94-1]

[1069-82-5, 56270-93-0, 60562-16-5] *Tetradecanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di*-O-*tetradecanoylglycerol. 1,2-Dimyristoylglycerol. α,β-Dimyristin*

$C_{31}H_{60}O_5$ 512.812
Cryst. Mp 58.5-60° (*S*-form) Mp 37.5° (racemate) Mp 54° (racemate) Mp 59° (racemate). Shows polymorphism.

3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside):1,2-Di*-O-*myristoyl-3*-O-*(6-sulfoquinovopyranosyl)glycerol*
$C_{37}H_{70}O_{12}S$ 739.019
Constit. of the leaves of craboo (*Byrsonima crassifolia*) (nance). $[\alpha]_D^{25}$ +43 (c, 1 in MeOH) (as Na salt).

Phosphate: See Glycerol 1,2-ditetradecanoate 3-phosphate in *The Combined Chemical Dictionary.*

Glycerol 1-hexadecanoate 2-tetradecanoate

$C_{33}H_{64}O_5$ 540.866

3-O-*β-D-Galactopyranoside:*
$C_{39}H_{74}O_{10}$ 703.008
Oil. $[\alpha]_D^{24}$ -2.8 (c, 0.5 in $CHCl_3$).

Glycerol 2-hexadecanoate 1-tetradecanoate

$C_{33}H_{64}O_5$ 540.866

1-O-*(6-Deoxy-6-sulfo-β-D-glucopyranoside):* ***Crassicaulisin***
$C_{39}H_{74}O_{12}S$ 767.072
Amorph. powder (as Na salt). $[\alpha]_D$ +43 (c, 0.13 in MeOH) (Na salt).

Glycerol 1,2-dihexadecanoate [761-35-3]

[6076-30-8, 26657-95-4, 30334-71-5, 109430-50-4, 128308-90-7] *Hexadecanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di*-O-*hexadecanoylglycerol. Glycerol 1,2-palmitate. 1,2-Dipalmitin. α,β-Dipalmitin. 1,2-Dipalmitoylglycerol*
$C_{35}H_{68}O_5$ 568.919
Cryst. ($CHCl_3$/petrol). Mp 68-69°. $[\alpha]_D^{23}$ -2.75 (c, 7.62 in $CHCl_3$).

3-Phosphate: See Glycerol 1,2-dihexadecanoate 3-phosphate in *The Combined Chemical Dictionary.*

3-O-*β-D-Glucopyranoside: 1*-O-*β-D-Glucopyranosyl-2,3-di*-O-*palmitoylglycerol*
$C_{41}H_{78}O_{10}$ 731.061
Constit. of the leaves of *Byrsonima crassifolia* (nance). $[\alpha]_D^{25}$ -4 (c, 1 in MeOH).

3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside):* [122991-48-4] *1,2-Di*-O-*palmitoyl-3*-O-*(6-sulfoquinovopyranosyl)glycerol*
$C_{41}H_{78}O_{12}S$ 795.126
Constit. of the leaves of *Byrsonima crassifolia* (nance). Cryst. ($CHCl_3$/MeOH) (as Na salt). $[\alpha]_D$ +41 (c, 0.1 in DMSO) (Na salt). C-2 Config. not determined.

Ac:
Mp 51-52°.

Glycerol 1-(9*Z*-hexadecenoate) 2-tetradecanoate
$C_{33}H_{62}O_5$ 538.85

3-O-*β-D-Galactopyranoside (2*S-*):* [133174-19-3]
$C_{39}H_{72}O_{10}$ 700.992
Oil. $[\alpha]_D^{24}$ -2.8 (c, 0.5 in $CHCl_3$).

Glycerol 1,2-di-(8*E*-hexadecenoate) *1,2-Di*-O-*(8*E-*hexadecenoyl)glycerol*
$C_{35}H_{64}O_5$ 564.888

3-O-*β-D-Glucopyranoside: 1*-O-*β-D-Glucopyranosyl-2,3-di*-O-*(8-hexadecenoyl)glycerol*
$C_{41}H_{74}O_{10}$ 727.03
Constit. of the leaves of *Byrsonima crassifolia* (nance). $[\alpha]_D^{25}$ -8 (c, 1 in MeOH).

3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside): 1,2-Di*-O-*(8-hexadecenoyl)-3*-O-*(6-sulfoquinovopyranosyl)glycerol*
$C_{41}H_{74}O_{12}S$ 791.094
Constit. of the leaves of *Byrsonima crassifolia* (nance). $[\alpha]_D^{25}$ +50 (c, 1 in MeOH).

Glycerol 1-octadecanoate 2-hexadecanoate *2*-O-*Hexadecanoyl-1*-O-*octadecanoylglycerol. α-Stearo-β-palmitin*
$C_{37}H_{72}O_5$ 596.973
Cryst. (hexane) (racemate). Mp 69-71° (racemate).

Glycerol 2-octadecanoate 1-hexadecanoate [20296-26-8] *Octadecanoic acid 1-(hydroxymethyl)-2-[(1-oxohexadecyl)oxy]ethyl ester, 9CI. 1*-O-*Hexadecanoyl-2*-O-*octadecanoylglycerol. α-Palmito-β-stearin*
$C_{37}H_{72}O_5$ 596.973
Cryst. (hexane) (racemate). Mp 59-61° (racemate).

Glycerol 1,2-dioctadecanoate [1188-58-5]

[1323-83-7, 1429-59-0, 10567-21-2, 51063-97-9] *Octadecanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di*-O-*hexadecanoylglycerol. Glycerol 1,2-distearate. α,β-Distearin. Cithrol EDS. E471*
$C_{39}H_{76}O_5$ 625.026
Emulsifier, stabiliser, wetting agent and antistatic agent. Cryst. Mp 74-76° (*S*-form) Mp 59.5° (racemate) Mp 71-72° (racemate). Shows polymorphism.

3-Phosphate: See Glycerol 1,2-dioctadecanoate 3-phosphate in *The Combined Chemical Dictionary.*

Glycerol 1-(9*Z*-octadecenoate) 2-tetradecanoate *1*-O-*(9Z-Octadecenoyl)-2*-O-*tetradecanoylglycerol. 1*-O-*Oleoyl-2*-O-*palmitoylglycerol*
$C_{35}H_{66}O_5$ 566.903

3-Phosphate:
$C_{35}H_{67}O_8P$ 646.883
No phys. props. reported.

3-O-*β-D-Galactopyranoside (2*S-*):* [133174-21-7]
$C_{41}H_{76}O_{10}$ 729.045
Oil. $[\alpha]_D^{24}$ -2.5 (c, 0.5 in $CHCl_3$).

Glycerol 1-(9*E*-octadecenoate) 2-hexadecanoate
$C_{37}H_{70}O_5$ 594.957

3-O-*(6-Deoxy-6-sulfo-α-D-glucopyranoside):* [222991-63-1] *1-Oleoyl-2-palmitoyl-3-(6-sulfoquinovopyranosyl)glycerol*
$C_{43}H_{80}O_{12}S$ 821.164
Amorph. solid. Incorrect struct. assigned in CA.

Glycerol 1-(9*Z*-octadecenoate) 2-hexadecanoate

[38991-91-2] *9-Octadecenoic acid 3-hydroxy-2-[(1-oxohexadecyl)oxy]propyl ester. 2*-O-*Hexadecanoyl-1-(9Z-octadecenoyl)glycerol*
$C_{37}H_{70}O_5$ 594.957
Oil. *R*-enantiomer prepd..

3-Phosphate: [10015-87-9] *9-Octadecenoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-*

2-(phosphonoxy)ethyl ester
$C_{37}H_{71}O_8P$ 674.937
Racemate prepd..

Glycerol 2-(9*Z*-octadecenoate) 1-hexadecanoate [29541-66-0]

[3123-73-7] *9-Octadecenoic acid 1-(hydroxymethyl)-2-[(1-oxohexadecyl)oxy]ethyl ester. 1-*O*-Hexadecanoyl-2-*O*-(9Z-octadecenoyl)glycerol. 2-Oleoyl-1-palmitoylglycerol. α-Palmito-β-olein*
$C_{37}H_{70}O_5$ 594.957

3-Phosphate:
$C_{37}H_{71}O_8P$ 674.937
Mp 192-194° (as NH_4 salt). $[\alpha]_D$ +4.5 (c, 3 in $CHCl_3$) (NH_4 salt).

*3-*O*-β-D-Galactopyranoside: 1-*O*-β-D-Galactopyranosylglycerol 3-hexadecanoate 2-(9-octadecenoate)*
$C_{43}H_{80}O_{10}$ 757.099
Stereochem. not confirmed.

*3-*O*-[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:*
$C_{49}H_{90}O_{15}$ 919.241
Stereochem. not confirmed.

Glycerol 1-(9*Z*-octadecenoate) 2-octadecanoate [38635-46-0]

[73788-95-1] *9-Octadecenoic acid 3-hydroxy-2-[(1-oxooctadecyl)oxy]propyl ester, 9CI. 2-*O*-Octadecanoyl-1-*O*-(9Z-octadecenoyl)-glycerol. 1-*O*-Oleoyl-2-*O*-stearoylglycerol. α-Oleo-β-stearin*
$C_{39}H_{74}O_5$ 623.011
Mp 19-20° (racemate).

Glycerol 2-(9*Z*-octadecenoate) 1-octadecanoate [53702-48-0]

[21059-30-3] *9-Octadecenoic acid 1-(hydroxymethyl)-2-[(1-oxooctadecyl)oxy]ethyl ester, 9CI. 1-*O*-Octadecanoyl-2-*O*-(9Z-octadecenoyl)glycerol. 2-*O*-Oleoyl-1-*O*-stearoylglycerol. α-Stearo-β-olein*
$C_{39}H_{74}O_5$ 623.011
Mp 39.5-40° (racemate). $[\alpha]_D$ -2.8 (c, 9.2 in $CHCl_3$) (*S*-form).

Glycerol 1,2-di-(9*E*-octadecenoate) *1,2-Di-*O*-9*E*-octadecenoylglycerol. 1,2-Dielaidoylglycerol*
$C_{39}H_{72}O_5$ 620.995
Mp 25°. $[\alpha]_D^{25}$ -1.85 (c, 1.0 in $CHCl_3$).

Glycerol 1,2-di-(9*Z*-octadecenoate) [24529-88-2]

[2442-61-7, 3738-74-7, 25637-84-7, 33735-55-6] *1,2-Di-9*E*-octadecenoylglycerol. 1,2-Dioleoylglycerol. α,β-Diolein*
$C_{39}H_{72}O_5$ 620.995
Emulsifier, stabiliser, wetting agent and lubricant. Oil. $[\alpha]_D^{25}$ -1.91 (c, 6.2 in $CHCl_3$).

► RK1250000

3-Phosphate: [61617-08-1]

[5487-64-9, 14268-17-8] *9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester, 9CI. Dioleoylphosphatidic acid*
$C_{39}H_{73}O_8P$ 700.975
$[\alpha]_D^{22}$ +3.8 (c, 5 in $CHCl_3$) (*R*-form).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-tetradecanoate
$C_{35}H_{64}O_5$ 564.888

*3-*O*-β-D-Galactopyranoside (2*S*-):*
[133174-20-6]
$C_{41}H_{74}O_{10}$ 727.03
Oil. $[\alpha]_D^{24}$ -2.3 (c, 0.8 in $CHCl_3$).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-hexadecanoate
$C_{37}H_{68}O_5$ 592.941

*3-*O*-β-D-Galactopyranoside (2*S*-):*
$C_{43}H_{78}O_{10}$ 755.083
Oil. $[\alpha]_D^{24}$ -3.4 (c, 0.6 in $CHCl_3$).

Glycerol 2-(9*Z*,12*Z*-octadecadienoate) 1-hexadecanoate [51621-26-2]

[73649-99-7, 96613-82-0] *9,12-Octadecadienoic acid 1-(hydroxymethyl)-2-[(1-oxohexadecyl)oxy]ethyl ester. 1-O-Hexadecanoyl-2-*O*-(9Z,12Z-octadecadienoyl)glycerol. 1-*O*-Palmitoyl-2-*O*-linoleoylglycerol*
$C_{37}H_{68}O_5$ 592.941
Oil. $[\alpha]_D^{25}$ +2.5 (neat).

*3-*O*-[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:* [145033-48-3]
$C_{49}H_{88}O_{15}$ 917.225
Constit. of wheat flour.

*3-*O*-β-D-Galactopyranoside:* [28069-27-4]
*1-*O*-β-D-Galactopyranosylglycerol 3-hexadecanoate 2-(9,12-octadecadienoate)*
$C_{43}H_{78}O_{10}$ 755.083

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-(4*Z*-hexadecenoate)

*3-*O*-β-D-Galactopyranoside:*
$C_{43}H_{76}O_{10}$ 753.067
Viscous solid. $[\alpha]_D$ -6 (c, 0.2 in $CHCl_3$).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-octadecanoate *2-*O*-Octadecanoyl-1-*O*-(9Z,12Z-octadecadienoyl)glycerol. 1-*O*-Linoleoyl-2-*O*-stearoylglycerol. α-Linoleo-β-stearin*
$C_{39}H_{72}O_5$ 620.995
Oil. Mp 18.5° (*S*-form) Mp 9-10° (racemate).

Glycerol 2-(9*Z*,12*Z*-octadecadienoate) 1-octadecanoate [34487-26-8] *9,12-Octadecadienoic acid 1-(hydroxymethyl)-2-[(1-oxooctadecyl)oxy]ethyl ester. 2-*O*-(9Z,12Z-octadecadienoyl)-1-*O*-octadecanoylglycerol. 2-*O*-Linoleoyl-1-*O*-stearoylglycerol. α-Stearo-β-linolein*
$C_{39}H_{72}O_5$ 620.995
Mp 17.5° (*S*-form) Mp 13.5° (racemate).

*3-*O*-[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:*
$C_{51}H_{92}O_{15}$ 945.279

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-(9*Z*-octadecenoate) *9,12-Octadecadienoic acid 3-hydroxy-2-[(1-oxo-9-octadecenyl)oxy]propyl ester. 1-*O*-(9Z,12Z-Octadecadienoyl)-2-*O*-(9Z-octadecenoyl)glycerol. 1-*O*-Linoleoyl-2-*O*-oleoylglycerol*
$C_{39}H_{70}O_5$ 618.979
$[\alpha]_D^{20}$ -4.47 (*R*-form).

*3-*O*-β-D-Galactopyranoside: 1-*O*-β-D-Galactopyranosylglycerol 2-(9,12-octadecadienoate) 3-(9-octadecenoate)*
$C_{45}H_{80}O_{10}$ 781.121
Has 2*S*-config.

Glycerol 2-(9*Z*,12*Z*-octadecadienoate) 1-(9*Z*-octadecenoate) *2-*O*-(9Z,12Z-octadecadienoyl)-1-*O*-(9Z-octadecenoyl)glycerol. 2-Linoleoyl-1-oleoylglycerol. α-Oleo-β-linolein*
$C_{39}H_{70}O_5$ 618.979
Oil. $[\alpha]_D^{20}$ -2.6 (c, 2.0 in $CHCl_3$) (*R*-form).

Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) [24529-89-3]

[2442-62-8, 68069-29-4, 125356-49-2] *9,12-Octadecadienoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. Glycerol 1,2-di-*O*-linoleoate. 1,2-Dilinoleoylglycerol*
$C_{39}H_{68}O_5$ 616.963
Oil. $[\alpha]_D^{25}$ -2 (c, 1.1 in $CHCl_3$).

3-Phosphate: [13397-95-0]

[17966-17-5]
$C_{39}H_{69}O_8P$ 696.943
No phys. props. reported.

*3-*O*-β-D-Galactopyranoside:* [88195-88-4]
*1-*O*-β-D-Galactopyranosylglycerol 2,3-di-(9,12-octadecadienoate)*
$C_{45}H_{78}O_{10}$ 779.105
$[\alpha]_D$ +26 (MeOH).

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-tetradecanoate
$C_{35}H_{62}O_5$ 562.872

*3-*O*-β-D-Galactopyranoside (2*S*-):*
[133174-17-1]
$C_{41}H_{72}O_{10}$ 725.014
Oil. $[\alpha]_D^{24}$ -2.7 (c, 0.7 in $CHCl_3$).

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-hexadecanoate
$C_{37}H_{66}O_5$ 590.925

*3-*O*-β-D-Galactopyranoside (2*S*-):*
$C_{43}H_{76}O_{10}$ 753.067
Obt. as a mixt. with 1-*O*-(9,12,15-octadecatrienoyl), 2-*O*-(9*E*-hexadecenoyl) ester.

Glycerol 1-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 2-(9*E*-hexadecenoate)
$C_{37}H_{64}O_5$ 588.91

*3-*O*-β-D-Galactopyranoside (2*S*-):*
[133174-18-2]
$C_{43}H_{74}O_{10}$ 751.052
Oil. $[\alpha]_D^{24}$ -3.4 (c, 0.8 in $CHCl_3$).

Glycerol 1,2-di-(9*Z*,12*Z*,15*Z*-octadecatrienoate) *1,2-Di-*O*-(9Z,12Z,15Z-octadecatrienoyl)glycerol. 1,2-Di-*O*-linolenoylglycerol. Glycerol 1,2-dilinolenoate*
$C_{39}H_{64}O_5$ 612.932

3-Phosphate: [94086-57-4]

[34961-23-4] *9,12,15-Octadecatrienoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester*
$C_{39}H_{65}O_8P$ 692.911
$[\alpha]_D^{20}$ +31 (c, 3.5 in $CHCl_3$).

*3-*O*-β-D-Galactopyranoside (2*S*-):*
$C_{45}H_{74}O_{10}$ 775.074

*3-*O*-(6-Amino-6-deoxy-α-D-glucopyranoside): **Strangulatoside A***
$C_{45}H_{75}NO_9$ 774.089
Gum. $[\alpha]_D^{24}$ +25.5 (c, 3 in MeOH). C2-config. unknown.

*3-*O*-[[3-(4-Hydroxyphenyl)propanoyl]-(→6)-6-amino-6-deoxy-α-D-glucopyranoside]: **Strangulatoside B***
$C_{54}H_{83}NO_{11}$ 922.25
Gum. $[\alpha]_D^{24}$ +25.8 (c, 2.7 in MeOH). C2-config. unknown.

*3-*O*-[β-D-Allopyranosyl-(1→6)-α-D-glucopyranoside]:*
$C_{51}H_{84}O_{15}$ 937.216
Gum. $[\alpha]_D^{24}$ +25.3 (c, 6 in MeOH). C2-Config. not known.

Glycerol 2-(9,12,15-octadecatrienoate) 1-hexadecanoate *1-*O*-Hexadecanoyl-2-*O*-(9Z,12Z,15Z-octadecatrienoyl)glycerol*
$C_{37}H_{66}O_5$ 590.925

3-O-*[α-D-Galactopyranosyl-(1→6)-β-D-galactopyranoside]:* [178174-88-4] ***Inulagalactolipid A***
$C_{49}H_{86}O_{15}$ 915.209

Glycerol 2-(9*Z*,12*Z*,15*Z*-octadecatrienoate) 1-octadecanoate *1*-O-*Octadecanoyl-2*-O-*(9Z,12Z,15Z-octadecatrienoyl)glycerol*
$C_{39}H_{70}O_5$ 618.979

3-O-*β-D-Galactopyranoside:* [178174-86-2]
$C_{45}H_{80}O_{10}$ 781.121

Glycerol 1,2-di-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{39}H_{60}O_5$ 608.9

3-O-*β-D-Galactopyranoside (2*R-*):* [121312-93-4] ***Heterosigma glycolipid I***
$C_{45}H_{70}O_{10}$ 771.042
Oil. $[\alpha]_D^{25}$ -4.5 (c, 1.3 in $CHCl_3$).

Glycerol 1-(3*Z*,6*Z*,9*Z*,12*Z*,15*Z*-octadecapentaenoate) 2-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{39}H_{58}O_5$ 606.884

3-O-*β-D-Galactopyranoside (2*R-*):* [144118-09-2] ***Heterosigma glycolipid III***
$C_{45}H_{68}O_{10}$ 769.026
Oil. $[\alpha]_D^{25}$ -4.5 (c, 1.3 in $CHCl_3$).

3-O-*(6*-O-*Octadecanoyl-β-D-glucopyranoside):*
$C_{63}H_{102}O_{11}$ 1035.492
OIL. $[\alpha]_D^{25}$ -3.9 (c, 0.4 in $CHCl_3$).

Glycerol 1-(5*Z*,8*Z*,11*Z*,14*Z*,17*Z*-eicosapentaenoate) 2-(6*Z*,9*Z*,12*Z*,15*Z*-octadecatetraenoate)
$C_{41}H_{62}O_5$ 634.938

3-O-*β-D-Galactopyranoside (2*R-*):* [121245-05-4] ***Heterosigma glycolipid II***
$C_{47}H_{72}O_{10}$ 797.08
Oil. $[\alpha]_D$ -4.1 (c, 1.3 in $CHCl_3$).

Glycerol 2-(5,8,11,14,17-eicosapentaenoate) 1-(6,9,12,15-octadecatetraenoate)
$C_{41}H_{62}O_5$ 634.938

3-O-*[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranoside]:* [144118-10-5] ***Heterosigma glycolipid IV***
$C_{53}H_{82}O_{15}$ 959.222

Glycerol 1,2-dioctacosanoate [52363-45-8]

[127039-57-0] *Octacosanoic acid 1-(hydroxymethyl)-1,2-ethanediyl ester. 1,2-Di-*O*-octacosanoylglycerol. α,β-Dimontanylglycerol*
$C_{59}H_{116}O_5$ 905.562
Constit. of *Morus alba* root (white mulberry) bark. Cryst. (EtOAc). Mp 82-82.5°. Abs. config. of nat. prod. not known.

Ac:
Cryst. ($MeOH/CHCl_3$). Mp 68-69.5°.

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Mattson, F.H. *et al., J. Lipid Res.*, 1962, **3**, 281-296 (*rev, acyl migration*)
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Dorset, D.L. *et al., Z. Naturforsch., C*, 1978, **33**, 39 (*dihexadecanoyl, cryst struct*)
Beier, R.C. *et al., Can. J. Chem.*, 1980, **58**, 2800 (*cmr*)
Virtanen, J.A. *et al., Chem. Phys. Lipids*, 1980, **27**, 185-190 (*uniform acyl isomers, synth*)
Pascher, I. *et al., J. Mol. Biol.*, 1981, **153**, 791 (*didodecanoyl, cryst struct*)
Froeling, A. *et al., Chem. Phys. Lipids*, 1984, **36**, 29-38 (*mixed acyl isomers, synth*)
Eibl, H. *et al., Chem. Phys. Lipids*, 1986, **41**, 53-63 (*mixed acyl isomers, synth*)
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Son, B.W. *et al., Phytochemistry*, 1990, **29**, 307 (*sulfoglycosides, isol*)
Kobayashi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1404-1410 (*Heterosigma glycolipids*)
Prieto, J.A. *et al., J. Am. Oil Chem. Soc.*, 1992, **69**, 1019-1022 (*3-O-galactopyranosylgalactopyranoside, isol, wheat*)
Rogalska, E. *et al., Chirality*, 1993, **5**, 24-30 (*metab*)
Vilcheze, C. *et al., J. Lipid Res.*, 1994, **35**, 734-738 (*uniform acyl isomers, synth*)
Martin, S.F. *et al., J.O.C.*, 1994, **59**, 4805-4820 (*mixed acyl isomers, synth*)
Zoellner, P. *et al., Org. Mass Spectrom.*, 1994, **29**, 253 (*ms*)
Amarquaye, A. *et al., Planta Med.*, 1994, **60**, 85 (*sulfoglycosides, isol*)
Boswinkel, G. *et al., J. Am. Oil Chem. Soc.*, 1996, **73**, 707-711 (*acyl migration*)
Rho, M.C. *et al., J. Nat. Prod.*, 1996, **59**, 308 (*hexadecanoyl galactoside*)
Jung, J.H. *et al., Phytochemistry*, 1996, **42**, 447 (*Arisaema glycosides*)
Rho, M.C. *et al., Planta Med.*, 1996, **62**, 473 (*9-hexadecenoyl galactoside*)
Barton, R.H. *et al., Aust. J. Chem.*, 1997, **50**, 355-361 (*acyl migration*)
Rastrelli, L. *et al., Phytochemistry*, 1997, **45**, 647 (*Byrsonima glycosides*)
Roodsari, F.S. *et al., J.O.C.*, 1999, **64**, 7727-7737 (*mixed acyl isomers, synth*)
Sonnet, P.E. *et al., Lipid Synthesis and Manufacture*, (ed. Gunstone, F.D.), Sheffield Academic Press/CRC Press, 1999, (*book, !rev, synth*)
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Intestinal Lipid Metabolism, (eds. Mansbach, C.M. *et al*), 2001, (*book*)
Iorizzi, M. *et al., J. Agric. Food Chem.*, 2001, **49**, 2022-2029 (*Capsoside A*)
Son, B.W. *et al., Lipids*, 2001, **36**, 427-429 (*Oscillatoria galactoside*)
Dai, J.Q. *et al., Phytochemistry*, 2001, **58**, 1305-1309 (*Strangulatosides*)
Shao, Z.Y. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 205-209 (*Crassicaulisin*)

Glycerol 1,3-dialkanoates G-240

*1,3-Di-*O*-acylglycerols*
$RCOOCH_2CH(OH)CH_2OOCR'$
Meso-compds. if the R groups are identical. Potentially opt. active if they are different. Data given here refers to racemates unless stated otherwise.Acyl migration, particularly under the influence of heat, acidic or alkaline conditions, can result in the interconversion of 1,2-di-*O*-acyl- and 1,3-di-*O*-acylglycerols. Commercial preparations, prepared by chemical glycerolysis of triacylglycerols, contain mixtures or mono- and diacylglycerols. The diacylglycerol component forms an equilibrium mixture with a mole ratio of approximately 1.5:1 of the 1,3- and 1,2(2,3)-regioisomers.

Glycerol 1,3-didecanoate [17598-93-5] *Decanoic acid 2-hydroxy-1,3-propanediyl ester. 1,3-Di-*O*-decanoylglycerol. α,α′-Dicaprin*
$C_{23}H_{44}O_5$ 400.598
Cryst. (hexane). Mp 44°.

Glycerol 1,3-didodecanoate [539-93-5] *Dodecanoic acid 2-hydroxy-1,3-propanediyl ester. 1,3-Di-*O*-dodecanoylglycerol. α,α′-Dilaurin*
$C_{27}H_{52}O_5$ 456.705
Cryst. (EtOH/hexane). Mp 57.8°.

Glycerol 1,3-ditridecanoate [59891-27-9] *Tridecanoic acid 2-hydroxy-1,3-propanediyl ester. α,α′-Ditridecanoin. 1,3-Di-*O*-tridecanoylglycerol*
$C_{29}H_{56}O_5$ 484.758
Cryst. (hexane). Mp 62°.

Glycerol 1,3-ditetradecanoate [7770-09-4] *Tetradecanoic acid 2-hydroxy-1,3-propanediyl ester. 1,3-Di-*O*-tetradecanoylglycerol. α,α′-Dimyristin*
$C_{31}H_{60}O_5$ 512.812
Cryst. (hexane). Mp 66-67°.

2-Phosphate:
$C_{31}H_{61}O_8P$ 592.792
Cryst. + 0.5 quinoline (EtOAc). Mp 96.5-97.5°.

Glycerol 1,3-dipentadecanoate [59891-25-7] *Pentadecanoic acid 2-hydroxy-1,3-propanediyl ester. 1,3-Di-*O*-pentadecanoylglycerol. α,α′-Dipentadecanoin*
$C_{33}H_{64}O_5$ 540.866
Cryst. (hexane). Mp 70°.

Glycerol 1-hexadecanoate 3-decanoate [59891-26-8] *Hexadecanoic acid 2-hydroxy-3-[(1-oxodecyl)oxy]propyl ester. 1-*O*-Decanoyl-3-*O*-hexadecanoylglycerol. α,α′-Palmitocaprin*
$C_{29}H_{56}O_5$ 484.758
Cryst. (hexane). Mp 54.5°.

Glycerol 1-hexadecanoate 3-dodecanoate [51604-53-6]

[5281-51-6] *Hexadecanoic acid 2-hydroxy-3-[(1-oxododecyl)oxy]propyl ester. 1-*O*-Dodecanoyl-3-*O*-hexadecanoylglycerol. α-Palmito-α′-laurin*
$C_{31}H_{60}O_5$ 512.812
Cryst. (hexane). Mp 54.5°.

Glycerol 1-hexadecanoate 3-tetradecanoate [17637-37-5] *1-*O*-Hexadecanoyl-3-*O*-tetradecanoylglycerol. α-Palmito-α′-myristin*
$C_{33}H_{64}O_5$ 540.866
Cryst. (petrol). Mp 63.5-64°.

Glycerol 1,3-dihexadecanoate [502-52-3]

[26657-95-4] *Hexadecanoic acid 2-hydroxy-1,3-propanediyl ester. 1,3-Di-*O*-hexadecanoylglycerol. Glycerol 1,3-dipalmitate. 1,3-Dipalmitin. α,α′-Dipalmitin*
$C_{35}H_{68}O_5$ 568.919
Constit. of *Panax ginseng* (ginseng).
Cryst. (Me_2CO/hexane at 0°). Mp 73-74°.

Ac:
$C_{37}H_{70}O_6$ 610.956
Mp 54°.

Glycerol 1-octadecanoate 3-dodecanoate *1-*O*-Dodecanoyl-3-*O*-hexadecanoylglycerol. α-Stearo-α′-laurin*

$C_{33}H_{64}O_5$ 540.866
Cryst. Mp 62°.

Glycerol 1-octadecanoate 3-tetradecanoate *1-O-Octadecanoyl-3-O-tetradecanoylglycerol. α-Stearo-α′-myristin*
$C_{35}H_{68}O_5$ 568.919
Cryst. (Et_2O/EtOH). Mp 66.5-67°.

Glycerol 1-octadecanoate 3-hexadecanoate [17708-08-6]

[5281-52-7, 5281-87-8] *1-O-Hexadecanoyl-3-O-octadecanoylglycerol. 1-Palmitoyl-3-stearoylglycerol. α-Stearo-α′-palmitin*
$C_{37}H_{72}O_5$ 596.973
Cryst. (Me_2CO). Both enantiomers and the racemate known.

Glycerol 1,3-dioctadecanoate [504-40-5] *2-Hydroxy-1,3-propanediyl octadecanoate, 9CI. 1,3-Di-O-octadecanoylglycerol. α,α′-Distearin*
$C_{39}H_{76}O_5$ 625.026
Cryst. (Me_2CO). Mp 80-81°.

2-Phosphate:
$C_{39}H_{77}O_8P$ 705.006
Cryst. Mp 68.5-69.5°.

2-Ac:
$C_{41}H_{78}O_6$ 667.064
Mp 64°.

Glycerol 1-(9*Z*-octadecenoate) 3-dodecanoate *1-O-Dodecanoyl-3-O-(9Z-octadecenoyl)-glycerol*
$C_{33}H_{62}O_5$ 538.85
Cryst. (Et_2O/EtOH). Mp 32°.

Glycerol 1-(9*Z*-octadecenoate) 3-tetradecanoate *1-O-(9Z-Octadecenoyl)-3-O-tetradecanoylglycerol. α-Oleo-α′-myristin*
$C_{35}H_{66}O_5$ 566.903
Cryst. (Et_2O/EtOH). Mp 41°.

Glycerol 1-(9*Z*-octadecenoate) 3-hexadecanoate [3343-30-4]

[2190-30-9, 36805-77-3] *1-O-Hexadecanoyl-3-O-(9Z-octadecenoyl)glycerol. 1-Oleoyl-3-palmitoylglycerol*
$C_{37}H_{70}O_5$ 594.957
Cryst. (EtOH/petrol). Mp 44-44.5°. (*S*)-enantiomer also known (1-Oleoyl-3-palmitoyl-*sn*-glycerol).

Glycerol 1-(9*E*-octadecenoate) 3-octadecanoate *α-Elaido-α′-stearin. 1-O-Octadecanoyl-3-O-(9E-octadecenoyl)glycerol. 1-Elaidoyl-3-stearoylglycerol*
$C_{39}H_{74}O_5$ 623.011
Cryst. (Et_2O/EtOH). Mp 65.5-66°. Exhibits polymorphism.

Glycerol 1-(9*Z*-octadecenoate) 3-octadecanoate [5568-23-0] *1-O-Octadecanoyl-3-O-(9Z-octadecenoyl)glycerol. 1-Oleoyl-3-stearoylglycerol. α-Oleo-α′-stearin*
$C_{39}H_{74}O_5$ 623.011
Cryst. (Me_2CO). Mp 48-49°. Exhibits polymorphism.

Glycerol 1-(9*E*-octadecenoate) 3-(9*Z*-octadecenoate) *1-O-(9E-Octadecenoyl)-3-O-(9Z-octadecenoyl)glycerol. α-Elaido-α′-olein*
$C_{39}H_{72}O_5$ 620.995
Cryst. (Et_2O/MeOH). Mp 28.8°. Exhibits polymorphism.

Glycerol 1,3-di-9*E*-octadecenoate

[2465-32-9] *1,3-Di-O-9E-octadecenoylglycerol. α,α′-Dielaidin*
$C_{39}H_{72}O_5$ 620.995
Cryst. (Et_2O/EtOH at 10°). Mp 50.1°.

Glycerol 1,3-di-9*Z*-octadecenoate [25637-84-7]

[2465-32-9] *1,3-Di-O-9Z-octadecenoylglycerol. α,α′-Diolein*
$C_{39}H_{72}O_5$ 620.995
Cryst. (Me_2CO). Mp 26-28°.

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 3-hexadecanoate [99032-71-0] *1-O-Hexadecanoyl-3-O-(9Z,12Z-octadecadienoyl)-glycerol. α-Linoleo-α′-palmitin*
$C_{37}H_{68}O_5$ 592.941
Cryst. Mp 27-28°.

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 3-(9*Z*-octadecenoate) [104346-53-4] *1-O-(9Z,12Z-Octadecadienoyl)-3-O-(9Z-octadecenoyl)glycerol. α-Linoleo-α′-olein*
Oil.

Glycerol 1,3-di-(9,12-octadecadienoate) [15818-46-9]

[59925-29-0] *1,3-Di-O-(9Z,12Z-octadecadienoyl)glycerol. Glycerol 1,3-dilinoleoate. α,α′-Dilinolein*
$C_{39}H_{68}O_5$ 616.963
Oil. Mp -2.6°.

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 3-nonadecanoate *1-O-(9Z,12Z-Octadecadienoyl)-3-O-nonadecanoylglycerol*
Oil.

Glycerol 1,3-di-(9*Z*,12*Z*,15*Z*-octadecatrienoate) [98242-77-4] *1,3-Di-O-(9Z,12Z,15Z-octadecatrienoyl)glycerol. α,α′-Dilinolenin. α,γ-Dilinolein*
$C_{39}H_{64}O_5$ 612.932
Oil. Mp -12.3°.

Glycerol 1-eicosanoate 3-octadecanoate [59891-28-0] *1-O-Eicosanoyl-3-O-octadecanoylglycerol. 1-Arachidonoyl-3-stearoylglycerol. αα′-Arachidostearin*
$C_{41}H_{80}O_5$ 653.08
Cryst. (Me_2CO). Mp 76°.

Glycerol 1-docosanoate 3-hexadecanoate [59891-35-9] *1-O-Docosanoyl-3-O-hexadecanoylglycerol. α,α′-Behenopalmitin*
$C_{41}H_{80}O_5$ 653.08
Cryst. (Me_2CO). Mp 76-77°.

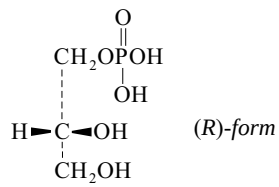
Glycerol 1-docosanoate 3-eicosanoate [57799-98-1] *1-O-Docosanoyl-3-O-eicosanoylglycerol. α,α′-Arachidobehenin*
$C_{45}H_{88}O_5$ 709.187
Cryst. (cyclohexane). Mp 70.5-71.5°.
Stereochem. of nat. prod. not known.

Crossley, A. *et al., J.C.S.*, 1959, 760-764 (*acyl migration*)
Mattson, F.H. *et al., J. Lipid Res.*, 1962, **3**, 281-296 (*rev, acyl migration*)
Serdavich, B. *et al., J. Am. Oil Chem. Soc.*, 1967, **44**, 381-393 (*acyl migration*)
Nilsson-Ehle, P. *et al., J. Biol. Chem.*, 1973, **248**, 6734-6737 (*metab*)
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Lok, C.M. *et al., Chem. Phys. Lipids*, 1985, **36**, 329-334 (*synth, mixed acyl*)
Eibl, H. *et al., Chem. Phys. Lipids*, 1986, **41**, 53-63 (*synth, mixed acyl isomers*)
Kodali, D.R. *et al., Chem. Phys. Lipids*, 1990, **52**, 163-170 (*acyl migration*)
Berger, M. *et al., J. Am. Oil Chem. Soc.*, 1992, **69**, 955-960 (*synth, uniform acyl isomers*)
Rogalska, E. *et al., Chirality*, 1993, **5**, 24-30 (*metab*)
Boswinkel, G. *et al., J. Am. Oil Chem. Soc.*, 1996, **73**, 707-711 (*acyl migration*)
Barton, R.H. *et al., Aust. J. Chem.*, 1997, **50**, 355-361 (*acyl migration*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1896-1906 (*use*)
Lipid Synthesis and Manufacture, (ed. Gunstone, F.D.) Sheffield Academic Press/CRC Press, 1999, 162-184; 288-320 (***rev, synth***)
Fat Digestion and Absorption, (eds. Christophe, A.B *et al*), AOCS Press, 2000, (*book*)
Lyubachevskaya, G. *et al., Lipids*, 2000, **35**, 1353-1358 (*acyl migration, metab*)
Intestinal Lipid Metabolism, (eds. Mansbach, C.M. *et al*), Kluwer, 2001, (*book*)
Ma, C.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 206-209 (*Hyoscyamus niger isolates*)

Glycerol 1-monophosphate G-241

[57-03-4]

[27082-31-1]
1,2,3-Propanetriol 1-(dihydrogen phosphate), 9CI. Glycerol 1-phosphate. α-Glycerophosphoric acid



(*R*)-*form*

$C_3H_9O_6P$ 172.074

Natural glycerophosphoric acid obt. from biol. sources is a mixt. of ca. 25% Glycerol 1-monophosphate, G-241 and 75% Glycerol 2-monophosphate, $[\alpha]_D$ ca. -0.5°. Synthetic glycerophosphoric acid prepd. by phosphorylation of glycerol has varying isomeric composition.

(*R*)-*form* [5746-57-6] *L-form*
Syrup. Dec. on dist. Slowly hydrol. by H_2O.

Ba salt (2:1):
$[\alpha]_D$ -1.45 (c, 10.3 in 2*N* HCl).

Di-Me ether:
$C_5H_{14}O_6P$ 201.136
$[\alpha]_D$ -7.2 (as Na salt).

Di-Me ether, di-Me ester:
$C_7H_{17}O_6P$ 228.181
$[\alpha]_D$ -4.78 (EtOH).

(*S*)-*form* [17989-41-2] *D-form*
Syrup. Dec. on dist. Slowly hydrol. by H_2O.

Li salt:
$[\alpha]_D^{28}$ +3.51 (H_2O).

Di-Me ether, di-Me ester:
$[\alpha]_D$ +5.1.

(±)-*form* [1509-81-5]
Syrup. pK_{a2} 6.66 (25°). Dec. on dist. Slowly hydrol. by H_2O.

K salt (1:2): [1319-69-3]

[1319-70-6]
$C_3H_7K_2O_6P$ 248.255
Dietary supplement. Pale yellow, syrupy liq. or aq. soln. (+ $3H_2O$). The K salt may be of either α- or β-glycerophosphoric acid for food use. CAS no. refers to trihydrate.

Mg salt (1:1): [927-20-8]
$C_3H_7MgO_6P$ 194.364
Plasticiser for food packaging materials.

Powder.

Mn salt (1:1): [1320-46-3]
$C_3H_7MnO_6P$ 224.997
Dietary supplement. White or pinkish white powder. The Mn salt may be of either α- or β-glycerophosphoric acid for food use.

Quinine salt:
Mp 155°.

[1334-74-3, 17603-42-8, 27214-00-2]

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Hossel, L.W. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1954, **73**, 150 (*derivs*)
Baer, E. *et al., J. Biol. Chem.*, 1955, **212**, 39 (*synth*)
Taga, T. *et al., Chem. Comm.*, 1972, 465 (*cryst struct*)
Harvey, D.J. *et al., J.C.S. Perkin 1*, 1972, 1074 (*trimethylsilyl, ms*)
Taguchi, Y. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1586 (*synth*)
Yeagle, P.L. *et al., J.A.C.S.*, 1975, **97**, 7175 (*cmr*)
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Weissman, J.D. *et al., J. Biol. Chem.*, 1982, **257**, 3618 (*synth*)
Gerothanassis, I.P. *et al., J. Magn. Reson.*, 1982, **46**, 423 (*O nmr*)
Crans, D.C. *et al., J.A.C.S.*, 1985, **107**, 7019 (*synth*)
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Glycerol triacetate G-242

[102-76-1]
1,2,3-Propanetriol triacetate, 9CI. Triacetylglycerol. ***Triacetin, 8CI, BAN, INN, USAN.*** *Fungacetin. Euzactin. Blekin. Enzacetin. Enzactin. Fungacet. Glyped. Motisil. Vanay. Estol 1581. FEMA 2007. E1518*

$AcOCH_2CH(OAc)CH_2OAc$

$C_9H_{14}O_6$ 218.206
Flavouring agent, adjuvant; formulation aid, humectant, solvent and vehicle. Present in papaya (*Carica papaya*). Oily liq. Sol. EtOH, Et_2O, C_6H_6, H_2O. d_4^{20} 1.16. Mp 3° Mp -78°. Bp 258-259° Bp_{40} 172°. n_D^{20} 1.4310. Log P 0.45 (calc).

▶ Eye irritant. LD_{50} (rat, orl) 3000 mg/kg. AK3675000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 620C (*ir*)
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Hancock, B. *et al., J.A.C.S.*, 1948, **70**, 424 (*cryst*)
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U.K. Pat., 1960, 845 029; *CA*, **55**, 9797h (*use*)
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Respondek, J. *et al., Org. Mass Spectrom.*, 1978, **13**, 618 (*ms*)
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Glycerol trialkanoates (diacid, symmetrical) G-243

Triacylglycerols (diacid, symmetrical)
$RCOOCH_2CH(OR')CH_2OOCR$
Meso-compds. For the unsymmetrical 1,2-R, 3-R′ isomers, see Glycerol trialkanoates (diacid, unsymmetrical), G-244. For triacid isomers 1R,2R′,3R″, see Glycerol trialkanoates (triacid), G-245. Monoacid triglycerides have individual entries, e.g. Glycerol trihexadecanoate, G-254. The average Western diet contains 100-160g triacylglycerols per day. Although about 100 fatty acids are associated with dietary triacylglyerols, the more important nutritional fatty acids are derived from a relatively small number of congeners, esp. hexanoyl, octanoyl and 9,12-octadecadienoyl. Widely used in food processing. Modified triacylglycerols are used for the production of zero-*trans* margarines and low-calorie fats. Structured medium-chain derivs. are used in diets where malabsorption prevents the utilisation of naturally-occurring long-chain triacylglycerols. Some short-chain derivs. are used as food flavours and as food formulation aids. Naturally occurring triacylglycerols are biosynthesised from a pool of five or more fatty acids, and derivs. with two or three different acyl groups are usually formed; symmetrical triacylglycerols are less often produced. The number of possible triacylglycerols increases rapidly with the number of different acids present in the fatty acid pool. With two acids, eight triacylglycerols (including enantiomers) are formed. The number of possible triacylglycerols that can be formed from 20 fatty acids, with all isomers distinguished (incl. optical isomers) is 8000.

Glycerol 1,3-didecanoate 2-dodecanoate
[60138-21-8]
Dodecanoic acid 1-[[(1-oxodecyl)oxy]methyl]-2-[(1-oxodecyl)oxy]ethyl ester. α,α′-Dicaprolaurin. β-Laurodidecoin
$C_{35}H_{66}O_6$ 582.903
Cryst. (EtOH). Mp 37.5°. Exhibits polymorphism.

Glycerol 1,3-didecanoate 2-tetradecanoate
α,α′-Dicapromyristin. Glycerol 2-tetradecanoate 1,3-didecanoate
$C_{37}H_{70}O_6$ 610.956
Cryst. (EtOH). Mp 34°. Exhibits polymorphism.

Glycerol 1,3-didecanoate 2-hexadecanoate
[93378-77-9]
α,α′-Dicapropalmitin
$C_{39}H_{74}O_6$ 639.01
Cryst. (EtOH). Mp 40°. Exhibits polymorphism.

Glycerol 1,3-didecanoate 2-octadecanoate
[139665-42-2]
α,α′-Dicaprostearin
$C_{41}H_{78}O_6$ 667.064
Cryst. (EtOH). Mp 44.5°. Exhibits polymorphism.

Glycerol 1,3-didecanoate 2-(9*Z*-octadecenoate) [22260-55-5]
α,α′-Dicaproolein
$C_{41}H_{76}O_6$ 665.048

Glycerol 1,3-didodecanoate 2-decanoate
[60138-22-9]
Dodecanoic acid 2-[(1-oxodecyl)oxy]-1,3-propanediyl ester, 9CI. α,α′-Dilaurocaprin. 2-Caprinyldilaurin. Glycerol 2-decanoate 1,3-didodecanoate
$C_{37}H_{70}O_6$ 610.956
Isol. from cocoa butter. Cryst. (C_6H_6). Mp 38.5°. Exhibits polymorphism (Lower Mp's reported 8°, 23°, 33°).

Glycerol 1,3-didodecanoate 2-tetradecanoate
[51464-76-7]
Tetradecanoic acid 2-[(1-oxododecyl)oxy]-1-[[(1-oxododecyl)oxy]methyl]ethyl ester. α,α′-Dilauromyristin
$C_{41}H_{78}O_6$ 667.064
Cryst. (EtOH). Mp 48°. Exhibits polymorphism.

Glycerol 1,3-didodecanoate 2-hexadecanoate
[93378-79-1]
α,α′-Dilauropalmitin
$C_{43}H_{82}O_6$ 695.117
Cryst. (EtOH). Mp 45.5°. Exhibits polymorphism.

Glycerol 1,3-didodecanoate 2-octadecanoate
[93378-74-6]
α,α′-Dilaurostearin
$C_{45}H_{86}O_6$ 723.171
Cryst. (EtOH). Mp 47°. Exhibits polymorphism.

Glycerol 1,3-didodecanoate 2-(9*Z*-octadecenoate) [51067-90-4]
α,α′-Dilauroolein
$C_{45}H_{84}O_6$ 721.155
Cryst. (petrol at -30°). Exhibits polymorphism.

Glycerol 1,3-ditetradecanoate 2-(2*E*,4*E*-hexadienoate) [7175-63-5]
Glycerol 2-(2E,4E-hexadienoate) 1,3-ditetradecanoate. 2-Sorbo-1,3-dimyristin
$C_{37}H_{66}O_6$ 606.925
Cryst. (MeOH). Mp 54-54.5°.

Glycerol 1,3-ditetradecanoate 2-decanoate
α,α′-Dimyristocaprin. Glycerol 2-decanoate 1,3-ditetradecanoate
$C_{41}H_{78}O_6$ 667.064
Cryst. (EtOH). Mp 43.5°. Exhibits polymorphism.

Glycerol 1,3-ditetradecanoate 2-dodecanoate
[60138-24-1]
Tetradecanoic acid 2-[(1-oxododecyl)oxy]-1,3-propanediyl ester. α,α′-Dimyristolaurin. Glycerol 2-dodecanoate 1,3-ditetradecanoate. β-Laurodimyristin
$C_{43}H_{82}O_6$ 695.117
Cryst. (EtOH). Mp 50°. Exhibits polymorphism.

Glycerol 1,3-ditetradecanoate 2-hexadecanoate [60138-26-3]

Hexadecanoic acid 1-[[(1-oxotetradecyl)oxy]methyl]-2-[(1-oxotetradecyl)oxy]ethyl ester. α,α′-Dimyristopalmitin. Glycerol 2-hexadecanoate 1,3-ditetradecanoate. β-Palmitodimyristin

$C_{47}H_{90}O_6$ 751.224
Cryst. (EtOH/C_6H_6). Mp 60°. Exhibits polymorphism.

Glycerol 1,3-ditetradecanoate 2-octadecanoate [93378-75-7]
α,α′-Dimyristostearin. Glycerol 2-octadecanoate 1,3-ditetradecanoate

$C_{49}H_{94}O_6$ 779.278
Cryst. (EtOH/C_6H_6). Mp 55.5°. Exibits polymorphism.

Glycerol 1,3-ditetradecanoate 2-(9*Z*-octadecenoate) [66908-04-1]
α,α′-Dimyristoolein. Glycerol 2-(9Z-octadecenoate) 1,3-ditetradecanoate

$C_{49}H_{92}O_6$ 777.262
Minor component of sunflower and other vegetable oils. Cryst. (EtOH/C_6H_6). Mp 28.5°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-hexanoate [56588-23-9]
Hexadecanoic acid 2-[(1-oxohexyl)oxy]-1,3-propanediyl ester. α,α′-Dipalmitocaproin

$C_{41}H_{78}O_6$ 667.064
Cryst. (EtOH/Et_2O). Mp 44.5° Mp 45.8°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-(2*E*,4*E*-hexadienoate) [65236-61-5]
Glycerol 1,3-dipalmitate 2-sorbate

$C_{41}H_{74}O_6$ 663.032
Cryst. Mp 62-62.5°.

Glycerol 1,3-dihexadecanoate 2-decanoate [67826-14-6]
Hexadecanoic acid 2-[(1-oxodecyl)oxy]-1,3-propanediyl ester. α,α′-Dipalmitocaprin. Glycerol 2-decanoate 1,3-dihexadecanoate

$C_{45}H_{86}O_6$ 723.171
Cryst. (EtOH). Mp 52°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-dodecanoate [56599-90-7]
Hexadecanoic acid 2-[(1-oxododecyl)oxy]-1,3-propanediyl ester. α,α′-Dipalmitolaurin. Glycerol 2-dodecanoate 1,3-dihexadecanoate

$C_{47}H_{90}O_6$ 751.224
Cryst. (EtOH/C_6H_6). Mp 53.5° Mp 55°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-tetradecanoate [56599-89-4]
Hexadecanoic acid 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester. α,α′-Dipalmitomyristin. β-Myristodipalmitin

$C_{49}H_{94}O_6$ 779.278
Cryst. (EtOH/C_6H_6). Mp 60°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-octadecanoate [2177-97-1]
Octadecanoic acid 2-[(1-oxohexadecyl)oxy]-1-[[(1-oxohexadecyl)oxy]methyl]ethyl ester. α,α′-Dipalmitostearin. β-Stearodipalmitin

$C_{53}H_{102}O_6$ 835.385
Cryst. (C_6H_6/EtOH). Mp 68°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-(9*E*-octadecenoate) [32221-51-5]
α,α′-Dipalmitoelaidin

$C_{53}H_{100}O_6$ 833.369
Cryst. (Me_2CO). Mp 56.5°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-(9*Z*-octadecenoate) [2190-25-2]

[28409-94-1]
α,α′-Dipalmitoolein. 2-Oleodipalmitin

$C_{53}H_{100}O_6$ 833.369
Constit. of cocoa butter. Cryst. (Me_2CO). Mp 37.2°. Exhibits polymorphism.

Glycerol 1,3-dihexadecanoate 2-(9*Z*,12*Z*-octadecadienoate) [2442-56-0]

[26836-30-6]
9,12-Octadecadienoic acid 2-[(1-oxohexadecyl)oxy]-1-[[(1-oxohexadecyl)oxy]methyl]ethyl ester. α,α′-Dipalmitolinolein

$C_{53}H_{98}O_6$ 831.354
Minor component of sunflower and other vegetable oils. Cryst. Mp 25.5-26°.

Glycerol 1,3-dihexadecanoate 2-docosanoate *α,α′-Dipalmitobehenin. Glycerol 2-docosanoate 1,3-dihexadecanoate*

$C_{57}H_{110}O_6$ 891.492
Cryst. (petrol/Et_2O). Mp 66.6°. Exhibits polymorphism.

Glycerol 1,3-dioctadecanoate 2-hexanoate [66411-62-9]
Octadecanoic acid 2-[(1-oxohexyl)oxy]-1,3-propanediyl ester. α,α′-Distearocaproin. Glycerol 2-hexanoate 1,3-dioctadecanoate

$C_{45}H_{86}O_6$ 723.171
Cryst. (EtOH/Et_2O). Mp 53°.

Glycerol 1,3-dioctadecanoate 2-decanoate [56968-93-5]
Octadecanoic acid 2-[(1-oxodecyl)oxy]-1,3-propanediyl ester. α,α′-Distearocaprin. Glycerol 2-decanoate 1,3-dioctadecanoate

$C_{49}H_{94}O_6$ 779.278
Cryst. (EtOH). Mp 57°. Exhibits polymorphism.

Glycerol 1,3-dioctadecanoate 2-dodecanoate [56183-45-0]
Octadecanoic acid 2-[(1-oxododecyl)oxy]-1,3-propanediyl ester. α,α′-Distearolaurin. Glycerol 2-dodecanoate 1,3-dioctadecanoate

$C_{51}H_{98}O_6$ 807.332
Cryst. (EtOH/C_6H_6). Mp 60.5°. Exhibits polymorphism.

Glycerol 1,3-dioctadecanoate 2-tetradecanoate [57396-99-3]
Octadecanoic acid 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester. α,α′-Distearomyristin

$C_{53}H_{102}O_6$ 835.385
Cryst. (C_6H_6/EtOH). Mp 62-63°. Exhibits polymorphism.

Glycerol 1,3-dioctadecanoate 2-hexadecanoate [2190-24-1]
Octadecanoic acid 2-[(1-oxohexadecyl)oxy]-1,3-propanediyl ester, 9CI. α,α′-Distearopalmitin. 2-Palmitodistearin. Glycerol 2-hexadecanoate 1,3-dioctadecanoate

$C_{55}H_{106}O_6$ 863.439
Isol. from cocoa butter. Cryst. (EtOH/petrol). Mp 68°. Exhibits polymorphism.

Glycerol 1,3-dioctadecanoate 2-(9*E*-octadecenoate)
α,α′-Distearoelaidin

$C_{57}H_{108}O_6$ 889.477
Cryst. (Me_2CO, petrol, Et_2O). Mp 59.5°. Exhibits polymorphism.

Glycerol 1,3-dioctadecanoate 2-(9*Z*-octadecenoate) [2846-04-0]
α,α′-Distearoolein. 2-Oleodistearin

$C_{57}H_{108}O_6$ 889.477
Present in oils of *Dipterocarpus* spp., *Allanblackia* spp. and others and cocoa butter. Cryst. (hexane). Mp 40.5-42.5°. Exhibits polymorphism.

Glycerol 1,3-dioctadecanoate 2-(9*Z*,12*Z*-octadecadienoate) [2190-13-8]
9,12-Octadecadienoic acid 2-[(1-oxooctadecyl)oxy]-1-[[(1-oxooctadecyl)oxy]methyl]ethyl ester. α,α′-Distearolinolein. Glycerol 2-(9Z,12Z-octadecadienoate) 1,3-dioctadecanoate

$C_{57}H_{106}O_6$ 887.461
Cryst. Mp 36.3-37°.

Glycerol 1,3-di-(9*E*-octadecenoate) 2-hexadecanoate
α,α′-Dielaidopalmitin

$C_{55}H_{102}O_6$ 859.407
Cryst. Mp 44.5°. Exhibits polymorphism.

Glycerol 1,3-di-(9*Z*-octadecenoate) 2-hexadecanoate [151911-06-7]

[1716-07-0, 27071-84-7]
α,α′-Dioleopalmitin

$C_{55}H_{102}O_6$ 859.407
Minor component of sunflower oil and other vegetable oils. Oil. Mp 5-6° Mp 19°. Exhibits polymorphism.

Glycerol 1,3-di-(9*E*-octadecenoate) 2-octadecanoate [107242-02-4]
α,α′-Dielaidostearin. Glycerol 2-octadecanoate 1,3-di-(9E-octadecenoate)

$C_{57}H_{106}O_6$ 887.461
Cryst. (Me_2CO). Mp 50.1°. Exhibits polymorphism.

Glycerol 1,3-di-(9*Z*-octadecenoate) 2-octadecanoate [29590-02-1]

[2410-29-9]
α,α′-Dioleostearin. Glycerol 2-octadecanoate 1,3-di-(9Z-octadecenoate)

$C_{57}H_{106}O_6$ 887.461
Minor component of sunflower and other vegetable oils. Cryst. (Et_2O). Mp 10.5-12.5° (14-15°). Exhibits polymorphism.

Glycerol 1,3-di-(9*Z*-octadecenoate) 2-(9*Z*,12*Z*-octadecadienoate) [2190-19-4]

[79517-08-1, 83148-24-7]
9,12-Octadecadienoic acid 2-[(1-oxo-9-octadecenyl)oxy]-1-[[(1-oxo-9-octadecenyl)oxy]methyl]ethyl ester. α,α′-Dioleolinolein. Glycerol 2-(9Z,12Z-octadecadienoate) 1,3-di-(9Z-octadecenoate)

$C_{57}H_{102}O_6$ 883.429
Minor component of sunflower and other vegetable oils.

Glycerol 1,3-di-(9*Z*,12*Z*-octadecadienoate)

2-hexadecanoate [2190-16-1]
9,12-Octadecadienoic acid 2-[(1-oxohexadecyl)oxy]-1,3-propanediyl ester. α,α′-Dilinoleopalmitin. Berulide. Glycerol 2-hexadecanoate 1,3-di-(9Z,12Z-octadecadienoate)

$C_{55}H_{98}O_6$ 855.376
Minor component of sunflower and other vegetable oils. Oil. Mp -3°.

Glycerol 1,3-di-(9*Z*,12*Z*-octadecadienoate) 2-octadecanoate [2190-18-3]
9,12-Octadecadienoic acid 2-[(1-oxooctadecyl)oxy]-1,3-propanediyl ester. α,α′-Dilinoleostearin

$C_{57}H_{102}O_6$ 883.429
Minor component of sunflower and other vegetable oils. Oil.

Glycerol 1,3-di-(9*Z*,12*Z*-octadecadienoate) 2-(9*Z*-octadecenoate) [2190-22-9]
9,12-Octadecadienoic acid 2-[(1-oxo-9-octadecenyl)oxy]-1,3-propanediyl ester. α,α′-Dilinoleoolein

$C_{57}H_{100}O_6$ 881.413
Minor component of sunflower and other vegetable oils. Mp -40°.

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Glycerol trialkanoates (diacid, unsymmetrical) G-244

Triacyglycerols (diacid, unsymmetrical). Unsymmetrical diacid triglcerides
$ROOCCH_2CH(OR)CH_2COOR'$
Chiral molecules. Cahn-Ingold-Prelog config. depends on the priorities of R and R′. For other triglycerides see Glycerol trialkanoates (diacid, symmetrical), G-243 and Glycerol trialkanoates (triacid), G-245 plus individual entries for the monoacid triglycerides. The average Western diet contains 100-160g triacylglycerols per day. Although about 100 fatty acids are associated with dietary triacylglycerols, the more important nutritional fatty acids are derived from a relatively small number of congeners, esp. hexenoyl, octanoyl and 9,12-octadecadienoyl. Widely used in food processing. Modified triacylglycerols are used for the production of zero-*trans* margarines and low calorie fats. Structured medium-chain derivs. are used in diets where malabsorption prevents the utilisation of naturally-occurring long-chain triacylglycerols. Some short-chain derivs. are used as food flavours and as food formulation aids. Naturally occurring triacylglycerols are biosynthesised from a pool of five or more fatty acids, and derivs. with two or three different acyl groups are usually formed; symmetrical triacylglycerols are less often produced. The number of possible triacylglycerols increases rapidly with the number of different acids present in the fatty acid pool. With two acids, eight triacylglycerols (including enantiomers) are formed. The number of possible triacylglycerols that can be formed from 20 fatty acids, with all isomers distinguished (incl. optical isomers) is 8000.

Glycerol 1,2-diacetate 3-octadecanoate [33599-07-4]

[57416-08-7, 60485-62-3, 60562-71-2]
Octadecanoic acid 2,3-bis(acetyloxy)propyl ester. α,β-Diacetostearin. 1,2-Diacetyl-3-stearoylglycerol

$C_{25}H_{46}O_6$ 442.635
Cryst. Mp 39-40° (*R*-form) Mp 48° (racemate). $[\alpha]_{300}^{25}$ +102 (C_6H_6). Exhibits polymorphism.

Glycerol 1,2-didecanoate 3-dodecanoate [60138-10-5]
Dodecanoic acid 2,3-bis[(1-oxodecyl)oxy]propyl ester. α,β-Dicaprolaurin

$C_{35}H_{66}O_6$ 582.903
Cryst. (C_6H_6). Mp 30° (racemate). Exhibits polymorphism.

Glycerol 1,2-didecanoate 3-tetradecanoate [62833-19-6]

[57416-11-2]
Tetradecanoic acid 2,3-bis[(1-oxodecyl)oxy]propyl ester. α,β-Dicapromyristin. 1,2-Didecanoyl-3-tetradecanoylglycerol

$C_{37}H_{70}O_6$ 610.956
Cryst. Mp 26-26.5° (*R*-form) Mp 34.5° (racemate). $[\alpha]_{300}^{27}$ +17.7 (C_6H_6). Exhibits polymorphism.

Glycerol 1,2-didecanoate 3-hexadecanoate [93378-76-8]

[158070-08-7]
α,β-Dicapropalmitin

$C_{39}H_{74}O_6$ 639.01
Mp 35° (racemate). Exhibits polymorphism.

Glycerol 1,2-didodecanoate 3-octanoate
α,β-Dilaurocaprylin

$C_{35}H_{66}O_6$ 582.903
Cryst. (EtOH/Me_2CO). Mp 28.5° (racemate).

Glycerol 1,2-didodecanoate 3-decanoate [60138-11-6]
Dodecanoic acid 1-[[(1-oxodecyl)oxy]methyl]-1,2-ethanediyl ester. α,β′-Dilaurocaprin. Glycerol 1-decanoate 2,3-didodecanoate

$C_{37}H_{70}O_6$ 610.956
Cryst. (C_6H_6). Mp 35.5° (racemate). Exhibits polymorphism.

Glycerol 1,2-didodecanoate 3-tetradecanoate [60175-30-6]

[57416-12-3, 65376-23-0]
Tetradecanoic acid 2,3-bis[(1-oxododecyl)oxy]propyl ester. α,β-Dilauromyristin. 1-Myristodilaurin. 1,2-Dilauroyl-3-myristoylglycerol

$C_{41}H_{78}O_6$ 667.064
Isol. from lipids of *Attalea speciosa* (babassu). Cryst. Mp 39.5-40° (*R*-form) Mp 19° (racemate) Mp 33.5° (racemate) Mp 39° (racemate) Mp 43.5° (racemate). $[\alpha]_{300}^{27}$ +5.4 (C_6H_6). Exhibits polymorphism.

Glycerol 1,2-didodecanoate 3-hexadecanoate [25708-03-6]

[57416-16-7]
Hexadecanoic acid 2,3-bis[(1-oxododecyl)oxy]propyl ester. α,β-Dilauropalmitin. 1,2-Dilauroyl-3-palmitoylglycerol

$C_{43}H_{82}O_6$ 695.117
Cryst. Mp 42.5-43° (*R*-form) Mp 46.5° (racemate). $[\alpha]_D^{27}$ +13.9 (C_6H_6). Exhibits polymorphism.

Glycerol 1,2-didodecanoate 3-octadecanoate [35405-56-2]

[57416-17-8]
Octadecanoic acid 2,3-bis[(1-oxododecyl)oxy]propyl ester. α,β-Dilaurostearin. 1,2-Dilauroyl-3-stearoylglycerol

$C_{45}H_{86}O_6$ 723.171
Cryst. Mp 43.5-44.5° (*R*-form) Mp 45° (racemate). $[\alpha]_{300}^{27}$ +13 (*R*-form). Exhibits polymorphism.

Glycerol 1,2-didodecanoate 3-(9*E*-octadecenoate)
α,β-Dilauroelaidin. 1,2-Dilauroyl-3-elaidylglycerol. 1-Elaidyl-2,3-dilauroylglycerol
Cryst. (EtOH). Mp 27° (racemate).

Glycerol 1,2-didodecanoate 3-(9*Z*-octadecenoate) [158112-13-1]

[20299-66-5, 67254-18-6]
1,2-Dilauroyl-3-oleoylglycerol. α,β-Dilauroolein

$C_{45}H_{84}O_6$ 721.155
Oil (*R*-form), cryst (Et_2O)(racemate). Mp 16° (racemate) Mp 20° (racemate). $[\alpha]_{300}$ +32.4 (C_6H_6) (*R*-form). Exhibits polymorphism.

Glycerol 1,2-ditetradecanoate 3-decanoate [60138-16-1]
Tetradecanoic acid 1-[[(1-oxodecyl)oxy]methyl]-1,2-ethanediyl ester. α,β-Dimyristocaprin

$C_{41}H_{78}O_6$ 667.064
Cryst. Mp 43.5° (racemate). Exhibits polymorphism.

Glycerol 1,2-ditetradecanoate 3-dodecanoate [60138-12-7]
Tetradecanoic acid 1-[[(1-oxododecyl)oxy]methyl]-1,2-ethanediyl ester. α,β-Dimyristolaurin. Laurodimyristin. Glycerol 1-dodecanoate 2,3-ditetradecanoate. Glycerol 1,2-dimyristate 3-palmitate

$C_{43}H_{82}O_6$ 695.117
Cryst (C_6H_6). Mp 46.5° (racemate) Mp 48.5° (racemate). Exhibits polymorphism.

Glycerol 1,2-ditetradecanoate 3-hexadecanoate [60138-13-8]
Hexadecanoic acid 2,3-bis[(1-oxotetradecyl)oxy]propyl ester. α,β-Dimyristopalmitin. Glycerol 1-hexadecanoate 2,3-tetradecanoate. Glycerol 1,2-dimyristate 3-palmitate

$C_{47}H_{90}O_6$ 751.224
Cryst. (Me_2CO or EtOH/Et_2O). Mp 54° (racemate). Exhibits polymorphism.

Glycerol 1,2-ditetradecanoate 3-octadecanoate [56846-96-9]
α,β-Dimyristostearin

$C_{49}H_{94}O_6$ 779.278
Cryst. (EtOH/C_6H_6). Mp 56° (racemate). Exhibits polymorphism.

Glycerol 1,2-dihexadecanoate 3-decanoate [93378-78-0]
α,β-Dipalmitocaproin. Glycerol 1-decanoate 2,3-dihexadecanoate

$C_{45}H_{86}O_6$ 723.171
Cryst. (EtOH/C_6H_6). Mp 45.5° (racemate). Exhibits polymorphism.

Glycerol 1,2-dihexadecanoate 3-dodecanoate
Hexadecanoic acid 1-[[(1-oxododecyl)oxy]methyl]-1,2-ethanediyl ester. α,β-Dipalmitolaurin. Glycerol 1-dodecanoate 2,3-dihexadecanoate. 1-Lauroyl-2,3-dipalmitoylglycerol

$C_{47}H_{90}O_6$ 751.224
Cryst. Mp 53.6-53.9° (*S*-form) Mp 54° (racemate). $[\alpha]_D$ -0.07 (C_6H_6) (*S*-form).

Glycerol 1,2-dihexadecanoate 3-octadecanoate [2177-98-2]

[5281-84-5, 5568-22-9, 65376-21-8]
Octadecanoic acid 2,3-bis[(1-oxohexadecyl)oxy]propyl ester. 1,2-Dipalmitoyl-3-stearoylglycerol. α,β-Dipalmitostearin

$C_{53}H_{102}O_6$ 835.385
Cryst. Mp 58° (*S*-form) Mp 62.5-63.5° (racemate). Exhibits polymorphism.

Glycerol 1,2-dihexadecanoate 3-(9*E*-octadecenoate)
α,β-Dipalmitoelaidin
Cryst. Mp 51.7° (racemate).

Glycerol 1,2-dihexadecanoate 3-(9*Z*-octadecenoate) [37179-82-1]

[28409-94-1, 53023-10-2, 53023-11-3]
α,β-Dipalmitoolein. 2,3-Dipalmito-1-olein. 3-Oleo-1,2-dipalmitin. 1-Oleoyl-2,3-dipalitoylglycerol
Found in palm oil and other vegetable oils. Cryst. (Et_2O). Mp 37° (*R*- or *S*-form) Mp 34.5° (racemate). $[\alpha]_D$ 0 (*R*- or *S*- form). n_D^{40} 1.4556.

Glycerol 1,2-dihexadecanoate 3-(6*Z*,9*Z*-octadecadienoate)
$C_{53}H_{98}O_6$ 831.354
Abs. config. of nat. prod. not determined.

Glycerol 1,2-dihexadecanoate 3-(9*Z*,12*Z*-octadecadienoate) [2535-35-5]

[26836-30-6, 84234-82-2, 102491-55-4]
9,12-Octadecadienoic acid 2,3-bis[(1-oxohexadecyl)oxy]propyl ester. α,β-Dipalmitolinolein

$C_{53}H_{98}O_6$ 831.354
Minor component of sunflower oil and other vegetable oils. Cryst. Mp 36.5-38°.

Glycerol 1,2-dihexadecanoate 3-(8*Z*,11*Z*-eicosadienoate)
$C_{55}H_{102}O_6$ 859.407
Abs. config. of nat. prod. not determined.

Glycerol 1,2-dioctadecanoate 3-acetate [13382-52-0]

[20236-49-1, 60562-72-3]
Octadecanoic acid 1-[(acetyloxy)methyl]-1,2-ethanediyl ester. α,β-Distearoacetin. 1-Acetyl-2,3-distearoylglycerol. Glycerol 1-acetate 2,3-dioctadecanoate

$C_{41}H_{78}O_6$ 667.064
Cryst, (Me_2CO). Mp 53° (49°)(*S*-form). $[\alpha]_{300}^{27}$ -400 (C_6H_6).

Glycerol 1,2-dioctadecanoate 3-propanoate [144979-56-6]

[60456-30-6, 60562-73-4]
Octadecanoic acid 1-[(1-oxopropoxy)-methyl]-1,2-ethanediyl ester. α,β-Distearopropionin. 1-Propionyl-2,3-distearoylglycerol

$C_{42}H_{80}O_6$ 681.09
Cryst. (Me_2CO). Mp 48° (*S*-form).

Glycerol 1,2-dioctadecanoate 3-butanoate [139665-43-3]

[60456-31-7, 60562-74-5]
Octadecanoic acid 1-[(1-oxobutoxy)-methyl]-1,2-ethanediyl ester. α,β-Distearobutyrin. Glycerol 1-butanoate 2,3-dioctadecanoate. 1-Butyryl-2,3-distearoylglycerol

$C_{43}H_{82}O_6$ 695.117
Cryst. Mp 49° (*S*-form).

Glycerol 1,2-dioctadecanoate 3-dodecanoate [35405-55-1]
Octadecanoic acid 3-[(1-oxododecyl)oxy]-1,2-propanediyl ester. α,β-Distearolaurin. Glycerol 1-dodecanoate 2,3-dioctadecanoate

$C_{51}H_{98}O_6$ 807.332
Cryst. (EtOH/C_6H_6). Mp 52°. Exibits polymorphism.

Glycerol 1,2-dioctadecanoate 3-tetradecanoate

[57416-14-5, 60138-19-4]
Octadecanoic acid 1-[[(1-oxotetradecyl)oxy]methyl]-1,2-ethanediyl ester. 1-Myristoyl-2,3-distearoylglycerol. 1,2-Distearoyl-3-myristoylglycerol. α,β-Distearomyristin

$C_{53}H_{102}O_6$ 835.385
Cryst. Mp 60-61° (*S*-form) Mp 62° (racemate). $[\alpha]_{300}^{27}$ -11.7 (C6 H6). Exhibits polymorphism.

Glycerol 1,2-dioctadecanoate 3-hexadecanoate [2177-99-3]

[5281-50-5, 5281-85-6]
Octadecanoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester. α,β-Distearopalmitin. 1-Palmitoyl-2,3-distearoylglycerol. Glycerol 1-hexadecanoate 2,3-dioctadecanoate

$C_{55}H_{106}O_6$ 863.439
Cryst. Mp 61° (*S*-form) Mp 65.2° (racemate). Exhibits polymorphism.

Glycerol 1,2-dioctadecanoate 3-(9*Z*-octadecenoate) [28880-75-3]

[51195-71-2]
9-Octadecenoic acid 2,3-bis[(1-oxooctadecyl)oxy]propyl ester. 1-Oleodistearin. 1,2-Distearoyl-3-oleoylglycerol. 1-Oleoyl-2,3-distearoylglycerol. α,β-Distearoolein

$C_{57}H_{108}O_6$ 889.477
Isol. from cocoa butter. Cryst. Mp 45-46° (*R*-form) Mp 42.1° (racemate). $[\alpha]_{300}$ +30.2 (C_6H_6) (*R*-form). Exhibits polymorphism.

Glycerol 1,2-dioctadecanoate 3-(9*Z*,12*Z*-octadecadienoate) [2442-53-7]
9,12-Octadecadienoic acid 2,3-bis[(1-oxooctadecyl)oxy]propyl ester. Glycerol 1-(9Z,12Z-octadecadienoate) 2,3-dioctadecanoate

$C_{57}H_{106}O_6$ 887.461
Cryst. Mp 39.5-40.8° (racemate).

Glycerol 1,2-dioctadecanoate 3-docosanoate [38280-88-5]
Docosanoic acid 2,3-bis[(1-oxooctadecyl)oxy]propyl ester. α,β-Distearobehenin. Glycerol 1-docosanoate 2,3-dioctadecanoate

$C_{61}H_{118}O_6$ 947.6
Cryst. (hexane/Me_2CO)(racemate). Mp 49° (racemate) Mp 75.5° (racemate).

Glycerol 1,2-di-(9*E*-octadecenoate) 3-dodecanoate [51067-89-1]

[95672-17-6, 95672-19-8]
α,β-Dielaidolaurin. Glycerol 1-dodecanoate 2,3-di-(9E-octadecenoate)
Cryst. (EtOH). Mp 35.5° (racemate).

Glycerol 1,2-di-(9*E*-octadecenoate) 3-tetradecanoate
α,β-Dielaidomyristin
$C_{53}H_{98}O_6$ 831.354
Cryst. (petrol or EtOH)(racemate). Mp 40° (racemate).

Glycerol 1,2-di-(9*Z*-octadecenoate) 3-tetradecanoate [35804-98-9]
α,β-Dioleomyristin
Minor component of palm oil and other vegetable oils. Cryst. (Et_2O at -20°)(ra-

cemate). Mp 12-13° (racemate).

Glycerol 1,2-di-(9*E*-octadecenoate) 3-hexadecanoate [68069-77-2]
*α,β-Dielaidopalmitin. Glycerol 1-hexadecanoate 2,3-di-(9*E*-octadecenoate)*
Cryst. Mp 40.3° Mp 46°. Exhibits polymorphism.

Glycerol 1,2-di-(9*E*-octadecenoate) 3-octadecanoate
*α,β-Dielaidostearin. Glycerol 1-octadecanoate 2,3-di-(9*E*-octadecenoate). 1,2-Dielaidoyl-3-stearoylglycerol*
Cryst. (Me_2CO). Mp 49.9°. Exhibits polymorphism.

Glycerol 1,2-di-(9*Z*-octadecenoate) 3-dodecanoate [4016-52-8]

[95672-17-6, 95672-19-8]
α,β-Dioleolaurin. Glycerol 1-dodecanoate 2,3-di-(9Z-octadecenoate)
Oil, cryst. (Et_2O at -20°). Mp 5-6° (racemate).

Glycerol 2,3-di-(9*Z*-octadecenoate) 1-hexadecanoate [14960-35-1]

[27071-84-7]
sn-*Glyceryl 1,2-dioleate 3-palmitate. Glycerol 1-hexadecanoate 2,3-di-(9Z-octadecenoate). 1-Palmitodiolein. α,β-Dioleopalmitin*
Isol. from cocoa butter, olive oil and palm oil. Oil. Mp 18.5-19° (*S*-form). $[\alpha]_{300}$ -28.3 (C_6H_6) (*S*-form).

Glycerol 1,2-di-(9*Z*-octadecenoate) 3-octadecanoate [2410-28-8]

[29590-02-1]
*α,β-Dioleostearin. Glycerol 1-octadecanoate 2,3-di-(9*E*-octadecenoate). 1,2-Dioleoyl-3-octadecanoylglycerol*
Minor component of sunflower oil and other vegetable oils. Cryst. Mp 22.5-23.5°. Exhibits polymorphism.

Glycerol 1,2-di-(9*Z*-octadecenoate) 3-(9*Z*,12*Z*-octadecadienoate) [2190-20-7]

[28880-78-6]
Glycerol 1-(9Z,12Z-octadecadienoate) 2,3-di-(9Z-octadecenoate). α,β-Dioleolinolein

$C_{57}H_{102}O_6$ 883.429
No phys. props. reported.

Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-dodecanoate [145135-15-5]
9,12-Octadecadienoic acid 1-[[(1-oxododecyl)oxy]methyl]-1,2-ethanediyl ester. Glycerol 1-dodecanoate 2,3-di-(9Z,12Z-octadecadienoate). α,β-Dilinoleolaurin

$C_{51}H_{90}O_6$ 799.268
Oil. Mp -12° (racemate).

Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-tetradecanoate [119963-42-7]
α,β-Dilinoleomyristin

$C_{53}H_{94}O_6$ 827.322
Oil. Mp -9° (racemate).

Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-hexadecanoate [26836-36-2]

[2190-15-0, 64550-34-1, 66964-28-1]
9,12-Octadecadienoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester. Glycerol 1-hexadecanoate 2,3-di-(9Z,12Z-octadecadienoate). α,β-Dilinoleopalmitin

$C_{55}H_{98}O_6$ 855.376
Minor component of sunflower oil and other vegetable oils. Oil. Mp -4° (racemate).

Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-octadecanoate [2190-17-2]
α,β-Dilinoleostearin. Glycerol 1-octadecanoate 2,3-di-(9Z,12Z-octadecadienoate)

$C_{57}H_{102}O_6$ 883.429
Minor component of sunflower oil and other vegetable oils. Oil (racemate).

Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-(9*Z*-octadecenoate) [28409-91-8]

[2190-21-8, 64550-35-2, 66964-27-0, 145986-52-3]
9,12-Octadecadienoic acid 1-[[(1-oxo-9-octadecenyl)oxy]methyl]-1,2-ethanediyl ester. 1,2-Dilinoleoyl-3-oleoylglycerol. α,β-Dilinoleoolein

$C_{57}H_{100}O_6$ 881.413
Minor component of sunflower oil and other vegetable oils. Oil. Mp -14° (racemate). $[\alpha]_{300}$ 0 (*S*-form).

Glycerol 1,2-di-(9*Z*,11*E*,13*Z*-octadecatrienoate) 3-(8*Z*,11*Z*,13*E*-octadecatrienoate) [189164-13-4]

$C_{57}H_{92}O_6$ 873.35
Constit. of the seeds of *Punica granatum* (pomegranate). Abs. config. not determined.

Glycerol 1,2-didocosanoate 3-octadecanoate
α,β-Dibehenostearin

$C_{65}H_{126}O_6$ 1003.707
Crys. (Et_2O/petrol). Mp 73.5° (racemate). Exhibits polymorphism.

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Glycerol trialkanoates (triacid) G-245

Triacylglycerols (triacid). Triacid triglycerides

$ROOCCH_2CH(OR')CH_2COOR''$

Chiral molecules, Cahn-Ingold-Prelog notation depends on the relative priorities of R and R''. Most data refers to racemates. For other triglycerides, see Glycerol trialkanoates (diacid, symmetrical), G-243, Glycerol trialkanoates (diacid, unsymmetrical), G-244 and individual entries for the monoacid triglycerides. The average Western diet contains 100-160g triacylglycerols per day. Although about 100 fatty acids are associated with dietary triacylglyerols, the more important nutritional fatty acids are derived from a relatively small number of congeners, esp. hexanoyl, octanoyl and 9,12-octadecadienoyl. Widely used in food processing. Modified triacylglycerols are used for the production of zero-*trans* margarines and low-calorie fats. Structured medium-chain derivs. are used in diets where malabsorption prevents the utilisation of naturally-occurring long-chain triacylglycerols. Some short-chain derivs. are used as food flavours and as food formulation aids. Naturally occurring triacylglycerols are biosynthesised from a pool of five or more fatty acids, and derivs. with two or three different acyl groups are usually formed; symmetrical triacylglycerols are less often produced. The number of possible triacylglycerols increases rapidly with the number of different acids present in the fatty acid pool. With two acids, eight triacylglycerols (including enantiomers) are formed. The number of possible triacylglycerols that can be formed from 20 fatty acids, with all isomers distinguished (incl. optical isomers) is 8000.

Glycerol 1-dodecanoate 2-tetradecanoate 3-octanoate
2-Myristocaprylolaurin. α-Caprylo-β-myristo-α'-laurin. Glycerol 1-dodecanoate 3-octanoate 2-tetradecanoate

$C_{37}H_{70}O_6$ 610.956
Isol. from coconut oil. Cryst. Mp 14.1°.

Glycerol 1-hexadecanoate 2-tetradecanoate 3-dodecanoate [60138-25-2]

[90827-55-7]
Hexadecanoic acid 3-[(1-oxododecy-

l)oxy]-2-[(1-oxotetradecyl)oxy]propyl ester. α-Palmito-β-myristolaurin. Glycerol 1-dodecanoate 3-hexadecanoate 2-tetradecanoate

$C_{45}H_{86}O_6$ 723.171
Cryst. (Me_2CO). Mp 49° (racemate). Exhibits polymorphism.

Glycerol 1-hexadecanoate 2-octadecanoate 3-tetradecanoate [55256-01-4]
Octadecanoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-2-[(1-oxotetradecyl)oxy]ethyl ester. α-Palmito-β-stearomyristin

$C_{51}H_{98}O_6$ 807.332
Cryst. ($EtOH/C_6H_6$). Mp 58.5-59° (racemate).

Glycerol 1-octadecanoate 2-butanoate 3-hexadecanoate
Octadecanoic acid 2-(1-oxobutoxy)-3-[(1-oxohexadecyl)oxy]propyl ester. α-Stearo-β-butyropalmitin. 2-Butyryl-1-palmitoyl-3-stearoylglycerol. Glycerol 2-butanoate 1-hexadecanoate 3-octadecanoate

$C_{41}H_{78}O_6$ 667.064
Cryst. Mp 49° (*S*-form) Mp 45.5-46° (racemate).

Glycerol 1-octadecanoate 2-decanoate 3-dodecanoate
α-Stearo-β-caprolaurin. Glycerol 2-decanoate 1-dodecanoate 3-octadecanoate

$C_{43}H_{82}O_6$ 695.117
Cryst. (Me_2CO). Mp 41.8°. Exhibits polymorphism.

Glycerol 1-octadecanoate 2-decanoate 3-tetradecanoate
α-Stearo-β-capromyristin. Glycerol 2-decanoate 1-octadecanoate 3-tetradecanoate

$C_{45}H_{86}O_6$ 723.171
Cryst. (Me_2CO). Mp 52.5° (racemate). Exhibits polymorphism.

Glycerol 1-octadecanoate 2-decanoate 3-hexadecanoate
α-Stearo-β-capropalmitin. Glycerol 2-decanoate 1-hexadecanoate 3-octadecanoate

$C_{47}H_{90}O_6$ 751.224
Cryst. (Me_2CO). Mp 55° (racemate). Exhibits polymorphism.

Glycerol 1-octadecanoate 2-dodecanoate 3-tetradecanoate
α-Stearo-β-lauromyristin. Glycerol 2-dodecanoate 1-octadecanoate 3-tetradecanoate

$C_{47}H_{90}O_6$ 751.224
Cryst. (Me_2CO). Mp 55° (racemate). Exhibits polymorphism.

Glycerol 1-octadecanoate 2-dodecanoate 3-hexadecanoate
α-Stearo-β-lauropalmitin. Glycerol 2-dodecanoate 1-hexadecanoate 3-octadecanoate

$C_{49}H_{94}O_6$ 779.278
Cryst. Mp 57.5° (racemate). Exhibits polymorphism.

Glycerol 1-octadecanoate 2-tetradecanoate 3-dodecanoate [66907-98-0]
α-Stearo-β-myristolaurin. Glycerol 1-dodecanoate 3-octadecanoate 2-tetradecanoate

$C_{47}H_{90}O_6$ 751.224
Cryst. (Me_2CO). Mp 49.5° (racemate). Exhibits polymorphism.

Glycerol 1-octadecanoate 2-tetradecanoate 3-hexadecanoate [56554-26-8]
Octadecanoic acid 3-[(1-oxohexadecyl)oxy]-2-[(1-oxotetradecyl)oxy]propyl ester. α-Stearo-β-myristopalmitin. Glycerol 1-hexadecanoate 3-octadecanoate 2-tetradecanoate

$C_{51}H_{98}O_6$ 807.332
Cryst. (Me_2CO). Mp 59.5°. Exhibits polymorphism.

Glycerol 1-octadecanoate 2-hexadecanoate 3-butanoate
[60456-33-9, 62833-21-0]
Octadecanoic acid 3-(1-oxobutoxy)-2-[(1-oxohexadecyl)oxy]propyl ester. α-Stearo-β-palmitobutyrin. 1-Butyryl-2-palmitoyl-3-stearoylglycerol. Glycerol 1-butanoate 2-hexadecanoate 3-octadecanoate

$C_{41}H_{78}O_6$ 667.064
Cryst. Mp 49° (*S*-form) Mp 47.5-48° (racemate).

Glycerol 1-octadecanoate 2-hexadecanoate 3-dodecanoate
α-Stearo-β-palmitolaurin. Glycerol 1-dodecanoate 2-hexadecanoate 3-octadecanoate

$C_{49}H_{94}O_6$ 779.278
Cryst. (Me_2CO). Mp 52° (racemate). Exhibits polymorphism.

Glycerol 1-octadecanoate 2-hexadecanoate 3-tetradecanoate [60138-20-7]
Octadecanoic acid 2-[(1-oxohexadecyl)oxy]-3-[(1-oxotetradecyl)oxy]propyl ester. α-Stearo-β-palmitomyristin. Glycerol 2-hexadecanoate 1-octadecanoate 3-tetradecanoate

$C_{51}H_{98}O_6$ 807.332
Cryst. (Me_2CO). Mp 56°. Exhibits polymorphism.

Glycerol 1-octadecanoate 2-(9*Z*-octadecenoate) 3-hexadecanoate [2190-27-4]

[26836-31-7]
9-Octadecenoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-2-[(1-oxooctadecyl)oxy]ethyl ester. α-Stearo-β-oleopalmitin. Glycerol 1-hexadecanoate 3-octadecanoate 2-(9Z-octadecenoate)

$C_{55}H_{104}O_6$ 861.423
Constit. of cocoa butter and confectionery fats. Derived from palm oil. Coating agent. Cryst. (Me_2CO). Mp 32-33° (racemate) Mp 37-38° (racemate). Exhibits polymorphism.

Glycerol 1-octadecanoate 2-(9*Z*,12*Z*-octadecadienoate) 3-hexadecanoate [2190-12-7]
9,12-Octadecadienoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-2-[[(1-oxooctadecyl)oxy]ethyl] ester. α-Stearo-β-linoleopalmitin. Glycerol 1-hexadecanoate 2-(9Z,12Z-octadecadienoate) 3-octadecanoate

$C_{55}H_{102}O_6$ 859.407

Glycerol 1-(9*E*-octadecenoate) 2-octadecanoate 3-(9*Z*-octadecenoate) [30465-28-2]
α-Elaido-α′-oleostearin. Glycerol 2-octadecanoate 1-(9E-octadecenoate) 3-(9Z-octadecenoate)

$C_{57}H_{106}O_6$ 887.461
Cryst. Mp 26-28°.

Glycerol 1-(9*E*-octadecenoate) 2-(9*Z*-octadecenoate) 3-octadecanoate [35219-91-1]
α-Oleo-β-elaidostearin. Glycerol 1-octadecanoate 3-(9E-octadecenoate) 2-(9Z-octadecenoate)

$C_{57}H_{106}O_6$ 887.461
Cryst. Mp 27-28.5° (racemate).

Glycerol 1-(9*Z*-octadecenoate) 2-octanoate 3-tetradecanoate
2-Caprylooleomyristin. α-Oleo-β-caprylo-α′-myristin. Glycerol 2-octanoate 1-(9Z-octadecenoate) 3-tetradecanoate

$C_{43}H_{80}O_6$ 693.101
Isol. from palm kernel oil. Cryst. Mp 14.8°.

Glycerol 1-(9Z-octadecenoate) 2-hexadecanoate 3-dodecanoate [120932-38-9]
α-Oleao-β-palmitolaurin. Glycerol 1-dodecanoate 2-hexadecanoate 3-(9Z-octadecenoate)

$C_{49}H_{92}O_6$ 777.262
Crys. (Me_2CO/petrol). Mp 29.5° (racemate).

Glycerol 1-(9*Z*-octadecenoate) 2-hexadecanoate 3-octadecanoate [59891-29-1]

[26836-31-7]
9-Octadecenoic acid 2-[(1-oxohexadecyl)oxy]-3-[(1-oxooctadecyl)oxy]propyl ester, 9CI. α-Oleo-β-palmitostearin. Glycerol 2-hexadecanoate 1-octadecanoate 3-(9Z-octadecenoate)

$C_{55}H_{104}O_6$ 861.423
Isol. from cocoa butter. Cryst. Mp 40-41° (racemate).

Glycerol 1-(9*Z*-octadecenoate) 2-octadecanoate 3-hexadecanoate [2190-28-5]

[26836-31-7]
9-Octadecenoic acid 3-[(1-oxohexadecyl)oxy]-2-[(1-oxooctadecyl)oxy]propyl ester. α-Oleo-β-stearopalmitin. Glycerol 1-hexadecanoate 2-octadecanoate 3-(9Z-octadecenoate)

$C_{55}H_{104}O_6$ 861.423
Cryst. Mp 41-41.5° (racemate). Exhibits polymorphism.

Glycerol 1-(9*Z*-octadecenoate) 2-(9*E*-octadecenoate) 3-octadecanoate [30465-26-0]
α-Elaido-β-oleostearin. Glycerol 1-octadecanoate 2-(9E-octadecenoate) 3-(9Z-octadecenoate)

$C_{57}H_{106}O_6$ 887.461
Cryst. Mp 29-31° (racemate).

Glycerol 1-(9*Z*-octadecenoate) 2-(9*Z*,12*Z*-octadecadienoate) 3-hexadecanoate [2579-00-2]

[26836-35-1]
9,12-Octadecadienoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-2-[(1-oxo-9-octadecenyl)oxy]ethyl ester. α-Oleo-β-linoleopalmitin. Glycerol 1-hexadecanoate 2-(9Z,12Z-octadecadienoate) 3-(9Z-octadecenoate)

$C_{55}H_{100}O_6$ 857.391
Mp 13-14° (racemate).

Glycerol 1-(9*Z*-octadecenoate) 2-(9*Z*,12*Z*-octadecadienoate) 3-octadecanoate [7162-26-7]

[26836-38-4]
9,12-Octadecadienoic acid 1-[[(1-oxo-9-octadecenyl)oxy]methyl]-2-[(1-oxooctadecyl)oxy]ethyl ester. α-Oleo-β-linoleostearin. Glycerol 2-(9Z,12Z-octadecadienoate) 1-octadecanoate 3-(9Z-

octadecenoate)

$C_{57}H_{104}O_6$ 885.445
Mp 8.5-9° (14-14.5°)(racemate).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-hexadecanoate 3-(9*Z*-octadecenoate) [2534-97-6]
9,12-Octadecadienoic acid 2-[(1-oxohexadecyl)oxy]-3-[(1-oxo-9-octadecenyl)oxy]propyl ester. Glycerol 2-hexadecanoate 1-(9Z,12Z-octadecadienoate) 3-(9Z-octadecenoate)

$C_{55}H_{100}O_6$ 857.391
Oil. Mp -10° (racemate).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-octadecanoate 3-hexadecanoate [2534-96-5]
α-Linoleo-β-stearopalmitin. Glycerol 1-hexadecanoate 3-(9Z,12Z-octadecadienoate) 2-octadecanoate

$C_{55}H_{102}O_6$ 859.407
Cryst. Mp 36-37° (racemate).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-octadecanoate 3-(9*Z*-octadecenoate) [2410-30-2]

[26836-38-4]
9,12-Octadecadienoic acid 3-[(1-oxo-9-octadecenyl)oxy]-2-[(1-oxooctadecyl)oxy]-propyl ester. α-Linoleo-β-stearoolein

$C_{57}H_{104}O_6$ 885.445
Mp -20–12° (racemate).

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-(9*Z*-octadecenoate) 3-hexadecanoate [2680-59-3]

[26836-35-1]
9,12-Octadecadienoic acid 3-[(1-oxohexadecyl)oxy]-2-[(1-oxo-9-octadecenyl)oxy]-propyl ester. α-Linoleo-β-oleopalmitin. Glycerol 1-hexadecanoate 3-(9Z,12Z-octadecadienoate) 2-(9Z-octadecenoate)

$C_{55}H_{100}O_6$ 857.391
Mp 13-13.5° (racemate). Exhibits polymorphism.

Glycerol 1-(9*Z*,12*Z*-octadecadienoate) 2-(9*Z*-octadecenoate) 3-octadecanoate [2190-14-9]

[26836-38-4]
9,12-Octadecadienoic acid 2-[(1-oxo-9-octadecenyl)oxy]-3-[(1-oxooctadecyl)oxy]-propyl ester. α-Linoleo-β-oleostearin. Glycerol 1-(9Z,12Z-octadecadienoate) 3-octadecanoate 2-(9Z-octadecenoate)

$C_{57}H_{104}O_6$ 885.445
Mp -17° (racemate) Mp -4–2° (racemate).

Glycerol 1-eicosanoate 2-(9*Z*-octadecenoate) 3-octadecanoate [59891-33-7]

[67877-82-1]
2-[(1-Oxo-9-octadecenyl)oxy]-3-[(1-oxooctadecyl)oxy]propyl eicosanoate. α-Stearo-β-oleoarachidin. Glycerol 1-eicosanoate 3-octadecanoate 2-(9Z-octadecenoate)

$C_{59}H_{112}O_6$ 917.53
Minor component of vegetable oils. Cryst. (Me_2CO). Mp 41-42° (racemate).

Hilditch, T.P. *et al., The Chemical Constitution of Natural Fats*, 4th edn., Chapman & Hall, 1964, (*book*)
Nilsson-Ehle, P. *et al., J. Biol. Chem.*, 1973, **248**, 6734-6737 (*metab*)
Jensen, R.G. *et al., Adv. Lipid Res.*, 1976, **14**, 213-247 (*rev, synth*)
The Lipid Handbook, (eds. Gunstone, F.D. *et al*), Chapman & Hall, 1986, (*book*)
High-performance Liquid Chromatography and Lipids, Christie, W.W., *et al*, Pergamon, 1987, (*book*)
Eibl, H. *et al., Chem. Phys. Lipids*, 1988, **47**, 47-53 (*synth*)
Sonnet, P.E. *et al., Chem. Phys. Lipids*, 1991, **58**, 35-39; 1994, **72**, 185-191 (*synth*)
Lipid Analysis: A Practical Approach, (eds. Hamilton, R.J. *et al*), IRL Press/Oxford University Press, 1992, (*book*)
Rogalska, E. *et al., Chirality*, 1993, **5**, 24-30 (*metab*)
Murphy, R.C. *et al., Handb. Lipid Res.*, 1993, **7**, (*book*)
Sassano, G.J. *et al., J. Am. Oil Chem. Soc.*, 1993, **70**, 1111-1114 (*gc*)
Villeneuve, P. *et al., Chem. Phys. Lipids*, 1994, **72**, 135-141; 1995, **76**, 109-113 (*synth*)
Lie Ken Jie, M.S.F. *et al., Chem. Phys. Lipids*, 1995, **77**, 155-171; **78**, 1-13 (*pmr, cmr*)
Gunstone, F.D. *et al., Fatty Acid and Lipid Chemistry*, Blackie Academic, 1996, (*book*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 650; 1221; 1227; 1229-1231; 2822
Lie Ken Jie, M.S.F. *et al., Lipids*, 1997, **32**, 1019 (*rev, pmr, cmr*)
Food Lipids, (eds. Akoh, C.C. *et al*), M. Dekker, 1998, (*book*)
Lie Ken Jie, M.S.F. *et al., Nat. Prod. Rep.*, 1998, **15**, 607-629 (*rev, occur, synth, anal*)
Structural Modified Food Fats: Synthesis, Biochemistry and Use, (ed. Christophe, A.B.), AOCS Press, 1998, (*book*)
Summers, L.K.M. *et al., J. Lipid Res.*, 1999, **40**, 1890-1898 (*metab*)
Lipid Synthesis and Manufacture, (ed. Gunstone, F.D.), Sheffield Academic Press/CRC Press, 1999, 162-184; 288-320 (***rev, synth***)
Fat Digestion and Absorption, (eds. Christophe, A.B. *et al*), AOCS Press, 2000, (*book*)
Intestinal Lipid Metabolism, (eds. Mansbach, C.M. *et al*), Kluwer, 2001, (*book*)
Beare-Rogers, J. *et al., Pure Appl. Chem.*, 2001, **73**, 685-744 (*rev*)
Structured and Modified Lipids, (ed. Gunstone, F.D.), M. Dekker, 2001, (*book*)
www.chem.qmw.ac.uk/iupac/lipid, (*IUPAC nomenclature*)
www.lipid.co.uk/mainhome.html,

Glycerol tributanoate G-246

[60-01-5]
1,2,3-Propanetriyl tributanoate. Glycerol tributyrate. Tributyrin. NSC 661583. FEMA 2223

$H_3CCH_2CH_2COOCH(CH_2OOCCH_2CH_2CH_3)_2$

$C_{15}H_{26}O_6$ 302.367
Flavouring agent. Liq. with bitter taste. Bp 305-310° Bp_{15} 190°.

▶ LD_{50} (mus, ivn) 320 mg/kg. Fl. p. >66°, autoignition temp. 407°. ET7350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 620D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 950B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 647D (*ir*)
Weatherby, L.S. *et al., J.A.C.S.*, 1925, **47**, 2249 (*synth*)
Wathelet, J.P. *et al., J. Chromatogr.*, 1975, **110**, 157 (*tlc*)
Mityushova, N.M. *et al., Dokl. Akad. Nauk SSSR*, 1976, **230**, 992
Lamberet, G. *et al., Lait*, 1976, **56**, 119
Hildebrand, D.C. *et al., Plant Dis. Rep.*, 1976, **60**, 7 (*tox*)
Prager, R.H. *et al., Aust. J. Chem.*, 1989, **42**, 1003-1005 (*synth*)
Drackley, J.K. *et al., J. Dairy Sci.*, 1989, **72**, 1986-1995 (*metab*)
Chen, Z.X. *et al., Cancer Res.*, 1994, **54**, 3494-3499 (*pharmacol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1221; 2824 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TIG750

Glycerol tridecanoate G-247

[621-71-6]
1,2,3-Propanetriyl decanoate, 9CI. Tricaprin. Caprin. Dynasan® 110

$H_3C(CH_2)_8COOCH[CH_2OOC(CH_2)_8CH_3]_2$

$C_{33}H_{62}O_6$ 554.849
Used in dietary food products. Cryst. (petrol/EtOH). Mp 32°. Exhibits polymorphism.

▶ HD9410000

[11139-88-1]

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90 (*synth*)

Glycerol tridocosanoate G-248

[18641-57-1]
1,2,3-Propanetriyl tridocosanoate, 9CI. Tribehenin. Compritol 888

$H_3C(CH_2)_{20}COOCH[CH_2OOC(CH_2)_{20}CH_3]_2$

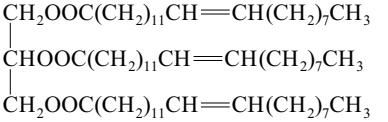
$C_{69}H_{134}O_6$ 1059.814
Probable constit. of fats. Cryst. (hexane). Mp 82.5°. Exhibits polymorphism.

▶ JR1305000

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90 (*synth*)
Hagemann, J.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 118

Glycerol tri-13-docosenoate G-249

13-Docosenoic acid 1,2,3-propanetriyl ester, 9CI



$C_{69}H_{128}O_6$ 1053.767

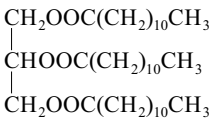
(all-*E*)-*form* [37635-44-2]
Tribrassidin
Mp 58°. Exhibits polymorphism.

(all-*Z*)-*form* [2752-99-0]
Trierucin. Erucin†
Widespread in seed oils. Mp 32°. Exhibits polymorphism.

Hagemann, J.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 118

Glycerol tridodecanoate G-250

[538-24-9]
1,2,3-Propanetriyl tridodecanoate. Trilaurin. Glycerol trilaurate. Laurin



$C_{39}H_{74}O_6$ 639.01
Mp 46.5°. Exists in polymorphic forms.

[37318-95-9]

Hilditch, T.P. *et al., The Chemical Constitution of Natural Fats*, 4th edn., Chapman & Hall, 1964,
Lutton, E.S. *et al., Lipids*, 1970, **5**, 90 (*polymorphism*)

Glycerol trieicosanoate G-251

[620-64-4]
1,2,3-Propanetriyl trieicosanoate, 9CI. Triarachidin. Triarachin
$H_3C(CH_2)_{18}COOCH[CH_2OOC(CH_2)_{18}CH_3]_2$
$C_{63}H_{122}O_6$ 975.653
Probable constit. of fats. Cryst. (hexane). Mp 78°. Exhibits polymorphism.

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90 (*synth*)
Hagemann, J.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 118

Glycerol triheneicosanoate G-252

[26536-14-1]
1,2,3-Propanetriyl triheneicosanoate. Triheneicosanoin
$H_3C(CH_2)_{19}COOCH[CH_2OOC(CH_2)_{19}CH_3]_2$
$C_{66}H_{128}O_6$ 1017.734
Probable constit. of fats. Cryst. (hexane). Mp 75.9°. Exhibits polymorphism.

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90

Glycerol triheptadecanoate G-253

[2438-40-6]
1,2,3-Propanetriyl triheptadecanoate. Triheptadecanoin, 8CI. Trimargarin
$H_3C(CH_2)_{15}COOCH[CH_2OOC(CH_2)_{15}CH_3]_2$
$C_{54}H_{104}O_6$ 849.412
Probable constit. of fats. Cryst. (hexane). Mp 64°. Exhibits polymorphism.

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90
Simpson, T.D. *et al., J. Am. Oil Chem. Soc.*, 1983, **60**, 19 (*polymorphism*)

Glycerol trihexadecanoate G-254

[555-44-2]
1,2,3-Propanetriyl hexadecanoate, 9CI. ***Tripalmitin, INN****. Palmitin. Glycerol tripalmitate*
$H_3C(CH_2)_{14}COOCH[CH_2OOC(CH_2)_{14}CH_3]_2$
$C_{51}H_{98}O_6$ 807.332
Present in palm oil. Cryst. (Et_2O). Mp 66.4°. Polymorphic.
► Fl. p. >66°.

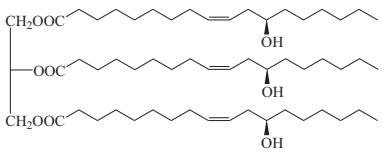
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 621A (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 525C (*nmr*)
Hilditch, T.P. *et al., The Chemical Constitution of Natural Fats*, 4th edn., Chapman & Hall Chapman and Hall, London, 4th Ed., 1964, 664
Chapman, D. *et al., The Structure of Lipids*, Methuen and Co., London, 1965, 268
Dorset, D.L. *et al., Z. Naturforsch., C*, 1978, **33**, 50 (*cryst struct*)
Saroja, M. *et al., Synth. Commun.*, 1986, **16**, 1423 (*synth*)
Nishida, Y. *et al., Agric. Biol. Chem.*, 1989, **53**, 2319 (*cmr*)
Kellens, M. *et al., Chem. Phys. Lipids*, 1991, **58**, 131 (*polymorphism*)
Jie, M. *et al., J. Chem. Res., Synop.*, 1992, 12 (*cmr*)

Glycerol trihexanoate G-255

[621-70-5]
1,2,3-Propanetriyl hexanoate, 9CI. Tricaproin
$H_3C(CH_2)_4COOCH[CH_2OOC(CH_2)_4CH_3]_2$
$C_{21}H_{38}O_6$ 386.528
Probable constit. of fats. Mp -25°.
► LD_{50} (mus, ivn) 122 mg/kg. MB2700000

Scheij, L.T.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1899, **18**, 169
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GGK000

Glycerol tri-12-hydroxy-9-octadecenoate G-256



$C_{57}H_{104}O_9$ 933.443
all*-[*R*-(*Z*)]-*form [2540-54-7]
Triricinolein. Ricinolein
Isol. from castor oil (*Ricinus communis*). Oil. d^{29} 0.96. n_D^{29} 1.4763.

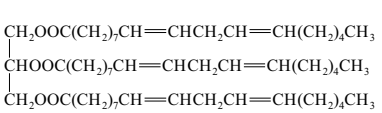
Meyer, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1897, **235**, 189 (*synth*)
Subrahmanyan, V.V.R. *et al., J. Chem. Eng. Data*, 1961, **6**, 548 (*props*)
Subrahmanyan, V.V.R. *et al., J. Sci. Ind. Res., Sect. D*, 1961, **20**, 45 (*isol*)
Rashkes, Y.V. *et al., Khim. Prir. Soedin.*, 1986, **22**, 551; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 516 (*ms*)

Glycerol trinonadecanoate G-257

1,2,3-Propanetriyl trinonadecanoate. Trinonadecanoin, 8CI
$H_3C(CH_2)_{17}COOCH[CH_2OOC(CH_2)_{17}CH_3]_2$
$C_{60}H_{116}O_6$ 933.573
Probable constit. of fats. Cryst. (hexane). Mp 71°. Exhibits polymorphism.

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90

Glycerol tri-9,12-octadecadienoate G-258

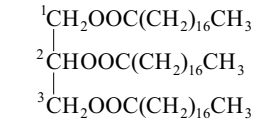


$C_{57}H_{98}O_6$ 879.398
(9*Z*,12*Z*)-*form* [537-40-6]
Glycerol trilinoleate. Trilinolein
Constit. of seed oils rich in linoleic acid, e.g., sunflower oil. Oil. Mp -11°. Exists in polymorphic forms.

Hilditch, T.P. *et al., The Chemical Constitution of Natural Fats*, 4th edn., Chapman & Hall, 1964,
Hagemann, J.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 118 (*polymorphism*)
Frost, D.J. *et al., Chem. Phys. Lipids*, 1975, **14**, 189 (*pmr*)

Glycerol trioctadecanoate G-259

[555-43-1]
Glycerol tristearate. Tristearin. Stearin. Hardened oil. Glycowax S 932

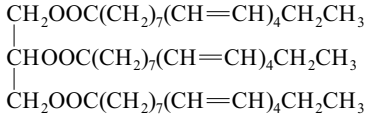


$C_{57}H_{110}O_6$ 891.492
Cryst. (Et_2O or hexane). Mp 73.5°. Exhibits polymorphism (lower Mp's reported 54.5°, 54.9°, 64°).
► Fl. p. >66°.

Lutton, E.S. *et al., J.A.C.S.*, 1955, **77**, 2646 (*synth*)
Markley, K.S. *et al., Fatty Acids*, 2nd Ed,. Interscience, London, 1960, 326
Barber, M. *et al., Tet. Lett.*, 1964, 1063 (*ms*)
Hilditch, T.P. *et al., The Chemical Constitution of Natural Fats*, 4th edn., Chapman & Hall, 1964, 664
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GGU000

Glycerol tri-9,11,13,15-octadecatetraenoate G-260

Triparinarin

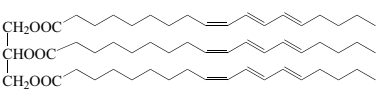


$C_{57}H_{86}O_6$ 867.303
Isol. from the seed fat of *Parinarium laurinium*. Cryst. Mp 49-50°.

Riley, J.P. *et al., J.C.S.*, 1951, 291 (*isol*)

Glycerol tri-9,11,13-octadecatrienoate G-261

[110300-19-1]



(9*Z*,9'*Z*,9"*Z*,11*E*,11'*E*,11"*E*,13*E*,13'*E*,13"*E*)-*form*

$C_{57}H_{92}O_6$ 873.35
(9*Z*,9′*Z*,9″*Z*,11*E*,11′*E*,11″*E*,13*E*,13′*E*,13′-″*E*)-*form* [159099-33-9]

[171269-41-3]
Glycerol tri-α-eleostearate. Tri-α-eleostearoylglycerol. Trieleostearin
Constit. of *Momordica charantia* (bitter melon).

(9*Z*,9′*Z*,9″*Z*,11*E*,11′*E*,11″*E*,13*Z*,13′*Z*,13-

,13′′Z)-form [168252-51-5]
Glycerol tripunicate. Tripunicylglycerol
Constit. of *Punica granatum* (pomegranate).

[136134-08-2, 145544-13-4]

Chang, M.-K. *et al., J. Am. Oil Chem. Soc.*, 1994, **71**, 1173; 1996, **73**, 263 (*Trielostearin*)
Joh, Y.-G. *et al., J. Am. Oil Chem. Soc.*, 1995, **72**, 1037 (*isol*)
Kapseu, C. *et al., J. Food Lipids*, 1995, **2**, 87 (*isol*)
Yusuph, M. *et al., Phytochemistry*, 1997, **44**, 1391 (*isol*)

Glycerol tri-6-octadecenoate G-262

6-Octadecenoic acid 1,2,3-propanetriyl ester, 9CI. Tripetroselin

$CH_2OOC(CH_2)_4CH = CH(CH_2)_{10}CH_3$
$CHOOC(CH_2)_4CH = CH(CH_2)_{10}CH_3$
$CH_2OOC(CH_2)_4CH = CH(CH_2)_{10}CH_3$

$C_{57}H_{104}O_6$ 885.445

(all-E)-form [35017-28-8]
Tripetroselaidin
Mp 52°. Exhibits polymorphism.

(all-Z)-form [3296-43-3]
Tripetroselinin
Constit. of some Umbelliferae seed oils, e.g. parsley (*Petroselinum*) spp.. Mp 28°. Exhibits polymorphism.

Hagemann, J.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 118 (*synth*)
Batchelor, J.G. *et al., J.O.C.*, 1974, **39**, 1698 (*cmr*)

Glycerol tri-9-octadecenoate G-263

$C_{57}H_{104}O_6$ 885.445

(E,E,E)-form [537-39-3]
Glycerol trielaidate. Trielaidin
Mp 41°. Exists in polymorphic forms.

(Z,Z,Z)-form [122-32-7]
Glycerol trioleate. Triolein. Olein
Constit. of olive oil and other vegetable oils. Oil. Mp 5°. Bp_{18} 235-240° part. dec.. Exists in polymorphic forms.

▶ Fl. p. >66°.

Hilditch, T.P. *et al., The Chemical Constitution of Natural Fats*, 4th edn., Chapman & Hall, 1964,
Hagemann, J.W. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 118 (*polymorphism*)

Glycerol trioctanoate G-264

[538-23-8]
1,2,3-Propanetriyl octanoate, 9CI. Tricaprylin. Panacet 800. Captex® 8000

$H_3C(CH_2)_6COOCH[CH_2OOC(CH_2)_6CH_3]_2$

$C_{27}H_{50}O_6$ 470.688
Used in bakery products. Carrier for essential oils and flavours. Cryst. (Me_2CO/EtOH at -35°). d_4^{20} 0.95. Mp 10°. Bp_1 233°. Exhibits polymorphism.

▶ LD_{50} (rat, orl) *ca.* 33000 mg/kg. Exp. reprod. effects (large dose). YJ7700000

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TMO000

Glycerol tripentadecanoate G-265

[30719-27-8]
1,2,3-Propanetriyl tripentadecanoate, 9CI. Tripentadecanoin, 8CI

$H_3C(CH_2)_{13}COOCH[CH_2OOC(CH_2)_{13}CH_3]_2$

$C_{48}H_{92}O_6$ 765.251
Probable constit. of fats. Cryst. (hexane). Mp 55°. Exhibits polymorphism.

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90

Glycerol tripropanoate G-266

[139-45-7]
1,2,3-Propanetriol tripropanoate, 9CI. Tripropionin, 8CI. FEMA 3286

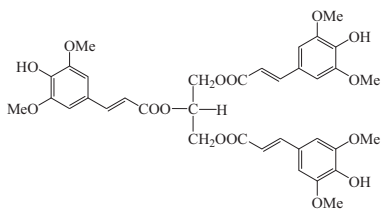
$H_3CCH_2COOCH(CH_2OOCCH_2CH_3)_2$

$C_{12}H_{20}O_6$ 260.286
Flavouring ingredient. d_{18}^{20} 1.1. Bp_{20} 176-177°. n_D^{20} 1.4339.

Prager, R.H. *et al., Aust. J. Chem.*, 1989, **42**, 1003-1005 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 306
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1230-1231

Glycerol tris(4-hydroxy-3,5-dimethoxyphenyl-2-propenoate) G-267

*Glycerol trisinapate. Tri-*O*-sinapoylglycerol*



$C_{36}H_{38}O_{15}$ 710.687
Constit. of *Raphanus sativus* (radish).

Traditional Chinese Medicines, (ed. Milne, G.A.), Ashgate, 1999, 2694

Glycerol tritetracosanoate G-268

[56933-26-7]
1,2,3-Propanetriyl tetracosanoate, 9CI. Trilignocerin

$H_3C(CH_2)_{22}COOCH[CH_2OOC(CH_2)_{22}CH_3]_2$

$C_{75}H_{146}O_6$ 1143.975
Probable constit. of fats. Cryst. (hexane). Mp 86°. Exhibits polymorphism.

Simpson, T.D. *et al., J. Am. Oil Chem. Soc.*, 1975, **52**, 303 (*struct*)

Glycerol tritetradecanoate G-269

[555-45-3]
Glycerol trimyristate. Trimyristin. Myristin

$^1CH_2OOC(CH_2)_{12}CH_3$
$^2CHOOC(CH_2)_{12}CH_3$
$^3CH_2OOC(CH_2)_{12}CH_3$

$C_{45}H_{86}O_6$ 723.171
Constit. of nutmegs. Mp 58.5°. Exists in polymorphic forms.

Hilditch, T.P. *et al., The Chemical Constitution of Natural Fats*, 4th edn., Chapman & Hall, 1964,
Lutton, E.S. *et al., Lipids*, 1970, **5**, 90 (*polymorphism*)
Frank, F. *et al., J. Chem. Educ.*, 1971, **48**, 255 (*isol*)

Glycerol tritridecanoate G-270

[26536-12-9]
1,2,3-Propanetriyl tritridecanoate, 9CI. Tritridecanoin, 8CI

$H_3C(CH_2)_{11}COOCH[CH_2OOC(CH_2)_{11}CH_3]_2$

$C_{42}H_{80}O_6$ 681.09
Probable constit. of fats. Cryst. (hexane). Mp 44.5°. Exhibits polymorphism.

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90

Glycerol triundecanoate G-271

[13552-80-2]
1,2,3-Propanetriyl undecanoate, 9CI. Triundecanoin. Captex 8227

$H_3C(CH_2)_9COOCH[CH_2OOC(CH_2)_9CH_3]_2$

$C_{36}H_{68}O_6$ 596.93
Carrier for flavours and fragrances. Cryst. (hexane). Mp 31.2°. Exhibits polymorphism.

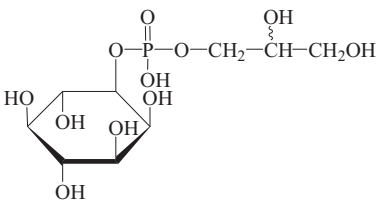
▶ YQ2581000

Lutton, E.S. *et al., Lipids*, 1970, **5**, 90

Glycerylphosphoinositol G-272

[129830-95-1]

[966-66-5, 2816-11-7, 27082-28-6, 37449-91-5, 62776-82-3, 138382-57-7]
myo-*Inositol 1-(2,3-dihydroxypropyl hydrogen phosphate), 9CI. Glycerophosphoinositol. Lysoplasmanylinositol*



$C_9H_{19}O_{11}P$ 334.216

It is not clear whether the name Lysoplasmanylinositol refers to the parent struct. or to *O*-alkyl derivs. See also 1-[7-(2-Hexyl-3-methylcyclopropyl)heptyl]lysoplasmanylinositol and 1-(9-Methylhexadecyl)lysoplasmanylinositol. Isol. from beef liver. Mp 145-150° dec. $[\alpha]_D$ -17.37 (c, 2 in H_2O). Parent structure of 3-Phosphatidylinositol, P-326. Not a recognised intermed. on the phospholipid pathway. Prob. an artifact of hydrol. Monoacyl derivs (Lysophosphatidylinositols) are encountered in biol. systems as prods. of enzymic or other hydrol. of phosphatidylinositols.

Cyclohexylamine salt: [98975-46-3]
Cryst. (EtOH). Mp 124-126°. $[\alpha]_D$ -13.2 (c, 2.09 in H_2O).

Ca salt: [135821-52-2]
$[\alpha]_D$ -15.46 (c, 2.07 in H_2O).

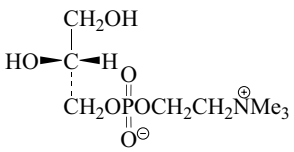
Ba salt: [138382-56-6]

$[\alpha]_D$ -14.8 (c, 3.79 in H_2O).

Brockerhoff, H. *et al., J.A.C.S.*, 1959, **81**, 2591-2592 (*isol*)
Brown, D.M. *et al., J.C.S.*, 1959, 3547-3552 (*synth*)
Brockerhoff, H. *et al., J. Biol. Chem.*, 1961, **236**, 1907-1911 (*isol*)
Dawson, R.M.C. *et al., Biochem. J.*, 1977, **162**, 241-245 (*synth*)
Filthuth, E. *et al., Chem. Phys. Lipids*, 1992, **60**, 253-261 (*lysophosphatidylinositols, synth*)
Bruzik, K.S. *et al., J.A.C.S.*, 1996, **118**, 7679-7688 (*synth*)

Glycerylphosphorylcholine G-273

[563-24-6]
2-[[(2,3-Dihydroxypropoxy)hydroxyphosphinyl]oxy]-N,N,N-trimethylethanaminium inner salt, 9CI. Choline glycerophosphate



(*R*)-form

$C_8H_{20}NO_6P$ 257.223

Lanched 1990(***R*)-form** [28319-77-9]
Choline alfoscerate, INN. sn-*Glycero-3-phosphocholine*
Hygroscopic viscous liq. or solid. $[\alpha]_D^{23}$ -2.85 (c, 2.2 in H_2O).

Compd. with $CdCl_2$: [64681-08-9]
Needles (EtOH). Mp 100-102°. $[\alpha]_D^{24}$ -1.4 (c, 5.5 in H_2O). Sinters >97°.

(*S*)-form [4217-84-9]
sn-*Glycero-1-phosphocholine*
$[\alpha]_{546}^{22}$ +3 (c, 2.5 in H_2O). Intermediate for synth of 'unnatural' 1-*sn*-phosphatidylcholines.

(±)-form [34688-34-1]
Sol. H_2O, EtOH, MeOH. Mp 152-153°. Described as visc. liq. (Baer) and v. hygroscopic powder (Mushika).

[71861-27-3, 73289-29-9]

Baer, E. *et al., J.A.C.S.*, 1948, **70**, 1394-1399 (*synth, bibl*)
Brockerhoff, H. *et al., Can. J. Biochem.*, 1965, **43**, 1777 (*synth*)
Abrahamsson, S. *et al., Acta Cryst.*, 1966, **21**, 79-87 (*cryst struct*)
Chadha, J.S. *et al., Chem. Phys. Lipids*, 1970, **4**, 104-108 (*synth*)
Mushika, Y. *et al., Chem. Pharm. Bull.*, 1971, **19**, 696-704 (*synth, bibl, pmr*)
Patel, K.M. *et al., J. Lipid Res.*, 1979, **20**, 674-677 (*synth, $CdCl_2$ complex*)
Kanda, P. *et al., J. Lipid Res.*, 1981, **22**, 879-882 (*synth, S-form*)
Lacey, C.J. *et al., J.O.C.*, 1983, **48**, 5214-5421 (*synth, cmr*)
Nakanishi, T. *et al., Am. J. Physiol.*, 1989, **257**, C795-C801 (*biol activity*)
Sigala, S. *et al., Eur. J. Pharmacol.*, 1992, **211**, 351-358 (*pharmacol*)
Govoni, S. *et al., Ann. N.Y. Acad. Sci.*, 1993, **695**, 307-310 (*pharmacol*)
Amenta, F. *et al., Ann. N.Y. Acad. Sci.*, 1993, **695**, 311-313 (*pharmacol*)
Abbiati, G. *et al., Eur. J. Drug Metab. Pharmacokinet.*, 1993, **18**, 173-180 (*pharmacokinet*)
Burt, C.T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **108**, 11-20 (*rev*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1419

Glycine G-274

[56-40-6]
Aminoacetic acid, 9CI. Glycocoll. Glue sugar. Gly. FEMA 3287. E640
H_2NCH_2COOH
$C_2H_5NO_2$ 75.067

Certain derivs. of importance in peptide synth. have been listed separately under the name of the *N*-protecting group.. Flavouring ingredient; dietary additive, nutrient. Cryst. (EtOH aq.). V. sol. H_2O (25g/100g at 25°); sol. H_2O; sl. sol. EtOH. Mp 292° (262°) dec. pK_{a1} 2.35; pK_{a2} 9.78 (25°). Isoelectric point 5.97. Sweet taste. The name E640 is also used for the Na salt.

▶ LD_{50} (rat, orl) 7930 mg/kg. Adverse effects of irrigation solutions observed.
MB7600000

Hydrochloride: [6000-43-7]
Mp 185°.

▶ MC0560000

Benzyl ester, 4-methylbenzenesulfonate salt: [1738-76-7]
Antioxidant in foodstuffs. Cryst. (MeOH/petrol). Mp 79-81° Mp 132-134°.

[920-25-2, 2184-96-5, 4896-77-9, 6000-44-8, 7299-33-4, 23297-34-9, 104403-70-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 563A-563B; 563C; 671C; 671D; **2**, 250B; 379A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 867A; 1067A; 1067B; 1067C (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 298 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 310 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 26), Wiley, N.Y., 1961, **3**, 1955 (*bibl, synth*)
Junk, G. *et al., J.A.C.S.*, 1963, **85**, 839 (*ms*)
Leipert, T.K. *et al., J.A.C.S.*, 1975, **97**, 269 (*N-15 nmr*)
Power, L.F. *et al., Acta Cryst. B*, 1976, **32**, 11 (*cryst struct*)
Szyper, M. *et al., Anal. Chim. Acta*, 1976, **85**, 357 (*uv*)
Hexem, J.G. *et al., J.A.C.S.*, 1981, **103**, 224 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, GHA000
Cheng, J.-P. *et al., J.A.C.S.*, 1993, **115**, 2655 (*conformn*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 589
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 307
Godfrey, P.D. *et al., J.A.C.S.*, 1995, **117**, 2019 (*conformn, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1233-1234
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GHA000; GHK000

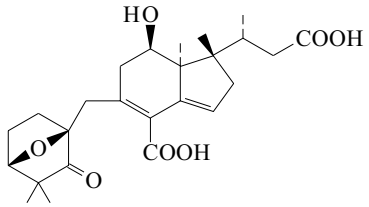
Glycinin G-275

The major storage protein in soybeans comprising *ca*. 35% of total protein. Plays an important role in tofu gel production.

Staswick, P.E. *et al., J. Biol. Chem.*, 1984, **259**, 13431-13435 (*struct*)
Yagasaki, K. *et al., J. Agric. Food Chem.*, 1997, **45**, 656-660 (*props*)
Cai, T. *et al., J. Agric. Food Chem.*, 1999, **47**, 720-727 (*use*)

Glycinoeclepin A G-276

[83216-10-8]



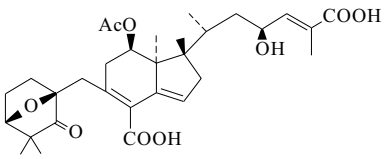
$C_{25}H_{34}O_7$ 446.539

A secocycloartane. Isol. from kidney bean roots. Struct. is incorrectly drawn in the reference λ_{max} 251 (ϵ 8300) (MeOH) (Derep).

Fukuzawa, A. *et al., Chem. Comm.*, 1985, 222
Corey, E.J. *et al., J.A.C.S.*, 1990, **112**, 8997 (*synth*)
Watanabe, H. *et al., J.C.S. Perkin 1*, 1991, 2919 (*synth*)

Glycinoeclepin B G-277

[103847-17-2]

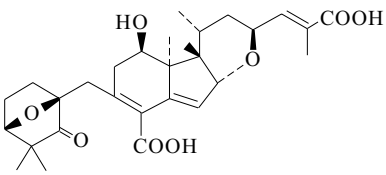


$C_{31}H_{42}O_9$ 558.667

Constit. of root of *Phaseolus vulgaris* (kidney bean). λ_{max} 252 (ϵ 9500) (MeOH) (Derep).

Fukuzawa, A. *et al., Tet. Lett.*, 1985, **26**, 5539
Corey, E.J. *et al., J.A.C.S.*, 1990, **112**, 8997 (*synth*)

Glycinoeclepin C G-278



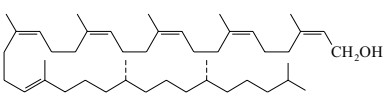
$C_{29}H_{38}O_8$ 514.614

Constit. of root of *Phaseolus vulgaris* (kidney bean). λ_{max} 252 (ϵ 9500) (MeOH) (Derep).

Fukuzawa, A. *et al., Tet. Lett.*, 1985, **26**, 5539

Glycinoprenol 9 G-279

[121254-96-4]



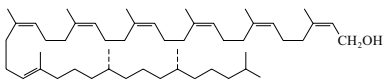
$C_{45}H_{80}O$ 637.126

Constit. of *Glycine max* (soybean). Oil.

Suga, T. *et al., J.O.C.*, 1989, **54**, 3390 (*isol, pmr, cmr*)
Ohnumo, S.-I. *et al., Tet. Lett.*, 1991, **32**, 241 (*synth*)

Glycinoprenol 10 G-280

[121254-97-5]

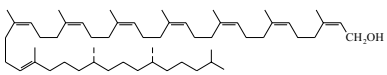


$C_{50}H_{88}O$ 705.245
Constit. of *Glycine max* (soybean). Oil.

Suga, T. *et al., J.O.C.*, 1989, **54**, 3390 (*isol, pmr, cmr*)
Ohnumo, S.-I. *et al., Tet. Lett.*, 1991, **32**, 241 (*synth*)

Glycinoprenol 11 G-281

[121254-98-6]

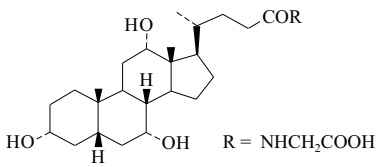


$C_{55}H_{96}O$ 773.363
Constit. of *Glycine max* (soybean). Oil.

Suga, T. *et al., J.O.C.*, 1989, **54**, 3390 (*isol, pmr, cmr*)
Ohnuma, S.-I. *et al., Tet. Lett.*, 1991, **32**, 241 (*synth*)

Glycocholic acid G-282

[475-31-0]
Cholylglycine

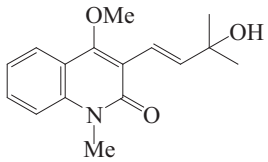


$C_{26}H_{43}NO_6$ 465.629
Small needles (EtOH aq.). Mp 140-142° Mp 154-155° dec. $[\alpha]_D^{13}$ +27.8 (EtOH). pK_a 4.4.

Na salt: [863-57-0]
Used in foodstuffs as a detergent to solubilize fats for absorption and is itself absorbed. Cryst. (EtOH/Et_2O). Mp 230-240°. $[\alpha]_D^{23}$ +29.2 (H_2O).
▶ MB9265100

Cortese, F. *et al., J.A.C.S.*, 1935, **57**, 1393 (*synth*)
Cortese, F. *et al., J.A.C.S.*, 1937, **59**, 2532 (*synth*)
Begemann, F. *et al., Z. Klin. Chem. Klin. Biochem.*, 1972, **10**, 29 (*isol*)
Games, D.E. *et al., Tet. Lett.*, 1974, **27**, 2377 (*ms*)
Tserng, K.-Y. *et al., J. Lipid Res.*, 1977, **18**, 404 (*synth*)
Shaw, R. *et al., Biomed. Mass Spectrom.*, 1978, **5**, 433 (*ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1234-1235

Glycocitlone A G-283



$C_{16}H_{19}NO_3$ 273.331
Yellow oil. λ_{max} 230 (log ϵ 4.46); 286 (sh) (log ϵ 3.93); 296 (log ϵ 4.02); 309 (log ϵ 4) (MeOH).

3′-Deoxy, 3′,4′-didehydro: [149998-43-6] **N-*Methylschinifoline***
$C_{16}H_{17}NO_2$ 255.316
Alkaloid from roots of *Zanthoxylum simulans* (Szechuan pepper). Oil.

3′-Deoxy, 3′,4′-didehydro, N-*de-Me:* [149998-56-1] *4-Methoxy-3-(3-methyl-1,3-butadienyl)-2(1*H*)-quinolinone.* ***Schinifoline*†**
$C_{15}H_{15}NO_2$ 241.289
Alkaloid from roots of *Zanthoxylum simulans* (Szechuan pepper). Cryst. Mp 171-174° dec.

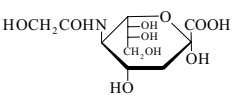
8-Hydroxy: ***Glycocitlone B***
$C_{16}H_{19}NO_4$ 289.33
Amorph. yellow powder. λ_{max} 202 (log ϵ 4.41); 225 (log ϵ 4.25); 267 (log ϵ 4.21); 296 (log ϵ 4.23); 307 (log ϵ 4.25); 410 (log ϵ 3.3) (MeOH).

8-Methoxy: ***Glycocitlone C***
$C_{17}H_{21}NO_4$ 303.357
Yellow oil. λ_{max} 230 (log ϵ 4.1); 258 (log ϵ 4.05); 307 (log ϵ 3.88); 321 (sh) (log ϵ 3.81); 350 (log ϵ 3.39) (MeOH).

Brader, G. *et al., Annalen*, 1993, 355 (*Schinifoline, N-Methylschinifoline*)
Wurz, G. *et al., Nat. Prod. Lett.*, 1993, **3**, 177 (*Schinifoline, isol*)
Ito, C. *et al., Chem. Pharm. Bull.*, 2000, **48**, 65-70 (*Glycocitlones*)

N-Glycolylneuraminic acid G-284

[1113-83-3]
*3,5-Dideoxy-5-[(hydroxyacetyl)amino]-*D-glycero-D-galacto-*2-nonulosonic acid, 9CI. Porcine sialic acid. NGNA*



α-D-Pyranose-*form*

$C_{11}H_{19}NO_{10}$ 325.272
Isol. from beef serum. Mp 185-187°. $[\alpha]_D$ -32 (H_2O). $[\alpha]_D^{22}$ -26.9 (c, 1.34 in H_2O) (1h, equilib.).

Blix, G. *et al., Nature (London)*, 1955, **175**, 340 (*isol*)
Zilliken, F. *et al., Adv. Carbohydr. Chem.*, 1958, **13**, 237 (*rev*)
Gottschalk, A. *et al., The Chemistry and Biology of Sialic Acids and Related Substances*, Cambridge Univ. Press, 1960, (*rev*)
Schoop, H.J. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1969, **350**, 155
Schauer, R. *et al., Angew. Chem., Int. Ed.*, 1973, **12**, 127
Corfield, A.P. *et al., Eur. J. Biochem.*, 1976, **68**, 597 (*biosynth*)
Codington, J.F. *et al., Methods Carbohydr. Chem.*, 1976, **7**, 226 (*occur, purifn*)

Kuboki, A. *et al., Tetrahedron*, 1997, **53**, 2387-2400 (*synth, pmr, cmr*)

Glycylalanylprolylmethionyl-phenylalanylvalinamide G-285

[115525-99-0]
H-Gly-^{2}Ala-Pro-^{4}Met-Phe-Val-NH_2
$C_{29}H_{45}N_7O_6S$ 619.784
Isol. from the pedal ganglion of *Mytilus edulis* (blue mussel).

*2-*L*-Serine analogue:* [115525-98-9] *Glycylserylprolylmethionylphenylalanylvalinamide*
$C_{29}H_{45}N_7O_7S$ 635.783
Isol. from *Mytilus edulis* (blue mussel).

Hirata, T. *et al., Biochem. Biophys. Res. Commun.*, 1988, **152**, 1376-1382 (*isol*)
Ikeda, T. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1992, **101**, 245-249 (*isol*)
Ikeda, T. *et al., CA*, 1994, **120**, 50479e (*isol*)

Glycylglycylglycine G-286

[556-33-2]
Diglycylglycine. Triglycine
$H_2NCH_2CONHCH_2CONHCH_2COOH$
$C_6H_{11}N_3O_4$ 189.171
Isol. from the seeds of *Blighia sapida* (akee apple). Needles (EtOH aq.). Mp 246° dec. pK_{a1} 3.27; pK_{a2} 7.9 (25°, 0.1*M* KNO_3).

Me ester:
$C_7H_{13}N_3O_4$ 203.197
Needles or prisms ($CHCl_3$/Et_2O). Mp 111°.

Me ester, hydrochloride:
Leaflets (MeOH). Mp 204° dec.

Me ester, hydrobromide:
Mp 205-207°.

Et ester:
$C_8H_{15}N_3O_4$ 217.224
Plates (EtOH) (as hydrochloride). Mp 214-219° (hydrochloride).

3,5-Dinitrobenzoyl:
Needles (H_2O). Mp 236° dec.

N-*Benzyloxycarbonyl, Me ester:*
Mp 158°.

Weygand, F. *et al., Chem. Ber.*, 1957, **90**, 639 (*synth*)
Elias, H.G. *et al., Makromol. Chem.*, 1967, **102**, 161 (*synth*)
Nekrasova, V.A. *et al., Zh. Obshch. Khim.*, 1968, **37**, 1761; *CA*, **68**, 78604y (*synth*)
Fowden, L. *et al., Phytochemistry*, 1969, **8**, 1043 (*isol*)
Nagai, M. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 1323 (*nmr*)
Feairheller, W.R. Jr. *et al., Appl. Spectrosc.*, 1971, **25**, 176 (*ir*)
Handelsman-Benory, E. *et al., Acta Cryst. C*, 1995, **51**, 2362 (*cryst struct, Me ester*)

N-Glycylphenylalanine G-287

$H_2NCH_2CONHCH(COOH)CH_2Ph$
$C_{11}H_{14}N_2O_3$ 222.243

L-***form*** [3321-03-7]
Needles (EtOH aq.). Mp 264-268°. $[\alpha]_D^{25}$ +41.8 (c, 2.5 in H_2O).

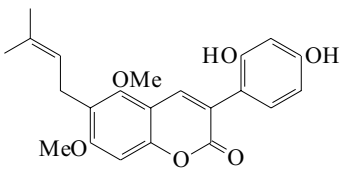
N^2-*(4-Hydroxy-3-methoxycinnamoyl):* [40747-82-8] N-*Feruloylglycyl-*L*-phenylalanine*
$C_{21}H_{22}N_2O_6$ 398.415
Constit. of *Medicago sativa* (alfalfa). $[\alpha]_D$ +34.5 (c, 0.4 in EtOH).

[62697-32-9]

van Rompaey, L. *et al., Bull. Soc. Chim. Belg.*, 1976, **85**, 657 (*synth, N-feruloyl*)
van Sumere, C.F. *et al., Phytochemistry*, 1980, **19**, 704 (*N-feruloyl*)

Glycyrin G-288

[66056-18-6]
*3-(2,4-Dihydroxyphenyl)-5,7-dimethoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, 9CI. 3-(2,4-Dihydroxyphenyl)-5,7-dimethoxy-6-prenylcoumarin*



$C_{22}H_{22}O_6$ 382.412
Isol. from roots of *Glycyrrhiza* sp. (licorice). Yellow needles. Mp 209-211°.

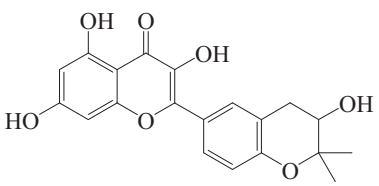
Di-Me ether: [66056-33-5]
Needles (MeOH aq.). Mp 78-80°.

7-O-De-Me: [94805-82-0] *3-(2,4-Dihydroxyphenyl)-7-hydroxy-5-methoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, 9CI.* ***Glycycoumarin***
$C_{21}H_{20}O_6$ 368.385
From licorice (*Glycyrrhiza glabra*). Yellow plates (C_6H_6/Me_2CO). Mp 243.5-244.5° (231°). Log P 4.35 (calc).

Kinoshita, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 135 (*Glycyrin*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2090 (*Glycycoumarin*)
Demizu, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3474 (*Glycycoumarin*)
Hwang, J.O. *et al., Nat. Prod. Sci.*, 1998, 130-135; *CA*, **130**, 63528b

Glycyrrhizaflavonol A G-289

[197304-01-1]

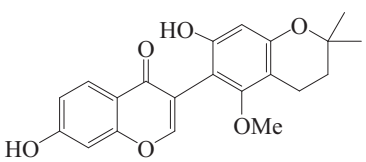


$C_{20}H_{18}O_7$ 370.358
Constit. of licorice (*Glycyrrhiza* sp.). Yellow needles. Mp 163°. Racemic λ_{max} 226 (sh) ; 250 (log ϵ 4.34); 267 (log ϵ 4.31); 367 (log ϵ 4.41) (MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1485-1492

Glycyrrhizaisoflavone C G-290

[161014-35-3]

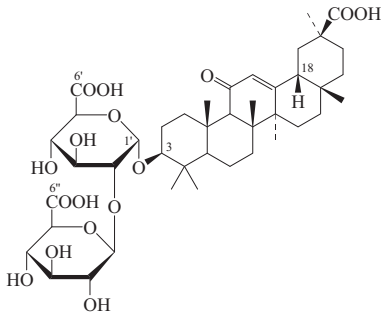


$C_{21}H_{20}O_6$ 368.385
Constit. of licorice (*Glycyrrhiza* sp.). Needles. Mp 159°. λ_{max} 211 (log ϵ 4.69); 248 (log ϵ 4.45); 288 (log ϵ 4.18); 302 (sh) (MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1485-1492

Glycyrrhizic acid G-291

[1405-86-3]
Glycyrrhetic acid 3-O-[β-D-glucuronopyranosyl-(1→2)-α-D-glucuronopyranoside]. Glycyrrhizinic acid. Dermacrin. Glycyrrhitin. ***Glycyrrhizin, JAN***



$C_{42}H_{62}O_{16}$ 822.942
Diglucuronide of 3-Hydroxy-11-oxo-12-oleanen-30-oic acid, H-694. Isol. from *Glycyrrhiza glabra* (liquorice). Nutriceutical with anticancer props.. Cryst. (AcOH) or hygroscopic powder. Mp 220° approx. $[\alpha]_D^{17}$ +46.2 (c, 1.5 in EtOH). Log P 2.09 (uncertain value) (calc). λ_{max} 249 (MeOH).

▶ Adverse effects of hypermineralocorticoidism result from excessive intake. LD_{Lo} (rat, orl) 3000 mg/kg. LD_{Lo} (rat, ipr) 2000 mg/kg. MD2025000

NH_4 salt: [53956-04-0]

[1407-03-0] *Ammonium glycyrrhizinate. Ammoniated glycyrrhizin. Glycyrram. Rizinsan A. Glycamil. Chiyorhizin AN. Glyciram. FEMA 2528*
Nonnutritive sweetener and flavour enhancer. Needles + $5H_2O$ (EtOH aq.). $[\alpha]_D^{20}$ +46.9 (EtOH aq.). Dec. at 212-217°.

▶ Exp. embryotoxic effects. LZ6500000

Di-K salt: [68797-35-3] ***Glycyrrhizinate dipotassium, JAN***

1′-Epimer: [103000-77-7] *Glycyrrhetic acid 3-O-[β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside].* ***Uralsaponin A****. Glycyrrhezinic acid. β-Glycyrrhizic acid*
$C_{42}H_{62}O_{16}$ 822.942
Cryst. Mp 235°. $[\alpha]_D^{18}$ +42.7. λ_{max} 252 (log ϵ 3.99) (MeOH).

1′-Epimer, 6′-butyl, 6″-Me ester: [388109-94-2]
$C_{47}H_{72}O_{16}$ 893.076

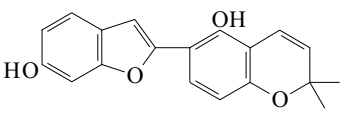
1′-Epimer, 6′-butyl, 6″-Et ester: [171980-73-7]
$C_{48}H_{74}O_{16}$ 907.103

[42294-03-1, 56649-78-6]

Karrer, P. *et al., Helv. Chim. Acta*, 1921, **4**, 100 (*isol*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1936, **19**, 1402 (*isol*)
Lythgoe, B. *et al., J.C.S.*, 1950, 1983 (*struct*)
Louis, L.H. *et al., J. Lab. Clin. Med.*, 1956, **47**, 20
Gilbert, R.J. *et al., J. Pharm. Pharmacol.*, 1964, **16**, 359; 394 (*salts*)
Essman, E.J. *et al., Fitoterapia*, 1984, **55**, 279 (*rev, use*)
Zhang, R. *et al., Yaoxue Xuebao*, 1986, **21**, 510; *CA*, **105**, 187603 (*Uralsaponin A*)
Ito, M. *et al., Antiviral Res.*, 1987, **7**, 127; 1988, **10**, 289; 1989, **11**, 255 (*anti-HIV activity*)
Mantovani, A. *et al., Food Chem. Toxicol.*, 1988, **26**, 435 (*tox*)
Stormer, F.C. *et al., Food Chem. Toxicol.*, 1993, **31**, 303 (*tox, rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 888
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1994, **30**, 772; *Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 720 (*pmr, cmr*)
Krähenbuhl, S. *et al., Steroids*, 1994, **59**, 121 (*hplc, pharmacokinet*)
Shim, S.-B. *et al., Planta Med.*, 2000, **66**, 40-43 (*isol, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 694-695 (*NH_4 salt, use*)
Xuan, C. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2001, **13**, 8-10; *CA*, **136**, 99121b (*Uralsaponin A esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GIE100; GIG000

Glyinflanin H G-292

[164123-54-0]
*6-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, 9CI. Glabrocoumarone B*

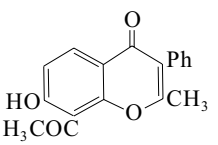


$C_{19}H_{16}O_4$ 308.333
Constit. of *Glycyrrhiza glabra* (licorice). Needles (MeOH aq.). Mp 168-169°. λ_{max} 237 (log ϵ 4.39); 277 (log ϵ 4.54); 286 (sh) (log ϵ 4.46) (MeOH).

Fukai, T. *et al., Phytochemistry*, 1995, **38**, 759 (*isol, uv, pmr, cmr, ms*)
Kinoshita, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1218 (*isol, uv, ir, pmr, cmr, ms*)

Glyzarin G-293

[62820-28-4]
*8-Acetyl-7-hydroxy-2-methyl-3-phenyl-4*H*-1-benzopyran-4-one, 9CI. 8-Acetyl-7-hydroxy-2-methylisoflavone*



$C_{18}H_{14}O_4$ 294.306
Constit. of *Glycyrrhiza glabra* (licorice). Yellow needles (EtOH). Mp 207-208°.

Bhardwaj, D.K. *et al., Phytochemistry*, 1977, **16**, 402 (*isol, struct*)
Jha, H.N. *et al., Org. Mass Spectrom.*, 1982, **17**, 350 (*ms*)

Gold G-294

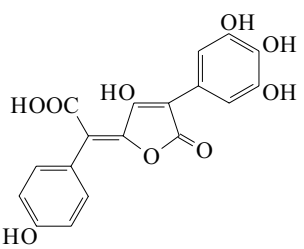
[7440-57-5]
Aurum (L.). E175
Au
Au 196.967
Atomic No. 79. Ground state electron config. [Xe]$4f^{14}5d^{10}6s^1$. 27 Isotopes are known of which only one, ^{197}Au, is stable. Known to ancient civilisations. Has no biological role. The most electronegative metal. Abundance: 0.004 ppm (earth's crust), 4×10^{-6} pm (sea water). Has fcc struct.. Used in food decoration and colouring esp. in Europe. Not permitted for food use in U.S.A.. Soft, yellow, malleable, ductile metal. Forms red, blue or violet colloidal suspensions. Physical props. depend on mechanical treatment. Mp 1064°. Bp 2808°. Stable in dry air at r.t.; and to H_2O, acids (except HNO_3/HCl) and alkalis. Sol. in aq. $CN^{\ominus}$. Unreactive to O_2, S, Se but reacts with Te.
▶ Non toxic. MD5070000

[16065-91-1, 19498-55-6, 20681-14-5]

Mellor Compr. Treat. Inorg. Theor. Chem., 1923, **3**, 491 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 62, 1954, (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **3**, 129 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **11**, 972 (*rev, bibl*)
Puddephatt, R.J. *et al., The Chemistry of Gold*, Elsevier, 1978, (*book*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 1364 (*rev*)
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1996, 88; 241
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1236 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GIS000

Gomphidic acid G-295

[25328-77-2]
4-Hydroxy-α-[3-hydroxy-5-oxo-4-(3,4,5-trihydroxyphenyl)-2(5H)-furanylidene]-benzeneacetic acid, 9CI



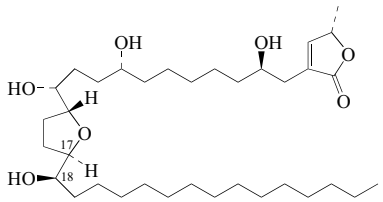
$C_{18}H_{12}O_9$ 372.287
Pigment from the lichen *Gomphidius glutinosus* (spike cap). Orange-red. Mp 300-302° dec. (205-215°) (unsharp). Closely related to Variegatic acid and Xerocomic acid, X-9.

O-*Tetra-Ac:*
Mp 198°.

Steglich, W. *et al., Z. Naturforsch., B*, 1969, **24**, 941; 1974, **29**, 96 (*isol, uv, ir, struct, pmr*)
Gedge, D.R. *et al., J.C.S. Perkin 1*, 1986, 2127 (*synth*)

Goniothalamicin G-296

[113817-64-4]



$C_{35}H_{64}O_7$ 596.886
Closely related to Annonacin, A-349.Wax. Sol. MeOH, hexane; poorly sol. H_2O. Mp 91-92° (86-88°). $[\alpha]_D^{25}$ +15.5 (c, 0.2 in $CHCl_3$). λ_{max} 210 (ϵ 10700) (MeOH) (Derep). λ_{max} 209 (ϵ 9000); 215 (E1%/1cm 3.86) (MeOH) (Berdy).

4-Deoxy: [177534-99-5] ***Longifolicin***
$C_{35}H_{64}O_6$ 580.887
Waxy solid. Mp 83°. $[\alpha]_D$ +13 (c, 0.001 in $CHCl_3$). λ_{max} 228 (log ϵ 3.7) (MeOH). λ_{max} 228 (ϵ 5000) (MeOH) (Berdy).

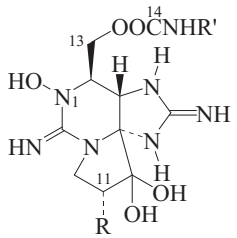
18-Epimer: [170902-34-8] ***Longicin***
$C_{35}H_{64}O_7$ 596.886
Wax. Mp 83°. $[\alpha]_D^{25}$ +13 (c, 1 in CH_2Cl_2).

17,18-Diepimer: [172586-14-0] **cis-*Goniothalamicin***
$C_{35}H_{64}O_7$ 596.886
Constit. of *Annona muricata* (soursop). Amorph. powder. Mp 80°. $[\alpha]_D^{25}$ +7.2 (c, 0.03 in $CHCl_3$). λ_{max} 213 (ϵ 10500) (MeOH).

Alkofahi, A. *et al., Experientia*, 1988, **44**, 83-85
Yu, J.G. *et al., J.O.C.*, 1992, **57**, 6198-6202 (*isol, pmr, cmr, ir, uv, ms*)
Ye, Q. *et al., J. Nat. Prod.*, 1995, **58**, 1398-1406 (*isol,, Goniothalamicin, Longicin*)
Ye, Q. *et al., Bioorg. Med. Chem.*, 1996, **4**, 537-545 (*Longifolicin*)
Rieser, M.J. *et al., J. Nat. Prod.*, 1996, **59**, 100 (*cis-Goniothalamicin*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)
Marshall, J.A. *et al., Tet. Lett.*, 1998, **39**, 1493-1496 (*synth, Longifolicin*)

Gonyautoxin I G-297

[60748-39-2]



R = OSO_3H, R' = H

$C_{10}H_{17}N_7O_9S$ 411.352
Prod. by *Gonyaulax* and *Protogonyaulax* spp. and isol. from shellfish. Neurotoxin, causal agent, with Saxitoxin, of shellfish poisoning. Sol. H_2O. Closely related to Saxitoxin, S-50. The Gonyautoxins, esp. the *N*-sulfates, show reduced toxicity compared with Saxitoxin.
▶ Toxic.

N^{14}-*Sulfonic acid (R' = SO_3H):* [89614-45-9] ***Toxin C₃***. *Protogonyautoxin 3. Toxin PX₃*
$C_{10}H_{17}N_7O_{12}S_2$ 491.416
From *Gonyaulax* and *Protogonyaulax* spp..
▶ Toxic.

1-Deoxy: [60508-89-6] ***Gonyautoxin II***
$C_{10}H_{17}N_7O_8S$ 395.352
From *Gonyaulax* and *Protogonyaulax* spp.. Sol. H_2O.
▶ Toxic.

1-Deoxy, N^{14}*-sulfonic acid:* [80173-30-4] ***Protogonyautoxin I***. *Toxin C_1. Toxin PX_1*
$C_{10}H_{17}N_7O_{11}S_2$ 475.417
From *Gonyaulax* and *Protogonyaulax* spp.. Prisms + H_2O (MeOH aq.).
▶ Toxic.

1-Deoxy, decarbamoyl: [86996-87-4] ***Decarbamoylgonyautoxin II***
$C_9H_{16}N_6O_7S$ 352.327
Isol. from various shellfish.

*1-Deoxy, decarbamoyl, 13-*O*-Ac:* [200816-97-3] ***13-Acetyldecarbamoylgonyautoxin II***
$C_{11}H_{18}N_6O_8S$ 394.365

11-Epimer: [64296-26-0] ***Gonyautoxin IV***
$C_{10}H_{17}N_7O_9S$ 411.352
From *Gonyaulax* and *Protogonyaulax* spp.. Sol. H_2O.
▶ Toxic.

11-Epimer, N^{14}*-sulfonic acid:* [89674-98-6] ***Toxin C₄***. *Protogonyautoxin 4. Toxin PX_4*
$C_{10}H_{17}N_7O_{12}S_2$ 491.416
From *Gonyaulax* and *Protogonyaulax* spp..
▶ Toxic.

11-Epimer, 1-deoxy: [60537-65-7] ***Gonyautoxin III***
$C_{10}H_{17}N_7O_8S$ 395.352
From *Gonyaulax* and *Protogonyaulax* spp.. Sol. H_2O.
▶ Toxic.

11-Epimer, 1-deoxy, N^{14}*-sulfonic acid:* [80226-62-6] ***Gonyautoxin VIII***. *Toxin C_2. Protogonyautoxin 2. Toxin PX_2*
$C_{10}H_{17}N_7O_{11}S_2$ 475.417
From *Gonyaulax* and *Protogonyaulax* spp.. Large cryst. + H_2O (H_2O).
▶ Toxic. UU6858700

11-Epimer, 1-deoxy, decarbamoyl: [87038-53-7] ***Decarbamoylgonyautoxin III***
$C_9H_{16}N_6O_7S$ 352.327
Isol. from various shellfish.

*11-Epimer, 1-deoxy, decarbamoyl, 13-*O*-Ac:* [200816-96-2] ***13-Acetyldecarbamoylgonyautoxin III***
$C_{11}H_{18}N_6O_8S$ 394.365

*11-Epimer, 12-deoxy, decarbamoyl, 13-*O*-Ac:* [200816-95-1]
$C_{11}H_{18}N_6O_7S$ 378.365

Harada, T. *et al., Agric. Biol. Chem.*, 1982, **46**, 1861 (*struct*)
Onoue, Y. *et al., J. Agric. Food Chem.*, 1983, **31**, 420 (*props*)
Oshima, Y. *et al., Agric. Biol. Chem.*, 1984, **48**, 1707 (*chromatog, struct, bibl*)
Maruyama, J. *et al., Agric. Biol. Chem.*, 1984, **48**, 2783 (*ms*)
Hall, S. *et al., Tet. Lett.*, 1984, **25**, 3537 (*isol, struct*)

Shimizu, Y. *et al., Tetrahedron*, 1984, **40**, 539 (*props*)
Onodera, H. *et al., Nat. Toxins*, 1997, **5**, 146-151 (*Lyngbya wollei derivs*)

Gonyautoxin VI G-298

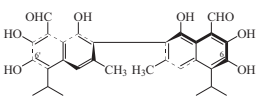
[82810-44-4]
Toxin B_2
As Gonyautoxin I, G-297 with
R = H, R′ = SO_3H
$C_{10}H_{17}N_7O_8S$ 395.352
Prod. by *Gonyaulax* and *Protogonyaulax* spp., isol. from shellfish. Neurotoxin; causal agent with Saxitoxin, of shellfish poisoning.
▶ Toxic.

1-Deoxy: [64296-25-9] ***Gonyautoxin V.*** *Toxin B_1*
$C_{10}H_{17}N_7O_7S$ 379.353
Prod. by *Gonyaulax* and *Protogonyaulax* spp..
▶ Toxic.

Harada, T. *et al., Agric. Biol. Chem.*, 1982, **46**, 1861 (*struct*)
Onoue, Y. *et al., J. Agric. Food Chem.*, 1983, **31**, 420 (*props*)
Oshima, Y. *et al., Agric. Biol. Chem.*, 1984, **48**, 1707 (*chromatog, struct, bibl*)
Maruyama, J. *et al., Agric. Biol. Chem.*, 1984, **48**, 2783 (*ms*)
Shimizu, Y. *et al., Tetrahedron*, 1984, **40**, 539 (*props*)
Hall, S. *et al., Tet. Lett.*, 1984, **25**, 3537 (*isol, structs*)

Gossypol G-299

[303-45-7]
1,1′,6,6′,7,7′-Hexahydroxy-3,3′-dimethyl-5,5′-bis(1-methylethyl)-[2,2′-binaphthalene]-8,8′-dicarboxaldehyde, 9CI. Thespesin



Absolute Configuration

$C_{30}H_{30}O_8$ 518.562
Atropisomeric compd., occurs naturally in both (+)- and (±)-forms. Tautomeric in polar solvents with intramolecular bis-lactol and bis-ketol tautomers.Has undergone widespread trials in Peoples Republic of China. Toxicity and poor therapeutic potential has precluded further interest as a male contraceptive. Poorly sol. H_2O. Log P 7.06 (uncertain value) (calc). λ_{max} 237 (ϵ 60250); 277 (ϵ 26300); 375 (ϵ 15850) (MeOH) (Berdy).
▶ DU3100000

(+)-*form* [20300-26-9]
Pale yellow needles (petrol), deep-yellow prisms + Me_2CO (Me_2CO), large elongated plates (Me_2CO aq.). Mp 181-183°. $[\alpha]_D^{19}$ +445 (c, 0.15 in $CHCl_3$).
▶ LD_{50} (mus, ipr) 35 mg/kg. Exp. reprod. effects. DU3101000

Hexa-Me ether: [17273-30-2]
Mp 242-244°. $[\alpha]_D$ +177 ($CHCl_3$).

(-)-*form* [90141-22-3]
Constit. of *Gossypium hirsutum* (cotton). Cryst. Mp 178-183°. $[\alpha]_D^{26}$ -360 (86% ee). More pharmacol. active isomer.
▶ DU3103500

(±)-*form* [40112-23-0]
Cryst. in three forms (Et_2O, $CHCl_3$, petrol). Mp 184° Mp 199° Mp 214°.
▶ Adverse effects reported when used therapeutically. Exp. reprod. effects. DU3104000

2-Aminoethylsulfonate: [87606-98-2] *Metaphin*. *GSN*Names refer to Na salt.

Hexa-Ac: [30719-67-6]
Mp 276-279°.
▶ Exp. reprod. effects. DU3103000

Bisphenylhydrazone:
Yellow plates (C_6H_6). Mp 303°.

6-Me ether: [54302-42-0]
$C_{31}H_{32}O_8$ 532.589
Yellow cryst. (C_6H_6/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 146-149°. λ_{max} 235 (ϵ 77100); 288 (ϵ 31200); 369 (ϵ 13900) (EtOH) (Berdy). λ_{max} 240 (ϵ 63500); 340 (ϵ 9000); 380 (ϵ 14600) (EtOH-NaOH) (Berdy).

6,6′-Di-Me ether: [1110-58-3]
$C_{32}H_{34}O_8$ 546.616
Golden-yellow cryst. (C_6H_6/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 181-184°. λ_{max} 231 (ϵ 69900); 253 (ϵ 48200); 287 (ϵ 32200); 360 (ϵ 11200) (EtOH) (Berdy). λ_{max} 239 (ϵ 61200); 271 (ϵ 32000); 348 (ϵ 10700) (EtOH-NaOH) (Berdy).

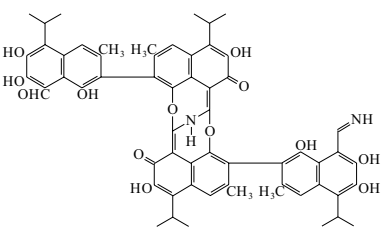
Hexa-Me ether:
Cryst. in three forms, two colourless and one red. Mp 158-160° (red) Mp 221° Mp 231-232°.

[62770-38-1]

Vioque-Pizarro, A. *et al., Anal. Chim. Acta*, 1951, **5**, 529 (*detn, Sn*)
Adams, R. *et al., Chem. Rev.*, 1960, **60**, 555 (*rev*)
Bell, A. *et al., Phytopathology*, 1967, **57**, 759
Bhakuni, D.S. *et al., Experientia*, 1968, **24**, 109 (*isol*)
King, T.J. *et al., Tet. Lett.*, 1968, 261 (*isol*)
Wood, A.B. *et al., Chem. Ind. (London)*, 1969, 1738 (*conformn*)
Edwards, J.D. *et al., J. Am. Oil Chem. Soc.*, 1970, **47**, 441 (*synth*)
Abou-Donia, M.B. *et al., Lipids*, 1970, **5**, 938 (*metab*)
Talipov, S.T. *et al., Zh. Anal. Khim.*, 1970, **25**, 1420 (*detn, Ge*)
Stipanovic, R.D. *et al., Phytochemistry*, 1975, **14**, 1077
O'Brien, D.H. *et al., J.O.C.*, 1978, **43**, 1105 (*nmr*)
Aripov, U.A. *et al., Khim.-Farm. Zh.*, 1983, **17**, 908 (*pharmacol, deriv*)
Masciadri, R. *et al., Chem. Comm.*, 1985, 1573 (*biosynth*)
Matlin, S.A. *et al., Contraception*, 1985, **31**, 141; 1988, **37**, 229 (*activity*)
Segal, S.J. *et al., Gossypol*, Plenum Press, N.Y., 1985, (*book*)
Talipov, S.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 835; 1986, **22**, 112; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 797; 1986, **22**, 108 (*cryst struct*)
Ibragimov, B.T. *et al., Khim. Prir. Soedin.*, 1985, **21**, 837; 1986, **22**, 113; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 799; 1986, **22**, 110 (*cryst. struct*)
Stipanovic, R.D. *et al., Chem. Comm.*, 1986, 100 (*biosynth*)
Sampath, D.S. *et al., Chem. Comm.*, 1986, 649 (*cd, resoln*)
Wu, D.F. *et al., Clin. Pharmacol. Ther. (St. Louis)*, 1986, **39**, 613 (*pharmacol*)
Lacombe, L. *et al., J. Nat. Prod.*, 1987, **50**, 277 (*cmr*)
Tyson, R. *et al., Chem. Ind. (London)*, 1988, 118 (*hplc, resoln*)
Huang, L. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 2664 (*cd, abs config, bibl*)
Lin, T.-S. *et al., Antimicrob. Agents Chemother.*, 1989, **33**, 2149 (*anti-HIV activity*)
Wu, D.F. *et al., Drugs*, 1989, **38**, 333 (*pharmacol*)
Brzezinski, B. *et al., J. Mol. Struct.*, 1990, **239**, 23 (*tautom, ir*)
Marciniak, B. *et al., J.C.S. Perkin 2*, 1991, 1359 (*pmr, tautom*)
Jaroszewski, J.W. *et al., Chirality*, 1992, **4**, 216 (*props*)
Ibragimov, B.T. *et al., Khim. Prir. Soedin.*, 1992, **28**, 186; 191; 330; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 159; 163; 288 (*cryst struct*)
Jaroszewski, J.W. *et al., Planta Med.*, 1992, **58**, 454 (*occur*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1375
Akhila, A. *et al., Phytochemistry*, 1993, **33**, 335 (*biosynth*)
Matlin, S.A. *et al., Drugs*, 1994, **48**, 851 (*pharmacol, rev*)
Coyle, T. *et al., J. Neuro-Oncol.*, 1994, **19**, 25 (*pharmacol*)
Meyers, A.I. *et al., Chem. Comm.*, 1997, 1573-1574 (*synth*)
Meyers, A.I. *et al., Tetrahedron*, 1998, **54**, 10493-10511 (*bibl, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GJM000; GJM025; GJM030; GJM035

Gossypurpurin G-300

[21891-57-6]

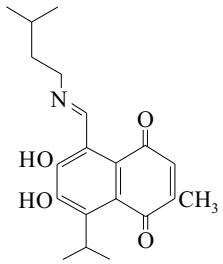


$C_{60}H_{56}N_2O_{13}$ 1013.108
Constit. of cotton seed (*Gossypium* sp.). Dark violet cryst. (C_6H_6). Prod. by the hydrol. of water-soluble gossypetin glycosides including a substance known as Gossyfiolin.

Manevich, E.F. *et al., CA*, 1965, **62**, 16154; 16551 (*isol, synth*)
Glushenkova, A.I. *et al., Khim. Prir. Soedin.*, 1988, **24**, 707; *Chem. Nat. Compd. (Engl. Transl.)*, 1988, **24**, 601 (*synth*)
Nazarova, I.P. *et al., Khim. Prir. Soedin.*, 1989, **75**, 63; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 54 (*isol*)

Gossyrubilone G-301

[69734-70-9]
6,7-Dihydroxy-2-methyl-5-[[(3-methylbutyl)imino]methyl]-8-(1-methylethyl)-1,4-naphthalenedione. 6,7-Dihydroxy-5-(isobutyliminomethyl)-8-isopropyl-2-methyl-1,4-naphthoquinone



$C_{20}H_{25}NO_4$ 343.422
Isol. from terminal leaves of *Gossypium hirsutum* (cotton). Red cryst. Mp 140-142°.

Bell, A.A. *et al., Phytochemistry*, 1978, **17**, 1297 (*isol, uv, ir, pmr, ms*)

Graecunin I G-302

[71123-81-4]

Spirostanol saponin of unknown struct.. Constit. of the seeds of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 193-194°. $[\alpha]_D$ -84 (EtOH).

Varshney, I.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1134 (*isol*)

Graecunin A G-303

[67621-48-1]

Spirostanol saponin of unknown struct.. Constit. of the leaves of *Trigonella foenum-graecum* (fenugreek). Amorph. powder.

Varshney, I.P. *et al., J. Indian Chem. Soc.*, 1977, **54**, 1135 (*isol*)
Varshney, I.P. *et al., J. Nat. Prod.*, 1984, **47**, 44 (*isol*)

Graecunin B G-304

[67621-49-2]

Spirostanol saponin of unknown struct.. Constit. of the leaves of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 154-156°. $[\alpha]_D$ -46 (EtOH).

Varshney, I.P. *et al., J. Indian Chem. Soc.*, 1977, **54**, 1135 (*isol*)
Varshney, I.P. *et al., J. Nat. Prod.*, 1984, **47**, 44 (*isol*)

Graecunin C G-305

[67621-50-5]

Spirostanol saponin of unknown struct.. Constit. of the leaves of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 147-149°. $[\alpha]_D$ +9.5 (EtOH).

Varshney, I.P. *et al., J. Indian Chem. Soc.*, 1977, **54**, 1135 (*isol*)
Varshney, I.P. *et al., J. Nat. Prod.*, 1984, **47**, 44 (*isol*)

Graecunin D G-306

[74350-29-1]

Spirostanol saponin of unknown struct.. Constit. of the leaves of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 141-142°. $[\alpha]_D$ +49 (EtOH).

Varshney, I.P. *et al., J. Nat. Prod.*, 1984, **47**, 44

Graecunin F G-307

[89899-79-6]

Spirostanol saponin of unknown struct.. Constit. of the leaves of *Trigonella foenum-graecum* (fenugreek). Amorph. powder.

Varshney, I.P. *et al., J. Nat. Prod.*, 1984, **47**, 44 (*isol*)

Graecunin H G-308

[71123-80-3]

Spirostanol saponin of unknown struct.. Constit. of the seeds of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 181-182°. $[\alpha]_D$ -72 (EtOH).

Varshney, I.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1134 (*isol*)

Graecunin J G-309

[71123-82-5]

Spirostanol saponin of unknown struct.. Constit. of the seeds of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 186-187°. $[\alpha]_D$ -25.2 (EtOH).

Varshney, I.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1134 (*isol*)

Graecunin K G-310

[71123-83-6]

Spirostanol saponin of unknown struct.. Constit. of the seeds of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 195-196°. $[\alpha]_D$ -44 (EtOH).

Varshney, I.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1134 (*isol*)

Graecunin L G-311

[71123-84-7]

Spirostanol saponin of unknown struct.. Constit. of the seeds of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 252-253°.

Varshney, I.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1134 (*isol*)

Graecunin M G-312

Spirostanol saponin of unknown struct.. Constit. of the seeds of *Trigonella foenum-graecum* (fenugreek). Amorph. powder.

Varshney, I.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1134 (*isol*)

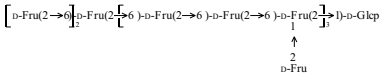
Graecunin N G-313

[71123-86-9]

Spirostanol saponin of unknown struct.. Constit. of the seeds of *Trigonella foenum-graecum* (fenugreek). Amorph. struct. Mp 238-239°. $[\alpha]_D$ -45.7 (EtOH).

Varshney, I.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 1134 (*isol*)

Graminin B G-314



A polyfructosan attached to a single glucose unit. Isol. from rye. $[\alpha]_D^{20}$ -31.7 (c, 1.0 in H_2O).

Poly-Ac:
$[\alpha]_D^{20}$ +7.9 (c, 1.0 in $CHCl_3$).

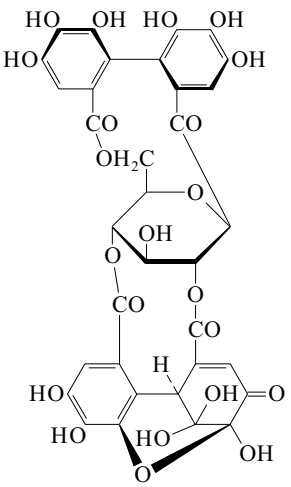
Poly-Me:
$[\alpha]_D^{20}$ -35.7 (c, 0.8 in $CHCl_3$).

Schlubach, H.H. *et al., Annalen*, 1952, **578**, 198; 1958, **614**, 123 (*isol*)

Granatin A G-315

[73683-70-2]

1,6-(S)-Hexahydroxydiphenoyl-2,4-(S)-dehydrohexahydroxydiphenoyl-β-D-glucopyranose

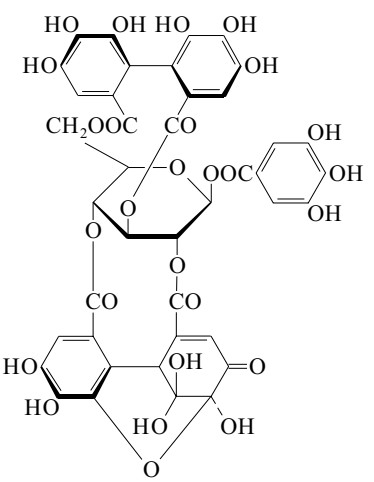


$C_{34}H_{24}O_{22}$ 784.55
Exists as an equilibrated mixt. of two isomers, the other being the alternative debenzofuranoid ketal. Major tannin constit. isol. from the leaves of *Punica granatum* (pomegranate). Yellow amorph. powder + $1H_2O$. $[\alpha]_D^{20}$ +9.5 (c, 0.5 in MeOH).

Haddock, E.A. *et al., J.C.S. Perkin 1*, 1982, 2535 (*pmr, cmr*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2424 (*struct*)

Granatin B G-316

[77322-54-4]



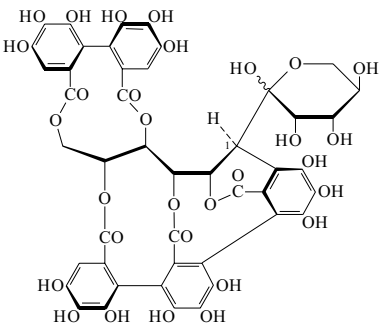
$C_{41}H_{28}O_{27}$ 952.656

Tautomeric. One tautomer shown. Isol. from pomegranate *Punica granatum*. Yellow cryst. + $8H_2O$ (H_2O). Mp 285° dec. $[\alpha]_D^{28}$ -109 → -123 (4h, 90% Me_2CO aq.).

Okuda, T. *et al., Tet. Lett.*, 1980, **21**, 4361
Haddock, E.A. *et al., J.C.S. Perkin 1*, 1982, 2535 (*pmr, cmr*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2424 (*struct*)

Grandinin G-317

[115166-32-0]



$C_{46}H_{34}O_{30}$ 1066.757

In equilib. with the furanose isomer.Pale brown amorph. powder + $6H_2O$. $[\alpha]_D^{24}$ -33 (c, 1.2 in 50% Me_2CO aq.). λ_{max} 220 ; 280 (MeOH) (Berdy).

1-Deglycosyl, 1α-hydroxy: [24312-00-3] ***Castalagin***
$C_{41}H_{26}O_{26}$ 934.641
Isol. from sweet chestnut. Off-white amorph. powder. $[\alpha]_D^{26}$ -99.9 (c, 0.52 in MeOH).

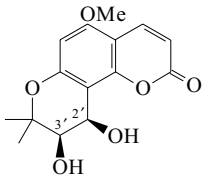
1-Deglycosyl, 1α-(3,4,5-trihydroxybenzoyloxy): [108449-60-1] ***1-O-Galloylcastalagin***
$C_{48}H_{30}O_{30}$ 1086.747
Needles + $7H_2O$ (H_2O). Mp 230° dec. $[\alpha]_D^{28}$ -105 (c, 1.0 in MeOH).

1-Deglycosyl, 1β-hydroxy: [36001-47-5] ***Vescalagin***
$C_{41}H_{26}O_{26}$ 934.641
Isol. from sweet chestnut *Castanea sativa*. Prisms (H_2O). Mp 200° dec. $[\alpha]_D^{25}$ -109.6 (c, 2 in H_2O).

1-Deglycosyl, 1β-carboxy: [118964-19-5] ***Vescalagincarboxylic acid***
$C_{42}H_{26}O_{27}$ 962.651
Needles + $1^1/_2H_2O$. Mp 180° dec. $[\alpha]_D^{23}$ -59.3 (c, 0.60 in MeOH aq.).

Mayer, W. *et al., Annalen*, 1967, **707**, 177; 1969, **721**, 186; 1971, **751**, 60 (*isol, struct, pmr*)
Nonaka, G. *et al., J.C.S. Perkin 1*, 1985, 165 (*pmr, cmr*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 217; 1989, **37**, 2071; 1990, **38**, 2151 (*struct, pmr, cmr, synth*)
Ishimaru, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3319 (*Vescalagincarboxylic acid*)
Vivas, N. *et al., Phytochemistry*, 1995, **39**, 1193 (*Castalagin, Vescalagin*)

Grandmarin G-318



(2′*R**,3′*R**)-*form*

$C_{15}H_{16}O_6$ 292.288

(2′*R*,3′*R*)-*form* [119139-64-9]
cis-*form*
Constit. of *Citrus natsudaidai*. Prisms (Et_2O/hexane). Mp 229-231°. $[\alpha]_D$ +5.41 (c, 0.074 in $CHCl_3$).

(2′*R*,3′*S*)-*form* [119239-48-4]
trans-*form*
Constit. of *Citrus* hybrids. Oil. $[\alpha]_D$ +7.69 (c, 0.078 in $CHCl_3$).

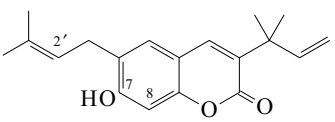
2′-Me ether: **trans-O-*Methylgrandmarin***
$C_{16}H_{18}O_6$ 306.315
Constit. of satsuma mandarins (*Citrus unshiu*). Amorph. solid. $[\alpha]_D$ -13.4 ($CHCl_3$).

3′-O-(3-Methylbutanoyl): **trans-*Grandmarin isovalerate***
$C_{20}H_{24}O_7$ 376.405
Constit. of citron (*Citrus medica*). Oil. $[\alpha]_D$ +24.1 (c, 0.071 in $CHCl_3$).

Ito, C. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3805; 1989, **37**, 2217; 1990, **38**, 2586

Gravelliferone G-319

[21316-80-3]
*3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, 9CI. 3-(1,1-Dimethylallyl)-7-hydroxy-6-(3-methyl-2-butenyl)coumarin, 8CI*



$C_{19}H_{22}O_3$ 298.381
Isol. from *Ruta graveolens* (rue). Mp 166-168°.

Me ether: [20958-62-7]
$C_{20}H_{24}O_3$ 312.408
Cryst. (hexane or EtOH aq.). Mp 70-72° (67-70°).

8-Methoxy: [30430-91-2]
$C_{20}H_{24}O_4$ 328.407
Constit. of *Ruta graveolens* (rue). Mp 131-133°.

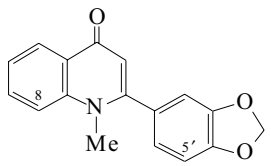
Me ether, 2′,3′-dihydro, 2′,3′-dihydroxy: [76960-88-8] ***Swietenocoumarin I***
$C_{20}H_{26}O_5$ 346.422
Gum.

Reisch, J. *et al., Experientia*, 1968, **24**, 992 (*isol, ir, uv*)
Reisch, J. *et al., Tet. Lett.*, 1968, 4395; 1970, 4305 (*deriv*)
Gonzalez, A.G. *et al., An. Quim.*, 1972, **68**, 415; 1977, **73**, 1015 (*isol, uv, ir*)
Bergenthal, D. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1978, **311**, 1026 (*cmr*)
Rao, A.V.R. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 1046 (*Swietenocoumarin I*)
Sharma, R.B. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 538 (*synth*)

Massanet, G.M. *et al., Heterocycles*, 1987, **26**, 1541 (*synth*)
Cairns, N. *et al., J.C.S. Perkin 1*, 1994, 3095; 3101 (*synth*)

Graveoline G-320

[485-61-0]
*2-(1,3-Benzodioxol-5-yl)-1-methyl-4(1*H*)-quinolinone, 9CI. 1-Methyl-2-(3,4-methylenedioxyphenyl)-4(1*H*)-quinolinone. Rutamine. Foliosine*



$C_{17}H_{13}NO_3$ 279.295
Alkaloid from *Ruta graveolens* (rue). Needles (EtOH). Mp 186-187° Mp 205-205.5° (dimorph.). Rutamine was the metastable lower-melting modification.

N-*De-Me:* [74054-38-9] *2-(3,4-Methylenedioxyphenyl)-4(1*H*)-quinolinone.* ***Norgraveoline***
Mp 288-290° (246-248°).

5′-Hydroxy: [107316-96-1] *2-(3-Hydroxy-4,5-methylenedioxyphenyl)-1-methyl-4(1*H*)-quinolinone.* ***3′-Hydroxygraveoline***
$C_{17}H_{13}NO_4$ 295.294
Amorph. Incorrect name in CA.

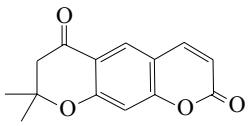
5′-Methoxy: [173180-39-7] *2-(3-Methoxy-4,5-methylenedioxyphenyl)-1-methyl-4(1*H*)-quinolinone.* ***3′-Methoxygraveoline***
$C_{18}H_{15}NO_4$ 309.321
Amorph. solid (EtOAc). Mp 193-194°. Numbering systems vary.

5′,8-Dimethoxy: [173180-40-0] *8-Methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-1-methyl-4(1*H*)-quinolinone.* ***3′,8-Dimethoxygraveoline***
$C_{19}H_{17}NO_5$ 339.347
Amorph. solid (MeOH). Mp 201-203°. Numbering systems vary.

Arthur, H.R. *et al., Aust. J. Chem.*, 1960, **13**, 510-513 (*isol, uv, ir, pmr, struct*)
Arthur, H.R. *et al., J.C.S.*, 1961, 4360-4361 (*synth*)
Schneider, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1967, **300**, 953-954 (*Rutamine*)
Reisch, J. *et al., Naturwissenschaften*, 1967, **54**, 200 (*synth*)
Razakova, D.M. *et al., Khim. Prir. Soedin.*, 1979, **15**, 810-812; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 716 (*Norgravoline*)
Kasahara, A. *et al., Chem. Ind. (London)*, 1981, 121 (*synth, Norgraveoline*)
Ulubelen, A. *et al., Phytochemistry*, 1986, **25**, 2692-2693 (*3′-Hydroxygraveoline*)
Koyama, J. *et al., Chem. Express*, 1992, **7**, 321-324 (*synth*)
Oliviera, F.M. *et al., Phytochemistry*, 1996, **41**, 647-649 (*3′-Methoxygraveoline, 3′,8-Dimethoxygraveoline*)
Annunziata, R. *et al., Synth. Commun.*, 1996, **26**, 495-501 (*synth*)
Koyama, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1038-1039 (*synth, ir, pmr*)

Graveolone G-321

[16499-05-1]
*6,7-Dihydro-8,8-dimethyl-2*H,*8*H-*benzo[1,2*-b:*5,4*-b′*]dipyran-2,6-dione*

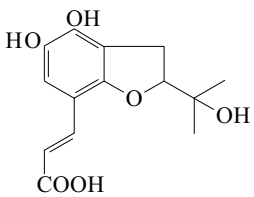


$C_{14}H_{12}O_4$ 244.246
Constit. of *Anethum graveolens* (dill). Cryst. (MeOH). Mp 177.5-178°.

Aplin, R.T. *et al., J.C.S.(C)*, 1967, 2593 (*isol*)
Mujumdar, A.S. *et al., J.C.S. Perkin 1*, 1974, 2236 (*synth*)
Talapatra, B. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 129 (*synth*)
Shinde, A.G. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 570 (*isol*)
Kavinde, M.N. *et al., Synth. Commun.*, 1990, **20**, 3259 (*synth*)

Gravolenic acid G-322

[13781-46-9]

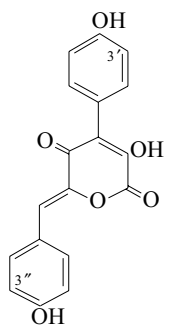


$C_{14}H_{16}O_6$ 280.277
Isol. from above-ground parts of *Ruta graveolens* (rue). Light-yellow cryst. (EtOAc or Me_2CO aq.). Mp 194°.

Reisch, J. *et al., Acta Pharm. Suec.*, 1966, **3**, 423 (*pmr, ord*)
Novák, I. *et al., Planta Med.*, 1966, **14**, 151 (*isol, uv, ir, struct*)

Grevilline A G-323

[41744-32-5]
*3-Hydroxy-4-(4-hydroxyphenyl)-6-[(4-hydroxyphenylmethylene)]-2*H-*pyran-2,5(6*H*)-dione, 9CI*



$C_{18}H_{12}O_6$ 324.289
Pigment from *Suillus grevillei* (larch bolete). Mp 197-199° (as tri-Ac). λ_{max} 268 (log ϵ 4.27); 389 (log ϵ 4.23) (MeOH).

3″-Hydroxy: [41744-33-6] ***Grevilline B***
$C_{18}H_{12}O_7$ 340.289
Pigment from *Suillus grevillei* (larch bolete). λ_{max} 280 (log ϵ 4.2); 396 (log ϵ 4.2) (MeOH).

3″-Hydroxy, tetra-Ac:
Mp 180-181°.

3′,3″-Dihydroxy: [41744-34-7] ***Grevilline C***
$C_{18}H_{12}O_8$ 356.288
Pigment from *Suillus grevillei* (larch bolete). λ_{max} 287 (log ϵ 4.24); 406 (log ϵ 4.23) (MeOH).

3′,3″-Dihydroxy, penta-Ac:
Mp 175-178°.

2′,3″,5′-Trihydroxy, 4′-deoxy: [54707-49-2] ***Grevilline D***
$C_{18}H_{12}O_8$ 356.288
Pigment from *Suillus grevillei* (larch bolete). Mp 300° dec. λ_{max} 288 (log ϵ 4.14); 409 (log ϵ 4.18) (MeOH).

Steglich, W. *et al., Tet. Lett.*, 1972, 4895 (*struct, pmr, uv*)
Besl, H. *et al., Z. Naturforsch., C*, 1974, **29**, 784 (*isol, struct*)
Lohrisch, H.J. *et al., Tet. Lett.*, 1975, 2905 (*synth*)
Lohrisch, H.J. *et al., Annalen*, 1986, 177 (*synth*)
Gill, M. *et al., Prog. Chem. Org. Nat. Prod.*, 1987, **51**, 4 (*rev*)
Pattenden, G. *et al., Tet. Lett.*, 1987, **28**, 4749 (*synth*)
Gill, M. *et al., Aust. J. Chem.*, 1990, **43**, 1497 (*synth*)

Grifolan 7N G-324

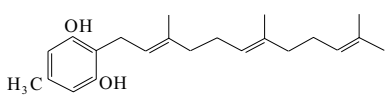
[98037-03-7]
A (1→3)-β-D-glucan having a β-D-glucopyranosyl group attached to the 6-position of almost every third backbone unit. MW *ca*. 1,200,000. Other similar polymers of smaller size isol. from this sp.. Isol. from *Grifola frondosa* (maitake). $[\alpha]_D$ +1.8 (c, 1 in H_2O).

[37361-00-5, 100358-66-5, 104074-36-4, 113189-33-6]

Iino, K. *et al., Carbohydr. Res.*, 1985, **141**, 111-119 (*isol*)

Grifolin G-325

[6903-07-7]
5-Methyl-2-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,3-benzenediol, 9CI. 2-Farnesyl-5-methylresorcinol

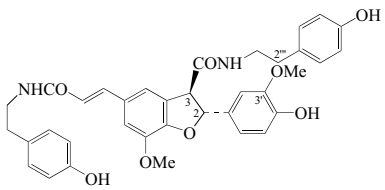


$C_{22}H_{32}O_2$ 328.494
Isol. from the edible maitake mushroom (*Grifola confluens*). Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 43°. λ_{max} 272 (ϵ 871) (MeOH) (Derep). λ_{max} (solvent not reported) (Derep). λ_{max} 273 (ϵ 2190); 275 (E1%/1cm 800); 281 (ϵ 2040) (MeOH) (Berdy). λ_{max} 272 (ϵ 1107); 275 (E1%/1cm 935); 281 (E1%/1cm 906) (EtOH) (Berdy). λ_{max} 223 ; 291 (MeOH-NaOH) (Berdy).
▶ LD_{50} (mus, scu) 1600 mg/kg.

Goto, T. *et al., Tetrahedron*, 1963, **19**, 2079 (*isol, ir, uv, ms, nmr, struct*)
Isobe, M. *et al., Tetrahedron*, 1968, **24**, 945 (*ir, uv, nmr, synth*)
Ima-ye, K. *et al., J.C.S. Perkin 1*, 1973, 2591 (*synth, ir, pmr*)
Yamada, S. *et al., Synth. Commun.*, 1978, 241 (*synth*)
Zechlin, L. *et al., Annalen*, 1981, 2099 (*isol, props*)
Marquet, J. *et al., Chem. Lett.*, 1981, 173 (*synth*)
DeMarch, P. *et al., An. Quim., Ser. C*, 1983, **79**, 15 (*synth*)
Ohta, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2239 (*synth, bibl*)
Misasa, H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1660 (*isol, ir, pmr*)
Saimoto, H. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 1178 (*synth*)
Mahioa, V. *et al., J. Nat. Prod.*, 1995, **58**, 324 (*isol, pmr, cmr*)
Nukata, M. *et al., Phytochemistry*, 2002, **59**, 731-737 (*isol, pmr, cmr*)

Grossamide G-326

[80510-06-1]



$C_{36}H_{36}N_2O_8$ 624.689
Isol. from *Capsicum annuum* var. *grossum*. Cryst. (MeOH/$CHCl_3$/cyclohexane). Mp 174-175° (133-135°).

3′-O-*De-Me:* [170171-94-5] ***Demethylgrossamide***
$C_{35}H_{34}N_2O_8$ 610.662
Amorph. powder.

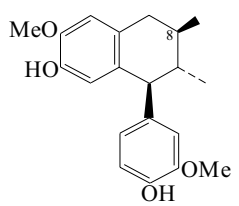
2-Epimer: ***Tribulusamide A***
$C_{36}H_{36}N_2O_8$ 624.689
Amorph. solid. $[\alpha]_D^{25}$ -10.9 (c, 0.1 in MeOH). λ_{max} 220 (log ϵ 4.22); 287 (log ϵ 4.01); 340 (log ϵ 4.07) (MeOH).

2-Epimer, 2‴-oxo: ***Tribulusamide B***
$C_{36}H_{34}N_2O_9$ 638.673
Amorph. solid. $[\alpha]_D^{25}$ -4.9 (c, 0.2 in MeOH). λ_{max} 220 (log ϵ 4.38); 285 (log ϵ 4.32); 320 (log ϵ 4.18) (MeOH).

Yoshihara, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 2593; 1983, **47**, 217 (*isol, synth, struct*)
Sakakibara, I. *et al., Phytochemistry*, 1991, **30**, 3013-3016 (*isol*)
Lajide, L. *et al., Phytochemistry*, 1995, **40**, 1105-1112 (*Demethylgrossamide*)
Li, J.-X. *et al., Planta Med.*, 1998, **64**, 628-631 (*Tribulusamides*)
Seca, A.M.L. *et al., Phytochemistry*, 2001, **58**, 1219-1223 (*isol, pmr, cmr*)

Guaiacin G-327

[36531-08-5]
5,6,7,8-Tetrahydro-8-(4-hydroxy-3-methoxyphenyl)-3-methoxy-6,7-dimethyl-2-naphthalenol, 9CI. 4,4′-Dihydroxy-3′,5-dimethoxy-2,7′-cyclolignan



$C_{20}H_{24}O_4$ 328.407

Lignan numbering shown. Constit. of *Myristica fragrans* (nutmeg). Cryst. (C_6H_6). Mp 204-206° (198-200°). $[\alpha]_D^{25}$ +46 ($CHCl_3$).

Di-Me ether: See Galbulin in *The Combined Chemical Dictionary.*

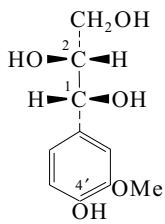
8-Epimer: [78341-26-1] ***Isoguaiacin***
$C_{20}H_{24}O_4$ 328.407
Cryst. $[\alpha]_D^{26}$ +89.7 (c, 0.39 in $CHCl_3$).

3-Epimer, di-Et ether:
Long needles (MeOH). Mp 108°. $[\alpha]_D^{23}$ -32 (c, 4.7 in $CHCl_3$).

King, F.E. *et al., J.C.S.*, 1964, 4011 (*isol*)
Majumder, P.L. *et al., Phytochemistry*, 1972, **11**, 811 (*isol*)
Gottlieb, O.R. *et al., Phytochemistry*, 1976, **15**, 773
Rao, K.V. *et al., J. Nat. Prod.*, 1982, **45**, 393
Fo, R.B. *et al., Planta Med.*, 1984, 53
Wang, B.-G. *et al., Planta Med.*, 2000, **66**, 511-515 (*Isoguaiacin*)

Guaiacylglycerol G-328

[1208-42-0]
1-(4-Hydroxy-3-methoxyphenyl)-1,2,3-propanetriol, 9CI, 8CI. α-(4-Hydroxy-3-methoxyphenyl)glycerol



(1*R*,2*R*)-*form*

$C_{10}H_{14}O_5$ 214.218

(1*RS*,2*RS*)-*form* [27391-16-8]
(±)-threo-*form*
Syrup.

1-O-*β*-D-*Glucopyranoside:*
$C_{16}H_{24}O_{10}$ 376.36
Isol. from *Pinus sylvestris* (Scotch pine) needles. Cryst. Mp 162-166°. $[\alpha]_D^{22}$ +45.

2-O-*β*-D-*Glucopyranoside:*
$C_{16}H_{24}O_{10}$ 376.36
Isol. from *Pinus sylvestris* (Scotch pine) needles. Amorph. $[\alpha]_D^{22}$ -16.

(1ξ,2ξ)-*form*

2-O-*β*-D-*Glucopyranoside:* [7162-98-3]
$C_{16}H_{24}O_{10}$ 376.36
Constit. of *Pinus sylvestris* (Scotch pine). Config. unknown.

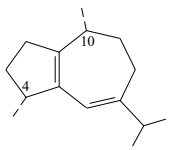
3-O-*β*-D-*Glucopyranoside:* [7094-73-7]
$C_{16}H_{24}O_{10}$ 376.36
Constit. of *Pinus sylvestris* (Scotch pine). Config. unknown.

[38916-91-5, 62078-66-4]

Adler, E. *et al., Acta Chem. Scand.*, 1963, **17**, 27 (*synth, config, bibl*)
Theander, O. *et al., Acta Chem. Scand.*, 1965, **19**, 1792 (*isol, glucosides*)
Rudloff, E. *et al., Chem. Ind. (London)*, 1965, 180 (*isol*)
Sano, Y. *et al., CA*, 1970, **73**, 121683r (*isol*)
Brezny, R. *et al., Chem. Zvesti*, 1978, **32**, 684 (*synth*)
Lundgren, L.N. *et al., Acta Chem. Scand., Ser. B*, 1982, **36**, 695; 1985, **39**, 241 (*synth, isol, pmr, bibl*)
Kikuchi, M. *et al., CA*, 1986, **105**, 206286t (*4′-glucoside*)
Deyama, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 523 (*isol*)
Sugiyama, M. *et al., Phytochemistry*, 1993, **33**, 1215 (*4′-glucoside*)
Fuzzati, N. *et al., Phytochemistry*, 1995, **39**, 409
Okuyama, E. *et al., Chem. Pharm. Bull.*, 1998, **46**, 655-662 (*isol, pmr, cmr*)
Greca, M.D. *et al., Phytochemistry*, 1998, **49**, 1299-1304 (*isol, pmr, cmr*)

1(5),6-Guaiadiene G-329

1,2,3,4,5,6-Hexahydro-1,4-dimethyl-7-(1-methylethyl)azulene, 9CI. 1,2,3,4,5,6-Hexahydro-7-isopropyl-1,4-dimethylazulene



(4α,10α)-*form*

$C_{15}H_{24}$ 204.355
λ_{max} 268 (ε 6700) ($CHCl_3$) (Derep). λ_{max} 208 (ε 6700) ($CHCl_3$) (Berdy).

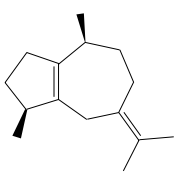
(4α,10α)-*form* [111900-51-7]
Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ +80 (c, 0.25 in $CHCl_3$).

(4β,10α)-*form* [111900-50-6]
Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ +36.2 (c, 0.16 in $CHCl_3$).

Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1616

1(5),7(11)-Guaiadiene G-330

[88-84-6]
β-Guaiene. *Guaiene. 1,2,3,4,5,6,7,8-Octahydro-1,4-dimethyl-7-(1-methylethylidene)azulene, 9CI*



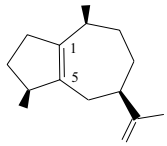
$C_{15}H_{24}$ 204.355
Flavouring ingredient. Constit. of sweet flag oil. Oil. d^{20} 0.91. $Bp_{15.5}$ 137-139°. $[\alpha]_D^{20}$ +13.

▶ ME6344000

Takeda, K. *et al., Tetrahedron*, 1961, **13**, 308 (*synth*)
Bates, R.B. *et al., J.A.C.S.*, 1962, **84**, 1307 (*struct*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 309
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1247-1248
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GKO000

1(5),11-Guaiadiene G-331

[3691-12-1]
α-Guaiene

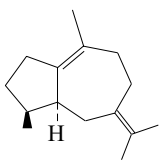


$C_{15}H_{24}$ 204.355
Constit. of guaiac wood oil (*Bulnesia sarmienti*). Oil. $Bp_{2.5}$ 78-79°. $[\alpha]_D^{19}$ -64.5 (c, 3.6 in dioxan).

1α,5α-Epoxide: [10410-05-6] *1α,5α-Epoxy-11-guaiene.* ***Epoxyguaiene***
$C_{15}H_{24}O$ 220.354
Constit. of the essential oil of *Cyperus rotundus* (nutgrass). Oil. Bp_1 102-104°. $[\alpha]_D$ +11.

Takeda, K. *et al., Tetrahedron*, 1961, 13 (*isol, struct*)
Kapadia, V.H. *et al., Tet. Lett.*, 1967, 4661

1(10),7(11)-Guaiadiene G-332

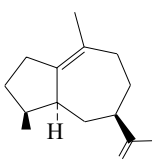


$C_{15}H_{24}$ 204.355

(4β,5α)-*form* [3772-93-8]
β-Bulnesene
Constit. of guaiac wood oil (*Bulnesia sarmienti*).

Heathcock, C.H. *et al., J.A.C.S.*, 1971, **93**, 1746 (*isol*)
Oppolzer, W. *et al., Helv. Chim. Acta*, 1980, **63**, 1198 (*synth*)
Sammes, P.G. *et al., Chem. Comm.*, 1983, 666 (*synth*)
Bromidge, S.M. *et al., J.C.S. Perkin 1*, 1985, 1725 (*synth*)

1(10),11-Guaiadiene G-333



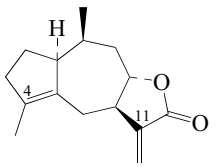
$C_{15}H_{24}$ 204.355

(4β,5α,10β)-*form* [3691-11-0]
α-Bulnesene. *δ-Guaiene*
Constit. of guaiac wood oil (*Bulnesia sarmienti*). Oil. Bp_8 118°. $[\alpha]_D$ +8.28. n_D^{20} 1.5046.

(4ξ,5ξ,10ξ)-*form*
α-Chigadmarene
Oil. Bp_9 117-118°. $[\alpha]_D^{28}$ -150 ($CHCl_3$).

Somasekar, A. *et al., J. Indian Chem. Soc.*, 1952, **29**, 604; 620 (*α-Chigadmarene*)
Bates, R.B. *et al., J.A.C.S.*, 1962, **84**, 1307 (*struct*)
Minyard, J.B. *et al., J. Agric. Food Chem.*, 1966, **14**, 332 (*isol*)
Francis, N.J.O. *et al., Planta Med.*, 1972, **22**, 201 (*biosynth*)
Mehta, G. *et al., Tet. Lett.*, 1975, 4495 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 371 (*rev, tox*)

4,11(13)-Guaiadien-12,8-olide G-334



(1α,8α,10β)-*form*

$C_{15}H_{20}O_2$ 232.322

(1α,8α,10β)-*form*

4α,5α-Epoxide: [68776-54-5] ***4,5-Epoxy-11(13)-guaien-12,8-olide***
$C_{15}H_{20}O_3$ 248.321
Constit. of *Inula helenium* (elecampane). Oil. $[\alpha]_D^{24}$ +39.7 (c, 1.4 in $CHCl_3$).

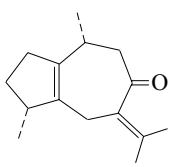
(1α,8β,10β)-*form* [117824-98-3]
3-Desoxoachalensolide
Oil. $[\alpha]_D^{24}$ +162 (c, 1.55 in $CHCl_3$).

11β,13-Dihydro: [117825-17-9] *4-Guaien-12,8-olide.* ***11,13-Dihydrodesoxoachalensolide***
$C_{15}H_{22}O_2$ 234.338

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172 (*isol, pmr, epoxide*)
Zdero, C. *et al., Phytochemistry*, 1988, **27**, 2835-2842 (*Desoxoachalensolide, Dihydrodesoxoachalensolide*)

1(5),7(11)-Guaiadien-8-one G-335

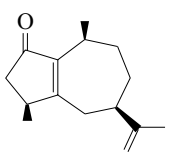
[71305-96-9]
Calamusenone



$C_{15}H_{22}O$ 218.338
Constit. of *Acorus calamus* (sweet flag). Oil. $Bp_{0.01}$ 90°. $[\alpha]_D^{22}$ +137 (c, 0.83 in $CHCl_3$).

Rohr, M. *et al., Phytochemistry*, 1979, **18**, 279-281

1(5),11-Guaiadien-2-one G-336

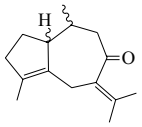


$C_{15}H_{22}O$ 218.338

(4β,7β,10β)-*form* [18374-76-0]
Rotundone
Constit. of the essential oil of *Cyperus rotundus* (nutgrass). Oil. Bp_1 128-129°. $[\alpha]_D$ -92.7.

Kapadia, V.H. *et al., Tet. Lett.*, 1967, 4661
Paknikar, S.K. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 1060 (*synth*)

4,7(11)-Guaiadien-8-one G-337

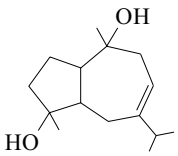


$C_{15}H_{22}O$ 218.338
Constit. of *Acorus calamus* (sweet flag). Oil. $Bp_{0.01}$ 90°. $[\alpha]_D^{22}$ -178 (c, 1 in $CHCl_3$).

Rohr, M. *et al., Phytochemistry*, 1979, **18**, 279

7-Guaiene-4,10-diol G-338

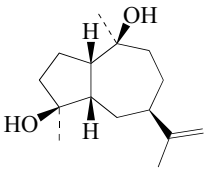
[31946-48-2]
Curcumadiol



$C_{15}H_{26}O_2$ 238.369
Constit. of *Curcuma zedoaria* (zedoary). Cryst. (EtOAc). Mp 145-145.5°. $[\alpha]_D$ -11.6 (c, 1.7 in EtOH).

Hinkino, H. *et al., Chem. Pharm. Bull.*, 1971, **19**, 93

11-Guaiene-4,10-diol G-339

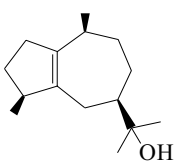


$C_{15}H_{26}O_2$ 238.369

(1β,4β,5β,10β)-*form* [217817-10-2]
Guaidiol
Constit. of *Curcuma zedoaria* (zedoary). Cryst. (C_6H_6/hexane). Mp 134-136°. $[\alpha]_D^{25}$ +30 (c, 1 in EtOH).

Syu, W.-J. *et al., J. Nat. Prod.*, 1998, **61**, 1531-1534 (*isol, pmr, cmr, cryst struct*)

1(5)-Guaien-11-ol G-340



$C_{15}H_{26}O$ 222.37

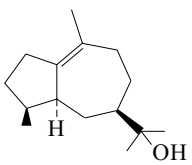
(4β,7β,10β)-*form* [489-86-1]
Guaiol. Champacol
Cryst. (Me_2CO at -15°). Mp 89-90°. $[\alpha]_D$ -41 (c, 3.5 in $CHCl_3$).

Ac: [134-28-1]

[17431-48-0] *Guaiol acetate*
$C_{17}H_{28}O_2$ 264.407
Flavouring ingredient with a sweet taste suggestive of currant. Liq. with a sweet currant-like taste.

Minato, H. *et al., Tetrahedron*, 1961, **13**, 308 (*struct*)
Marshall, J.A. *et al., J.O.C.*, 1972, **37**, 982 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1916 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Buchanan, G.L. *et al., J.C.S. Perkin 1*, 1973, 2404 (*synth*)
Andersen, N.H. *et al., Tet. Lett.*, 1973, 2079 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1248-1249 (*Ac*)

1(10)-Guaien-11-ol G-341

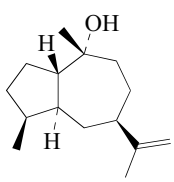


$C_{15}H_{26}O$ 222.37

(4β,5α,7β)-*form* [22451-73-6]
Bulnesol
Constit. of guaiac wood oil (*Bulnesia sarmienti*). Also from *Ferula* spp.. Cryst. Mp 69-70°. Bp_4 136-138°. $[\alpha]_D$ +3.8 (EtOH).

Heathcock, C.H. *et al., J.A.C.S.*, 1971, **93**, 1746 (*synth*)
Andersen, N.H. *et al., Synth. Commun.*, 1973, **3**, 115 (*synth*)
Teisseire, P. *et al., Recherches*, 1974, **19**, 8 (*isol*)

11-Guaien-10-ol G-342



$C_{15}H_{26}O$ 222.37

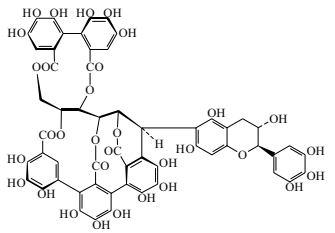
(1β,4β,5α,10α)-*form* [21698-41-9]
Pogostol
Constit. of patchouli oil from *Pogostemon cablin*. Oil. $[\alpha]_D$ -20.2 (c, 8.7 in $CHCl_3$).

Me ether: [197158-56-8] ***10-Methoxy-11-guaiene***
$C_{16}H_{28}O$ 236.397
Oil. $[\alpha]_D$ -33.3 (c, 0.066 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1608 (*isol*)
Bruns, K. *et al., Parfuem. Kosmet.*, 1978, **59**, 109 (*isol*)
Fleischer, T.C. *et al., J. Nat. Prod.*, 1997, **60**, 1054-1056 (*Me ether*)

Guajavin B G-343

[145826-23-9]



$C_{56}H_{38}O_{32}$ 1222.897

Isol. from the bark of *Psidium guajava* (guava). Pale brown amorph. powder + $8H_2O$. $[\alpha]_D^{21}$ +27.5 (c, 1.1 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2092 (*synth, pmr, cmr*)

4-Guanidinobutanoic acid G-344

[463-00-3]

4-[(Aminoiminomethyl)amino]butanoic acid, 9CI. 4-(1-Guanidino)butyric acid, 8CI. GGBA

$HN{=}C(NH_2)NHCH_2CH_2CH_2COOH$

$C_5H_{11}N_3O_2$ 145.161

Found in soybean, tea and *Citrus* spp.. Cryst. + $2H_2O$ (H_2O).

▶ Toxic to chick embryos.

Hydrochloride: [13890-14-7] Mp 184°.

Amide: [4210-97-3] *4-Guanidinobutyramide.* ***Tiformin, INN****. Tyformin, BAN* $C_5H_{12}N_4O$ 144.176Log P -2.9 (calc).

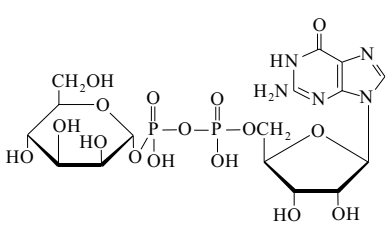
Amide; hydrochloride: [23256-39-5] *HL 523. Augmentin*† Cryst. (MeOH). Mp 108°.

Robin, Y. *et al., Bull. Soc. Chim. Biol.*, 1953, **35**, 285 (*biosynth*)
Irreverre, F. *et al., Nature (London)*, 1957, **80**, 704 (*occur*)
Makisumi, S. *et al., J. Biochem. (Tokyo)*, 1961, **49**, 284 (*isol*)
Pant, R. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1964, **335**, 272 (*synth*)
Reinbothe, H. *et al., Phytochemistry*, 1964, **3**, 327 (*biosynth*)
Tomita, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3628 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13387
Okabe, N. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1992 (*cryst struct*)

Guanosine diphosphate mannose G-345

[3123-67-9]

Guanosine 5′-(trihydrogen diphosphate)-mono-α-D-mannopyranosyl ester, 9CI. Guanosine 5′-(trihydrogen pyrophosphate)mono-α-D-mannopyranosyl ester, 8CI. GDP-mannose



$C_{16}H_{25}N_5O_{16}P_2$ 605.345

Present in egg white. Presumed intermed. in formation of mannan in yeast. Also isol. from green gram (*Phaseolus aureus*) seedlings. λ_{max} 260 ; 280 (H_2O).

K salt: λ_{max} 252 (ϵ 13700) (H_2O)).

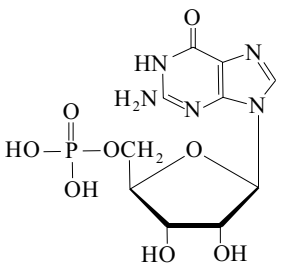
Cabib, E. *et al., J. Biol. Chem.*, 1954, **206**, 779
Munch-Petersen, A. *et al., Arch. Biochem. Biophys.*, 1955, **55**, 592 (*synth*)
Grégoire, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1963, **257**, 3508 (*isol*)
Donovan, J.W. *et al., Arch. Biochem. Biophys.*, 1967, **122**, 17
Braell, W.A. *et al., Anal. Biochem.*, 1976, **74**, 484 (*synth*)
Lee, C. *et al., Biochemistry*, 1976, **15**, 697 (*conformn, pmr*)
Pallanca, J.E. *et al., J.C.S. Perkin 1*, 1993, 3017

5′-Guanylic acid, 9CI, 8CI G-346

[85-32-5]

[661-20-1]

Guanosine 5′-(dihydrogen phosphate). Guanosine monophosphate. Guanosine 5′-phosphoric acid. GMP. E626



$C_{10}H_{14}N_5O_8P$ 363.223

Widely distributed in plants and animals, occurs in the hydrolysates of RNA. Mp 190-200° dec. pK_{a3} 6.66 (25°). λ_{max} 256 (ϵ 12400) (aq. buffer) (pH 2). λ_{max} 260 (ϵ 12100) (aq. buffer) (pH 12).

▶ MF9283000

Di-Na salt: [5550-12-9] *Disodium guanylate. E628* Flavour enhancer. Hygroscopic monohydrate. Mp 250° dec.

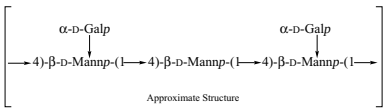
▶ LD_{50} (mus, orl) 15000 mg/kg. MF9290000

Chambers, R.W. *et al., J.A.C.S.*, 1957, **79**, 3747 (*synth*)
Tener, G.M. *et al., J.A.C.S.*, 1961, **83**, 159
Takaku, O. *et al., Agric. Biol. Chem.*, 1975, **39**, 2373 (*pmr*)
Simoncsits, A. *et al., Biochim. Biophys. Acta*, 1975, **395**, 74 (*synth*)
Norton, R.S. *et al., J.A.C.S.*, 1976, **98**, 1007 (*cmr*)
Barnes, C.L. *et al., Acta Cryst. B*, 1982, **38**, 812 (*cryst struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, GLS800
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1362
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 892 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GLS800

Guar gum G-347

[9000-30-0]

Guar flour. Cyanopsis gum. Burtonite V-7-E. Dealea TPI. Decorpa. Galactasol. Glucotard. Guarina. Guarem. E412. Many other names



Used in foods as emulsifier, stabiliser, thickener, gelling agent, formulation aid and firming agent; ice-cream stabiliser, used to improve the yield of curds in soft cheese, to increase the yield of doughs and baked products, as a binder and lubricant in sausages, and as thickener or viscosity control agent in beverages, salad dressings and relishes. Yellowish-white to white powder. Sol. H_2O; insol. org. solvs.

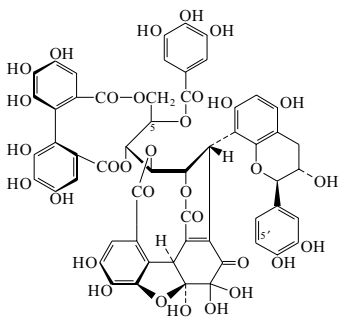
[2-Hydroxy-3-(trimethylammonio)propyl] ether: [65497-29-2] *Hi-Care® 1000*

2-Hydroxypropyl ether: [39421-75-5] *Jaguar® HP-11*

Goldstein, A.M. *et al., Ind. Gums*, 2nd edn., (eds. Whistler, R.L. *et al*), Academic Press, 1973, 303-321 (*rev*)
Busch, P. *et al., Parfuem. Kosmet.*, 1984, **65**, 756; 758-760 (*2-hydroxy-3-(trimethylammonio)propyl ether*)
Prabhanjan, H. *et al., Carbohydr. Polym.*, 1989, **11**, 279-292 (*2-hydroxypropyl ether*)
Todd, P.A. *et al., Drugs*, 1990, **39**, 917-928 (*rev, clinical use*)
Food Chemicals Codex, 4th edn., *National Academy Press*, 1996, 187-188 (*use, props*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 349
Merck Index, 12th edn., 1996, 780 (*props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1250-1255

Guavin A G-348

[105581-34-8]



$C_{56}H_{40}O_{32}$ 1224.913

Flavano-ellagitannin. A tannin constit. of the leaf of *Psidium guajava* (guava). Light brown amorph. powder + $9H_2O$. $[\alpha]_D^{20}$ -36 (c, 0.5 in MeOH).

O⁵-Degalloyl, O⁵-Ac: [107937-15-5] ***Guavin D***

$C_{51}H_{38}O_{29}$ 1114.844

Isol. from leaves of *Psidium guajava* (guava). Light brown amorph. powder + $6H_2O$. $[\alpha]_D^{20}$ -97 (c, 0.5 in MeOH).

O⁵-Degalloyl, O⁵-Ac, 5′-OH: [105581-31-5] ***Guavin C***

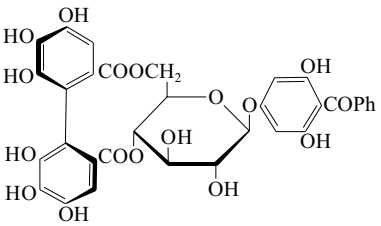
$C_{51}H_{38}O_{30}$ 1130.843

Isol. from *Psidium guajava* (guava). Pale brown powder + $5H_2O$. $[\alpha]_D$ -52 (c, 0.5 in MeOH).

Okuda, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 443; 1988, **36**, 3849 (*struct, pmr*)

Guavin B G-349

[94530-90-2]



$C_{33}H_{26}O_{17}$ 694.558

Ellagitanin constit. of *Psidium guajava* (guava). Light-brown amorph. powder. $[\alpha]_D$ -71 (c, 0.5 in MeOH).

Okuda, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3787

Gum karaya G-350

[9000-36-6]

Karaya gum. Sterculia gum. FEMA 2605

A partially acetylated polysaccharide containing D-galactouronic acid, D-galactose and L-rhamnose units. Emulsifier, thickener, foam stabiliser, flavouring ingredient, gelling agent.

Merck Index, 12th edn., 1996, 5296

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1510-1517

Gum tragacanth G-351

[9000-65-1]

Tragacanth gum. FEMA 3079

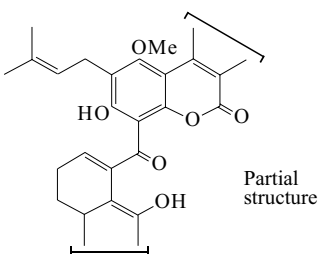
Complex mixt. of polysaccharides; contains two primary constituents, water-sol. Tragacanthin and water-insol. Bassorin. Stabiliser, thickener, emulsifier.

Merck Index, 12th edn., 1996, 4609

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2818-2822

α-Guttiferin G-352

[11048-92-3]



$C_{33}H_{38}O_8$ 562.658

In *CA*, α-Guttiferin is confused with α_2-Guttiferin which is identical with Morellic acid. See Morellin, M-759. Constit. of Gamboge the resinous exudation of *Garcinia morella* (batuan). Mp 113-115°. $[\alpha]_D^{26}$ -475 (c, 1.5 in $CHCl_3$).

► MG1578700

Py complex:

Mp 115-117°. $[\alpha]_D^{26}$ -561.2 (c, 1.496 in $CHCl_3$).

Nageswara Rao, K.V. *et al., Experientia*, 1961, **17**, 213 (*struct*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GME300

δ-Guttiferinic acid G-353

$C_{28}H_{34}O_8$ 498.572

Coumarinic acid. Struct. unknown. Constit. of the seeds of *Garcinia morella* (batuan). Yellow powder. Sol. MeOH, $CHCl_3$, bases; poorly sol. H_2O. Mp 122-128°. $[\alpha]_D^{25}$ -140.6 (c, 0.48 in $CHCl_3$). λ_{max} 245 (log ϵ 1.38) (MeOH). λ_{max} 278 ; 359 (MeOH) (Berdy).

Gupta, V.S. *et al., Indian J. Chem.*, 1963, **1**, 259-266 (*isol*)

γ-Guttiferinic acid G-354

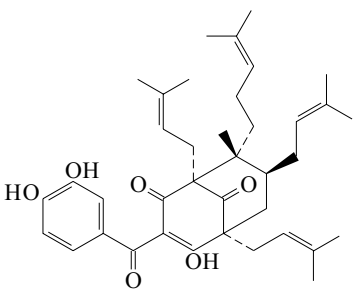
$C_{32}H_{40}O_9$ 568.663

Coumarinic acid. Struct. unknown. Constit. of the seeds of *Garcinia morella* (batuan). Pale yellow powder. Sol. MeOH, $CHCl_3$, bases; poorly sol. H_2O. Mp 80-84°. $[\alpha]_D^{25}$ -172.5 (c, 0.56 in $CHCl_3$). λ_{max} 220 (log ϵ 1.54); 275 (log ϵ 1.57); 318 (sh) (log ϵ 1.21) (MeOH). λ_{max} 278 ; 359 (MeOH) (Berdy).

Gupta, V.S. *et al., Indian J. Chem.*, 1963, **1**, 259-266

Guttiferone A G-355

[147687-34-1]



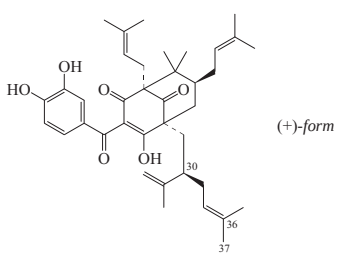
$C_{38}H_{50}O_6$ 602.809

Constit. of *Garcinia livingstonei* (imbe). Yellow oil. $[\alpha]_D$ +34 (c, 1.7 in $CHCl_3$). Log P 10.2 (uncertain value) (calc). λ_{max} 228 (ϵ 22500); 280 (ϵ 27300) (MeOH) (Derep).

Gustafson, K.R. *et al., Tetrahedron*, 1992, **48**, 10093 (*isol, pmr, cmr*)

Guttiferone E G-356

Camboginol. Garcinol†



(+)-*form*

$C_{38}H_{50}O_6$ 602.809

Guttiferone E was the name given originally to the (+)-form and Camboginol/Garcinol referred to the (-)-form. The identity of Camboginol is tentative. λ_{max} 228 (ϵ 22500); 280 (ϵ 27300) (MeOH) (Derep).

(+)-*form* [147782-04-5]

Yellow oil. $[\alpha]_D$ +101 (c, 0.5 in $CHCl_3$). Log P 10.07 (uncertain value) (calc). λ_{max} 228 (ϵ 19200); 280 (ϵ 22600) (MeOH) (Berdy). λ_{max} 230 ; 277 ; 346 (EtOH) (Berdy).

$\Delta^{36,37}$-Isomer: [52617-32-0] ***Xanthochymol***

$C_{38}H_{50}O_6$ 602.809

Constit. of the famine food *Garcinia xanthochymus*. Cryst. Mp 135°. λ_{max} 276 (ϵ 19952); 351 (MeOH) (Berdy). λ_{max} 230 (ϵ 8800); 277 (ϵ 10000); 346 (EtOH) (Berdy). λ_{max} 252 ; 363 (EtOH/HCl) (Berdy).

► LD_{50} (mus, ipr) 1000 mg/kg.

(-)-*form* [78824-30-3]

[75088-61-8]

Constit. of *Garcinia indica* (kokam). Camboginol isol. from *Garcinia cambogia*. Cryst. (hexane). Sol. MeOH, hexane; poorly sol. H_2O. Mp 132° (122°). $[\alpha]_D^{22}$ -143 (c, 0.01 in $CHCl_3$). λ_{max} 228 (ϵ 22500); 280 (ϵ 27300) (MeOH) (Derep). λ_{max} 278 (ϵ 26900) (MeOH) (Berdy). λ_{max} 229 (ϵ 18620); 286 (ϵ 14450) (EtOH) (Berdy). λ_{max} 244 (ϵ 13180); 354 (ϵ 10470) (hexane) (Berdy).

30-Epimer: ***Guttiferone F***

$C_{38}H_{50}O_6$ 602.809

$[\alpha]_D$ -293 (c, 0.37 in $CHCl_3$). λ_{max} 230 (ϵ 22500); 270 (ϵ 23000) (MeOH).

Karanjgoakar, C.G. *et al., Tet. Lett.*, 1973, 4977 (*Xanthochymol*)

Rao, A.V.R. *et al., Tet. Lett.*, 1980, **21**, 1975 (*isol, uv, pmr, cmr, Camboginol*)

Rao, A.V.R. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 983 (*struct, Camboginol*)

Krishnamurthy, N. *et al., Tet. Lett.*, 1981, **22**, 793; 1982, **23**, 2233 (*Garcinol*)

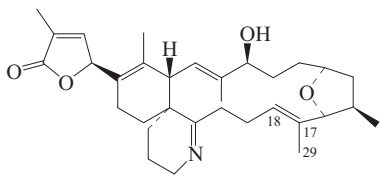
Sahu, A. *et al., Phytochemistry*, 1989, **28**, 1233 (*Garcinol*)

Gustafson, K.R. *et al., Tetrahedron*, 1992, **48**, 10093 (*isol, pmr, cmr*)

Fuller, R.W. *et al., J. Nat. Prod.*, 1999, **62**, 130-132 (*Guttiferone F*)

Gymnodimine G-357

[173792-58-0]



$C_{32}H_{45}NO_4$ 507.712

Isol. from New Zealand oysters (*Tiostrea chilensis*) and the dinoflagellate *Gymnodinium* cf. *mikimotoi*. Amorph. solid. $[\alpha]_D^{25}$ -10.4 (c, 0.13 in MeOH).

*$\Delta^{17,29}$-Isomer, 18*S*-hydroxy:* ***Gymnodimine B***

$C_{32}H_{45}NO_5$ 523.711

Seki, T. *et al., Tet. Lett.*, 1995, **36**, 7093 (*isol, pmr, cmr, struct*)

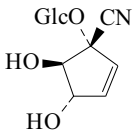
Stewart, M. *et al., Tet. Lett.*, 1997, **38**, 4889 (*cryst struct, abs config*)

Miles, C.O. *et al., J. Agric. Food Chem.*, 2000, **48**, 1373-1376 (*Gymnodimine B*)

Gynocardin G-358

[14332-17-3]

1-(β-D-Glucopyranosyloxy)-4,5-dihydroxy-2-cyclopentene-1-carbonitrile, 8CI



$C_{12}H_{17}NO_8$ 303.268

Glucoside from *Pangium edule* (football fruit). Prismatic needles + 1½ H_2O (H_2O). Mp 165-166° (anhyd.). $[\alpha]_D^{28}$ +72.9 (c, 0.96 in H_2O).

Hexa-Ac:

Mp 119-120°. $[\alpha]_D^{25}$ +40.2 (c, 1.69 in $CHCl_3$).

Hexa-Me ether:

Oil. $[\alpha]_D^{27}$ +87.1 (c, 1.54 in $CHCl_3$).

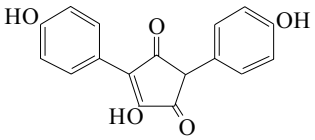
Coburn, R.A. *et al., J.O.C.*, 1966, **31**, 4312 (*isol, struct*)

Kim, H.S. *et al., Chem. Comm.*, 1970, 381 (*cryst struct*)

Gyrocyanin G-359

[52591-12-5]

4-Hydroxy-2,5-bis(4-hydroxyphenyl)-4-cyclopentene-1,3-dione, 9CI. 3,5-Bis(4-hydroxyphenyl)-1,2,4-cyclopentanetrione



$C_{17}H_{12}O_5$ 296.279

Several tautomers possible. Constit. of the mushroom *Gyroporus cyanescens* (cornflower bolete). Lemon-yellow prisms (EtOH aq.). Mp 240° (darkens). Readily oxidises to Gyroporin.

Besl, H. *et al., Chem. Ber.*, 1973, **106**, 3223

Steglich, W. *et al., Z. Naturforsch., C*, 1977, **32**, 46

Gyromitrin G-360

[16568-02-8]

Ethylidenemethylhydrazinecarboxaldehyde, 9CI. N′-*Ethylidene*-N-*formyl*-N-*methylhydrazine. Acetaldehyde* N-*formyl*-N-*methylhydrazone*

$H_3CCH{=}NNMeCHO$

$C_4H_8N_2O$ 100.12

Toxin from the fungus *Gyromitra esculenta*. Freq. cause of mushroom poisoning. Unstable cryst. Mp 19.5° (5°).

▶ Toxic, carcinogenic. Toxicity varies greatly between individuals. LQ8500000

List, P.H. *et al., Tet. Lett.*, 1967, 1893 (*isol*)

Zinner, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1971, **304**, 706 (*synth*)

Pyysalo, H. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 235; 792 (*isol, ms*)

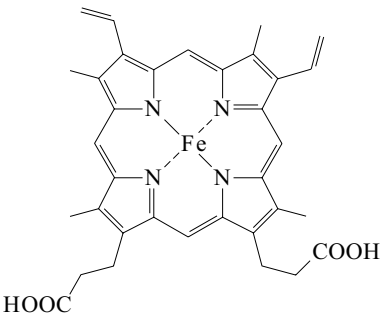
Zelenin, K.N. *et al., Zh. Org. Khim.*, 1978, **14**, 490 (*pmr, conformn*)

Meier-Bratschi, A. *et al., J. Agric. Food Chem.*, 1983, **31**, 1117 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAH000

Haem H-1

[14875-96-8]
[7,12-Diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-N^{21},N^{22},N^{23},N^{24}]dihydrogenferrate(2-), 9CI. Heme b. Heme. Protohaem IX



$C_{34}H_{32}FeN_4O_4$ 616.498

Prosthetic group of the blood pigments haemoglobin and myoglobin, and of a range of cytochrome, peroxidase and catalase enzymes.

Protein conjugate (1):

[100684-32-0] ***Myoglobin***
Isol. from skeletal muscles and some heart muscles of many animal spp.. O_2-carrying globular haem-protein consisting of a single polypeptide chain of 153 residues. MW *ca*. 17500.

Protein conjugate (2): [9008-02-0] ***Haemoglobin***. *Hemoglobin*
Found in mammalian blood. O_2-carrying globular protein containing 4 haem units. MW *ca.* 64,450. Reversibly binds O_2 to form oxyhaemoglobin (low spin, diamagnetic, Fe atom co-planar with porphyrin ring). Deoxyhaemoglobin is high spin, paramagnetic with Fe atom above plane of porphyrin ring.

Haemoglobin deriv.: [142261-03-8] ***Haemoglobin crosfumaril, INN, USAN***. *Haemoglobin Ao (human $\alpha_2\beta_2$ tetrameric subunit) α-chain 99,99′-diamide with (*E*)-2-butenoic acid. HemAssist. DCLHb*

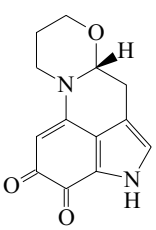
Fe-*Nitrosyl:*
$C_{34}H_{32}FeN_5O_5$ 646.504
Pigment responsible for the pink colouration of cooked cured meat. Characterised spectroscopically.

[9034-60-0, 9034-72-4, 9050-29-7, 37294-39-6, 51142-53-1, 56363-95-2, 56451-61-7, 56690-69-8, 59650-79-2, 67312-26-9, 70699-68-2, 73561-33-8, 73561-34-9, 76082-69-4, 79585-70-9, 83745-26-0, 86753-08-4, 87491-40-5, 89700-67-4, 95329-61-6, 104200-15-9, 104200-17-1, 104716-92-9]

Caughey, W.S. *et al., Inorg. Biochem.*, 1973, **2**, 795 (*rev*)
Wuethrich, K. *et al., Pure Appl. Chem.*, 1974, **40**, 127 (*cmr*)
Fairbanks, V.F. *et al., Fundam. Clin. Chem.*, (Tietz, N.W., Ed.), 2nd Edn., Saunders (Philadelphia), 1976, 401 (*rev*)
Kaplan, B.H. *et al., Hematology*, 2nd Edn., 1977, 149 (*rev, synth*)
De Matteis, F. *et al., Handb. Exp. Pharmacol.*, 1978, **44**, 1 (*book*)
Rothgeb, T.M. *et al., Methods Enzymol.*, 1978, **52**, 473 (*rev, isol, anal*)
The Porphyrins, (Ed. Dolphin, D.H.), Academic Press, N.Y., 1979, (*book*)
Elder, G.H. *et al., Iron Biochem. Med. 1974-1980*, 1980, **2**, 245 (*rev*)
Rothgeb, T.M. *et al., J. Biol. Chem.*, 1981, **256**, 1432 (*pmr*)
Sykes, A.G. *et al., Adv. Inorg. Bioinorg. Mech.*, 1982, **1**, 121 (*rev*)
Clerico, A. *et al., J. Nucl. Med. Allied Sci.*, 1982, **26**, 117 (*anal*)
Dickinson, L.C. *et al., Chem. Soc. Rev.*, 1983, **12**, 387 (*rev, epr*)
Scheidt, W.R. *et al., Phys. Bioinorg. Chem. Ser.*, 1983, **1**, 89 (*rev*)
Moore, G.R. *et al., Biochim. Biophys. Acta*, 1984, **788**, 147 (*pmr*)
Perutz, M. *et al., Methods Enzymol.*, 1985, **114**, 3 (*rev, cryst struct*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*revs, biosynth*)
Brunori, M. *et al., Top. Mol. Struct. Biol.*, 1985, **7**, 263 (*rev, struct, props*)
Dawson, J.H. *et al., Adv. Inorg. Bioinorg. Mech.*, 1986, **4**, 1 (*rev*)
Porstmann, B. *et al., Z. Klin. Med.*, 1986, **41**, 5 (*rev*)
Frauenfelder, H. *et al., Ann. N.Y. Acad. Sci.*, 1987, **504**, 151 (*rev*)
Smith, K.M. *et al., Heterocycles*, 1987, **26**, 1947 (*rev, synth*)
Biological Applications of Raman Spectroscopy; Vol. 3 Resonance Raman Spectra of Heme and Metalloproteins, (Ed. Spiro, T.G.), John Wiley, N.Y., 1988, (*Raman*)
Gadsby, P.M.A. *et al., J.A.C.S.*, 1990, **112**, 5003 (*epr, mcd*)
Pickelmann, S. *et al., Chir. Forum Exp. Klin. Forsch.*, (Suppl. 1), 1996, 97-100 (*haemoglobin crosfumaril*)
Pegg, R.B. *et al., J. Agric. Food Chem.*, 1996, **44**, 416-421 (*nitrosyl*)

Haematopodin H-2

[151964-21-5]

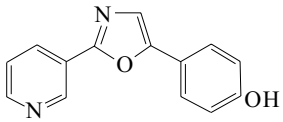


$C_{13}H_{12}N_2O_3$ 244.249
Pigment from fruiting bodies of the toadstool *Mycena haematopus* (blood mycena). Black cryst. +1 H_2O (CH_2Cl_2/MeOH). Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ +571 (c, 0.14 in MeOH). Mp >350°. Artifact formed during workup λ_{max} 208 (ϵ 9900); 242 (ϵ 18600); 344 (ϵ 10700); 514 (ϵ 890) (MeOH) (Berdy).

Baumann, C. *et al., Angew. Chem., Int. Ed.*, 1993, **32**, 1087 (*isol, uv, ir, pmr, cmr, cd, cryst struct*)
Hopmann, C. *et al., Annalen*, 1996, 1117 (*synth*)

Halfordinol H-3

[4210-82-6]
4-[2-(3-Pyridinyl-5-oxazolyl)]phenol, 9CI. 5-(4-Hydroxyphenyl)-2-(3-pyridyl)oxazole. Aegelenine



$C_{14}H_{10}N_2O_2$ 238.245
Fine cream needles. Mp 255-256°.

Ac:
Mp 167-180°.

Me ether: [33864-03-8] *3-[5-(4-Methoxyphenyl)-2-oxazolyl]pyridine, 9CI.* ***Methylhalfordinol***. *2-(3-Pyridyl)-5-(4-methoxyphenyl)oxazole*
$C_{15}H_{12}N_2O_2$ 252.272
Alkaloid from ripe fruits of *Aegle marmelos* (bael fruit) and the aerial parts of *Triphasia trifolia* (limeberry). Needles (C_6H_6/petrol or EtOH). Mp 100-101° (98-99°).

O-*(3-Methyl-2-butenyl):* [17190-80-6] **O-*Isopentenylhalfordinol***. *3-[5-[4-[(3-Methyl-2-butenyl)oxy]phenyl]-2-oxazolyl]pyridine, 9CI.* O-*(3,3-Dimethylallyl)halfordinol.* O-*Prenylhalfordinol*
$C_{19}H_{18}N_2O_2$ 306.363
Alkaloid from *Aegle marmelos* (bael fruit). Cryst. (EtOAc/hexane). Mp 118-119° (109-111°).

O-*(3-Methyl-3-butenyl):* [17190-81-7] **O-*(3-Methyl-3-butenyl)halfordinol***
$C_{19}H_{18}N_2O_2$ 306.363Obt. only in admixture with the isomeric *O*-Isopentenylhalfordinol. Alkaloid not named in the paper.

O-*(2,3-Dihydroxy-3-methylbutyl):* [21059-65-4] ***Halfordine***†
$C_{19}H_{20}N_2O_4$ 340.378
Cream needles (MeOH). Mp 163-164°.

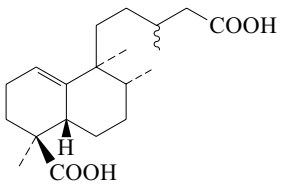
O-*(2,3-Dihydroxy-3-methylbutyl),* N-*Me:***N-*Methylhalfordinium***
$C_{20}H_{23}N_2O_4^{\oplus}$ 355.413
Fine yellow needles (EtoAc/MeOH)(as chloride). Mp 235° dec. (chloride). Methylated on the pyridine nitrogen.

O-*(3-Methyl-2-oxobutyl):* [21144-32-1] ***Halfordinone***
$C_{19}H_{18}N_2O_3$ 322.363
Needles (Me_2CO/petrol). Mp 132-133°.

O-*(3,7-Dimethyl-2,6-octadienyl)* (E-*):* [89764-17-0] **O-*Geranylhalfordinol***
$C_{24}H_{26}N_2O_2$ 374.482

Crow, W.D. *et al., Aust. J. Chem.*, 1964, **17**, 119; 1965, **18**, 1433 (*ir, ms, pmr, isol, struct*)
Dreyer, D.L. *et al., J.O.C.*, 1968, **33**, 3658 (*derivs*)
Onaka, T. *et al., Tet. Lett.*, 1971, 4393 (*synth*)
Manandhar, M.D. *et al., Phytochemistry*, 1978, **17**, 1814 (*derivs*)
Burke, B.A. *et al., Tet. Lett.*, 1978, 2723 (*deriv*)
Sharma, B.R. *et al., Planta Med.*, 1981, **43**, 102 (*Methylhalfordinol*)
Bowen, I.H. *et al., Phytochemistry*, 1982, **21**, 433 (*Methylhalfordinol*)
Philip, S. *et al., Heterocycles*, 1984, **22**, 9 (*O-Geranylhalfordinol*)
Velez, H. *et al., Rev. Cubana Quim.*, 1986, **2**, 22; *CA*, **109**, 20246g (*Methylhalfordinol*)
Dominguez, X.A. *et al., Heterocycles*, 1988, **27**, 35 (*derivs*)
Molina, P. *et al., Heterocycles*, 1993, **36**, 2255 (*synth, Methylhalfordinol*)

1(10)-Halimene-15,19-dioic acid H-4



$C_{20}H_{32}O_4$ 336.47

***ent*-form**

Isol. (as di-Me ester) from seed-pod resin of *Hymenaea courbaril*.

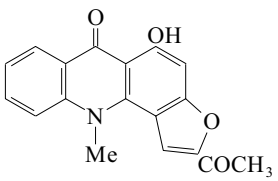
[52591-97-6, 52591-98-7]

Khoo, S.F. *et al., Tetrahedron*, 1973, **29**, 3379 (*isol*)

Hallacridone H-5

[109897-77-0]

2-Acetyl-5-hydroxy-11-methylfuro[2,3-c]acridin-6(11H)-one, 9CI



$C_{18}H_{13}NO_4$ 307.305

Struct. revised in 1989. Minor alkaloid from *Ruta graveolens* (rue) tissue cultures. Yellow needles ($CHCl_3$). Mp 295-298°.

Baumert, A. *et al., Pharmazie*, 1987, **42**, 67; *CA*, **107**, 93537w

Baumert, A. *et al., Fitoterapia*, 1988, **59**, 83; *CA*, **109**, 226730u

Reisch, J. *et al., J.C.S. Perkin 1*, 1989, 1047 (*synth, ir, struct*)

Halocins H-6

[120501-02-2]

Polypeptides. Prod. by *Haloferax* spp. Bacteriocins with potential food uses.

Halocin H1 [179393-68-1]

Prod. by *Haloferax mediterranei* Xia3.

Halocin H4 [81775-78-2]

Prod. by *Haloferax mediterranei* ATCC 33500. Comprises a single polypeptide chain.

Halocin H6 [127120-77-8]

Prod. by *Haloferax gibbonsii*.

Rodriguez-Valera, F.G. *et al., Can. J. Microbiol.*, 1982, **28**, 151-154 (*isol*)

Meseguer, I. *et al., FEMS Microbiol. Lett.*, 1985, **28**, 177-182 (*Halocin H4*)

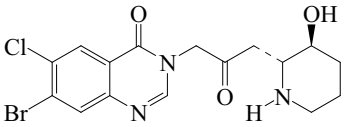
Torreblanca, M. *et al., J. Gen. Microbiol.*, 1989, **135**, 2655-2661 (*Halocin H6*)

Platas, G. *et al., Microbiologia (Madrid)*, 1996, **12**, 75-84 (*Halocin H1*)

Halofuginone, BAN, INN H-7

[55837-20-2]

7-Bromo-6-chloro-3-[3-(3-hydroxy-2-piperidinyl)-2-oxopropyl]-4(3H)-quinazolinone, 9CI



$C_{16}H_{17}BrClN_3O_3$ 414.685

Veterinary antiprotozoal agent. Poultry feed additive for prevention of coccidiosis. Log P 0.99 (calc). Analogue of Febrifugine. USA coccidiostat market share 5-10% in 1995-6.

Hydrobromide: [64924-67-0] *Halofuginone hydrobromide, USAN. Stenorol. RU 19110*

Cryst. Mp 247° dec.

U.S. Pat., 1967, 3 320 124; *CA*, **68**, 39647 (*synth, pharmacol*)

Ger. Pat., 1977, 2 703 652; *CA*, **87**, 184543e (*synth, pharmacol*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 514

Beier, R.C. *et al., J. Agric. Food Chem.*, 1998, **46**, 1049-1054 (*anal*)

Pines, M. *et al., Drug Dev. Res.*, 2000, **50**, 371-378 (*pharmacol, rev*)

Drugs of the Future, 2000, **25**, 635-636 (*rev*)

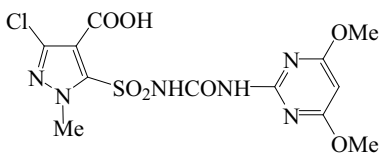
McGaha, T.L. *et al., J. Invest. Dermatol.*, 2002, **118**, 461-470 (*pharmacol*)

Gavish, Z. *et al., The Prostate*, 2002, **51**, 73-83 (*pharmacol*)

Halosulfuron, BSI H-8

[135397-30-7]

3-Chloro-5-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-1-methyl-1H-pyrazole-4-carboxylic acid, 9CI. 3-Chloro-5-(4,6-dimethoxypyrimidin-2-ylcarbamoylsulfamoyl)-1-methylpyrazole-4-carboxylic acid



$C_{12}H_{13}ClN_6O_7S$ 420.789

Me ester: [100784-20-1] ***Halosulfuron-methyl, BSI***. *Manage. Permit. Sempra. A 841101. MON 12000. NC 319. MON 12037*

$C_{13}H_{15}ClN_6O_7S$ 434.816

Herbicide used on maize, sugarcane and rice. Powder. Mp 176-177°. pK_a 3.44 (22°).

▶ LD_{50} (rat, orl) 8865 mg/kg.

Eur. Pat., 1985, 281 582, (*Nissan*); *CA*, **104**, 148871w (*Halosulfuron-methyl, synth, activity*)

Japan. Pat., 1985, 60 208 977; *CA*, **104**, 148871w (*synth, activity*)

Suzuki, K. *et al., Brighton Crop Prot. Conf. - Weeds*, 1991, **1**, 31-37 (*Halosulfuron-methyl, activity*)

Yamamoto, S. *et al., ACS Symp. Ser.*, 1992, **504**, 34-42 (*Halosulfuron-methyl, rev, synth, activity, analogues*)

Derr, J.F. *et al., Weed Technol.*, 1996, **10**, 95-99 (*Halosulfuron-methyl, activity*)

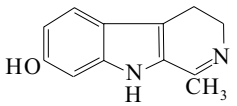
Dubelman, A.M. *et al., J. Agric. Food Chem.*, 1997, **45**, 2314-2321 (*metab*)

Pesticide Manual, 12th edn., 2000, No. 414

Harmalol, 8CI H-9

[525-57-5]

4,9-Dihydro-1-methyl-3H-pyrido[3,4-b]indol-7-ol, 9CI. 3,4-Dihydro-7-hydroxy-1-methyl-β-carboline



$C_{12}H_{12}N_2O$ 200.24

Alkaloid from *Passiflora incarnata* (maypops). Fine orange-yellow or red needles + $3H_2O$ (EtOH aq.). Sol. Me_2CO, $CHCl_3$; poorly sol. H_2O. Mp 100-105°. Log P 1.31 (uncertain value) (calc). Readily oxid. in air λ_{max} 218 ; 260 ; 376 (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 175 mg/kg.

Hydrochloride: [6028-00-8]

Green cryst. (EtOH), red needles (EtOH). Mp 264-267° dec.

Me ether: [304-21-2] *4,9-Dihydro-7-methoxy-1-methyl-3H-pyrido[3,4-b]indole. 3,4-Dihydro-7-methoxy-1-methyl-β-carboline.* ***Harmaline****. Dihydroharmine. Harmidine*

$C_{13}H_{14}N_2O$ 214.266

Alkaloid from *Passiflora incarnata* (maypops). Sol. Et_2O. Mp 250-251° (227-229°). Log P 1.91 (uncertain value) (calc). λ_{max} 218 (ϵ 17700); 260 (ϵ 7950); 376 (ϵ 10050) (MeOH) (Berdy).

▶ LD_{50} (rat, scu) 120 mg/kg. UU9800000

Me ether, hydrochloride: [6027-98-1]

Mp 212° Mp 239-240° (dihydrate).

▶ MG8750000

Me ether, N-*Ac:*

Mp 204-205°.

Me ether, 1,2-dihydro: See Tetrahydroharmine in *The Combined Chemical Dictionary.*

[6028-07-5]

Fischer, O. *et al., Ber.*, 1889, **22**, 637 (*synth*)

Späth, E. *et al., Ber.*, 1930, **63**, 120 (*Me ether, synth*)

Konovalova, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1935, **273**, 156 (*synth*)

Spenser, I.D. *et al., Can. J. Chem.*, 1959, **37**, 1851 (*derivs, synth, uv, ir*)

Robinson, B. *et al., Chem. Ind. (London)*, 1965, 605 (*Me ether, pmr*)

Phillipson, J.D. *et al., J. Chromatogr.*, 1975, **105**, 163 (*Me ether, uv, tlc, glc*)

Allen, J.R.F. *et al., Phytochemistry*, 1980, **19**, 1573 (*occur, bibl*)

Coune, C.A. *et al., Phytochemistry*, 1980, **19**, 2009 (*cmr*)

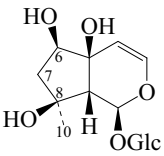
Verpoorte, R. *et al., Org. Magn. Reson.*, 1984, **22**, 328 (*cmr*)

Biondic, M.C. *et al., J.C.S. Perkin 2*, 1992, 1049 (*Me ether, uv*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1376 (*Me ether*)

Harpagide H-10

[6926-08-5]



$C_{15}H_{24}O_{10}$ 364.349
Log P -6.4 (uncertain value) (calc).

6′-O-α-D-Glucopyranosyl: [131862-10-7] ***Stachyoside A***
$C_{21}H_{34}O_{15}$ 526.491
Isol. from *Stachys sieboldii* (Chinese artichoke). Amorph.

[79549-53-4, 133645-38-2]

Miyase, T. *et al., CA*, 1991, **114**, 78651e (*Stachyoside A*)

Hederagenin bisdesmosides H-11

Derivs. of Hederagenin (see D-582) both glycosylated at C-3 and with a glycosyl ester group at C-28.

Triglycosides

3-O-[β-D-Glucopyranosyl-(1→2)-α-L-arabinopyranoside], 28-O-β-D-glucopyranosyl ester: [141492-08-2] ***Medicoside F***
$C_{47}H_{76}O_{18}$ 929.107
Constit. of *Medicago sativa* (alfalfa). Amorph. powder. $[\alpha]_D^{23}$ +30 (c, 2.37 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-xylopyranoside], 28-O-β-D-glucopyranosyl ester: [169397-84-6] ***Medicoside E***
$C_{47}H_{76}O_{18}$ 929.107
Constit. of *Medicago sativa* (alfalfa). $[\alpha]_D^{20}$ +51.9 (c, 1.31 in MeOH).

3-O-[(2-Carboxy-1-carboxymethoxy-2-hydroxyethyl)-(→3)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [178535-50-7] ***Betavulgaroside VI***
$C_{47}H_{72}O_{21}$ 973.073
Constit. of *Beta vulgaris* (sugar beet). Cryst. ($CHCl_3$/MeOH). Mp 210-212°. $[\alpha]_D^{30}$ +14.8 (c, 0.1 in MeOH).

Tetraglycosides

3-O-[α-L-Arabinopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-α-L-arabinopyranoside], 28-O-β-D-glucopyranosyl ester: [107241-23-6] ***Medicoside I***
$C_{52}H_{84}O_{22}$ 1061.222
Isol. from *Medicago sativa* (alfalfa). $[\alpha]_D$ +31 (c, 1.05 in $CHCl_3$).

3-O-[β-D-Xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [178894-84-3] ***Tuberoside C***
$C_{53}H_{84}O_{24}$ 1105.232
Constit. of *Ullucus tuberosus* (ulluco).

Massiot, G. *et al., J.C.S. Perkin 1*, 1988, 3071-3079 (*Medicosides, pmr, ms*)
Timbekova, A.E. *et al., Khim. Prir. Soedin.*, 1993, **29**, 701-705; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 622 (*Medicoside E, Medicoside F*)
Espada, A. *et al., Annalen*, 1996, 781-784 (*Tuberoside C*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1758-1763 (*Betavulgaroside VI*)

Hederagenin 3-glycosides H-12

Derivs. of, Hederagenin (see D-582) glycosylated at C-3 only.

Diglycosides

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucuronopyranoside]: [25406-62-6] ***Spinasaponin B***
$C_{42}H_{66}O_{15}$ 810.974
Saponin from roots of spinach (*Spinacia* spp.).

3-O-[(2-Carboxy-1-carboxymethoxy-2-hydroxyethyl)-(→3)-β-D-glucuronopyranoside]: [178535-51-8] ***Betavulgaroside VII***
$C_{41}H_{62}O_{16}$ 810.931
Constit. of *Beta vulgaris* (sugar beet). Cryst. ($CHCl_3$/MeOH). Mp 190-192°. $[\alpha]_D^{30}$ +59.4 (c, 0.1 in MeOH).

Triglycosides

3-O-[α-L-Arabinopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-α-L-arabinopyranoside]: [102349-43-9] ***Medicoside C***
$C_{46}H_{74}O_{17}$ 899.08
Isol. from alfalfa (*Medicago sativa*). Mp 227-229°. $[\alpha]_D^{21}$ +34 (c, 0.41 in EtOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]: [171828-79-8] ***Congmuyenoside A***. *Elatoside J*
$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. (MeOH aq.). Mp 231-236° Mp 262-264°. $[\alpha]_D^{25}$ +25.7 (c, 0.1 in $CHCl_3$/MeOH aq.).

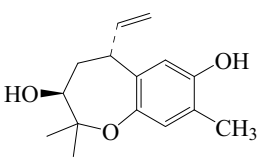
Tetraglycosides

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]: [184427-82-5] ***Congmuyenoside B***
$C_{54}H_{88}O_{24}$ 1121.275
Constit. of *Aralia elata* (Japanese angelica tree). Needles (MeOH). Mp 283-284°. $[\alpha]_D$ +30 (Py).

Tschesche, R. *et al., Annalen*, 1976, **726**, 125-135 (*Spinasaponin B*)
Timbekova, A.E. *et al., Khim. Prir. Soedin.*, 1985, **21**, 805-806; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 763 (*Medicoside C*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1878-1882 (*Elatoside J*)
Kuang, H.-X. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2183-2185 (*Congmuyenosides A and B*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1758-1763 (*Betavulgaroside VII*)

Heliannuol C H-13

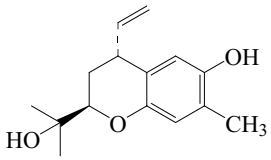
[161730-08-1]



$C_{15}H_{20}O_3$ 248.321
A rearranged bisabolane sesquiterpenoid. Constit. of *Helianthus annuus* (sunflower). Oil. $[\alpha]_D^{25}$ -38 (c, 0.1 in $CHCl_3$).
Macías, F.A. *et al., J.O.C.*, 1994, **59**, 8261-8266 (*isol, pmr, cmr*)

Heliannuol E H-14

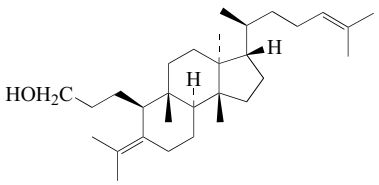
[241139-49-1]



$C_{15}H_{20}O_3$ 248.321
Constit. of *Helianthus annuus* (sunflower). Yellow oil. $[\alpha]_D^{25}$ -68.6 (c, 0.1 in $CHCl_3$).
Macías, F.A. *et al., Tet. Lett.*, 1999, **40**, 4725-4728 (*isol, pmr, cmr*)

Helianol H-15

[178330-51-3]
19(10→9)-Abeo-3,4-secotirucalla-4,24-dien-3-ol



$C_{30}H_{52}O$ 428.74
Constit. of *Helianthus annuus* (sunflower). Gum. Struct revised in 1998.

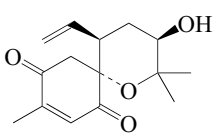
Octanoyl: [290305-83-8] ***Helianyl octanoate***
$C_{38}H_{66}O_2$ 554.938
Constit. of *Helianthus annuus* (sunflower).

20-Epimer: [203570-12-1] *19(10→9)-Abeo-3,4-secoeupha-4,24-dien-3-ol.* ***Isohelianol***
$C_{30}H_{52}O$ 428.74
Constit. of *Camellia sasanqua*. Amorph. solid. $[\alpha]_D^{25}$ +34.6 (c, 0.3 in $CHCl_3$).

Akihisa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1255-1257 (*isol, pmr, cmr*)
Akihisa, T. *et al., J. Nat. Prod.*, 1998, **61**, 409-412 (*isol, pmr, cmr, struct*)
Schulz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*Helianyl octanoate*)

Heliespirone A H-16

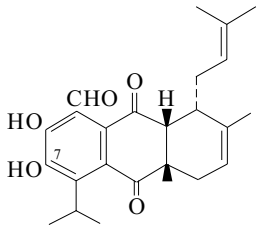
[202533-71-9]



$C_{15}H_{20}O_4$ 264.321
Constit. of *Helianthus annuus* (sunflower). Yellow oil. $[\alpha]_D^{25}$ -29 (c, 0.1 in $CHCl_3$).
Marías, F.A. *et al., Tet. Lett.*, 1998, **39**, 427-430 (*isol, pmr, cmr*)

Heliocide H_1 H-17

[65024-84-2]



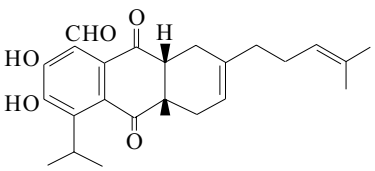
$C_{25}H_{30}O_5$ 410.509
Constit. of *Gossypium hirsutum* (cotton).

7-Me ether: [64872-35-1] ***Heliocide B_1***
$C_{26}H_{32}O_5$ 424.536

Stipanovic, R.D. *et al., J. Agric. Food Chem.*, 1977, **26**, 115 (*isol*)
Bell, A.A. *et al., Phytochemistry*, 1978, **17**, 1297 (*isol*)

Heliocide H_2 H-18

[63525-06-4]



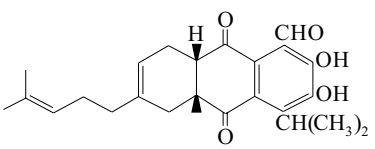
$C_{25}H_{30}O_5$ 410.509
Constit. of *Gossypium hirsutum* (cotton).
Cryst. Mp 123-126°.

3-Me ether: [69734-89-0] ***Heliocide B_2***
$C_{26}H_{32}O_5$ 424.536
Constit. of *Gossypium* sp..

Stipanovic, R.D. *et al., Tet. Lett.*, 1977, 567
Bell, A.A. *et al., Phytochemistry*, 1978, **17**, 1297 (*Heliocide B_2*)

Heliocide H_3 H-19

[64960-69-6]
*5,8,8*a,*9,10,10*a-*Hexahydro-2,3-dihydroxy-10*a*-methyl-4-(1-methylethyl)-6-(4-methyl-3-pentenyl)-9,10-dioxo-1-anthracenecarboxaldehyde, 9CI*



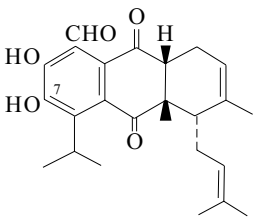
$C_{25}H_{30}O_5$ 410.509
Constit. of *Gossypium hirsutum* (cotton).
Mp 128-134°.

3-Me ether: [69734-90-3] ***Heliocide B_3***
$C_{26}H_{32}O_5$ 424.536

Bell, A.A. *et al., Phytochemistry*, 1978, **17**, 151; 1297 (*isol, struct*)

Heliocide H_4 H-20

[64960-68-5]



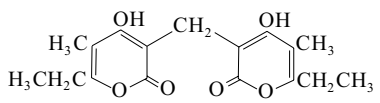
$C_{25}H_{30}O_5$ 410.509
Constit. of *Gossypium hirsutum* (cotton).

7-Me ether: [69734-91-4] ***Heliocide B_4***
$C_{26}H_{32}O_5$ 424.536
Cryst. (hexane). Mp 86-89°. Mod. unstable in soln., stable in cryst. state.

Stipanovic, R.D. *et al., J. Agric. Food Chem.*, 1977, **26**, 115 (*isol*)
Bell, A.A. *et al., Phytochemistry*, 1978, **17**, 1297 (*isol, struct, uv, ms, pmr, synth*)

Helipyrone H-21

[29902-01-0]
*3,3′-Methylenebis[6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one], 9CI. Helipyrone A*



$C_{17}H_{20}O_6$ 320.341
Constit. of *Helichrysum italicum* (curry plant). Cryst. ($CHCl_3$/petrol). Mp 218-220°. λ_{max} 293 (ϵ 14400) (MeOH) (Berdy).

Di-Ac: [57103-54-5]
Mp 151-152°.

Hansel, R. *et al., Tet. Lett.*, 1970, 3369 (*isol, struct*)
Kappe, T. *et al., Tet. Lett.*, 1970, 5105 (*synth*)
Budějšinský, M. *et al., Phytochemistry*, 1975, **14**, 1383 (*deriv*)
Ali, E. *et al., Phytochemistry*, 1982, **21**, 243 (*isol, cmr, synth*)

Helium, 11CI H-22

[7440-59-7]
E939

He

He 4.003

Atomic No. 2. Ground state electron config. $1s^2$. Isol. in 1900 from atmospheric neon by Sir W. Ramsey and M.W. Travers (London). 5 Isotopes are known of which 2 are natural, ^3He, ^4He. Second most abundant element in the cosmos, 0.003 ppm (earth's crust); 5 ppm (v/v) in atm. At 2K, He(I) transforms into He(II) which is a superfluid. With increasing pressure: α-He (hcp) → β-He (fcc) → γ-He (bcc). Food processing aid. Colourless, odourless, tasteless, monatomic, non-toxic gas. Sol. 8.61 cm^3 kg^{-1} in H_2O. Mp -272.2° (under pressure). Bp -269°. Forms no normal chemical compds..

► MH6520000

[12184-98-4, 12184-99-5, 12596-21-3, 12631-81-1, 14234-48-1, 14452-58-5, 15644-29-8]

Mellor Compr. Treat. Inorg. Theor. Chem., 1927, **7**, 889 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 1, *Suppl.*, 1970, 16; 132 (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 213 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 249 (*rev, bibl*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 1042 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1257-1258
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 94; 241
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HAM500

Helveticins H-23

Proteins. Prod. by *Lactobacillus helveticus*. Bacteriocins with possible food uses.

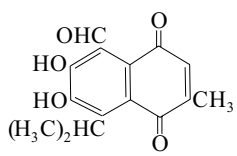
Helveticin J [104708-98-7]
Prod. by *Lactobacillus helveticus* 481. MW 37 KDa.

Helveticin V1829 [147230-06-6]
Prod. by *Lactobacillus helveticus* 1829.

Juerger, M.C. *et al., J. Bacteriol.*, 1986, **167**, 439-446 (*Helveticin J*)
Vaughan, E.E. *et al., J. Appl. Bacteriol.*, 1992, **73**, 299-308 (*Helveticin V1829*)

Hemigossypolone H-24

5,8-Dihydro-2,3-dihydroxy-6-methyl-4-(1-methylethyl)-5,8-dioxo-1-naphthalenecarboxaldehyde, 9CI. 5-Formyl-6,7-dihydroxy-8-isopropyl-2-methyl-1,4-naphthoquinone.
para-*Hemigossypolone*



$C_{15}H_{14}O_5$ 274.273
Constit. of *Gossypium hirsutum* (cotton).
Yellow cryst. ($CHCl_3$). Mp 166.5-169°.

Me ether: ***Hemigossypolone methyl ether****. 5-Formyl-6-hydroxy-8-isopropyl-7-methoxy-2-methyl-1,4-naphthoquinone*
$C_{16}H_{16}O_5$ 288.299
Yellow cryst. Mp 57-59° Mp 72-75°. Incorrectly stated to occur also in *Bombax malabaricum*. This was Isohemigossypolone methyl ether.

Butta, K. *et al., Curr. Sci.*, 1971, **40**, 630 (*isol*)
Bell, A.A. *et al., Chem. Comm.*, 1976, 109 (*struct, synth*)
Bell, A.A. *et al., Phytochemistry*, 1978, **17**, 1297 (*deriv*)

1,21-Heneicosanediol H-25

$HOH_2C(CH_2)_{19}CH_2OH$

$C_{21}H_{44}O_2$ 328.577
Constit. of apple wax. Cryst. (EtOH). Mp 105-105.5°. $Bp_{1.5}$ 223-224°.

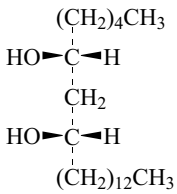
Di-O-*sulfate:* [189822-33-1]
$C_{21}H_{44}O_8S_2$ 488.706

Di-Ac:
$C_{25}H_{48}O_4$ 412.652

Cryst. (petrol). Mp 60°.

Chuit, P. *et al., Helv. Chim. Acta*, 1929, **12**, 850 (*synth*)
Lukes, R. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1719 (*synth*)
Mazliak, P. *et al., Phytochemistry*, 1962, **1**, 79 (*occur*)
Ahmed, Z.F. *et al., J. Nat. Prod.*, 1964, **27**, 115 (*occur*)
Aiello, A. *et al., Tetrahedron*, 1997, **53**, 5877 (*isol, sulfate*)

6,8-Heneicosanediol H-26



$C_{21}H_{44}O_2$ 328.577

(6*R,8*S**)-*form*** [155800-82-1]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 66-68°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, pmr, ms*)

4,6-Heneicosanedione H-27

$H_3C(CH_2)_{14}COCH_2COCH_2CH_2CH_3$

$C_{21}H_{40}O_2$ 324.546
Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-heneicosanone
$C_{21}H_{42}O_2$ 326.562
Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-4-heneicosanone
$C_{21}H_{42}O_2$ 326.562
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

6,8-Heneicosanedione H-28

$H_3C(CH_2)_{12}COCH_2CO(CH_2)_4CH_3$

$C_{21}H_{40}O_2$ 324.546
Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-8-heneicosanone
$C_{21}H_{42}O_2$ 326.562
Constit. of the pollen of *Helianthus annuus* (sunflower).

8-Alcohol:8-Hydroxy-6-heneicosanone
$C_{21}H_{42}O_2$ 326.562
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

Heneicosanoic acid, 9CI H-29

[2363-71-5]

$H_3C(CH_2)_{19}COOH$

$C_{21}H_{42}O_2$ 326.562
Isol. from olive oil (*Olea europaea*). Needles (Me_2CO). Sol. Me_2CO, hexane; poorly sol. H_2O. Mp 73-74°.

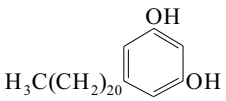
Me ester: [6064-90-0]
$C_{22}H_{44}O_2$ 340.588
Mp 48-50°. Bp_4 207°.

[28898-67-1, 59252-40-3]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 758B; 927B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 486B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 632C (*ir*)
Le Sueur, H.R. *et al., J.C.S.*, 1915, **107**, 736 (*synth*)
Cocker, W. *et al., Perfum. Essent. Oil Res.*, 1963, **54**, 235 442 (*isol*)
Org. Synth., 1981, **60**, 11 (*synth*)

5-Heneicosyl-1,3-benzenediol H-30

[70110-59-7]
5-Heneicosylresorcinol



$C_{27}H_{48}O_2$ 404.675
Constit. of wheat bran. Cryst. (hexane). Mp 99.5-100.5°.

Di-Ac:
Cryst. (EtOH). Mp 72.5-73°.

Di-Me ether:1-Heneicosyl-3,5-dimethoxybenzene
Cryst. (EtOAc). Mp 63.5-64.5°.

*3,4,6,7,9,10,12,13,15,16,18,19-Dodecakisdehydro(*all-*Z-):* [138168-61-3] ***5-(3,6,9,12,15,18-Heneicosahexaenyl)-1,3-benzenediol***
Oil. Darkens in air.

12′,13′-Didehydro(Z-): [189562-00-3] *5-(12-Heneicosenyl)-1,3-benzenediol. 5-(12-Heneicosenyl)resorcinol*
$C_{27}H_{46}O_2$ 402.659
Constit. of wheat and rye flour.

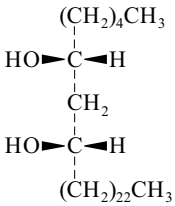
14′,15′-Didehydro(Z-):5-(14-Heneicosenyl)-1,3-benzenediol. 5-(14-Heneicosenyl)resorcinol
$C_{27}H_{46}O_2$ 402.659
Constit. of wheat and rye flour.

16′,17′-Didehydro(Z-): [189562-08-1] *5-(16-Heneicosenyl)-1,3-benzenediol. 5-(16-Heneicosenyl)resorcinol*
$C_{27}H_{46}O_2$ 402.659
Constit. of wheat and rye flour.

12′,13′,15′,16′-Tetradehydro(Z,Z-): [189562-03-6] *5-(12,15-Heneicosadienyl)-1,3-benzenediol. 5-(12,15-Heneicosadienyl)resorcinol*
$C_{27}H_{44}O_2$ 400.643
Constit. of wheat and rye flour.

Wenkert, E. *et al., J.O.C.*, 1964, **29**, 435 (*anal, synth*)
Reusch, R.N. *et al., J. Bacteriol.*, 1979, **139**, 448; 1981, **145**, 889 (*isol*)
Gohil, S. *et al., J. Sci. Food Agric.*, 1988, **45**, 43 (*isol*)
Barrow, R.A. *et al., Aust. J. Chem.*, 1991, **44**, 1393 (*deriv*)
Suzuki, Y. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 480-486 (*isol, ms*)

6,8-Hentriacontanediol H-31

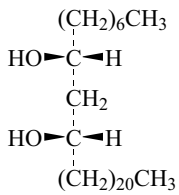


$C_{31}H_{64}O_2$ 468.845

(6*R,8*S**)-*form*** [155800-88-7]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 80-81°. $[\alpha]_D$ -0.5 (c, 0.09 in $CHCl_3$).

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ir, pmr, cmr, ms*)

8,10-Hentriacontanediol H-32



$C_{31}H_{64}O_2$ 468.845

(8*R,10*S**)-*form*** [193419-78-2]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 64-66°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

8,10-Hentriacontanedione H-33

$H_3C(CH_2)_{20}COCH_2CO(CH_2)_6CH_3$

$C_{31}H_{60}O_2$ 464.814
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

15-Hentriacontanol H-34

[27759-56-4]

$H_3C(CH_2)_{15}CH(OH)(CH_2)_{13}CH_3$

$C_{31}H_{64}O$ 452.846
Constit. of *Pisum sativum* (pea). Mp 81.5°.

Sulzbacher, M.J. *et al., J. Appl. Chem.*, 1955, **5**, 637-641 (*synth*)
Macey, M.J.K. *et al., Phytochemistry*, 1970, **9**, 5 (*isol*)

9-Hentriacontanone H-35

[34136-52-2]

$H_3C(CH_2)_{21}CO(CH_2)_7CH_3$

$C_{31}H_{62}O$ 450.83
Constit. of the waxes of coffee leaves and rose flowers.

Stoianova-Ivanova, B. *et al., Phytochemistry*, 1971, **10**, 1391 (*isol*)
Ablanque, E. *et al., CA*, 1989, **110**, 209458q (*isol*)

16-Hentriacontanone H-36

[502-73-8]

Palmitone

$H_3C(CH_2)_{14}CO(CH_2)_{14}CH_3$

$C_{31}H_{62}O$ 450.83

Constit. of *Piper nigrum* (pepper). Cryst. (EtOH). Mp 82-83°.

Oxime:

$C_{31}H_{63}NO$ 465.845

Cryst. (EtOH or AcOH). Mp 59°.

Chibnall, A.C. *et al., Biochem. J.*, 1937, **31**, 1981 (*isol*)

Asselineau, J. *et al., Biochim. Biophys. Acta*, 1961, **54**, 359 (*isol*)

Hayashi, N. *et al., J. Indian Chem. Soc.*, 1971, **48**, 288 (*isol*)

Singh, J.K. *et al., J. Indian Chem. Soc.*, 1976, **53**, 1162 (*isol*)

Dhav, D.N. *et al., Planta Med.*, 1976, **29**, 91 (*isol*)

Gonzalez-Trujano, M.E. *et al., Planta Med.*, 2001, **67**, 136-141 (*isol,ir,pmr,cmr,ms*)

22-Hentriacontene-2,4-dione H-37

$H_3C(CH_2)_7CH$
$=CH(CH_2)_{17}COCH_2COCH_3$

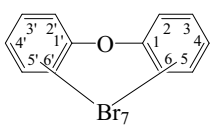
$C_{31}H_{58}O_2$ 462.798

(Z)-form

Constit. of the epicuticular waxes of *Vanilla fragrans* (vanilla) and *Vanilla tahitensis* (Tahitian vanilla).

Ramaroson-Raonizafinimanana, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 4739-4743 (*isol*)

Heptabromodiphenyl ethers H-38



$C_{12}H_3Br_7O$ 722.483

Environmental pollutant, detected in breast milk.

2,2′,3,4,4′,5′,6-Heptabromodiphenyl ether

[207122-16-5]

1,2,3,5-Tetrabromo-4-(2,4,5-tribromophenoxy)benzene. PBDE 183. BDE 183

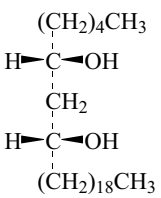
No phys. props. reported.

Environ. Health Criter., No. 162, Polybrominated Diphenyl Ethers, WHO, 1994, (*rev, tox, occur*)

Sjodin, A. *et al., Environ. Health Perspect.*, 1999, **107**, 643-648 (*occur, tox*)

Ryan, J.J. *et al., Organohalogen Compd.*, 2000, **47**, 57-60 (*anal*)

6,8-Heptacosanediol H-39



$C_{27}H_{56}O_2$ 412.738

(6S,8R)-form [155800-85-4]

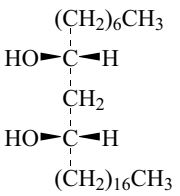
erythro-*form*

Constit. of the flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 66-68°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105-108 (*isol, ms*)

Ukiya, M. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1187-1189 (*abs config*)

8,10-Heptacosanediol H-40



$C_{27}H_{56}O_2$ 412.738

(8R*,10S*)-form [193419-76-0]

erythro-*form*

Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 54-56°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

4,6-Heptacosanedione H-41

$H_3C(CH_2)_{20}COCH_2COCH_2CH_2CH_3$

$C_{27}H_{52}O_2$ 408.707

Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-heptacosanone

$C_{27}H_{54}O_2$ 410.722

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

6,8-Heptacosanedione H-42

$H_3C(CH_2)_{18}COCH_2CO(CH_2)_4CH_3$

$C_{27}H_{52}O_2$ 408.707

Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-8-heptacosanone

$C_{27}H_{54}O_2$ 410.722

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

8,10-Heptacosanedione H-43

$H_3C(CH_2)_{16}COCH_2CO(CH_2)_6CH_3$

$C_{27}H_{52}O_2$ 408.707

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

10,12-Heptacosanedione H-44

[95605-27-9]

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_8CH_3$

$C_{27}H_{52}O_2$ 408.707

Constit. of *Helianthus annuus* (sunflower). Cryst. (Me_2CO). Mp 50-51°.

Tulloch, A.P. *et al., Phytochemistry*, 1985, **24**, 131-137 (*synth, cmr*)

Matsuzaki, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 2341-2342 (*isol, uv, pmr, ms*)

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol*)

12,14-Heptacosanedione H-45

$H_3C(CH_2)_{12}COCH_2CO(CH_2)_{10}CH_3$

$C_{27}H_{52}O_2$ 408.707

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

14-Heptacosanol H-46

[32116-10-2]

Dimyrstylcarbinol

$H_3C(CH_2)_{12}CH(OH)(CH_2)_{12}CH_3$

$C_{27}H_{56}O$ 396.739

Found in traces in apple skin wax. Mp 80-81°.

Kipping, F. *et al., J.C.S.*, 1893, 452; 459 (*synth*)

Grun, A. *et al., Angew. Chem.*, 1926, **39**, 421

Al-Mamun, M.A. *et al., J. Am. Oil Chem. Soc.*, 1974, **51**, 229

Bennett, R.L. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1976, **14**, 3021

18-Heptacosene-2,4-dione H-47

$H_3C(CH_2)_7CH$
$=CH(CH_2)_{13}COCH_2COCH_3$

$C_{27}H_{50}O_2$ 406.691

(Z)-form

Nervonoylacetone

Constit. of the epicuticular waxes of *Vanilla fragrans* (vanilla) and *Vanilla tahitensis* (Tahitian vanilla).

Ramaroson-Raonizafinimanana, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 4739-4743 (*isol, synth*)

1,8-Heptadecadiene-4,6-diyne-3,10-diol, 9CI H-48

[63910-76-9]

$H_2C{=}CHCH(OH)C{\equiv}CC{\equiv}CCH$
$=CHCH(OH)(CH_2)_6CH_3$

$C_{17}H_{24}O_2$ 260.375

Isol. from *Panax quinquefolium* (American ginseng).

(+)-(Z)-form [132075-01-5]

Seselidiol

Yellowish oil. $[\alpha]_D^{23}$ +192 (c, 0.53 in Et_2O). λ_{max} 232 (ϵ); 246 (ϵ); 256 (ϵ); 270 (ϵ); 286 (ϵ) (MeOH) (Derep).

Di-Ac: [131989-87-2]

$C_{21}H_{28}O_4$ 344.45

Yellowish oil.

Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1977, **310**, 285; 945 (*isol, struct, uv, ir, ms, pmr*)

Shim, S.C. *et al., Phytochemistry*, 1987, **26**, 2849 (*isol, pmr, cmr*)

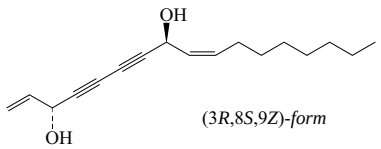
Hu, C.-Q. *et al., J. Nat. Prod.*, 1990, **53**, 932 (*isol, struct*)

Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 521 (*isol*)

Bernart, M.W. *et al., J. Nat. Prod.*, 1996, **59**, 748 (*isol*)

1,9-Heptadecadiene-4,6-diyne-3,8-diol, 9CI H-49

[30779-95-4]



(3*R*,8*S*,9*Z*)-*form*

$C_{17}H_{24}O_2$ 260.375
Log P 2.49 (calc).

(3*R*,8*S*,9*Z*)-*form* [55297-87-5]
Falcarindiol
Constit. of roots of several plants including the common carrot (*Daucus carota*) and *Angelica acutiloba* (Dong Dang Gui). Pale yellow oil. Sol. MeOH, Et_2O. $[\alpha]_D$ +204.8 (c, 1 in $CHCl_3$). Log P 2.49 (calc). Pharmacol. active isomer λ_{max} 231 ; 244 ; 256 (MeOH) (Berdy). λ_{max} 233 (ϵ 1000); 245 (ϵ 1000); 259 (ϵ 800) (EtOH) (Berdy). λ_{max} 232 (ϵ 400); 244 (ϵ 400); 258 (ϵ 200) (Et_2O) (Berdy).

3-Ac: [111264-34-7]
$C_{19}H_{26}O_3$ 302.413
Constit. of carrots *Daucus carota*.

3-Ketone: [18089-23-1] *8-Hydroxy-1,9-heptadecadien-4,6-diyn-3-one.* ***Falcarinolone***
$C_{17}H_{22}O_2$ 258.36
Isol. from carrot (*Daucus carota*) and caraway seed *(Carum carvi)*. Unstable pale yellow oil. $[\alpha]_D^{20}$ +255 (c, 5.1 in Et_2O).

Diketone: [65892-84-4] *1,9-Heptadecadiene-4,6-diyne-3,8-dione.* ***Falcarindione***
$C_{17}H_{20}O_2$ 256.344
Isol. from roots of *Carum carvi* (caraway). Unstable yellowish oil.

(3*R,8*R**)-*form***

9,10-Epoxide: [133921-58-1] *1-(3-Heptyloxiranyl)-7-octene-2,4-diyne-1,6-diol, 9CI. 9,10-Epoxy-1-heptadecene-4,6-diyne-3,8-diol.* ***Panaquinquecol 2***. *PQ 2*
$C_{17}H_{24}O_3$ 276.375
Constit. of *Panax quinquefolium* (American ginseng). Oil. $[\alpha]_D$ +86.9 (c, 0.64 in MeOH).

9,10-Epoxide, 8-Ac: [145400-15-3] ***Panaquinquecol 6***. *PQ 6*
$C_{19}H_{26}O_4$ 318.412
Constit. of *Panax quinquefolium* (American ginseng). Oil. $[\alpha]_D$ -27 (c, 1 in $CHCl_3$).

Bohlmann, F. *et al., Chem. Ber.*, 1961, **94**, 958; 3189; 1967, **100**, 3450; 3454; 1971, **104**, 2033; 1975, **108**, 511 (*isol, derivs*)
Bentley, R.K. *et al., J.C.S.(C)*, 1969, 685 (*isol, ir, uv, pmr*)
Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1977, **310**, 945 (*synth, ir, uv, pmr*)
Tanaka, S. *et al., Arzneim.-Forsch.*, 1977, **27**, 2039 (*pharmacol*)
Garrod, B. *et al., Physiol. Plant Pathol.*, 1978, **13**, 241 (*ir, uv, pmr, ms*)
Kemp, M.S. *et al., Phytochemistry*, 1978, **17**, 1002 (*isol, props*)
Lemmich, E. *et al., Phytochemistry*, 1981, **20**, 1419 (*abs config*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 521-522 (*PQ 2*)
Fujimoto, Y. *et al., Phytochemistry*, 1992, **31**, 3499 (*PQ 6*)
Satoh, A. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 152 (*isol, pmr, ms*)
Bernart, M.W. *et al., J. Nat. Prod.*, 1996, **59**, 748-753 (*isol, props*)
Zheng, G. *et al., J. Nat. Prod.*, 1999, **62**, 626-628 (*synth, ir, pmr, cmr*)
Xu, L. *et al., Chin. Chem. Lett.*, 2000, **11**, 213-216 (*synth, Oplopandiol, Ac*)

2,9-Heptadecadiene-4,6-diyne-1,8-diol, 8CI H-50

$H_3C(CH_2)_6CH{=}CHCH(OH)C{\equiv}CC{\equiv}CCH{=}CHCH_2OH$

$C_{17}H_{24}O_2$ 260.375

(2*Z*,8*S*,9*Z*)-*form* [32768-89-1]
Oil. $[\alpha]_D^{20}$ +270 (c, 0.7 in $CHCl_3$). 8*S*-Config. of *Azorella trifurcata* isolate not establ. λ_{max} 228 (ϵ 8000); 270 (ϵ 14000); 288 (ϵ 20000); 316 (ϵ 17000) (EtOH) (Berdy).

1-Ac: [144790-29-4]
$C_{19}H_{26}O_3$ 302.413
Constit. of *Daucus carota* (carrot). Oil. Struct. revised in 1992.

[32768-88-0]

Bohlmann, F. *et al., Chem. Ber.*, 1971, **104**, 1322
Lund, E.D. *et al., Phytochemistry*, 1992, **31**, 3621 (*struct, bibl*)
Estevez-Braun, A. *et al., J. Nat. Prod.*, 1994, **57**, 1178 (*isol, pmr, cmr, abs config*)

1,16-Heptadecadiene-4,6-diyne-3,9,10-triol, 9CI H-51

[139163-35-2]
Ginsenoyne C

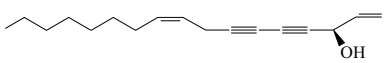
$H_2C{=}CHCH(OH)C{\equiv}CC{\equiv}CCH_2CH(OH)CH(OH)(CH_2)_5CH{=}CH_2$

$C_{17}H_{24}O_3$ 276.375
Present in ginseng root. Amorph. powder. $[\alpha]_D$ -16.5 (c, 1.5 in $CHCl_3$). λ_{max} 201 ; 231 ; 243 ; 257 (MeOH) (Berdy).

Tri-Ac: [139035-33-9]
Oil. $[\alpha]_D$ +13.3 (c, 1.49 in $CHCl_3$).

Hirakura, K. *et al., Phytochemistry*, 1991, **30**, 3327 (*isol, ir, uv, ms, pmr, cmr*)

1,9-Heptadecadiene-4,6-diyn-3-ol H-52



$C_{17}H_{24}O$ 244.376

(*R*)-(*Z*)-*form* [21852-80-2]
Carotatoxin. Carrotatoxin
Sol. Et_2O, MeOH. $Bp_{0.02}$ 115°. $[\alpha]_D$ -36.9 (c, 0.77 in $CHCl_3$). n_D^{18} 1.5018. λ_{max} 230 (ϵ 400); 242 (ϵ 400); 256 (ϵ 200) (Et_2O) (Berdy). λ_{max} 230 (ϵ 986); 247 (ϵ 739); 256 (ϵ 445) (hexane) (Berdy).
▶Toxic.

(*S*)-(*Z*)-*form* [81203-57-8]
Panaxynol. *Falcarinol*
Isol. from ginseng. $[\alpha]_D^{25}$ +29.4 (c, 1.7 in $CHCl_3$). $[\alpha]_D$ +33.8 (c, 0.53 in $CHCl_3$).

(Z,Z)-(9,12-Octadecadienoyl): [155551-18-1] *Panaxynol linoleate*
$C_{35}H_{54}O_2$ 506.81
Isol. from ginseng. Oil. $[\alpha]_D$ +18.7 (c, 6.8 in $CHCl_3$).

[155475-74-4]

Bohlmann, F. *et al., Chem. Ber.*, 1965, **98**, 3010; 1966, **99**, 3552 (*isol, synth*)
Crosby, D.G. *et al., Tetrahedron*, 1967, **23**, 465 (*ir, uv*)
Bentley, R.K. *et al., J.C.S.(C)*, 1969, 685 (*isol, ir, uv, nmr*)
Kim, Y.S. *et al., Arch. Pharmacal Res.*, 1989, **12**, 207-213 (*activity*)
Terada, A. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 2977 (*isol, bibl*)
Matsunaga, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3480-3488 (*activity*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 521 (*isol*)
Hirakura, K. *et al., Phytochemistry*, 1992, **31**, 899-904 (*Panaxynol, Panaxynol linoleate, isol*)
Bernast, M.W. *et al., Tet. Lett.*, 1994, **35**, 993 (*abs config*)
Kobaisy, M. *et al., J. Nat. Prod.*, 1997, **60**, 1210-1213 (*isol, abs config*)
Zheng, G. *et al., Tet. Lett.*, 1999, **40**, 2181-2182 (*synth, abs config, nmr, props*)
Mayer, S.F. *et al., J.O.C.*, 2002, **67**, 9115-9121 (*Panaxynol, synth*)

9,16-Heptadecadiene-4,6-diyn-3-ol, 8CI H-53

$H_2C{=}CH(CH_2)_5CH{=}CHCH_2C{\equiv}CC{\equiv}CCH(OH)CH_2CH_3$

$C_{17}H_{24}O$ 244.376

(*Z*)-*form* [24587-16-4]
Oil.

9,10-Epoxide, Ac: [142465-54-1] ***Ginsenoyne H***
$C_{19}H_{26}O_3$ 302.413
Isol. from ginseng. Oil. $[\alpha]_D$ -208.9 (c, 2.27 in $CHCl_3$).

Bohlmann, F. *et al., Chem. Ber.*, 1969, **102**, 1691
de Pascual, T.J. *et al., An. Quim.*, 1977, **73**, 1525; *CA*, **89**, 176303c
Hirakura, K. *et al., Phytochemistry*, 1991, **30**, 4053 (*Ginsenoyne H*)

1,9-Heptadecadiene-4,6-diyn-3-one H-54

$H_3C(CH_2)_6CH{=}CHCH_2C{\equiv}CC{\equiv}CCOCH{=}CH_2$

$C_{17}H_{22}O$ 242.36

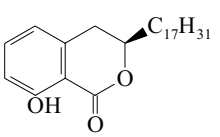
(*Z*)-*form* [4117-11-7]
Falcarinone
Isol. from *Sium sisarum* (skirret). Pale yellow oil.

9,10-Epoxide: See Ginsenoyne in P-17

Bohlmann, F. *et al., Chem. Ber.*, 1961, **94**, 958; 1962, **95**, 1320; 1965, **98**, 3010

3-Heptadecadienyl-3,4-dihydro-8-hydroxy-1*H*-2-benzopyran-1-one H-55

3-Heptadecadienyl-3,4-dihydro-8-hydroxyisocoumarin



$C_{26}H_{38}O_3$ 398.584
Posn. of double bonds in side chain not

determined.

(R)-form [158681-29-9]
Constit. of the fruit of *Ginkgo biloba* (ginkgo).

Choukchou-Braham, N. *et al., Tet. Lett.*, 1994, **35**, 3949 (*isol*)

Heptadecanal H-56

[629-90-3]

$H_3C(CH_2)_{15}CHO$

$C_{17}H_{34}O$ 254.455

Isol. from lemon oil (*Citrus limon*). Cryst. (petrol). Mp 36°. Bp_{26} 204°.

Oxime: [24435-10-7]
$C_{17}H_{35}NO$ 269.47
Mp 89.5°.

Semicarbazone:
Mp 108°.

Ikeda, R.M. *et al., J. Agric. Food Chem.*, 1962, **10**, 98 (*isol*)
Rao, P.V. *et al., J. Lipid Res.*, 1967, **8**, 380 (*synth, glc*)
Org. Synth., 1971, **51**, 39 (*synth*)

1,17-Heptadecanediol, 9CI H-57

[66577-59-1]

$HOCH_2(CH_2)_{15}CH_2OH$

$C_{17}H_{36}O_2$ 272.47

Occurs in leaf cutin of *Limonia acidissima* (wood apple). Cryst. (C_6H_6). Mp 96-96.5° (93-94°). Bp_2 204-205°.

Chuit, P. *et al., Helv. Chim. Acta*, 1929, **12**, 850 (*synth*)
Percec, V. *et al., Macromolecules*, 1990, **23**, 3509 (*synth, pmr*)
Patwardhan, S.A. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 647 (*rev*)

2,4-Heptadecanedione, 9CI H-58

[64042-18-8]

Tetradecanoylacetone. Myristoylacetone

$H_3C(CH_2)_{12}COCH_2COCH_3$

$C_{17}H_{32}O_2$ 268.439

Acetogenin. Constit. of *Ruta graveolens* (rue). Oil. Mp 42.5° (39°).

Morgan, G.T. *et al., J.C.S.*, 1925, **127**, 2891 (*synth*)
Douglas, D.E. *et al., Lipids*, 1977, **12**, 635 (*synth*)
Douglas, D.E. *et al., Can. J. Biochem.*, 1978, **56**, 691 (*occur*)
Tattje, D.H.E. *et al., Pharm. Weekbl.*, 1978, **113**, 1169 (*isol*)
Amico, V. *et al., J. Nat. Prod.*, 1990, **53**, 1379 (*isol*)

2-Heptadecanone H-59

[2922-51-2]

$H_3C(CH_2)_{14}COCH_3$

$C_{17}H_{34}O$ 254.455

Constit. of aroma compounds of white bread. Cryst. Mp 48°. Bp 319-320° Bp_{110} 246°.

Keskin, H. *et al., CA*, 1946, **40**, 1822^7 (*synth*)
Bente, P.F. *et al., J. Phys. Chem.*, 1975, **79**, 713 (*synth, ms*)
Obretenov, T. *et al., Z. Lebensm.-Unters. - Forsch.*, 1977, **165**, 195 (*isol, glc, ms*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 828

8,11,14-Heptadecatrienal H-60

[112209-66-2]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_6CHO$

$C_{17}H_{28}O$ 248.408

(all-Z)-form [56797-44-5]
Constit. of cucumber and wheat.

14,15-Dihydro: [56797-42-3] *8,11-Heptadecadienal*
$C_{17}H_{30}O$ 250.423
Constit. of cucumber.

11,12,14,15-Tetrahydro: [56797-41-2] *8-Heptadecenal, 9CI*
$C_{17}H_{32}O$ 252.439
Constit. of cucumber. Oil.

[1191-86-2, 96360-10-0, 123350-64-1]

Kemp, T.R. *et al., J. Am. Oil Chem. Soc.*, 1975, **52**, 300-302 (*occur*)
Takagi, Y. *et al., Agric. Biol. Chem.*, 1981, **45**, 769
Stoessl, A. *et al., Can. J. Microbiol.*, 1985, **31**, 129 (*isol*)
Hamilton-Kemp, T.R. *et al., Phytochemistry*, 1986, **25**, 241 (*isol*)
Kajiwara, T. *et al., Phytochemistry*, 1989, **28**, 407; 1990, **29**, 745; 2193; 1991, **30**, 1805 (*isol*)
Poigny, S. *et al., J.C.S. Perkin 1*, 1997, 2175-2177 (*tetrahydro, synth, ir, pmr, cmr*)

1,5,8-Heptadecatriene H-61

$H_3C(CH_2)_7CH{=}CHCH_2CH{=}CHCH_2CH_2CH{=}CH_2$

$C_{17}H_{30}$ 234.424

(5Z,8Z)-form [145297-96-7]
Constit. of the essential oil of *Tussilago farfara* (coltsfoot).

Suzuki, N. *et al., Yakugaku Zasshi*, 1992, **112**, 571 (*isol*)

1,8,15-Heptadecatriene-11,13-diyne, 9CI H-62

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH_2CH{=}CH(CH_2)_5CH{=}CH_2$

$C_{17}H_{22}$ 226.361

8,9-Epoxide: [95925-05-6] *8,9-Epoxy-1,15-heptadecadiene-11,13-diyne. 2-(6-Heptenyl)-3-(6-octene-2,4-diynyl)oxirane, 9CI*
$C_{17}H_{22}O$ 242.36

(8E,15E)-form [28834-02-8]
Constit. of the plant *Silybum marianum* (milk thistle).

(8Z,15E)-form
Oil.

(8Z,15Z)-form [6386-16-9]
Occurs in *Silybum marianum* (milk thistle).

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 586; 3201; 1968, **101**, 532; 1969, **102**, 1691 (*isol, uv, ir, pmr, ms, struct, synth*)
Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1970, **303**, 7 (*isol, pmr, ir, uv*)
Lam, J. *et al., Phytochemistry*, 1971, **10**, 647 (*epoxide*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 201 (*epoxide*)

1,8,10-Heptadecatriene-4,6-diyne-3,12-diol H-63

$H_3C(CH_2)_4CH(OH)CH{=}CHCH{=}CHC{\equiv}CC{\equiv}CCH(OH)CH{=}CH_2$

$C_{17}H_{22}O_2$ 258.36

(all-E)-form [143966-10-3]
Constit. of ginseng.

Lutomski, J. *et al., Herba Pol.*, 1991, **37**, 113 (*isol*)

1,9,16-Heptadecatriene-4,6-diyn-3-ol H-64

[88153-63-3]

$H_2C{=}CH(CH_2)_5CH{=}CHCH_2C{\equiv}CC{\equiv}CCH(OH)CH{=}CH_2$

$C_{17}H_{22}O$ 242.36

(-)-(Z)-form [36150-08-0]
Dehydrofalcarinol
Pale yellow oil. $[\alpha]_D^{23}$ -5 (c, 13.9 in Et_2O).

Ac: [78516-98-0]
$C_{19}H_{24}O_2$ 284.397
Oil. λ_{max} 232 (ϵ 1230); 244 (ϵ 1047); 258 (ϵ 692); 285 (ϵ 234); 306 (ϵ 170) (EtOH) (Berdy).

9,10-Epoxide: [139163-34-1] *9,10-Epoxy-1,16-heptadecadiene-4,6-diyn-3-ol*. ***Ginsenoyne A***
$C_{17}H_{22}O_2$ 258.36
Isol. from ginseng. Oil. $[\alpha]_D$ -121.9 (c, 1.0 in $CHCl_3$). λ_{max} 201 ; 230 ; 243 ; 256 (EtOH).

9,10-Epoxide, Ac: [142449-71-6] ***Ginsenoyne F***
$C_{19}H_{24}O_3$ 300.397
Isol. from ginseng. Oil. $[\alpha]_D$ -54.2 (c, 2.35 in $CHCl_3$).

9,10-Epoxide, 9,12-octadecadienoyl(Z,Z-): [155551-20-5] ***Ginsenoyne A linoleate***
$C_{35}H_{52}O_3$ 520.794
Isol. from ginseng. Oil. $[\alpha]_D$ -13.9 (c, 6 in $CHCl_3$).

[13894-97-8, 155475-73-3]

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 3552 (*isol, ir, pmr, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 113 (*isol*)
Harada, R. *et al., Phytochemistry*, 1982, **21**, 2009 (*isol*)
Wang, Y. *et al., Phytochemistry*, 1990, **29**, 3101 (*isol, struct, bibl, pmr, cmr*)
Hirakura, K. *et al., Phytochemistry*, 1991, **30**, 3327; 4053 (*isol, ir, uv, ms, pmr, cmr*)
Hirakura, K. *et al., Phytochemistry*, 1994, **35**, 963 (*Ginsenoyne A linoleate*)
Bernart, M.W. *et al., J. Nat. Prod.*, 1996, **59**, 748 (*isol, pmr, cmr, abs config, props*)

2,9,16-Heptadecatriene-4,6-diyn-8-ol H-65

$H_2C{=}CH(CH_2)_5CH{=}CHCH(OH)C{\equiv}CC{\equiv}CCH{=}CHCH_3$

$C_{17}H_{22}O$ 242.36

(Z,Z)-form [13894-72-9]
Isol. from fresh roots of *Silybum marianum* (milk thistle). Oil. λ_{max} 247 (ϵ 4000); 254 (ϵ 7200); 269 (ϵ 10400); 284 (ϵ 8000) (Et_2O).

9,10-Epoxide: [13030-79-0] *9,10-Epoxy-2,16-heptadecadiene-4,6-diyn-8-ol*
$C_{17}H_{22}O_2$ 258.36
$[\alpha]_{Hg}^{20}$ +153 (c, 1.5 in Et_2O).

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 2096; 3201 (*isol, uv, ir, pmr, struct*)
Schulz, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1970, **301**, 7 (*isol*)
Lam, J. *et al., Phytochemistry*, 1971, **10**, 647 (*epoxide*)

Yano, K. *et al., Phytochemistry*, 1980, **19**, 1864 (*epoxide*)

1,7,9-Heptadecatriene-11,13,15-triyne, 9CI H-66

[20252-54-4]
Centaur X₃
$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH{=}CH(CH_2)_4CH{=}CH_2$
$C_{17}H_{18}$ 222.329

(*all-E*)-*form* [41688-30-6]
Constit. of *Artemisia vulgaris* (mugwort). Mp 17.5°.

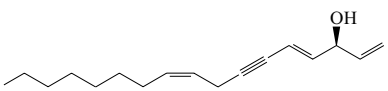
(7*Z*,9*E*)-*form*
Cryst. (petrol). Mp -12°.
Bohlmann, F. *et al., Chem. Ber.*, 1957, **90**, 1661 (*synth*)
Bentley, R.K. *et al., J.C.S.(C)*, 1969, 1096 (*isol*)
Bedford, C.T. *et al., J.C.S. Perkin 1*, 1976, 735 (*synth*)

1,4,9-Heptadecatrien-6-yne-3,8-diol H-67

$H_3C(CH_2)_6CH{=}CHCH(OH)C{\equiv}CCH{=}CHCH(OH)CH{=}CH_2$
$C_{17}H_{26}O_2$ 262.391

(3ξ,4*E*,8ξ,9*Z*)-*form*
Crithmumdiol
Constit. of *Crithmum maritimum* (rock samphire). Oil. $[\alpha]_D$ +43 (c, 0.6 in MeOH). λ_{max} 231 (ε 5270); 277 (ε 1025) (EtOH).
Ruberto, G. *et al., Planta Med.*, 1999, **65**, 681-682

1,4,9-Heptadecatrien-6-yn-3-ol, 9CI H-68



$C_{17}H_{26}O$ 246.392

(3*S*,4*E*,9*Z*)-*form* [141947-41-3]
Ginsenoyne J
Constit. of the roots of *Panax ginseng*. Oil. $[\alpha]_D$ -24.6 (c, 2.2 in $CHCl_3$). λ_{max} 198 (ε 10300); 230 (ε 18200) (EtOH) (Berdy).

Ketone: [141947-45-7] *1,4,9-Heptadecatrien-3-one*
$C_{17}H_{24}O$ 244.376
λ_{max} 232 (ε 13000) (EtOH) (Berdy).

Japan. Pat., 1992, 04 352 742; *CA*, **119**, 48933j (*ketone*)
Hirakura, K. *et al., Phytochemistry*, 1992, **31**, 899 (*isol, pmr, cmr*)

1-Heptadecene-4,6-diyne-3,9-diol, 9CI H-69

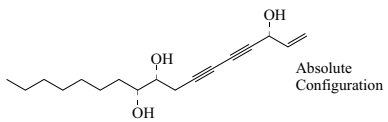
[77084-19-6]
$H_3C(CH_2)_7CH(OH)CH_2C{\equiv}CC{\equiv}CCH(OH)CH{=}CH_2$
$C_{17}H_{26}O_2$ 262.391
Present in ginseng root. Cryst. (hexane). Mp 80-85° dec.
Dabrowski, Z. *et al., Phytochemistry*, 1980, **19**, 2464 (*isol, struct*)

8-Heptadecene-4,6-diyne-3,10-diol H-70

$H_3C(CH_2)_6CH(OH)CH{=}CHC{\equiv}CC{\equiv}CCH(OH)CH_2CH_3$
$C_{17}H_{26}O_2$ 262.391

(*E*)-*form*
10-Ac: [143966-09-0] *10-Acetoxy-8-heptadecene-4,6-diyn-3-ol*
$C_{19}H_{28}O_3$ 304.428
Constit. of *Panax ginseng* (ginseng).
Lutomski, J. *et al., Herba Pol.*, 1991, **37**, 113 (*isol*)

1-Heptadecene-4,6-diyne-3,9,10-triol, 9CI H-71



$C_{17}H_{26}O_3$ 278.391
λ_{max} 231 (ε 711); 243 (ε 627); 256 (ε 376) (H_2O) (Derep).

(3*R*,9*R*,10*R*)-*form* [87005-03-6]
Panaxytriol. *Falcarintriol*
Found in ginseng. Needles (H_2O). $[\alpha]_D$ -19 (c, 1 in $CHCl_3$). Abs. config. finally confirmed in 2002.

10-Ac: [122855-48-5] ***10-Acetylpanaxytriol***
$C_{19}H_{28}O_4$ 320.428
Found in ginseng roots.

10-Me ether: [133921-57-0] *10-Methoxy-1-heptadecene-4,6-diyne-3,9-diol, 9CI*. ***Panaquinquecol 1***. *PQ 1*
$C_{18}H_{28}O_3$ 292.417
Found in American ginseng (*Panax quinquefolium*). Oil. $[\alpha]_D$ -21.7 (c, 0.58 in MeOH).

Matsunaga, H. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1279 (*isol, uv, pmr, cmr, synth*)
Kim, S.I. *et al., Yakhak Hoeji*, 1989, **33**, 118; *CA*, **111**, 146363 (*10-Acetylpanaxytriol*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 521 (*isol, ms, cmr, struct*)
Kobayashi, M. *et al., Tetrahedron*, 1997, **53**, 15691-15700 (*abs config*)
Lu, W. *et al., Tetrahedron*, 1999, **55**, 7157-7168 (*synth, abs config*)
Gurjar, M.K. *et al., Tetrahedron*, 1999, **55**, 12563-12576 (*synth*)
Satoh, M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 126-128 (*abs config*)
Mayer, S.F. *et al., J.O.C.*, 2002, **67**, 9115-9121 (*synth*)
Yadav, J.S. *et al., Tetrahedron*, 2002, **58**, 4955-4961 (*synth*)

9-Heptadecene-4,6-diyn-3-one H-72

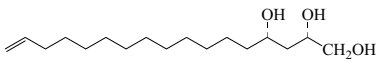
1,2-Dihydrofalcarinone
$H_3C(CH_2)_6CH{=}CHCH_2C{\equiv}CC{\equiv}CCOCH_2CH_3$
$C_{17}H_{24}O$ 244.376

(*Z*)-*form* [32768-86-8]
Oil.
9R,*10*S-*Epoxide, 3-alcohol:9,10-Epoxy-4,6-heptadecadiyn-3-ol*. ***Ginsenoyne D***
$C_{17}H_{26}O_2$ 262.391
Isol. from roots of *Panax ginseng* (ginseng). Oil. $[\alpha]_D$ -90.7 (c, 3.0 in $CHCl_3$). λ_{max} 200 ; 230 ; 241 ; 255 (EtOH).

9R,*10*S-*Epoxide, 3-alcohol, Ac:* [142449-72-7] ***Ginsenoyne G***
$C_{19}H_{28}O_3$ 304.428
Isol. from ginseng root. Oil. $[\alpha]_D$ -182.6 (c, 3.77 in $CHCl_3$).
Bohlmann, F. *et al., Chem. Ber.*, 1971, **104**, 1322 (*isol*)
Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1977, **310**, 945 (*synth*)
Hirakawa, K. *et al., Phytochemistry*, 1991, **30**, 3327; 4053 (*Ginsenoynes*)

16-Heptadecene-1,2,4-triol, 9CI H-73

[83797-45-9]
Avocadene



$C_{17}H_{34}O_3$ 286.454
Constit. of avocado (*Persea americana*). Mp 68°. $[\alpha]_D^{25}$ -6.7 ($CHCl_3$).

(2*S*,4*S*)-*form*
1-Ac: [24607-09-8]
$C_{19}H_{36}O_4$ 328.491
Constit. of avocado (*Persea americana*). Mp 58-59°. $[\alpha]_D^{25}$ -6.7 ($CHCl_3$).

2-Ac: [51352-69-3]
$C_{19}H_{36}O_4$ 328.491
Constit. of avocado (*Persea americana*).

4-Ac: [59499-18-2]
$C_{19}H_{36}O_4$ 328.491
Constit. of avocado (*Persea americana*).

Kashman, Y. *et al., Tetrahedron*, 1969, **25**, 4617
Alves, H.M. *et al., Ann. Acad. Bras. Ci&eenc.*, 1970, **425**, 45 (*ir, ms, pmr, uv*)
Bittner, S. *et al., Phytochemistry*, 1971, **10**, 1417
Brown, B.I. *et al., J. Chromatogr.*, 1973, **86**, 239
Adikaram, N.K.B. *et al., Phytochemistry*, 1992, **31**, 93 (*isol, pmr, cmr, props*)
Oberlies, N.H. *et al., J. Nat. Prod.*, 1998, **61**, 781-785 (*isol, pmr, cmr, ms*)
Domergue, F. *et al., Phytochemistry*, 2000, **54**, 183-189 (*abs config*)

9-Heptadecenoic acid H-74

[10136-52-4]

[26265-99-6]
$H_3C(CH_2)_6CH{=}CH(CH_2)_7COOH$
$C_{17}H_{32}O_2$ 268.439

(*E*)-*form* [76261-97-7]
Mp 38°.

Et ester:
$C_{19}H_{36}O_2$ 296.492
$Bp_{0.5}$ 150°.

(*Z*)-*form* [1981-50-6]

[28040-00-8]
Minor constit. of several animal and vegetable fats. Mp 11.4-12.2° Mp 14.5°. $Bp_{0.5}$ 175°.

Me ester: [14101-91-8]
$C_{18}H_{34}O_2$ 282.465
Mp -26.3°. Bp_2 149-152°.

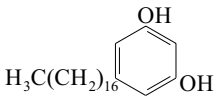
Et ester:
$Bp_{0.1}$ 139°.

Ames, D.H. *et al., J.C.S.*, 1951, 1079
Vauer, V.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1966, 2241 (*synth, ir*)
Boon, J.J. *et al., Lipids*, 1977, **12**, 717 (*synth, ms*)

Benyagoub, M. *et al., J. Chem. Ecol.*, 1996, **22**, 405 (*isol, activity*)

5-Heptadecyl-1,3-benzenediol, 9CI H-75

[41442-57-3]
5-Heptadecylresorcinol



$C_{23}H_{40}O_2$ 348.568
Isol. from cereal grains. Plates (cyclohexane). Mp 91-93°.

2′,3′-Didehydro(Z-): [94751-34-5] ***5-(2-Heptadecenyl)-1,3-benzenediol, 9CI***. *5-(2-Heptadecenyl)resorcinol*
$C_{23}H_{38}O_2$ 346.552
Isol. from mango (*Mangifera indica*) latex.

10′,11′-Didehydro(Z-): [52483-21-3] *5-(10-Heptadecenyl)-1,3-benzenediol, 9CI. 5-(10-Heptadecenyl)resorcinol*. ***Irisresorcinol***
$C_{23}H_{38}O_2$ 346.552
Isol. from *Ginkgo biloba* (ginkgo). Powder. Mp 35-36°.

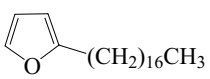
12′,13′-Didehydro(Z-): [103462-06-2]

[103462-07-3] *5-(12-Heptadecenyl)-1,3-benzenediol, 9CI. 5-(12-Heptadecenyl)resorcinol*
$C_{23}H_{38}O_2$ 346.552
Constit. of peel of mango fruit (*Mangifera indica*). Oil. λ_{max} 233 (ϵ 1900); 274 (ϵ 920); 290 (ϵ 860) (EtOH) (Berdy). λ_{max} 244 (ϵ 1400); 292 (ϵ 920) (EtOH-NaOH) (Berdy).

Cirigottis, K.A. *et al., Aust. J. Chem.*, 1974, **27**, 345-355 (*isol, synth, uv, pmr, derivs*)
Cojocaru, M. *et al., Phytochemistry*, 1986, **25**, 1093 (*12′,13′-didehydro*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3016 (*Irisresorcinol*)
Gohil, S. *et al., J. Sci. Food Agric.*, 1988, **45**, 43-52 (*isol*)
Arisawa, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2431-2434 (*synth*)
Bouillant, M.L. *et al., Phytochemistry*, 1994, **35**, 769 (*12′,13′-didehydro*)

2-Heptadecylfuran H-76

[208329-97-9]

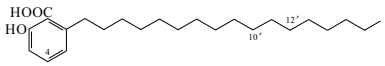


$C_{21}H_{38}O$ 306.531
Constit. of avocado pear, *Persea americana*.

Rodriguez-Saona, C.R. *et al., J. Chem. Ecol.*, 1998, **24**, 867-889 (*isol*)
Rodriguez-Saona, C.R. *et al., J. Nat. Prod.*, 1999, **62**, 191-193 (*synth, activity*)

2-Heptadecyl-6-hydroxybenzoic acid, 9CI H-77

[20261-39-6]
6-Heptadecylsalicylic acid



$C_{24}H_{40}O_3$ 376.578
Cryst. (EtOAc/cyclohexane). Mp 90-91.5°.

8′,9′-Didehydro(Z-): [69506-63-4] *2-(8-Heptadecenyl)-6-hydroxybenzoic acid. 6-(8-Heptadecenyl)salicylic acid*. ***Merulinic acid C***. *Δ$^{8'}$-Merulinic acid C. Geranicardic acid*
$C_{24}H_{38}O_3$ 374.562
Isol. from pistachio shells. Cryst. (Me_2CO). Mp 33-33.5°.

10′,11′-Didehydro(Z-): [111047-30-4]

[76261-15-9] *2-(10-Heptadecenyl)-6-hydroxybenzoic acid, 9CI. 6-(10-Heptadecenyl)salicylic acid*
$C_{24}H_{38}O_3$ 374.562
Isol. from *Ginkgo biloba* (ginkgo). Powder. Mp 45-46°.

10′,11′-Didehydro, Me ester: [111047-31-5]
$C_{25}H_{40}O_3$ 388.589
Isol. from *Ginkgo biloba* (ginkgo). Oil.

12′,13′-Didehydro(Z-): [20261-41-0] *6-(12-Heptadecenyl)-6-hydroxybenzoic acid, 9CI. 6-(12-Heptadecenyl)salicylic acid*
$C_{24}H_{38}O_3$ 374.562

8′,9′,11′,12′-Tetradehydro(Z,Z-): [141545-69-9] *2-Hydroxy-6-(8,11-heptadecadienyl)benzoic acid*. ***Pelandjauic acid***. *Pentaspadonic acid*
$C_{24}H_{36}O_3$ 372.547
Cryst. (Et_2O). Mp 23-26°.

8′,9′,11′,12′,14′,15′-Hexadehydro(all-Z-): [83173-24-4] *2-(8,11,14-Heptadecatrienyl)-6-hydroxybenzoic acid*. ***Antibiotic SB 202742***. *SB 202742*
$C_{24}H_{34}O_3$ 370.531
Constit. of *Spondias mombin* (yellow mombin). Oil. λ_{max} 205 (ϵ 22497); 241 (ϵ 3532); 308 (ϵ 2160) (MeOH) (Berdy).

4-Hydroxy: [69493-39-6] *2-Heptadecyl-4,6-dihydroxybenzoic acid, 9CI*. ***Dihydromerulinic acid A***
$C_{24}H_{40}O_4$ 392.578
Amorph. powder. Mp 105-107°. λ_{max} 217 (log ϵ 3.8); 262 (log ϵ 3.47); 297 (log ϵ 3.16) (MeOH).

4-Hydroxy, 8′,9′-didehydro(Z-): [69506-65-6] *2-(8-Heptadecenyl)-4,6-dihydroxybenzoic acid*. ***Merulinic acid A***. *Δ$^{8'}$-Merulinic acid A*
$C_{24}H_{38}O_4$ 390.562
Isol. from pistachio shells. Cryst. (Me_2CO). Sol. bases. Mp 116-117° (95-97°). λ_{max} 217 (log ϵ 4.35); 262 (log ϵ 4.03); 300 (log ϵ 3.67) (MeOH) (Derep). λ_{max} 225 (ϵ 24300); 259 (ϵ 9797); 299 (ϵ 4187) (MeOH) (Berdy).

4-Hydroxy, 10′,11′-didehydro: [69506-66-7] *2-(10-Heptadecenyl)-4,6-dihydroxybenzoic acid*
$C_{24}H_{38}O_4$ 390.562

4-Hydroxy, 8′,9′,11′,12′-tetradehydro(Z,Z-): [229469-23-2] *2-(8,11-Heptadecadienyl)-4,6-dihydroxybenzoic acid*. ***Dehydromerulinic acid A***
$C_{24}H_{36}O_4$ 388.546
Amorph. powder. Mp 90-92°. λ_{max} 217 (log ϵ 4.69); 263 (log ϵ 4.37); 301 (log ϵ 3.98) (MeOH).

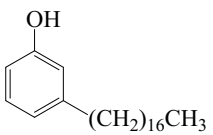
16′-Hydroxy, 8′,9′-didehydro(Z-): [69506-64-5] *2-Hydroxy-6-(16-hydroxy-8-heptadecenyl)benzoic acid*. ***Merulinic acid B***. *Δ$^{8'}$-Merulinic acid B*
$C_{24}H_{38}O_4$ 390.562
Waxy solid. Sol. bases; poorly sol. H_2O. Mp 31-32°. λ_{max} 210 (ϵ 19000); 243 (ϵ 5100); 309 (ϵ 3190) (MeOH) (Derep). λ_{max} 210 (ϵ 19000); 243 (ϵ 5098); 309 (ϵ 3190) (MeOH) (Berdy).

[111047-30-4, 114849-34-2, 124576-72-3, 129296-77-1, 129296-79-3]

Lamberton, J.A. *et al., Aust. J. Chem.*, 1959, **12**, 234 (*Pelandjauic acid*)
Giannetti, B.M. *et al., Z. Naturforsch., C*, 1978, **33**, 807-816 (*Merulinic acids*)
Durrani, A.A. *et al., J.C.S. Perkin 1*, 1979, 2069 (*synth*)
Spencer, G.F. *et al., J. Nat. Prod.*, 1980, **43**, 724 (*isol*)
Reffstrup, T. *et al., Acta Chem. Scand., Ser. B*, 1982, **36**, 291 (*SB 202742, isol, pmr, ir*)
Yalpani, M. *et al., Phytochemistry*, 1983, **22**, 2263 (*isol, cmr*)
Gerhold, D.L. *et al., J. Chem. Ecol.*, 1984, **10**, 713 (*isol*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3016 (*isol, ms, ir, pmr, deriv*)
Navarrete, A. *et al., Planta Med.*, 1989, **55**, 579 (*occur*)
Walters, D.P. *et al., Phytochemistry*, 1990, **29**, 1815 (*biosynth*)
Coates, N.J. *et al., J. Nat. Prod.*, 1994, **57**, 654 (*SB 202742, isol, pmr*)
Zehnter, R. *et al., Annalen*, 1995, 2209-2220 (*synth, ir, pmr, cmr*)
Sontag, B. *et al., Eur. J. Org. Chem.*, 1999, 1051-1055 (*Merulinic acids A*)

3-Heptadecylphenol H-78

[78636-94-9]
Cardanol$_{17:0}$



$C_{23}H_{40}O$ 332.568
Mp 60.4-60.8°.

7′,8′-Didehydro(Z-): ***3-(7-Heptadecenyl)-phenol***
$C_{23}H_{38}O$ 330.553

8′,9′-Didehydro: ***3-(8-Heptadecenyl)phenol***
$C_{23}H_{38}O$ 330.553

10′,11′-Didehydro(Z-): [111047-33-7] ***3-(10-Heptadecenyl)phenol***. *Cardanol $C_{17:1}$*
Isol. from *Ginkgo biloba* (ginkgo). Oil.

12′,13′-Didehydro: ***3-(12-Heptadecenyl)-phenol***
$C_{23}H_{38}O$ 330.553

14′,15′-Didehydro: ***3-(14-Heptadecenyl)-phenol***

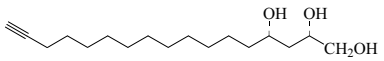
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3016 (*3-(10-Heptadecenyl)phenol*)
Asakawa, Y. *et al., Phytochemistry*, 1987, **26**, 735-738 (*isol*)
Jinno, S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1688-1694 (*synth, pmr*)

Correia, S.J. *et al., Phytochemistry*, 2001, **56**, 781-784 (*isol*)
Franke, K. *et al., Planta Med.*, 2001, **67**, 477-479 (*isol*)

16-Heptadecyne-1,2,4-triol, 9CI H-79

[24607-05-4]

[34524-38-4]



$C_{17}H_{32}O_3$ 284.438

(2*S*,4*S*)-*form* [129099-96-3]
Avocadyne
Constit. of avocado (*Persea americana*). Mp 76°. $[\alpha]_D^{25}$ -4.9 ($CHCl_3$). λ_{max} 203 (MeOH).

1-Ac: [24607-06-5]
$C_{19}H_{34}O_4$ 326.475
Constit. of avocado (*Persea americana*). Mp 73°. $[\alpha]_D^{25}$ -4.6 ($CHCl_3$).

2-Ac: [37139-04-1]
$C_{19}H_{34}O_4$ 326.475
Constit. of avocado (*Persea americana*).

4-Ac: [28884-46-0]
$C_{19}H_{34}O_4$ 326.475
Constit. of avocado (*Persea americana*).

Kashman, Y. *et al., Tetrahedron*, 1969, **25**, 4617; 1970, **26**, 1943 (*isol, struct*)
Alves, H.M. *et al., Ann. Acad. Bras. Ci&eenc.*, 1970, **425**, 45
Brown, B.I. *et al., J. Agric. Food Chem.*, 1972, **20**, 753
Adikaram, N.K.B. *et al., Phytochemistry*, 1992, **31**, 93 (*isol, pmr, cmr, props*)
Oberlies, N.H. *et al., J. Nat. Prod.*, 1998, **61**, 781-785 (*isol, pmr, cmr, ms*)
Domergue, F. *et al., Phytochemistry*, 2000, **54**, 183-189 (*abs config*)

2,4-Heptadienal, 9CI H-80

[5910-85-0]
$H_3CCH_2CH{=}CHCH{=}CHCHO$
$C_7H_{10}O$ 110.155

(*E,E*)-*form* [4313-03-5]
Bp_{12} 78° $Bp_{0.06}$ 27-29°.

2,4-Dinitrophenylhydrazone:
Purple needles. Mp 157-159°.

Di-Et acetal:1,1-Diethoxy-2,4-heptadiene
$C_{11}H_{20}O_2$ 184.278
Bp_{12} 96.5-97.5°.

*4*R,*5*S-*Epoxide:* [78307-41-2]

[69511-21-3] *3-(3-Ethyloxiranyl)-2-propenal, 9CI. 4,5-Epoxy-2-heptenal*
$C_7H_{10}O_2$ 126.155
Lipid peroxidation product implicated in nonenzymic browning reactions of aminoacids and proteins. Reacts with lysine and lysine groups to form pyrrole adducts.

(2*E*,4*Z*)-*form* [4313-02-4]
Bp_{18} 65°. n_D^{25} 1.4990.

(2*Z*,4*E*)-*form* [59121-26-5]
No phys. props. reported.

*(*E*)-Oxime:* [53937-30-7]
Mp -11°. $Bp_{0.01}$ 60-70°.

2,4-Dinitrophenylhydrazone: [42022-67-3]
Mp 141-143°.

(*Z,Z*)-*form* [108793-60-8]
No phys. props. reported.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 474D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 742A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 564C (*ir*)
Bricont, J. *et al., Helv. Chim. Acta*, 1967, **50**, 1517-1522 (*E,Z-form, ms, ir*)
Schiess, P. *et al., Helv. Chim. Acta*, 1974, **57**, 1676-1691 (*Z,E-form*)
Jaenicke, L. *et al., Chem. Ber.*, 1975, **108**, 225-232 (*E,Z-form, synth*)
Nishida, S. *et al., Chem. Lett.*, 1976, 1297 (*synth*)
Swoboda, P.A.T. *et al., J. Sci. Food Agric.*, 1978, **29**, 803-807 (*isol, synth, pmr, uv, ms, epoxide*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1983, **21**, 855 (*rev, tox*)
Zimmermann, B. *et al., Chem. Ber.*, 1986, **119**, 2848 (*synth, ir, pmr*)
Josephson, D.B. *et al., J. Food Sci.*, 1987, **52**, 328-331 (*glc*)
Hayes, R. *et al., Tet. Lett.*, 1991, **32**, 2953-2954 (*Z,E-form*)
Zamora, R. *et al., Lipids*, 1994, **29**, 243-249 (*epoxide*)
Hidalgo, F.J. *et al., J. Agric. Food Chem.*, 1995, **43**, 1023-1028 (*epoxide*)

2,5-Heptadien-1-ol H-81

[62237-90-5]
$H_3CCH{=}CHCH_2CH{=}CHCH_2OH$
$C_7H_{12}O$ 112.171
Constit. of the flowers of *Viola odorata* (sweet violet).

(*E,E*)-*form* [66618-63-1]
Oil. Bp_{14} 93-95°.

[35120-05-9, 41368-47-2]

Binet du Jassonneix, C. *et al., Bull. Soc. Chim. Fr.*, 1977, 1223 (*synth, ir, Raman*)
Chin, S.K. *et al., J. Chem. Res., Synop.*, 1985, 71 (*synth*)
Furukawa, J. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1229 (*synth*)
Jacoby, D. *et al., Synthesis*, 1990, 301 (*synth*)
Cu, J.Q. *et al., Phytochemistry*, 1992, **31**, 571 (*occur*)

4,6-Heptadiyne-1,3-diol H-82

$HC{\equiv}CC{\equiv}CCH(OH)CH_2CH_2OH$
$C_7H_8O_2$ 124.139
Isol. from aerial parts of *Artemisia dracunculus* (tarragon).

Di-Ac:
$C_{11}H_{12}O_4$ 208.213
Oil.

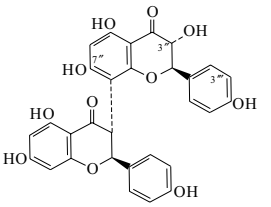
1-O-*β*-D-*Glucopyranoside:*

[139051-29-9, 139051-30-2]
$C_{13}H_{18}O_7$ 286.281
Isol. from aerial parts of *Artemisia dracunculus* (tarragon). Oil. Isol. as a mixt. of 3-epimers.

Jakupovic, J. *et al., Planta Med.*, 1991, **57**, 450 (*isol, struct, ir, ms, pmr, cmr*)

3″,4′,4‴,5,5″,7,7″-Heptahydroxy-3,8″-biflavanone, 8CI H-83

[14736-58-4]
*2,2′,3,3′-Tetrahydro-3′,5,5′,7,7′-pentahydroxy-2,2′-bis(4-hydroxyphenyl)[3,8′-bi-4*H*-1-benzopyran]-4,4′-dione, 9CI.* ***GB 1***.
4′,5,7-Trihydroxyflavanone(3→8)-3,4′,5,7-tetrahydroxyflavanone



Absolute configuration

$C_{30}H_{22}O_{11}$ 558.497
Cryst. (C_6H_6/Me_2CO) or amorph. powder. Mp 210°.

3‴-Hydroxy: [18412-96-9]

[18913-18-3] *3″,3‴,4′,4‴,5,5″,7,7″-Octahydroxy-3,8″-biflavanone, 8CI.* ***GB 2***
$C_{30}H_{22}O_{12}$ 574.497
Amorph. solid. Mp 230°. $[\alpha]_D$ -10.5 (c, 0.35 in MeOH).

3‴-Hydroxy, 4‴-Me ether: [68705-66-8] *3″,3‴,4′,5,5″,7,7″-Heptahydroxy-4‴-methoxy-3,8″-biflavanone.* ***Kolaflavanone***
$C_{31}H_{24}O_{12}$ 588.523
Amorph. powder.

3′,3‴-Dihydroxy: [73428-17-8] *3′,3″,3‴,4′,4‴,5,5″,7,7″-Nonahydroxy-3,8″-biflavanone.* ***Manniflavanone****. Garciniflavanone*
$C_{30}H_{22}O_{13}$ 590.496
Yellow amorph. solid. Mp 220-225°. Manniflavanone and Garciniflavanone appear to be identical with the same struct. (including stereochem.) registered twice in CA.

3′,3‴-Dihydroxy, 4′-Me ether: [110605-18-0] ***GB 3***
$C_{31}H_{24}O_{13}$ 604.523
Amorph. $[\alpha]_D^{20}$ -29.9 (c, 1 in Me_2CO).

3″-Deoxy: [19360-72-6] *4′,4‴,5,5″,7,7″-Hexahydroxy-3,8″-biflavanone. 3,8″-Binaringenin.* ***GB 1a***
$C_{30}H_{22}O_{10}$ 542.498
Amorph. $[\alpha]_D$ -28.1 (c, 0.22 in MeOH).

*3″-Deoxy, 7″-*O*-β-*D*-glucopyranoside:* [56663-56-0] ***3,8″-Binaringenin 7-glucoside***
$C_{36}H_{32}O_{15}$ 704.64
Cryst. Mp 218-221°. $[\alpha]_D^{20}$ -31.7 (c, 2.5 in EtOH).

*3″-Deoxy, 3‴-hydroxy, 7″-*O*-β-*D*-glucopyranoside:* [31654-49-6] ***Xanthochymuside***
$C_{36}H_{32}O_{16}$ 720.639
Isol. from the famine food *Garcinia xanthochymus*. Amorph. powder + $2H_2O$. Mp 223-225° (anhyd.) Mp 219° (hydrate). $[\alpha]_D^{20}$ -40 (c, 0.3 in MeOH). λ_{max} 227 (log ϵ 3.46); 250 (sh) (log ϵ 4.01); 290 (log ϵ 4.4); 337 (sh) (log ϵ 3.8) (MeOH).

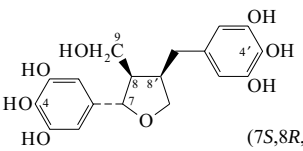
2″-Epimer, 3″-deoxy: ***GB 2b***
$C_{30}H_{22}O_{10}$ 542.498
$[\alpha]_D$ +8.2 (c, 0.22 in MeOH).

[111186-59-5, 132435-50-8]

Pelter, A. *et al., Tet. Lett.*, 1967, 1767 (*struct*)
Konashima, M. *et al., Tet. Lett.*, 1970, 4203 (*Xanthochymusside*)

Jackson, B. *et al., J.C.S.(C)*, 1971, 3791 (*isol, ir, uv, pmr, ms*)
Fa-Ching Chen, *et al., Phytochemistry*, 1975, **14**, 818 (*Xanthochymuside*)
Chen, F.-C. *et al., Phytochemistry*, 1975, **14**, 818-820 (*3,8″-Binaringenin 7-glucoside*)
Bandaranyake, W.M. *et al., Phytochemistry*, 1975, **14**, 1878 (*isol, ir, uv, pmr, ms*)
Cotterill, P.J. *et al., J.C.S. Perkin 1*, 1978, 532 (*Kolaflavanone*)
Duddeck, H. *et al., Phytochemistry*, 1978, **17**, 1369 (*cd*)
Crichton, E.G. *et al., Phytochemistry*, 1979, **18**, 1553 (*Manniflavanone*)
Iwu, M. *et al., J. Nat. Prod.*, 1982, **45**, 650 (*isol*)
Kabangu, K. *et al., Planta Med.*, 1987, **53**, 275 (*GB 3*)
Sonnenbichler, J. *et al., Z. Naturforsch., C*, 1987, **42**, 855 (*abs config, cd, pmr*)
Iwu, M.M. *et al., Fitoterapia*, 1990, **61**, 178 (*Garciniflavanone*)
Terashima, K. *et al., Heterocycles*, 1999, **50**, 283-290 (*isol, uv, pmr, cmr*)

3,3′,4,4′,5,5′,9-Heptahydroxy-7,9′-epoxylignan H-84



(7*S*,8*R*,8′*R*)-*form*

$C_{18}H_{20}O_8$ 364.351

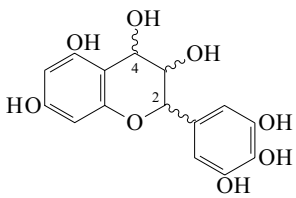
(7*S*,8*R*,8′*R*)-*form*

3,3′,5,5′-Tetra-Me ether, 9-O-*β*-D-*xylopyranoside:* [126882-52-8] ***Prupaside***
$C_{27}H_{36}O_{12}$ 552.574
Isol. from *Prunus padus* (bird cherry). Powder. $[\alpha]_D^{24}$ -38 (c, 0.87 in MeOH).

Yoshinari, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3301 (*Prupaside*)

3,3′,4,4′,5,5′,7-Heptahydroxyflavan H-85

[491-52-1]
*3,4-Dihydro-2-(3,4,5-trihydroxyphenyl)-2*H*-1-benzopyran-3,4,5,7-tetrol, 9CI. 3,3′,4,4′,5,5′,7-Flavanheptol, 8CI.* ***Leucodelphinidin***



$C_{15}H_{14}O_8$ 322.271
Small prisms +1H_2O (Me_2CO). Mp 300° dec. Log P -1.15 (uncertain value) (calc). Stereochem. of isolates undefined.

*3-*O-*β*-D-*Glucopyranoside:* [27838-81-9] *Leucodelphinidin 3-glucoside.* ***Diospyrin***†
$C_{21}H_{24}O_{13}$ 484.413
Isol. from *Diospyros kaki* (Japanese persimmon). Powder. $[\alpha]_D^{13}$ +288 (c, 0.5 in H_2O).

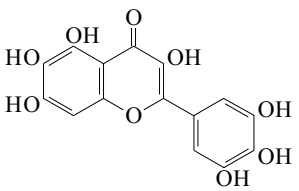
*3-*O-*[β-*D-*Galactopyranosyl-(1→4)-β-*D-*glucopyranoside]:* [189890-19-5]
$C_{27}H_{34}O_{18}$ 646.555
Constit. of *Moringa oleifera* (horseradish tree). Cryst. (EtOAc). Mp 158°. λ_{max} 282 (EtOH).

[98919-67-6, 117404-67-8, 126721-83-3, 126721-84-4]

Nakayama, T. *et al., Nature (London)*, 1963, **199**, 72 (*Diospyrin*)
Khare, G.C. *et al., J. Indian Chem. Soc.*, 1997, **74**, 247-248 (*3-galactosylglucoside*)

3,3′,4′,5,5′,6,7-Heptahydroxyflavone H-86

*3,5,6,7-Tetrahydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,5′,6,7-Hexahydroxyflavonol. 6-Hydroxymyricetin*



$C_{15}H_{10}O_9$ 334.239

*6,7-Methylene, 4′-Me ether, 3-*O-*β*-D-*glucuronopyranoside:*
$C_{23}H_{20}O_{15}$ 536.402
Constit. of *Spinacia oleracea* (spinach).

Edenharder, R. *et al., J. Agric. Food Chem.*, 2001, **49**, 2767-2773 (*6,7-methylene 4′-Me 3-glucuronide*)

3,3′,4′,5,5′,7,8-Heptahydroxyflavone, 8CI H-87

*3,5,7,8-Tetrahydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,5′,7,8-Hexahydroxyflavonol.* ***Hibiscetin****. 8-Hydroxymyricetin*

$C_{15}H_{10}O_9$ 334.239
Light yellow platelets (EtOH). Mp 350° dec.

*3-*O-*β*-D-*Glucopyranoside:* ***Hibiscitrin***
$C_{21}H_{20}O_{14}$ 496.381
Glycoside from *Hibiscus sabdariffa* (roselle). Cryst. (EtOH). Mp 238-240°.

3,3′,7,8-Tetra-Me, 4′,5′-methylene ether: [161697-25-2] *5-Hydroxy-3,3′,7,8-tetramethoxy-4′,5′-methylenedioxyflavone*
$C_{20}H_{18}O_9$ 402.357
Constit. of the dried fruit of *Citrus reticulata* (mandarin).

Rao, P.S. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1942, **15**, 148; 1948, **27**, 209 (*isol*)
Chow, P.W. *et al., Aust. J. Chem.*, 1968, **21**, 2529 (*isol, uv*)
Nakayama, M. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 3276 (*synth, uv*)
Chakraborty, J. *et al., J. Indian Chem. Soc.*, 1971, **48**, 80
Whalen, M.D. *et al., Phytochemistry*, 1979, **18**, 263 (*derivs*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1081 (*isol, uv, ir, pmr*)
Whalen, M.D. *et al., Phytochemistry*, 1983, **22**, 2107 (*isol, pmr, uv, ms*)
Fang, N. *et al., Phytochemistry*, 1985, **24**, 2693; 1986, **25**, 927 (*isol*)
Horie, T. *et al., Phytochemistry*, 1988, **27**, 1491 (*synth, struct*)
Saxena, V.K. *et al., J. Inst. Chem. (India)*, 1994, **66**, 62 (*3,3′,7,8-tetra-Me, 4′,5′-methylene ether*)

3,3′,4′,5,6,7,8-Heptahydroxyflavone H-88

[87926-83-8]
*2-(3,4-Dihydroxyphenyl)-3,5,6,7,8-pentahydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,6,7,8-Hexahydroxyflavonol. 8-Hydroxyquercetagetin*

$C_{15}H_{10}O_9$ 334.239
Isol. from petals of African marigold (*Tagetes erecta*). Yellow needles (EtOH). Mp >330°.

3′,6,8-Tri-Me ether: [549-10-0] *3,4′,5,7-Tetrahydroxy-3′,6,8-trimethoxyflavone.* ***Limocitrol***
$C_{18}H_{16}O_9$ 376.319
Constit. of citrus fruits. Fine yellow needles (MeOH or EtOH). Mp 221-222° (210-211°).

*3′,6,8-Tri-Me ether, 3-*O-*β*-D-*glucopyranoside:* [77133-42-7] *Limocitrol 3-glucoside*
$C_{24}H_{26}O_{14}$ 538.461
Isol. from lemon (*Citrus limon*). Yellow prisms (H_2O). Mp 163° Mp 203-204° (dimorph.).

*4′,6,8-Tri-Me ether, 3-*O-*β*-D-*glucopyranoside:Isolimocitrol 3-glucoside*
$C_{24}H_{26}O_{14}$ 538.461
Isol. from *Citrus limon*. Cryst. (MeOH aq.). Mp 220-225°.

*3′,5,6,8-Tetra-Me ether, 3-*O-*β*-D-*glucopyranoside:* [118694-40-9]
$C_{25}H_{28}O_{14}$ 552.488
Constit. of *Citrus* spp..

3,3′,4′,5,6,8-Hexa-Me ether: [185678-89-1] *7-Hydroxy-3,3′,4′,5,6,8-hexamethoxyflavone*
$C_{21}H_{22}O_9$ 418.399
Constit. of the peel of tangerine (*Citrus* sp.).

3,3′,4′,5,7,8-Hexa-Me ether: [167416-97-9] *6-Hydroxy-3,3′,4′,5,7,8-hexamethoxyflavone*
$C_{21}H_{22}O_9$ 418.399
Constit. of satsuma orange, *Citrus unshiu*.

3,3′,4′,6,7,8-Hexa-Me ether: [1176-88-1] *5-Hydroxy-3,3′,4′,6,7,8-hexamethoxyflavone*
$C_{21}H_{22}O_9$ 418.399
Isol. from peel of orange (*Citrus sinensis*). Yellow cryst. (MeOH). Mp 110-111°.

*3′,4′,5,6,7,8-Hexa-Me ether, 3-*O-*β*-D-*glucopyranoside:* [98891-93-1] *Natsudaidain 3-glucoside*
$C_{27}H_{32}O_{14}$ 580.541
Constit. of *Citrus* spp..

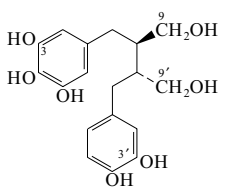
*3′,4′,5,6,7,8-Hexa-Me ether, 3-*O-*(4-*O-*3-hydroxy-3-methylglutaroyl-β-*D-*glucopyranoside):* [149402-86-8]
$C_{33}H_{40}O_{18}$ 724.668
Constit. of *Citrus* sp. Amorph. powder. $[\alpha]_D$ -6.3 (c, 0.32 in MeOH). Me ester also isol. from same source as a possible artifact.

Hepta-Me ether: [1178-24-1] *3,3′,4′,5,6,7,8-Heptamethoxyflavone*

$C_{22}H_{24}O_9$ 432.426
Isol. from *Citrus* spp. peels. Cryst. (EtOH). Mp 129-131°.

Sastry, G.P. *et al., Tetrahedron*, 1961, **15**, 111 (*synth*)
Row, L.R. *et al., Indian J. Chem.*, 1963, **1**, 207 (*synth*)
Gentili, B. *et al., Tetrahedron*, 1964, **20**, 2313 (*Limocitrol, Isolimocitrol, 3-glucoside*)
Dreyer, D.L. *et al., Tetrahedron*, 1964, **20**, 2977 (*synth*)
Walther, K. *et al., Planta Med.*, 1966, **14**, 453 (*Heptamethoxyflavone*)
Tatum, J.H. *et al., Phytochemistry*, 1972, **11**, 2283 (*isol, uv*)
Murphy, S.T. *et al., Aust. J. Chem.*, 1974, **27**, 187
Higa, T. *et al., J.C.S. Perkin 1*, 1974, 1350
Martino, V.S. *et al., Phytochemistry*, 1976, **15**, 1086 (*3′,4′,5,7-Tetrahydroxy-3,6,8-trimethoxyflavone*)
Calvert, D.J. *et al., Org. Magn. Reson.*, 1979, **12**, 583 (*cmr*)
Bittner, M. *et al., Phytochemistry*, 1983, **22**, 1523 (*isol*)
Bhardwaj, D.K. *et al., Proc. Indian Natl. Sci. Acad., Part A*, 1983, **49**, 408 (*isol*)
Roitman, J.N. *et al., Phytochemistry*, 1985, **24**, 835 (*derivs*)
Fang, N. *et al., Phytochemistry*, 1985, **24**, 2693; 1986, **25**, 235 (*derivs*)
Yu, S. *et al., Phytochemistry*, 1988, **27**, 171 (*isol*)
Jong, T.-T. *et al., Phytochemistry*, 1989, **28**, 245 (*isol*)
Sugiyama, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 714 (*deriv*)
Agrawal, B. *et al., Int. J. Pharmacogn.*, 1993, **31**, 305 (*3′,6,8-tri-Me ether 3-arabinosylgalactoside*)
Chkhikvishvili, I.D. *et al., Khim. Prir. Soedin.*, 1994, **30**, 821 (*6-Hydroxy-3,3′,4′,5,7,8-hexamethoxyflavone*)
Chen, J. *et al., J. Agric. Food Chem.*, 1997, **45**, 364-368 (*3,3′,4′,5,6,8-hexa-Me ether, hepta-Me ether*)

3,3′,4,4′,5,9,9′-Heptahydroxylignan H-89



(8*R*,8′*R*)-*form*

$C_{18}H_{22}O_7$ 350.368

(8*R*,8′*R*)-*form*

3′,4′-Methylene, 3,4,5-tri-Me ether: [73149-51-6] *9,9′-Dihydroxy-3,4,5-trimethoxy-3′,4′-methylenedioxylignan.* ***Dihydroclusin***
$C_{22}H_{28}O_7$ 404.459
Constit. of *Piper cubeba* (cubeb pepper). Cryst. Mp 97-98°. $[\alpha]_D^{25}$ -27.13 (c, 0.24 in $CHCl_3$).

Prabhu, B.R. *et al., Phytochemistry*, 1985, **24**, 329 (*Dihydroclusin*)
Kato, M.J. *et al., Phytochemistry*, 1990, **29**, 1799

Heptanal, 9CI, 8CI H-90

[111-71-7]
Heptaldehyde. Enanthal. Oenanthal. Enanthole. Oenanthole. Oenanthaldehyde. Enanthaldehyde. FEMA 2540

$H_3C(CH_2)_5CHO$
$C_7H_{14}O$ 114.187
Found in essential oils of ylang-ylang, clary sage, California orange, bitter orange and others. Flavouring agent. Liq. with a pungent odour and an unpleasant, fatty taste. d^{20} 0.82. Mp -43.3°. Bp 152.8° Bp_{30} 59.6°. n_D^{20} 1.4133.
▶ Low oral toxicity; flammable, fl. p. 35°. MI6900000

Oxime: [629-31-2]
$C_7H_{15}NO$ 129.202
Plates (EtOH). Mp 57-58°. Bp 195° Bp_{14} 100.5°.

Semicarbazone: [6033-21-2]
Cryst. (MeOH). Mp 108-109°.

Di-Me acetal: [10032-05-0] *1,1-Dimethoxyheptane. FEMA 2541*
$C_9H_{20}O_2$ 160.256
Flavouring ingredient. Oil with a pleasant odour reminiscent of walnut and cognac. Bp 182° Bp_{17} 75°.

Di-Et acetal: [688-82-4] *1,1-Diethoxyheptane*
$C_{11}H_{24}O_2$ 188.309
Bp_{774} 204-205°.

Enol acetate(E-): [17574-85-5] *1-Acetoxy-1-heptene*
$C_9H_{16}O_2$ 156.224
Bp_{17} 87°.

Enol acetate(Z-):
$C_9H_{16}O_2$ 156.224
Bp_{16} 73°.

[5775-78-0, 5784-69-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 468B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 731B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 554D (*ir*)
Org. Synth., Coll. Vol., 3, 1955, 127 (*enol acetate*)
Freytag, W. *et al., Chem. Ber.*, 1967, **100**, 3457 (*enol acetate*)
Org. Synth., 1971, **51**, 31; 1977, **56**, 36 (*synth*)
Cossé-Barbi, A. *et al., Spectrochim. Acta A*, 1972, **28**, 561 (*uv*)
Brown, P. *et al., Org. Mass Spectrom.*, 1973, **7**, 305 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 701 (*rev, tox*)
Norasaka, K. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 2773 (*synth*)
Hojo, M. *et al., Tet. Lett.*, 1977, 3883 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HBB500
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 312-313
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1262-1264
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

2,3-Heptanedione, 9CI H-91

[96-04-8]
2,3-Dioxoheptane. FEMA 2543
$H_3CCOCO(CH_2)_3CH_3$
$C_7H_{12}O_2$ 128.171
Flavour ingredient. Found in tomato, beer, rum, soybean, mushroom and shoyu. Liq. with pungent cheese odour and sweet buttery taste. Bp_{10} 44-45°.

Bis-2,4-dinitrophenylhydrazone:
Mp 226-227°.

Cuvigny, T. *et al., C. R. Hebd. Seances Acad. Sci.*, 1953, **237**, 815
Unanyon, M.P. *et al., CA*, 1968, **69**, 2472d (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1265 (*occur, props*)

3,4-Heptanedione, 9CI H-92

[13706-89-3]
$H_3CCH_2CH_2COCOCH_2CH_3$
$C_7H_{12}O_2$ 128.171
Constit. of coffee. Bp_{732} 147°.

3-Oxime: [32818-77-2]
$C_7H_{13}NO_2$ 143.185
Insol. H_2O. Bp_{60} 145°.

Dioxime: [42563-88-2]
$C_7H_{14}N_2O_2$ 158.2
Cryst. (EtOH). Mp 167-168°.

Wassermann, H.H. *et al., J.A.C.S.*, 1976, **98**, 7868 (*synth*)

Heptanoic acid, 9CI, 8CI H-93

[111-14-8]
Hexane-1-carboxylic acid. Heptoic acid. Enanthic acid. Oenanthic acid. Heptylic acid. Oenanthylic acid. Enanthylic acid. FEMA 3348
$H_3C(CH_2)_5COOH$
$C_7H_{14}O_2$ 130.186
Present in essential oils, e.g. violet leaf oil, palm oil. Also present in apple, feijoa fruit, strawberry jam, clove bud, ginger, black tea, morello cherry, grapes, rice bran and other foodstuffs. Flavouring ingredient. Used as one of the components in washing solns. used to assist lye peeling of fruit and vegetables. Oil. Sol. hexane; poorly sol. H_2O. d_4^{20} 0.92. Mp -9°. Bp 222-245° Bp_{11} 115-116°. n_D^{20} 1.4216.
▶ LD_{50} (rat, orl) 7000 mg/kg. MJ1575000

Me ester: [106-73-0] *Methyl heptanoate. FEMA 2705*
$C_8H_{16}O_2$ 144.213
Flavouring agent. Liq. with currant-like flavour and orris-like odour. d_4^{20} 0.87. Fp -55.8. Bp 172.1° Bp_{100} 113-116°. n_D^{20} 1.4133.
▶ MJ2297500

Et ester: [106-30-9] *Ethyl heptanoate. FEMA 2437*
$C_9H_{18}O_2$ 158.24
Found in fruits, e.g. apple, apricot, grapefruit, strawberry etc. Also present in pea, Parmesan cheese, butter, fish oil, hop oil, wine, Bantu beer, apple brandy. Flavouring agent; used in fruit aroma compositions. Fp -66.1. Bp 188.6° Bp_{14} 78°. n_D^{15} 1.4144.
▶ MJ2087000

Propyl ester: [7778-87-2] *Propyl heptanoate. FEMA 2948*
$C_{10}H_{20}O_2$ 172.267
Used in imitation brandy flavouring. d 0.87. Bp 206°.

Butyl ester: [5454-28-4] *Butyl heptanoate. FEMA 2199*
$C_{11}H_{22}O_2$ 186.294

Flavouring agent used in imitation fruit and beer flavouring. Present in apples. Liq. with fruity odour and taste. d_4^{20} 0.86. Fp -68.4. Bp 226°. n_D^{20} 1.4228.

2-Methylpropyl ester: [7779-80-8] *Isobutyl enanthate. 2-Methylpropyl heptanoate. FEMA 2200*
$C_{11}H_{22}O_2$ 186.294
Used in imitation brandy flavouring.

Pentyl ester: [7493-82-5] *Pentyl heptanoate. Amyl enanthate. FEMA 2073*
$C_{12}H_{24}O_2$ 200.32
Flavouring ingredient. Liq. with fruity odour and taste. d^{20} 0.85. Mp -49.5°. Bp 245-246°. n_D^{20} 1.4263.

2-Propenyl ester: [142-19-8] *2-Propenyl heptanoate. Allyl enanthate. FEMA 2031*
$C_{10}H_{18}O_2$ 170.251
Used in fruit flavours. Liq. with fruity odour and banana taste. $d_4^{15.5}$ 0.89. Bp 210°. n_D^{20} 1.4290.

► MJ1750000

[10051-45-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 482D; 607A; 712C; 729D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 753B; 920C; 921A; 1168A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 574D; 623A; 623B; 770B (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 315 (*synth*)
Ho, T.-S. *et al., Synthesis*, 1972, 562 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1977, **15**, 619 (*2-propenyl ester*)
Couperus, P.A. *et al., Org. Magn. Reson.*, 1978, **11**, 590 (*cmr*)
Odinokov, V.N. *et al., Zh. Org. Khim.*, 1978, **14**, 60 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EKN050
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 41 (*pentyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 89; 161; 341; 989; 1265; 1769 (*occur, props, esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGH250; HBE000; EKN050

1-Heptanol, 9CI H-94

[111-70-6]

[53535-33-4]
Heptyl alcohol, 8CI. FEMA 2548

$H_3C(CH_2)_5CH_2OH$

$C_7H_{16}O$ 116.203
Found in a few essential oils, e.g. *Rosa rugosa*. Also present in roasted peanut, roasted filbert, plum brandy, rice bran, cooked rice, peated malt, Bourbon vanilla, banana, morello cherry, orange, guava fruit, pineapple and plum. Flavouring ingredient. Liq. with pungent spicy taste. d_4^{20} 0.82. Fp -34.1. Bp 176.3° Bp_{15} 78-79°. n_D^{20} 1.4241.

► LD_{50} (rat, orl) 500 mg/kg. Fl. p. 63/74°. MK0350000

Formyl: [112-23-2] *Heptyl formate. FEMA 2552*
$C_8H_{16}O_2$ 144.213
Food flavour. d 0.88. Bp 178°.

Ac: [112-06-1] *Heptyl acetate. Acetate C7. FEMA 2547*
$C_9H_{18}O_2$ 158.24
Present in apple, apricot, banana, orange peel, lemon peel, melon, Bartlett pears, other fruits, heated beef fat, ginger, wines and spirits. Flavouring ingredient. Liq. with sweet apricot-like taste. d_4^{15} 0.88. Fp -50. Bp 191.5°. n_D^{20} 1.4150.

► Eye, skin and mucous membrane irritant. AH9901000

Butanoyl: [5870-93-9] *Heptyl butanoate. FEMA 2549*
$C_{11}H_{22}O_2$ 186.294
Used in food flavouring. d 0.88. Bp 225°.

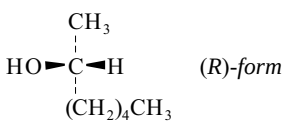
Heptanoyl: [624-09-9] *Heptyl heptanoate*
$C_{14}H_{28}O_2$ 228.374
Used in food flavouring. d 0.86. Bp 274°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 110D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 165A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 157A (*ir*)
Gartenmeister, R. *et al., Annalen*, 1886, **233**, 255; 266; 271; 276; 280; 284; 288 (*esters*)
Org. Synth., Coll. Vol., 1, 1932, 304 (*synth, bibl*)
Cambie, R.C. *et al., J.C.S.(C)*, 1966, 72 (*isol*)
Burgess, A.R. *et al., J.C.S.(B)*, 1969, 341 (*ms*)
Doyle, M.P. *et al., J.A.C.S.*, 1972, **94**, 3659 (*synth*)
Merz, A. *et al., Angew. Chem., Int. Ed.*, 1973, **12**, 845 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 697 (*rev, tox*)
Bascetta, E. *et al., Chem. Phys. Lipids*, 1985, **36**, 253 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HBL500
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1277; 1278 (*occur, props, Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBL000; HBL500

2-Heptanol, 9CI H-95

[543-49-7]

[53535-33-4]
1-Methylhexanol. FEMA 3288



(*R*)-*form*

$C_7H_{16}O$ 116.203

► Eye and skin irritant. LD_{50} (rat,orl) 2580 mg/kg. Fl. p. 71°. MJ2975000

(*R*)-*form* [6033-24-5]
Bp_{23} 74.5°. $[\alpha]_D^{25}$ -3.78 (neat).

(*S*)-*form* [6033-23-4]
Bp 150° Bp_{20} 73.5°. $[\alpha]_D^{25}$ +4.12 (neat). $[\alpha]_D^{20}$ +11.45 (EtOH).

O-*β*-D-*Glucopyranoside:* [117074-18-7]
$C_{13}H_{26}O_6$ 278.345

Ac:
$C_9H_{18}O_2$ 158.24
Bp_{17} 71°. $[\alpha]_D^{20}$ +8.23.

(±)-*form* [52390-72-4]
Flavouring ingredient. Sol. EtOH, Et_2O, C_6H_6; sl. sol. H_2O. d^{20} 0.82. Bp 158-160° $Bp_{16.5}$ 66.7°.

3,5-Dinitrobenzoyl:
Mp 49.4°.

(ξ)-*form*
Occurs in oil of ginger (*Zingiber officinale*) and strawberries (*Fragaria vesca*).

O-*β*-D-*Glucopyranoside:*
Occurs in oil of ginger (*Zingiber officinale*).

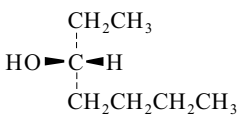
[5921-82-4, 54638-12-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 119D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 179B; 179C; 180A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 168A (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 317 (*synth*)
Lukes, R. *et al., Coll. Czech. Chem. Comm.*, 1960, **25**, 483 (*abs config*)
Nigam, N.C. *et al., Can. J. Chem.*, 1964, **42**, 2610 (*isol*)
Zweifel, G. *et al., Tet. Lett.*, 1966, 6021 (*synth*)
Carlson, R.M. *et al., Tet. Lett.*, 1971, 3661 (*synth*)
Keinan, E. *et al., J.A.C.S.*, 1986, **108**, 162 (*synth*)
Jolad, S.D. *et al., Phytochemistry*, 1988, **27**, 2199 (*isol, glucoside*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 315
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1267-1268
Sekiwa, Y. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 384-389 (*glucoside*)
Nakamura, K. *et al., J.C.S. Perkin 1*, 2000, 3205-3211 (*S-form, synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBE500

3-Heptanol, 9CI H-96

[589-82-2]

[53535-33-4]
FEMA 3547



(*R*)-*form*

$C_7H_{16}O$ 116.203

► Eye and skin irritant. LD_{50} (rat,orl) 1870 mg/kg. Fl. p. 60°. MJ3150000

(*R*)-*form* [62701-49-9]
Bp_{18} 66°. $[\alpha]_D^{23}$ -0.9.

α-*Naphthylurethane:*
Mp 74-75°. $[\alpha]_D^{20}$ 0.

(*S*)-*form* [26549-25-7]
Bp_{117} 104-106° Bp_{18} 66°.

(±)-*form* [40617-58-1]
Flavouring agent. Oily liq. with a powerful herbaceous odour and a pungent taste. Insol. H_2O, sol. EtOH. Bp_{750} 156.5-157°.

Et ether:3-Ethoxyheptane
$C_9H_{20}O$ 144.256
Bp_{750} 151°.

(ξ)-*form*
Present in strawberry, mint and banana.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 120A (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 180B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 168B (*ir*)
Seebach, D. *et al., Angew. Chem., Int. Ed.*, 1969, **8**, 982
Zweifel, G. *et al., Synthesis*, 1973, 37 (*synth*)
Keinan, E. *et al., J.A.C.S.*, 1986, **108**, 162 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 315
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1268-1269
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBF000

2-Heptanone, 9CI H-97

[110-43-0]
Methyl pentyl ketone. Amyl methyl ketone. FEMA 2544

$H_3C(CH_2)_4COCH_3$

$C_7H_{14}O$ 114.187

Present in apple, morello cherry, feijoa fruit, grapes, quince, clove bud, cheeses, wines, black tea, raw shrimp, Ceylon cinnamon, rancid coconut oil and other foodstuffs. Also a minor constit. of plant oils. Flavour ingredient. Light yellow oil with characteristic slightly spicy banana odour. d_4^{20} 0.82. Fp -35.5. Bp 151.45° Bp_{21} 111°. n_D^{20} 1.4110.

► Flammable. Skin irritant. LD_{50} (rat, orl) 1670 mg/kg. OES: long-term 50 ppm; short-term 100 ppm (Sk). MJ5075000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 408D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 636C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 492B (*ir*)
Young, F.G. *et al., J.A.C.S.*, 1950, **72**, 3635
Posner, G.H. *et al., Tet. Lett.*, 1970, 4647 (*synth*)
Brown, C.A. *et al., J.O.C.*, 1974, **39**, 1324
Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1976, 1941 (*synth, ir*)
Friedrich, E. *et al., Synthesis*, 1977, 893 (*synth*)
Anderson, M.W. *et al., J.C.S. Perkin 1*, 1986, 1995 (*synth, pmr, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1269-1270 (*occur, props*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 827
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MGN500

3-Heptanone, 9CI H-98

[106-35-4]
Butyl ethyl ketone. FEMA 2545

$H_3C(CH_2)_3COCH_2CH_3$

$C_7H_{14}O$ 114.187

Flavouring ingredient. Liq. with a powerful green, fatty, fruity odour and a melon/banana flavour. d^{20} 0.82. Bp 149-152°. n_D^{20} 1.4115.

► Flammable. Eye and skin irritant. LD_{50} (rat, orl) 2760 mg/kg. OES: long-term 50 ppm; short-term 75 ppm (Sk) (current); short-term 100 ppm (Sk) (proposed). MJ5250000

Oxime: [2108-81-8]
$C_7H_{15}NO$ 129.202
Bp_1 56°.

2,4-Dinitrophenylhydrazone: [64739-11-3]
Mp 70.2°.

Semicarbazone: [3622-67-1]
Mp 99-100° Mp 111°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 409A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 637A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 492C (*ir*)
Michel, J. *et al., Bull. Soc. Chim. Fr.*, 1968, 4898 (*synth*)
Collman, J.P. *et al., J.A.C.S.*, 1972, **94**, 1788 (*synth*)
Olah, G.A. *et al., Synthesis*, 1977, 677 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 316
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1270-1271
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 201
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EHA600

4-Heptanone, 9CI, 8CI H-99

[123-19-3]
Dipropyl ketone. Butyrone. FEMA 2546

$H_3C(CH_2)_2CO(CH_2)_2CH_3$

$C_7H_{14}O$ 114.187

Flavouring ingredient. Refractive liq. with a penetrating odour and burning taste. Insol. H_2O, sol. EtOH, Et_2O. d^{20} 0.81. Mp -32.6°. Bp 142-144°. n_D^{20} 1.4069.

► Flammable, fl. p. 49°. LD_{50} (rat,orl) 3730 mg/kg. MJ5600000

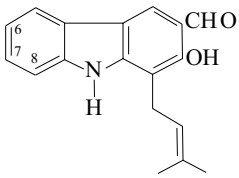
Oxime: [1188-63-2]
$C_7H_{15}NO$ 129.202
Cryst. Sol. $CHCl_3$. Mp 187-188°. Bp_{772} 196°.

2,4-Dinitrophenylhydrazone: [1655-41-0]
Mp 75°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 409B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 637B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 492D (*ir*)
Goldsmith, D.J. *et al., Tetrahedron, Suppl.* 7, 1966, 145 (*ms*)
Holland, W.J. *et al., Mikrochim. Acta*, 1972, 183 (*synth*)
Dubois, J.E. *et al., Spectrochim. Acta A*, 1972, **28**, 528 (*uv*)
Org. Synth., Coll. Vol., 5, 1973, 589 (*synth*)
Walker, R. *et al., Mikrochim. Acta*, 1974, 105; 1975, **2**, 249; 541 (*detn, Au, Pd*)
Dunn, P. *et al., Mikrochim. Acta*, 1975, **2**, 129; 1977, **1**, 363 (*detn, Pd*)
Kirchoff, R. *et al., Tet. Lett.*, 1976, 2533 (*synth*)
Shono, T. *et al., Tet. Lett.*, 1977, 3625 (*synth*)
Jorgensen, J.W. *et al., Science (Washington, D.C.)*, 1978, **199**, 796
Whitten, W.K. *et al., J. Chem. Ecol.*, 1980, **6**, 49
Dupuis, L.T. *et al., Mikrochim. Acta*, 1980, **1**, 29 (*detn, Ag*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 317
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1271-1272
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DWT600

Heptaphylline H-100

[17750-35-5]
2-Hydroxy-1-(3-methyl-2-butenyl)-9H-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-2-hydroxy-1-prenylcarbazole



$C_{18}H_{17}NO_2$ 279.338

Alkaloid from the leaves of *Clausena lansium* (wampee). Bright yellow needles (Et_2O or $CHCl_3$/hexane). Mp 171-172°.

7-Hydroxy: [170663-15-7] *2,7-Dihydroxy-1-(3-methyl-2-butenyl)-9H-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-2,7-dihydroxy-1-prenylcarbazole.* ***7-Hydroxyheptaphylline***
$C_{18}H_{17}NO_3$ 295.337
Alkaloid from root bark of *Clausena lansium* (wampee). Yellow needles (CH_2Cl_2/MeOH). Mp 194-196°.

Joshi, B.S. *et al., Phytochemistry*, 1972, **11**, 2065 (*isol, uv, ir, pmr, struct, synth*)
Anwer, F. *et al., Experientia*, 1977, **33**, 412 (*isol*)
Prakash, D. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 1075 (*isol*)
Wu, T.-S. *et al., J. Nat. Prod.*, 1982, **45**, 718 (*isol*)
Kumar, V. *et al., Phytochemistry*, 1995, **40**, 1563 (*7-Hydroxyheptaphylline*)
Yenjai, C. *et al., Planta Med.*, 2000, **66**, 277-281 (*activity*)

2-Heptenal, 9CI H-101

[2463-63-0]
FEMA 3165

$H_3C(CH_2)_3CH{=}CHCHO$

$C_7H_{12}O$ 112.171

Isol. from soya bean oil (*Glycine max*). Flavouring constit. of many foods. Oil with pungent, green, somewhat fatty odour, pleasant only in extreme dilution.

► MJ8794000

(E)-form [18829-55-5]
d 0.86. Bp 165-167° Bp_{15} 61-62°. $[\alpha]_D^{20}$ +1.45.

► MJ8795000

2,4-Dinitrophenylhydrazone: [2122-10-3]
Mp 132-133°.

(Z)-form [57266-86-1]
Bp_{16} 64-65°.

Di-Et acetal:1,1-Diethoxy-1-heptene
$C_{11}H_{22}O_2$ 186.294
Bp_{15} 90-92°.

[20810-22-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 473A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 737B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 560D (*ir*)
Fujimaki, M. *et al., Agric. Biol. Chem.*, 1965, **29**, 855 (*isol*)
Tadema, G. *et al., CA*, 1976, **85**, 5141m (*synth*)
Wada, M. *et al., Chem. Lett.*, 1977, 345 (*synth*)
Yamamoto, K. *et al., Synthesis*, 1977, 721 (*synth, ir, pmr*)

Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth*)
Huang, Y.-Z. *et al., J.O.C.*, 1987, **52**, 3558 (*synth, ir, ms, pmr*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 331 (*rev, tox, E-form*)
Fortes, C.C. *et al., Synth. Commun.*, 1997, **27**, 3917-3941 (*synth, ir, pmr, cmr, ms*)

4-Heptenal, 9CI H-102

[62238-34-0]
$H_3CCH_2CH{=}CHCH_2CH_2CHO$
$C_7H_{12}O$ 112.171

(*E*)-*form* [929-22-6]
Oil with nauseous odour. Bp 112-113°.

2,4-Dinitrophenylhydrazone:
Dull-orange needles (EtOH). Mp 120°.

(*Z*)-*form* [6728-31-0] *FEMA 3289*
Flavouring agent. Used in cream and butter flavourings. Component of butter. Widespread trace constit. of food flavours. Liq. with creamy odour. Bp_{12} 42-44°. n_D^{20} 1.4343.

Di-Et acetal: [18492-65-4] *7,7-Diethoxy-3-heptene. FEMA 3349*
$C_{11}H_{22}O_2$ 186.294
Flavouring ingredient used to impart cream or butter-like flavour. Liq.

Mukerji, S.K. *et al., Tet. Lett.*, 1966, 2479 (*synth*)
Stetter, H. *et al., Synthesis*, 1975, 379 (*synth*)
Cardinale, G. *et al., Tetrahedron*, 1984, **40**, 1881-1883 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 318
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1272-1274

2-Heptenoic acid, 9CI H-103

[18999-28-5]
Hex-1-ene-1-carboxylic acid
$H_3C(CH_2)_3CH{=}CHCOOH$
$C_7H_{12}O_2$ 128.171
► LD_{50} (mus, ipr) 1600 mg/kg. MJ9650000

Me ester: [22104-69-4]
[38693-91-3, 66618-64-2]
$C_8H_{14}O_2$ 142.197
Both (*E*)- and (*Z*)-forms present in wine and pomace from Muscat de Frontignan grapes. Bp_{16} 77-79°. Phys. props. are for material of unspecified geometry.

(*E*)-*form* [10352-88-2]
FEMA 3920
Flavouring ingredient. Liq. Mp -12–11°. $Bp_{0.3}$ 89°. n_D^{22} 1.4560.

Et ester: [54340-72-6]
$C_9H_{16}O_2$ 156.224
Bp_3 58°. n_D^{23} 1.4375.

Amide: [22031-62-5]
$C_7H_{13}NO$ 127.186
Mp 125°.

Nitrile: [22031-56-7] *2-Heptenenitrile. 1-Cyanohexene*
$C_7H_{11}N$ 109.171
Bp 186-187° Bp_{14} 72-73°. n_D^{20} 1.4428.

(*Z*)-*form* [1577-31-7]
Liq. d_4^{22} 0.94. Mp -19°. Bp 225-228° Bp_{11} 120-122°. n_D^{25} 1.4515.

Et ester: [35066-42-3]
$C_9H_{16}O_2$ 156.224
Bp_{20} 80°.

Nitrile: [66478-41-9]
Bp 171-172° Bp_{20} 112-114°.

[2351-88-4, 22629-47-6]

Okamoto, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 543-545 (*nitrile*)
Zweifel, G. *et al., J.A.C.S.*, 1977, **99**, 3184-3185 (*synth*)
Coutrot, P. *et al., Synthesis*, 1978, 133-134 (*E-form, synth*)
Nakayama, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 184-185 (*Me ester, synth*)
Alexaxis, A. *et al., Tetrahedron*, 1980, **36**, 1961-1969 (*Z-form, synth, ir, pmr*)
Etievant, P.X. *et al., J. Sci. Food Agric.*, 1983, **34**, 393-403 (*Me ester, detn, wine*)
Newcomb, M. *et al., J.A.C.S.*, 1986, **108**, 240-244 (*nitrile*)
Org. Synth., Coll. Vol., 6, 1988, 711-714 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBK500

4-Heptenoic acid, 9CI H-104

[35194-37-7]
Hex-3-ene-1-carboxylic acid
$H_3CCH_2CH{=}CHCH_2CH_2COOH$
$C_7H_{12}O_2$ 128.171
Isol. as the Me ester from oil of *Humulus lupulus* (hops).

(*E*)-*form* [51193-78-3]
Bp_8 105°. n_D^{20} 1.4400.

Chloride: [74132-57-3]
$C_7H_{11}ClO$ 146.616
Bp_{12} 69-71°.

(*Z*)-*form* [41653-95-6]
Yellow oil. Bp_{12} 116°.

Me ester: [39924-30-6]
$C_8H_{14}O_2$ 142.197
Bp_4 106.5°.

Chloride:
Bp_{35} 72-76°. n_D^{20} 1.4400.

Nitrile:1-Cyano-3-hexene
$C_7H_{11}N$ 109.171
Oil. Bp_{40} 75°.

[80639-52-7]

Hunsdiecker, H. *et al., Ber.*, 1942, **75**, 460-468 (*synth*)
Crombie, L. *et al., J.C.S.*, 1952, 869-875 (*synth*)
Buttery, R.G. *et al., CA*, 1965, **62**, 1050 (*isol*)
Furukawa, Y. *et al., CA*, 1976, **84**, 150153a (*synth*)
Sato, T. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 505-508 (*synth, ir, pmr*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255-3264 (*synth, pmr*)
Udding, J.H. *et al., J.O.C.*, 1994, **59**, 6671-6682 (*synth, nitrile, ir, pmr, cmr*)
Favino, T.F. *et al., J.O.C.*, 1996, **61**, 8975-8979 (*nitrile synth, pmr*)

3-Hepten-1-ol, 9CI H-105

[10606-47-0]
$H_3C(CH_2)_2CH{=}CHCH_2CH_2OH$
$C_7H_{14}O$ 114.187

(*E*)-*form* [2108-05-6]
Bp 170-171°.

Diphenylurethane:
Cryst. (petrol). Mp 105°.

Ac: [1576-77-8] *FEMA 3493*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient. Liq. d^{15} 1.43.
Bp_3 55-57°. n_D^{20} 1.4302.

2-Methylpropanoyl: [57859-47-9] *FEMA 3494*
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient. Liq. d^{25} 0.88.
Bp_3 85-90°. n_D^{20} 1.4296.

(*Z*)-*form* [1708-81-2]
Bp_{18} 80-82°.

Diphenylurethane:
Needles (petrol). Mp 84-85°.

Stapp, P.R. *et al., J.O.C.*, 1971, **36**, 2505-2507 (*Ac, synth*)
Warwel, S. *et al., Synthesis*, 1975, 632 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 320 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1276-1277 (*esters*)
Satoh, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 18-22 (*Z-form, synth, ir, pmr*)

4-Hepten-1-ol H-106

$H_3CCH_2CH{=}CHCH_2CH_2CH_2OH$
$C_7H_{14}O$ 114.187

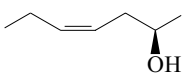
(*E*)-*form* [24469-79-2]
Bp_{20} 83-85° Bp_{11} 74-76°.

(*Z*)-*form* [6191-71-5]
FEMA 3841
Food flavourant. Liq. with fruity odour. d^{25} 0.85. Bp_{20} 84-86°.

Crombie, L. *et al., J.C.S.*, 1950, 1707 (*synth*)
Joshi, N.N. *et al., J.C.S. Perkin 1*, 1983, 2963 (*synth, ir, pmr*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1994, 673 (*synth, pmr*)
Udding, J.H. *et al., J.O.C.*, 1994, **59**, 6671 (*synth, ir, pmr, cmr*)

4-Hepten-2-ol H-107

[66642-85-1]



(2*R*,4*Z*)-*form*

$C_7H_{14}O$ 114.187

(2*R*,4*Z*)-*form* [124753-74-8]
Found in bananas.

(2*S*,4*Z*)-*form* [124753-75-9]
Found in bananas.

(±)-(4*E*)-*form* [58927-81-4]
Oil.

(±)-(4*Z*)-*form* [80357-56-8]
Oil. Bp_6 45°.

[34146-55-9, 94088-33-2, 143731-68-4, 143731-69-5]

Alexakis, A. *et al., Tetrahedron*, 1980, **36**, 1961 (*synth*)
Barluenga, J. *et al., Synthesis*, 1987, 318 (*synth, pmr, cmr, ms*)
Mosandl, A. *et al., J. Agric. Food Chem.*, 1991, **39**, 1131 (*occur*)
Zhu, J. *et al., J. Chem. Ecol.*, 1995, **21**, 29 (*isol*)

2-Hepten-4-one, 9CI H-108

[4643-25-8]
Propenyl propyl ketone. FEMA 3399
$H_3C(CH_2)_2COCH{=}CHCH_3$
$C_7H_{12}O$ 112.171
Flavouring ingredient.

(*E*)-*form* [32397-56-1]
Bp_{15} 53-54°.

Bierling, B. *et al., J. Prakt. Chem.*, 1972, **314**, 170 (*synth*)
Reich, H.J. *et al., J.A.C.S.*, 1975, **97**, 5434 (*synth, pmr*)
Jung, M.E. *et al., J.O.C.*, 1977, **42**, 3961 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 319
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1274-1275

3-Hepten-2-one, 9CI H-109

[1119-44-4]
FEMA 3400
$H_3C(CH_2)_2CH{=}CHCOCH_3$
$C_7H_{12}O$ 112.171
Flavouring ingredient. Bp_{23} 66°.

(*E*)-*form* [5609-09-6]
d^{20} 0.85. Bp_{11} 51-52°. n_D^{20} 1.4436.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 124.5-125°.

Semicarbazone:
Mp 128°.

(*Z*)-*form*
d^{20} 0.88. Bp_{11} 34-39°. n_D^{20} 1.4325.

Semicarbazone:
Mp 107.5-108.5°.

Sturtz, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 2477 (*synth*)
Sharpless, K.B. *et al., J.A.C.S.*, 1973, **95**, 6137 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 319
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1275

4-Hepten-2-one, 9CI H-110

[24332-22-7]
$H_3CCOCH_2CH{=}CHCH_2CH_3$
$C_7H_{12}O$ 112.171
Sweet-smelling liq. Bp_{20} 61-62°.

Semicarbazone:
Plates. Mp 109-110°.

(*E*)-*form* [36678-43-0]
Constit. of bananas.

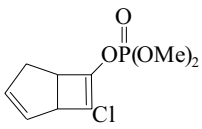
2,4-Dinitrophenylhydrazone: [36756-48-6]
Mp 121°.

(*Z*)-*form* [90605-45-1]
Constit. of bananas.

Uehara, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1570 (*synth, ir, uv, pmr*)
Bierling, B. *et al., J. Prakt. Chem.*, 1972, **314**, 170 (*synth*)
Zhu, J. *et al., J. Chem. Ecol.*, 1995, **21**, 29 (*isol, synth*)

Heptenophos, BSI, ISO H-111

[23560-59-0]
7-Chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl phosphate, 9CI, 8CI. Hostaquick. Ragadan



$C_9H_{12}ClO_4P$ 250.618
Agricultural and veterinary insecticide. Used for treatment of ectoparasites in cattle, pigs, sheep and domestic pets. Also for control of aphids in glasshouse crops. Pale-amber liq. Misc. most org. solvs. d_4^{20} 1.29. $Bp_{0.001}$ 94-95°.

▶ LD_{50} (rat, orl) 96 mg/kg; LD_{50} (rat, skn) 2000 mg/kg. TB8545000

U.K. Pat., 1966, 1 194 603; *CA*, **70**, 106068p (*synth, use*)
Agrochemicals Handbook, Royal Society of Chemistry, 1983, A226
Stan, H.-J. *et al., J. Chromatogr.*, 1983, **279**, 173 (*glc*)
Prinsloo, S.M. *et al., J. Assoc. Off. Anal. Chem.*, 1985, **68**, 1100; 1987, **70**, 878 (*detn*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A226
Pesticide Manual, 11th edn., 1997, No. 395
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBK700

6-Heptenyl glucosinolate H-112

1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)-7-octenimidate]
$H_2C{=}CH(CH_2)_5C(SGlc){=}NOSO_3H$
$C_{14}H_{25}NO_9S_2$ 415.485
Present in Japanese horseradish (*Wasabia japonica*).

Kojima, M. *et al., Yakugaku Zasshi*, 1973, **93**, 453; *CA*, **80**, 130475w (*occur*)

3-(2-Heptenyloxy)-1,2-propanediol H-113

Glycerol 1-(2-heptenyl) ether. 1-O-(2-Heptenyl)glycerol
$H_3C(CH_2)_3CH$
$=CHCH_2OCH_2CH(OH)CH_2OH$
$C_{10}H_{20}O_3$ 188.266

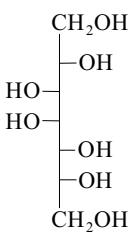
(*Z*)-*form*

3-Undecanoyl:3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate
$C_{21}H_{40}O_4$ 356.545
Constit. of the pods of *Moringa oleifera* (horseradish tree). $[\alpha]_D^{24}$ -2.5 (c, 0.004 in $CHCl_3$). C-2 config. not determined
λ_{max} 201 ; 217 (MeOH).

Faizi, S. *et al., Planta Med.*, 1998, **64**, 225-228

D-*glycero*-D-*galacto*-Heptitol, 9CI, 8CI H-114

[527-06-0]
Perseitol. Persitol. α-Mannoheptitol. L-glycero-D-manno-Heptitol



$C_7H_{16}O_7$ 212.199
Isol. from leaves, fruit and particularly seeds of the avocado *Persea gratissima* or *Persea dymifolia*. Needles. Mp 187-188°. $[\alpha]_D^{20}$ +1 (H_2O). Oxidised by *B. xylinum*.

Hepta-Ac: [19147-10-5]
$C_{21}H_{30}O_{14}$ 506.46
Mp 119°. $[\alpha]_D^{20}$ -13.4 ($CHCl_3$).

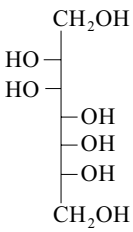
1,2:4,5:6,7-Tri-O-isopropylidene:
$C_{16}H_{28}O_7$ 332.393
Mp 58-60°. $[\alpha]_D^{20}$ -7 (c, 2.4 in $CHCl_3$).

[30635-52-0]

Peirce, G. *et al., J. Biol. Chem.*, 1915, **23**, 327
Hann, R.M. *et al., J.A.C.S.*, 1939, **61**, 336 (*struct*)
Szafranek, J. *et al., Anal. Lett.*, 1973, **6**, 479 (*glc*)
Okuda, T. *et al., Carbohydr. Res.*, 1975, **39**, 237 (*synth*)
Angyal, S. *et al., Carbohydr. Res.*, 1984, **126**, 15 (*cmr*)
Brimacombe, J.S. *et al., Carbohydr. Res.*, 1986, **150**, 35 (*synth*)
Kanters, J.A. *et al., Acta Cryst. C*, 1990, **46**, 71 (*cryst struct*)
Kopf, J. *et al., Acta Cryst. C*, 1991, **47**, 2186 (*cryst struct*)
Jorgensen, M. *et al., J.O.C.*, 2001, **66**, 4630-4634 (*synth, cmr*)
Ishizu, T. *et al., Tet. Lett.*, 2001, **42**, 6887-6889 (*isol*)
Ishizu, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 489-492 (*pmr, cmr, struct*)

D-*glycero*-D-*manno*-Heptitol, 9CI, 8CI H-115

[488-38-0]
D-glycero-D-talo-Heptitol. Volemitol. α-Sedoheptitol. β-Mannoheptitol



$C_7H_{16}O_7$ 212.199
Occurs in the edible chichitake mushroom (*Lactarius volemus*). Widely distributed in plants. Needles (EtOH). Mp 152-153°. $[\alpha]_D^{20}$ +2.2 (H_2O).

Hepta-Ac:1,2,3,4,5,6,7-Hepta-O-acetyl-D-glycero-D-manno-heptitol
$C_{21}H_{30}O_{14}$ 506.46
Mp 63°. $[\alpha]_D^{20}$ +36.1 (c, 2 in $CHCl_3$).

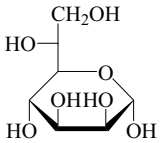
Tri-O-benzylidene:
$C_{28}H_{28}O_7$ 476.525
Needles. Mp 214-215°. $[\alpha]_D^{20}$ +1.7 ($CHCl_3$). Exact struct. apparently not detd..

[30635-52-0]

La Forge, F.B. *et al., J. Biol. Chem.*, 1917, **30**, 61; 1920, **42**, 375; 1928, **79**, 1 (*isol, tribenzylidene*)
Maclay, W.D. *et al., J.O.C.*, 1944, **9**, 293 (*occur, synth, hepta-Ac*)
Merrill, A.T. *et al., J.A.C.S.*, 1947, **69**, 70 (*synth, hepta-Ac*)
Adams, G.A. *et al., Can. J. Microbiol.*, 1967, **13**, 1605 (*isol, glc*)
Mills, J.A. *et al., Aust. J. Chem.*, 1974, **27**, 1433 (*conformn*)
Angyal, S. *et al., Carbohydr. Res.*, 1984, **126**, 15 (*cmr*)
Brimacome, J.S. *et al., Carbohydr. Res.*, 1986, **150**, 35 (*synth*)
Köll, P. *et al., Carbohydr. Res.*, 1991, **218**, 55; 1993, **247**, 111 (*cryst struct, hepta-Ac*)

D-*glycero*-D-*manno*-Heptose, 9CI, 8CI H-116

[1961-73-5]
D-altro-D-manno-*Heptose*



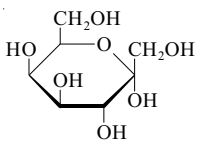
α-D-Pyranose-*form*

$C_7H_{14}O_7$ 210.183
Found combined in baker's yeast. $[\alpha]_D^{22}$ +21.5 (c, 3.2 in MeOH).

Ginsberg, V. *et al., J. Biol. Chem.*, 1962, **237**, 497 (*occur*)
Bagdien, G. *et al., Biochem. Z.*, 1966, **344**, 197 (*occur*)
Brimacombe, J.S. *et al., Carbohydr. Res.*, 1986, **152**, 329 (*synth*)
Paulsen, H. *et al., Annalen*, 1994, 389 (*methylphosphonate, synth*)

galacto-2-Heptulose H-117

Perseulose. Galactoheptulose



α-D-Pyranose-*form*

$C_7H_{14}O_7$ 210.183
An aq. soln. at 22°C contains 78% α-pyr, 16% α-fur, and 6% β-fur.

D-*form* [13403-16-2]
Mp 102-103°. $[\alpha]_D^{25}$ +90.6 → +75.3 (c, 2.2 in H_2O).

Hexa-Ac:1,3,4,5,6,7-Hexa-O-*acetyl*-D-galacto-*2-heptulose*
$C_{19}H_{26}O_{13}$ 462.407
Mp 102°. $[\alpha]_D^{27}$ -1.6 (c, 3. in $CHCl_3$).

L-*form* [29325-35-7]
Isol. from leaves of *Medicago sativa* (alfalfa). Mp 110-115°.

Phenylosazone:
Mp 190-202° dec. $[\alpha]_D^{20}$ -114 → -35 (c, 1 in Py).

Phenylosazone, 3,4,5,6,7-penta-Ac:
Mp 117-118°. $[\alpha]_D^{20}$ -86.8 (c, 1.2 in $CHCl_3$).

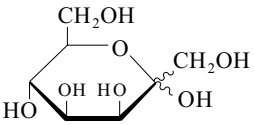
β-L-Pyranose-*form*

2,7-Anhydro:
$C_7H_{12}O_6$ 192.168
Fluffy needles (Me_2CO aq.). Mp 134-135°. $[\alpha]_D^{20}$ -20.7 (c, 1.8 in H_2O).

Bertrand, G. *et al., Bull. Soc. Chim. Fr.*, 1928, **43**, 663
Hann, R.M. *et al., J.A.C.S.*, 1939, **61**, 336-340 (*struct*)
Wolfrom, M.L. *et al., J.A.C.S.*, 1943, **65**, 1021-1027 (*D-form, synth*)
McComb, E.A. *et al., Arch. Biochem. Biophys.*, 1961, **95**, 316; 1962, **99**, 409 (*isol, biosynth*)
Wolfrom, M.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 171 (*synth, L-form*)
Stewart, L.C. *et al., J.O.C.*, 1963, **28**, 1842-1844 (*β-L-pyr-2,7-anhydro*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)

manno-2-Heptulose, 9CI H-118

[654-29-5]
Mannoheptulose. Mannoketoheptose



$C_7H_{14}O_7$ 210.183
An aq. soln. at 22° contains >99% α-pyr.

D-*form* [3615-44-9]
Occurs in *Persea gratissima* (avocado) and *Medicago sativa* (alfalfa). Mp 151-152°. $[\alpha]_D^{20}$ +29.7 (c, 4 in H_2O).

Phenylosazone:
Mp 200°.

Hexa-Ac:
$C_{19}H_{26}O_{13}$ 462.407
Prisms (Et_2O). Mp 110°. $[\alpha]_D^{20}$ +39 (c, 2 in $CHCl_3$).

5,6-O-*Ethylidene:5,6*-O-*Ethylidene*-D-manno-*2-heptulose*
$C_9H_{16}O_7$ 236.221
Mp 201°. $[\alpha]_D^{20}$ +4.4 (c, 3 in H_2O).

1-Deoxy: [35016-85-4]
$C_7H_{14}O_6$ 194.184
Cryst. (EtOH/petrol). Mp 110-112°. $[\alpha]_D^{25}$ +27.1 (c, 2 in H_2O).

α-D-Pyranose-*form*

Me glycoside:Methyl α-D-manno-*2-heptulopyranoside*
$C_8H_{16}O_7$ 224.21
Prisms (MeOH). Mp 142°. $[\alpha]_D^{20}$ +69 (c, 2 in H_2O).

Me glycoside, penta-Ac:Methyl penta-O-*acetyl-α-D*-manno-*2-heptulopyranoside*
$C_{18}H_{26}O_{12}$ 434.396
Needle-like prisms (Et_2O). Mp 64°. $[\alpha]_D^{20}$ +49.5 (c, 2 in $CHCl_3$).

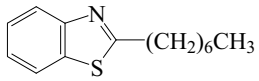
β-D-Pyranose-*form*

2,7-Anhydro: [7739-21-1] *2,7-Anhydro-β-D-manno-2-heptulopyranoside*
$C_7H_{12}O_6$ 192.168
Prisms (EtOH aq.). Mp 159-160°. $[\alpha]_D^{20}$ -80.4 (c, 2 in H_2O).

La Forge, F.B. *et al., J. Biol. Chem.*, 1916, **28**, 511 (*isol*)
Montgomery, E.M. *et al., J.A.C.S.*, 1939, **61**, 1654 (*isol, synth, α-D-Me pyr, α-D-Me pyr penta-Ac, hexa-Ac*)
Zissis, E. *et al., J.A.C.S.*, 1957, **79**, 2593-2597 (*anhydro*)
Sowden, J.C. *et al., J.A.C.S.*, 1958, **80**, 2532 (*synth*)
Richtmyer, N.K. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 173 (*isol*)
Montgomery, E.M. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 175 (*synth*)
Rendig, V.V. *et al., J. Agric. Food Chem.*, 1964, **12**, 421 (*isol*)
Kampf, A. *et al., Carbohydr. Res.*, 1972, **21**, 1 (*1-deoxy*)
Kanters, J.A. *et al., Acta Cryst. B*, 1979, **35**, 1152 (*cryst struct*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)

2-Heptylbenzothiazole, 9CI H-119

[69938-51-8]

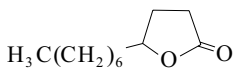


$C_{14}H_{19}NS$ 233.377
Volatile flavour component of roasted peanuts. Liq. Mp 101° (as picrate). Bp_7 147°.

Metzger, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 1692-1696 (*synth*)
Ho, C.T. *et al., Lebensm.-Wiss. Technol.*, 1982, **15**, 340-342 (*synth*)

5-Heptyldihydro-2(3*H*)-furanone, 9CI H-120

[104-67-6]
γ-Undecalactone. 5-Heptylbutyrolactone. 5-Hydroxyundecanoic acid γ-lactone. 1,4-Undecanolide. Peach lactone. Persicol. FEMA 3091



$C_{11}H_{20}O_2$ 184.278
► YQ2485000

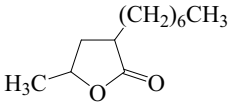
(±)-*form*
Flavouring ingredient. Liq. with a strong fruity peach-like odour. d_{25}^{25} 0.94. Bp 286° $Bp_{1.5}$ 117-118°.

(ξ)-*form*
Present in fresh apple, peach, apricot (*Prunus armeniaca*), yellow passion fruit, blackberry and other fruits. Also present in animal fats, e.g. butter, beef fat, pork fat and chicken fat, and in origanum and cooked rice. Flavouring agent.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1130C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 751D (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 408C (*ir*)
Honkanen, E. *et al., Acta Chem. Scand.*, 1965, **19**, 370 (*ms*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037; *CA*, **80**, 30604u (*ir, pmr*)
Modina, P. *et al., Ion (Madrid)*, 1974, **34**, 357; *CA*, **81**, 169065h (*synth*)
Pyysalo, H. *et al., Finn. Chem. Lett.*, 1975, 136; *CA*, **84**, 69088m (*synth, pmr, cmr, ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, (Suppl.), 1975, **13**, 921; *CA*, **86**, 161072r (*rev*)
Sotaro, M. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 770 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 780
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2867-2868

3-Heptyldihydro-5-methyl-2(3*H*)-furanone, 9CI H-121

[40923-64-6]
FEMA 3350

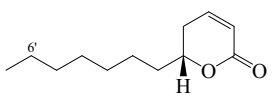


$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. with nutty, pecan odour. Bp_{17} 170°.

U.S. Pat., 1993, 5 231 192; *CA*, **114**, 101 715q (*synth, pmr*)
Adams, T.B. *et al., Food Chem. Toxicol.*, 1998, **36**, 249-278 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 732 (*use, props*)
Arakelyan, S.V. *et al., CA*, **78**, 135585a (*synth*)

6-Heptyl-5,6-dihydro-2*H*-pyran-2-one H-122

[16400-72-9]
2-Dodecen-5-olide. 5-Hydroxy-2-dodecenoic acid lactone. FEMA 3802



(*R*)-*form*

$C_{12}H_{20}O_2$ 196.289
(*R*)-*form* [152398-49-7]

[152398-50-0]
$Bp_{0.001}$ 135°. $[\alpha]_D^{20}$ -78 (c, 1 in $CHCl_3$).

*6′*R-*Hydroxy:* [125564-58-1] *5,6-Dihydro-6-(6-hydroxyheptyl)-2*H*-pyran-2-one, 9CI.* ***Gamahonolide A***
$C_{12}H_{20}O_3$ 212.288
Syrup. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ -66.1 (c, 0.23 in MeOH). λ_{max} 205 (ε 12000) (EtOH) (Derep).

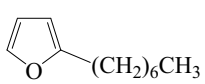
*6′*R-*Hydroxy, 6′*-O-*(3-ethoxycarbonylpropanoyl):* [125585-99-1] ***Gamahonolide B***
$C_{18}H_{28}O_6$ 340.416
Syrup. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{23}$ -24 (c, 0.15 in MeOH). λ_{max} 205 (ε 12000) (EtOH) (Derep).

(±)-*form*
Flavouring ingredient. Liq. with fatty/milky odour. Bp_9 148-153°. n_D 1.4617.

Nobuhara, A. *et al., Agric. Biol. Chem.*, 1968, **32**, 1016 (*synth*)
Cavill, G.W.K. *et al., Aust. J. Chem.*, 1968, **21**, 2819 (*isol*)
Urbach, G. *et al., Agric. Biol. Chem.*, 1972, **36**, 1217 (*ms*)
Koshino, H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1096 (*Gamahonolides*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 818

2-Heptylfuran, 9CI, 8CI H-123

[3777-71-7]
FEMA 3401

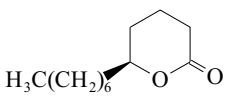


$C_{11}H_{18}O$ 166.263
Lipid-derived Maillard prod. Flavouring ingredient. Present in French fried potato, fried or roasted chicken, roast guinea hen, cooked beef, heated beef fat, used frying oils, roast filbert, endive, avocado fruit and fresh ripe tomatoes. Bp_{44} 110-111°.

Ho, C.T. *et al., Lebensm.-Wiss. Technol.*, 1982, **15**, 340-342 (*occur*)
Kelly, S.M. *et al., Helv. Chim. Acta*, 1983, **66**, 1850-1859 (*synth*)
Farmer, L.J. *et al., J. Sci. Food Agric.*, 1992, **60**, 489-497 (*occur*)
Takeoka, G. *et al., J. Agric. Food Chem.*, 1996, **44**, 654-660 (*occur*)
Elmore, J.S. *et al., J. Agric. Food Chem.*, 1999, **47**, 1619-1625 (*occur*)

6-Heptyltetrahydro-2*H*-pyran-2-one, 9CI H-124

[713-95-1]
δ-Dodecalactone. 5-Dodecanolide. FEMA 2401



(*S*)-*form*

$C_{12}H_{22}O_2$ 198.305
► UQ0850000
(*S*)-*form* [108943-47-1]
$[\alpha]_D$ -47.5 (c, 2.0 in THF).
(±)-*form* [3051-22-7]
Used in food flavouring. Liq. Mp -12°. $Bp_{0.03}$ 100-103°. n_D^{25} 1.4684. n_D^{25} 1.4571.
(ξ)-*form*
Isol. from coconut oil, peach, raspberry, strawberry and other fruits, peppermint oil, cheeses, cooked meats and white wine.

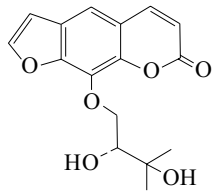
[16400-73-0]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1153A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 756C (*ir*)
Taylor, R.J. *et al., CA*, 1961, **55**, 390 (*synth*)
Allen, R.R. *et al., Chem. Ind. (London)*, 1965, 1560 (*isol, ir*)
Parliament, T.H. *et al., Chem. Ind. (London)*, 1966, 1845 (*synth*)
Lamberti, V. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 504 (*synth*)
Kohver, O. *et al., Tetrahedron*, 1970, **26**, 2391 (*abs config, ord, cd*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 773 (*rev, tox*)
Bianco, L. *et al., Tet. Lett.*, 1988, **29**, 1915-1918 (*resoln*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBP450

Heraclenol H-125

[2817-09-6]

[118407-74-2]
*9-(2,3-Dihydroxy-3-methylbutoxy)-7*H*-furo[3,2-g][1]benzopyran-7-one, 9CI. Isosaxalin. Komalin. Prangenin hydrate. Heraclenin hydrate*



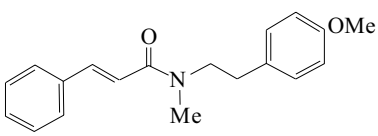
$C_{16}H_{16}O_6$ 304.299
(*R*)-*form* [26091-76-9]
Obt. from roots of *Angelica* spp.. Mp 117-118°. $[\alpha]_D^{32}$ +16.5 (Py).
2′-O-*(3-Methylbutanoyl):*
$C_{21}H_{24}O_7$ 388.416
Constit. of *Angelica archangelica* (angelica). Gum.
2′-O-*(3-Methyl-2-butenoyl):*
$C_{21}H_{22}O_7$ 386.401
Constit. of *Angelica archangelica* (angelica). Gum.

[31575-93-6]

Gupta, B.D. *et al., Indian J. Chem.*, 1964, **2**, 464 (*isol*)
Sharma, Y.N. *et al., Naturwissenschaften*, 1964, **51**, 537 (*isol*)
Nielsen, B.E. *et al., Acta Chem. Scand.*, 1969, **23**, 962 (*config*)
Bandopadhyay, M. *et al., Indian J. Chem.*, 1970, **8**, 855; 1146; 1973, **11**, 530 (*isol, synth*)
González, A.G. *et al., An. Quim.*, 1974, **70**, 856; 1976, **72**, 584; 1977, **73**, 858 (*derivs*)
Ivie, G.W. *et al., J. Agric. Food Chem.*, 1978, **26**, 1394 (*isol*)
Razdan, T.K. *et al., Phytochemistry*, 1982, **21**, 923 (*isol, ir, uv, pmr, ms*)
Harkar, S. *et al., Phytochemistry*, 1984, **23**, 419 (*isol, ir, ms*)
Sun, H. *et al., Pharmazie*, 1986, **41**, 888

Herclavine H-126

N-*[2-(4-Methoxyphenyl)ethyl]*-N-*methyl-3-phenyl-2-propenamide, 9CI.* N-*(*p-*Methoxyphenethyl)*-N-*methylcinnamamide.* N-*(2-*p-*Anisylethyl)*-N-*methylcinnamamide. Cinnamic acid* p-*methoxyphenethylamide*

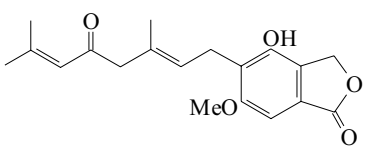


$C_{19}H_{21}NO_2$ 295.38
(*E*)-*form* [539-18-4]
Alkaloid from the bark of *Zanthoxylum clava-herculis* (Hercules' club). Cryst. (Et_2O or petrol). Mp 76°.

LaForge, F.B. *et al., J.O.C.*, 1944, **9**, 250 (*isol, struct, synth*)
Crombie, L. *et al., J.C.S.*, 1955, 995 (*isol, uv, ir*)
Chatterjee, A. *et al., J.O.C.*, 1959, **24**, 687 (*ir*)

Hericenone A H-127

[126654-52-2]



$C_{19}H_{22}O_5$ 330.38

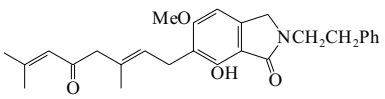
Struct. revised in 1992. Constit. of the edible lions mane mushroom (*Hericium erinaceum*). Cryst. ($CHCl_3$). Mp 100-102°. λ_{max} 214 (ϵ 28600); 241 (sh) (ϵ 8600); 253 (ϵ 9000); 289 (sh) (ϵ 3000); 299 (ϵ 3200) (MeOH) (Derep).

Kawagishi, H. *et al., Tet. Lett.*, 1990, **31**, 373-376 (*isol, pmr*)

Rao, A.V.R. *et al., Tet. Lett.*, 1992, **33**, 4061-4064 (*synth, struct*)

Hericenone B H-128

[126654-53-3]



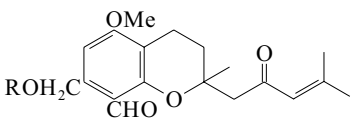
$C_{27}H_{31}NO_4$ 433.546

Isol. from the edible lions mane mushroom (*Hericium erinaceum*). Cryst. ($CHCl_3$). Mp 136-138°. λ_{max} 214 (ϵ 45000); 235 (sh) (ϵ 16800); 248 (ϵ 17800) (MeOH) (Derep).

Kawagishi, H. *et al., Tet. Lett.*, 1990, **31**, 373 (*isol, pmr*)

Hericenone F H-129

[141996-36-3]



R = $-CO(CH_2)_{14}CH_3$

$C_{35}H_{54}O_6$ 570.808

Constit. of the edible lion's mane mushroom *Hericium erinaceum*. Pale yellow oil. Racemic.

Kawagishi, H. *et al., Phytochemistry*, 1993, **32**, 175 (*isol, pmr, cmr*)

Hericenone G H-130

[141973-36-6]

As Hericenone F, H-129 with

R = $-CO(CH_2)_{16}CH_3$

$C_{37}H_{58}O_6$ 598.862

Constit. of the edible lion's mane mushroom (*Hericium erinaceum*). Pale yellow plates ($CHCl_3$/EtOH). Mp 56-58°.

Kawagishi, H. *et al., Phytochemistry*, 1993, **32**, 175 (*isol, pmr, cmr*)

Hericenone H H-131

[141973-37-7]

As Hericenone F, H-129 with

R = $-CO(CH_2)_7CH{=}CHCH_2CH{=}CH(CH_2)_4CH_3$

$C_{37}H_{54}O_6$ 594.83

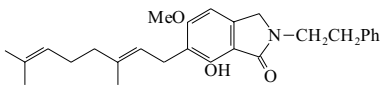
Constit. of the edible lion's mane mushroom (*Hericium erinaceum*). Pale yellow oil.

Kawagishi, H. *et al., Phytochemistry*, 1993, **32**, 175 (*isol, pmr, cmr*)

Hericerin H-132

[140381-53-9]

*6-(3,7-Dimethyl-2,6-octadienyl)-2,3-dihydro-7-hydroxy-5-methoxy-2-(2-phenylethyl)-1*H*-isoindol-1-one, 9CI*



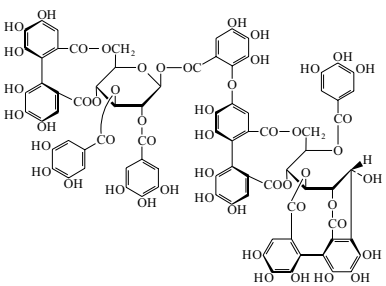
$C_{27}H_{33}NO_3$ 419.563

Isol. from the edible lions mane mushroom (*Hericium erinaceum*). Needles + $^1/_2H_2O$ (C_6H_6/EtOAc). Mp 138-140°.

Kimura, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 2673 (*isol, pmr, cmr*)

Heterophylliin B H-133

[135329-62-3]



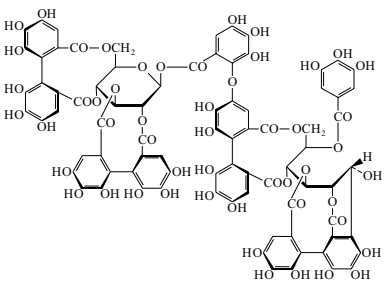
$C_{82}H_{56}O_{52}$ 1873.313

An ellagitannin constit. of *Corylus heterophylla* (Siberian filbert). Off-white amorph. powder + $12H_2O$. $[\alpha]_D^{20}$ +141 (c, 1.0 in MeOH).

Yoshida, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 49 (*struct, cd, pmr, cmr*)

Heterophylliin C H-134

[135308-98-4]



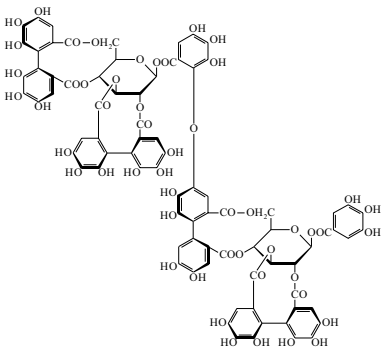
$C_{82}H_{54}O_{52}$ 1871.297

An ellagitannin from the leaf of *Corylus heterophylla* (Siberian filbert). Light brown amorph. powder + $15H_2O$. $[\alpha]_D^{20}$ +101 (c, 1.0 in MeOH).

Yoshida, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 49 (*struct, uv, cd, pmr, cmr*)

Heterophylliin D H-135

[135308-99-5]



$C_{82}H_{54}O_{52}$ 1871.297

Tannin constit. of *Corylus heterophylla* (Siberian filbert). Off-white amorph. powder. $[\alpha]_D^{20}$ +78 (c, 1.0 in MeOH).

O-*Degalloyl:* [109742-47-4] ***Roxbin A***

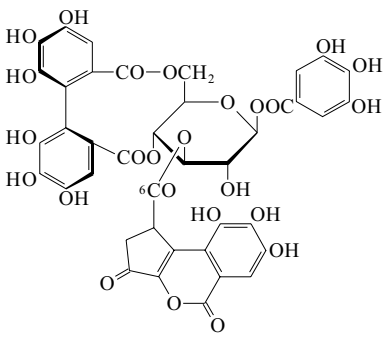
$C_{75}H_{50}O_{48}$ 1719.191

Off-white amorph. powder + $4H_2O$. $[\alpha]_D^{20}$ +46.5 (c, 1.0 in MeOH). Mixt. of equilibrating α- and β-anomers.

Yoshida, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1817; 1991, **39**, 49 (*struct, uv, cd, pmr, cmr*)

Heterophylliin E H-136

[135309-00-1]



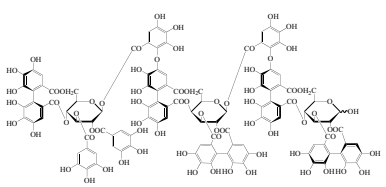
$C_{40}H_{28}O_{25}$ 908.646

Isol. from the leaf of *Corylus heterophylla* (Siberian filbert). Off-white amorph. powder + $7H_2O$. $[\alpha]_D^{20}$ -36 (c, 1.0 in MeOH).

Yoshida, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 49 (*struct, uv, cd, pmr, cmr*)

Heterophylliin G H-137

[211190-41-9]



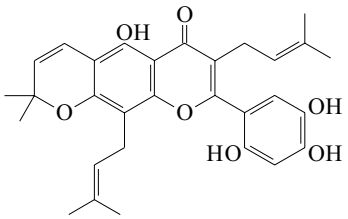
$C_{116}H_{78}O_{74}$ 2655.848

Constit. of *Corylus heterophylla* (Siberian filbert). Amorph. pale brown powder. $[\alpha]_D$ +91.7 (c, 1 in MeOH). λ_{max} 210 (log ϵ

5.58); 285 (log ϵ 5.24) (MeOH).

Jin, Z.-X. *et al., Phytochemistry*, 1998, **48**, 333-338 (*isol, uv, cd, pmr, cmr, ms*)

Heterophyllin H-138

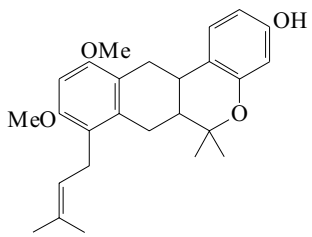


$C_{30}H_{32}O_7$ 504.579
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow needles. Mp 202-204°. λ_{max} 206 (log ϵ 4.6); 283 (log ϵ 4.59); 342 (log ϵ 4.03) (MeOH). λ_{max} 206 (ϵ 11480); 283 (ϵ 38900); 342 (ϵ 17000) (MeOH) (Berdy).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 1447-1453 (*isol, uv, ir, pmr*)

Heterophylol H-139

[152841-81-1]
6a,7,12,12a-Tetrahydro-9,11-dimethoxy-6,6-dimethyl-8-(3-methyl-2-butenyl)-6H-benzo[b]naphtho[2,3-d]pyran-3-ol, 9CI

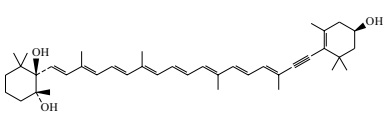


$C_{26}H_{32}O_4$ 408.536
Not the same as Heterophyllol (1,12-Dihydroxy-5,11(13)-eudesmadien-3-one). Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Needles ($CHCl_3$/MeOH). Mp 217-218°. $[\alpha]_D^{24}$ -3 (c, 0.1 in Me_2CO). λ_{max} 204 (ϵ 66070); 228 (sh) (ϵ 19500); 284 (ϵ 8710) (MeOH).

Lin, C.-N. *et al., Phytochemistry*, 1995, **39**, 1447 (*isol, uv, ir, pmr, cmr*)

Heteroxanthin H-140

[29488-00-4]
7′,8′-Didehydro-5,6-dihydro-β,β-carotene-3,3′,5,6-tetrol

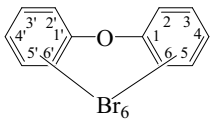


$C_{40}H_{56}O_4$ 600.88
Constit. of *Mytilus edulis* (blue mussel). Cryst.

Strain, H.H. *et al., Tet. Lett.*, 1971, 733 (*struct*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1984, **67**, 2043 (*abs config*)

Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv, ms*)

Hexabromodiphenyl ethers H-141



$C_{12}H_4Br_6O$ 643.587
Persistent environmental pollutant, detected in human breast milk and fish.

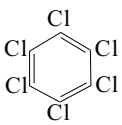
2,2′,4,4′,5,5′-Hexabromodiphenyl ether
[68631-49-2]
1,1′-Oxybis[2,4,5-tribromo]benzene, 9CI. PBDE 153. BDE 153
$C_{12}H_4Br_6O$ 643.587
Mp 157.6°.

2,2′,4,4′,5,6′-Hexabromodiphenyl ether
[207122-15-4]
1,3,5-Tribromo-2-(2,4,5-tribromophenoxy)benzene. PBDE 154. BDE 154
$C_{12}H_4Br_6O$ 643.587
Mp 142-143°.

Environ. Health Criter., No. 162, Polybrominated Diphenyl Ethers, WHO, 1994, (*rev, tox, occur*)
Oern, U. *et al., Acta Chem. Scand.*, 1996, **50**, 802-807 (*synth, uv, pmr, ms*)
Marsh, G. *et al., Environ. Sci. Technol.*, 1999, **33**, 3033-3037 (*synth, uv, pmr, ms*)
Ryan, J.J. *et al., Organohalogen Compd.*, 2000, **47**, 57-60; 61-64 (*occur*)
Hale, R.C. *et al., Nature (London)*, 2001, **412**, 140-141 (*occur*)

Hexachlorobenzene, 9CI, 8CI, BSI, ISO H-142

[118-74-1]
Perchlorobenzene. HCB



C_6Cl_6 284.782
Agricultural fungicide. Needles (2-propanol). Mp 226°.
▶ Fl. p. 242°. Possible human carcinogen. Exp. carcinogenic and reprod. effects. Chronic exposure in humans is associated with development of a type of porphyria, enlarged liver, painless arthritis, enlarged thyroid and neurological symptoms.
DA2975000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1016B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 135B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 949C (*ir*)
Schnepp, O. *et al., J. Chem. Phys.*, 1959, **30**, 868 (*uv*)
Bullester, M. *et al., J.A.C.S.*, 1960, **82**, 4259 (*uv*)
Ware, J. *et al., J.O.C.*, 1961, **26**, 2267 (*synth*)
Solomon, W. *et al., J.O.C.*, 1966, **31**, 1551 (*synth*)
Delorme, P. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1967, **64**, 591 (*ir*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Clark, J. *et al., J.C.S. Perkin 2*, 1976, 73 (*ms*)
Takeuchi, Y. *et al., J.C.S. Perkin 2*, 1985, 175 (*cmr*)
Dobson, S. *et al., IARC Sci. Publ.*, 1986, **77**, 203-209; 231-242; 575-579; 585-589; 621-628 (*rev*)
Renner, G. *et al., Toxicol. Environ. Chem.*, 1988, **18**, 51 (*rev, metab*)
van Ommen, B. *et al., Drug Metab. Drug Interact.*, 1989, **7**, 213 (*tox, rev*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A227
Pesticide Manual, 11th edn., 1997, No. 397
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 320
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HCC500

1,1,1,3,3,3-Hexachloro-2-propanone, 9CI H-143

[116-16-5]
Hexachloroacetone. HCA, WSSA
$Cl_3CCOCCl_3$
C_3Cl_6O 264.749
Constit. of *Osmanthus fragrans* (sweet osmanthus). Liq. Sl. sol. H_2O. d_{12}^{12} 1.74. Fp -2. Bp 202-204° Bp_{26} 99-101.5°.
▶ LD_{50} (rat, orl) 1290 mg/kg; LD_{50} (rat, skn) 2980 mg/kg. UC2100000

Tetrahydrate:
Unstable cryst. Mp 39.5-40.5° (incongruent). Unstable. Previously thought to be a covalent monohydrate.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 418A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 653C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 506C (*ir*)
Ambrus, T. *et al., Rev. Roum. Chim.*, 1963, **14**, 506; *CA*, **60**, 6739 (*manuf*)
Andersen, P. *et al., Acta Chem. Scand., Ser. A*, 1974, **28**, 239 (*struct*)
Hawkes, G.E. *et al., J.O.C.*, 1974, **39**, 1276 (*cmr*)
Japan. Pat., 1974, 7 424 909; *CA*, **80**, 145423b (*synth*)
Schulman, E.M. *et al., J.A.C.S.*, 1976, **98**, 3793 (*hydrate*)
Lee, E.K.C. *et al., Adv. Photochem.*, 1980, **12**, 1 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 239
Ding, D. *et al., J. Essent. Oil Res.*, 1989, **1**, 295 (*isol*)
Pesticide Manual, 9th edn., 1991, No. 7060
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2642-2643 (*use*)
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HCL500

Hexacosanal H-144

[26627-85-0]
$H_3C(CH_2)_{24}CHO$
$C_{26}H_{52}O$ 380.696
Isol. from *Vitis vinifera* var. *sultana*. Cryst. (MeOH). Mp 73-73.5°.

Crabbé, P. *et al., Bull. Soc. Chim. Belg.*, 1961, **70**, 168 (*synth, ir*)
Radler, F. *et al., Aust. J. Chem.*, 1965, **18**, 1059 (*isol*)

1,26-Hexacosanediol H-145

[15541-01-2]

$HOCH_2(CH_2)_{24}CH_2OH$

$C_{26}H_{54}O_2$ 398.711

Isol. from apple wax. Cryst. (C_6H_6/EtOAc). Mp 110.5° (102-105°).

Di-Ac: [15541-04-5]
$C_{30}H_{58}O_4$ 482.786
Mp 77.5°.

Dibenzoyl:
$C_{40}H_{62}O_4$ 606.927
Cryst. (MeOH). Mp 67-70°.

Bis(3,4-dihydroxycinnamoyl):1,26-Hexacosanediol dicaffeate. 1,26-Dicaffeoylhexacosanediol
$C_{44}H_{66}O_8$ 723.001
Isol. from oats (*Avena sativa*). Mp 140-141°. Occurs mixed with the corresponding octacosanediol homologue.

Bis(4-hydroxy-3-methoxycinnamoyl):1,26-Hexacosanediol diferulate
$C_{46}H_{70}O_8$ 751.054
Isol. from oats (*Avena sativa*). Cryst. (Et_2O/petrol). Mp 91-93.5°. A mixt. with the octacosanediol homologue.

Musgrave, O.C. *et al., J.C.S.*, 1952, 4393 (*isol, synth*)
Murray, K.E. *et al., Aust. J. Chem.*, 1955, **8**, 432 (*isol*)
Mazliak, P. *et al., Phytochemistry*, 1962, **1**, 79 (*isol*)
Daniels, D.G.H. *et al., Chem. Ind. (London)*, 1964, 2058; 1965, 1763 (*isol, dicinnamoyl, dicaffeoyl*)

4,6-Hexacosanedione H-146

$H_3C(CH_2)_{19}COCH_2COCH_2CH_2CH_3$

$C_{26}H_{50}O_2$ 394.68

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

5,7-Hexacosanedione H-147

$H_3C(CH_2)_{18}COCH_2CO(CH_2)_3CH_3$

$C_{26}H_{50}O_2$ 394.68

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

6,8-Hexacosanedione H-148

$H_3C(CH_2)_{17}COCH_2CO(CH_2)_4CH_3$

$C_{26}H_{50}O_2$ 394.68

Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-8-hexacosanone
$C_{26}H_{52}O_2$ 396.696
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

7,9-Hexacosanedione H-149

$H_3C(CH_2)_{16}COCH_2CO(CH_2)_5CH_3$

$C_{26}H_{50}O_2$ 394.68

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

10,12-Hexacosanedione H-150

$H_3C(CH_2)_{13}COCH_2CO(CH_2)_8CH_3$

$C_{26}H_{50}O_2$ 394.68

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

11,13-Hexacosanedione H-151

$H_3C(CH_2)_{12}COCH_2CO(CH_2)_9CH_3$

$C_{26}H_{50}O_2$ 394.68

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

Hexacosanoic acid, 9CI H-152

[506-46-7]

Cerinic acid. Cerotic acid. Ceric acid. Ceratinic acid. EB 82B

$H_3C(CH_2)_{24}COOH$

$C_{26}H_{52}O_2$ 396.696
Mp 88-89°.

Me ester: [5802-82-4]
$C_{27}H_{54}O_2$ 410.722
Mp 63-68°. Bp_{15} 286° $Bp_{3.5}$ 248°.

Et ester: [29030-81-7]
$C_{28}H_{56}O_2$ 424.749
Mp 59.5-59.8°.

Nonyl ester:Nonyl hexacosanoate
$C_{35}H_{70}O_2$ 522.937
Cryst. (C_6H_6). Mp 83°.

Amide: [22715-86-2]
$C_{26}H_{53}NO$ 395.711
Mp 105-107°.

2-Methylpropylamide: [119736-87-7] N-*(2-Methylpropyl)hexacosanamide, 9CI. Hexacosanoic acid isobutylamide.* ***Longamide***
$C_{30}H_{61}NO$ 451.818
Minor constit. of fruits of *Piper longum* (long pepper). Amorph. powder. Mp 72°.

Levene, P.A. *et al., J. Biol. Chem.*, 1924, **59**, 905 (*synth*)
Helz, G.E. *et al., J. Biol. Chem.*, 1936, **116**, 203
Bernhard, K. *et al., Helv. Chim. Acta*, 1948, **31**, 977
Asselineau, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1953, **237**, 1804
Tember, G.A. *et al., CA*, 1974, **80**, 47410a (*synth*)
Watanabe, S. *et al., Z. Naturforsch., C*, 1975, **30**, 825 (*ms*)
Koul, S.K. *et al., Phytochemistry*, 1988, **27**, 3523 (*Longamide*)
Mehta, B.K. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1304-1306 (*Nonyl hexacosanoate*)

1-Hexacosene H-153

[18835-33-1]

$H_3C(CH_2)_{23}CH{=}CH_2$

$C_{26}H_{52}$ 364.697

Constit. of *Aralia elata* (Japanese angelica tree).

Dreisbach, R.R. *et al., Adv. Chem. Ser.*, 1959, **22**, 1 (*props*)
Streibl, M. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 2522 (*synth*)
Watanabe, S. *et al., Z. Naturforsch., C*, 1975, **30**, 825 (*isol*)
Tembe, G.L. *et al., Ind. Eng. Chem. Res.*, 1991, **30**, 2247 (*synth*)
Nesterov, G.A. *et al., J. Mol. Catal.*, 1991, **66**, 367 (*synth*)

17-Hexacosenoic acid H-154

[544-84-3]

$H_3C(CH_2)_7CH{=}CH(CH_2)_{15}COOH$

$C_{26}H_{50}O_2$ 394.68

(Z)-form [66274-43-9]
Ximenic acid
Isol. from seed fat of *Ximenia* spp. and fish oil lipids. Mp 50.5-50.9°.

Me ester:
$C_{27}H_{52}O_2$ 408.707
Oil.

Lightelm, S.P. *et al., J. Sci. Food Agric.*, 1954, **5**, 281 (*isol, config, bibl*)
Litchfield, C. *et al., Lipids*, 1970, **5**, 144; 1978, **13**, 199 (*isol*)
Kling, M.R. *et al., J.C.S. Perkin 1*, 1993, 1183 (*synth, ir, ms*)

2,4-Hexadecadienoic acid, 9CI H-155

[25377-52-0]

$H_3C(CH_2)_{10}CH{=}CHCH{=}CHCOOH$

$C_{16}H_{28}O_2$ 252.396

(all-E)-form [59404-48-7]

2-Methylpropylamide: **N-*Isobutyl-2,4-hexadecadienamide***
$C_{20}H_{37}NO$ 307.518
Noncryst. Mp 78.5-84° (refers to synthetic material).

(2E,4Z)-form

Me ester: [54977-89-8]
$C_{17}H_{30}O_2$ 266.423
Used as aroma compd. in the food industry.

Et ester:
$C_{18}H_{32}O_2$ 280.45
Aroma compd..

[28933-88-2]

Okogun, J.I. *et al., J.C.S. Perkin 1*, 1974, 2195 (*pmr, ms*)
Swiss Pat., 1974, 557 645; *CA*, **82**, 138023 (*synth*)
Vig, O.P. *et al., Indian J. Chem.*, 1975, **13**, 1358 (*synth*)
Reisch, J. *et al., J. Nat. Prod.*, 1985, **48**, 862 (*isol, uv, ir, pmr, ms, struct, isobutylamide*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419 (*synth, isobutylamide*)

Hexadecanal, 9CI H-156

[629-80-1]

Palmitic aldehyde. Palmitaldehyde

$H_3C(CH_2)_{14}CHO$

$C_{16}H_{32}O$ 240.428

Isol. from lemon oil (*Citrus limon*). Mp 34°. Bp_{29} 200-202°. Polymerises on standing to the trimer (Mp 73°).

Oxime:
$C_{16}H_{33}NO$ 255.443
Mp 88°.

Di-Me acetal: [2791-29-9] *1,1-Dimethoxyhexadecane*
$C_{18}H_{38}O_2$ 286.497
Mp 10°. Bp_{15} 139-146°.

Le Sueur, H.R. *et al., J.C.S.*, 1905, **87**, 1888

(*synth*)
Ikeda, R.M. *et al., J. Agric. Food Chem.*, 1962, **10**, 98 (*isol*)
Goldfine, H. *et al., J. Biol. Chem.*, 1964, **239**, 2130 (*isol*)
Christiansen, K. *et al., Lipids*, 1969, **4**, 421 (*ms, acetal*)
Degani, I. *et al., J.C.S. Perkin 1*, 1976, 323 (*synth*)
Gung, B.W. *et al., Synth. Commun.*, 2002, **32**, 2733-2740 (*synth, pmr*)

Hexadecane H-157

[544-76-3]
Cetane
$H_3C(CH_2)_{14}CH_3$
$C_{16}H_{34}$ 226.445
Isol. from oil of *Piper longum* (long pepper). Mp 18.17°. Bp_{160} 287° $Bp_{0.1}$ 105-110°.
▶ Fl. p. >71°, autoignition temp. 202/205°.
ML9200000
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 4C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 4A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 5A (*ir*)
Corey, P.C. *et al., J.C.S.*, 1933, 346 (*synth*)
Org. Synth., 1935, **15**, 27 (*synth*)
Cocher, W. *et al., J.C.S.*, 1963, 677 (*isol*)
Niwa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1746 (*ms*)
Tosi, C. *et al., Spectrochim. Acta A*, 1972, **28**, 585 (*ir*)
Fritz, H. *et al., Chem. Ber.*, 1976, **109**, 1258 (*cmr, pmr*)

Hexadecanedioic acid, 9CI H-158

[505-54-4]
Thapsic acid
$HOOC(CH_2)_{14}COOH$
$C_{16}H_{30}O_4$ 286.411
Cryst. (EtOH or EtOAc). Mp 126°.

Nitrile, mono-Me ester: Methyl 15-cyanopentadecanoate
$C_{17}H_{31}NO_2$ 281.437
Constit. of the leaves of *Moringa oleifera* (horseradish tree).

Faizi, S. *et al., J. Nat. Prod.*, 1997, **60**, 1317-1321 (*nitrile mono-Me ester*)

Hexadecanoic acid H-159

[57-10-3]
Palmitic acid, USAN. Aethalic acid. FEMA 2832
$H_3C(CH_2)_{14}COOH$
$C_{16}H_{32}O_2$ 256.428
Occurs in the form of esters (glycerides) in oils and fats of vegetable and animal origin. Usually obt. from palm oil. Widely distributed in plants. Defoaming agent, lubricant and fruit coating constit.. Cryst. Mp 63-64°. Bp 390° Bp_{100} 268.5° Bp_{15} 215°.
▶ Skin irritant. LD_{50} (mus, ivn) 57 mg/kg.
RT4550000

Et ester: [628-97-7] *Ethyl hexadecanoate. Ethyl palmitate. FEMA 2451*
$C_{18}H_{36}O_2$ 284.481
Present in various fruits, e.g. apricot, sour cherry, grapefruit, bilberry, guava fruit, melon, pineapple, Chinese quince, ceriman (*Monstera deliciosa*) etc. Also present in crispbread, clary sage, blackcurrant buds, wines, rice bran, plum brandy, fruit brandy, Bourbon vanilla, beans and salted/pickled plums. Cryst. (EtOH or petrol). Mp 19.3° Mp 24° (dimorph.). Bp 303° Bp_{10} 191°.

Amide: [629-54-9] *Hexadecanamide, 9CI. Palmitamide, 8CI*
$C_{16}H_{33}NO$ 255.443
Release agent migrating from food packaging. Isol. from seeds of Mexican apple (*Casimiroa edulis*). Cryst. (EtOH). Mp 106-107°. Bp_{12} 235-236°.

[408-35-5, 542-42-7, 2624-31-9, 4991-47-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 485A; 609B; 731D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 756B; 1169B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 577B; 629D; 630A (*ir*)
Whitby, G.S. *et al., J.C.S.*, 1926, 1458-1465 (*synth, esters*)
Smith, J.C. *et al., J.C.S.*, 1931, 802 (*Et ester*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, NY, 1947, **2**, 72 (*use*)
Kincl, F.A. *et al., J.C.S.*, 1956, 4163 (*isol, amide*)
Bailey, A.V. *et al., J. Am. Oil Chem. Soc.*, 1971, **48**, 775 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 703 (*occur*)
Hill, I.R. *et al., J. Chem. Phys.*, 1979, **70**, 842 (*ir, Raman*)
Bengsch, E. *et al., J. Magn. Reson.*, 1986, **68**, 1 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PAE250
Gross, M.L. *et al., Org. Mass Spectrom.*, 1992, **27**, 423 (*ms*)
Yokoyama, I. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 400 (*ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1029-1030; 2080-2082 (*use, Et ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IQW000; PAE250

1-Hexadecanol H-160

[36653-82-4]

[29354-98-1]
Cetyl alcohol, USAN. *Cetanol. Palmityl alcohol. Hexadecyl alcohol. Hyfatol 16. FEMA 2554*
$H_3C(CH_2)_{14}CH_2OH$
$C_{16}H_{34}O$ 242.444
Flavouring ingredient. Mp 50°. Bp 334° Bp_{12} 178-182°.
▶ Eye and skin irritant. LD_{50} (rat, orl) 6400 mg/kg. MM0225000

Hydrogen sulfate: [1120-01-0] *Hexadecyl sulfate. Cetyl sulfate*
$C_{16}H_{34}O_4S$ 322.508
Trimorphic cryst. (Na salt). Mp 25-26° Mp 30-31° Mp 40-41°. CAS no. refers to Na salt (sodium dodecyl sulfate).

O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{40}H_{74}O_{19}$ 859.013
$[\alpha]_D$ -37.2 (c, 0.49 in MeOH).

O-*[α-L-Rhamnopyranosyl-(1→2)[α-L-arabinopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{45}H_{82}O_{23}$ 991.129
$[\alpha]_D$ -26.7 (c, 0.22 in MeOH).

Ac: [629-70-9]
$C_{18}H_{36}O_2$ 284.481
Dimorphous. Mp 24.2°. Bp_{205} 220-225° Bp_{15} 200°.

4-Nitrobenzoyl:
Mp 68.4°.

Vinyl ether: [822-28-6] *1-(Ethenyloxy)-hexadecane, 9CI. Hexadecyl vinyl ether, 8CI*
$C_{18}H_{36}O$ 268.482
Liq. d_4^{20} 0.83. Bp_1 142°. n_D^{20} 1.4468.

[124-29-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 113A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 168A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 159B (*ir*)
Org. Synth., 1930, **10**, 62 (*synth*)
Rawlings, F.F. *et al., J.A.C.S.*, 1955, **77**, 870-872 (*sodium dodecyl sulfate, synth, cryst struct*)
Reppe, A. *et al., Annalen*, 1956, **601**, 84 (*vinyl ether*)
Meinwald, J. *et al., J.A.C.S.*, 1966, **88**, 1305
Dolejs, L. *et al., Org. Mass Spectrom.*, 1968, **1**, 563 (*ms*)
Geiseler, G. *et al., Spectrochim. Acta A*, 1968, **24**, 1007 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 683 (*rev, tox*)
Rossi, R. *et al., Tetrahedron*, 1982, **38**, 639 (*cmr*)
Kartha, V.B. *et al., Can. J. Chem.*, 1984, **62**, 128-132 (*sodium dodecyl sulfate, synth, ir, Raman*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HCP000
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 99-103
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 326
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1408
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1286-1288
Voutquenne, L. *et al., Phytochemistry*, 1999, **50**, 63-69 (*Dimocarpus glycosides*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HCP000

2-Hexadecanone H-161

[18787-63-8]
Methyl tetradecyl ketone
$H_3C(CH_2)_{13}COCH_3$
$C_{16}H_{32}O$ 240.428
Isol. from hop oil (*Humulus lupulus*). Cryst. Mp 43-43.5°. Bp_{100} 130-131°.
▶ MM0300000

Semicarbazone:
Cryst. (EtOH). Mp 117-118°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 642C (*nmr*)
Jahnsen, V.J. *et al., Nature (London)*, 1962, **196**, 474 (*isol*)
Klein, D.A. *et al., Appl. Microbiol.*, 1969, **17**, 676

Bailey, A.V. *et al., J. Chem. Eng. Data*, 1970, **15**, 542
Wyrick, S.D. *et al., J. Med. Chem.*, 1976, **19**, 219 (*synth*)

3-Hexadecenoic acid, 9CI H-162

[25447-95-4]

$H_3C(CH_2)_{11}CH{=}CHCH_2COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [1686-10-8]
Constit. of many plant systems including spinach leaves and red clover (*Trifolium pratense*). Mp 53-54°.

[28039-99-8]

Klenk, E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1963, **334**, 44 (*isol*)
Weenik, R.O. *et al., Biochim. Biophys. Acta*, 1964, **84**, 613
Hopkins, C.Y. *et al., Can. J. Chem.*, 1964, **42**, 2224 (*isol*)
Haverkate, F. *et al., Experientia*, 1964, **20**, 511
Kleiman, R. *et al., Lipids*, 1966, **1**, 301 (*isol*)
Knipprath, W. *et al., Lipids*, 1966, **1**, 81 (*synth*)
Kannan, R. *et al., Fette, Seifen, Anstrichm.*, 1974, **76**, 344 (*pmr*)

5-Hexadecenoic acid, 9CI H-163

[20057-14-1]

[25447-95-4]

$H_3C(CH_2)_9CH{=}CH(CH_2)_3COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [7056-84-0]
(*Z*)-*form* [7056-90-8]

[28039-99-8]
Isol. from *Dioscoreophyllum cumminsii* (serendipity berry). Oil.

Me ester:
$C_{17}H_{32}O_2$ 268.439
Oil.

Fulco, A.J. *et al., J. Biol. Chem.*, 1964, **239**, 998 (*isol*)
Bhatty, M.K. *et al., Can. J. Biochem.*, 1966, **44**, 311 (*isol*)
Spencer, G.F. *et al., Lipids*, 1972, **7**, 435 (*isol*)
Starratt, A.N. *et al., Chem. Phys. Lipids*, 1976, **16**, 215 (*synth*)
Henkel, B. *et al., Annalen*, 1995, 921 (*Z-form, Me ester, synth, cmr*)

6-Hexadecenoic acid, 9CI H-164

[2197-46-8]

[25447-95-4]

$H_3C(CH_2)_8CH{=}CH(CH_2)_4COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [28290-76-8]
Constit. of parsley oil.
(*Z*)-*form* [17004-51-2]

[28039-99-8]

Spencer, G.F. *et al., Lipids*, 1971, **6**, 712 (*isol*)

9-Hexadecenoic acid, 9CI H-165

[2091-29-4]

[25447-95-4]
Hypogaic acid

$H_3C(CH_2)_5CH{=}CH(CH_2)_7COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [10030-73-6]
Palmitelaidic acid
Mp 32-33°.
► LD_{50} (mus, iabd) 300-700 mg/kg.
(*Z*)-*form* [373-49-9]

[28039-99-8]
Palmitoleic acid. Zoomaric acid. Physeteleic acid
A major component of lipids of marine plants and animals, also found in plant oils, e.g. *Macadamia ternifolia* (small-fruited Macadamia nut) seed oil (20%). Mp 0.5°. Bp_1 180-183° $Bp_{0.6}$ 162°. n_D^{20} 1.4582.

Me ester: [1120-25-8]
$C_{17}H_{32}O_2$ 268.439
Liq. Bp_5 140-141°.

Isopropyl ester: [68862-23-7] *Isopropyl 9-hexadecenoate*
$C_{19}H_{36}O_2$ 296.492

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 782B; 986C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 587D (*ir*)
Armstrong, E.F. *et al., J. Soc. Chem. Ind., London*, 1925, **44**, 182T
Bridge, R.E. *et al., J.C.S.*, 1950, 2396 (*isol*)
Boughton, B.W. *et al., J.C.S.*, 1952, 671 (*synth*)
Hofmann, K. *et al., J. Biol. Chem.*, 1955, **213**, 415
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 734 (*occur*)
Suzuki, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 2269 (*ir, ms*)
Batchelor, J.G. *et al., J.O.C.*, 1974, **39**, 1698 (*cmr*)
Francke, W. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 796-797 (*isopropyl ester, isol*)
Mannan, A. *et al., Chem. Ind. (London)*, 1984, 851 (*isol, occur*)
Peschke, K. *et al., Chemoecology*, 1999, **9**, 47-54 (*isopropyl ester, isol*)

11-Hexadecenoic acid H-166

[2271-34-3]

[25447-95-4]
Lycopodiumoleic acid. Tanacetumoleic acid. Palmitvaccenic acid

$H_3C(CH_2)_3CH{=}CH(CH_2)_9COOH$

$C_{16}H_{30}O_2$ 254.412

(*E*)-*form* [73292-39-4]
Isol. from *Chrysanthemum vulgare* (tansy). Bp_{18} 235-240°.
(*Z*)-*form* [2416-20-8]

[28039-99-8]
Sol. MeOH, hexane; poorly sol. H_2O.

Ackman, R.G. *et al., Lipids*, 1966, **1**, 341 (*occur*)
Walker, R.W. *et al., Lipids*, 1969, **4**, 15 (*occur*)
Nichols, P.D. *et al., J. Microbiol. Methods*, 1986, **5**, 49

13-Hexadecenoic acid H-167

[14134-46-4]

[25447-95-4]

$H_3CCH_2CH{=}CH(CH_2)_{11}COOH$

$C_{16}H_{30}O_2$ 254.412

(*Z*)-*form*

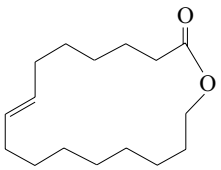
[28039-99-8]
Isol. from herring oil.

[92661-08-0]

Ackman, R.G. *et al., Lipids*, 1966, **1**, 341

7-Hexadecen-1,16-olide H-168

Oxacycloheptadec-8-en-2-one, 9CI. Ambrettolide. Ambrettolic acid lactone

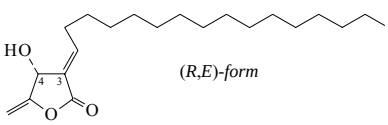


$C_{16}H_{28}O_2$ 252.396

(*E*)-*form* [51155-12-5]
Oil.
(*Z*)-*form* [123-69-3]
FEMA 2758
Once used in fruit flavouring; its use has been discontinued due to its toxic nature. Oil with strong musk-like odour. Bp_1 154-156°.
► RN9740000

Baudart, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1945, **221**, 205 (*synth*)
Sabnis, S.D. *et al., J.C.S.*, 1963, 2477 (*synth, ir*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir, pmr*)
Bergström, G. *et al., Chem. Scr.*, 1974, **5**, 39
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 707 (*rev, tox, Ambrettolide*)
Sanz, V. *et al., J.C.S. Perkin 1*, 1982, 1837 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1916

3-Hexadecylidenedihydro-4-hydroxy-5-methylene-2(3*H*)-furanone H-169



(*R,E*)-*form*

$C_{21}H_{36}O_3$ 336.514

(*S,E*)-*form* [139559-06-1]
Isolinderanolide
Constit. of *Lindera benzoin* (spicebush) berries. Oil. $[\alpha]_D$ -49.5 (c, 0.002 in $CHCl_3$).

11′,12′-Didehydro(Z-): [139328-80-6] *3-(11-Hexadecenylidene)dihydro-4-hydroxy-5-methylene-2(3H)-furanone.* ***Isolinderenolide***
$C_{21}H_{34}O_3$ 334.498
Constit. of *Lindera benzoin* (spicebush) berries. Oil. $[\alpha]_D$ -22.3 (c, 0.0026 in $CHCl_3$).

(*S,Z*)-*form* [139559-07-2]
Linderanolide
Constit. of *Lindera benzoin* (spicebush) berries. Oil. Mp -10°. $[\alpha]_D$ -46 (c, 0.01 in $CHCl_3$).

Anderson, J.E. *et al., J. Nat. Prod.*, 1992, **31**, 71 (*Linderanolide, Isolinderanolide, Isolinderenolide*)
Seki, K. *et al., Phytochemistry*, 1995, **40**, 1175-1181 (*Linderanolides, Isolinderanolides*)

2,4-Hexadienal, 9CI H-170

[142-83-6]

[80466-34-8]
Sorbic aldehyde. Sorbaldehyde

$H_3CCH{=}CHCH{=}CHCHO$

C_6H_8O 96.129

►Polymerizes explosively on heating. Severe eye and skin irritant. LD_{50} (rat, orl) 300 mg/kg. LD_{50} (rbt, skn) 270 mg/kg. WG1925000

(*E*,*E*)-*form*
FEMA 3429
Flavouring ingredient. Present in olives, roasted peanuts, tomato, caviar, fish, and tea. d^{22} 0.91. Bp 173-174° Bp_{11} 64-66°. n_D^{20} 1.5372.

►Fl. p. 68° (oc).

Oxime: [1515-97-5]
C_6H_9NO 111.143
Needles (EtOH). Mp 159.5-160.5° dec.

Phenylhydrazone:
Yellow plates (EtOH). Mp 101-102°.

Semicarbazone:
Plates (EtOH). Mp 206°.

(2*Z*,4*E*)-*form* [54716-12-0]
Pale yellow malodorous liq. Bp *ca.* 180°.

2,4-Dinitrophenylhydrazone:
Mp 161-163°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 474C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 741C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 564B (*ir*)
Albriktsen, P. *et al., Acta Chem. Scand.*, 1973, **27**, 3993 (*pmr, config*)
Shiess, P. *et al., Helv. Chim. Acta*, 1974, **57**, 2583 (*synth*)
Corey, E.J. *et al., Chem. Ber.*, 1978, **111**, 1362 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 337 (*rev, tox*)
Furber, M. *et al., J.C.S. Perkin 1*, 1989, 683 (*synth, ir, pmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 327
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1290-1291
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2238
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKT500

2,4-Hexadienedial, 9CI, 8CI H-171

[3249-28-3]
Muconic dialdehyde. Mucondialdehyde

OHCCH=CHCH=CHCHO

$C_6H_6O_2$ 110.112

►MM2010000

(*E*,*E*)-*form* [18409-46-6]
Stress metab. isol. from the leaves of the pseudocereal *Chenopodium album*. Pale-yellow needles (petrol). Mp 120.5-121°.

►MM2020000

(*E*,*Z*)-*form* [53042-85-6]
Yellow leaflets (hexane). Mp 58.5-59°.

(*Z*,*Z*)-*form* [64330-65-0]
Yellow needles (C_6H_6/hexane). Mp 99°.

Nakajima, M. *et al., Chem. Ber.*, 1959, **92**, 163 (*synth, ir*)
Kossmehl, G. *et al., Chem. Ber.*, 1974, **107**, 710 (*synth, bibl*)
Hinshaw, J.C. *et al., J.O.C.*, 1974, **39**, 3951 (*synth*)
Davies, S.G. *et al., J.C.S. Perkin 1*, 1977, 1346 (*synth, pmr*)
Tahara, S. *et al., Experientia*, 1994, **50**, 137 (*isol*)
Murray, M.M. *et al., J.A.C.S.*, 1994, **116**, 8152 (*synth*)
Maruta, Y. *et al., Phytochemistry*, 1995, **38**, 1169 (*isol*)

2,4-Hexadienoic acid, 9CI H-172

[22500-92-1]
1,3-Pentadiene-1-carboxylic acid. Sorbic acid, 8CI. E200

$H_3CCH{=}CHCH{=}CHCOOH$

$C_6H_8O_2$ 112.128

(2*E*,4*E*)-*form* [110-44-1]
Panosorb. FEMA 3921
Preservative for many foodstuffs. Generally used as K salt or (less frequently) as Ca salt. Antimicrobial agent against a wide variety of microorganisms, esp. yeasts and moulds. Preservative action more efficient in acidic foods. Typical usage levels 500-2000 ppm. Needles (EtOH aq.). Mod. sol. hot H_2O. Mp 134.5°. Bp 228° dec.. pK_{a1} 4.51 (25°, 0.1*M* NaCl). Undergoes radiation-induced radical polym..

►Skin and eye irritant, contact sensitiser. LD_{50} (rat, orl) 7360 mg/kg. WG2100000

Na salt: [7757-81-5] *Sodium sorbate*
$C_6H_7NaO_2$ 134.11
Antimicrobial agent; preservative.

K salt:Potassium sorbate. Sorbistat K. Unistat K. FEMA 2921. E202
$C_6H_7KO_2$ 150.218
Mould inhibitor, preservative for cheese, fruit preserves, baked goods, wine and other foodstuffs. Also for paper and board food packaging materials. Flavouring ingredient. Cryst. Dec. >270°.

Ca salt: [7492-55-9] *Calcium sorbate*
$C_{12}H_{14}CaO_4$ 262.318
Preservative for foods, e.g. margarine. Fine cryst. powder. Dec. 400°.

Me ester: [689-89-4] *Methyl sorbate. FEMA 3714*
$C_7H_{10}O_2$ 126.155
Flavouring ingredient. Liq. with a fruity-anise odour. Mp 5°. Bp 180° Bp_{20} 70°. n_D^{20} 1.0521.

Et ester: [5941-48-0]

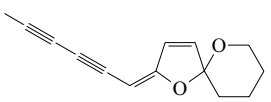
[2396-84-1] *Ethyl sorbate. FEMA 2459*
$C_8H_{12}O_2$ 140.182
Flavouring ingredient. d^{20} 0.96. Bp_{20} 85°. n_D^{20} 1.5020.

2-Propenyl ester: [7493-75-6] *2-Propenyl 2,4-hexadienoate. Allyl sorbate. FEMA 2041*
$C_9H_{12}O_2$ 152.193
Flavouring ingredient.

[821-00-1, 1515-80-6, 1516-01-4, 24634-61-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 502A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 784C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 588D (*ir, EE-form*)
Eisner, U. *et al., J.C.S.*, 1953, 1372 (*synth, uv, EE-form, ZE-form*)
Woodford, R. *et al., CA*, 1970, **72**, 136 312x (*rev*)
Bonjouklian, R. *et al., J.O.C.*, 1977, **42**, 4095 (*synth*)
Frighetto, N. *et al., Chem. Phys. Lipids*, 1978, **22**, 115 (*cmr, EE-form*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 402 (*rev*)
Lombardo, L. *et al., Synthesis*, 1978, 131 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, SKU000
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 296 (*use*)
Vinczer, P. *et al., Org. Prep. Proced. Int.*, 1991, **23**, 441 (***synth, pmr***)
Cox, P.J. *et al., Acta Cryst. C*, 1994, **50**, 1620 (*cryst struct*)
Kaschabek, S.R. *et al., J.O.C.*, 1994, **59**, 4001 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 31; 267; 562 (*esters*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1146
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 100; 423-424; 1041-1042; 1857-1858; 2319-2321; 2607-2608; 2618-2619 (*esters, K salt, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1520-1521 (*K salt, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKU000

2-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene H-173



(*E*)-*form*

$C_{14}H_{14}O_2$ 214.263

(*E*)-*form* [3306-40-9]
Constit. of roots of *Tanacetum vulgare* (tansy). Mp 83°. $[\alpha]_{Hg}^{20}$ +29 (c, 2.0 in Et_2O). Also descr. as resinous liq..

8-O-*Ac:8-Acetoxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene*
$C_{16}H_{16}O_4$ 272.3Not obt. pure
λ_{max} 240 ; 254 ; 310 ; 318 (no solvent reported).

8-O-*(3-Methylbutanoyl):8-Isovaleryloxy-2-(2,4-hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene*
$C_{19}H_{22}O_4$ 314.38
Cryst. (petrol). Mp 93-94°. $[\alpha]_D^{23}$ +7.7 (c, 1.71 in Et_2O).

(*Z*)-*form* [5535-87-5]
Mp 78°. $[\alpha]_D$ 0. Both isomers also descr. as resinous liquids.

8-O-*Ac:*
Cryst. (Et_2O/petrol). Mp 127°. $[\alpha]_D^{23}$ +15.2 (c, 3.08 in Et_2O).

8-O-*(3-Methylbutanoyl):*
Cryst. (petrol). Mp 87-88°. $[\alpha]_D^{23}$ -35.1 (c, 2.45 in Et_2O).

Deoxy, 3,4-epoxy:2-(2,4-Hexadiynylidene)-3,4-epoxy-1,6-dioxaspiro[4.5]decane

$C_{14}H_{14}O_3$ 230.263No stereochem. λ_{max} 224 ; 264 ; 277 ; 292 (no solvent reported).

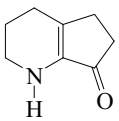
Bohlmann, F. *et al., Chem. Ber.*, 1960, **93**, 1937; 1961, **94**, 3193; 1963, **96**, 226; 1964, **97**, 1179; 1966, **99**, 990; 1830; 2416

Yano, K. *et al., Phytochemistry*, 1972, **11**, 2577

1,2,3,4,5,6-Hexahydro-7*H*-cyclopenta[*b*]pyridin-7-one, 13CI H-174

[104704-30-5]

*1,2,3,4,5,6-Hexahydro-7*H*-1-pyrindin-7-one, 12CI*



$C_8H_{11}NO$ 137.181

Proline-derived Maillard product. Constit. of wort and beer. Flavouring ingredient. Cryst. with bread-like aroma. Mp 68°. $Bp_{0.2}$ 100° (Kugelrohr).

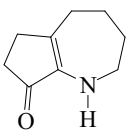
Tressl, R. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404; 1993, **41**, 547-553 (*isol, ms, ir, pmr*)

Ger. Pat., 1992, 4 217 395; *CA*, **120**, 217293d (*synth, use*)

Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

2,3,4,5,6,7-Hexahydrocyclopent[*b*]azepin-8(1*H*)-one H-175

[81978-77-0]



$C_9H_{13}NO$ 151.208

Proline-specific Maillard product. Flavouring ingredient. Cryst. with bread-like aroma. Mp 82°. $Bp_{0.15}$ 100-120° (Kugelrohr).

Tressl, R. *et al., Annalen*, 1985, 2017-2027 (*isol, pmr, ms*)

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137; 1993, **41**, 547-553 (*isol, ms, pmr*)

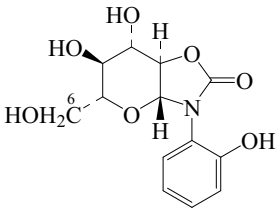
Ger. Pat., 1992, 4 217 395; *CA*, **120**, 217293d (*synth, use*)

Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

Hexahydro-6,7-dihydroxy-5-(hydroxymethyl)-3-(2-hydroxyphenyl)-2*H*-pyrano[2,3-*d*]oxazol-2-one, 9CI H-176

[396714-67-3]

1-(2-Hydroxyphenylamino)-1-deoxyglucoside 1,2-carbamate



$C_{13}H_{15}NO_7$ 297.264

Struct. revised in 2001. Originally thought to be the *N*-glycoside of 2-Benzoxazolol, B-40. Isol. from the roots of oats *(Avena sativa)* and corn *(Zea mays)*. Cryst. Mp 125-128°. $[\alpha]_D^{26}$ +30 (c, 1 in MeOH).

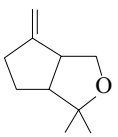
6-O-β-D-Glucopyranoside: [396714-64-0] *1-(2-Hydroxyphenylamino)-1-deoxy-β-D-gentiobioside 1,2-carbamate*
$C_{19}H_{25}NO_{12}$ 459.406
Trace metab. of corn.

Sicker, D. *et al., Phytochemistry*, 2001, **58**, 819-825

Hexahydro-1,1-dimethyl-4-methylene-1*H*-cyclopenta[*c*]furan, 9CI H-177

[19901-95-2]

2,2-Dimethyl-6-methylene-3-oxabicyclo[3.3.0]octane. ***Hop ether***



$C_{10}H_{16}O$ 152.236

Volatile constit. of Japanese hops. Oil. Bp_{15} 50-53°.

Naya, Y. *et al., Nippon Kagaku Kaishi*, 1968, **89**, 1113 (*isol*)

Naya, Y. *et al., Tet. Lett.*, 1968, 1645 (*isol*)

Imagawa, T. *et al., Tet. Lett.*, 1979, 1691 (*synth*)

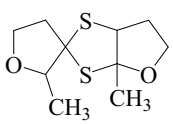
Johnson, C.R. *et al., Tet. Lett.*, 1982, **23**, 5005 (*synth*)

Billington, D.C. *et al., J. Organomet. Chem.*, 1987, **328**, 223

Tanimori, S. *et al., Agric. Biol. Chem.*, 1990, **54**, 1875 (*synth*)

Hexahydro-2′,3*a*-dimethylspiro[1,3-dithiolo[4,5-*b*]furan-2,3′(2′*H*)-furan], 9CI H-178

[38325-25-6]



$C_{10}H_{16}O_2S_2$ 232.367

Major component (65%) of the meaty flavour ingredient FEMA 3270.

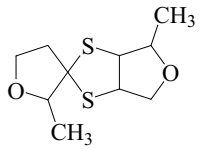
Netherlands Pat., 1972, 7 100 235; *CA*, **77**, 125041k (*synth, use*)

Guentert, M. *et al., ACS Symp. Ser.*, 1992, **490**, 140-163 (*occur, pmr, glc*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 203 (*use*)

Hexahydro-2′,4-dimethylspiro[1,3-dithiolo[4,5-*c*]furan-2,3′(2′*H*)-furan], 9CI H-179

[38325-26-7]



$C_{10}H_{16}O_2S_2$ 232.367

Minor component (35%) of the meaty flavouring ingredient FEMA 3270.

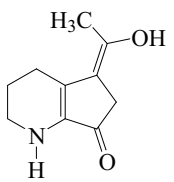
Netherlands Pat., 1972, 7 100 235; *CA*, **77**, 125041k (*synth, use*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 203 (*use*)

1,2,3,4,5,6-Hexahydro-5-(1-hydroxyethylidene)-7*H*-cyclopenta[*b*]pyridin-7-one, 13CI H-180

[118355-70-7]

*1,2,3,4,5,6-Hexahydro-5-(1-hydroxyethylidene)-7*H*-1-pyrindin-7-one, 12CI*



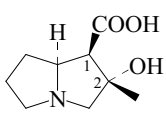
$C_{10}H_{13}NO_2$ 179.218

Proline-derived Maillard product. Unstable. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*isol, ir, ms, pmr*)

Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

Hexahydro-2-hydroxy-2-methyl-1*H*-pyrrolizine-1-carboxylic acid, 9CI H-181



(1*R*,2*S*,7a*S*)-*form*

$C_9H_{15}NO_3$ 185.222

(1*R*,2*S*,7a*S*)-*form* [147634-91-1] ***Neotussilaginic acid***

Me ester: [147730-89-0] ***Neotussilagine.*** *Isotussilaginine*
$C_{10}H_{17}NO_3$ 199.249
Alkaloid artifact from *Tussilago farfara* (coltsfoot) resulting from the use of MeOH during isol..

(1*R*,2*R*,7a*S*)-*form* [147634-92-2] ***Neoisotussilagic acid***

Me ester: [147730-90-3] ***Neoisotussilagine.*** *Tussilaginine*

$C_{10}H_{17}NO_3$ 199.249
Alkaloid artifact from *Tussilago farfara* (coltsfoot) resulting from the use of MeOH during isol..

(1*S*,2*S*,7a*S*)-*form* [147634-89-7]
Tussilagic acid

Me ester: [80151-77-5] ***Tussilagine***
Alkaloid artifact from *Tussilago farfara* (coltsfoot) resulting from the use of MeOH during isol.. Mp 193° (dec.). $[\alpha]_D^{25}$ -2.7 (c, 0.15 in EtOH).

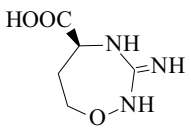
(1*S*,2*R*,7a*S*)-*form* [147634-90-0]
Isotussilaginic acid

Me ester: [91108-32-6] ***Isotussilagine***
$C_{10}H_{17}NO_3$ 199.249
Alkaloid artifact from *Tussilago farfara* (coltsfoot) resulting from the use of MeOH during isol.. $[\alpha]_D^{25}$ +129 (C, 0.17 in $CHCl_3$).

Röder, E. *et al., Planta Med.*, 1981, **43**, 99 (*ir, pmr, cmr, ms, struct*)
Weidenfeld, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 367 (*cryst struct, abs config*)
Röder, E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1984, **317**, 403 (*synth*)
Passreiter, C.M. *et al., Phytochemistry*, 1992, **31**, 4135 (*stereoisomers*)
Passreiter, C.M. *et al., Planta Med.*, 1992, **58**, 556-557 (*isol*)
Ma, D. *et al., Tet. Lett.*, 1998, **39**, 9067-9068 (*synth, pmr*)
Ma, D. *et al., J.C.S. Perkin 1*, 1999, 1703-1707 (*synth*)

Hexahydro-3-imino-1,2,4-oxadiazepine-3-carboxylic acid, 9CI H-182

Desaminocanavanine. Deaminocanavanine



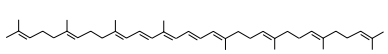
$C_5H_9N_3O_3$ 159.144
Cyclic anhydride of Canavanine, C-72 the name Desaminocanavanine is rather misleading.

(*S*)-*form* [21539-44-6]
L-form
May occur with Canavanine, C-72 in Jack bean meal (*Canavalia ensiformis*) and other plants. Cryst. Mp 257-258° dec. $[\alpha]_D$ +25. Unreactive to ninhydrin.

Rosenthal, G.A. *et al., Phytochemistry*, 1972, **11**, 2827 (*synth, bibl*)

7,7′,8,8′,11,12-Hexahydrolycopene H-183

[540-05-6]
7,7′,8,8′,11,12-Hexahydro-ψ,ψ-carotene



$C_{40}H_{62}$ 542.93
Pale yellow oil with brilliant green fluorescence. The (all-*E*) and several mono- and di-Z isomers appear to occur naturally.

1,2-Epoxide: [51598-36-8] *1,2-Epoxy-1,2,7,7′,8,8′,11,12-octahydro-ψ,ψ-carotene*
$C_{40}H_{62}O$ 558.929
Isol. from tomatoes (*Lycopersicon esculentum*). Not separated from the 1′,2′-epoxide.

1′,2′-Epoxide: [51599-11-2] *1,2-Epoxy-1,2,7,7′,8,8′,11′,12′-octahydro-ψ,ψ-carotene*
$C_{40}H_{62}O$ 558.929
Isol. from tomatoes (*Lycopersicon esculentum*). λ_{max} 331 ; 348 ; 367 (petrol).

9*Z*-*form* [151767-13-4]
Pale yellow liq. λ_{max} 332 ; 348 ; 367 (hexane).

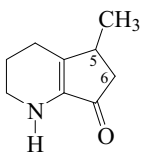
15*Z*-*form* [27664-65-9]
Phytofluene
Pale yellow oil.

(15*Z*,9′*Z*)-*form* [72746-34-0]
Isol. from tomato (*Lycopersicon esculentum* var. 'Tangella'). Yellow oil with intense blue-green fluorescence. λ_{max} 249 ; 257 ; 331 ; 348 ; 367 (hexane).

Zechmeister, L. *et al., Arch. Biochem. Biophys.*, 1953, **47**, 160 (*occur*)
Jungawala, F.B. *et al., Arch. Biochem. Biophys.*, 1965, **110**, 291-299 (*config, Phytofluene*)
Davis, J.B. *et al., J.C.S.(C)*, 1966, 2154 (*isol, struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1817 (*occur*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759 (*epoxides*)
Brown, D.J. *et al., Biochem. Soc. Trans.*, 1975, **3**, 741 (*biosynth*)
Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*15Z,9′Z-form, ir, pmr, cmr*)
Frecknall, E.A. *et al., Phytochemistry*, 1984, **23**, 1707 (*occur*)
Ebenezer, W.J. *et al., J.C.S. Perkin 1*, 1993, 1869 (*9Z-isomer*)

1,2,3,4,5,6-Hexahydro-5-methyl-7*H*-cyclopenta[*b*]pyridin-7-one, 13CI H-184

[104704-29-2]
*1,2,3,4,5,6-Hexahydro-5-methyl-7*H*-1-pyrindin-7-one, 12CI*



$C_9H_{13}NO$ 151.208
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404; 1993, **41**, 547-553 (*isol, ir, ms, pmr*)
Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

1,2,3,4,5,6-Hexahydro-6-methyl-7*H*-cyclopenta[*b*]pyridin-7-one, 13CI H-185

[104704-38-3]
*1,2,3,4,5,6-Hexahydro-6-methyl-7*H*-1-pyrindin-7-one, 12CI*

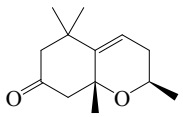
$C_9H_{13}NO$ 151.208
Proline-derived Maillard product. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*isol, ir, ms, pmr*)
Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

2,3,5,6,8,8*a*-Hexahydro-2,5,5,8*a*-tetramethyl-7*H*-1-benzopyran-7-one, 9CI H-186

[20194-67-6]

[165523-62-6, 165523-63-7, 165523-64-8, 165523-65-9]
3,4-Dihydro-3-oxoedulan



(2*RS*,8*aRS*)-*form*

$C_{13}H_{20}O_2$ 208.3
Constit. of purple passion fruit, Riesling wine, grapes and grape leaf, quince, dried kukoshi berries (*Lycium chinense*) and sweet osmanthus (*Osmanthus fragrans*) flowers. Generally present in nature as an unequal mixture of diasteroisomers.

(2*RS*,8*aRS*)-*form* [157784-98-0]

[128660-64-0]
(±)-cis-*form*
Mp 85°.

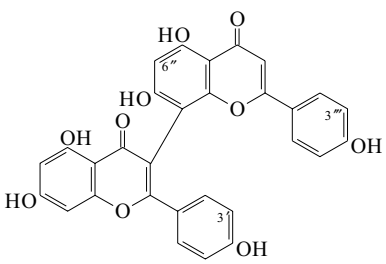
(2*RS*,8*aSR*)-*form* [157785-09-6]

[128660-65-1]
(±)-trans-*form*
Mp 42-45°. $Bp_{0.1}$ 70-75°.

Enzell, C.R. *et al., Mass Spectrom. Rev.*, 1986, **5**, 39-72 (*ms*)
Weyerstahl, P. *et al., Annalen*, 1994, 415-427 (*synth, cmr, pmr*)
Schmidt, G. *et al., J. Agric. Food Chem.*, 1995, **43**, 1898-1902 (*occur, synth, uv, pmr, cmr*)
Chassagne, D. *et al., Food Chem.*, 1999, **66**, 281-288 (*occur, passion fruit*)

4′,4‴,5,5″,7,7″-Hexahydroxy-3,8″-biflavone H-187

[101140-06-1]
*5,5′,7,7′-Tetrahydroxy-2,2′-bis(4-hydroxyphenyl)-[3,8′-bi-4*H*-1-benzopyran]-4,4′-dione, 9CI. 3,8″-Biapigenin*



$C_{30}H_{18}O_{10}$ 538.466
Isol. from *Fagopyrum esculentum* (buckwheat). Cryst. ($MeOH/CHCl_3$). Mp 259-261°.

Hexa-Me ether:4′,4‴,5,5″,7,7″-Hexamethoxy-3,8″-biflavone
$C_{36}H_{30}O_{10}$ 622.627
Needles ($CHCl_3$/MeOH). Mp 175°.

3‴-Hydroxy: [28570-47-0]

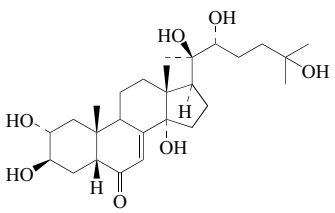
3‴,4′,4‴,5,5″,7,7″-Heptahydroxy-3,8″-biflavone. Saharanflavone
$C_{30}H_{18}O_{11}$ 554.466

3‴-Hydroxy, hepta-Me ether: [39727-25-8]
3‴,4′,4‴,5,5″,7,7″-Heptamethoxy-3,8″-biflavone
Needles ($CHCl_3$/MeOH). Mp 152°.

6″-Hydroxy: [114312-08-2]
4′,4‴,5,5″,6″,7,7″-Heptahydroxy-3,8‴-biflavone. ***Sumaflavone***
$C_{30}H_{18}O_{11}$ 554.466

Pelter, A. *et al., Tetrahedron*, 1971, **27**, 1625 (*Saharanflavone*)
Ikeshiro, Y. *et al., Tet. Lett.*, 1972, 4383 (*Saharanflavone*)
Berghoefer, R. *et al., Planta Med.*, 1987, **53**, 216 (*isol, cmr*)
Van Loo, P. *et al., Chromatographia*, 1988, **25**, 15 (*Sumaflavone*)
Kitanov, G. *et al., Khim. Prir. Soedin.*, 1988, **24**, 454; *Chem. Nat. Compd. (Engl. Transl.)*, 1988, **24**, 390 (*isol*)
Cardona, M.L. *et al., Heterocycles*, 1989, **29**, 2297 (*isol*)
Terashima, K. *et al., Heterocycles*, 1999, **50**, 283-290 (*isol, uv, pmr, cmr*)

2,3,14,20,22,25-Hexahydroxycholest-7-en-6-one, 9CI H-188



(2α,3β,5β,20*R*,22*R*)-*form*

$C_{27}H_{44}O_7$ 480.64

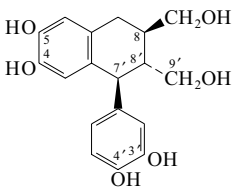
(2β,3β,5β,20*R*,22*R*)-*form* [5289-74-7]
Crustecdysone*. Commisterone. β-Ecdysone. Ecdysterone. 20-Hydroxy-α-ecdysone. Isoinokosterone. Polypodine A. Viticosterone*
Isol. from the marine crayfish *Jasus lalandei* in low yield (2 mg/ton). Plates (EtOAc/THF). Mp 237.5-239.5° (243°). $[\alpha]_D$ +61.8 ($CHCl_3$). Log P -1.91 (uncertain value) (calc).

► LD_{50} (mus, ipr) 6400 mg/kg. Exp. reprod. effects. FZ8060000

[35241-82-8]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 574C (*nmr*)
Galbraith, M.N. *et al., Chem. Comm.*, 1966, 905-906 (*isol, Crustecdysone*)
Hüppi, G. *et al., J.A.C.S.*, 1967, **89**, 6790-6792 (*Crustecdysone, synth*)
Horn, D.H.S. *et al., Biochem. J.*, 1968, **109**, 399-406 (*20-Hydroxyecdysone*)
Kerb, U. *et al., Tet. Lett.*, 1968, 4277-4280 (*20-Hydroxyecdysterone, synth*)
Dammeier, B. *et al., Chem. Ber.*, 1971, **104**, 1660-1673 (*Ecdysterone, struct, abs config*)
Zatsny, I. *et al., Khim. Prir. Soedin.*, 1975, **11**, 155-158; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 170-172 (*ms*)
Kametani, T. *et al., Tet. Lett.*, 1980, 4855-4856 (*20-Hydroxyecdysterone, synth*)
Kubo, I. *et al., Agric. Biol. Chem.*, 1985, **49**, 243-244 (*pmr*)
Bandara, B.M. *et al., Phytochemistry*, 1989, **28**, 1073-1075 (*isol, cmr*)
Hedtmann, U. *et al., Tetrahedron*, 1991, **47**, 3753-3772 (*synth*)
Nagakari, M. *et al., Chem. Comm.*, 1994, 1761-1762 (*biosynth*)
Kusamba, C. *et al., Fitoterapia*, 1995, **66**, 175-178 (*cmr*)
Pathak, A.K. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 674-676 (*20-Hydroxyecdysone, pmr, cmr*)
Suksamrarn, A. *et al., Phytochemistry*, 1995, **38**, 473-476 (*cmr*)
Devarenne, T.P. *et al., Phytochemistry*, 1995, **40**, 1125-1131 (*biosynth*)
Calcagno, M.-P. *et al., Tetrahedron*, 1996, **52**, 10137-10146 (*pmr, cmr*)
Fujimoto, Y. *et al., Tet. Lett.*, 1997, **38**, 2697-2700; 2701-2704 (*biosynth*)
Nomura, K. *et al., Chem. Pharm. Bull.*, 2000, **48**, 344-348 (*biosynth*)
Hyodo, R. *et al., Phytochemistry*, 2000, **53**, 733-737 (*biosynth*)

3′,4,4′,5,9,9′-Hexahydroxy-2,7′-cyclolignan H-189



(7′*S*,8*R*,8′*R*)-*form*

$C_{18}H_{20}O_6$ 332.352

(7′*S*,8*R*,8′*R*)-*form*

*3′,5-Di-Me ether, 4′-*O*-β-D-glucopyranoside:* [145748-07-8] *Isolariciresinol 4′-O-β-D-glucoside*
$C_{26}H_{34}O_{11}$ 522.548
Constit. of Riesling wine. Amorph. solid.

*3′,5-Di-Me ether, 9′-*O*-α-L-arabinofuranoside:* [63358-10-1]

[62080-75-5] *Isolariciresinol 9′-O-α-L-arabinofuranoside*
$C_{25}H_{32}O_{10}$ 492.522
Constit. of Scots pine (*Pinus sylvestris*) needles. Amorph. $[\alpha]_D^{20}$ -36.8 (c, 1 in EtOH).

*3′,5-Di-Me ether, 9-*O*-β-D-glucopyranoside:* [63358-11-2]

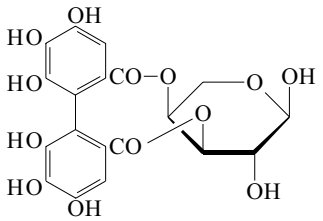
[62080-76-6] *Isolariciresinol 9-O-β-D-glucoside*
$C_{26}H_{34}O_{11}$ 522.548
Constit. of Scots pine (*Pinus sylvestris*) needles. Amorph. $[\alpha]_D^{20}$ +8 (c, 0.9 in EtOH).

*3′,5-Di-Me ether, 9′-*O*-β-D-glucopyranoside:* [63358-12-3] *Isolariciresinol 9′-O-β-D-glucoside*
$C_{26}H_{34}O_{11}$ 522.548
Constit. of Scots pine (*Pinus sylvestris*) needles. Needles (MeOH). Mp 135-138°. $[\alpha]_D^{23}$ +45.4 (c, 0.8 in MeOH).

Popoff, T. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 329-337 (*Isolariciresinol glycosides*)
Lundgren, L.N. *et al., Acta Chem. Scand., Ser. B*, 1985, **39**, 241-248 (*Isolariciresinol glycosides*)
Marinos, V.A. *et al., Phytochemistry*, 1992, **31**, 4307 (*Isolariciresinol 4′-glucoside*)

3,4-Hexahydroxydiphenoylarabinose H-190

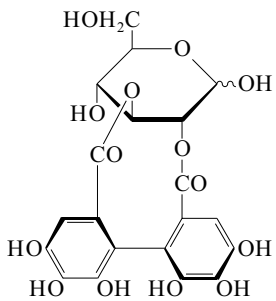
[19833-16-0]
Arabinopyranose cyclic 3,4-(4,4′,5,5′,6,6′-hexahydroxydiphenate), 8CI



$C_{19}H_{16}O_{13}$ 452.328
Isol. from fruits of *Psidium guajava* (guava). Plates (EtOH aq.). Mp 230-235° dec. $[\alpha]_D^{25}$ -24.2 (c, 0.4 in Py).

Misra, K. *et al., Phytochemistry*, 1968, **7**, 641

2,3-Hexahydroxydiphenoylglucose H-191



(*R*)$_{axial}$-β-D-Pyranose-*form*

$C_{20}H_{18}O_{14}$ 482.354

(*S*)$_{axial}$-D-Pyranose-*form*
Light brown amorph. powder + $1H_2O$. $[\alpha]_D^{20}$ +50.5 (c, 0.8 in MeOH).

*4-*O*-(3,4,5-Trihydroxybenzoyl):* [115356-04-2] ***Pterocaryanin B***
$C_{27}H_{22}O_{18}$ 634.46
Constit. of *Castanea mollissima* (Chinese chestnut).

(*S*)$_{axial}$-α-D-Pyranose-*form*

*1-*O*-(3,4,5-Trihydroxybenzoyl):* [84316-77-8] *1-*O*-Galloyl-2,3-(S)-hexahydroxydiphenoyl-α-D-glucopyranose.* ***Sanguiin H4***
$C_{27}H_{22}O_{18}$ 634.46
Isol. from *Sanguisorba officinalis* (burnet bloodwort). Light buff amorph. powder + $1H_2O$. $[\alpha]_D^{20}$ +86 (c, 0.6 in MeOH).

1,6-Bis(3,4,5-trihydroxybenzoyl): [82202-99-1] *1,6-Di-*O*-galloyl-2,3-(S)-hexahydroxydiphenoyl-α-D-glucopyranose.* ***Sanguiin H1***
$C_{34}H_{26}O_{22}$ 786.566
Isol. from the underground parts of *Sanguisorba officinalis* (burnet bloodwort). Tan amorph. powder. $[\alpha]_D^{20}$ +93.5 (c, 0.7 in Me_2CO).

(*S*)$_{axial}$-β-D-Pyranose-*form*

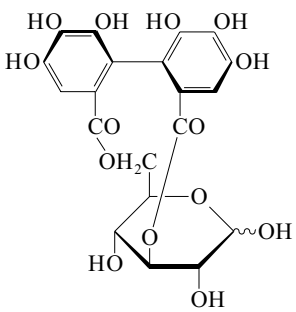
*1-*O*-(3,4,5-Trihydroxybenzoyl):* [87392-

62-9] *1*-O-*Galloyl-2,3-(*S*)-hexahydroxydiphenoyl-β-D-glucopyranose.* ***Isostrictinin***. *Sanguiin H5*
$C_{27}H_{22}O_{18}$ 634.46
Tannin constit. isol. from the leaf of *Psidium guajava* (guava) and from underground parts of *Sanguisorba officinalis* (burnet bloodwort). Off-white amorph. powder + $2H_2O$. $[\alpha]_D^{17}$ -11.5 (c, 0.4 in MeOH). $[\alpha]_D^{20}$ +122.3 (c, 0.9 in Me_2CO). Large discrepancy in opt. rotns. may indicate non-identity of Isostrictinin and Sanguiin H5 despite different solvs..

[81571-73-5]

Nonaka, G.-I. *et al., J.C.S. Perkin 1*, 1982, 1067 (*Sanguiin H1*)
Gupta, R.K. *et al., J.C.S. Perkin 1*, 1982, 2525 (*Sanguiins*)
Okuda, T. *et al., Phytochemistry*, 1982, **21**, 2871 (*Isostrictinin*)
Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*Sanguiins*)
Yoshida, T. *et al., J.C.S. Perkin 1*, 1985, 315 (*Sanguiins*)
Nonaka, G. *et al., Phytochemistry*, 1988, **27**, 1185 (*Pterocaryanins*)
Saijo, R. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2063 (*Pterocaryanins*)
Feldman, K.S. *et al., J.O.C.*, 1995, **60**, 8171 (*synth, Isostrictinin*)

3,6-Hexahydroxydiphenoylglucose H-192



$C_{20}H_{18}O_{14}$ 482.354

$(R)_{axial}$-β-D-pyranose-*form*

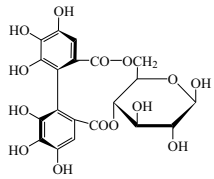
1,4-Bis-(3,4,5-trihydroxybenzoyl): [103744-87-2] *1,4-Di*-O-*galloyl-3,6-(*R*)-hexahydroxydiphenoyl-β-D-glucopyranose.* ***Tercatain***
$C_{34}H_{26}O_{22}$ 786.566
A tannin constit. isol. from *Punica granatum* (pomegranate). Amorph. powder + $1H_2O$. $[\alpha]_D^{19}$ -71.1 (c, 1.0 in MeOH).

1,2,4-Tris-(3,4,5-trihydroxybenzoyl): [88847-11-4] *1,2,4-Tri*-O-*galloyl-3,6-(*R*)-hexahydroxydiphenoyl-β-D-glucopyranose.* ***Punicafolin***
$C_{41}H_{30}O_{26}$ 938.672
Isol. from the leaf of *Punica granatum* (pomegranate). Cryst. powder + $2H_2O$ (H_2O). Mp 235-237° dec. $[\alpha]_D^{20}$ -59.5 (c, 0.4 in MeOH).

Tanaka, T. *et al., Phytochemistry*, 1985, **24**, 2075 (*Punicafolin*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1039 (*Tercatain*)
Hussein, S.A.M. *et al., Phytochemistry*, 1997, **45**, 819 (*Tercatain*)

4,6-Hexahydroxydiphenoylglucose H-193

[36378-48-0]



$C_{20}H_{18}O_{14}$ 482.354

$(S)_{axial}$-α-D-Pyranose-*form*

1,3-Bis-(3,4,5-trihydroxybenzoyl): [87687-52-3] *1,3-Di*-O-*galloyl-4,6-(*S*)-hexahydroxydiphenoyl-α-D-glucopyranose.* ***Heterophylliin A***
$C_{34}H_{26}O_{22}$ 786.566
Isol. from the leaf of *Corylus heterophylla* (Siberian filbert). Off-white amorph. powder + $6H_2O$. $[\alpha]_D^{20}$ +117 (c, 0.6 in MeOH).

$(S)_{axial}$-β-D-pyranose-*form*

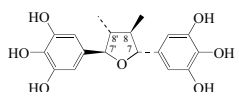
1,2,3-Tris(3,4,5-trihydroxybenzoyl): [58970-75-5] *1,2,3-Tri*-O-*galloyl-4,6-(*S*)-hexahydroxydiphenoyl-β-D-glucopyranose.* ***Tellimagrandin II***. *Eugeniin. Cornustannin 2*
$C_{41}H_{30}O_{26}$ 938.672
Isol. from *Eugenia caryophyllata* (clove) and *Filipendula ulmaria* (meadowsweet). Light brown amorph. powder + $1H_2O$. $[\alpha]_D^{20}$ +62.2 (c, 0.8 in Me_2CO). $[\alpha]_D^{20}$ +10 (c, 0.85 in MeOH). Log P 1.92 (calc). Cornustannin 2 and Eugeniin appear to be identical. Phys. props. refer to Eugeniin.

[79786-08-6, 81571-72-4]

Wilkins, C.K. *et al., Phytochemistry*, 1976, **15**, 211-214 (*Tellimagrandins*)
Gupta, R.K. *et al., J.C.S. Perkin 1*, 1982, 2525-2534 (*Tellimagrandins, occur, pmr, cmr*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 49-54; 2849-2854 (*Heterophylliin A, β-D-isomer*)
Nelson, T.D. *et al., J.O.C.*, 1994, **59**, 2577-2580 (*synth, Tellimagrandins*)
Feldman, K.S. *et al., J.O.C.*, 1999, **64**, 209-216 (*synth, Tellimagrandin II*)
Khanbabaee, K. *et al., Tetrahedron*, 2002, **58**, 1159-1163 (*1,3-DigalloylHHDP-β-D-glucose, synth, pmr, cmr*)

3,3′,4,4′,5,5′-Hexahydroxy-7,7′-epoxylignan H-194

Tetrahydro-3,4-dimethyl-2,5-bis(3,4,5-trihydroxyphenyl)furan



$C_{18}H_{20}O_7$ 348.352

(7*R*,7′*R*,8*R*,8′*R*)-*form*

3,3′,5,5′-Tetra-Me ether: [112572-55-1] *4,4′-Dihydroxy-3,3′,5,5′-tetramethoxy-7,7′-epoxylignan.* ***Fragransin B_2***
$C_{22}H_{28}O_7$ 404.459
Isol. from *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ 0 ($CHCl_3$).

(7*R,7′*S**,8*R**,8′*S**)-*form***

3,3′,5,5′-Tetra-Me ether: [112516-03-7] ***Fragransin B_1***
$C_{22}H_{28}O_7$ 404.459
Isol. from *Myristica fragrans* (nutmeg). Cryst. Mp 100-102°. Opt. inactive (*meso*-).

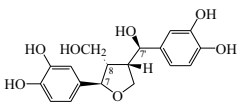
(7*R,7′*S**,8*S**,8′*S**)-*form***

3,3′,5,5′-Tetra-Me ether: [112572-56-2] ***Fragransin B_3***
$C_{22}H_{28}O_7$ 404.459
Isol. from *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +12.5 (c, 1.02 in $CHCl_3$).

[50393-98-1, 63284-54-8]

Hattori, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3315 (*Fragransins*)

3,3′,4,4′,7′,9-Hexahydroxy-7,9′-epoxylignan H-195



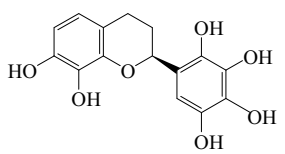
$C_{18}H_{20}O_7$ 348.352

(7*S*,7′*S*,8*R*,8′*R*)-*form*

7′-Ketone, 3,4:3′,4′-bis(methylene) ether: ***8′-Episesaminone***
$C_{20}H_{18}O_7$ 370.358
Constit. of the seeds of *Sesamum indicum* (sesame). $[\alpha]_D$ +126.2 (c, 0.1 in $CHCl_3$). λ_{max} 230 (log ε 4.76); 280 (log ε 3.75); 312 (log ε 2.87) (MeOH).

Marchand, P.A. *et al., J. Nat. Prod.*, 1997, **60**, 1189-1192 (*8′-Episesaminone*)

2′,3′,4′,5′,7,8-Hexahydroxyflavan H-196



$C_{15}H_{14}O_7$ 306.271

(*S*)-*form*

3′,4′,5′,7-Tetra-Me ether: [133342-95-7] *2′,8-Dihydroxy-3′,4′,5′,7-tetramethoxyflavan*
$C_{19}H_{22}O_7$ 362.379
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Oil. $[\alpha]_D^{20}$ -7.3 (c, 0.55 in $CHCl_3$). λ_{max} 226 (log ε 4.18); 286 (log ε 3.66) (MeOH).

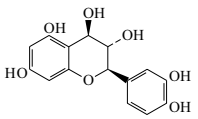
3′,4′,5′,7,8-Penta-Me ether: [133342-92-4] *2′-Hydroxy-3′,4′,5′,7,8-pentamethoxyflavan*
$C_{20}H_{24}O_7$ 376.405
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Oil. $[\alpha]_D^{20}$ -15.4 (c, 0.74 in $CHCl_3$). λ_{max} 227 (log ε 4.2); 284 (log ε 3.8); 289 (sh) (log ε 3.74) (MeOH).

Kaneda, N. *et al., J. Nat. Prod.*, 1991, **54**, 196-

206 (*isol, uv, ir, cd, pmr, cmr, ms*)

3,3′,4,4′,5,7-Hexahydroxyflavan H-197

[480-17-1]
*2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-benzopyran-3,4,5,7-tetrol, 9CI. **Leucocyanidin**. Leucanthocyanidol. Leucocyanidol. Leucocianidol, INN. Pygnoforton. Pyknogenol. Procyanidol*



(*2R,3S,4R)-form*

$C_{15}H_{14}O_7$ 306.271
Stereochem. of naturally occurring isomers has not been fully worked out
λ_{max} 285 (MeOH) (Berdy).

(2ξ,3ξ,4ξ)-*form*

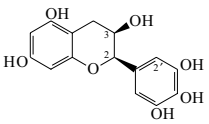
3-O-α-L-Arabinopyranoside: [74046-15-4] ***Loquatoside***
$C_{20}H_{22}O_{11}$ 438.387
Constit. of the fruit of *Eriobotrya japonica* (loquat). Cryst. (EtOAc/petrol). Mp 208°. $[\alpha]_D^{25}$ -22 (EtOH).

[15963-96-9, 17912-82-2, 20408-92-8, 29913-80-2, 29913-81-3, 98856-47-4, 104371-01-9]

Agrawal, S. *et al., Planta Med.*, 1980, **38**, 277 (*Loquatoside*)

3,3′,4′,5,5′,7-Hexahydroxyflavan H-198

[13425-13-3]
3,4-Dihydro-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3,5,7-triol, 9CI



(*2R,3R)-form*

$C_{15}H_{14}O_7$ 306.271

(2*R*,3*R*)-*form* [970-74-1]
*(-)-*cis-*form*. ***Epigallocatechin***. *Epigallocatechol. Antiscurvy factor C_2. Teacatechin II*
Widespread in plants; broad beans are an esp. good source; present in green and black tea. Potential nutriceutical. Cryst. (H_2O). Mp 219-221° dec. $[\alpha]_D$ -60.3 (c, 0.3 in EtOH). Early isolates are often referred to as (-)-Catechin.

► KB5100000

3-O-(3,4,5-Trihydroxybenzoyl): [989-51-5] ***3-O-Galloylepigallocatechin***. *Teatannin II. Epigallocatechin 3-gallate*
$C_{22}H_{18}O_{11}$ 458.378
Present in black tea and green tea (*Thea sinensis*). Cryst. (H_2O). Mp 217° Mp 245-247°. $[\alpha]_D$ -179 (c, 0.3 in EtOH). Log P 1.16 (uncertain value) (calc).

► LD_{50} (mus, orl) 2170 mg/kg. KB5200000

3,3′-Bis(3,4,5-trihydroxybenzoyl): [89013-66-1] ***3,3′-Di-O-galloylepigallocatechin***
$C_{29}H_{22}O_{15}$ 610.484
Isol. from green tea (*Thea sinensis*). Off-white amorph. powder. $[\alpha]_D^{23}$ -28.6 (c, 1.0 in Me_2CO). Obt. as an equilibrated mixt. with the 3,4′-isomer.

3,5-Bis(3,4,5-trihydroxybenzoyl): [37484-73-4] ***3,5-Di-O-galloylepigallocatechin***
$C_{29}H_{22}O_{15}$ 610.484
Isol. from tea (*Thea sinensis*). Powder. $[\alpha]_D^{23}$ -13 (EtOH).

3,4′-Bis(3,4,5-trihydroxybenzoyl): [89013-67-2] ***3,4′-Di-O-galloylepigallocatechin***
$C_{29}H_{22}O_{15}$ 610.484
Isol. from tea (*Thea sinensis*). Off-white amorph. powder. $[\alpha]_D^{23}$ -32.7 (c, 1.0 in Me_2CO). Obt. as equilib. mixt. with the 3,3′-isomer.

3-O-(3,4-Dihydroxy-5-methoxybenzoyl): [83104-87-4] ***3-O-(3-O-Methylgalloyl)epigallocatechin***
$C_{23}H_{20}O_{11}$ 472.404
Isol. from green tea (*Thea sinensis*) and oolong tea (*Camellia sinensis*). Powder. $[\alpha]_D^{14}$ -162 (c, 1 in EtOH).

3-O-(3,5-Dihydroxy-4-methoxybenzoyl):3-O-(4-O-Methylgalloyl)epigallocatechin
$C_{23}H_{20}O_{11}$ 472.404
Constit. of oolong tea (*Camellia sinensis*).

3-O-Cinnamoyl: [108907-46-6] *3-Cinnamoylepigallocatechin*
$C_{24}H_{20}O_8$ 436.417
Isol. from Assam tea (*Camellia sinensis* var. *assamica*). Off-white powder + $1^1/_3H_2O$. $[\alpha]_D^{23}$ -144.1 (c, 1 in Me_2CO).

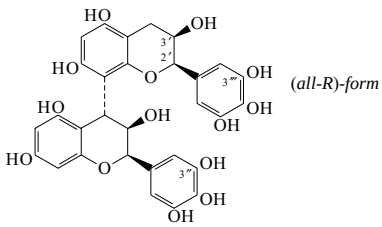
3-O-(4-Hydroxycinnamoyl):3-O-p-Coumaroylepigallocatechin
$C_{24}H_{20}O_9$ 452.417
Isol. from leaves of green tea (*Thea sinensis*). Powder + $1^1/_2H_2O$. $[\alpha]_D^{22}$ -158.3 (c, 0.6 in Me_2CO).

(2*R*,3*S*)-*form* [970-73-0]
*(+)-*trans-*form*. ***Gallocatechin***. *Gallocatechol. Casuarin*
Widespread in plants; found esp. in green tea, redcurrants, gooseberries and marrowfat peas. Potential nutriceutical. Cryst. + $2H_2O$ (H_2O). Sol. H_2O. Mp 189-191°. $[\alpha]_D$ +14.7 (Me_2CO aq.).

(2*S*,3*R*)-*form*
ent-*Gallocatechin*

Mayer, W. *et al., Annalen*, 1960, **630**, 19 (*3-O-, 4-O-Methylgalloyl epigallocatechin*)
Korver, O. *et al., Tetrahedron*, 1971, **27**, 5459 (*cd*)
Coxon, D.T. *et al., Tetrahedron*, 1972, **28**, 2819 (*3,5-digallate*)
Gazave, J.M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1974, **278**, 525
Czochanska, Z. *et al., J.C.S. Perkin 1*, 1980, 2278 (*cmr*)
Saijo, R. *et al., Agric. Biol. Chem.*, 1982, **46**, 1969 (*3-O-methylgallate*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3906 (*3-coumarate, gallates*)
Ayoub, S.M.H. *et al., Planta Med.*, 1984, **50**, 532 (*7-gallates*)
Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1987, **35**, 611 (*Cinnamoylepigallocatechin*)
Sun, D. *et al., Phytochemistry*, 1988, **27**, 579 (*gallates*)
Nakane, H. *et al., Biochemistry*, 1990, **29**, 2841 (*anti-HIV activity*)
Lee, M.W. *et al., Phytochemistry*, 1992, **31**, 2117 (*gallates*)
Fujiki, H. *et al., Prev. Med.*, 1992, **21**, 503 (*gallate, pharmacol, rev*)
Shirai, T. *et al., Chest*, 1994, **106**, 1801 (*tox*)
Davis, A.L. *et al., Magn. Reson. Chem.*, 1996, **34**, 887-890 (*pmr, cmr, gallates*)
de Mello, J.P. *et al., Phytochemistry*, 1996, **41**, 807 (*benzoylepigallocatechins*)
Seto, R. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1434-1439 (*isol, pmr, cmr*)
Miketova, P. *et al., J. Nat. Prod.*, 1998, **61**, 461-467 (*ms*)
Sano, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 1906-1910 (*3-3-Methylgalloylepigallocatechin, 3-4-Methylgalloylepigallocatechin*)

3,3′,4′,5,5′,7-Hexahydroxyflavan-(4→8)-3,3′,4′,5,5′,7-hexahydroxyflavan H-199



(*all-R*)-*form*

$C_{30}H_{26}O_{14}$ 610.527

(*all-R*)-*form* [87392-61-8] ***Prodelphinidin B_2***. *Epigallocatechin(4β→8)epigallocatechin*
Amorph. powder. $[\alpha]_D^{18}$ +35.3 (c, 0.55 in Me_2CO).

3′-O-(4-Hydroxybenzoyl):3′-O-(4-Hydroxybenzoyl)prodelphinidin B_2
$C_{37}H_{30}O_{16}$ 730.634

3′-(3,4,5-Trihydroxybenzoyl): [86588-88-7] ***3′-Galloylprodelphinidin B_2***
$C_{37}H_{30}O_{18}$ 762.633
Isol. from *Thea sinensis* tea and Chinese arbutus *Myrica rubra* bark. Pale brown amorph. powder + $1^1/_2H_2O$. $[\alpha]_D^{20}$ -52.7 (c, 0.62 in Me_2CO). $[\alpha]_D^{18}$ +73.2 (c, 0.93 in MeOH).

3,3′-Bis(3,4,5-trihydroxybenzoyl): [86588-89-8] ***3,3′-Digalloylprodelphinidin B_2***. *Rhodisin*
$C_{44}H_{34}O_{22}$ 914.739
Isol. from *Myrica rubra* (Chinese bayberry). Off-white amorph. powder. $[\alpha]_D^{25}$ -60.9 (c, 0.87 in Me_2CO).

3,3′-Bis(3,4,5-trihydroxybenzoyl), 7-O-gentiotrioside: [125579-38-6] ***Rhodisinoside***
$C_{62}H_{64}O_{37}$ 1401.165

3′′-Deoxy, 3′-O-(3,4,5-trihydroxybenzoyl): [126715-89-7] ***Epicatechin(4β→8)epi-8)epigallocatechin 3-O-gallate***
$C_{37}H_{30}O_{17}$ 746.634
Isol. from commercial oolong tea (*Camellia sinensis* var. *viridis*). Tan amorph. powder + $2H_2O$. $[\alpha]_D^{20}$ -52.6 (c, 0.9 in Me_2CO).

3′′-Deoxy, 3,3′-bis(3,4,5-trihydroxybenzoyl): [126715-90-0] ***Epicatechin 3-O-gallate(4β→8)epigallocatechin-3-O-gallate***
$C_{44}H_{34}O_{21}$ 898.74
Isol. from commercial oolong tea (*Camellia sinensis* var. *viridis*). Tan amorph. powder + $2H_2O$. $[\alpha]_D^{21}$ -55.8 (c, 0.8 in Me_2CO).

*3′′-Deoxy, 4′′′-Me ether:**Epicatechin(4β→8)-4′-O-methylepigallocatechin***
$C_{31}H_{28}O_{13}$ 608.554

Amorph. light brown powder. $[\alpha]_D$ +22.7 (c, 0.72 in MeOH). λ_{max} 220 (log ϵ 4.3); 280 (log ϵ 3.39) (MeOH).

3‴-Deoxy:Epigallocatechin(4β→8)epicatechin
$C_{30}H_{26}O_{13}$ 594.528

3‴-Deoxy, 3′-(3,4,5-trihydroxybenzoyl): ***Epigallocatechin(4β→8)epicatechin 3-O-gallate***
$C_{37}H_{30}O_{17}$ 746.634
Isol. from tea *Thea sinensis*. Off-white amorph. powder + $2H_2O$. $[\alpha]_D^{24}$ -71.8 (c, 1 in Me_2CO).

(2*R*,2′*R*,3*R*,3′*S*,4*R*)-*form* [78362-04-6] ***Prodelphinidin B₁***. *Epigallocatechin(4β→8)gallocatechin*

3-O-(3,4,5-Trihydroxybenzoyl): [152100-01-1] ***3-Galloylprodelphinidin B₁***
$C_{37}H_{30}O_{18}$ 762.633

3,3′-Bis(3,4,5-trihydroxybenzoyl): [87392-65-2] ***3,3′-Digalloylprodelphinidin B₁***
$C_{44}H_{34}O_{22}$ 914.739
Isol. from Chinese arbutus (*Myrica rubra*) bark. Off-white amorph. powder. $[\alpha]_D^{14}$ +26.6 (c, 0.25 in Me_2CO).

3″-Deoxy: ***Epicatechin(4β→8)gallocate-8)gallocatechin***
$C_{30}H_{26}O_{13}$ 594.528
Constit. of *Phyllanthus emblica* (emblic). Tan powder + 3½ H_2O. $[\alpha]_D^{16}$ +17 (c, 0.4 in MeOH).

3‴-Deoxy: [77983-30-3] ***Epigallocatechin(4β→8)catechin***
$C_{30}H_{26}O_{13}$ 594.528
Isol. from *Hordeum vulgare* (barley) grains and *Pinus sylvestris* (Scotch pine). Buff powder + $1H_2O$. $[\alpha]_D$ +22 (c, 0.4 in EtOH).

3‴-Deoxy, undeca-Ac:
Small rosettes (MeOH). Mp 236-240° (softens at 130-140°). $[\alpha]_D$ +96 (c, 0.5 in MeCN).

3‴-Deoxy, 3-O-(3,4,5-trihydroxybenzoyl):
$C_{37}H_{30}O_{17}$ 746.634

(2*R*,2′*R*,3*R*,3′*R*,4*S*)-*form* [86631-36-9] ***Prodelphinidin B₉***. *Epigallocatechin(4α→8)epigallocatechin*
Isol. from beer.

(2*R*,2′*R*,3*S*,3′*R*,4*S*)-*form* [68964-95-4] ***Prodelphinidin B₄***. *Gallocatechin(4α→8)epigallocatechin*
Isol. from leaves of Assam tea (*Camellia sinensis assamica*).

Dodeca-Ac:
Cryst. (MeOH). Mp 154-156°. $[\alpha]_D^{25}$ -77 (c, 0.2 in $CHCl_3$).

3-O-(4-Hydroxybenzoyl):Gallocatechin(4α→8)epigallocatechin 3-O-(4-hydroxybenzoate)
$C_{37}H_{30}O_{16}$ 730.634

3′-O-(3,4,5-Trihydroxybenzoyl): [126786-49-0] ***3′-Galloylprodelphinidin B4***
$C_{37}H_{30}O_{18}$ 762.633
Isol. from commercial oolong tea (*Camellia sinensis* var. *viridis*). Tan amorph. powder + $6H_2O$. $[\alpha]_D^{23}$ -262.2 (c, 1.2 in Me_2CO).

3″-Deoxy: [121958-00-7] ***Catechin(4α→8)epigallocatechin***
$C_{30}H_{26}O_{13}$ 594.528
Isol. from *Camellia sinensis assamica* (Assam tea). Tan powder + 1½H_2O. $[\alpha]_D^{17}$ -168.9 (c, 1 in Me_2CO).

3″-Deoxy, 3′-O-(3,4,5-trihydroxybenzoyl): ***Catechin(4α→8)epigallocatechin 3-O-gallate***
$C_{37}H_{30}O_{17}$ 746.634
Isol. from *Camellia sinensis* var. *viridis* (oolong tea). Tan amorph. powder + $6H_2O$. $[\alpha]_D^{23}$ -236.6 (c, 1 in Me_2CO).

3‴-Deoxy: [79199-56-7] ***Gallocatechin(4α→8)epicatechin***
$C_{30}H_{26}O_{13}$ 594.528
Isol. from *Camellia sinensis assamica* (Assam tea). Tan powder + 1½H_2O. $[\alpha]_D^{17}$ -216.4 (c, 1 in Me_2CO).

(2*R*,2′*R*,3*S*,3′*S*,4*S*)-*form* [110115-59-8] *Gallocatechin(4α→8)gallocatechin.* ***Prodelphinidin B₃***
$[\alpha]_D^{20}$ -146 (c, 0.05 in MeOH aq.).

Dodeca-Ac:
Cryst. (EtOH). Mp 184-186°. $[\alpha]_D^{20}$ -98.9 (c, 1 in Me_2CO).

4″,4‴-Di-Me ether: ***4″,4‴-Di-O-methylprodelphinidin B₃***
$C_{32}H_{30}O_{14}$ 638.581

3″-Deoxy:Catechin(4α→8)gallocatechin
$C_{30}H_{26}O_{13}$ 594.528

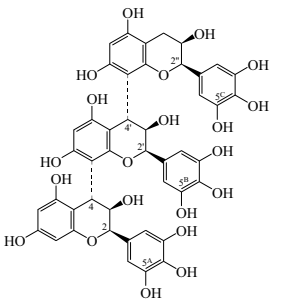
3‴-Deoxy: [78392-25-3] ***Prodelphinidin C***. *Gallocatechin(4α→8)catechin*
$C_{30}H_{26}O_{13}$ 594.528
$[\alpha]_D^{20}$ -247 (c, 0.07 in MeOH aq.).

3‴-Deoxy, undeca-Ac:
Powder. $[\alpha]_D^{20}$ -68.8 (c, 0.61 in $CHCl_3$).

Krishnamurty, V. *et al., Tetrahedron*, 1966, **22**, 2367 (*isol, deriv*)
Gandhi, P. *et al., Experientia*, 1977, **33**, 1272 (*isol, deriv*)
Foo, L.Y. *et al., J.C.S. Perkin 1*, 1978, 1186 (*Prodelphinidin C, Prodelphinidin B₄*)
Gupta, R.K. *et al., J.C.S. Perkin 1*, 1981, 1148 (*isol, 3‴-deoxy*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3906 (*deriv*)
Nonaka, G. *et al., J.C.S. Perkin 1*, 1983, 2139 (*derivs*)
Nonaka, G. *et al., Phytochemistry*, 1983, **22**, 237; 1984, **23**, 1753 (*Prodelphinidin B₂*)
Delcour, K.A. *et al., J. Inst. Brewing*, 1984, **90**, 153 (*Prodelphinidin B₉*)
Sun, D. *et al., Phytochemistry*, 1987, **26**, 1825; 1988, **27**, 579 (*derivs*)
Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 77; 3255 (*derivs, isol, tea*)
Kim, K.H. *et al., Khim. Prir. Soedin.*, 1989, **25**, 723; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 618 (*Rhodisin, Rhodisinoside*)
Danne, A. *et al., Phytochemistry*, 1993, **34**, 1129; 1994, **37**, 533 (*isol*)
Weinges, K. *et al., Phytochemistry*, 1995, **38**, 505 (*Prodelphinidin B₃*)
De Mello, J.P. *et al., Phytochemistry*, 1996, **41**, 807 (*isol*)
Hartisch, C. *et al., Phytochemistry*, 1996, **42**, 191 (*isol, pmr, derivs*)
Hussein, G. *et al., Phytochemistry*, 1999, **50**, 689-694 (*Epicatechin-4′-methylepigallocatechin*)
Palazzo de Mello, J.C. *et al., Phytochemistry*, 1999, **51**, 1105-1107 (*4″,4‴-di-Me ether*)
Zhang, Y.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1507-1510 (*Epicatechin-4β→8-gallocatechin*)

3,3′,4′,5,5′,7-Hexahydroxyflavan(4→8)-3,3′,4′,5,5′,7-hexahydroxyflavan(4→8)-3,3′,4′,5,5′,7-hexahydroxyflavan H-200

[102491-62-3]



(*all-R*)-*form*

$C_{45}H_{38}O_{21}$ 914.783

(2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*R*,4*R*,4′*R*)-*form* *Epigallocatechin(4β→8)epigallocatechin(4β→8)epigallocatechin(4β→8)epigallocatechin*

3,3′,3″-Tris(3,4,5-trihydroxybenzoyl), 7-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Rhodichimoside***
$C_{90}H_{90}O_{53}$ 2019.669
Amorph. pale brown powder. $[\alpha]_D^{22}$ -16 (c, 0.32 in EtOH). λ_{max} 220 ; 245 ; 278 ; 301 (EtOH).

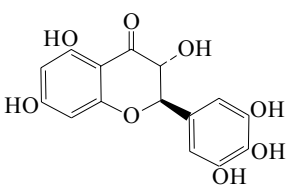
(2*R*,2′*R*,2″*R*,3*S*,3′*S*,3″*R*,4*S*,4′*S*)-*form* [135820-76-7] *Gallocatechin(4α→8)gallocatechin(4α→8)epigallocatechin(4α→8)epigallocatechin*
Pale brown amorph. powder. Sol. H_2O. λ_{max} 205 ; 275 ; 460 (H_2O) (Berdy).

(2*R*,2′*R*,2″*R*,3*S*,3′*S*,3″*S*,4*S*,4′*S*)-*form* [87402-90-2] *Gallocatechin(4α→8)gallocatechin(4α→8)gallocatechin*
Found in barley.

Brandon, M.J. *et al., Phytochemistry*, 1982, **21**, 2953 (*isol*)
Cal, Y. *et al., Phytochemistry*, 1991, **30**, 2033 (*isol*)
Tits, M. *et al., Phytochemistry*, 1992, **31**, 971 (*isol, struct*)
Kuliev, Z.A. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2000, **36**, 60-64 (*Rhodichimoside*)

3,3′,4′,5,5′,7-Hexahydroxyflavanone H-201

*2,3-Dihydro-3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Ampelopsin***† *. Ampeloptin. Dihydromyricetin*



$C_{15}H_{12}O_8$ 320.255

(2*R*,3*R*)-*form* [27200-12-0]
trans-*form*
Isol. from flowers of *Eugenia jambolana* (jambolan). Needles (H_2O). Mp 245-

246°. $[\alpha]_D^{20}$ +41.7. (2*R*,3*R*)-abs. config. assumed in most cases, opt. rotns. not reported.

3-O-*(3,4,5-Trihydroxybenzoyl), 3′-sulfate:* [87388-96-3] ***Myricatin***
$C_{22}H_{16}O_{15}S$ 552.425
Isol. from *Myrica rubra* (Chinese bayberry). Pale yellow needles (H_2O) (as K salt). Mp 235-237° (K salt). $[\alpha]_D^{17}$ +78.2 (c, 0.87 in Me_2CO).

3′-Me ether: [71106-82-6] *3,4′,5,5′,7-Pentahydroxy-3′-methoxyflavanone. 4′,5,5′,7-Tetrahydroxy-3′-methoxydihydroflavonol.* ***Hovenitin I***
$C_{16}H_{14}O_8$ 334.282
Constit. of the seeds and fruit of *Hovenia dulcis* (raisin tree).

(2*R*,3*S*)-*form* [119439-94-0] ***Hovenitin III***
Constit. of the seed and fruit of *Hovenia dulcis* (raisin tree).

3′-Me ether: [188838-86-0] ***Hovenitin II***
$C_{16}H_{14}O_8$ 334.282
Constit. of the seeds and fruit of *Hovenia dulcis* (raisin tree).

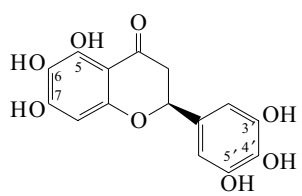
(2*RS*,3*RS*)-*form* [119565-96-7] *(±)*-trans-*form*
Constit. of *Camellia sinensis* (Chinese green tea). Needles (H_2O). Mp 195-198° dec.

[87338-96-3]

Kubota, T. *et al., Nippon Kagaku Kaishi*, 1939, **60**, 604; 607; *CA*, **36**, 4118 (*isol, struct*)
Fujise, S. *et al., Nippon Kagaku Kaishi*, 1961, **82**, 891; *CA*, **57**, 12416 (*synth*)
Harborne, J.B. *et al., Phytochemistry*, 1971, **10**, 2727 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 587 (*occur*)
Rao, M.M. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 178 (*isol, pmr*)
Kho, K.F.F. *et al., Pharm. Weekbl.*, 1979, **114**, 325 (*biosynth*)
Miller, J.M. *et al., Phytochemistry*, 1979, **18**, 1412 (*isol*)
Chauhan, J.J. *et al., Planta Med.*, 1979, **35**, 373 (*deriv*)
Nonaka, G.-I. *et al., Phytochemistry*, 1983, **22**, 237 (*Myricatin*)
Sakushima, A. *et al., Phytochemistry*, 1983, **22**, 1677
Onda, M. *et al., J. Nat. Prod.*, 1989, **52**, 1100 (*synth*)
Li, S. *et al., J. Het. Chem.*, 1990, **27**, 2029 (*synth*)
Shen, C.-C. *et al., Phytochemistry*, 1993, **34**, 843 (*pmr, cmr*)
Yoshikawa, M. *et al., Yakugaku Zasshi*, 1997, **117**, 108-118 (*Hovenitins*)

3′,4′,5,5′,6,7-Hexahydroxyflavanone H-202

*2,3-Dihydro-5,6,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one*



$C_{15}H_{12}O_8$ 320.255

(*S*)-*form*

3′,6-Di-Me ether, 4′,5′-methylene ether: [143381-59-3] *5,7-Dihydroxy-3′,6-dimethoxy-4′,5′-methylenedioxyflavanone.* ***Agamanone***
$C_{18}H_{16}O_8$ 360.32
Isol. from the famine food *Agave americana*. Cryst. ($MeOH/CHCl_3$). Mp 237°.

Parmar, V.S. *et al., Phytochemistry*, 1992, **31**, 2567 (*Agamanone*)

3′,4′,5,6,7,8-Hexahydroxyflavanone H-203

$C_{15}H_{12}O_8$ 320.255

6,7,8-Tri-Me ether: [99759-28-1] *3′,4′,5-Trihydroxy-6,7,8-trimethoxyflavanone*
$C_{18}H_{18}O_8$ 362.335
Yellow needles (MeOH).

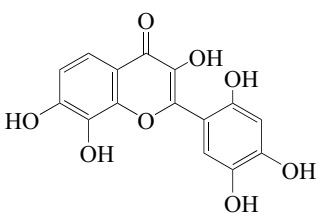
3′,4′,6,7,8-Penta-Me ether:5-Hydroxy-3′,4′,6,7,8-pentamethoxyflavanone. Norcitromitin
$C_{20}H_{22}O_8$ 390.389Was descr. as a nat. prod. from *Citrus mitis* but subsequent work showed that it was prob. identical with the flavone 5-Demethylnobiletin (see 3′,4′,5,6,7,8-Hexahydroxyflavone, H-211).

Hexa-Me ether:3′,4′,5,6,7,8-Hexamethoxyflavanone. Citromitin
$C_{21}H_{24}O_8$ 404.416
Constit. of *Citrus* sp. (Dancy tangerine). Isol. from Xinhui citrus peel. Pale yellow needles (MeOH). Mp 164-165°. Was descr. as a nat. prod. from *C. mitis* but subsequent work showed that this was prob. 3′,4′,5,6,7,8-Hexamethoxyflavone, H-223.

Tatum, J.H. *et al., Phytochemistry*, 1978, **17**, 447
Silva, G.A.B. *et al., J. Nat. Prod.*, 1985, **48**, 861 (*3′,4′,5-Trihydroxy-6,7,8-trimethoxyflavanone*)
Cai, K. *et al., Fenxi Huaxue*, 1997, **25**, 1270-1273; *CA*, **128**, 45899c (*Hexamethoxyflavanone, isol, activity*)
Chen, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 1235-1238 (*Hexamethoxyflavanone*)

2′,3,4′,5′,7,8-Hexahydroxyflavone H-204

*3,7,8-Trihydroxy-2-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 2′,4′,5′,7,8-Pentahydroxyflavonol*



$C_{15}H_{10}O_8$ 318.239
λ_{max} 248 (log ϵ 4.28); 307 (log ϵ 3.93); 347 (log ϵ 3.92) (MeOH).

3,4′,5′,7,8-Penta-Me ether:2′-Hydroxy-3,4′,5′,7,8-pentamethoxyflavone
$C_{20}H_{20}O_8$ 388.373
Constit. of the leaves of the famine food *Parkia clappertoniana*. Yellow cryst. Mp 183.5-184°.

Lemmich, E. *et al., Phytochemistry*, 1996, **42**, 1011-1013 (*isol, uv, ir, pmr, cmr, deriv*)

3,3′,4′,5,5′,7-Hexahydroxyflavone H-205

[529-44-2]
*3,5,7-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,5′,7-Pentahydroxyflavonol.* ***Myricetin****. Cannabiscetin. Myricetol*

$C_{15}H_{10}O_8$ 318.239
Flavanol found in a wide variety of foodstuffs especially in red table wine, bee pollen, bilberries, blueberries, bog whortleberries, broad beans, Chinese bayberry, corn poppy leaves, cranberries, crowberries, blackcurrants, dock leaves, fennel, grapes, parsley, perilla, rutabaga, dill weed and tea (green and black). Glycosides are also widely distributed. Potential nutriceutical showing anti-HIV activity. Light yellow needles (EtOH aq.). Sol. Me_2CO, DMF. Mp 357-360° dec. Log P -0.95 (calc). λ_{max} 252 ; 374 (MeOH) (Berdy). λ_{max} 255 ; 375 (EtOH) (Berdy). λ_{max} 285 ; 437 (MeOH/NaOH) (Berdy).

▶ LK8646000

3-O-*(4*-O-*Acetyl-α-L-rhamnopyranoside):4″*-**O-Acetylmyricitrin***
$C_{23}H_{22}O_{13}$ 506.419
Constit. of the leaves of *Eugenia jambolana* (jambolan). Yellow cryst. Mp 174-176°.

3-O-*(3,4-Di*-O-*acetyl-α-L-rhamnopyranoside):* [184533-13-9]
$C_{25}H_{24}O_{14}$ 548.456
Constit. of *Myrsine africana* (cape myrtle). Greenish-yellow powder. λ_{max} 258 ; 302 ; 352 (MeOH).

3-O-*[3,4,5-Trihydroxybenzoyl-(→2)-4*-O-*acetyl-α-L-rhamnopyranoside]:* ***Eujambin***
$C_{30}H_{26}O_{17}$ 658.525
Constit. of *Eugenia jambolana* (jambolan). Amorph. yellow powder. λ_{max} 222 ; 264 ; 284 ; 300 (sh) ; 351 (MeOH).

7-O-*α-L-Rhamnopyranoside:* [184533-14-0] *Myricetin 7-rhamnoside*
$C_{21}H_{20}O_{12}$ 464.382
Constit. of *Myrsine africana* (cape myrtle). No exptl. data given in ref. (Arot, *et al*, 1996).

3-O-*β-D-Galactopyranoside:* [15648-86-9]
$C_{21}H_{20}O_{13}$ 480.381
Occurs in *Thea sinensis* (tea) and other plants. Dark orange cryst. Mp 198-201°.

3-O-*(6*-O-*Acetyl-β-D-galactopyranoside):-Myricetin 3-(6-acetylgalactoside)*
$C_{23}H_{22}O_{14}$ 522.418
Constit. of the flowers of *Trifolium repens* (white clover). Powder.

3,3′-Di-O-*galactoside:* [28454-81-1]
$C_{27}H_{30}O_{18}$ 642.523
Isol. from *Myrica gale* (bog myrtle).

3′-O-*β-D-Glucopyranoside:* [520-14-9] ***Cannabiscitrin***
$C_{21}H_{20}O_{13}$ 480.381
Occurs in green tea (*Thea sinensis*) and blackcurrant (*Ribes nigrum*). Yellow cryst. Mp 220° (softens at 210°).

7-O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:*
$C_{28}H_{24}O_{17}$ 632.487
Constit. of the pods of *Acacia farnesiana* (sweet acacia). Yellow cryst. Mp 238°.

3-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-galactopyranoside]:* [145544-43-0] *Myricetin 3-robinobioside*
$C_{27}H_{30}O_{17}$ 626.524
Constit. of the roots of *Syzygium cumini* (jambolan).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: Myricetin 3-neohesperidoside*
$C_{27}H_{30}O_{17}$ 626.524
Constit. of the leaves of the famine food *Physalis angulata* (cutleaf ground cherry). Amorph. yellow powder. Mp 174-175°. $[\alpha]_D^{25}$ -79.4 (c, 0.7 in MeOH). λ_{max} 266 (log ϵ 4.23); 299 (sh) (log ϵ 3.8); 356 (log ϵ 4.12) (MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranoside], 7*-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [128701-39-3]
$C_{39}H_{50}O_{26}$ 934.808
Isol. from *Cyamopsis tetragonoloba* (guar).

[6822-41-9, 28454-80-0, 29662-78-0, 36116-88-8, 39049-12-2, 79191-63-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 97D (*ir*)
Perkin, A.G. *et al., J.C.S.*, 1902, **81**, 203-210 (*struct*)
Kalff, J. *et al., J.C.S.*, 1925, **127**, 181-184 (*synth*)
Seshadri, T.R. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1946, **23**, 296-304; *CA*, **40**, 6447 (*struct*)
Kagan, J. *et al., Phytochemistry*, 1967, **6**, 317-318 (*3-galactoside*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1575; 1576 (*occur*)
Gaydou, E.M. *et al., Ann. Chim. (Paris)*, 1977, **2**, 303-308 (*synth, uv, cmr*)
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1978, **14**, 806; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 689 (*galloylglycosides*)
Markham, K.R. *et al., Tetrahedron*, 1978, **34**, 1389 (*cmr*)
Bohm, B.A. *et al., Phytochemistry*, 1979, **18**, 1079-1080 (*galloylglucoside*)
Nair, R.A.G. *et al., Phytochemistry*, 1983, **22**, 318 (*3,3′,5,5′-Tetrahydroxy-4′,7-dimethoxyflavone, glycoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Vaishnava, M.M. *et al., Fitoterapia*, 1992, **63**, 259-260 (*3-robinobioside*)
Hertog, M.G.L. *et al., Food and Cancer Prevention: Chemical and Biological Aspects*, Royal Society of Chemistry, 1993, 198 (*anal*)
Shen, C.-C. *et al., Phytochemistry*, 1993, **34**, 843-845 (*pmr, cmr*)
Arot, L.O.M. *et al., Phytochemistry*, 1996, **43**, 1107-1109 (*7-rhamnoside, 3-diacetylrhamnoside*)
Barakat, H.H. *et al., Phytochemistry*, 1999, **51**, 139-142 (*7-6-galloylglucoside*)
Norbaek, R. *et al., Phytochemistry*, 1999, **51**, 1139-1146 (*3-glucosylrhamnoside 7-glucoside*)
Foo, L.Y. *et al., Phytochemistry*, 2000, **54**, 539-548 (*3-6-acetylgalactoside, 3-galactoside*)
Ismail, N. *et al., Fitoterapia*, 2001, **72**, 676-679 (*3-neohesperidoside*)
Mahmoud, I.I. *et al., Phytochemistry*, 2001, **58**, 1239-1244 (*Eujambin*)
Timbola, A.K. *et al., Fitoterapia*, 2002, **73**, 174-176 (*4′′-O-Acetylmyricitrin*)

3,3′,4′,5,5′,8-Hexahydroxyflavone H-206

[90332-28-8]
*3,5,8-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,5′,8-Pentahydroxyflavonol*

$C_{15}H_{10}O_8$ 318.239
Isol. from *Cassia tora* (charota). Yellow prisms (EtOAc/petrol). Mp 297-300° dec.

Hexa-Ac:
Mp 238-240°.

Chakrabarty, K. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 1165 (*isol, ir*)

3,3′,4′,5,6,7-Hexahydroxyflavone H-207

[90-18-6]
*2-(3,4-Dihydroxyphenyl)-3,5,6,7-tetrahydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,6,7-Pentahydroxyflavonol. **Quercetagetin**. 6-Hydroxyquercetin*

$C_{15}H_{10}O_8$ 318.239
Pale yellow cryst. + $2H_2O$ (EtOH aq.). Sol. EtOH, alkalis; sl. sol. H_2O. Mp 325° (318-320°). Log P -0.88 (calc). λ_{max} 259 (ϵ 16982); 361 (ϵ 21877) (MeOH) (Berdy).

3-O-*β-D-Glucopyranoside:* [60671-81-0] ***Tagetiin***. *Quercetagetin 3-glucoside*
$C_{21}H_{20}O_{13}$ 480.381
Isol. from *Tagetes erecta* (African marigold). Needles + $3H_2O$. Mp 203° dec. (195-198°). $[\alpha]_D^{19}$ -109.6.

7-O-*β-D-Glucopyranoside:* [548-75-4] ***Quercetagitrin***. *Quercetagetin 7-glucoside*
$C_{21}H_{20}O_{13}$ 480.381
Isol. from petals of *Tagetes erecta* (African marigold). Cryst. (Py aq.). Mp 236-238° dec.

3′,7-Di-Me ether, 3-O-*β-D-glucuronopyranoside:*
$C_{23}H_{22}O_{14}$ 522.418
Isol. from spinach.

4′,7-Di-Me ether, 3-O-*β-D-glucuronopyranoside:*
$C_{23}H_{22}O_{14}$ 522.418
Constit. of spinach.

3′,4′,7-Tri-Me ether: [99499-83-9] *3,5,6-Trihydroxy-3′,4′,7-trimethoxyflavone*
$C_{18}H_{16}O_8$ 360.32
Constit. of fingered citron fruits (*Citrus medica*).

3′,4′,7-Tri-Me ether, 3-O-*β-D-glucuronopyranoside:*
$C_{24}H_{24}O_{14}$ 536.445
Constit. of spinach.

Hexa-Me ether: [1251-84-9] *3,3′,4′,5,6,7-Hexamethoxyflavone*. ***Hexamethylquercetagetin***
$C_{21}H_{22}O_8$ 402.4
Isol. from peel of *Citrus* spp.. Cryst. (Me_2CO). Mp 142-143°.

6,7-Methylene, 3-Me ether, 4′-O-*β-D-glucuronopyranoside:*
$C_{23}H_{20}O_{14}$ 520.403
Isol. from spinach (*Spinacia oleracea*). Yellow needles + $4H_2O$ (dioxan aq.). Mp 197-198°. $[\alpha]_D^{22}$ -74.9 (c, 0.14 in dioxan aq.).

6,7-Methylene, 4′-Me ether, 3-O-*β-D-glucuronopyranoside:*
$C_{23}H_{20}O_{14}$ 520.403
Constit. of spinach.

6,7-Methylene, 3,3′-di-Me ether, 4′-O-*β-D-glucuronopyranoside:*
$C_{24}H_{22}O_{14}$ 534.429
Isol. from spinach (*Spinacia oleracea*). Yellow needles + $2H_2O$ (dioxan aq.). Mp 165-168° (softens at 140-145°). $[\alpha]_D^{22}$ -74.5 (c, 0.1 in dioxan aq.).

6,7-Methylene, 3′,4′-di-Me ether, 3-O-*β-D-glucuronopyranoside:*
$C_{24}H_{22}O_{14}$ 534.429
Constit. of spinach.

[100363-98-2]

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Jain, A.C. *et al., J.C.S.*, 1955, 3908 (*synth*)
Morita, N. *et al., Yakugaku Zasshi*, 1957, **77**, 31 (*Tagetiin*)
Farkas, L. *et al., Chem. Ber.*, 1964, **97**, 610 (*isol*)
Harborne, J.B. *et al., Phytochemistry*, 1965, **4**, 647 (*derivs*)
Bate-Smith, E.C. *et al., Phytochemistry*, 1969, **8**, 1035 (*isol*)
Nakayama, M. *et al., Nippon Kagaku Zasshi*, 1970, **91**, 739 (*uv*)
González, A.G. *et al., An. Quim.*, 1971, **67**, 795 (*isol*)
Tarpo, E. *et al., CA*, 1971, **19**, 25 (*isol*)
Hensch, M. *et al., Helv. Chim. Acta*, 1972, **55**, 1610 (*deriv*)
Rodriguez, E. *et al., Phytochemistry*, 1972, **11**, 1507 (*isol*)
Tatum, J.H. *et al., Phytochemistry*, 1972, **11**, 2283 (*Hexamethoxyflavone*)
Ickes, G.R. *et al., J. Pharm. Sci.*, 1973, **62**, 1009 (*isol*)
Nair, A.G.R. *et al., Phytochemistry*, 1975, **14**, 1135 (*isol*)
Herz, W. *et al., Tetrahedron*, 1975, **31**, 1577 (*deriv*)
Oganesyan, E.S. *et al., Khim. Prir. Soedin.*, 1976, **12**, 599; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 537 (*isol*)
Wagner, H. *et al., Tet. Lett.*, 1976, 67 (*synth*)
Wagner, H. *et al., Tetrahedron*, 1977, **33**, 1405 (*derivs, synth*)
Bacon, J.D. *et al., Phytochemistry*, 1978, **17**, 1939 (*isol*)
Kiso, Y. *et al., Heterocycles*, 1982, **19**, 1615 (*isol*)
Aritomi, M. *et al., Phytochemistry*, 1984, **23**, 2043 (*6,7-methylene ether, 4′-glucuronosides*)
He, H. *et al., Yaoxue Xuebao*, 1985, **20**, 433-435 (*3′,4′,7-tri-Me ether, isol*)
Kulkarni, M.M. *et al., Phytochemistry*, 1987, **26**, 2079 (*isol*)
Ahmed, A.A. *et al., Phytochemistry*, 1989, **28**, 665 (*isol*)
Shilin, Y. *et al., Phytochemistry*, 1989, **28**, 1509 (*isol*)
Tominaga, H. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 2668
Edenharder, R. *et al., J. Agric. Food Chem.*, 2001, **49**, 2767-2773 (*Spinacia glucuronides*)

3,3′,4′,5,6,8-Hexahydroxyflavone H-208

*2-(3,4-Dihydroxyphenyl)-3,5,6,8-tetrahydroxy-4*H*-1-benzopyran-4-one. 3′,4′,5,6,8-Pentahydroxyflavonol*

$C_{15}H_{10}O_8$ 318.239

Hexa-Me ether: [218945-14-3] *3,3′,4′,5,6,8-Hexamethoxyflavone*
$C_{21}H_{22}O_8$ 402.4
Constit. of *Citrus reticulata* (mandarin).

Abdel-Alim, M.A. *et al., Egypt. J. Pharm. Sci.*, 1997, **38**, 131-136 (*hexa-Me ether*)

3,3′,4′,5,7,8-Hexahydroxyflavone H-209

[489-35-0]
*2-(3,4-Dihydroxyphenyl)-3,5,7,8-tetrahydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,7,8-Pentahydroxyflavonol.* ***Gossypetin****. Articulatidin. Equisporol*

$C_{15}H_{10}O_8$ 318.239
Yellow needles (EtOH aq.). Mp 310-314° (305°).

*3-*O*-β-D-Glucopyranoside, 8-*O*-β-D-glucuronopyranoside:* [135010-45-6]
$C_{27}H_{28}O_{19}$ 656.507
Isol. from leaves of mallow (*Malva sylvestris*).

*8-*O*-β-D-Glucopyranoside, 3-*O*-sulfate:*
$C_{21}H_{20}O_{16}S$ 560.445
Isol. from apple leaves.

*8-*O*-β-D-Glucuronopyranoside, 3-*O*-sulfate:* [81074-98-8]
$C_{21}H_{18}O_{17}S$ 574.429
Isol. from mallow leaves (*Malva sylvestris*). Mp 239° dec. Incorrect struct. given in CA.

*4′,8-Di-Me ether, 3-*O*-β-D-glucopyranoside:* [90456-57-8]
$C_{23}H_{24}O_{13}$ 508.435
Isol. from *Citrus* spp..

3′,4′,7-Tri-Me ether: [89971-05-1] *3,5,8-Trihydroxy-3′,4′,7-trimethoxyflavone*
$C_{18}H_{16}O_8$ 360.32
Constit. of citron peel (*Citrus medica*). Cryst. (DMF/MeOH). Mp 277-278.5° dec. Struct. recently revised (1993).

3,3′,4′,7-Tetra-Me ether: [7380-44-1] *5,8-Dihydroxy-3,3′,4′,7-tetramethoxyflavone*
$C_{19}H_{18}O_8$ 374.346
Isol. from sweet orange oil.

Hexa-Me ether: [7741-47-1] *3,3′,4′,5,7,8-Hexamethoxyflavone*
$C_{21}H_{22}O_8$ 402.4
Isol. from Valencia orange peel (*Citrus sinensis*) and shepherds purse (*Capsella bursa-pastoris*). Cryst. (MeOH). Mp 170-172°.

7,8-Methylene, 3-Me ether:3′,4′,5-Trihydroxy-3-methoxy-7,8-methylenedioxyflavone. ***Wharangin***
$C_{17}H_{12}O_8$ 344.277
Isol. from spinach (*Spinacia oleracea*). Yellow needles (Me_2CO). Mp 277-278°.

[11084-66-5, 27215-32-3, 28454-90-2, 63109-35-3]

Cambie, R.C. *et al., J.C.S.*, 1960, 2376 (*Wharangin*)
Tatum, J.H. *et al., Phytochemistry*, 1972, **11**, 2283 (*Hexamethoxyflavone*)
Nauwar, M.A.M. *et al., Phytochemistry*, 1977, **16**, 145; 1981, **20**, 2446-2448 (*8-glycoside 3-sulfates*)
Tominaga, H. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 2668 (*3′,4′,7-tri-Me ether*)

3′,4′,5,5′,7,8-Hexahydroxyflavone, 8CI H-210

[89473-44-9]
*5,7,8-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 8-Hydroxytricetin*

$C_{15}H_{10}O_8$ 318.239
Yellow needles +1H_2O (MeOH). Mp 300°.

*5-*O*-β-D-Glucopyranoside:* [150226-16-7]
$C_{21}H_{20}O_{13}$ 480.381
Yellow needles ($CHCl_3$). Mp 325°.

*5-*O*-α-L-Rhamnopyranoside:* [150226-15-6]
$C_{21}H_{20}O_{12}$ 464.382
Pale yellow cryst. Mp 350°.

*7-*O*-β-D-Glucuronoside:* [119262-69-0] *8-Hydroxytricetin 7-glucuronide*
$C_{21}H_{18}O_{14}$ 494.365
Yellow needles (MeOH aq.). Mp 300°.

8-Me ether: [641-87-2] *3′,4′,5,5′,7-Pentahydroxy-8-methoxyflavone.* ***3′,4′,5′-Trihydroxywogonin***
$C_{16}H_{12}O_8$ 332.266
Cryst. (EtOH), brown platelets. Mp 300° Mp 335-340°. This struct. was prev. given to Acrammerin but this appears to be erroneous.

4′,8-Di-Me ether: [64251-86-1] *3′,5,5′,7-Tetrahydroxy-4′,8-dimethoxyflavone*
$C_{17}H_{14}O_8$ 346.293
Yellow needles (EtOH). Mp 254-256°.

3′,4′,8-Tri-Me ether: [164122-10-5] *3′,5,7-Trihydroxy-4′,5′,8-trimethoxyflavone*
$C_{18}H_{16}O_8$ 360.32

4′,5,8-Tri-Me ether: [64251-91-8] *3′,5′,7-Trihydroxy-4′,5,8-trimethoxyflavone*
$C_{18}H_{16}O_8$ 360.32
Yellow cubes (EtOAc). Mp 264-266°.

3′,4′,5′,8-Tetra-Me ether: [32348-78-0] *5,7-Dihydroxy-3′,4′,5′,8-tetramethoxyflavone*
$C_{19}H_{18}O_8$ 374.346
Pale yellow needles (EtOH). Mp 226-227°.

3′,5′,7,8-Tetra-Me ether: [111670-54-3] *4′,5-Dihydroxy-3′,5′,7,8-tetramethoxyflavone*
$C_{19}H_{18}O_8$ 374.346
Isol. from *Lepidium sativum* (garden cress). Cryst. ($CHCl_3$/petrol). Mp 208-210°.

4′,5′,7,8-Tetra-Me ether: [63529-08-8] *3′,5-Dihydroxy-4′,5′,7,8-tetramethoxyflavone*
$C_{19}H_{18}O_8$ 374.346
Yellow cryst. (MeOH). Mp 141-146°.

Hexa-Me ether: [80324-51-2] *3′,4′,5,5′,7,8-Hexamethoxyflavone.* ***Bannamurpanisin***
$C_{21}H_{22}O_8$ 402.4
Mp 196-197°.

Balasubramanian, S.K. *et al., CA*, 1956, **50**, 2558e
Gupta, S.R. *et al., Indian J. Chem.*, 1975, **13**, 785 (*derivs*)
Chhabra, S.C. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 651
Le Quesne, P.W. *et al., J. Nat. Prod.*, 1976, **39**, 391 (*3′,5-Dihydroxy-4′,5′,7,8-tetramethoxyflavone*)
Chhabra, S.C. *et al., Phytochemistry*, 1977, **16**, 1109 (*3′,5,5′,7-Tetrahydroxy-4′,8-dimethoxyflavone, 3′,5′,7-Trihydroxy-4′,5,8-trimethoxyflavone*)
Cavalcante, S. de H. *et al., Acta Amazonica*, 1982, **12**, 377 (*Bannamurpanisin*)
De Silva, L.B. *et al., CA*, 1982, **96**, 31647 (*Bannamurpanisin*)
Horie, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 3773 (*synth, pmr, uv*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv, derivs*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1984, **32**, 551 (*ms, Bannamurpanisin*)
Chandra, S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 82 (*derivs*)
Kawasaki, T. *et al., Phytochemistry*, 1988, **27**, 3709 (*7-Glucuronide*)
Ahmad, M. *et al., J. Chem. Res., Synop.*, 1993, 248 (*5-glycosides*)
Zhang, X. *et al., Yaoxue Xuebao*, 1995, **30**, 211-214 (*3′,4′,8-tri-Me ether*)

3′,4′,5,6,7,8-Hexahydroxyflavone H-211

[2192-25-8]
*2-(3,4-Dihydroxyphenyl)-5,6,7,8-tetrahydroxy-4*H*-1-benzopyran-4-one. Majoranetin. Nornobiletin. 6,8-Dihydroxyluteolin*

$C_{15}H_{10}O_8$ 318.239
Yellow prisms (EtOH). Mp 310-312° dec.

3′-Me ether: [181020-34-8] *4′,5,6,7,8-Pentahydroxy-3′-methoxyflavone. Annagenin*
$C_{16}H_{12}O_8$ 332.266
Aglycone from *Artemisia dracunculus* (tarragon). Bright yellow cryst. (EtOH aq.). Mp 256-258°. λ_{max} 258 ; 271 (sh) ; 376 (EtOH).

*3′-Me ether, 8-*O*-α-L-rhamnopyranoside:* [181020-33-7] ***Estragonoside***
$C_{22}H_{22}O_{12}$ 478.409
Constit. of *Artemisia dracunculus* (tarragon). Yellow cryst. (EtOH). Mp 192-195°. λ_{max} 258 ; 267 (sh) ; 348 (EtOH).

3′,4′-Di-Me ether:5,6,7,8-Tetrahydroxy-3′,4′-dimethoxyflavone
$C_{17}H_{14}O_8$ 346.293
Isol. from Seville orange (*Citrus aurantium*).

6,7,8-Tri-Me ether: [70360-12-2] *3′,4′,5-Trihydroxy-6,7,8-trimethoxyflavone.* ***Sideritiflavone***
$C_{18}H_{16}O_8$ 360.32
Isol. from *Mentha piperita*. Light yellow needles (EtOH). Mp 197-198°. λ_{max} 258 (ε 58894); 279 (ε 66070); 348 (ε 77624) (MeOH) (Berdy).

3′,4′,7,8-Tetra-Me ether: [13509-93-8] *5,6-Dihydroxy-3′,4′,7,8-tetramethoxyflavone.* ***Pebrellin***
$C_{19}H_{18}O_8$ 374.346
Constit. of *Mentha piperita* and *Thymus piperella*.

3′,4′,5,6,8-Penta-Me ether: [149402-88-0] *7-Hydroxy-3′,4′,5,6,8-pentamethoxyflavone*
$C_{20}H_{20}O_8$ 388.373
Constit. of mandarin orange (*Citrus reticulata*). Needles (MeOH). Mp 190-191°.

3′,4′,6,7,8-Penta-Me ether: [2174-59-6] *5-Hydroxy-3′,4′,6,7,8-pentamethoxyflavone.* ***Demethylnobiletin****. 5-Desmethoxynobiletin (incorr.)*
$C_{20}H_{20}O_8$ 388.373
Isol. from *Citrus* spp., *Mentha piperita* and *Thymus* sp.. Mp 145-146°.

3′,5,6,7,8-Penta-Me ether: [34810-62-3] *4′-Hydroxy-3′,5,6,7,8-pentamethoxyflavone*
$C_{20}H_{20}O_8$ 388.373
Constit. of mandarin orange peel (*Citrus reticulata*). Cryst. (MeOH aq.) (also descr. as gum). Mp 147-148°.

4′,5,6,7,8-Penta-Me ether: [112448-39-2] *3′-Hydroxy-4′,5,6,7,8-pentamethoxyflavone*
$C_{20}H_{20}O_8$ 388.373
Constit. of mandarin orange (*Citrus reticulata*). Cryst. (EtOAc/hexane). Mp 139-140°.

Sarin, P.S. *et al., Tetrahedron*, 1960, **8**, 64 (*Demethylnobiletin*)
Wagner, H. *et al., Chem. Ber.*, 1971, **104**, 3357 (*4′-Hydroxy-3′,5,6,7,8-pentamethoxyflavone*)
Tatum, J.H. *et al., Phytochemistry*, 1972, **11**, 2283-2288 (*5-Desmethoxynobiletin*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **23**, 717 (*4′-Hydroxy-3′,5,6,7,8-pentamethoxyflavone*)
Bhardwaj, D.K. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 800 (*Sideritiflavone*)
Jullien, F. *et al., Phytochemistry*, 1984, **23**, 2972-2973 (*Sideritiflavone*)
Silva, G.A.B. *et al., J. Nat. Prod.*, 1985, **48**, 861 (*Sideritiflavone*)
Bohlmann, F. *et al., Phytochemistry*, 1985, **24**, 1027-1030 (*5-Desmethoxynobiletin*)
Barberan, F.A.T. *et al., Planta Med.*, 1985, 452 (*5,6-Dihydroxy-3′,4′,7,8-tetramethoxyflavone*)
Mizuno, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3125 (*3′-Hydroxy-4′,5,6,7,8-pentamethoxyflavone*)
Sugiyama, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 714 (*7-Hydroxy-3′,4′,5,6,8-pentamethoxyflavone*)
Kurkin, V.A. *et al., Khim. Prir. Soedin.*, 1997, **33**, 61-65; *Chem. Nat. Compd. (Engl. Transl.)*, 1997, **33**, 46-49 (*Estragonoside*)

3,4′,5,6,7,8-Hexahydroxyflavone H-212

[4431-48-5]
*3,5,6,7,8-Pentahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 4′,5,6,7,8-Pentahydroxyflavonol.* ***Calycopteretin***

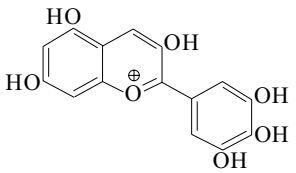
$C_{15}H_{10}O_8$ 318.239
Yellow plates (EtOAc). Mp 318-320° dec.

3,4′,6,7,8-Penta-Me ether: [50439-46-8] *5-Hydroxy-3,4′,6,7,8-pentamethoxyflavone.* ***5-Hydroxyauranetin****. 4′-*O*-Methylcalycopterin*
$C_{20}H_{20}O_8$ 388.373
Constit. of *Citrus aurantium* (Seville orange). Yellow prisms (MeOH or EtOH). Mp 125-127° (120°). λ_{max} 225 (sh) (ϵ 16200); 282 (ϵ 17000); 336 (ϵ 17400) (EtOH) (Derep).

Sarin, P.S. *et al., Tetrahedron*, 1960, **8**, 64 (*5-Hydroxyauranetin*)
Gupta, S.R. *et al., Phytochemistry*, 1973, **12**, 2539 (*5-Hydroxyauranetin*)
Kingston, D.G.I. *et al., J. Nat. Prod.*, 1979, **42**, 496 (*5-Hydroxyauranetin*)
Imre, S. *et al., Planta Med.*, 1984, 360 (*5-Hydroxyauranetin*)
Paula, V.F. *et al., J. Braz. Chem. Soc.*, 2002, **13**, 276-280 (*5-Hydroxyauranetin, pmr, cmr, cryst struct*)

3,3′,4′,5,5′,7-Hexahydroxyflavylium(1+) H-213

[528-53-0]
3,5,7-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-1-benzopyrilium(1+), 9CI. ***Delphinidin****. Delphinidol*



$C_{15}H_{11}O_7^{\oplus}$ 303.248
Widespread anthocyanidin found esp. in blueberries, raspberries and red table wine. Glycosides also widespread. Dark red-brown cryst. (as chloride). Mp 250° (chloride). Forms mono-, di- and trihydrates.

*3-*O*-Arabinoside:* [28500-01-8] *Delphinidin 3-arabinoside*
$C_{20}H_{19}O_{11}^{\oplus}$ 435.363
Isol. from *Vaccinium* spp. and other plant spp..

*3-*O*-α-*L*-Rhamnopyranoside, 5-*O*-β-*D*-glucopyranoside:* [53925-31-8] *Delphinidin 5-glucoside 3-rhamnoside*
$C_{27}H_{31}O_{16}^{\oplus}$ 611.532
Isol. from peas and beans.

*3-*O*-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-*D*-galactopyranoside]:Delphinidin 3-(6-*p*-coumaroylgalactoside)*
$C_{30}H_{27}O_{14}^{\oplus}$ 611.535
Constit. of the leaves of red flower tea, *Camellia sinensis*.

Galactoside: ***Myrtillin B***
Isol. from whortleberries. No MF detd..

*3-*O*-β-*D*-Glucopyranoside:* [6906-38-3] ***Myrtillin****. Delphinidin 3-glucoside. Myrtillin A*
$C_{21}H_{21}O_{12}^{\oplus}$ 465.39
Isol. from grapes and many other plant spp. Present in red wine. Deep purple cryst. (HCl aq.).

*3-*O*-(*O*-Acetyl-β-*D*-glucopyranoside):* [66594-00-1] *Delphinidin 3-(acetylglucoside)*
$C_{23}H_{23}O_{14}^{\oplus}$ 523.426
Isol. from grapes.

*3-*O*-[4-Hydroxycinnamoyl-(→6)-β-*D*-glucopyranoside]:* [51939-70-9] *Delphinidin 3-(6-coumaroylglucoside)*
$C_{30}H_{27}O_{14}^{\oplus}$ 611.535
Isol. from grapes.

*3-*O*-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-*D*-glucopyranoside], 5-*O*-β-*D*-glucopyranoside:* [64615-55-0] ***Awobanin****. Awobannin*
$C_{36}H_{37}O_{19}^{\oplus}$ 773.677
Isol. from grapes. Red needles (as chloride). Dec. >200° (chloride).

*3-*O*-[4-Hydroxycinnamoyl-(→?)-[3,4,5-trihydroxybenzoyl-(→?)]-β-*D*-glucopyranoside]:* [83063-59-6]
$C_{37}H_{31}O_{18}^{\oplus}$ 763.641
Isol. from *Hibiscus sabdariffa* (roselle).

*3,5-Di-*O*-β-*D*-glucopyranoside:* [17670-06-3] ***Delphin****. Hyacin. Delphoside*†*. C.I. Natural blue. Aurobanin A*
$C_{27}H_{31}O_{17}^{\oplus}$ 627.532
Isol. from pomegranate. Cryst. with bronze reflex (as chloride). Mp 202-203° dec. (chloride).

*3,5-Bis-*O*-(6-*O*-malonyl-β-*D*-glucopyranoside):* [104078-09-3] *Delphinidin 3,5-di(6-*O*-malonylglucoside)*
$C_{33}H_{35}O_{23}^{\oplus}$ 799.626
Isol. from chicory (*Chicorium intybus*).

*3-*O*-[β-*D*-Xylopyranosyl-(1→2)-β-*D*-galactopyranoside], 5-*O*-β-*D*-glucopyranoside:Delphinidin 5-glucoside 3-lathyroside*
$C_{32}H_{39}O_{21}^{\oplus}$ 759.648
Isol. from purple pea pods.

*3-*O*-[β-*D*-Xylopyranosyl-(1→2)-β-*D*-galactopyranoside], 5-*O*-[6-*O*-acetyl-β-*D*-glucopyranoside]:Delphinidin 5-(6-acetylglucoside) 3-lathyroside*
$C_{34}H_{41}O_{22}^{\oplus}$ 801.685
Isol. from purple pea pods.

*3-*O*-[β-*D*-Xylopyranosyl-(1→2)-β-*D*-glucopyranoside]:* [53158-73-9] *Delphinidin 3-sambubioside*
$C_{26}H_{29}O_{16}^{\oplus}$ 597.505
Isol. from *Hibiscus sabdariffa* (roselle).

*3-*O*-[β-*D*-Xylopyranosyl-(1→2)-β-*D*-glucopyranoside], 5-*O*-β-*D*-glucopyranoside:* [36415-91-5] *Delphinidin 5-glucoside 3-sambubioside*
$C_{32}H_{39}O_{21}^{\oplus}$ 759.647
Isol. from peas and beans.

*3-*O*-[α-*L*-Rhamnopyranosyl-(1→?)-β-*D*-glucopyranoside], 7-*O*-*D*-xyloside:* [76865-36-6]
$C_{32}H_{39}O_{20}^{\oplus}$ 743.648
Isol. from olives (*Olea europaea*).

*7-*O*-[α-*L*-Rhamnopyranosyl-(1→?)-β-*D*-glucopyranoside], 3-*O*-*D*-xyloside:* [80148-77-2]
$C_{32}H_{39}O_{20}^{\oplus}$ 743.648
Isol. from olives (*Olea europaea*).

*3-*O*-[β-*D*-Glucopyranosyl-(1→2)-β-*D*-glucopyranoside]:* [59212-40-7] *Delphinidin 3-sophoroside*
$C_{27}H_{31}O_{17}^{\oplus}$ 627.532
Isol. from blackcurrant juice.

*3-*O*-[β-*D*-Glucopyranosyl-(1→2)-β-*D*-glucopyranoside], 5-*O*-β-*D*-glucopyranoside:* [36547-37-2] *Delphinidin 5-glucoside 3-sophoroside*
$C_{33}H_{41}O_{22}^{\oplus}$ 789.674
Isol. from peas and beans.

*3-*O*-[β-*D*-Glucopyranosyl-(1→6)-β-*D*-glucopyranoside]:* [55169-25-0] *Delphinidin 3-gentiobioside*
$C_{27}H_{31}O_{17}^{\oplus}$ 627.532
Isol. from *Eugenia jambolana* (jambolan).

*3-*O*-[Glucosyl-(→?)-glucoside]:* ***Nasunin A****. Delphinidin 3-bioside. Eichhornin*
$C_{27}H_{31}O_{17}^{\oplus}$ 627.532
Isol. form *Solanum melongena* (aubergine). Golden needles (MeOH or HCl aq.) (as chloride). Mp 197° dec. (chloride). Almost certainly identical with one of the 3-glycosides of defined struct. but this cannot be detd. from the lit. Also it is not clear whether Nasunin A, Eichhornin and the other samples are identical. Phys. props. refer to Delphinidin 3-bioside.

Glycoside: ***Hibiscin***
$C_{26}H_{29}O_{16}^{\oplus}$ 597.505
Isol. from fruits of *Hibiscus sabdariffa* (roselle). Red-brown needles or prisms (as chloride). Mp 178° (chloride). Hydrol. gives Delphinidin + 1 Glc and 1 pentose.

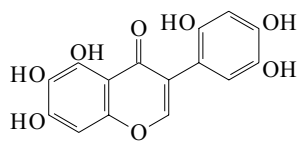
3-O-(6-O-Malonyl-β-D-glucopyranoside), 5-O-β-D-glucopyranoside:
$C_{30}H_{33}O_{20}^{\oplus}$ 713.579
Constit. of the flowers of *Cichorium intybus* (chicory).

[58091-00-2, 126417-61-6, 127254-37-9, 127304-90-9, 127337-94-4, 128508-49-6, 144607-76-1, 144921-63-1]

Pratt, D.D. *et al., J.C.S.*, 1925, **127**, 166 (*isol*)
Bradley, W. *et al., J.C.S.*, 1930, 793 (*synth*)
Reynolds, T.M. *et al., J.C.S.*, 1934, 1235 (*isol*)
Carmack, M. *et al., J.A.C.S.*, 1959, **81**, 4110 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1727; 1730; 1734; 1735; 1737; 1739 (*Delphinidin, Myrtillin B, Hibiscin, Nasunin A, Gentianin, Delphinin*)
Yoshitama, K. *et al., Phytochemistry*, 1977, **16**, 591 (*Delphin*)
Ishikura, N. *et al., Bot. Mag.*, 1978, **91**, 25
Karawya, M.S. *et al., Fitoterapia*, 1981, **52**, 175 (*coumaroylgalloylglucoside, sambubioside*)
Hoshino, T. *et al., Tet. Lett.*, 1981, **22**, 3621 (*cd, conformn*)
Iacobucci, G.A. *et al., Tetrahedron*, 1983, **39**, 3005 (*rev*)
Hosino, T. *et al., Phytochemistry*, 1986, **25**, 829 (*cd*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Brandt, K. *et al., Phytochemistry*, 1993, **33**, 209 (*derivs*)
Markham, K.R. *et al., Phytochemistry*, 1993, **34**, 679 (*derivs*)
Merlin, J.-C. *et al., Phytochemistry*, 1994, **35**, 227 (*Raman*)
Hosokawa, K. *et al., Phytochemistry*, 1995, **38**, 1293 (*derivs, uv, pmr, cmr*)

2′,4′,5,5′,6,7-Hexahydroxyisoflavone H-214

5,6,7-Trihydroxy-3-(2,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one, 9CI



$C_{15}H_{10}O_8$ 318.239

2′,4′,5′,6-Tetra-Me ether: [4935-92-6] *5,7-Dihydroxy-2′,4′,5′,6-tetramethoxyisoflavone. 5,7-Dihydroxy-6-methoxy-3-(2,4,5-trimethoxyphenyl)-4H-1-benzopyran-4-one, 9CI.* ***Caviunin***
$C_{19}H_{18}O_8$ 374.346
Needles (EtOH). Mp 191-193°.

2′,4′,5′,6-Tetra-Me ether, 7-O-glucopyranoside: [50299-68-8]
$C_{25}H_{28}O_{13}$ 536.488
Fibrous cryst. (EtOH). Mp 236-237°.

2′,4′,5′,6-Tetra-Me ether, 7-O-(rhamnosylglucoside): [75883-12-4]
$C_{31}H_{38}O_{17}$ 682.631
Dihydrate. Mp 138-139°.

2′,4′,5′,6-Tetra-Me ether, 7-O-gentiobioside: [72578-98-4]
$C_{31}H_{38}O_{18}$ 698.63
Mp 210-212°.

2′,6-Di-Me, 4′,5′-methylene ether:5,7-Dihydroxy-2′,6-dimethoxy-4′,5-methylenedioxyisoflavone. ***Dalpalatin***
$C_{18}H_{14}O_8$ 358.304
Cryst. (C_6H_6/$CHCl_3$). Mp 228-230°.

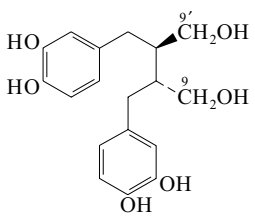
4′,5′-Methylene, 2′,5,6-tri-Me ether: [158591-68-5] *7-Hydroxy-2′,5,6-trimethoxy-4′,5′-methylenedioxyisoflavone*
$C_{19}H_{16}O_8$ 372.331
Needles. Mp 177°.

4′,5′-Methylene, 2′,5,6-tri-Me ether, 7-O-(2-O-p-coumaroyl-β-D-glucopyranoside): [158591-66-3]
$C_{34}H_{32}O_{15}$ 680.618
Constit. of the seeds of *Trichosanthes anguina* (snake gourd). Brown needles (MeOH). Mp 165°.

Farkas, L. *et al., Chem. Ber.*, 1961, **94**, 2501 (*synth*)
Gottlieb, O.R. *et al., J.O.C.*, 1961, **26**, 2449 (*isol*)
Dyke, S.F. *et al., J.O.C.*, 1961, **26**, 2453 (*synth*)
Várady, J. *et al., Tet. Lett.*, 1965, 4273 (*synth*)
Gottlieb, H.E. *et al., Phytochemistry*, 1977, **16**, 1811 (*cmr*)
Radhakrishniah, M. *et al., J. Indian Chem. Soc.*, 1979, **46**, 81 (*glucoside*)
Sharma, A. *et al., Phytochemistry*, 1979, **18**, 1253 (*gentiobioside*)
Rajulu, K.G. *et al., Phytochemistry*, 1980, **19**, 1563 (*rhamnosylglucoside*)
Rao, J.R. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 78 (*Dalpalitin*)
Yadava, R.N. *et al., Phytochemistry*, 1994, **36**, 1519 (*deriv*)

3,3′,4,4′,9,9′-Hexahydroxylignan H-215

2,3-Bis(3,4-dihydroxybenzyl)-1,4-butanediol



(8*R*,8′*R*)-form

$C_{18}H_{22}O_6$ 334.368

(8R,8′R)-form

3,4:3′,4′-Bis(methylene) ether: [24563-03-9] *2,3-Bis(1,3-benzodioxol-5-ylmethyl)-1,4-butanediol, 9CI.* ***Dihydrocubebin***
$C_{20}H_{22}O_6$ 358.39
Isol. from *Piper cubeba* (cubeb pepper). Cryst. Mp 112°. $[\alpha]_D$ -42.

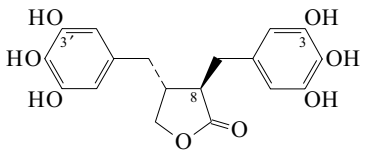
3,4:3′,4′-Bis(methylene) ether, 9-Ac: [112448-60-9] ***Hemiariensin***
$C_{22}H_{24}O_7$ 400.427
Constit. of *Piper cubeba* (cubeb pepper). Viscous gum. λ_{max} 232 (log ϵ 4.42); 286 (log ϵ 4.39) (MeOH).

[40516-27-6]

Dwuma-Badu, D. *et al., J. Nat. Prod.*, 1975, **38**, 343 (*Dihydrocubebin*)
Anjaneyulu, A.S.R. *et al., Tet. Lett.*, 1975, 2961 (*Dihydrocubebin*)
Mahalanabis, K.K. *et al., Tet. Lett.*, 1982, **23**, 3975 (*synth*)
Badheka, L.P. *et al., Phytochemistry*, 1987, **26**, 2033 (*Hemiariensin*)
Brown, E. *et al., Tetrahedron*, 1989, **45**, 141 (*synth*)

3,3′,4,4′,5,5′-Hexahydroxylignan-9,9′-olide H-216

4,5-Dihydro-3,4-bis(3,4,5-trihydroxybenzyl)-2(3H)-furanone



$C_{18}H_{18}O_8$ 362.335
Lignan numbering shown.

(8R,8′R)-form

3′,4′-Methylene, 3,4,5,5′-tetra-Me ether: [94359-20-3] ***5-Methoxyyatein***
$C_{23}H_{26}O_8$ 430.454
Amorph. powder. $[\alpha]_D$ -21 (c, 1 in $CHCl_3$).

4,5-Methylene, 3,3′,4′,5′-tetra-Me ether: [101751-71-7] ***Cubebinone***
$C_{23}H_{26}O_8$ 430.454
Constit. of *Piper cubeba* (cubeb pepper). Cryst. Mp 108-110°. $[\alpha]_D^{25}$ -36.1 (c, 0.083 in $CHCl_3$).

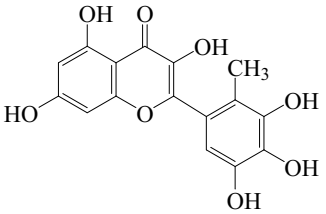
3,3′,4′,5,5′-Penta-Me ether: [112667-54-6] ***Hernolactone***
$C_{23}H_{28}O_8$ 432.469
Pale yellow solid. $[\alpha]_D$ -30 (c, 0.36 in $CHCl_3$). λ_{max} 225 (ϵ 15490); 272 (ϵ 1950) (EtOH) (Berdy).

Hexa-Me ether: [93395-16-5] *3,3′,4,4′,5,5′-Hexamethoxylignan-9,9′-olide.* ***Cubebininolide****. Cordigerin*
$C_{24}H_{30}O_8$ 446.496
Constit. of *Piper cubeba* (cubeb pepper). $[\alpha]_D$ -42.4 (MeOH).

Richomme, P. *et al., J. Nat. Prod.*, 1984, **47**, 879-881 (*Cordigerin*)
Koul, S.K. *et al., Phytochemistry*, 1984, **23**, 2099-2101 (*Cubebininolide*)
Richomme, P. *et al., Heterocycles*, 1985, **23**, 309 (*5-Methoxyyatein*)
Badheka, L.P. *et al., Phytochemistry*, 1986, **25**, 487 (*isol, struct, Cubebinone*)
Tanoguchi, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4162; 1989, **37**, 68; 1991, **39**, 1873 (*isol, struct, cd, synth, Hernolactone*)
Lalami, K. *et al., Heterocycles*, 1988, **27**, 1131 (*synth, Cubebinone*)

3,3′,4′,5,5′,7-Hexahydroxy-2′-methylflavone H-217

2′-C-Methylmyricetin

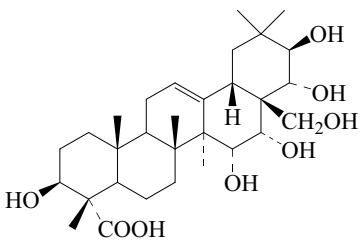


$C_{16}H_{12}O_8$ 332.266

5′-O-(3,4,5-Trihydroxybenzoyl), 3-O-α-L-rhamnopyranoside: [244137-68-6]
$C_{29}H_{26}O_{16}$ 630.515
Constit. of *Syzygium samarangense* (Java apple) leaves. Yellow needles. Mp 192° dec. $[\alpha]_D^{30}$ -126 (MeOH). λ_{max} 264 ; 300 (sh) (MeOH).

Nair, A.G.R. *et al., Fitoterapia*, 1999, **70**, 148-151 (*isol, uv, pmr, cmr*)

3,15,16,21,22,28-Hexahydroxy-12-oleanen-23-oic acid H-218



$C_{30}H_{48}O_8$ 536.704

(3β,15α,16α,21β,22α)-*form*

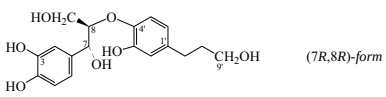
21,22-Diangeloyl, 3-O-[α-L-arabinopyranosyl-(1→3)-6-O-methyl-β-D-glucuronopyranoside], 23-Me ester: [288153-01-5] ***TR-saponin A***
$C_{53}H_{80}O_{20}$ 1037.203
Constit. of *Camellia sinensis* var. *assamica* (Assam tea).

21-Angeloyl, 22-(2-methylbutanoyl), 3-O-[α-L-arabinopyranosyl-(1→3)-6-O-methyl-β-D-glucuronopyranoside], 23-Me ester: [288153-02-6] ***TR-saponin B***
$C_{53}H_{82}O_{20}$ 1039.219
Constit. of *Camellia sinensis* var. *assamica* (Assam tea).

21-Angeloyl, 22-(2-methylbutanoyl), 16-Ac, 3-O-[α-L-arabinopyranosyl-(1→3)-6-O-methyl-β-D-glucuronopyranoside], 23-Me ester: [288153-03-7] ***TR-saponin C***
$C_{55}H_{84}O_{21}$ 1081.256
Constit. of *Camellia sinensis* var. *assamica* (Assam tea).

Lu, Y. *et al., Phytochemistry*, 2000, **53**, 941-946 (*isol, pmr, cmr*)

3,3′,4,7,9,9′-Hexahydroxy-8,4′-oxyneolignan H-219



(7*R*,8*R*)-*form*

$C_{18}H_{22}O_7$ 350.368
Lignan numbering shown.

(7*R,8*R**)-*form***

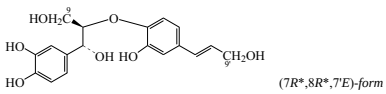
3-Me ether: [62137-27-3]
Constit. of *Pinus sylvestris* (Scotch pine). $[\alpha]_D^{20}$ +35.4 (c, 0.7 in EtOH).

3-Me ether, 4-O-β-D-xylopyranoside: [62223-56-7]
$C_{24}H_{32}O_{11}$ 496.51
Constit. of *Pinus sylvestris* (Scotch pine). Amorph. Obt. as a mixt. of *erythro*- and *threo*-isomers.

[57701-87-8, 62137-27-3, 112295-60-0, 126253-43-8, 171261-40-8]

Popoff, T. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 329
Higuchi, R. *et al., Phytochemistry*, 1977, **16**, 1587
Lundgren, L.N. *et al., Acta Chem. Scand., Ser. B*, 1985, **39**, 241
Fang, J.-M. *et al., Phytochemistry*, 1992, **31**, 3659
Pan, H. *et al., Phytochemistry*, 1995, **39**, 1423 (*isol, derivs*)
Seca, A.M.L. *et al., Phytochemistry*, 2001, **56**, 759-767

3,3′,4,7,9,9′-Hexahydroxy-8,4′-oxyneolign-7′-ene H-220



(7*R**,8*R**,7′E)-*form*

$C_{18}H_{20}O_7$ 348.352

(7*R*,8*R*,7′*E*)-*form*
trans-erythro-*form*

9,9′-Bis-O-(4-hydroxy-E-cinnamoyl): ***Dadahol B***
$C_{38}H_{36}O_{11}$ 668.696
Oil. Isol. as a mixt. of *erythro*- and *threo*- stereoisomers, to which uv spectrum refers λ_{max} 210 (log ε 4.11); 224 (log ε 3.96); 311 (log ε 3.98) (MeOH).

3,3′-Di-Me ether: [1103-58-8]

[181514-29-4, 181514-30-7] *Guaiacylglycerol β-coniferyl ether*
$C_{20}H_{24}O_7$ 376.405
Syrup. $[\alpha]_D^{22}$ -6.7 (c, 0.53 in MeOH). The *B. javanica* isolate was assigned an isomeric struct. in 1996 and then reassigned as this compd..

3,3′-Di-Me ether, 4-O-β-D-glucopyranoside: [157446-63-4] ***Alaschanioside A***
$C_{26}H_{34}O_{12}$ 538.547
Amorph. powder. $[\alpha]_D^{23}$ -10.8 (c, 0.4 in MeOH).

3,3′-Di-Me ether, 9,9′-di-Ac: [210161-55-0]
$C_{24}H_{28}O_9$ 460.48
Oil. $[\alpha]_D^{25}$ +8.8 (c, 0.63 in CH_2Cl_2). λ_{max} 268 (log ε 4.49); 300 (log ε 4.2) (no solvent reported).

5-Methoxy, 3,3′-di-Me ether, 4-O-β-D-glucopyranoside: [175556-09-9] ***Longifloroside B***
$C_{27}H_{36}O_{13}$ 568.574
Amorph. powder. $[\alpha]_D^{14}$ +16.5 (c, 0.4 in MeOH).

5′-Methoxy, 3,3′-di-Me ether, 9,9′-bis-O-(4-hydroxy-E-cinnamoyl): ***Dadahol A***
$C_{39}H_{38}O_{12}$ 698.722
Oil. $[\alpha]_D^{20}$ +20 (c, 0.07 in MeOH). λ_{max} 205 (log ε 4.02); 224 (log ε 3.98); 289 (log ε 3.78); 311 (log ε 3.81) (MeOH).

9′-Carboxylic acid, 3,3′-di-Me ether, 4-O-β-D-glucopyranoside: ***Glehlinoside C***
$C_{26}H_{32}O_{13}$ 552.531
Off-white amorph. solid. $[\alpha]_D^{25}$ -34.3 (c, 0.09 in MeOH). Possesses *erythro*-config. λ_{max} 230 ; 275 (MeOH).

(7*R*,8*R*,7′*Z*)-*form*

3-Me ether, 9′-O-β-D-glucopyranoside: ***Semitortoside B***
$C_{25}H_{32}O_{12}$ 524.521

(7*R*,8*S*,7′*E*)-*form* trans-threo-*form*

9-O-(4-Hydroxy-3-methoxy-E-cinnamoyl), 9′-O-(4-hydroxy-E-cinnamoyl): ***Carolignan K***
$C_{39}H_{38}O_{12}$ 698.722
Yellowish oil.

3,3′-Di-Me ether, 4-O-β-D-glucopyranoside: [105279-09-2] ***Citrusin A***
$C_{26}H_{34}O_{12}$ 538.547
Isol. from lemon (*Citrus limon*) and round kumquat (*Fortunella japonica*) peels. Mp 108-109°. $[\alpha]_D^{20}$ -17.2 (c, 0.3 in MeOH).

3,3′-Di-Me ether, 9,9′-di-Ac: [210161-56-1]
$C_{24}H_{28}O_7$ 428.481
Oil. $[\alpha]_D^{25}$ -15.6 (c, 0.85 in CH_2Cl_2). λ_{max} 268 (log ε 4.16); 300 (log ε 3.86) (MeOH).

3,3′-Di-Me ether, 9,9′-bis-O-(4-hydroxy-E-cinnamoyl):
$C_{38}H_{36}O_{11}$ 668.696

5,5′-Dimethoxy, 3,3′-di-Me ether, 4-O-β-D-glucopyranoside: [169312-06-5] ***Picraquassioside C***
$C_{28}H_{38}O_{14}$ 598.6
Amorph. powder. $[\alpha]_D^{20}$ -9.7 (c, 1 in MeOH).

(7*R*,8*S*,7′*Z*)-*form* cis-threo-*form*

3-Me ether, 9′-O-β-D-glucopyranoside: [190520-35-5] ***Semitortoside A***
$C_{25}H_{32}O_{12}$ 524.521

(7ξ,8ξ,7′*E*)-*form*

3,3′-Di-Me ether, 9′-O-β-D-glucopyranoside: [214778-46-8]

[249292-62-4] ***Hyuganoside III***. *Terebinthacoside III*
$C_{26}H_{34}O_{12}$ 538.547

5′-Methoxy, 3,3′-di-Me ether, 4-O-β-D-glucopyranoside: [105279-10-5] ***Citrusin B***
$C_{27}H_{36}O_{13}$ 568.574
Isol. from lemon (*Citrus limon*) and the round kumquat (*Fortunella japonica*). Mp 105-106°. $[\alpha]_D^{20}$ -11.3 (c, 0.3 in MeOH).

Freudenberg, K. *et al., Chem. Ber.*, 1955, **88**, 617; 626 (*synth, uv, ir*)
Nimz, H. *et al., Chem. Ber.*, 1965, **98**, 533 (*isol*)

Miki, K. *et al., Phytochemistry*, 1980, **19**, 449 (*isol, pmr*)
Sawabe, A. *et al., Nippon Kagaku Kaishi*, 1986, **60**, 593 (*Citrusins*)
Deyama, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1803-1807 (*Citrsuin B*)
Matsubara, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 647 (*Citrusin A*)
Della Greca, M. *et al., Phytochemistry*, 1994, **35**, 777-779 (*isol*)
Gao, J. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 466-468 (*Alaschanioside A*)
Yoshikawa, K. *et al., Phytochemistry*, 1995, **40**, 253 (*Picraquassioside C*)
Gellerstedt, G. *et al., Phytochemistry*, 1995, **40**, 263-265 (*Arum italicum isolate*)
Wang, C.Z. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 150-153 (*Semitortosides*)
Wang, C.-Z. *et al., Planta Med.*, 1997, **63**, 241-244 (*Longifloroside B*)
Matsuda, H. *et al., Bioorg. Med. Chem. Lett.*, 1998, **8**, 2191-2196 (*Hyuganoside III*)
Valcic, S. *et al., J. Nat. Prod.*, 1998, **61**, 771-775 (*9,9′-di-Ac*)
Li, S. *et al., Phytochemistry*, 1998, **49**, 2125-2128 (*synth, pmr, cmr*)
Seca, A.M.L. *et al., Phytochemistry*, 2001, **56**, 759-767 (*Carolignan K*)
Su, B.-N. *et al., J. Nat. Prod.*, 2002, **65**, 163-169 (*Dadahols*)

Hexakis(cyano-*C*)ferrate(4-), 11CI H-221

[13408-63-4]
*Hexacyanoferrate(*II*)(4-). Ferrocyanide*
$[Fe(CN)_6]^{4\ominus}$ (O_h)
$C_6FeN_6^{\ominus}$ 211.953
Alkali and alkaline earth (except Ba) salts sol. H_2O; insol. EtOH. Low spin Fe^{II} but crosses over to high spin at 2×10^5 atm. pressure.

Tetra-Na salt: [13601-19-9] *Sodium ferrocyanide. E535*
$C_6FeN_6Na_4$ 303.912Becomes anhyd. at 81°.

Tetra-Na salt, decahydrate: [14434-22-1]

[59299-99-9] *Yellow prussiate of soda*
Acidity regulator, anticaking agent for salt. Pale yellow monoclinic cryst. V. sol. H_2O. Mp 82° (anhyd.). Sl. efflorescent. Dehydrates above 50° and becomes anhyd. at 81.5°; dec. at 435°.

Tetra-K salt: [13943-58-3] *Potassium ferrocyanide. E536*
$C_6FeK_4N_6$ 368.346
Acidity regulator.
► LJ8219000

Di-Ca salt:Calcium ferrocyanide. E538
Acidity regulator.

[25869-98-1, 38670-32-5]

Shriver, D.F. *et al., Inorg. Chem.*, 1965, **4**, 725 (*synth, ir, uv*)
Shriver, D.F. *et al., Struct. Bonding (Berlin)*, 1966, **1**, 32 (*rev, bibl*)
Tullberg, A. *et al., Acta Chem. Scand., Ser. A*, 1974, **28**, 551-562 (*tetra-Na salt, cryst struct*)
Sharpe, A.G. *et al., The Chemistry of Cyano Complexes of the Transition Metals*, Academic Press, 1976, 103
Compr. Coord. Chem., Pergamon, 1987, **4**, 1204 (*rev, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2978 (*tetra-Na decahydrate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANH875; IGY000; PLH100; TEC500

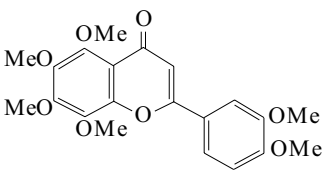
Hexakis(2-methyl-2-phenylpropyl)distannoxane, 9CI H-222

[13356-08-6]
Fenbutatin oxide, BSI. Bis[tris(2-methyl-2-phenylpropyl)tin] oxide. Hexaneophyldistannoxane. Bis(trineophyltin) oxide. Vendex. Torque
$(Me_2CPhCH_2)_3Sn{-}O{-}Sn(CH_2CPhMe_2)_3$
$C_{60}H_{78}OSn_2$ 1052.696
Miticide for use on fruit and vegetable crops. Cryst. powder. Sol. $CHCl_3$, C_6H_6, sl. sol. Me_2CO, insol. H_2O.
► JN8770000

U.S. Pat., 1970, 3 657 451; *CA*, **76**, 69178a
Pesticide Manual, 11th edn., 1997, No. 303
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BLU000

3′,4′,5,6,7,8-Hexamethoxyflavone H-223

[478-01-3]
*2-(3,4-Dimethoxyphenyl)-5,6,7,8-tetramethoxy-4*H*-1-benzopyran-4-one, 9CI. **Nobiletin***

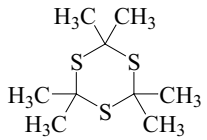


$C_{21}H_{22}O_8$ 402.4
Isol. from peel of king orange (*Citrus nobilis*), Seville orange (*Citrus aurantium*) and other *Citrus* spp., and the round kumquat (*Fortunella japonica*). Pale yellow cryst. (MeOH). Mp 134°.

Robinson, R. *et al., J.C.S.*, 1938, 1004 (*isol, struct*)
Schneider, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1968, **301**, 785 (*isol*)
Talapatra, S.K. *et al., Phytochemistry*, 1975, **14**, 309 (*isol*)
Yinon, J. *et al., Org. Mass Spectrom.*, 1978, **13**, 167 (*ms*)
Tatum, J.H. *et al., Phytochemistry*, 1978, **17**, 447 (*isol*)
Ngo, Le-Van, *et al., Phytochemistry*, 1979, **18**, 1859 (*isol*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 708 (*cmr*)
Herz, W. *et al., Phytochemistry*, 1982, **21**, 2363 (*isol*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1984, **32**, 551 (*ms*)
Chen, W.M. *et al., Indian J. Heterocycl. Chem.*, 1997, **6**, 221-222 (*synth*)

2,2,4,4,6,6-Hexamethyl-1,3,5-trithiane H-224

[828-26-2]
Trithioacetone. FEMA 3475



$C_9H_{18}S_3$ 222.439
Flavouring ingredient. Mp 21.8°. Bp_{10} 105-107°. n_D^{24} 1.5400.

1,1-Dioxide: [18784-16-2]
$C_9H_{18}O_2S_3$ 254.438
Mp 102°.

1,1,3,3-Tetraoxide: [18798-11-3]
$C_9H_{18}O_4S_3$ 286.437
Mp 209°.

1,1,3,3,5,5-Hexaoxide: [18784-17-3]
$C_9H_{18}O_6S_3$ 318.436
Mp 316°.

Douglass, I.B. *et al., J.O.C.*, 1950, **15**, 795-799 (*synth*)
Ettinghausen, O.G. *et al., Polymer*, 1966, **7**, 469-474 (*purifn, ms, pmr*)
Burnop, V.C.E. *et al., Polymer*, 1967, **8**, 589-607 (*oxides*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1744 (*use*)

Hexanal, 9CI, 8CI H-225

[66-25-1]
Caproaldehyde. Caproic aldehyde. Aldehyde C6. FEMA 2557
$H_3C(CH_2)_4CHO$
$C_6H_{12}O$ 100.16
Constit. of many foodstuffs. A prod. of aerobic enzymatic transformations of plant constits. Used in fruit flavours and in perfumery. Liq. with green, unripe-fruit odour. Bp 131° Bp_{12} 28°. n_D^{20} 1.4039. Autoxidises rapidly.
► Skin and eye irritant. LD_{50} (rat, orl) 4890 mg/kg. MN7175000

Oxime: [6033-61-0]
$C_6H_{13}NO$ 115.175
Mp 51°.

2,4-Dinitrophenylhydrazone: [1527-97-5]
Orange-yellow needles (EtOH). Mp 104°.

Semicarbazone: [6033-78-9]
Mp 106° Mp 115°.

Di-Ac: [64847-81-0]
$C_{10}H_{18}O_4$ 202.25
Bp_{10} 115-117°.

Di-Me acetal: [1599-47-9] *1,1-Dimethoxyhexane*
$C_8H_{18}O_2$ 146.229
Bp 158° Bp_{12} 52-53°.

Di-Et acetal: [3658-93-3] *1,1-Diethoxyhexane*
$C_{10}H_{22}O_2$ 174.283
Bp 155-158° Bp_{30} 90°.

Me enol ether: [37617-02-0] *1-Methoxy-1-hexene*
$C_7H_{14}O$ 114.187
Bp_{27} 48-50°.

[78227-51-7, 78227-52-8]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 359C (*pmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 468A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 554A (*ir*)
Drawert, F. *et al., Annalen*, 1966, **694**, 200 (*occur*)
Liedtke, R.J. *et al., J.A.C.S.*, 1969, **91**, 6814 (*ms*)
Org. Synth., 1971, **51**, 11; 39 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 111 (*rev, tox*)
Sosnina, I.E. *et al., CA*, 1977, **87**, 133810g (*synth*)
Cole, T.E. *et al., Tet. Lett.*, 1977, 781 (*synth*)
Callot, H.J. *et al., Bull. Soc. Chim. Fr.*, 1983, 317 (*Me enol ether*)
Newcomb, M. *et al., J.A.C.S.*, 1986, **108**, 240 (*Me enol ether*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HEM000
Fleming, I. *et al., J.C.S. Perkin 1*, 1998, 2687-2700 (*deriv, synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Hexane, 9CI H-226

[110-54-3]

$H_3C(CH_2)_4CH_3$

C_6H_{14} 86.177

Extraction solvent used in food production. Present in volatile fractions of various plant spp. e.g. apples, orange juice, guava fruit, roasted filberts, porcini (*Boletus edulis*), shiitake (*Lentinus edodes*), heated sweet potato and sage. Also present in scallops. Liq. d_4^{25} 0.66. Fp -93.5. Bp 68.95°. n_D^{25} 1.3723.

▶ Highly flammable, fl. p. -23°, autoignition temp. 223°. Eye irritant. Symptoms of acute exposure incl. headache, drowsiness, dizziness and unconsciousness. Chronic exposure (and abuse) associated with development of peripheral neuropathies. OES: long-term 20 ppm. MN9275000

[21666-38-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 2B (*ir*)
Michael, A. *et al., Am. Chem. J.*, 1901, **25**, 421
Albright, M.J. *et al., J. Organomet. Chem.*, 1977, **125**, 1-8 (*cmr*)
Sato, F. *et al., J. Organomet. Chem.*, 1977, **142**, 71-79 (*synth*)
Gussoni, M. *et al., J. Mol. Struct.*, 1980, **61**, 355-359 (*ir*)
Mikaya, A.I. *et al., Org. Mass Spectrom.*, 1984, **19**, 428-432 (*ms*)
Riddick, J.A. *et al., Tech. Chem. (N.Y.)*, 4th edn., Wiley-Interscience, 1986, **2**, 92; 824 (*props, purifn*)
Battershill, J.M. *et al., HSE Toxicity Review 18: n-Hexane*, HMSO, London, 1987, (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HEN000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1103
Boese, R. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 988-992 (*cryst struct*)
Graham, D.G. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 327 (*rev, tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 670
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HEN000

Hexanedioic acid, 9CI H-227

[124-04-9]

Adipic acid. Butane-1,4-dicarboxylic acid. E355. FEMA 2011

$HOOCCH_2CH_2CH_2CH_2COOH$

$C_6H_{10}O_4$ 146.143

Constit. of beet juice, pork fat, guava fruit (*Psidium guajava*), papaya (*Carica papaya*) and raspberry (*Rubus idaeus*). Food acidulant. Monoclinic cryst. (HNO_3). Sol. EtOH; spar. sol. Et_2O; mod. sol. H_2O. Mp 153° (149-150°). Bp 337.5° Bp_{100} 265° Bp_{15} 216°. pK_{a1} 4.41; pK_{a2} 5.41 (20°). pK_{a1} 4.44; pK_{a2} 5.44 (25°). Sublimes. Does not readily form a monomeric anhydride; forms a polymeric anhydride which gives the unstable monomer on dist..

▶ Fl. p. 196°, autoignition temp. 420°. Severe eye and mucous membrane irritant. LD_{50} (mus, orl) 1900 mg/kg. AU8400000

Bis(2-ethylhexyl) ester: [103-23-1] *Bis(2-ethylhexyl) adipate. Diethylhexyl adipate. DEHA. Flexol A26. Vestinol OA. Wickenol 158*

$C_{22}H_{42}O_4$ 370.571

Indirect food additive arising from contact with polymers and adhesives. Liq. Sol. Me_2CO, Et_2O, EtOH. d^{25} 0.92. Mp -67.8°. Bp 417° Bp_1 180°. n_D^{20} 1.4474.

▶ Fl. p. 196°. Low oral tox. but high doses produce liver tumours in rodents. Relevance to man under investigation. AU9700000

Anhydride: [2035-75-8] *2,7-Oxepanedione, 9CI. Adipic anhydride*

$C_6H_8O_3$ 128.127

Food starch esterification agent. Tablets. Mp 22°. $Bp_{0.1}$ 98-100°. Adipic acid also forms a polymeric anhydride.

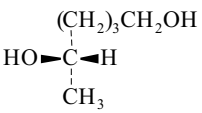
[110-29-2, 3385-41-9, 19090-60-9, 23311-84-4, 27178-16-1, 29254-17-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 495B; 618A; 618B; 642D; 695D; 696A; 741A; 770C; 841C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 770B; 942C; 943A; 943B; 943C; 1120B; 1120C; 1357A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 582A; 642B; 642C; 642D; 643A; 746C; 746D; 800D (*ir*)
Hill, J.W. *et al., J.A.C.S.*, 1930, **52**, 4110-4114 (*anhydride*)
Org. Synth., Coll. Vol., 1, 1932, 18-19 (*synth*)
Henne, A.L. *et al., J.A.C.S.*, 1943, **65**, 752-754 (*synth*)
Welcher, F. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **2**, 22 (*synth, standard*)
Jain, B.D. *et al., Curr. Sci.*, 1963, **32**, 66 (*pptn*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 15; 766 (*use*)
Holmes, J.L. *et al., Org. Mass Spectrom.*, 1970, **3**, 1505-1518 (*ms*)
Tanaka, K. *et al., Hydrocarbon Process.*, 1974, **53**, 114 (*rev*)
Williamson, K.L. *et al., J. Magn. Reson.*, 1978, **30**, 367-383 (*cmr*)
Marco, J.A. *et al., Phytochemistry*, 1978, **17**, 1438 (*occur*)
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499-508 (*pmr*)
IARC Monog., 1982, **29**, 257; *Suppl.* 7, 62 (*diethylhexyl ester, rev, tox*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH-Weinheim, 1985, **A1**, 269 (*rev*)
Venturello, C. *et al., J.O.C.*, 1986, **51**, 1599-1602 (*synth*)
Castle, L. *et al., J. Assoc. Off. Anal. Chem.*, 1988, **71**, 394-396 (*diethylhexyl ester, gc, ms*)
Food Surveill. Pap., Ministry Agriculture, Fisheries and Food, HMSO, London, 1990, **30**, 28 (*diethylhexyl ester*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 466 (*rev*)
Smith, J.R.L. *et al., J.C.S. Perkin 2*, 1992, 605-611 (*rev, synth*)
Draths, K.M. *et al., J.A.C.S.*, 1994, **116**, 399-400 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 49-53 (*use*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 22
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEN000; AEO000; AEN250; AEQ250; AER250; DOQ300; AEO750; AEP750

1,5-Hexanediol, 9CI H-228

[928-40-5]

[26762-52-7]



(*S*)-*form*

$C_6H_{14}O_2$ 118.175

▶ MO2080000

(S)-form [109784-17-0]

Oil. $[\alpha]_D^{20}$ +8 (c, 0.55 in MeOH).

Bis-4-nitrobenzoyl:

Cryst. (CH_2Cl_2/pentane). Mp 107-108°. $[\alpha]_D^{20}$ +43 (c, 0.43 in $CHCl_3$).

(±)-form

Food additive. Bp_{17} 140-141° $Bp_{0.5}$ 89-91°.

Bis-4-nitrobenzoyl:

Mp 89-90°.

[71401-68-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 134C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 202C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 196A (*ir*)
Perkin, W.H. *et al., J.C.S.*, 1887, **51**, 702 (*synth*)
Sigg, H.P. *et al., Helv. Chim. Acta*, 1964, **47**, 1401 (*abs config, ir, pmr*)
Voitsekhovskoya, A.L. *et al., CA*, 1967, **66**, 55320x (*synth*)
Moore, B.P. *et al., Aust. J. Chem.*, 1976, **29**, 1365 (*synth*)
Davies, S.G. *et al., J.C.S. Perkin 1*, 1996, 2467 (*synth*)

2,3-Hexanedione, 9CI H-229

[3848-24-6]

Methyl propyl diketone. Methyl propyl glyoxal. FEMA 2558

$H_3CCOCO(CH_2)_2CH_3$

$C_6H_{10}O_2$ 114.144

Constit. of coffee, peach, roast chicken, beer, shoyu and clam. Flavour ingredient. Buttery, cheese tasting and creamy buttery odour. d_4^{19} 0.93. Bp 128°.

▶ Skin irritant. MO3140000

3-Oxime: [42563-83-7]
$C_6H_{11}NO_2$ 129.158
Cryst. (EtOH). Mp 49.5° Mp 60°.

▶ MO3350000

Dioxime: [4481-42-9] *Methyl propyl glyoxime*
$C_6H_{12}N_2O_2$ 144.173
Needles (Et_2O). Mp 175°.

Bisphenylhydrazone:
Yellow needles (C_6H_6). Mp 137-138°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 424C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 510B (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 387B (*nmr*)
Dufraise, *et al., Bull. Soc. Chim. Fr.*, 1927, **41**, 1370
Bestman, H.-J. *et al., Chem. Ber.*, 1969, **102**, 2259 (*synth*)
Yamashita, M. *et al., Chem. Comm.*, 1977, 691 (*synth*)
Schroeder, F. *et al., Annalen*, 1994, 1211 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HEQ200

3,4-Hexanedione, 9CI H-230

[4437-51-8]
Bipropionyl. FEMA 3168
$H_3CCH_2COCOCH_2CH_3$
$C_6H_{10}O_2$ 114.144
Flavouring ingredient. Yellow oil with a pungent, unpleasant odour. d^{21} 0.94. Fp -10. Bp 130° Bp_{10} 32°. n_D^{21} 1.4130.

Dioxime: [4437-52-9] *Diethylglyoxime*
$C_6H_{12}N_2O_2$ 144.173
Needles (C_6H_6). Spar. sol. H_2O, $CHCl_3$, insol. petrol. Mp 185° (part. subl.).

Bisphenylhydrazone:
Mp 161°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 660C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 510C (*ir*)
Urion, *et al., Ann. Chim. (Paris)*, 1934, **1**, 54 (*synth*)
Yamashita, M. *et al., Chem. Comm.*, 1977, 691 (*synth*)
Olah, G.A. *et al., Synthesis*, 1991, 1177 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 329
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1296-1297

1,6-Hexanedithiol, 9CI, 8CI H-231

[1191-43-1]
Hexamethylendithiol. 1,6-Dimercaptohexane. FEMA 3495
$HSCH_2(CH_2)_4CH_2SH$
$C_6H_{14}S_2$ 150.309
Present in boiled and cooked beef. Flavouring ingredient. Liq. Bp_{44} 139-142°. n_D^{20} 1.5110.

▶ MO3500000

Bis-2,4-dinitrophenyl:
Cryst. (butanone/MeOH). Mp 221.5-222.3°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 261B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 420C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 343A (*ir*)
Grogan, C.H. *et al., J.O.C.*, 1955, **20**, 50 (*synth, bibl, deriv*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 330
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1297-1298

Hexanethioic acid H-232

[7530-91-8]
$H_3C(CH_2)_4COSH \Leftrightarrow H_3C(CH_2)_4C(S)OH$
$C_6H_{12}OS$ 132.226
Bp_9 62-63°.

SH-form

Me ester: [2432-77-1] S-*Methyl hexanethioate. Methanethiol caproate. FEMA 3862*
$C_7H_{14}OS$ 146.253
Present in durian fruit (*Durio zibethinus*), fish oil, beer and hop oil. Flavouring ingredient. Liq. with sulphurous odour. Bp_{15} 50°.

Propyl ester: [2432-78-2]
$C_9H_{18}OS$ 174.307
Present in leek oil. Characterised spectroscopically.

2-Propenyl ester: [156420-69-8]
$C_9H_{16}OS$ 172.291
Aroma constit. of fried garlic. Characterised spectroscopically.

McFadden, W.H. *et al., Anal. Chem.*, 1965, **37**, 560-566 (*S-Me ester, synth, ms*)
Kobayashi, Y. *et al., Synthesis*, 1985, 671-672 (*synth, ir*)
Vinokurov, V.A. *et al., Zh. Org. Khim.*, 1987, **23**, 2250-2251; *J. Org. Chem. USSR (Engl. Transl.)*, 1987, **23**, 1990-1991 (*S-Me ester, synth, uv*)
Stephani, A. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **194**, 21-25 (*S-Propyl ester*)
Shin, H.C. *et al., Lipids*, 1993, **28**, 73-74 (*synth*)
Weenen, H. *et al., J. Agric. Food Chem.*, 1996, **44**, 3291-3293 (*S-Me ester, occur, durian*)
Eri, S. *et al., J. Agric. Food Chem.*, 2000, **48**, 1140-1149 (*S-Me ester, occur, hops*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1134 (*S-Me ester, use*)
Hsu, J.P. *et al., CA*, **121**, 81405c (*S-2-propenyl ester*)

1-Hexanethiol, 9CI H-233

[111-31-9]
Hexyl mercaptan. 1-Mercaptohexane. FEMA 3842
$H_3C(CH_2)_4CH_2SH$
$C_6H_{14}S$ 118.243
Food additive listed in the EAFUS Food Additive Database (Jan. 2001). Present in cooked meats. Food flavouring agent. Liq. with burnt fat/meaty odour. d 0.84. Mp -81°. Bp 151-152°. n_D 1.4482.

▶ Flammable. MO4550000

S-*Me:* [20291-60-5] *1-(Methylthio)hexane, 9CI. Hexyl methyl sulfide, 8CI*
$C_7H_{16}S$ 132.269
Bp_{15} 61-62°.

S-*Et:* [7309-44-6] *1-(Ethylthio)hexane, 9CI. Ethyl hexyl sulfide, 8CI*
$C_8H_{18}S$ 146.296
d 0.78. Bp 183-185°. n_D^{20} 1.4541.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 256A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 412B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 336C (*ir*)
Von Braun, J. *et al., Annalen*, 1929, **472**, 138 (*synth*)
Backer, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1932, **51**, 1166 (*synth*)
Frank, R.L. *et al., J.A.C.S.*, 1946, **68**, 2103 (*synth*)
El Heweihi, Z. *et al., Chem. Ber.*, 1953, **86**, 862 (*synth*)
Parham, W.E. *et al., J.O.C.*, 1962, **27**, 2698 (*S-Et*)
Lissel, M. *et al., Synthesis*, 1986, 382 (*S-Me*)
Harpp, D.N. *et al., Tet. Lett.*, 1986, **27**, 3975 (*synth*)
Gingras, M. *et al., Tet. Lett.*, 1990, **31**, 1397 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HES000

Hexanoic acid, 9CI, 8CI H-234

[142-62-1]
Caproic acid. Pentane-1-carboxylic acid. Hexylic acid. Hexoic acid. FEMA 2559
$H_3C(CH_2)_4COOH$
$C_6H_{12}O_2$ 116.16
Present in apple, wine grapes, butter, licorice and cheeses, e.g. blue cheeses, Cheddar cheese, Swiss cheese, feta cheese, gruyere de comte cheese, etc. Also present in a few essential oils and fruit aromas. Secondary product of butyric acid fermentation. Flavouring ingredient. Oily liq. with acrid taste and unpleasant odour. Sol. alkalis, EtOH, Et_2O; spar. sol. H_2O. d_4^{15} 0.93. Fp -1.5. Bp 205°. n_D^{20} 1.4164. pK_{a1} 4.8 (25°).

▶ Skin and eye irritant. LD_{50} (rat, orl) 3000 mg/kg. Fl. p. 102° (oc), autoignition temp. 380/402°. MO5250000

Me ester: [106-70-7] *Methyl hexanoate. Methyl caproate. FEMA 2708*
$C_7H_{14}O_2$ 130.186
Present in wine grapes, melon, raspberry, blackberry, plum, quince, apple brandy, wines, Bourbon vanilla, coffee, black tea, potato, tomato, cheeses, rye bread, meats and other foodstuffs. Flavouring agent. Liq. with ether-like odour reminiscent of pineapple. d_4^{24} 0.89. Fp -71. Bp 150° Bp_{15} 52°. n_D^{20} 1.4049.

▶ Causes burns, flammable, fl. p. 32°. MO8401400

Et ester: [123-66-0] *Ethyl hexanoate. Ethyl caproate. FEMA 2439*
$C_8H_{16}O_2$ 144.213
Found in many fruits, clove bud, corn oil, Camembert cheese, milk, fruit brandies, sparkling wine and Bourbon vanilla. Used in perfumes and fruit flavours. Liq. with ether-like odour reminiscent of pineapple. d_4^{20} 0.87. Mp -67.5°. Bp 168° Bp_2 27°. n_D^{20} 1.4073.

▶ MO7735000

Propyl ester: [626-77-7] *Propyl hexanoate.*

Propyl caproate. FEMA 2949
$C_9H_{18}O_2$ 158.24
Flavouring ingredient. Constit. of apple, apricot, grapes, passion fruit, starfruit, mountain papaya, other fruits, cheeses and various alcoholic beverages. Liq. with sweet blackberry-plum flavour. d_4^{25} 0.86. Mp -69°. Bp 187° (185.5°). n_D^{25} 1.4109.

Isopropyl ester: [2311-46-8] *Isopropyl hexanoate. Isopropyl caproate. FEMA 2950*
$C_9H_{18}O_2$ 158.24
Present in wine grapes, strawberry, starfruit (*Averrhoa carambola*), blue cheeses, gruyere de comte cheese and Parmesan cheese. Flavouring ingredient. Liq. with fresh, sweet, berry-like taste. d_4^{20} 0.86. Bp 161° Bp_2 34°.

2-Propenyl ester: [123-68-2] *2-Propenyl hexanoate. Allyl caproate. FEMA 2032*
$C_9H_{16}O_2$ 156.224
Found in baked potato, pineapple and mushrooms. Used in artificial pineapple flavourings. Liq. with pineapple odour. d_4^{20} 0.89. Bp 185° Bp_{15} 75-76°. n_D^{20} 1.4243.

▶MO6125000

Butyl ester: [626-82-4] *Butyl hexanoate. Butyl caproate. FEMA 2201*
$C_{10}H_{20}O_2$ 172.267
Present in fruits and berries, e.g. apricot, banana, orange, wine grapes, papaya etc. Also present in beer, apple brandy and plum wine. Used in fruit flavourings. Liq. with powerful pineapple-like odour. d_4^{20} 0.86. Fp -68.4. Bp 208°. n_D^{15} 1.4160.

▶ET4203000

2-Methylpropyl ester: [105-79-3] *2-Methylpropyl hexanoate. Isobutyl caproate. FEMA 2202*
$C_{10}H_{20}O_2$ 172.267
Used in imitation pineapple flavouring. Liq. d 0.86.

Pentyl ester: [540-07-8] *Pentyl hexanoate. Amyl caproate. FEMA 2074*
$C_{11}H_{22}O_2$ 186.294
Flavouring ingredient. Liq. d_4^{25} 0.86. Mp -47°. Bp 226-227°. n_D^{25} 1.4202.

3-Methylbutyl ester: [2198-61-0] *3-Methylbutyl hexanoate. Isopentyl caproate. Isoamyl hexanoate. FEMA 2075*
$C_{11}H_{22}O_2$ 186.294
Used in fruit flavours and in fragrances. Present in fruits, cheeses and alcoholic beverages. d 0.86. Bp 222°.

Hexyl ester: [6378-65-0] *Hexyl hexanoate. Capryl caproate. Hexyl caproate. FEMA 2572*
$C_{12}H_{24}O_2$ 200.32
Used in fruit flavouring. Present in many fruits, Parmesan cheese, alcoholic beverages and black tea. Volatile component from fruit ripening. Liq. d_{20}^{20} 0.86. Bp 245-246° Bp 208° Bp_{13} 116-120°. n_D^{20} 1.4249.

[10051-44-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 482C; 606C; 606D; 712B; 729A; 838C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 753A; 918A; 918B; 1167C; 1194B; 1220B; 1353C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 574C; 621A; 621B; 778A; 797D (*ir*)
Gartenmeister, R. *et al., Annalen*, 1886, **233**, 249 (*esters*)
Org. Synth., Coll. Vol., 2, 1943, 474; Note 6 (*synth*)
Saunders, J.E. *et al., Appl. Spectrosc.*, 1968, **22**, 697-713 (*ir, esters*)
Von Sydow, E. *et al., Arch. Mass Spectral Data*, 1971, **2**, 76-77; 86-87 (*ms, esters*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 814 (*occur*)
Yarger, R.G. *et al., J. Chem. Ecol.*, 1975, **1**, 323
Caswell, L.R. *et al., J.O.C.*, 1976, **41**, 3312 (*uv*)
Sevrin, M. *et al., Tet. Lett.*, 1977, 3835 (*synth*)
Miyazaki, S. *et al., CA*, 1978, **89**, 129030b (*synth*)
Couperus, P.A. *et al., Org. Magn. Reson.*, 1978, **11**, 590 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 825 (*rev, use, tox*)
Nwaukwa, S.O. *et al., Tet. Lett.*, 1982, **23**, 35-38 (*synth, esters*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 341 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HEU000
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 43; 394 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 90; 161-162; 341; 989; 1453-1454; 1774 (*occur, props, esters*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 49; 201; 546; 745; 764; 785; 853; 1134; 1548 (*esters, use, occur, props*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 671
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGA500; EHF000; HEU000; HEM500; HER500; HFM700

1-Hexanol, 9CI H-235

[111-27-3]

[25917-35-5]
Hexyl alcohol, 8CI. Alcohol C6. Caproyl alcohol. FEMA 2567

$H_3C(CH_2)_4CH_2OH$
$C_6H_{14}O$ 102.176
Common constit. of essential oils e.g. orange peel oil. Present in various fruits, ginger, port wine, green tea, fruit brandies and unprocessed rice. Flavouring ingredient. Oil with fruity/aromatic odour and flavour. d_{20}^{20} 0.82. Fp -46.7. Bp 157°. n_D^{20} 1.4133.

▶Fl. p. 63°. Skin and eye irritant. LD_{50} (rat, orl) 720 mg/kg. MQ4025000

O-*β-D-Glucopyranoside:* [59080-45-4] *Hexyl glucoside*
$C_{12}H_{24}O_6$ 264.318
Constit. of *Citrus* spp. and apples (*Malus sylvestris*). Mp 51.5° (as tetra-Ac). $[\alpha]_D$ -24.6 ($CHCl_3$) (tetra-Ac).

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [124044-06-0]
$C_{17}H_{32}O_{10}$ 396.434
Constit. of apples (*Malus sylvestris*).

Formyl: [629-33-4] *Hexyl formate. FEMA 2570*
$C_7H_{14}O_2$ 130.186
Present in fruits e.g. apple, grape, peach, strawberry, black tea, licorice and other foods. Flavouring ingredient. Oil with fruity apple/unripe plum odour and sweet taste. d_4^{20} 0.88. Bp 155-156° (176.7°). n_D^{20} 1.4051.

Ac: [142-92-7] *Hexyl acetate. Acetate C6. FEMA 2565*
$C_8H_{16}O_2$ 144.213
Used in fruit essences and fruit aroma concentrates. Present in wines, black tea, soya bean and other foods. Oil with fruity odour and bittersweet taste. d_4^{20} 0.87. Fp -81. Bp 169.2°. n_D^{20} 1.4092.

▶AI0875000

Propanoyl: [2445-76-3] *Hexyl propionate. FEMA 2576*
$C_9H_{18}O_2$ 158.24
Flavouring ingredient. Liq. d_4^{15} 0.87. Mp -57.5°. Bp 185-186° (180°). n_D^{25} 1.4067.

Butanoyl: [2639-63-6] *Hexyl butyrate*
$C_{10}H_{20}O_2$ 172.267
Occurs in many fruits. Liq. d^{15} 0.87. Mp -78°. Bp 207.8°. n_D^{20} 1.4170.

Benzoyl: [6789-88-4] *Hexyl benzoate. FEMA 3691*
$C_{13}H_{18}O_2$ 206.284
Present in fruits of apricot, lingonberry, cowberry, feijoa, peach, sapodilla and other fruits. Also present in Parmesan cheese, butter and black tea. Flavouring ingredient. Apple-smelling liq. Bp 272° $Bp_{8.5}$ 138°.

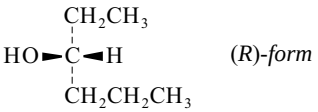
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 110C; 603A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 164C; 902C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 156D; 609D (*ir*)
Gartenmeister, R. *et al., Annalen*, 1886, **233**, 255 (*formyl*)
Org. Synth., Coll. Vol., 1, 1932, 306 (*synth*)
Bilterys, R. *et al., Bull. Soc. Chim. Belg.*, 1935, **44**, 567-586 (*butanoyl*)
Sharkey, A.G. *et al., Anal. Chem.*, 1959, **31**, 87-94 (*ms, butanoyl*)
Burgess, A.R. *et al., J.C.S.(B)*, 1969, 341 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, No. 72 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Org. Synth., 1973, **53**, 77 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 695 (*rev, tox*)
Kabalka, G.W. *et al., J.O.C.*, 1975, **40**, 1776 (*synth*)
Shokova, E.A. *et al., Zh. Org. Khim.*, 1984, **20**, 2312 (*cmr*)
Riddick, J.A. *et al., Tech. Chem. (N.Y.)*, 4th edn., Wiley-Interscience, 1986, **2**, 218; 892 (*props, purifn*)
Ford, R.A. *et al., Food Cosmet. Toxicol.*, 1988, **26**, 351 (*rev, formyl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HFI500; HFJ500
Schwab, W. *et al., J. Agric. Food Chem.*, 1990, **38**, 757 (*isol, glycosides*)
Nakamura, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1908 (*Hexyl glucoside*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1320; 1322; 1324; 1327 (*occur, use, esters*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 176 (*tox*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HFI500; HFJ500

3-Hexanol, 9CI H-236

[623-37-0]

[25917-35-5]
FEMA 3351



(*R*)-*form*

$C_6H_{14}O$ 102.176

(*R*)-*form* [13471-42-6]
Bp 133-134°. $[\alpha]_D^{20}$ -7.13.

(*S*)-*form* [6210-51-1]
Bp 131-133°. $[\alpha]_D^{20}$ +6.81 ($CHCl_3$).

(±)-*form* [17015-11-1]
Flavouring ingredient. Sl. sol. H_2O, sol. EtOH, Me_2CO, Et_2O. d^{20} 0.82. Bp 134.5-135.5°. n_D^{20} 1.4167.

[66585-24-8, 66585-38-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 119C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 179A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 167D (*ir*)
Lieben, A. *et al., Ber.*, 1875, **8**, 1017
Levene, P.A. *et al., J. Biol. Chem.*, 1929, **83**, 579; 591 (*abs config*)
Kenyon, J. *et al., J.C.S.*, 1945, 273 (*synth, resoln*)
Clarke, T.C. *et al., J.A.C.S.*, 1977, **99**, 2740 (*synth*)
Keinan, E. *et al., J.A.C.S.*, 1986, **108**, 162 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 331
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1299-1300

2-Hexanone, 9CI H-237

[591-78-6]
Butyl methyl ketone. Methyl butyl ketone

$H_3C(CH_2)_3COCH_3$

$C_6H_{12}O$ 100.16

Present in hop oil (*Humulus lupulus*), potato (*Solanum tuberosum*) and groundnuts (*Arachis hypogaea*). Liq. d^0 0.83. Bp 127°.

▶ Flammable, fl. p. 23°, autoignition temp. 423°. Eye and skin irritant. Chronic exposure associated with development of peripheral neuropathies. Earlier symptoms of exp. include headache and nausea. LD_{50} (rat, orl) 2590 mg/kg. OES: long-term 5 ppm (Sk). MP1400000

Oxime: [5577-48-0]
$C_6H_{13}NO$ 115.175
Bp 185° (slight dec.) Bp_{112} 138°.

2,4-Dinitrophenylhydrazone: [2348-17-6]
Mp 117-118° (106°).

Semicarbazone: [3622-64-8]
Mp 125°.

Di-Et ketal:2,2-Diethoxyhexane
$C_{10}H_{22}O_2$ 174.283
Bp_{18} 68-69°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 635B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 408A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 490B (*ir*)
Wagner, G. *et al., J. Prakt. Chem.*, 1891, **44**, 259
Grignard, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1926, **182**, 299
Suzuki, A. *et al., J.A.C.S.*, 1967, **89**, 5708 (*synth*)
Kurts, A.L. *et al., J. Organomet. Chem.*, 1969, **17**, 21 (*synth*)
Yamashita, M. *et al., Tet. Lett.*, 1978, 761 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1104
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HEV000
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 672

3-Hexanone, 9CI H-238

[589-38-8]
Ethyl propyl ketone. FEMA 3290

$H_3C(CH_2)_2COCH_2CH_3$

$C_6H_{12}O$ 100.16

Flavouring ingredient. Sl. sol. H_2O, sol. Me_2CO, EtOH, Et_2O. d^{20} 0.81. Bp 123-123.5°. n_D^{20} 1.4004.

▶ Highly flammable, fl. p. 14°. Eye and skin irritant. LD_{50} (rat, orl) 3360 mg/kg. MP1575000

Oxime: [28364-56-9]
$C_6H_{13}NO$ 115.175
Bp_{17} 86°.

2,4-Dinitrophenylhydrazone: [1655-39-6]
Mp 130° Mp 149-151°.

Semicarbazone: [3622-65-9]
Mp 112°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 408B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 635C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 490C (*ir*)
Lieben, A. *et al., Ber.*, 1875, **8**, 1017
Kurts, A.L. *et al., J. Organomet. Chem.*, 1969, **17**, 21 (*synth*)
Schwartz, J. *et al., J.A.C.S.*, 1974, **96**, 4721 (*synth*)
Yamashita, M. *et al., Tet. Lett.*, 1978, 761 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 332
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1300-1301
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HEV500

Hexasodium metaphosphate ($P_6O_{18}^{6\ominus}$), 9CI, 8CI H-239

[10124-56-8]
Hexasodium metaphosphate. Sodium hexametaphosphate. Sodium tetrapolyphosphate. Graham's salt. SHMP

$Na_6(P_6O_{18})$

$Na_6O_{18}P_6$ 611.77

Structure possesses 12-membered ring with alternate P and O atoms. Emulsifier, texturiser, dietary supplement, sequestrant, binding agent, pig/poultry scald agent, potential food contaminant arising from paper/board packaging. White solid + $6H_2O$.

▶ OY3675000

Hexahydrate: [15528-36-6]
Colourless cryst. (aq. EtOH). Ion consists of 12-membered $(P-O)_6$ ring of six PO_4 tetrahedra joined at corners.

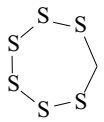
▶ Of relatively low toxicity; LD_{50} 3000-4300 mg/kg $^{-1}$ (small mammals).

[13478-98-3, 14550-21-1]

Jost, K.-H. *et al., Acta Cryst.*, 1965, **19**, 555 (*cryst struct*)
Griffith, E.J. *et al., Inorg. Chem.*, 1965, **4**, 549 (*synth, props*)
Kura, G. *et al., J. Chromatogr.*, 1971, **56**, 111 (*purifn*)
Fluck, E. *et al., Z. Naturforsch., B*, 1974, **29**, 603 (*pe*)
Griffiths, L. *et al., J.C.S. Dalton*, 1986, 2247 (*P-31 nmr*)
Watanobe, W. *et al., J. Mater. Sci.*, 1992, **27**, 5259-5261
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SHM500

Hexathiepane, 9CI H-240

[17233-71-5]
1,2,3,4,5,6-Hexathiacycloheptane



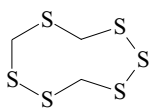
CH_2S_6 206.423

Minor constit. of *Lentinus edodes* (shiitake). Mp 90°.

Katsura, M. *et al., Chem. Pharm. Bull.*, 1967, **15**, 988 (*isol, synth*)
Fehér, F. *et al., Z. Naturforsch., B*, 1969, **24**, 1485 (*synth*)
Fehér, F. *et al., CA*, 1976, **85**, 54924c (*cryst struct*)

1,2,3,5,6,8-Hexathionane, 9CI H-241

[103439-80-1]
1,2,3,5,6,8-Hexathiacyclononane



$C_3H_6S_6$ 234.476

Constit. of the edible shiitake mushroom (*Lentinus edodes*).

Chen, C.C. *et al., ACS Symp. Ser.*, 1986, **317**, 176 (*occur*)
Chen, C.C. *et al., J. Agric. Food Chem.*, 1986, **34**, 830 (*occur*)

1,2,4,5,7,8-Hexathionane, 9CI H-242

[81531-38-6]
1,2,4,5,7,8-Hexathiacyclononane

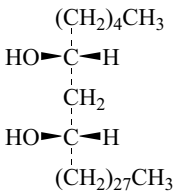
$C_3H_6S_6$ 234.476

Constit. of the seeds of petai (*Parkia speciosa*). Characteristic odour component of the beans. Yellow oil with strong odour. Poorly sol. hexane. Attempted recryst. from dioxan gave cryst. containing

only four S atoms.

Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521 (*isol*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)

6,8-Hexatriacontanediol H-243

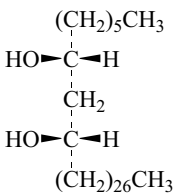


$C_{36}H_{74}O_2$ 538.979

(6*R,8*S**)-*form*** [193419-70-4]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 88-90°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, pmr, ms*)

7,9-Hexatriacontanediol H-244



$C_{36}H_{74}O_2$ 538.979

(7*R,9*S*)-*form*** [193419-75-9]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 81-84°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

5-Hexatriacontanone H-245

$H_3C(CH_2)_3CO(CH_2)_{30}CH_3$

$C_{36}H_{72}O$ 520.964

Appears to be indexed as the 6-isomer in CAS. Constit. of *Solanum torvum* (pea eggplant). Cryst. (Me_2CO). Mp 78°.

[87538-98-5]

Mahmood, U. *et al., Phytochemistry*, 1983, **22**, 167 (*isol, ir, pmr, ms*)

2-Hexenal, 9CI H-246

[505-57-7]

[1335-39-3]
3-Propylacrolein. FEMA 2560

$H_3CCH_2CH_2CH{=}CHCHO$

$C_6H_{10}O$ 98.144
Constit. of many foods. Flavouring ingredient.

► LD_{50} (mus, ipr) 290 mg/kg. MP5880000

(*E*)-*form* [6728-26-3]
Leaf aldehyde
Used in perfumery and flavourings. Liq. with sharp herbal pungency, apple-like in high dilution. Bp 146-147° Bp_{12} 43°. n_D^{20} 1.4480.

► Peroxidizable. Skin irritant. LD_{50} (rat, orl) 780 mg/kg. LD_{50} (rbt, skn) 600 mg/kg. MP5900000

2,4-Dinitrophenylhydrazone: [2122-02-3]
Red needles. Mp 147°.

Semicarbazone:
Cryst. (MeOH). Mp 179°.

Di-Et acetal: [67746-30-9] *1,1-Diethoxy-2-hexene*
$C_{10}H_{20}O_2$ 172.267
d 0.85. Bp_{55} 95-98°. n_D^{20} 1.4210.

(*Z*)-*form* [16635-54-4]
Fruit flavour/aroma constituent. Bp 140° Bp_{20} 46°.

2,4-Dinitrophenylhydrazone:
Mp 142.2-142.7°.

[54306-00-2]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 736C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 472D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 560B (*ir*)
Curtius, T. *et al., Annalen*, 1913, **404**, 93 (*isol*)
Elkik, E. *et al., Bull. Soc. Chim. Fr.*, 1968, 283 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 453 (*rev, tox*)
Hatanaka, A. *et al., Phytochemistry*, 1976, **15**, 1125 (*biosynth*)
Ito, Y. *et al., J.O.C.*, 1978, **43**, 1011 (*synth*)
Zimmermann, B. *et al., Chem. Ber.*, 1986, **119**, 2848 (*synth, ir, pmr*)
Hatanaka, A. *et al., Z. Naturforsch., C*, 1992, **47**, 183 (*synth, pmr, cmr*)
Duffault, J.-M. *et al., Synth. Commun.*, 1996, **26**, 3257 (*Z-form*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2285
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HFA500; PNC500

3-Hexenal, 9CI H-247

[4440-65-7]

[1335-39-3]
FEMA 3923

$H_3CCH_2CH{=}CHCH_2CHO$

$C_6H_{10}O$ 98.144

(*E*)-*form* [69112-21-6]
Flavouring agent. Bp_{36} 51.5-52.5° Bp_{20} 35°.

► MP5920000

2,4-Dinitrophenylhydrazone:
Mp 99-101°.

Semicarbazone:
Mp 133-134°.

(*Z*)-*form* [6789-80-6] *FEMA 2561*
Flavouring ingredient. Present in apple, cucumber, grape, banana, raspberry, strawberry, black tea and tomato. Liq. with a powerful leafy odour. Sl. sol. H_2O, sol. EtOH. d_4^{22} 0.85. Bp_{730} 120° Bp_{20} 36°. n_D^{22} 1.4300.

► LD_{50} (rat, orl) 1560 mg/kg. MP5940000

2,4-Dinitrophenylhydrazone: [2121-99-5]
Mp 102.3-103.1° Mp 99.5-101°.

Semicarbazone:
Mp 128-130°.

Di-Et acetal: [73545-18-3] *1,1-Diethoxy-3-hexene, 9CI*
$C_{10}H_{20}O_2$ 172.267
Liq. Bp_1 40-43°.

Winter, M. *et al., Helv. Chim. Acta*, 1962, **45**, 2567 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 343 (*rev, tox, E-form*)
Hatanaka, A. *et al., Z. Naturforsch., C*, 1992, **47**, 183 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 333
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1301-1303
Sha, W. *et al., J.O.C.*, 2000, **65**, 5315-5326 (*di-Et acetal, synth, pmr, cmr*)
Wavrin, L. *et al., Synthesis*, 2002, 326-330 (*synth, ir, pmr, cmr*)

4-Hexenal H-248

[1335-39-3]

$H_3CCH{=}CHCH_2CH_2CHO$

$C_6H_{10}O$ 98.144

(*E*)-*form* [25166-87-4]
Oil. Bp_{50} 34° Bp_{20} 37°.

Oxime:
$C_6H_{11}NO$ 113.159
Bp_{13} 80°.

2,4-Dinitrophenylhydrazone:
Mp 122.7-123.1°.

(*Z*)-*form* [4634-89-3] *FEMA 3496*
Present in onion. Flavouring ingredient. Bp_{20} 38°. n_D^{20} 1.4315.

2,4-Dinitrophenylhydrazone:
Mp 99.5-99.8°.

Oppolzer, W. *et al., Tetrahedron*, 1985, **41**, 3497 (*synth, ir, pmr, ms*)
Hatanaka, A. *et al., Z. Naturforsch., C*, 1992, **47**, 183 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 334
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1302-1303

2-Hexenoic acid, 9CI H-249

[1191-04-4]

$H_3CCH_2CH_2CH{=}CHCOOH$

$C_6H_{10}O_2$ 114.144

(*E*)-*form* [13419-69-7]
FEMA 3169
Used as flavouring for tea and reverted soybean oil. Present in apple, banana, bilberry, guava fruit, loganberry, peppermint oil, pork fat, white wine and black or green tea. Needles (H_2O, EtOH). Mp 36-37°. Bp 216-217° Bp_8 100°. pK_{a1} 4.75 (25°).

Me ester: [2396-77-2] *FEMA 2709*
$C_7H_{12}O_2$ 128.171
Flavouring ingredient. Present in papaya (*Carica* spp.), peas and soursop (*Annona muricata*). Liq. with green-fruity flavour. Bp 169° Bp_{13} 56-58°.

Et ester: [27829-72-7]

[1552-67-6] *FEMA 3675*
$C_8H_{14}O_2$ 142.197
Flavouring agent. Liq. Bp_{10} 111°. n_D^{20} 1.1450.

Hexyl ester: [33855-57-1]

[16930-97-5] *FEMA 3692*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. Bp_{10} 122°. n_D^{20} 1.4423.

2-Propenyl ester:Allyl hexenoate
$C_9H_{14}O_2$ 154.208
Flavouring ingredient.

4-Bromophenacyl ester:
Mp 62-62.5°.

Chloride: [18802-95-4]
C_6H_9ClO 132.589
Bp_{23} 70°.

Anilide:
$C_{12}H_{15}NO$ 189.257
Needles. Mp 109-110°.

(*Z*)-*form* [1577-28-2]
Flavouring for reverted soybean oil. Mp 0-1°. $Bp_{0.2}$ 71-73°. pK_{a1} 4.63 (25°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 500B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 779A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 586A (*ir*)
Baker, C.F. *et al., Annalen*, 1894, **283**, 117 (*synth*)
Goldberg, A.A. *et al., J.C.S.*, 1928, 2343 (*synth*)
Cainelli, G. *et al., Chem. Comm.*, 1973, 94 (*synth*)
Org. Synth., 1973, **53**, 123 (*synth*)
Zimmermann, B. *et al., Chem. Ber.*, 1986, **119**, 2848 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 237; 351 (*esters*)
Black, T.H. *et al., Synth. Commun.*, 1995, **25**, 15 (*synth, ir, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 91; 993; 1305; 1330; 1776 (*occur, props, esters*)

3-Hexenoic acid, 9CI H-250

[4219-24-3]
2-Pentene-1-carboxylic acid. Hydrosorbic acid. FEMA 3170
$H_3CCH_2CH{=}CHCH_2COOH$
$C_6H_{10}O_2$ 114.144
Isol. from raspberry (*Rubus idaeus*), hop oil, beer, white wine, cocoa, kiwifruit and tea (*Thea sinensis*). Used in tea flavouring. Mp 12°. Bp 208° Bp_{22} 118-119°.
► MP7730000

(*E*)-*form* [1577-18-0]
Me ester: [2396-78-3] *FEMA 3364*
$C_7H_{12}O_2$ 128.171
Minor constit. of pineapples, also found in soursop (*Annona muricata*) and mountain papaya (*Carica pubescens*). Bp_{34} 67-68°. (*E*)-config. assumed.

Et ester: [2396-83-0] *FEMA 3342*
$C_8H_{14}O_2$ 142.197
Present in melon, yellow and purple passion fruits, quince, Chinese quince, prickly pear, kiwi fruit and Mexican breadfruit (*Monstera deliciosa*). Flavouring agent. Liq. with green, fruity aroma. Bp_{12} 63-64°. n_D^{20} 1.4260.

(*Z*)-*form* [1775-43-5]
Liq.

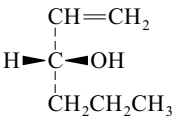
(Z)-3-Hexenyl ester: [61444-38-0] cis-*3-Hexenyl* cis-*3-hexenoate. FEMA 3689*
$C_{12}H_{20}O_2$ 196.289
Flavouring ingredient. Liq. with green grass, green tomato odour. Bp 194° Bp_{12} 112°. n_D^{20} 1.4515.

[1775-43-5]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 985A (*nmr*)
Boxer, J.E. *et al., J.C.S.*, 1931, 748 (*synth*)
Takei, S. *et al., Ber.*, 1935, **68**, 95 (*synth*)
Isaacs, E. *et al., J.C.S.*, 1936, 202 (*synth*)
Birch, A.J. *et al., Aust. J. Chem.*, 1976, **29**, 2737 (*synth*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 352 (*3-hexenyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 992; 1306; 1315-1316; 1777-1778 (*esters, occur, props, use*)

1-Hexen-3-ol, 9CI H-251

[4798-44-1]
Propyl vinyl carbinol. FEMA 3608


(*R*)-*form*

$C_6H_{12}O$ 100.16
Flavouring ingredient.

(*R*)-*form*
Bp_{90} 70-72°. $[\alpha]_D$ -28.2. $[\alpha]_D^{20}$ -14.7 (c, 1.9 in $CHCl_3$) (99% ee).

Strychnine salt:
Mp 170°.

Acid phthalate:
Mp 62-63°.

(±)-*form* [67928-93-2]
Food flavourant. Liq. with ethereal/rum-like odour. Bp 133.5-134° Bp_{20} 49-51°.

4-Nitrobenzoyl:
Mp 60-62°.

Me ether:3-Methoxy-1-hexene
$C_7H_{14}O$ 114.187
Liq. Bp 113-115° (88-91°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 143A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 215A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 207C (*ir*)
Niemann, C. *et al., J.O.C.*, 1943, **8**, 397 (*synth*)
Von Sydow, E. *et al., Arch. Mass Spectral Data*, 1971, **2**, 28 (*ms*)
Rappoport, Z. *et al., J.A.C.S.*, 1972, **94**, 2320 (*synth*)
Schurig, V. *et al., J. Essent. Oil Res.*, 1989, **1**, 209 (*resoln*)
Matsuda, M. *et al., CA*, 1991, **114**, 23370g (*synth, cmr*)
Francke, W. *et al., Annalen*, 1994, 1211 (*R-form, synth, pmr, cmr, ms*)
Bailey, W.F. *et al., J.O.C.*, 1994, **59**, 6528 (*Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1306-1307

2-Hexen-1-ol, 9CI H-252

[2305-21-7]
2-Hexenyl alcohol. FEMA 2562
$H_3C(CH_2)_2CH{=}CHCH_2OH$
$C_6H_{12}O$ 100.16

(*E*)-*form* [928-95-0]
Isol. from tea. Constit. of many fruits, e.g., apples, grapes. Also present in asparagus (cooked or raw), cooked potato, cooked beef, beer, cognac, white wine, soybean and olives. Flavouring agent. Bp 158-160° Bp_{95} 100.5-103.4° Bp_{20} 71.5-72°. n_D^{20} 1.4410.
► Skin irritant. LD_{50} (rat, orl) 3500 mg/kg. MP8390000

O-*β-D-Glucopyranoside:* [117017-90-0]
Erigeside B
$C_{12}H_{22}O_6$ 262.302
Syrup. $[\alpha]_D^{21}$ -28.3 (c, 0.43 in EtOH).

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [129277-35-6]
$C_{17}H_{30}O_{10}$ 394.418
Syrup. $[\alpha]_D^{23}$ -26.7 (c, 0.1 in H_2O).

O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [129277-34-5] *2-Hexenyl sophoroside*
$C_{18}H_{32}O_{11}$ 424.444
Powder. $[\alpha]_D^{24}$ -25.7 (c, 0.3 in H_2O).

Formyl: [53398-78-0] *2-Hexenyl formate. FEMA 3927*
$C_7H_{12}O_2$ 128.171
Flavouring ingredient.

Ac: [2497-18-9] trans-*2-Hexenyl acetate. FEMA 2564*
$C_8H_{14}O_2$ 142.197
Found in strawberry (*Fragaria*) and other fruits and essential oils. Used in artificial fruit flavours. Liq. with fresh, fruity odour. d_4^{20} 0.9. Bp 165-166° Bp_{15} 67-68°. n_D^{20} 1.4277.
► MP8425000

Propanoyl: [53398-80-4] *2-Hexenyl propionate. FEMA 3932*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient.

Butanoyl: [53398-83-7] *2-Hexenyl butanoate. FEMA 3926*
$C_{10}H_{18}O_2$ 170.251
Flavouring agent. Liq. with green, fruity odour. Bp 190°.

3-Methylbutanoyl: [68698-59-9] *2-Hexenyl isovalerate. FEMA 3930*
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient.

Pentanoyl: [56922-74-8] *2-Hexenyl valerate. FEMA 3935*
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient.

3,5-Dinitrobenzoyl:
Mp 64-65° (52°).

2-Naphthylurethane:
Mp 76°.

Me ether: [56052-83-6] *1-Methoxy-2-hexene*
$C_7H_{14}O$ 114.187
Liq. Bp_{721} 126-128°.

(*Z*)-*form* [928-94-9]
Constit. of currants and hops. Food flavouring for baked goods and candies producing a fresher note than the *E*-isomer. Bp 156-158° Bp_{56} 90-91° Bp_{20} 69-69.5°.

Ac: [56922-75-9]
Bp_{170} 116°.

3,5-Dinitrobenzoyl:
Mp 67° (52°).

[10094-40-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 141C; 141D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 213A; 213B; 964C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 204B; 205D; 664D (*ir*)
Bouis, M. *et al., Ann. Chim. (Paris)*, 1928, **9**, 402
Suzuki, A. *et al., J.A.C.S.*, 1971, **93**, 2792 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 911 (*rev, tox, E-form*)
Jacob, P. *et al., J.O.C.*, 1977, **42**, 579 (*synth*)
Hamilton, J.G.C. *et al., J. Chem. Ecol.*, 1985, **11**, 1399
Mori, K. *et al., Tetrahedron*, 1986, **42**, 6459 (*synth, ir, pmr*)
Mizutani, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2689 (*glucoside*)
Surender, P. *et al., Proc. Indian Natl. Sci. Acad., Part B*, 1988, **54**, 315-316 (*isol, butanoyl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HFD500
Yuda, M. *et al., Phytochemistry*, 1990, **29**, 1989 (*isol, glycosides*)
Hatanaka, A. *et al., Z. Naturforsch., C*, 1992, **47**, 183 (*synth, pmr, cmr*)
Yue, J. *et al., Phytochemistry*, 1994, **36**, 717 (*Erigeside B*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 336; 338
Crich, D. *et al., J.A.C.S.*, 1995, **117**, 8757 (*Me ether, synth, pmr, cmr*)
Duffault, J.-M. *et al., Synth. Commun.*, 1996, **26**, 3257 (*Z-form, Ac*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1307-1308; 1311-1312 (*use, occur, Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HFD500; HFE100

3-Hexen-1-ol, 9CI H-253

[544-12-7]
3-Hexenyl alcohol. Leaf alcohol
$H_3CCH_2CH{=}CHCH_2CH_2OH$
$C_6H_{12}O$ 100.16

(*E*)-*form* [928-97-2]
Used in blueberry flavouring. Bp 153-156° Bp_{22} 80-85° Bp_{20} 72.5-73°.

(*Z*)-*form* [928-96-1]
Phyllol. Verdalol. FEMA 2563
Used as tea flavourant. Preferred to (*E*)-isomer in perfumes and flavours to add natural 'green' notes. Occurs in geranium, tea, citrus and other oils, and many fruits, e.g. banana, concord grape, quince. Liq. with odour of fresh grass. Bp 156-157° Bp_{20} 73.5-74.3°. n_D^{20} 1.4384.
▶ Flammable, fl. p. 54°, low oral tox.. MP8400000

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [132278-37-6] cis-*3-Hexenyl β-primeveroside*
$C_{17}H_{30}O_{10}$ 394.418
Constit. of *Camellia sinensis*. Pale yellow powder. $[\alpha]_D$ -56.7 (c, 0.9 in MeOH).

Formyl: [33467-73-1] cis-*3-Hexenyl formate. FEMA 3353*
$C_7H_{12}O_2$ 128.171
Present in tea aroma, raspberry, cornmint oil and black chokeberry (*Aronia melanocarpa*). Used in flavour compositions. Liq. with green fruity odour. Bp 155°. n_D^{20} 1.4270.
▶ MP8550000

Ac: [3681-71-8] cis-*3-Hexenyl acetate. FEMA 3171*
$C_8H_{14}O_2$ 142.197
Present in green tea and fruit volatiles. Flavouring component. Bp_{12} 66°.
▶ MP8425050

Propanoyl: [33467-74-2] cis-*3-Hexenyl propanoate. 3-Hexenyl propionate. FEMA 3933*
$C_9H_{16}O_2$ 156.224
Present in thyme, black tea and mango. Flavouring ingredient for baked goods, candies etc.. Liq. with green, oily flavour. Bp_{20} 91°.

2-Methylpropanoyl: [41519-23-7] cis-*3-Hexenyl isobutyrate. FEMA 3929*
$C_{10}H_{18}O_2$ 170.251
Found in spearmint oil. Flavouring ingredient. Liq. with green, fruity odour.
▶ UA2470200

Butanoyl: [16491-36-4]

[2142-93-0] cis-*3-Hexenyl butyrate. FEMA 3402*
$C_{10}H_{18}O_2$ 170.251
Constit. of aroma from Ceylon tea. Also present in orange peel oil, lovage root and many fruits, e.g. feijoa fruit, nectarine, strawberry, guava, Chinese quince. Flavouring ingredient. Liq. with green, fruity odour. d_4^{25} 0.9. Bp 192° Bp_{20} 96°. n_D^{25} 1.4287.

2-Methylbutanoyl: [53398-85-9]

[10094-41-4] cis-*3-Hexenyl 2-methylbutanoate. FEMA 3497*
$C_{11}H_{20}O_2$ 184.278
Food flavour. Liq. with apple taste and apple/pineapple odour. Bp 212°.

3-Methylbutanoyl: [35154-45-1]

[10032-11-8] cis-*3-Hexenyl 3-methylbutanoate. 3-Hexenyl isovalerate. FEMA 3498*
$C_{11}H_{20}O_2$ 184.278
Food flavour. Present in tabasco pepper, bell pepper, black tea, sage, cherimoya, *Mentha* spp., nectarine, lamb's lettuce and other plants. Liq. with apple-like taste and odour. Bp 199°.

E-*2-Methyl-2-butenoyl:* [67883-79-8] cis-*3-Hexenyl tiglate. FEMA 3931*
$C_{11}H_{18}O_2$ 182.262
Flavouring ingredient. Bp 105°.

Pentanoyl: [35852-46-1] cis-*3-Hexenyl pentanoate.* cis-*3-Hexenyl valerate. FEMA 3936*
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient. Constit. of Spanish oregano (*Coridothymus capitatus*), tabasco pepper (*Capsicum frutescens*). Bp_{20} 108°.

Hexanoyl: [31501-11-8] cis-*3-Hexenyl hexanoate. FEMA 3403*
$C_{12}H_{22}O_2$ 198.305
Constit. of tabasco peppers (*Capsicum frutescens*). Aroma component of green tea. Also present in orange peel oil, guava fruit, feijoa fruit, purple passion fruit and other fruits. Flavouring agent. Liq. with green, fruity odour. Bp_{12} 122°.

E-*2-Hexenoyl:* [53398-87-1] cis-*3-Hexenyl* trans-*2-hexenoate. FEMA 3928*
$C_{12}H_{20}O_2$ 196.289
Flavouring ingredient.

E-*4-Hexenoyl:* [74638-19-0] cis-*3-Hexenyl* trans-*4-hexenoate*
$C_{12}H_{20}O_2$ 196.289
Constit. of Spanish oregano (*Coridothymus capitatus*).

2-Oxopropanoyl: [68133-76-6] cis-*3-Hexenyl pyruvate. FEMA 3934*
$C_9H_{14}O_3$ 170.208
Flavouring ingredient. Bp_5 76°.

Phenylacetyl: [42436-07-7] cis-*3-Hexenyl phenylacetate. FEMA 3633*
$C_{14}H_{18}O_2$ 218.295
Flavouring ingredient. Present in *Mentha* spp.. Liq. Bp 299°. n_D^{20} 1.5007.

Benzoyl: [25152-85-6]

[72200-74-9, 75019-52-2] cis-*3-Hexenyl benzoate. FEMA 3688*
$C_{13}H_{16}O_2$ 204.268
Constit. of black tea aroma. Also present in bilberry, lingonberry, cowberry and feijoa fruit and peel. Flavouring agent. d^{15} 1.01. Bp_6 134-135°. n_D^{20} 1.5056. Phys. props. refer to a preparation of undefined stereochem., prob. a mixt. of *E*- and *Z*-isomers.

[53398-84-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 142A; 142B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 213C; 214A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 206C; 206D (*ir*)
Walbaum, H. *et al., J. Prakt. Chem.*, 1917, **96**, 245-250 (*synth, benzoyl*)
Crombie, L. *et al., J.C.S.*, 1950, 873 (*synth, struct, occur*)
U.S. Pat., 1969, 3 485 868; *CA*, **72**, 66408g (*butanoyl*)
Sato, S. *et al., Agric. Biol. Chem.*, 1970, **34**, 1355-1367 (*Z-benzoyl, isol, ir*)
Hayman, L.W. *et al., J. Agric. Food Chem.*, 1971, **19**, 1131-1134 (*hexanoyl, isol, ms*)
Yamanishi, T. *et al., Agric. Biol. Chem.*, 1972, **36**, 1153-1158 (*butanoyl, isol, ir, ms*)
Dahill, R.T. Jr. *et al., J. Chem. Eng. Data*, 1972, **17**, 399 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 909 (*rev, tox, Z-form*)
Takei, Y. *et al., Agric. Biol. Chem.*, 1976, **40**, 2151-2157 (*hexanoyl, synth, ir, ms*)
Hattori, R. *et al., Agric. Biol. Chem.*, 1978, **42**, 1351-1356 (*Z-benzoyl, nmr, ir, ms*)
Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 89 (*isol, esters*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HFE000
Otsuka, H. *et al., Phytochemistry*, 1990, **29**, 3681 (*primeveroside*)
Morisaki, N. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2945 (*synth, pmr*)
Hatanaka, A. *et al., Z. Naturforsch., C*, 1992, **47**, 183 (*synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1309-1320
Nishikitani, M. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1631-1633 (*primeveroside*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 756; 759-773 (*esters, use, props, occur*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HFE000; HFE520

4-Hexen-1-ol, 9CI H-254

[6126-50-7]
FEMA 3430
$H_3CCH{=}CHCH_2CH_2CH_2OH$
$C_6H_{12}O$ 100.16
Flavouring ingredient.

(*E*)-*form* [928-92-7]
Constit. of bananas. Bp 159-159.4° Bp_{19} 70-74°.

1-Naphthylurethane:
Mp 74-75°.

3,5-Dinitrobenzoyl:
Mp 33.1-33.8°.

Ac: [72237-36-6]
$C_8H_{14}O_2$ 142.197
Bp_{16} 68°. Bp. presumably refers to *E*-form.

(*Z*)-*form* [928-91-6]
Constit. of bananas. Bp 158-159°.

1-Naphthylurethane:
Mp 74-75°.

3,5-Dinitrobenzoyl:
Mp 24.8-25.6°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 142C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 214B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 207A (*ir*)
Schlosser, M. *et al., Helv. Chim. Acta*, 1974, **57**, 1567 (*synth, ir*)
Čeković, Z. *et al., J.A.C.S.*, 1974, **96**, 3000 (*synth*)
Org. Synth., 1976, **55**, 62 (*synth, bibl*)
Taber, D.F. *et al., J.O.C.*, 1988, **53**, 2984 (*synth, pmr, cmr, ir, ms*)
Hatanaka, A. *et al., Z. Naturforsch., C*, 1992, **47**, 183 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 338
Denmark, S.E. *et al., J.O.C.*, 1995, **60**, 1391 (*synth, pmr, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1308-1309

4-Hexen-3-one H-255

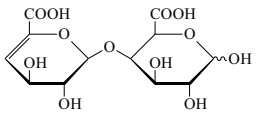
[2497-21-4]
FEMA 3352
$H_3CCH_2COCH{=}CHCH_3$
$C_6H_{10}O$ 98.144
Flavouring ingredient.
▶MP8659900

(*E*)-*form* [50396-87-7]
Bp 135-137° Bp_{55} 58-61°. n_D^{20} 1.4400.

2,4-Dinitrophenylhydrazone:
Red cryst. Mp 170°. This deriv. presumed here to belong to the (*E*)-isomer.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 645B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 501A (*ir*)
Coppens, *et al., Bull. Soc. Chim. Belg.*, 1929, **38**, 310
Stutsman, P.S. *et al., J.A.C.S.*, 1939, **61**, 3303 (*synth*)
Oare, D.A. *et al., J.O.C.*, 1990, **55**, 132 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 334
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1304-1305

α-L-*threo*-4-Hex-4-enopyranuronosyl-D-galacturonic acid H-256



Pyranose-*form*

$C_{12}H_{16}O_{12}$ 352.251
Isol. from the enzymic hydrolysate of pectin produced by the pectin-trans eliminase from *Bacillus polymyxa* or commercial pectinase. $[\alpha]_D$ +177.8 (H_2O).

Albersheim, P. *et al., Helv. Chim. Acta*, 1960, **43**, 1422 (*isol*)
Nagel, C.W. *et al., Arch. Biochem. Biophys.*, 1961, **94**, 328 (*isol*)
Hasegawa, S. *et al., J. Biol. Chem.*, 1962, **237**, 619 (*isol*)

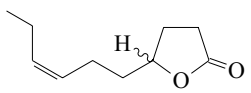
5-Hexenyl glucosinolate H-257

[76265-24-2]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)-6-heptenimidate]
$H_2C{=}CH(CH_2)_4C(SGlc){=}NOSO_3H$
$C_{13}H_{23}NO_9S_2$ 401.458
Present in horseradish (*Armoracia lapathifolia*) and Japanese horseradish (*Wasabia japonica*).

Kojima, M. *et al., Yakugaku Zasshi*, 1973, **93**, 453; *CA*, **80**, 130475w (*occur*)
Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)

5-(3-Hexenyl)dihydro-2(3*H*)-furanone, 9CI H-258

[67114-38-9]
***γ*-Jasmolactone**



(*Z*)-*form*

$C_{10}H_{16}O_2$ 168.235

(±)-(*Z*)-*form* [93787-95-2]
Liq. $Bp_{0.2}$ 165°.

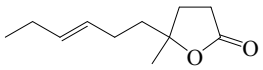
(ξ)-(*Z*)-*form*
Constit. of peppermint oil.

[63095-33-0]

Takahashi, K. *et al., Agric. Biol. Chem.*, 1980, **44**, 1535 (*isol*)
Naoshima, Y. *et al., Agric. Biol. Chem.*, 1981, **45**, 2639 (*synth*)
Ballini, R. *et al., Synth. Commun.*, 1989, **19**, 575 (*synth, pmr*)
Yamashita, M. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 1257 (*synth, pmr*)

5-(3-Hexenyl)dihydro-5-methyl-2(3*H*)-furanone, 9CI H-259

[93257-19-3]
4-Hydroxy-4-methyl-7-decenoic acid γ-lactone. γ-(3-Hexenyl)-γ-methylbutyrolactone



(*E*)-*form*

$C_{11}H_{18}O_2$ 182.262

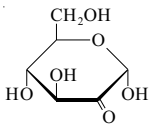
(±)-(*E*)-*form* [14252-84-7]
Bp_{13} 136°. n_D^{20} 1.4700.

(±)-(*Z*)-*form* [70851-61-5]
FEMA 3937
Flavouring agent for baked goods, candies and meat products. Liq. with creamy coconut/butter odour. d_4^{25} 0.97. Bp 150°.

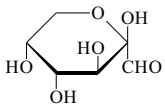
Stoll, M. *et al., Helv. Chim. Acta*, 1938, **21**, 1547-1553 (*synth*)
Keiichi, S. *et al., J.O.C.*, 1964, **29**, 2290-2293 (*synth, ir*)
Sisido, K. *et al., J.O.C.*, 1964, **29**, 2290-2293 (*synth, ir*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 43S (*Z-form, rev*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 821 (*use*)

arabino-Hexos-2-ulose H-260

Glucosone. Fructosone. Mannosone



α-D-Pyranose-form



β-D-2,6-Pyranose-form

$C_6H_{10}O_6$ 178.141

D-*form* [26345-59-5]
Formed during sterilisation of foods by irradiation. $[\alpha]_D^{20}$ -9.8.

Bayne, S. *et al., Adv. Carbohydr. Chem.*, 1956, **11**, 43 (*rev*)
Liu, T.E. *et al., Carbohydr. Res.*, 1983, **113**, 151 (*D-form, enzymic synth*)
Koths, K. *et al., Carbohydr. Res.*, 1992, **232**, 59 (*enzymic synth*)

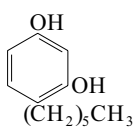
Hexyl glucosinolate H-261

[127929-25-3]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)heptanimidate], 9CI
$H_3C(CH_2)_5C(SGlc){=}NOSO_3H$
$C_{13}H_{25}NO_9S_2$ 403.474
Present in radish (*Raphanus sativus*) and in kohlrabi aroma.

Kjaer, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1715 (*occur*)
Macleod, G. *et al., Phytochemistry*, 1990, **29**, 1183 (*occur*)

4-Hexyl-1,3-benzenediol, 9CI H-262

[136-77-6]
4-Hexylresorcinol, 8CI. 1-(2,4-Dihydroxyphenyl)hexane. Caprokol. ***Hexylresorcinol, BAN, USAN.*** *Hexylresorcin. Everfresh®*



$C_{12}H_{18}O_2$ 194.273

Food additive for prevention of enzymic browning in shrimp and fruits. Needles (petrol). Mp 68-70°. $Bp_{6.5}$ 178-180° (lit. gives a pressure range). Log P 3.95 (calc).

▶ Conc. solns. corrosive and irritating to skin and mucous membranes. Alcoholic solns. show vesicant props. Eye irritant. LD_{50} (rat, orl) 550 mg/kg. Exp. reprod. effects. VH1575000

9-Aminoacridine complex: [7527-91-5] ***Acrisorcin, INN, USAN.*** *Akrinol. Aminacrine hexylresorcinate. Sch 7056*
Yellow cryst. Mp 189-190°.

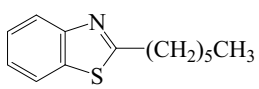
1-Ac:
$C_{14}H_{20}O_3$ 236.31
Oil.

3-Ac:
$C_{14}H_{20}O_3$ 236.31
Needles (heptane). Mp 62-63°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1105B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 301A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1040A (*ir*)
Dohme, A.R.L. *et al., J.A.C.S.*, 1926, **48**, 1691 (*synth*)
Cox, E.N. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1931, **50**, 848 (*synth*)
Shas, E.Y. *et al., Chem. Zentralbl.*, 1941, **2**, 636 (*rev*)
Cohen, I.R. *et al., Anal. Chem.*, 1961, **33**, 726 (*use*)
Seneca, H. *et al., Antibiot. Chemother. (Washington, D.C.)*, 1961, **11**, 587 (*Acrisorcin*)
U.S. Pat., 1964, 3 122 553, (*Bensen*); *CA*, **60**, 13231 (*Acrisorcin*)
Quercia, V. *et al., Boll. Chim. Farm.*, 1971, **110**, 428 (*ms*)
Hemenway, D.R. *et al., Am. Ind. Hyg. Assoc. J.*, 1980, **41**, 305; *CA*, **93**, 78676q (*use*)
Mizobuchi, S. *et al., Agric. Biol. Chem.*, 1985, **49**, 1327 (*synth, props*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2519
Chhabra, R.S. *et al., Fundam. Appl. Toxicol.*, 1988, **11**, 685 (*tox*)
King, J.M. *et al., J. Assoc. Off. Anal. Chem.*, 1991, **74**, 1003 (*hplc*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1134
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HFV500

2-Hexylbenzothiazole, 9CI H-263

[65718-88-9]

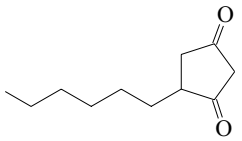


$C_{13}H_{17}NS$ 219.35
Volatile flavour component of roasted peanuts. Liq. Mp 107° (as picrate). Bp_7 141°.

Metzger, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 1692-1696 (*synth*)
Elderfield, R.C. *et al., J.A.C.S.*, 1960, **82**, 1982-1988 (*synth*)
Boger, D.L. *et al., J.O.C.*, 1978, **43**, 2296-2297 (*synth*)

4-Hexyl-1,3-cyclopentanedione, 9CI H-264

[126624-27-9]
Tsibulin 2



$C_{11}H_{18}O_2$ 182.262
Phytoalexin from *Allium cepa* bulbs (onion) infected with *Botrytis cinerea*. Pale-yellow oil. λ_{max} 207 ; 220 ; 246 (EtOH) (Berdy).

Tverskoy, L. *et al., Phytochemistry*, 1991, **30**, 799 (*isol*)

2-Hexyl-1-cyclopropaneacetic acid H-265

3,4-Methylenedecanoic acid. Cascarillic acid



$C_{11}H_{20}O_2$ 184.278

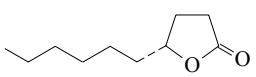
(3*R,4*S**)-*form*
trans-*form*
Component of cascarilla essential oil.

Me ester:
$C_{12}H_{22}O_2$ 198.305
Oil. $[\alpha]_D^{20}$ -10.5 (c, 0.55 in $CHCl_3$). The (±)-*cis*- and *trans*-forms have both been synthesised as their Me esters.

Motil, O. *et al., Phytochemistry*, 1972, **11**, 407 (*isol*)
Vig, B. *et al., J. Indian Chem. Soc.*, 1973, **50**, 557 (*synth*)
Wilson, S.R. *et al., Tet. Lett.*, 1976, 4231 (*synth, ir, nmr, ms*)

5-Hexyldihydro-2(3*H*)-furanone, 9CI H-266

[706-14-9]
4-Hydroxydecanoic acid lactone, 8CI. γ-Hexylbutyrolactone. γ-Decalactone. 4-Decanolide. Decanolactone



(*R*)-*form*

$C_{10}H_{18}O_2$ 170.251
▶ Skin irritant. LU4600000

(*R*)-*form* [107797-26-2]
Flavouring agent. Oil with peach-like odour. Bp 281° $Bp_{7.7}$ 140-145°. $[\alpha]_D^{20}$ +42.5 (c, 0.5 in MeOH).

(*S*)-*form* [107797-27-3]
$[\alpha]_D^{20}$ -39.2 (c, 0.4 in MeOH).

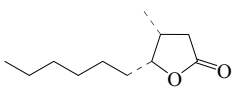
(±)-*form* [2825-92-5]
Liq. Bp 281°.

(ξ)-*form*
Component of apricot, plum and strawberry aromas.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 699A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1130B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 751C (*ir*)
Honkanen, E. *et al., Acta Chem. Scand.*, 1965, **19**, 370 (*ms*)
Sakurai, K. *et al., Yakugaku Zasshi*, 1968, **88**, 919-928 (*activity*)
Heiba, E.I. *et al., J.A.C.S.*, 1974, **96**, 7977 (*synth*)
Pyysalo, H. *et al., Finn. Chem. Lett.*, 1975, 136; *CA*, **84**, 69088m (*synth, pmr, cmr, ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, (Suppl.), 1976, **14**, 741 (*tox, rev*)
Grieco, P.A. *et al., Tet. Lett.*, 1978, 419 (*synth*)
Labows, J.N. *et al., Appl. Environ. Microbiol.*, 1979, **38**, 412; *CA*, **91**, 189438s (*isol*)
Thijs, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1986, **105**, 332 (*synth*)
Bravo, P. *et al., Tetrahedron*, 1987, **43**, 4635 (*synth*)
Flood, P.F. *et al., J. Chem. Ecol.*, 1989, **15**, 2207
Cardillo, R. *et al., Gazz. Chim. Ital.*, 1993, **122**, 489 (*stereochem*)
Yadav, J.S. *et al., Synth. Commun.*, 1993, **23**, 2731 (*synth*)
Haffner, T. *et al., J. Agric. Food Chem.*, 1996, **44**, 1218 (*biosynth*)
Kula, J. *et al., Tetrahedron*, 1996, **52**, 11321 (*synth*)
Parker, S.R. *et al., J. Agric. Food Chem.*, 1997, **45**, 2774-2776 (*activity*)
Maier, A. *et al., J. Antibiot.*, 1999, **52**, 952-959 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HKA500

5-Hexyldihydro-4-methyl-2(3*H*)-furanone H-267

[67663-01-8]
3-Methyl-4-decanolide



(4*R*,5*R*)-*form*

$C_{11}H_{20}O_2$ 184.278
Isol. from orange juice.

(4*R*,5*R*)-*form* [121644-12-0]
(+)-cis-*form*
$[\alpha]_D^{22}$ +59.8 (c, 0.4 in $CHCl_3$).

(4*RS*,5*SR*)-*form* [125133-98-4]
(±)-trans-*form*
Oil.

[147254-32-8, 147254-33-9, 252009-40-8]

Pratt, A.J. *et al., J.C.S. Perkin 1*, 1989, 1521-1527 (*synth, pmr*)
Naaf, R. *et al., J. Essent. Oil Res.*, 1996, **8**, 587-595 (*isol*)
Masuzawa, Y. *et al., Nat. Prod. Lett.*, 1999, **13**, 239-246 (*synth*)

5-Hexyldihydro-5-methyl-2(3*H*)-furanone, 9CI H-268

[7011-83-8]
4-Methyl-4-decanolide. γ-Methyldecalactone. 4-Hydroxy-4-methyldecanoic acid lactone

$C_{11}H_{20}O_2$ 184.278

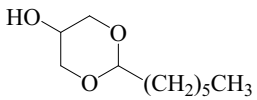
(±)-*form* [124099-86-1]
Flavouring ingredient. $Bp_{0.6}$ 110-115°. n_D^{27} 1.4470.

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 867 (*rev*)

Ho, T. *et al., Synth. Commun.*, 1982, **12**, 53-56 (*synth, ir, pmr*)
Baskaran, S. *et al., J.O.C.*, 1990, **55**, 891-895 (*synth, ir, pmr*)

2-Hexyl-1,3-dioxan-5-ol H-269

Heptanal 1,3-glyceryl acetal



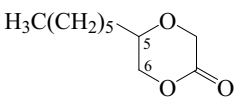
$C_{10}H_{20}O_3$ 188.266

The coml. prod. is a mixt. with 2-Hexyl-1,3-dioxolane-4-methanol, H-272. Flavouring agent for beverages, baked goods and candies.

Gj, S. *et al., Tet. Lett.*, 1967, 3153-3159 (*synth, pmr, ir*)
Pat. Coop. Treaty (WIPO), 1996, 96 29 895; *CA*, **125**, 326976c (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 715 (*use*)

5-Hexyl-1,4-dioxan-2-one, 9CI H-270

FEMA 2574



$C_{10}H_{18}O_3$ 186.25

The coml. prod. is a mixt. with the 6-hexyl isomer, H-271, to which the FEMA no. refers. Flavouring ingredient. Liq. with powerful, sweet, nut-like creamy odour.

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 789 (*use*)

6-Hexyl-1,4-dioxan-2-one, 9CI H-271

[59646-18-3]

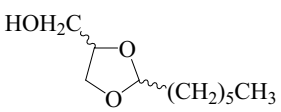
$C_{10}H_{18}O_3$ 186.25

Perfumery and flavour ingredient. Component of FEMA 2574. Liq. with aldehydic, woody, wholesome odour.

U.S. Pat., 1974, 3 959 185; *CA*, **85**, 46696q (*synth, use, ir*)

2-Hexyl-1,3-dioxolane-4-methanol H-272

[1708-35-6, 18445-09-5, 18445-22-2, 18550-94-2]
Heptanal 1,2-glyceryl acetal. FEMA 2542



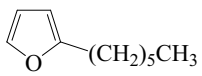
$C_{10}H_{20}O_3$ 188.266

The coml. prod. is a mixt. with 2-Hexyl-1,3-dioxan-5-ol, H-269, to which the phys. props. and FEMA no. refer. Flavouring ingredient for beverages, baked goods and candies. Viscous liq. $Bp_{0.5}$ 102-114°.

Gj, S. *et al., Tet. Lett.*, 1967, 3153-3159 (*synth, pmr, ir*)
Pat. Coop. Treaty (WIPO), 1996, 96 29 895; *CA*, **125**, 326976c (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 715 (*use*)

2-Hexylfuran H-273

[3777-70-6]



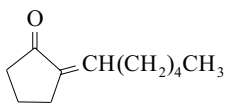
$C_{10}H_{16}O$ 152.236

Reported in roast chicken, roast lamb fat, roast peanut oil, roast guinea hen, fenugreek seed, cooked pork, coriander oil and used cooking fats. Liq. $Bp_{0.5}$ 34-36°.

Elix, J.A. *et al., J.C.S.(C)*, 1968, 595-596 (*synth, uv, pmr*)
Noleau, I. *et al., Lebensm.-Wiss. Technol.*, 1987, **20**, 37-41 (*occur*)
Sheu, J.H. *et al., J.O.C.*, 1989, **54**, 5126-5128 (*synth, pmr*)
Takeoka, G. *et al., J. Agric. Food Chem.*, 1996, **44**, 654-660 (*glc, occur, fats*)
Elmore, J.S. *et al., J. Chromatogr., A*, 2001, **905**, 233-240 (*occur, glc*)

2-Hexylidenecyclopentanone, 9CI H-274

[17373-89-6]
FEMA 2573



$C_{11}H_{18}O$ 166.263

Food flavourant. Oil with floral and green fruity odour, with spicy undertones. d_4^4 0.92. Bp 240° Bp_{17} 132.5-134° $Bp_{0.07}$ 62°.

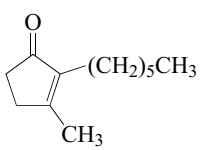
Semicarbazone: [16741-84-7]
Mp 182-183.5°.

2,4-Dinitrophenylhydrazone: [16424-97-8]
Mp 108.5-109.3°.

Fed. Regist., 1967, **32**, 7946; *CA*, **67**, 7946 (*use*)
Lardelli, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 4811 (*synth*)
Ijima, A. *et al., Chem. Pharm. Bull.*, 1973, **21**, 215 (*synth*)
Katsin, N. *et al., Synth. Commun.*, 1977, **7**, 185 (*synth*)
Sharp, D.W. *et al., Toxicology*, 1978, **9**, 261; *CA*, **89**, 101118n (*use*)
Nakamura, S. *et al., Tetrahedron*, 2001, **57**, 6703-6711 (*synth, ir, pmr*)

2-Hexyl-3-methyl-2-cyclopenten-1-one, 9CI H-275

[4868-24-0]
Homodihydrojasmone



$C_{12}H_{20}O$ 180.289

Occurs in ginger and other natural sources. Oily liq. with spicy floral odour. Bp_{20} 145-147°. n_D^{29} 1.4735.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 135°.

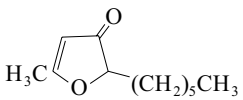
Semicarbazone:
Mp 174-175°.

Rai, C. *et al., J. Indian Chem. Soc.*, 1957, **34**, 178 (*synth*)
Jones, J.B. *et al., Can. J. Chem.*, 1972, **50**, 2718 (*synth, pmr*)
Salaün, J. *et al., Tetrahedron*, 1983, **39**, 2421 (*synth, pmr, ir*)

2-Hexyl-5-methyl-3(2*H*)-furanone, 9CI H-276

[33922-66-6]

[59462-25-8, 131320-78-0, 131320-79-1]
2-Hexyl-5-methyl-3-oxo-2,3-dihydrofuran.
Norcepanone



$C_{11}H_{18}O_2$ 182.262

(±)-*form*
Bp_3 79-81° ($Bp_{0.15}$ 78°).

(ξ)-*form*
Constit. of onions, leeks and shallots.

Boelens, M. *et al., J. Agric. Food Chem.*, 1971, **19**, 984-991 (*isol, ms, pmr, ir*)
De Rijke, D. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 731-738 (*synth, ir, pmr*)
Galetto, W.G. *et al., J. Agric. Food Chem.*, 1976, **24**, 854-856 (*synth*)
Andersen, S.H. *et al., Tetrahedron*, 1983, **39**, 2241-2245 (*synth, pmr*)
Thomas, A.F. *et al., Tet. Lett.*, 1986, **27**, 505-506 (*synth*)

2-Hexyl-3-phenyl-2-propenal H-277

[101-86-0]
2-(Phenylmethylene)octanal, 9CI. α-Hexylcinnamaldehyde, 8CI. 2-Benzylideneoctanal. FEMA 2569

$PhCH{=}C(CHO)(CH_2)_5CH_3$

$C_{15}H_{20}O$ 216.322

Flavouring agent. d_4^{25} 0.95. Mp 4°. Bp 252° Bp_{20} 169° Bp_{15} 174-176°. n_D^{25} 1.5268.

▶ Skin irritant. Fl. p. >100°. GD6560000

Semicarbazone:
Mp 111.2°.

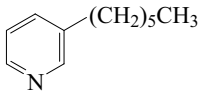
2,4-Dinitrophenylhydrazone:
Mp 149°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 927C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1282A (*ir*)
Shoruigin, P. *et al., Zh. Russ. Fiz.-Khim. Ova., Chast Khim.*, 1930, **62**, 2033; *CA*, **25**, 4247[6] (*synth*)
Seiichi, U. *et al., Nippon Kagaku Kaishi*, 1949, **52**, 142; *CA*, **45**, 2150c (*synth*)
Japan. Pat., 1971, 71 10 540; *CA*, **75**, 35424s (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, (Suppl.), 1974, **12**, 915 (*tox, rev*)

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HFO500
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

3-Hexylpyridine, 9CI H-278

[6311-92-8]

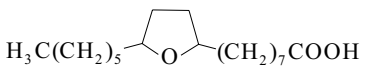


$C_{11}H_{17}N$ 163.262
Found in orange oil. Perfumery and flavouring ingredient. Liq. with sweet fragrance. $Bp_{0.08}$ 65-71°.

Eur. Pat., 1992, 470 391; *CA*, **116**, 194165 (*synth, use*)
Thomas, A.F. *et al., J. Agric. Food Chem.*, 1992, **40**, 2236-2243 (*synth, isol, ms, pmr*)
Tereshko, A.B. *et al., Zh. Org. Khim.*, 1995, **31**, 289-290; *J. Org. Chem. USSR (Engl. Transl.)*, 1995, **31**, 258-259 (*synth*)
Schwab, P.F.H. *et al., J.O.C.*, 2002, **67**, 443-449 (*synth, pmr*)

5-Hexyltetrahydro-2-furanoctanoic acid, 9CI H-279

[61781-98-4]
9,12-Epoxyoctadecanoic acid

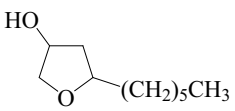


$C_{18}H_{34}O_3$ 298.465
Present in heat-treated soybean oil. Diastereoisomeric mixt..

Abbot, G.G. *et al., Chem. Phys. Lipids*, 1970, **4**, 351; 1971, **7**, 303 (*synth, ms*)
Doi, H. *et al., Yukagaku*, 1976, **25**, 831 (*isol*)

5-Hexyltetrahydro-3-furanol, 9CI H-280

2-Hexyl-4-hydroxytetrahydrofuran



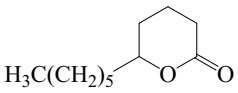
$C_{10}H_{20}O_2$ 172.267

Ac: [10039-39-1] *4-Acetoxy-2-hexyltetrahydrofuran*
$C_{12}H_{22}O_3$ 214.304
Liq. with sweet fruity odour/taste. Formerly designated ∗FEMA 2566∗. The material formerly given this struct. has been shown to be a mixture of several non-isomeric compounds. In view of this it has been removed from the GRAS list.

Hall, R.L. *et al., Food Technol. (Chicago)*, 1970, **24**, 533-542

6-Hexyltetrahydro-2*H*-pyran-2-one, 9CI H-281

[710-04-3]
5-Hydroxyundecanoic acid lactone, 8CI. 1,5-Undecanolactone. FEMA 3294



$C_{11}H_{20}O_2$ 184.278

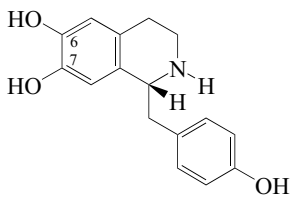
(±)-*form* [118100-37-1]
Flavouring reagent. d 0.97. $Bp_{10.5}$ 152-155°. Enantiomers also reported in the lit. but not well descr..

[108861-12-7, 108861-13-8]

Stoll, M. *et al., Helv. Chim. Acta*, 1938, **21**, 1547 (*synth*)

Higenamine H-282

[17072-47-8]
1,2,3,4-Tetrahydro-1-[(4-hydroxyphenyl)-methyl]-6,7-isoquinolinediol, 9CI. 1,2,3,4-Tetrahydro-6,7-dihydroxy-1-(4-hydroxybenzyl)isoquinoline. Demethylcoclaurine



(*R*)-*form*

$C_{16}H_{17}NO_3$ 271.315
Historically, Higenamine was the racemate and Demethylcoclaurine the opt. active form, probably the (*S*)-form.

(*R*)-*form* [106032-53-5]
Alkaloid from the seed embryo of *Nelumbo nucifera* (East India lotus). Prisms (EtOH). Mp 242-244° dec. $[\alpha]_D^{26.5}$ +16 (c, 1 in MeOH). Abs. config. not proven.

N-*Me,* N-*oxide(*R-*):* [240430-84-6] **N-*Methylhigenamine* N-*oxide***
$C_{17}H_{19}NO_4$ 301.341
Needles (H_2O). Mp 156-159°. $[\alpha]_D$ -9.6 (c, 0.12 in DMSO). λ_{max} 225 (sh) (log ε 4.35); 284 (log ε 3.64) (H_2O).

O^6-*Me:* [2196-60-3]

[486-39-5] ***Coclaurine***. *Sanjoinine K*
$C_{17}H_{19}NO_3$ 285.342
Mp 217-218°. $[\alpha]_D$ +47 (EtOH).

O^6-*Me,* N,O,O-*tri-Ac:*
Mp 199°. $[\alpha]_D$ -76 (EtOH).

O^6,N-*Di-Me:* [5096-70-8] **N-*Methylcoclaurine***
$C_{18}H_{21}NO_3$ 299.369
Mp 182-183°. $[\alpha]_D$ -80 (c, 0.17 in EtOH). $[\alpha]_D$ -62 (c, 0.13 in $CHCl_3$). Remarkably (+)-Coclaurine forms a (-)-*N*-methyl deriv..

O^7-*Me:* [574-75-4] ***Isococlaurine***
$C_{17}H_{19}NO_3$ 285.342
Plates (MeOH). Mp 216-217°. $[\alpha]_D$ +12 (MeOH).

O^7-*Me, hydrochloride:*
Plates + $1H_2O$ (H_2O). Mp 175-176°. $[\alpha]_D$ +28 (H_2O). $[\alpha]_D$ +16 (MeOH).

O^6,O^7-*Di-Me:* See Armepavine, A-410

O^6,N,N-*Tri-Me:* [6801-40-7] ***(-)-Magnocurarine***
$C_{19}H_{24}NO_3^{\oplus}$ 314.404
Mp 199-200° (as chloride). $[\alpha]_D$ -91 (H_2O).

O^7,N,N-*Tri-Me:* [6871-67-6] ***Lotusine***
$C_{19}H_{24}NO_3^{\oplus}$ 314.404
Quaternary alkaloid from the embryo of *Nelumbo nucifera* (East India lotus). Mp 213-215° (as chloride). $[\alpha]_D$ -15 (MeOH) (chloride). Another natural product (cyanogenic glycoside) reported in 1901 and named Lotusin was erroneous.

$O^{4'}$,N,N-*Tri-Me:* [107584-81-6] ***Luxandrine***
$C_{19}H_{24}NO_3^{\oplus}$ 314.404
Pale brown amorph. solid (as chloride). $[\alpha]_D$ +27 (c, 0.24 in $CHCl_3$/MeOH). Dec. in soln..

$O^{4'}$,O^6,N-*Tri-Me:* [19879-50-6] **N-*Demethylcolletine***. *4′-Methyl*-N-*methylcoclaurine*
$C_{19}H_{23}NO_3$ 313.396
Oil. $[\alpha]_D^{20}$ -74 (c, 0.7 in MeOH).

$O^{4'}$,O^6,N,N-*Tetra-Me:* [15500-51-3] ***Colletine***
$C_{20}H_{26}NO_3^{\oplus}$ 328.43
Cryst. + $1H_2O$ (EtOAc/EtOH) (as chloride). Mp 130-132° (chloride). $[\alpha]_D^{20}$ -132.8 (c, 1.07 in EtOH).

(*S*)-*form* [22672-77-1]

O^7-*Me:*
Cryst. (MeOH). Mp 195-197°. $[\alpha]_D$ -14 (c, 0.5 in MeOH).

O^7-*Me, hydrochloride:*
Needles (MeOH). Mp 242-243°. $[\alpha]_D$ -18 (c, 0.5 in MeOH). $[\alpha]_D$ -27.5 (c, 1.0 in H_2O).

O^6,N-*Di-Me:* [3423-07-2]
Mp 134-136° Mp 176-177°. $[\alpha]_D^{22}$ +82 (c, 0.496 in EtOH).

O^6,N-*Di-Me,* O^7-*α-D-xylopyranoside:* [93631-49-3] ***Latericine***
$C_{23}H_{29}NO_7$ 431.485
Needles + 1MeOH (MeOH). Mp 216-223°. $[\alpha]_D$ +93 (c, 0.555 in EtOH). $[\alpha]_D$ +40 (c, 0.521 in Py). Stereochem. incorrectly assigned in CAS.

O^6,N,N-*Tri-Me:* [63428-12-6] ***(+)-Magnocurarine***
$C_{19}H_{24}NO_3^{\oplus}$ 314.404
Mp 199-200° dec.(as chloride). $[\alpha]_D^{22}$ +106 (c, 1 in H_2O).

$O^{4'}$,O^7,N-*Tri-Me:* [131724-50-0] ***Roefractine***
$C_{19}H_{23}NO_3$ 313.396
Amorph. $[\alpha]_D$ +73 (c, 0.14 in MeOH).

O,O,O-*Tri-Me,* N-*oxide:***O-*Methylroefractine* N-*oxide***
$C_{20}H_{25}NO_4$ 343.422
$[\alpha]_D$ -2.3 (c, 1.7 in H_2O). λ_{max} 230 (log ε 4.4); 285 (log ε 3.61) (no solvent reported).

O,O,O,N,N-*Penta-Me:*
Mp 115° dec. (hydrate) (as iodide) Mp 139° dec (anhyd.) (iodide).

(±)-*form* [5843-65-2]

Hydrochloride:
Mp 265° (258° dec.).

Hydrobromide:
Mp 269-270°.

N-*Me:* [66277-20-1] **N-*Methylhigenamine***
$C_{17}H_{19}NO_3$ 285.342
Cryst. (EtOH). Mp 148-150°. λ_{max} 225 (sh) (log ϵ 4.6); 285 (log ϵ 4.08) (EtOH).

O^6-*Me:*
Mp 220-221°.

O^7-*Me:*
Mp 135-136°.

O^7-*Me, hydrochloride:*
Mp 215°.

O^6,N-*Di-Me:* [1472-62-4]
Mp 161-162° (anhyd.).

(ξ)-*form*

4′-O-*β*-D-*Glucopyranoside:* [192324-89-3]
$C_{22}H_{27}NO_8$ 433.457
$[\alpha]_D$ -2.3 (c, 0.4 in MeOH). λ_{max} 200 ; 222 ; 292 (no solvent reported).

N-*Me,* O^7-*β*-D-*glucopyranoside:* [154418-17-4] **N-*Methylhigenamine 7*-O-*β*-D-*glucopyranoside***
$C_{23}H_{29}NO_8$ 447.484
Pale brownish prisms + $2^1/_2H_2O$ (Py aq.). Mp 158-159°. $[\alpha]_D$ -35.8 (c, 1.0 in Py).

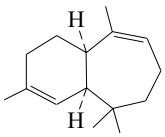
[94997-19-0]

King, H. *et al., J.C.S.*, 1940, 737 (*Isococlaurine*)
Finkelstein, J. *et al., J.A.C.S.*, 1951, **73**, 550 (*synth, Coclaurine*)
Tomita, M. *et al., Yakugaku Zasshi*, 1951, **71**, 1069; *CA*, **46**, 5059 (*Magnocurarine*)
McKenzie, A.K. *et al., Aust. J. Chem.*, 1953, **6**, 180 (*Magnocurarine*)
Arndt, R.R. *et al., J.C.S.*, 1963, 2547 (*deriv*)
Furukawa, H. *et al., Yakugaku Zasshi*, 1965, **85**, 335; 472; *CA*, **63**, 4351d; 5692d (*4′-Methyl-N-methylcoclaurine, Lotusine*)
Preininger, V. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 3345 (*Latericine*)
Albonico, S.M. *et al., J.C.S.(C)*, 1966, 1340 (*uv, ord, abs config, Colletine, Magnocurarine*)
Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 1729 (*isol, pmr, ms, Coclaurine*)
Sanchez, E. *et al., Tetrahedron*, 1967, **23**, 1139 (*Colletine*)
Fridrichsons, J. *et al., Tetrahedron*, 1968, **24**, 5785 (*cryst struct, Coclaurine*)
Koshiyama, H. *et al., Chem. Pharm. Bull.*, 1970, **18**, 2564 (*isol, uv, ir, pmr, ms, struct, synth, Demethylcoclaurine*)
Bhakuni, D.S. *et al., Tetrahedron*, 1972, **28**, 1093 (*abs config, Isococlaurine*)
Masaki, N. *et al., J.C.S. Perkin 1*, 1977, 717 (*cryst struct, Demethylcoclaurine*)
Torres, R. *et al., J. Nat. Prod.*, 1979, **42**, 430 (*N-Demethylcolletine*)
Saxena, N.K. *et al., J. Indian Chem. Soc.*, 1980, **57**, 773 (*uv, ir, pmr, Lotusine*)
Nishibe, S. *et al., J. Nat. Prod.*, 1986, **49**, 547 (*4′-Methyl-N-methylcoclaurine*)
Cortes, D. *et al., Phytochemistry*, 1986, **25**, 2693 (*Luxandrine*)
Han, B.H. *et al., Pure Appl. Chem.*, 1989, **61**, 443 (*isol, Coclaurine*)
Gozler, B. *et al., J. Nat. Prod.*, 1990, **53**, 666 (*Roefractine*)
Ida, Y. *et al., Phytochemistry*, 1994, **35**, 209 (*N-Methylhigenamine 7-glucoside*)
Hegde, V.R. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 1207-1212 (*glucoside*)
Xu, Q. *et al., J. Nat. Prod.*, 1999, **62**, 1025-1027 (*N-Methylhigenamine oxide*)

2,7-Himachaladiene H-283

[53111-25-4]

***γ*-Himachalene**

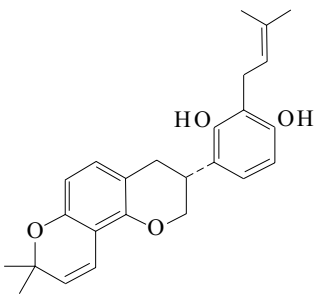


$C_{15}H_{24}$ 204.355
Constit. of the essential oil of anise (aniseed). Oil. $[\alpha]_D^{24}$ -9 (c, 0.24 in $CHCl_3$).

Plattier, M. *et al., Recherches*, 1974, **19**, 145 (*struct*)
Tabacchi, R. *et al., Helv. Chim. Acta*, 1974, **57**, 849 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1985, **24**, 505 (*isol*)

Hispaglabridin A H-284

*4-(3,4-Dihydro-8,8-dimethyl-2*H,*8*H-*benzo[1,2*-b:*3,4*-b′*]dipyran-3-yl)-2-(3-methyl-2-butenyl)-1,3-benzenediol, 9CI*



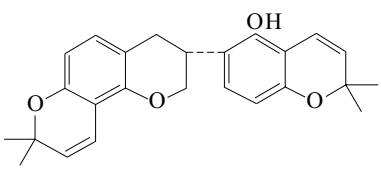
$C_{25}H_{28}O_4$ 392.494Log P 6.05 (calc).
λ_{max} 281 (ϵ 11600); 290 ; 312 (MeOH) (Berdy).

(*R*)-*form* [68978-03-0]
Isol. from *Glycyrrhiza glabra* (licorice). Cryst. (cyclohexane). Mp 132-133°. $[\alpha]_D^{25}$ -8.23 (c, 2.43 in $CHCl_3$). Pharmacol. active isomer.

Mitscher, L.A. *et al., Heterocycles*, 1978, **9**, 1533 (*isol, struct, synth*)
Mitscher, L.A. *et al., J. Nat. Prod.*, 1980, **43**, 259 (*isol, struct*)
Kinoshita, T. *et al., Heterocycles*, 1996, **43**, 581 (*isol, pmr, cmr, ms*)

Hispaglabridin B H-285

*6-(3,4-Dihydro-8,8-dimethyl-2*H,*8*H-*benzo[1,2*-b:*3,4*-b′*]dipyran-3-yl)-2,2-dimethyl-2*H-*1-benzopyran-5-ol, 9CI*



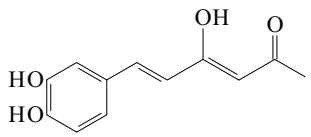
$C_{25}H_{26}O_4$ 390.478
Log P 6.09 (calc).
λ_{max} 280 (ϵ 14800); 290 ; 309 (MeOH) (Berdy).

(*R*)-*form* [68978-02-9]
Isol. from *Glycyrrhiza glabra* (licorice). Amorph. Mp 84-86°. $[\alpha]_D^{25}$ -32.4 (c, 0.2 in $CHCl_3$). Pharmacol. active isomer.

Mitscher, L.A. *et al., Heterocycles*, 1978, **9**, 1533 (*isol, struct, synth*)
Mitscher, L.A. *et al., J. Nat. Prod.*, 1980, **43**, 259 (*isol, struct*)
Kinoshita, T. *et al., Heterocycles*, 1996, **43**, 581 (*isol, pmr, cmr, ms*)

Hispolone H-286

[173933-40-9]
6-(3,4-Dihydroxyphenyl)-4-hydroxy-3,5-hexadien-2-one. 6-(3,4-Dihydroxyphenyl)-5-hexene-2,4-dione

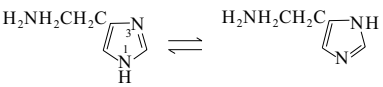


$C_{12}H_{12}O_4$ 220.224
Enolised β-diketone. Isol. from the mushroom *Inonotus hispidus*, of uncertain palatability. Sol. MeOH, EtOAc. Mp 137°. λ_{max} 258 (ϵ 4900); 373 (ϵ 22400) (MeOH). λ_{max} 258 (ϵ 4898); 373 (ϵ 22387) (MeOH) (Berdy).

Ali, N.A.A. *et al., Phytochemistry*, 1996, **41**, 927 (*isol, uv, ir, pmr, cmr, ms*)

Histamine H-287

[51-45-6]
*1*H-*Imidazole-4-ethanamine, 9CI. 4-(2-Aminoethyl)-1*H-*imidazole. Ergamine. Scombrotoxin*



$C_5H_9N_3$ 111.146
1*H*-form predominates *ca*. 4:1 in aq. soln. At physiological pH exists as a mixt. of base: monocation: dication in ratio 1:96:3 with both base and monocation capable of $1H \Leftrightarrow 3H$ tautom..Sol. H_2O, MeOH. Mp 86°. $Bp_{0.8}$ 167°. pK_{a1} 6.02; pK_{a2} 9.7 (25°, 0.1*M* KCl).
▶ Adverse human effects by subcutaneous (and other non-oral routes of) administration. Potent capillary dilator. Allergic skin effects. Exp. reprod. effects. LD_{50} (rat, ivn) 630 mg/kg; LD_{50} (mus, ims) 12 mg/kg. MS1050000

Hydrochloride (1:2): [56-92-8] ***Histamine dihydrochloride, USAN. Amin-Glaukosan. Histamyl. Imido. Peremin. Many other names***
Mp 244-246°.
▶ Exp. reprod. effects. LD_{50} (mus, ivn) 370 mg/kg. MS1575000

Phosphate (1:2): [6890-40-0]

[51-74-1] ***Histamine phosphate, USAN. Histapon***
Mp 140°.

Dipicrate:
Mp 239°.

ω-N-*Ac:* [673-49-4] **N-*Acetylhistamine***
$C_7H_{11}N_3O$ 153.183
Isol. from leaves of *Spinacia oleracea* (spinach). Prisms (EtOH/Et_2O or

EtOH/EtOAc). Mp 147-148°.

ω-N-*(4-Oxodecanoyl):* [7222-82-4] **N^{α}-*(4-Oxodecanoyl)histamine***
$C_{15}H_{25}N_3O_2$ 279.381
Cryst. ($CHCl_3$ or $CHCl_3$/EtOH). Mp 115-117°. Easily converted into Glochidine and Glochidicine.

ω-N-*(2-Methylbutanoyl):* See Dolichotheline in *The Combined Chemical Dictionary.*

ω-N-*Cinnamoyl:* See N^{α}-Cinnamoylhistamine in *The Combined Chemical Dictionary.*

ω-N-*Me:* [673-50-7] **N-*Methylhistamine***
$C_6H_{11}N_3$ 125.173
▶ NI7355000

ω-N-*Me; hydrochloride (1:2):*
Mp 176-177°.

ω-N-*Me, picrate (1:2):*
Mp 188°.

ω-N-*Me, 1*-N-*β*-D-*glucopyranosyl:* [490-41-5] *1-β-*D*-Glucosyl*-N-*methylhistamine. Casimidine*
$C_{12}H_{21}N_3O_5$ 287.315
Cryst. (MeOH). Mp 207-209°. $[\alpha]_D$ +11 (EtOH).

ω-N-*Di-Me:* See 4-[2-(Dimethylamino)ethyl]imidazole, D-752

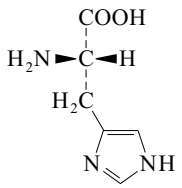
N^1-*Me:* [501-75-7] tele-*Methylhistamine*
$C_6H_{11}N_3$ 125.173
Cryst. (EtOH aq.). Mp 218-219° (as picrate). Metab. of histamine.

N^1-*Me, hydrochloride (1:2):* [6481-48-7]
Cryst. (EtOH). Mp 205-207°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 489B; 492C (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 617D; 623B (*ir*)
Koessler, K.K. *et al., J.A.C.S.*, 1918, **40**, 1716 (*synth*)
Tabor, H. *et al., J. Biol. Chem.*, 1949, **180**, 703 (*isol, synth, N-Acetylhistamine*)
Appel, W. *et al., Arzneim.-Forsch.*, 1959, **9**, 22 (*isol, derivs*)
Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 555 (*ω-N-(4-Oxodecanoyl)histamine*)
Reisch, J. *et al., J. Pharm. Pharmacol.*, 1968, **20**, 81 (*ms*)
Fales, H.M. *et al., Arch. Mass Spectral Data*, 1971, **2**, 650 (*ms*)
Milne, G.W.A. *et al., Anal. Chem.*, 1973, **45**, 1952 (*cims*)
Ganellin, C.R. *et al., J. Med. Chem.*, 1973, **16**, 610 (*pmr*)
Bonnet, J.J. *et al., J.A.C.S.*, 1973, **95**, 4829 (*cryst struct*)
Panzcia, R.P. *et al., J.A.C.S.*, 1973, **95**, 8737 (*Casimidine*)
Roseghini, M. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1976, **54**, 31 (*occur, derivs*)
Durant, G.J. *et al., J. Med. Chem.*, 1976, **19**, 923 (N^1-*Me*)
Bryn, S.R. *et al., J.O.C.*, 1976, **41**, 2283 (*conformn*)
Roseghini, M. *et al., Z. Naturforsch., C*, 1976, **31**, 118 (*occur, derivs*)
Reynolds, W.F. *et al., Can. J. Biochem.*, 1977, **55**, 576 (*cmr, tautom*)
Bertaccini, G. *et al., Handb. Exp. Pharmacol.*, 1982, **59**, 201 (*rev*)
Green, J.P. *et al., Agents Actions*, 1987, **22**, 1 (*rev, metab*)
Potvin, P.G. *et al., Chem. Comm.*, 1987, 672 (N^1-*Me*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 321
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 775
Worth, G.A. *et al., J.A.C.S.*, 1994, **116**, 239 (*tautom*)
Al-Badr, A.A. *et al., Anal. Profiles Drug Subst.*, 2001, **27**, 159-264 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HGD000; HGE000; HGD500

Histidine, INN, USAN H-288

[7006-35-1]
*α-Amino-1*H*-imidazole-4-propanoic acid, 9CI. 2-Amino-3-imidazolylpropionic acid. 3-(1-Imidazolyl)alanine. His*


(*S*)-*form*

$C_6H_9N_3O_2$ 155.156
The tautomerism of histidine in soln. does not appear very well documented. Both imidazole tautomers presumably present.

(*S*)-*form* [71-00-1]
L-*form. FEMA 3694*
Flavouring ingredient; dietary supplement, nutrient. Sol. H_2O (7.59 g per 100 cm^3 at 25°); sl. sol. EtOH. Mp 277° dec. $[\alpha]_D^{25}$ -59.8 (-38.5) (H_2O). $[\alpha]_D^{25}$ +18.3 (+11.8) (5*M* HCl). Isoelectric point pH 7.59. Bitter taste.
▶ Exp. reprod. effects (large dose). MS3070000

Hydrochloride: [645-35-2]

[1007-42-7, 5934-29-2, 6027-02-7, 7048-02-4]
Mp 254° dec. (as monohydrate).

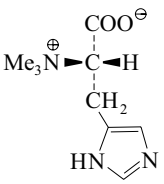
N^{α}-*Ac:* [2497-02-1]

[39145-52-3] N-*Acetylhistidine*
$C_8H_{11}N_3O_3$ 197.193
Constit. of the tissues of various fish and amphibian spp.. Cryst. (H_2O). Mp 169° (157-159° (dec.)) Mp 187° (hydrate). $[\alpha]_D^{25}$ +46.8 (c, 1 in H_2O).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 492D; 493A; 493B; 493C; 493D (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 621B; 621D; 622C; 623A; **2**, 621B; 621C; 621D; 622C; 622D; 623A (*ir*)
Org. Synth., 1938, **18**, 43 (*synth*)
Celander, D.R. *et al., J. Biol. Chem.*, 1953, **202**, 339 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., Vol. 3, 1961, 1971 (*rev*)
Martin, R.B. *et al., J.A.C.S.*, 1965, **87**, 1065 (*pmr*)
Bennett, I. *et al., Acta Cryst. B*, 1970, **26**, 1722 (*cryst struct, hydrochloride*)
Oda, K. *et al., Acta Cryst. B*, 1972, **28**, 639 (*cryst struct, hydrochloride*)
Madden, J.J. *et al., Acta Cryst. B*, 1972, **28**, 2377 (*cryst struct*)
Kistenmacher, T.L. *et al., Acta Cryst. B*, 1972, **28**, 3352 (*N-Ac, cryst struct*)
Shrager, R.I. *et al., Biochemistry*, 1972, **11**, 541 (*nmr*)
Kistenmacher, T.J. *et al., Cryst. Struct. Commun.*, 1973, **2**, 673 (*cryst struct*)
Reynolds, W.F. *et al., J.A.C.S.*, 1973, **95**, 328 (*cmr*)
Matthews, H.R. *et al., J.A.C.S.*, 1973, **95**, 2297-2303 (*synth, uv, pmr, ms*)
Edington, P. *et al., Acta Cryst. B*, 1974, **30**, 204 (*cryst struct*)
Schwerzer, B. *et al., J. Prakt. Chem.*, 1979, **321**, 1007-1016 (*cmr, N-15 nmr*)
Pedroso, E. *et al., J. Het. Chem.*, 1986, **23**, 921-924 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HGE700
Reddy, A.V. *et al., Synth. Commun.*, 1992, **22**, 257-264 (*N-Acetylhistidine*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 356
Mostad, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1995, **210**, 114 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1340-1341
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HGE700

Histidine trimethylbetaine H-289

[507-29-9]
α-Carboxy-N,N,N-*trimethyl-1*H*-imidazole-4-ethanaminium hydroxide inner salt, 9CI. (1-Carboxy-2-imidazol-4-ylethyl)trimethylammonium hydroxide inner salt, 8CI. Hercynin. Erzinine. Herzynine*



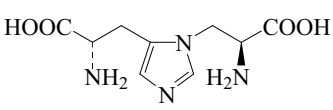
$C_9H_{15}N_3O_2$ 197.236

(*S*)-*form* [534-30-5]
L-*form*
Prod. by fungi, e.g. *Boletus edulis* (porcini), *Agaricus bisporus* (button mushroom). Mp 237-238° dec. $[\alpha]_D^{22}$ +44.5 (c, 1 in 5*M* HCl).

Barger, G. *et al., J.C.S.*, 1911, 2336 (*synth*)
Reinhold, V.N. *et al., J. Med. Chem.*, 1968, **11**, 258 (*synth*)
Tan, C.H. *et al., Phytochemistry*, 1968, **7**, 109 (*isol*)
Espersen, W.G. *et al., J. Phys. Chem.*, 1976, **80**, 741 (*cmr*)
Champavier, Y. *et al., Enzyme Microb. Technol.*, 2000, **26**, 243-251 (*activity*)

N^{π}-Histidinylalanine H-290

*α,α′-Diamino-1*H*-imidazole-1,5-dipropanoic acid.* N-*π-Histidinoalanine*



$C_9H_{14}N_4O_4$ 242.234

(*S,S*)-*form* [87047-17-4]
Isol. from heated milk and from the

extrapallial fluid of the estuarine clam (*Rangia cuneata*). Characterised spectroscopically.

Sass, R.L. *et al., Biochem. Biophys. Res. Commun.*, 1983, **114**, 304-309 (*isol, clam, pmr, cmr*)

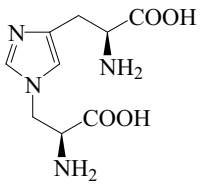
Henle, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1993, **197**, 114-117 (*occur, milk*)

N^{τ}-Histidinylalanine H-291

[103974-26-1]

[141949-35-1]

*α,α′-Diamino-1*H*-imidazole-1,4-dipropanoic acid.* N-*τ-Histidinoalanine. HAL*



$C_9H_{14}N_4O_4$ 242.234

(*S,S*)-*form* [65428-77-5]

Present in heated milk. Implicated in non-enzymic casein crosslinking of UHT milk and of yoghurts prepared from UHT milk. Also present in the extrapallial fluid of the estuarine clam (*Rangia cuneata*). Characterised spectroscopically.

Fujimoto, D. *et al., Biochem. Biophys. Res. Commun.*, 1982, **104**, 1102-1106 (*S,S-form, occur, synth, pmr*)

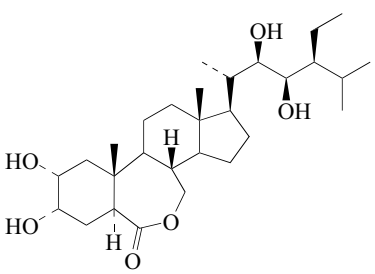
Sass, R.L. *et al., Biochem. Biophys. Res. Commun.*, 1983, **114**, 304-309 (*isol, clam, pmr, cmr*)

Friedman, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 1295-1319 (*rev, occur*)

Lauber, S. *et al., Nahrung*, 2001, **45**, 215-217 (*occur*)

28-Homobrassinolide H-292

[80483-89-2]



$C_{29}H_{50}O_6$ 494.71

Constit. of chinese cabbage (*Brassica rapa* ssp. *pekinensis*). Cryst. (EtOH). Mp 269-270°.

23-Epimer: [82373-95-3]

$C_{29}H_{50}O_6$ 494.71

Cryst. (EtOAc/hexane). Mp 195-196°. Two further stereoisomers also occur.

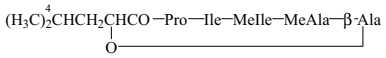
Hazra, B.G. *et al., Liebigs Ann./Recl.*, 1997, 1029-1034 (*synth, bibl*)

Yokota, T. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 526-531 (*stereoisomers*)

Homodestruxin B H-293

[110538-19-7]

*3-(*N*-Methyl-L-isoleucine)destruxin B, 9CI*



$C_{31}H_{53}N_5O_7$ 607.789

Cyclic depsipeptide antibiotic.Powder. Mp 202-204°. Analogue of Destruxins, D-95.

4-Hydroxy: ***Hydroxyhomodestruxin B***

$C_{31}H_{53}N_5O_8$ 623.788

Constit. of the leaves of *Sinapis alba* (white mustard). $[\alpha]_D^{24}$ -196 (c, 0.14 in MeOH).

Ayer, W.A. *et al., J. Nat. Prod.*, 1987, **50**, 400; 408 (*isol, ir, pmr*)

Krasnoff, S.B. *et al., J. Nat. Prod.*, 1996, **59**, 485 (*isol, pmr, cmr, ms*)

Pedras, M.S.C. *et al., Org. Lett.*, 1999, **1**, 1655-1658 (*Hydroxyhomodestruxin B*)

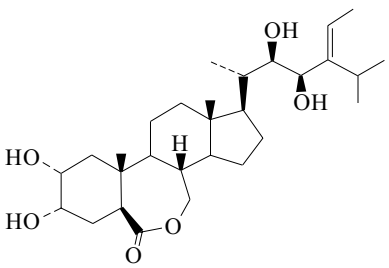
Ward, D.E. *et al., J.O.C.*, 2001, **66**, 7832-7840 (*synth*)

Pedras, M.S.C. *et al., Phytochemistry*, 2002, **59**, 579-596 (*rev*)

Homodolicholide H-294

[86630-40-2]

*2α,3α,22*R*,23*R*-Tetrahydroxy-B-homo-7-oxa-5α-stigmast-24(28)-en-6-one*



$C_{29}H_{48}O_6$ 492.695

Constit. of *Dolichos lablab* (hyacinth bean). Needles +1H_2O (MeCN aq.). Mp 227-228° (214-216° dec., sinters at 200°). $[\alpha]_D^{21}$ +35.4 (c, 0.48 in $CHCl_3$/MeOH).

Sakakibara, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 1407 (*synth*)

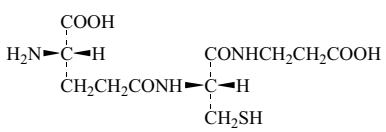
Yokota, T. *et al., Agric. Biol. Chem.*, 1983, **47**, 1409 (*isol, struct*)

Mori, K. *et al., Tetrahedron*, 1984, **40**, 1767 (*synth*)

Yokota, T. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 526-531 (*stereoisomer*)

Homoglutathione H-295

N-*[1-[(2-Carboxyethyl)carbamoyl]-2-mercaptoethyl]glutamine, 8CI. γ-Glutamylcysteinyl-β-alanine*



$C_{11}H_{19}N_3O_6S$ 321.354

L-L-*form* [18710-27-5]

Occurs in seeds of various legumes.

Hygroscopic. $[\alpha]_D^{20}$ -16.4 (c, 1.3 in H_2O).

S-*Me:* [102148-91-4] **S-*Methylhomoglutathione***. *γ-Glutamyl*-S-*methylcysteinyl-β-alanine*

$C_{12}H_{21}N_3O_6S$ 335.38

Constit. of the seeds of the mung bean (*Vigna radiata*).

Disulfide: ***Bis-γ-glutamylcysteinylbis-β-alanine***. N,N′-*[Dithiobis[1-[(2-carboxyethyl)carbamoyl]ethylene]]diglutamine*

$C_{22}H_{36}N_6O_{12}S_2$ 640.691

Peptide present in the seeds of the mung bean (*Vigna radiata*). Needles (H_2O). Mp 194-197°. $[\alpha]_D^{20.5}$ -59.5 (c, 0.5 in H_2O). The name Homoglutathione appears to be used for both the tripeptide and its disulfide.

Carnegie, P.R. *et al., Biochem. J.*, 1963, **89**, 459; 471 (*isol, struct*)

Neish, W.J.P. *et al., Tetrahedron*, 1963, **19**, 2031 (*synth*)

Camble, R. *et al., J.C.S.(C)*, 1968, 1219 (*synth*)

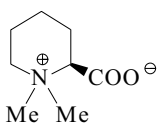
Kasai, T. *et al., Phytochemistry*, 1986, **25**, 679 (*S-Methylhomoglutathione*)

Klapheck, S. *et al., Physiol. Plant.*, 1988, **74**, 727; *CA*, **110**, 92132k (*isol, occur*)

Homostachydrine H-296

[1195-94-4]

2-Carboxy-1,1-dimethylpiperidinum hydroxide inner salt, 9CI. Pipecolic acid methylbetaine



(*S*)-*form*

$C_8H_{15}NO_2$ 157.212

(*S*)-*form* [472-22-0]

Isol. from seeds of *Medicago sativa* (alfalfa). Also from *Achillea millefolium* (yarrow). Fine needles. Mp 300° dec. $[\alpha]_D$ -9 (H_2O).

Hydrochloride:

Mp 216-217° dec. $[\alpha]_D$ -13.3 (c, 1.43 in EtOH).

(±)-*form*

V. hygroscopic cryst. Mp 207-208°.

Hydrochloride:

Mp 210-211° dec.

Wiehler, G. *et al., Can. J. Chem.*, 1958, **36**, 339 (*isol, struct, synth*)

Robertson, A.V. *et al., Can. J. Chem.*, 1959, **37**, 829 (*abs config*)

Beyerman, H.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1959, **78**, 134 (*abs config*)

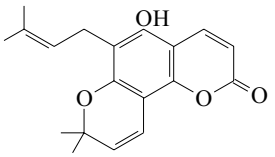
Pailer, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1960, **293**, 646 (*isol*)

Buechel, K.H. *et al., Chem. Ber.*, 1962, **95**, 2453 (*synth*)

Honyudisin H-297

[114542-45-9]

*5-Hydroxy-8,8-dimethyl-6-(3-methyl-2-butenyl)-2*H*,8*H*-benzo[1,2-*b*:3,4-*b′*]dipyran-2-one, 9CI*

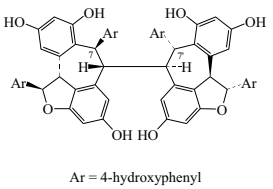


$C_{19}H_{20}O_4$ 312.365
Constit. of *Citrus grandis* (pummelo). Yellowish-green granules (EtOAc/hexane). Mp 179-180°.

Wu, T.-S. *et al., Phytochemistry*, 1988, **27**, 585

Hopeaphenol H-298

[17912-85-5]



Absolute Configuration

Ar = 4-hydroxyphenyl

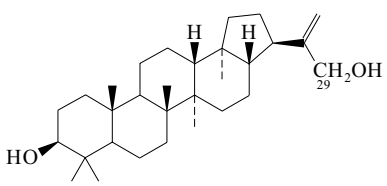
$C_{56}H_{42}O_{12}$ 906.941
Plates (MeOH/AcOH). Mp 351°. $[\alpha]_D$ -407 (EtOH).

Deca-Ac:
Needles (MeOH). Mp 249-250°. $[\alpha]_D$ -338 ($CHCl_3$).

7,7′-Diepimer: ***Isohopeaphenol***
$C_{56}H_{42}O_{12}$ 906.941
Isol. from *Vitis vinifera* (wine grape). Pale brown powder. $[\alpha]_D$ -114.5 (c, 0.4 in MeOH). λ_{max} 210 (ϵ 98800); 229 (ϵ 66600); 284 (ϵ 16800) (MeOH).

Coggan, P. *et al., J.C.S.*, 1965, 406 (*isol*)
Madhav, R. *et al., Tet. Lett.*, 1965, 2713 (*isol*)
Coggan, P. *et al., J.C.S.(B)*, 1970, 884 (*cryst struct, abs config*)
Kawabata, J. *et al., J.A.C.S.*, 1992, **114**, 1115 (*pmr, cmr*)
Kawabata, J. *et al., Magn. Reson. Chem.*, 1992, **30**, 6 (*pmr, cmr*)
Sotheeswaran, S. *et al., Phytochemistry*, 1993, **32**, 1083 (*rev, bibl*)
Ito, J. *et al., Heterocycles*, 1997, **45**, 1809-1813 (*Isohopeaphenol*)
Ohyama, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 663-668 (*isol*)
Ohyama, M. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3057-3060 (*activity*)

22(30)-Hopene-3,29-diol H-299



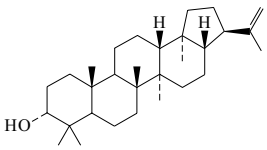
$C_{30}H_{50}O_2$ 442.724

(3β,21α*H*)-*form* [62498-82-2]
Constit. of *Rhodomyrtus tomentosa* (hill gooseberry). Cryst. Mp 253-254°. $[\alpha]_D$ +6.5 ($CHCl_3$).

29-Aldehyde: [62505-75-3] ***3β-Hydroxy-22(30)-hopen-29-al***
Constit. of *Rhodomyrtus tomentosa* (hill gooseberry). Cryst. (petrol). $[\alpha]_D$ +10.7 ($CHCl_3$).

Hui, W.-H. *et al., Phytochemistry*, 1976, **15**, 1741

22(29)-Hopen-3-ol H-300



(3α,21α*H*)-*form*

$C_{30}H_{50}O$ 426.724

(3α,21α*H*)-*form* [18610-71-4]
3-Epimoretenol. *3*-epi-*Moretenol*
Constit. of *Sapium sebiferum* (Chinese tallowtree). Cryst. Mp 223-224°. $[\alpha]_D$ -2.5.

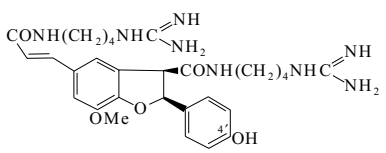
(3β,21α*H*)-*form* [1678-31-5]
Moretenol
Constit. of *Sapium sebiferum* (Chinese tallowtree). Cryst. ($CHCl_3$/MeOH). Mp 236°. $[\alpha]_D$ +27 (c, 2.3 in $CHCl_3$).

3-Ketone: [1812-63-1] *21α*H-*Hop-22(29)-en-3-one.* ***Moretenone***
$C_{30}H_{48}O$ 424.709
Constit. of *Sapium sebiferum* (Chinese tallowtree). Cryst. (Et_2O/MeOH). Mp 202-204°. $[\alpha]_D$ +54 (c, 2.7 in $CHCl_3$).

Galbraith, M.N. *et al., Aust. J. Chem.*, 1965, **18**, 226 (*isol*)
Khastgir, H.N. *et al., Chem. Comm.*, 1967, 1217 (*isol*)
Buckley, D.G. *et al., Chem. Ind. (London)*, 1971, 298 (*pmr*)
Hui, W.H. *et al., J.C.S. Perkin 1*, 1977, 897 (*isol*)
Matsunaga, S. *et al., Phytochemistry*, 1983, **22**, 605 (*isol*)
McLean, S. *et al., Can. J. Chem.*, 1987, **65**, 2519 (*isol, pmr, cmr*)
Rawan, D.D. *et al., Phytochemistry*, 1992, **31**, 702 (*isol, pmr, cmr*)

Hordatine B, 8CI H-301

[10502-21-3]



$C_{29}H_{40}N_8O_5$ 580.686
Alkaloid from *Hordeum vulgare* (barley). Sol. H_2O. Mp 132-135° (as dipicrate). $[\alpha]_D^{23}$ +54 (c, 1 in H_2O). λ_{max} 223 (ϵ 22000); 301 (ϵ 15500); 316 (ϵ 16200) (EtOH) (Berdy).

4′-O-*α*-*D*-*Glucopyranoside: Hordatine B glucoside*
$C_{35}H_{50}N_8O_{10}$ 742.828
Present in barley (*Hordeum vulgare*) as an inseparable mixt. with Hordatine A glucoside, known as Hordatine M (Gramineae). $[\alpha]_D^{23}$ +60 (c, 1 in H_2O).

O-*De-Me:* [7073-64-5] ***Hordatine A***
$C_{28}H_{38}N_8O_5$ 566.659
Alkaloid from barley (*Hordeum vulgare*). Sol. H_2O. Mp 132-135° (as dipicrate). $[\alpha]_D^{23}$ +69 (c, 1 in H_2O). λ_{max} 229 (ϵ 20700); 298 (ϵ 18400); 307 (ϵ 18400) (MeOH) (Berdy). λ_{max} 235 (ϵ 17000); 297 (ϵ 19400); 305 (ϵ 18700) (MeOH-NaOH) (Berdy).

O-*De-Me, 4′*-O-*α*-*D*-*glucopyranoside: Hordatine A glucoside*
$C_{34}H_{48}N_8O_{10}$ 728.801
Component of Hordatine M from barley (see above).

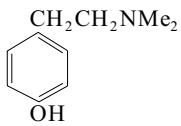
(±)-*form*
Mp 128-130° (as picrate).

[16995-91-8]

Stoessl, A. *et al., Can. J. Chem.*, 1967, **45**, 1745 (*isol, uv, ir, nmr, struct, synth*)
Smith, T.A. *et al., Phytochemistry*, 1978, **17**, 1093 (*occur*)

Hordenine H-302

[539-15-1]
4-(2-Dimethylaminoethyl)phenol, 9CI. 4-Hydroxy-N,N-*dimethylphenethylamine.* N-*Dimethyltyramine. Peyocactine. Anhaline. Cactine. Eremursine*



$C_{10}H_{15}NO$ 165.235
Alkaloid from *Hordeum vulgare* (barley). Mp 118°. Bp_{11} 173-174°. Log P 1.17 (calc).

Voswinckel, H. *et al., Ber.*, 1912, **45**, 1004 (*synth*)
Buck, J.S. *et al., J.A.C.S.*, 1938, **60**, 1789 (*synth, deriv*)
Badger, G.M. *et al., Aust. J. Chem.*, 1963, **16**, 734 (*isol, pmr*)
Rao, G.S. *et al., J. Pharm. Pharmacol.*, 1970, **22**, 545
Cherayil, G.D. *et al., J. Pharm. Sci.*, 1973, **62**, 2054 (*synth*)
Rao, K.V. *et al., Planta Med.*, 1975, **27**, 31 (*isol, deriv*)
Srinivasan, P.R. *et al., Org. Magn. Reson.*, 1976, **8**, 198 (*cmr*)
Kruger, T.L. *et al., J.O.C.*, 1977, **42**, 4161 (*ms*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*occur*)
Parvez, M. *et al., Acta Cryst. C*, 1991, **47**, 1450 (*cryst struct*)

Hordothionin H-303

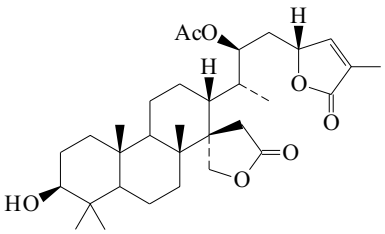
[96595-43-6]
Barley purothionin homolog. BPH-II
Peptide. A homologue of wheat purothionin. See Purothionin AII, P-585. Isol. from barley flour.

[73298-89-2]

Ozaki, Y. *et al., J. Biochem. (Tokyo)*, 1980, **87**, 549 (*isol, struct*)

Hovenidulcigenin A H-304

[171499-81-3]



$C_{32}H_{48}O_7$ 544.727
Sapogenin from *Hovenia dulcis* (raisin tree). Cryst. Mp 230-233°. $[\alpha]_D$ -23.1 (MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [171499-79-9] ***Hovenidulcioside A$_1$***
$C_{44}H_{68}O_{16}$ 853.012
Constit. of *Hovenia dulcis* (raisin tree). Cryst. Mp 183-186°. $[\alpha]_D$ -48.5 (MeOH).

3-O-*β-D-Glucopyranoside:* [171499-80-2] ***Hovenidulcioside A$_2$***
$C_{38}H_{58}O_{12}$ 706.869
Constit. of *Hovenia dulcis* (raisin tree). Cryst. Mp 157-160°. $[\alpha]_D$ -14 (MeOH).

24,25α-Dihydro: [182173-50-8] ***Hovenidulcigenin B***
$C_{32}H_{50}O_7$ 546.743
Sapogenin from *Hovenia dulcis* (raisin tree). Cryst. (MeOH/$CHCl_3$). Mp 205-208°. $[\alpha]_D^{27}$ +4.1 (c, 0.6 in MeOH).

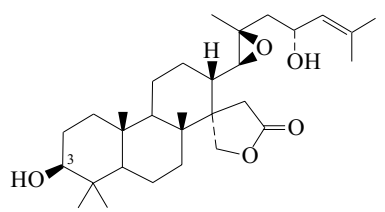
24,25α-Dihydro, 3-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [174902-16-0] ***Hovenidulcioside B$_1$***
$C_{44}H_{70}O_{16}$ 855.027
Constit. of *Hovenia dulcis* (raisin tree). Cryst. (MeOH aq.). Mp 177-180°. $[\alpha]_D^{27}$ -21.5 (c, 0.3 in MeOH).

24,25α-Dihydro, 3-O-*β-D-glucopyranoside:* [174902-17-1] ***Hovenidulcioside B$_2$***
$C_{38}H_{60}O_{12}$ 708.885
Constit. of *Hovenia dulcis* (raisin tree). Cryst. (MeOH aq.). Mp 133-136°. $[\alpha]_D^{25}$ -6 (c, 0.1 in MeOH).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 532; 1996, **44**, 1736 (*isol, pmr, cmr, cryst struct*)

Hovenolactone H-305

[85206-97-9]



$C_{30}H_{48}O_5$ 488.706
Sapogenin from *Hovenia dulcis* (raisin tree). Cryst. (MeOH). Mp 226-228°. $[\alpha]_D$ +12.3 (c, 0.57 in MeOH).

3-O-*(2*-O-*α-L-Rhamnopyranosyl-β-D-glucopyranoside):* [85191-73-7] ***Saponin E***
$C_{42}H_{68}O_{14}$ 796.991
Constit. of *Hovenia dulcis* (raisin tree). Cryst. Mp 167-169.5°. $[\alpha]_D$ -26.5 (c, 0.32 in MeOH).

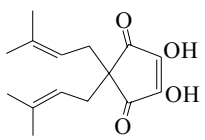
3-O-*β-D-Glucopyranoside:* [85202-26-2] ***Saponin H***
$C_{36}H_{58}O_{10}$ 650.848
Constit. of *Hovenia dulcis* (raisin tree). Cryst. Mp 171-172°. $[\alpha]_D$ -14.3 (c, 0.35 in MeOH).

3-O-*[α-L-Rhamnopyranosyl(1→2)-β-D-glucopyranoside], 23*-O-*β-D-glucopyranoside:* ***Hoduloside I***
$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Hovenia dulcis* (raisin tree). Amorph. powder. Mp 184-186°. $[\alpha]_D^{22}$ -19.5 (c, 4.9 in MeOH).

3-O-*[β-D-Glucopyranosyl(1→3)[α-L-rhamnopyranosyl(1→2)]-β-D-glucopyranoside]:* ***Hoduloside II***
$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Hovenia dulcis* (raisin tree). Amorph. powder. Mp 188-190°. $[\alpha]_D^{22}$ -14.6 (c, 1.9 in MeOH).

Kimura, Y. *et al., J.C.S. Perkin 1*, 1981, 1923 (*isol*)
Kobayashi, Y. *et al., J.C.S. Perkin 1*, 1982, 2795 (*struct*)
Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2287 (*Hodulosides*)

Hulupinic acid H-306

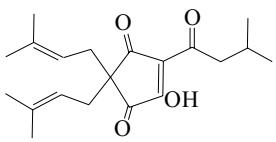


$C_{15}H_{20}O_4$ 264.321
Constit. of hops. Cryst. (Et_2O/petrol). Mp 167-168°.

Burton, J.S. *et al., J.C.S.*, 1964, 952

Hulupone H-307

[468-62-2]

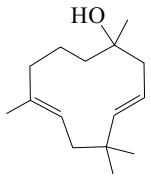


$C_{20}H_{28}O_4$ 332.439
Constit. of hops. Oil. $Bp_{0.0001}$ 110°.

Wright, D. *et al., J.C.S.*, 1963, 1769 (*synth*)
Gienapp, E. *et al., Nahrung*, 1975, **19**, 697 (*struct*)

2,9-Humuladien-7-ol H-308

[24405-58-1]
Humulol†

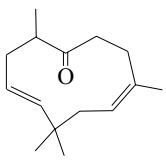


$C_{15}H_{26}O$ 222.37
Constit. of hop oil. Oil. $[\alpha]_D^{24}$ -1.2 (c, 0.9 in MeOH).

Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2405 (*isol*)
Naya, Y. *et al., Chem. Lett.*, 1973, 133 (*synth*)

2,9-Humuladien-6-one H-309

[24405-90-1]
Humuladienone

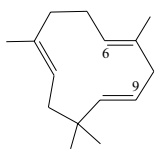


$C_{15}H_{24}O$ 220.354
Constit. of hops. Oil. $[\alpha]_D^{24}$ +5 (c, 0.7 in $CHCl_3$).

Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2088

2,6,9-Humulatriene H-310

[6753-98-6]
2,6,6,9-Tetramethyl-1,4,8-cycloundecatriene. ***α-Humulene****. α-Caryophyllene (obsol.). Humulene*



$C_{15}H_{24}$ 204.355
Farnesane numbering shown. Constit. of many essential oils including hops (*Humulus lupulus*) and cloves (*Syzygium aromaticum*). Oil. Bp_{10} 123°.

$AgNO_3$ complex:
Cryst. (EtOH). Mp 175°.

6,7-Episulfide: [65563-96-4] *1,5,5,8-Tetramethyl-12-thiabicyclo[9.1.0]dodeca-3,7-diene, 9CI*
$C_{15}H_{24}S$ 236.421
Constit. of hops. Oil.

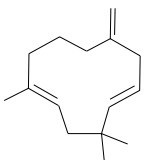
9,10-Episulfide: [74841-84-2] *3,7,7,10-Tetramethyl-12-thiabicyclo[9.1.0]dodeca-3,7-diene, 9CI*
$C_{15}H_{24}S$ 236.421
Constit. of hops. Oil.

McPhail, A.T. *et al., J.C.S.(B)*, 1966, 112 (*cryst struct*)
Dev, S. *et al., J.A.C.S.*, 1968, **90**, 1246 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1929 (*occur*)
Cradwick, M.E. *et al., J.C.S. Perkin 2*, 1973, 404 (*conformn*)

Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 855 (*synth*)
Kitagawa, Y. *et al., J.A.C.S.*, 1977, **99**, 3864 (*synth*)
Peppard, T.L. *et al., J.C.S. Perkin 1*, 1980, 311 (*isol*)
McMurry, J.E. *et al., Tet. Lett.*, 1982, **23**, 2723 (*synth*)
Shirahama, H. *et al., Chem. Lett.*, 1983, 281 (*synth*)
McMurry, J.E. *et al., Tetrahedron*, 1987, **43**, 5489 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 1993, **34**, 3675 (*synth*)
Hu, T. *et al., Org. Lett.*, 2002, **4**, 2441-2443 (*synth*)

2,7(14),9-Humulatriene H-311

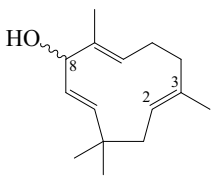
[116-04-1]
1,4,4-Trimethyl-8-methylene-1,5-cycloundecadiene. ***β-Humulene***



$C_{15}H_{24}$ 204.355
Constit. of hops. Oil.

Naya, Y. *et al., Chem. Lett.*, 1973, 727

2,6,9-Humulatrien-8-ol H-312



$C_{15}H_{24}O$ 220.354
Most refs. refer to Zerumbone.

(2*E*,6*E*,8ξ,9*E*)-*form*

Hydroperoxide: [228565-88-6] *8-Hydroperoxy-2,6,9-humulatriene.* ***Humulene-8-hydroperoxide***
$C_{15}H_{24}O_2$ 236.353
Constit. of *Curcuma zedoaria* (zedoary).

Ketone: [471-05-6] *2,6,9-Humulatrien-8-one.* ***Zerumbone***
$C_{15}H_{22}O$ 218.338
Constit. of the rhizomes of wild ginger (*Zingiber zerumbet*). Cryst. Mp 66-67°. Bp_{10} 165-167°.

Ketone, oxime:
Cryst. (EtOH aq.). Mp 178.5°.

Ketone, semicarbazone:
Cryst. (EtOH aq.). Mp 163°.

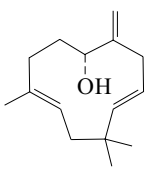
Ketone, 2ξ,3ξ-epoxide: [22471-70-1] *2,3-Epoxy-6,9-humuladien-8-one.* ***Zerumbone oxide***
$C_{15}H_{22}O_2$ 234.338
Constit. of ginger *Zingiber zerumbet*. Cryst. Mp 100°.

6,7-Dihydro, ketone: [125481-94-9] *2,9-Humuladien-8-one.* ***Buddledone A***
$C_{15}H_{24}O$ 220.354
Oil. λ_{max} 240 (log ϵ 3.12) ($CHCl_3$).

Dev, S. *et al., Tetrahedron*, 1960, **8**, 171 (*isol*)
Damodaran, N.P. *et al., Tet. Lett.*, 1965, 1977 (*struct*)
Dev, S. *et al., J.A.C.S.*, 1968, **90**, 1246 (*pmr*)
Chabra, B.R. *et al., Indian J. Chem.*, 1975, **13**, 222 (*Zerumbone oxide*)
Hall, S.R. *et al., Aust. J. Chem.*, 1981, **34**, 2243 (*cryst struct*)
Shirahama, H. *et al., Chem. Lett.*, 1981, 717 (*synth*)
Russel, M.A. *et al., J.C.S. Perkin 2*, 1982, 245 (*cryst struct*)
Kodama, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4039 (*synth*)
Dai, J.-R. *et al., Nat. Prod. Lett.*, 1997, **10**, 115-118 (*Zerumbone, pmr, cmr*)
Phan, M.G. *et al., CA*, 1998, **131**, 71211d (*hydroperoxides*)
Want, Q. *et al., Int. J. Biochem. Cell Biol.*, 1998, **37**, 599-600 (*cryst struct*)
Liao, Y.-H. *et al., J. Nat. Prod.*, 1999, **62**, 1241-1245 (*Buddledone A*)
Kitayama, T. *et al., J.O.C.*, 1999, **64**, 2667-2672 (***isol, bibl***)

2,7(14),9-Humulatrien-6-ol H-313

[19888-00-7]
Humulenol II

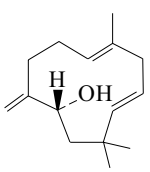


$C_{15}H_{24}O$ 220.354
Constit. of *Zingiber zerumbet* (wild ginger). Oil. Bp_1 115-116°. $[\alpha]_D^{30}$ +30 (c, 3.6 in $CHCl_3$).

Damodaran, N.P. *et al., Tetrahedron*, 1968, **24**, 4133 (*isol*)
Picket, J.A. *et al., Chem. Ind. (London)*, 1977, 30 (*synth*)
Namikawa, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 3616 (*synth*)

3(15),6,9-Humulatrien-2-ol H-314

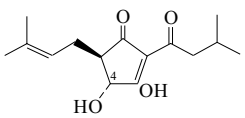
[19888-01-8]
Humulenol I



$C_{15}H_{24}O$ 220.354
Constit. of *Zingiber zerumbet* (wild ginger). Oil. $Bp_{3.5}$ 128-130°. $[\alpha]_D^{30}$ +25.9 (c, 1.8 in $CHCl_3$).

Damodaran, N.P. *et al., Tetrahedron*, 1968, **24**, 4133

Humulinic acid H-315



(4*R*,5*R*)-*form*
$C_{15}H_{22}O_4$ 266.336
λ_{max} 225 (E1%/1cm 400); 267 (MeOH) (Berdy). λ_{max} 225 (ϵ 9630); 266 (ϵ 9620) (EtOH-HCl) (Berdy). λ_{max} 250 (ϵ 20600) (EtOH-NaOH) (Berdy).

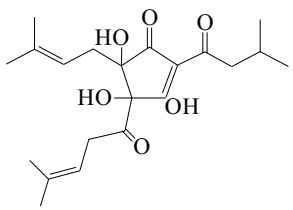
(4*R*,5*R*)-*form* [24184-12-1]
Humulinic acid A
Constit. of hops. Cryst. (cyclohexane). Mp 93°.

(4*S*,5*R*)-*form* [26892-78-4]
Humulinic acid B
Constit. of hops. Cryst. (cyclohexane). Mp 72-73°.

Anteunis, M. *et al., Bull. Soc. Chim. Belg.*, 1959, **68**, 102; 1962, **71**, 623; 1964, **73**, 275; 285 (*isol, struct, ir, pmr*)
de Keukeleire, D. *et al., Tetrahedron*, 1971, **27**, 4939 (*abs config*)
Cant, E. *et al., Org. Mass Spectrom.*, 1972, **6**, 977 (*ms*)
Borremans, F. *et al., Org. Magn. Reson.*, 1975, **7**, 415 (*cmr*)

Humulinone H-316

[981-03-3]

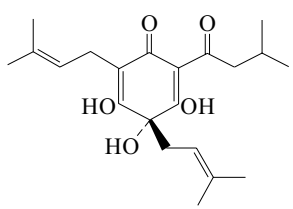


$C_{21}H_{30}O_6$ 378.464
Constit. of hops. Cryst. Sol. MeOH, hexane; fairly sol. H_2O. Mp 74°. λ_{max} 229 (E1%/1cm 330); 268 (E1%/1cm 250); 280 (E1%/1cm 300) (MeOH) (Berdy).

Meheus, J. *et al., Bull. Soc. Chim. Belg.*, 1964, **73**, 268 (*synth, pmr*)
Shaw, S.J. *et al., Org. Mass Spectrom.*, 1972, **6**, 873 (*ms*)

Humulone H-317

[26472-41-3]
α-Lupulinic acid. α-Bitter acid. α-Lupulic acid



$C_{21}H_{30}O_5$ 362.465
Log P 3.88 (calc).

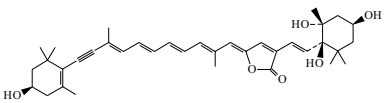
***(R)*-form**
Constit. of hops. Cryst. Sol. MeOH, hexane; fairly sol. acids; poorly sol. H_2O. Mp 66-66.5°. $[\alpha]_D^{20}$ -232.2. λ_{max} 236 (E1%/1cm 390); 283 ; 323 (MeOH) (Berdy). λ_{max} 235 (ϵ 10100); 281 (ϵ 8000); 320 (ϵ 5330) (EtOH-HCl) (Berdy). λ_{max} 228 (ϵ 14700); 324 (ϵ 11000); 368 (ϵ 8700) (EtOH-NaOH) (Berdy).

Riedl, W. *et al., CA*, 1952, **46**, 3508 (*synth*)

de Keukeleire, D. *et al., Tetrahedron*, 1970, **26**, 385 (*abs config*)
Schmabeck, A.F. *et al., Can. J. Microbiol.*, 1975, **21**, 205 (*pharmacol*)
Molyneux, R.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 1201 (*pmr*)
Borremans, F. *et al., Org. Mass Spectrom.*, 1975, **7**, 415 (*ms*)
Drawent, F. *et al., Phytochemistry*, 1976, **15**, 1689 (*biosynth*)
Obara, H. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3034 (*synth*)
Zuurbier, K.W.M. *et al., Phytochemistry*, 1995, **38**, 77 (*biosynth*)
Fung, S.-Y. *et al., Phytochemistry*, 1997, **44**, 1047 (*biosynth*)

Hydratopyrrhoxanthinol H-318

[120416-68-4]



$C_{37}H_{48}O_6$ 588.783

Struct. incorrectly drawn in paper. Abs. config. based on comparison with Heteroxanthin, H-140. Constit. of the edible mussel *Mytilus edulis*. λ_{max} 452 (Me_2CO).

Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv, ms*)

Hydrazine H-319

[302-01-2]
Diazane

$H_2N–NH_2$ (C_2)

H_4N_2 32.045

Hydrogen-bonded as liq. and solid. Self-ionising solv. Interatomic distances: N–H 102, N–N 145 pm. Food contaminant arising from its use as a boiler water additive in production of steam used in food processing. Colourless oily fuming liq. Misc. H_2O, alcohols; sl. sol. org. solvs. d^{25} 1. Mp 1.8°. Bp 113.5°. n_D^{25} 1.4640. pK_a 7.96.

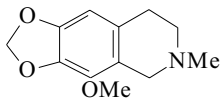
▶ Explosive in air if ignited or overheated. Highly toxic, corrosive. MU7175000

[7803-57-8, 13255-48-6, 18500-32-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1228C; 1228D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 363C (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., Longman, *Part* 2, 1967, **8/II**, 69 (*rev*)
Compr. Inorg. Chem., Pergamon, 1973, **2**, 250 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 734 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1351
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HGS000; HGV000; HGU500; HGW500

Hydrocotarnine H-320

[550-10-7]
5,6,7,8-Tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-g]isoquinoline, 9CI.
1,2,3,4-Tetrahydro-8-methoxy-2-methyl-6,7-methylenedioxyisoquinoline



$C_{12}H_{15}NO_3$ 221.255

Alkaloid from opium (*Papaver somniferum*). Plates (petrol). Mp 55.5-56.5°. Bp_{15} 182-183°.

▶ JI4825000

Hydrochloride:
Cryst. (EtOH). Mp 215-217° Mp 247-249° dec.

Hydrobromide:
Mp 237-238° (229°).

Picrate:
Mp 173°.

Hesse, O. *et al., Annalen*, (Suppl.), 1872, **8**, 261 (*isol*)
Beckett, G.H. *et al., J.C.S.*, 1875, **28**, 573 (*synth*)
Bandow, E. *et al., Ber.*, 1898, **31**, 1577 (*synth*)
Pyman, F.L. *et al., J.C.S.*, 1912, **101**, 1595 (*synth*)
Dey, B.B. *et al., J. Indian Chem. Soc.*, 1935, **12**, 421 (*synth*)
Clayson, D.B. *et al., J.C.S.*, 1949, 2016 (*synth*)
Schneider, W. *et al., Annalen*, 1958, **615**, 34 (*synth*)
Habermehl, G. *et al., Annalen*, 1970, **742**, 138 (*ms*)
Charnock, G.A. *et al., J.C.S. Perkin 2*, 1972, 856 (*synth, pmr, ms*)
Göber, B. *et al., Pharmazie*, 1973, **28**, 221 (*synth*)
Harsányi, K. *et al., Annalen*, 1975, 1201 (*synth*)
Minamikawa, J. *et al., Can. J. Chem.*, 1979, **57**, 1720 (*synth*)

Hydrocyanic acid, 9CI, 8CI H-321

[74-90-8]
Hydrogen cyanide. Prussic acid. Formonitrile

HC≡N ($C_{\infty v}$)

CHN 27.026

Interatomic distances: H–C 106.55, C–N 115.32 pm. Present in freshly distilled bitter almond oil (2-4%) prior to its removal by precipitation as calcium ferrocyanide to give food quality oil. V. volatile liq. or colourless gas smelling of bitter almonds. Misc. H_2O, EtOH, Et_2O. d^0 0.72. Mp -13°. Bp 25.7°. pK_a 9.89. Aq. solns. are unstable. Burns with violet flame. V. weak acid. Can condense to a tetramer or a black polymer. T_{crit} 183.5°.

▶ Extremely flammable, fl. p. -18°. Anhydrous liq. form stable ≤ r.t. if inhibited with acid. Lack of stabiliser or presence of alkali can lead to explosive polymn. Free acid, aq. solns. and salts very toxic by all routes of administration. Fatal dose of HCN for man is *ca.* 50 mg and of cyanides *ca.* 250 mg. Exposure to smaller toxic doses causes headache, dizziness, dyspnoea, nausea. MEL: short-term 10 ppm (Sk). MW6825000

[3017-23-0, 13127-85-0, 20722-83-2, 21107-92-6, 26746-21-4, 91280-07-8]

Org. Synth., Coll. Vol., 1, 1932, 314 (*synth*)
Andrussov, *et al., Angew. Chem.*, 1935, **48**, 593 (*synth*)
Webb, R.L. *et al., Encycl. Polym. Sci. Technol.*, 1967, **7**, 568 (*rev*)
Dibeler, V.H. *et al., J. Chem. Phys.*, 1968, **48**, 4765 (*ms*)
Winnewisser, G. *et al., J. Mol. Spectrosc.*, 1971, **39**, 149 (*struct*)
Feeney, J. *et al., Eur. J. Biochem.*, 1973, **34**, 107 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 252
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 628 (*synth*)
Sastry, G.R.N. *et al., Indian J. Chem.*, 1975, **10**, 33 (*rev*)
Weigert, W. *et al., CA*, 1978, **89**, 45705n (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 307 (*rev*)
Pesticide Manual, 6th edn., 1979, 300 (*use*)
Nagata, T. *et al., Chem. Phys.*, 1981, **57**, 45 (*uv*)
Wasylishen, R.E. *et al., Can. J. Chem.*, 1982, **60**, 2194 (*N-15 nmr*)
Yoshikawa, S. *et al., J. Biol. Chem.*, 1985, **260**, 3518 (*ir*)
Clinical and Experimental Toxicology of Cyanides, (eds., Ballantyne, B. *et al*) Wright, Bristol, 1987,
Chemical Warfare Agents, (eds., Somani, S.M), Academic Press, 1992, 209 (*toxicodynamics*)
Meredith, T.J. *et al., Antidotes for Poisoning by Cyanide*, IPCS/CEC Evaluation of Antidote Series, Volume 2, Cambridge University Press, 1993,
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1128
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2709-2711 (*use*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 166
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0362
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 690
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HHS000; HHU000

Hydrogen H-322

[1333-74-0]
Dihydrogen. Hydrogen 1. Protium. E949

H_2

H 1.008

Atomic No. 1. Ground state electron config. $1s^1$. H. Cavendish is regarded as the discoverer in 1766. 3 important isotopes. Deuterium (D) and radioactive Tritium (T) discovered in 1932 and 1934 respectively. Third most abundant element (after O and Si) on earth's surface. ^1H is stable with natural abundance 99.9975-99.9816 atom %. This isotope is the most important nucleus in nmr spectroscopy, but D and T are also nmr sensitive. Each isotope consists of equilib. mixt. of *ortho*- and *para*-forms (different nuclear spins). Solid H_2 is hcp normally but may be fcc under special conditions. Important in bonding (H-bonding) between the more electronegative elements. Used as a packaging gas. Stable, colourless, tasteless gas. V. low soly. most liqs. Mp -259°. Bp -252.6°. I = ½; μ = +2.7928456 μ_N. nmr relative sensitivity (^1H=1.00) 1.00 (by

definition); receptivity (^{13}C=1.00) 5680. Forms compounds with almost every other element.

▶ Not directly toxic but will cause asphyxiation. Forms explosive mixtures with air, O_2, halogens etc.. MW8900000

[12181-16-7, 12184-84-8, 12184-88-2, 12184-89-3, 12184-90-6, 12184-91-7, 12385-13-6, 12408-02-5, 12595-95-8, 12595-96-9, 14464-47-2, 14885-60-0, 14885-61-1, 15086-10-9, 28132-48-1]

Mellor Compr. Treat. Inorg. Theor. Chem., 1922, **1**, 122; 270 (*rev, bibl*)
Weeks, M.E. *et al., Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 183; 197 (*history*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 1 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 539; 554; **12**, 938; 1015 (*rev, bibl*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1186 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DBB800; HHW500; HHY500

Hydrogen chloride H-323

[7647-01-0]
Hydrochloric acid, 9CI. Muriatic acid. Chlorohydric acid. Hydrochloride. Spirits of salt. E507

HCl

ClH 36.461

H–Cl 127.4 pm. Acidifying agent, pH control agent. Auxiliary for inversion of sucrose and hydrolysis of starch or proteins. Processing aid in beer malting. Colourless, corrosive, nonflammable gas with a pungent odour. Fumes in air. Dissolves in H_2O to give a strong, highly-corrosive acid. V. sol. H_2O; sol. MeOH, EtOH, Et_2O. Mp -114°. Bp -85°. ΔH_f° -92.31 kJ mol^{-1}; ΔG_f° -95.3 kJ mol^{-1}; S_f 186.8 J K^{-1} mol^{-1}.

▶ Highly corrosive. Mildly toxic by inhalation. Irritant to the eyes and skin. MW4025000

Monohydrate: [32754-98-6]
Mp -15.35°.

Dihydrate: [13465-05-9]
Mp -17.7°.

Trihydrate: [13465-06-0]
Mp -24.9°.

Hexahydrate: [66326-44-1]
Mp -70°.

[7698-05-7, 13760-18-4, 13779-43-6]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 81A (*ir*)
Honigschmid, O. *et al., Z. Anorg. Allg. Chem.*, 1927, **163**, 315 (*synth*)
Inorg. Synth., 1939, **1**, 147 (*synth, gas*)
Yoon, Y.K. *et al., Acta Cryst.*, 1959, **12**, 17 (*cryst struct, monohydrate*)
Savoie, R. *et al., J. Chem. Phys.*, 1966, **44**, 548 (*ir, Raman*)
Lundgren, J.O. *et al., Acta Cryst.*, 1967, **23**, 966; 971 (*cryst struct, hydrates*)
Gilbert, A.S. *et al., Chem. Comm.*, 1971, 337 (*ir, hydrates*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1280 (*rev*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 294
Taesler, I. *et al., Acta Cryst. B*, 1978, **34**, 2424 (*cryst struct, hexahydrate*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 983 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 217-218
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2694-2699; 2707-2708 (*use*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1714
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HHL000; HHX000; HHX500

Hydrogen peroxide (H_2O_2), 11CI, USAN H-324

[7722-84-1]
Hydrogen dioxide. Hydroperoxide. Albone†. Genoxide. Hioxyl. Inhibine. Oxydol. Perhydrol. Peroxan. NSC 19892

H-O-O-H (C_2)

H_2O_2 34.015

Interatomic distances: H–O 95.0, O–O 147.5 pm; angle: HOO 94.8°. Used in foods as a bleaching agent, antimicrobial agent and oxidising agent. Unstable colourless liq. Misc. H_2O; insol. petrol. $d^{-1.7}$ 1.64. Mp -0.4°. Bp 150.2° (extrap.). pK_a 11.65. Used in comly. available dilute soln. Component of Hyperol (Ortizon, Perhydrate)..

▶ Potentially explosive in presence of org. matter, corrosive and irritating to all tissues when undil. Skin contact causes whitening or bleaching of the skin leading to erythema and vesiculation if not removed. Can injure eyes. Mutagenic props. Dangerous fire haz. Explosion haz. when highly conc. Solns. in Et_2O v. explosive. Dec. by some metals and alkalis. OES: long-term 1 ppm; OES: short-term 2 ppm. MX0900000

Monodeutero compd.: [34322-11-7]
DHO_2 35.021
Colourless liq. Interatomic distances: H–O 96.5, D–O 96.5, O–O 149 pm; angle: HOO 100°.

Dideutero compd.: [6909-54-2]
D_2O_2 36.027
Colourless liq. Shows strong tendency to supercool. d^{20} 1.54. Mp 1.5°.

Mellor Compr. Treat. Inorg. Theor. Chem., 1922, **1**, 877 (*bibl*)
Feher, F. *et al., Ber.*, 1939, **72**, 1789 (*ir, Raman, D_2O_2*)
Phibbs, M.K. *et al., Can. J. Chem.*, 1951, **29**, 173 (*synth, D_2O_2*)
Bain, O. *et al., Can. J. Chem.*, 1955, **33**, 45; 541 (*ir, DHO_2*)
Schumb, W.C. *et al., Hydrogen Peroxide*, Reinhold Publishing Corporation, New York, 1955, (*uses*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 3, 1966, **7**, (*bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 457; 1972, **3**, 154; 1979, **7**, 174; 1982, **10**, 201; 1969, **2**, 216; 1981, **9**, 241; 1986, **12**, 242; 1980, **8**, 247; 1974, **4**, 253; 1977, **6**, 286; 1975, **5**, 337 (*uses*)
Oelfke, W.C. *et al., J. Chem. Phys.*, 1969, **51**, 5336 (*struct*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 771 (*rev*)
Chen, H. *et al., Spectrochim. Acta A*, 1973, **29**, 1611 (*ir, Raman*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 156 (*synth*)
Sugawara, T. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 3391 (*O-17 nmr*)
Giguere, P.A. *et al., J. Raman Spectrosc.*, 1984, **15**, 199 (*Raman, DHO_2*)
Tso, T.L. *et al., J. Phys. Chem.*, 1985, **89**, 1618 (*ir, DHO_2*)
Koput, J. *et al., J. Mol. Spectrosc.*, 1986, **115**, 438 (*struct*)
Hess, W.T. *et al., Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley*, 1991, **13**, 961 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 798
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2731-3742 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1354-1357
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 4163
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 337
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 693
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HIB000; HIB010

10-Hydroperoxy-1,8-heptadecadiene-4,6-diyn-3-ol H-325

[141947-42-4]
Ginsenoyne K

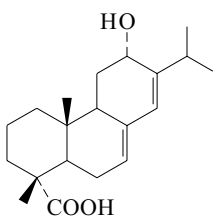
$H_3C(CH_2)_6CH(OOH)CH{=}CHC{\equiv}CC{\equiv}CCH(OH)CH{=}CH_2$

$C_{17}H_{24}O_3$ 276.375
Constit. of the roots of *Panax ginseng*. Pale yellow oil. $[\alpha]_D$ -27.2 (c, 3.78 in $CHCl_3$).

Hirakura, K. *et al., Phytochemistry*, 1992, **31**, 899 (*isol, pmr, cmr, struct*)

12-Hydroxy-7,13-abietadien-18-oic acid H-326

12-Hydroxyabietic acid



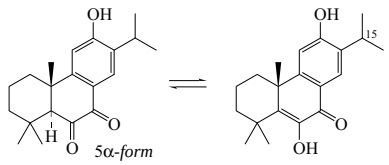
$C_{20}H_{30}O_3$ 318.455

12α-*form* [3484-61-5]
Constit. of *Pinus sylvestris* (Scotch pine).

Barrero, A.F. *et al., Phytochemistry*, 1990, **29**, 593 (*isol, pmr*)
San Feliciano, A. *et al., Magn. Reson. Chem.*, 1993, **31**, 841 (*cmr*)
Cheung, A.T. *et al., Tetrahedron*, 1993, **49**, 7903 (*isol, pmr, cmr*)

12-Hydroxy-8,11,13-abietatriene-6,7-dione H-327

6,12-Dihydroxy-5,8,11,13-abietatetraen-7-one



$C_{20}H_{26}O_3$ 314.424

Exists in dioxo form, since 5α- and 5β-epimers separately characterised.

5α-*form* [119817-27-5]

Prexanthoperol. *Hypargenin C*

Minor constit. of *Juniperus communis* (juniper). Yellow cryst. or orange amorph. solid. Mp 207-210°. Identity of Prexanthoperol and Hypargenin C not definitely establ. λ_{max} 218 (ϵ 3150); 320 (ϵ 12500); 333 (ϵ 15800); 403 (ϵ 5000) (MeOH) (Berdy).

5β-*form* [564-23-8]

Xanthoperol

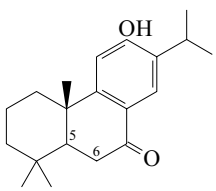
Constit. of *Juniperus communis* (juniper). Yellow cryst. (C_6H_6). Mp 255-270° dec. $[\alpha]_D^{20}$ +132.5 (c, 1.2 in EtOH).

Brendenberg, J.B. *et al., Acta Chem. Scand.*, 1956, **10**, 1511 (*isol*)
Nasipuri, D. *et al., J.C.S.*, 1962, 4248 (*synth*)
Kondo, Y. *et al., Chem. Pharm. Bull.*, 1963, **11**, 678 (*struct*)
Ulubelen, A. *et al., J. Nat. Prod.*, 1988, **51**, 1178 (*isol, pmr, cmr*)
Ghosal, M. *et al., Indian J. Chem., Sect. B*, 1992, **31**, 524 (*synth*)

12-Hydroxy-8,11,13-abietatrien-7-one H-328

[511-05-7]

Sugiol. *Isomicropinic acid. 7-Oxoferruginol*



$C_{20}H_{28}O_2$ 300.44

Constit. of *Juniperus communis* (juniper). Cryst. (AcOH). Mp 295-297°. $[\alpha]_D^{20}$ +22.6 (c, 1.2 in dioxan).

Me ether:12-Methoxy-8,11,13-abietatrien-7-one. Sugiol methyl ether

$C_{21}H_{30}O_2$ 314.467

Needles (MeOH). Mp 126-127°. $[\alpha]_D^{25}$ +42.9 (c, 0.8 in $CHCl_3$).

enol-form [128741-28-6] *6,8,11,13-Abietatetraene-7,12-diol*. ***Trilobinol***

Isol. from *Salvia triloba* (Greek sage). Yellow amorph. powder.

Kupchan, S.M. *et al., J.O.C.*, 1969, **34**, 3912 (*isol*)
Cambie, R.C. *et al., Aust. J. Chem.*, 1971, **24**, 217 (*isol*)
Meyer, W.L. *et al., J.O.C.*, 1975, **40**, 3686 (*synth, bibl*)
Matsumoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 1575 (*bibl*)
Chang, H.M. *et al., J.O.C.*, 1990, **55**, 3537 (*isol, pmr, cmr*)
Ulubelen, A. *et al., Planta Med.*, 1990, **56**, 82 (*Trilobinol*)
Das, S. *et al., Tet. Lett.*, 1994, **35**, 4027 (*synth*)
Kuo, Y.H. *et al., Phytochemistry*, 1996, **42**, 779 (*sugiol methyl ether*)
Gao, J. *et al., Phytochemistry*, 1997, **44**, 759 (*Sugiol, cmr*)

Hydroxyacetaldehyde, 9CI H-329

[141-46-8]

Glycolaldehyde, 8CI. Hydroxyethanal. Glycollic aldehyde. Diose

$HOCH_2CHO \Leftrightarrow HOCH{=}CHOH$

$C_2H_4O_2$ 60.052

In acid and alkaline media is in equilib. with enediol form. Fresh aq. solns. contain dimer which becomes monomolecular after 24h. Reduces Fehling's soln.. Occasional isolate from biol. systems, e.g. tomato volatiles, *Aspergillus niger* autolysate. Plates. Sol. H_2O, hot EtOH; spar. sol. Et_2O. Mp 96-97°.

▶ LD_{50} (rat, ipr) 280 mg/kg. MC2980000

[52856-11-8, 52856-12-9]

Biochem. Prep., 1955, **4**, 56 (*synth*)
Gebhardt, B. *et al., Z. Chem.*, 1964, **4**, 189 (*synth*)
George, W.O. *et al., J.C.S.(B)*, 1971, 1352 (*pmr*)
Brittain, E.F.H. *et al., J.C.S.(B)*, 1971, 2414 (*ms*)
Kobayashi, Y. *et al., J. Mol. Struct.*, 1976, **32**, 235 (*ir*)
Roth, J.A. *et al., J. Organomet. Chem.*, 1979, **172**, C27 (*synth*)
Fedoronko, M. *et al., Carbohydr. Res.*, 1980, **87**, 35 (*equilib*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 162 (*use*)

Hydroxyacetic acid, 9CI H-330

[79-14-1]

Glycollic acid. Glycolic acid

$HOCH_2COOH$

$C_2H_4O_3$ 76.052

Found in sugar cane (*Saccharum officinarum*). Needles (H_2O), leaflets (Et_2O). Sol. H_2O, org. solvs. Mp 80°. Bp 100° dec.. pK_a 3.82. Log P -1.07 (calc). Forms various anhydrides. Comly. available as a 70% soln. or as pure cryst..

▶ Fl. p. >74° (65-67%). Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 1950 mg/kg. MC5250000

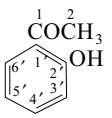
[2836-32-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 517A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 807B; 1033A; 1033B; 1122A; **2**, 1334B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 721A; 747D (*ir*)
Petersson, G. *et al., Tetrahedron*, 1970, **26**, 3413 (*ms*)
Pijper, W.P. *et al., Acta Cryst. B*, 1971, **27**, 344 (*cryst struct*)
Wu, J.-T. *et al., Petrochemia*, 1973, **12**, 36 (*rev*)
Szyper, M. *et al., Anal. Chim. Acta*, 1976, **85**, 357 (*uv*)
Barrelle, M. *et al., Org. Magn. Reson.*, 1982, **19**, 102 (*cmr*)
Kukla, M. *et al., J.O.C.*, 1984, **49**, 5003 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **13**, 1055 (*rev*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0714
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 650
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EKM500; GHO000; HIM500

2′-Hydroxyacetophenone, 8CI H-331

[118-93-4]

1-(2-Hydroxyphenyl)ethanone, 9CI. o-*Acetylphenol. 2-Hydroxyphenyl methyl ketone. FEMA 3548*



$C_8H_8O_2$ 136.15

Present in tomato, cassia (*Cinnamomum cassia*), fried beef, rum, whiskey, cocoa, coffee and black tea. Flavouring ingredient. Greenish-yellow oil. d^{20} 1.13. Mp 4-6°. Bp_{717} 213° Bp_{17} 106°. n_D^{20} 1.5593. pK_a 10.22 (25°).

▶ Fl. p. 98°. AM8575000

[54582-21-7, 54582-28-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 32B; 40A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 842B; 855C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1252B; 1258B (*ir*)
Norris, J.F. *et al., J.A.C.S.*, 1939, **61**, 1413 (*synth*)
Smith, W.B. *et al., J.A.C.S.*, 1972, **94**, 1959 (*pmr*)
Durmis, J. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 243 (*ir*)
Tomasik, P. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1974, **22**, 1065 (*uv*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 357
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1359-1360
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HIN500

4′-Hydroxyacetophenone, 8CI H-332

[99-93-4]

1-(4-Hydroxyphenyl)ethanone, 9CI. p-*Acetylphenol. 4-Hydroxyphenyl methyl ketone.* ***Piceol***. *Ameliarol*

$C_8H_8O_2$ 136.15

Needles (EtOH aq. or Et_2O). Mp 109°. Bp_3 148°. pK_a 8.05 (25°). pK_{a1} -4.73 (25°, H_2SO_4 aq.).

▶ LD_{50} (mus, orl) 1500 mg/kg. AM8750000

O-*[4-Hydroxybenzoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:*

[228405-07-0]

$C_{26}H_{30}O_{13}$ 550.515

Constit. of *Thymus vulgaris* (thyme). Powder.

O-*[4-Hydroxy-3,5-dimethoxybenzoyl-(*

→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]: [228405-06-9]
$C_{28}H_{34}O_{15}$ 610.568
Constit. of *Salvia officinalis* (sage) and *Thymus vulgaris* (thyme). Powder.

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [149475-53-6] ***Asterbatanoside A***. *Bungeiside C*
$C_{19}H_{26}O_{11}$ 430.408
Needles. Mp 226-228° Mp 234-235°. $[\alpha]_D$ -100.9 (c, 0.4 in MeOH). $[\alpha]_D^{28}$ -68.5 (c, 0.7 in Py).

Me ether: [100-06-1] *4′-Methoxyacetophenone. Acetanisole. Melitone. Linarodin. FEMA 2005*
$C_9H_{10}O_2$ 150.177
Trace constit. of oil of *Piper longum* (long pepper). Present in cranberry (*Vaccinium oxycoccus*) and other fruits, tomato, anise (*Pimpinella anisum*), grilled and roasted beef and sherry. Flavouring ingredient and adjuvant; useful in vanilla, nut, tobacco and butter flavours. Plates (EtOH). Mp 38-39°. Bp 258° Bp_{15} 138-139°. pK_{a1} -4.81 (25°, H_2SO_4 aq.).

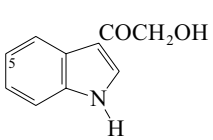
▶ Skin irritant. LD_{50} (rat, orl) 1720 mg/kg.
AM9240000

[26358-63-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 32D; 44B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 843C; 844B; 845C; 861B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1252D; 1253A; 1256B; 1259A (*ir*)
Norris, J.F. *et al., J.A.C.S.*, 1939, **61**, 1413 (*synth*)
Simons, J.H. *et al., J.A.C.S.*, 1939, **61**, 1795 (*synth*)
Miyajima, G. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2301 (*cmr*)
Durmis, J. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 243 (*ir*)
Sakurai, H. *et al., Org. Mass Spectrom.*, 1973, **7**, 1109 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1974, 927 (*rev, deriv*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 6 (*Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 11-12 (*Me ether*)
Wang, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 1911-1914; 2000, **48**, 235-238 (*benzoylapiosylglucosides*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HIO000; MDW750

3-(Hydroxyacetyl)-1*H*-indole H-333

[2400-51-3]
2-Hydroxy-1-(1H-indol-3-yl)ethanone, 9CI. Hydroxymethyl indol-3-yl ketone, 8CI



$C_{10}H_9NO_2$ 175.187
Alkaloid from liquid cultures of the fungus *Lactarius deliciosus*. Needles (EtOAc); cryst. (H_2O or C_6H_6). Mp 162-163° Mp 173-174°. λ_{max} 212 (ϵ 10232); 240 (ϵ 5500); 294 (ϵ 4466) (MeOH) (Berdy).

▶ KM5779000

Oxime:
$C_{10}H_{10}N_2O_2$ 190.201
Mp 116-118°.

O-*Ac:* [27536-15-8]
$C_{12}H_{11}NO_3$ 217.224
Cryst. (H_2O). Mp 140°.

O-*Benzoyl:* [2400-52-4]
$C_{17}H_{13}NO_3$ 279.295
Cryst. (MeOH). Mp 187-189°.

N,O-*Di-Ac:*
$C_{14}H_{13}NO_4$ 259.261
Oil. Mp 0° approx.

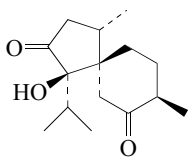
5-Hydroxy: [132922-98-6] *5-Hydroxy-3-(hydroxyacetyl)-1H-indole.* ***Hyrtiosin A***
$C_{10}H_9NO_3$ 191.186
Needles. Mp 196-197°. λ_{max} 215 (ϵ 59200); 252 (ϵ 35000); 270 (ϵ 22400); 303 (ϵ 23300) (MeOH) (Berdy).

[34951-71-8, 34951-79-6]

Suvorov, N.N. *et al., Khim. Geterotsikl. Soedin.*, 1965, 265; 1971, 778; *Chem. Heterocycl. Compd.*, 1965, 173; 1971, 725 (*synth, oxime, ir*)
U.K. Pat., 1970, 1 183 919; *CA*, **72**, 132517v (*synth, O-Ac*)
Vereshchagin, A.L. *et al., Khim. Geterotsikl. Soedin.*, 1983, 46; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1983, 40 (*O-Ac*)
Tsujii, S. *et al., J.O.C.*, 1988, **53**, 5446 (*synth*)
Bernart, M. *et al., Phytochemistry*, 1990, **29**, 3697 (*isol*)
Kobayashi, J. *et al., Tetrahedron*, 1990, **46**, 7699 (*Hyrtiosin A*)
Dillman, R.L. *et al., J. Nat. Prod.*, 1991, **54**, 1056 (*isol, uv, pmr, cmr, ms*)
Ayer, W.A. *et al., J. Nat. Prod.*, 1994, **57**, 839 (*isol, pmr, ms, struct*)
Böhlendorf, B. *et al., Annalen*, 1996, 49 (*isol, ir, pmr, cmr, ms*)

7-Hydroxy-3,8-acoranedione H-334

[185154-96-5]
1-Hydroxyepiacorone

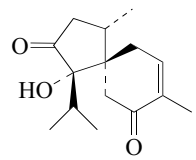


$C_{15}H_{24}O_3$ 252.353
Constit. of *Acorus calamus* (sweet flag). Needles (MeOH). Mp 128-131°. $[\alpha]_D$ -61 (c, 0.32 in MeOH).

Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175-1182 (*isol, pmr, cmr*)

7-Hydroxy-4-acorene-3,8-dione H-335

[185154-98-7]
1-Hydroxyacorenone

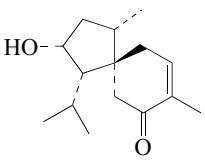


$C_{15}H_{22}O_3$ 250.337
Constit. of *Acorus calamus* (sweet flag). Oil. λ_{max} 234 (ϵ 6700) (MeOH).

Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175-1182 (*isol, pmr, cmr*)

8-Hydroxy-4-acoren-3-one H-336

[185154-94-3]
2-Hydroxyacorenone



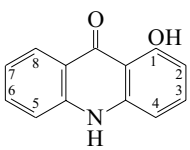
$C_{15}H_{24}O_2$ 236.353
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D$ -44.9 (c, 0.29 in MeOH). λ_{max} 240 (ϵ 6570) (MeOH).

Ac: [185154-95-4]
$C_{17}H_{26}O_3$ 278.391
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D$ -75.8 (c, 0.31 in MeOH). λ_{max} 240 (ϵ 7070) (MeOH).

Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175-1182 (*isol, pmr, cmr*)

1-Hydroxyacridone H-337

[65582-54-9]
1-Hydroxy-9(10H)-acridinone, 9CI



$C_{13}H_9NO_2$ 211.22
Yellow needles (Me_2CO). Mp 280° (subl., dec.).

N-*Me:* [16584-54-6] ***1-Hydroxy-10-methylacridone***
$C_{14}H_{11}NO_2$ 225.246
Alkaloid from the roots of *Ruta graveolens* (rue). Also isol. from the callus cultures obt. from the meristematic cells of *Ruta graveolens*. Yellow needles (Me_2CO). Mp 192-194°.

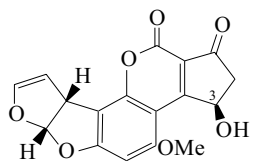
Me ether, N-*Me:* [16584-58-0] ***1-Methoxy-10-methylacridone***
$C_{15}H_{13}NO_2$ 239.273
Yellow amorph. solid. Mp 164°.

Hughes, G.K. *et al., Aust. J. Sci. Res., Ser. A*, 1952, **5**, 206 (*synth*)
Reisch, J. *et al., Experientia*, 1971, **27**, 1005 (*deriv, isol, pmr, struct*)
Scharlemann, W. *et al., Z. Naturforsch., B*, 1972, **27**, 806 (*deriv, isol, uv*)
Rózsa, Zs. *et al., Pharmazie*, 1975, **30**, 753 (*isol, deriv*)

Adams, J.H. *et al., J.C.S. Perkin 1*, 1977, 2173 (*deriv, synth, uv, ir, pmr*)
Rózsa, Zs. *et al., Phytochemistry*, 1978, **17**, 169 (*uv, ir, pmr, ms, deriv, isol, synth*)
Gibbons, S. *et al., Phytochemistry*, 1997, **44**, 1109 (*1-Methoxy-10-methylacridone*)
Coppola, G.M. *et al., Org. Prep. Proced. Int.*, 1999, **31**, 225-227 (*synth, ir, pmr*)

3-Hydroxyaflatoxin B_1 H-338

[55058-52-1]
2,3,6a,9a-Tetrahydro-3-hydroxy-4-methoxycyclopenta[c]furo[3′,2′:4,5]furo[2,3-h][1]benzopyran-1,11-dione, 9CI



(3*R*)-*form*

$C_{17}H_{12}O_7$ 328.278

(3*R*)-*form* [56648-94-3]
Epiaflatoxin Q_1
Mp 235° dec.

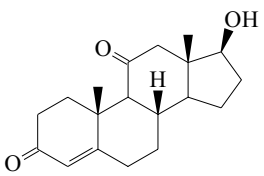
(3*S*)-*form* [52819-96-2]
Aflatoxin Q_1
Mycotoxin. Metab. of Aflatoxin B. Cryst. ($CHCl_3$). Mp 265° dec., 280° dec.

▶ Carcinogen. GY1800000

Ac:
Mp 305° dec.

Steyn, P.S. *et al., J.C.S. Perkin 1*, 1974, 2551
Büchi, G. *et al., J.O.C.*, 1975, **40**, 3458 (*synth*)
Toxicol. Aflatoxins, (eds. Eaton, D.L. *et al*), Academic Press, London, 1994,
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 345
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 20

17-Hydroxyandrost-4-ene-3,11-dione, 9CI H-339



$C_{19}H_{26}O_3$ 302.413

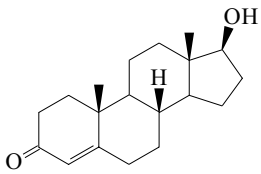
17β-*form* [564-35-2]
11-Oxotestosterone. 11-Ketotesterone
Cryst. (Me_2CO/hexane). Mp 187-187.5°. $[\alpha]_D^{20}$ +200 (c, 1.333 in $CHCl_3$).

Ac: [4271-84-5]
$C_{21}H_{28}O_4$ 344.45
Cryst. (Me_2CO/petrol). Mp 166.5-167.5°. $[\alpha]_D^{24}$ +173 ($CHCl_3$).

(±)-17β-*form* [87583-72-0]
Mp 192-195°.

Herzog, H.L. *et al., J.A.C.S.*, 1953, **75**, 266 (*synth*)
U.K. Pat., 1955, 738 629; *CA*, **51**, 509 (*synth,uv*)
Hanč, O. *et al., Arzneim.-Forsch.*, 1957, **7**, 175 (*synth*)
Baker, T.S. *et al., Steroids*, 1977, **29**, 429 (*synth*)
Van Royen, L.A. *et al., Tet. Lett.*, 1983, **24**, 3145 (*synth, pmr, (±)-17β-form*)

17-Hydroxyandrost-4-en-3-one H-340



17β-*form*

$C_{19}H_{28}O_2$ 288.429

17α-*form* [481-30-1]
epi-*Testosterone*. ***Epitestosterone***
Cryst. (EtOAc). Mp 220-221°. $[\alpha]_D$ +17 ($CHCl_3$).

Ac:
Cryst. (hexane). Mp 116°. $[\alpha]_D$ +110 ($CHCl_3$).

17β-*form* [58-22-0] ***Testosterone, BAN, INN, USAN***. *Andropatch. Atmos. Many other names*
Cryst. (Me_2CO aq.). Mp 155°. $[\alpha]_D$ +109 (c, 4 in EtOH).

▶ Adverse effects reported when used therapeutically (and for ester derivatives). Exp. neoplastic agent. Human teratogen, exp. reprod. effects. XA3030000

Ac: [1045-69-8] ***Testosterone acetate***. *Aceto-Sterandryl. Aceto-Testoviron. Amolisin. Androtest A. Deposteron. Farmatest. Perandren. Perandrone A. Testiculosterone. Testolent*
$C_{21}H_{30}O_3$ 330.466
Cryst. (Me_2CO aq.). Mp 140-141°. $[\alpha]_D^{20}$ +87.8 (EtOH).

▶ XA3061500No longer marketed

17-Chloral hemiacetal: [53608-96-1] *17β-(2,2,2-Trichloro-1-hydroxyethoxy)androst-4-en-3-one, 9CI*. ***Cloxotestosterone, INN***
$C_{21}H_{29}Cl_3O_3$ 435.816
Cryst. (EtOAc). Mp 200-201°. Log P 5.35 (uncertain value) (calc).

17-Chloral hemiacetal, Ac: [13867-82-8] *Caprosem*
$C_{23}H_{31}Cl_3O_4$ 477.854
Cryst. (EtOAc). Mp 192-193°. Log P 5.89 (uncertain value) (calc).

17-Cyclohexanecarboxylate: [14191-92-5] ***Testosterone hexahydrobenzoate***. *Many other names*
$C_{26}H_{38}O_3$ 398.584
Mp 126-128°. $[\alpha]_D$ +8.8. Log P 6.2 (uncertain value) (calc).

▶ XA3065000

17-Cyclohexanemethoxycarboxylate: [2697-92-9] ***Testosterone hexahydrobenzyl carbonate***. *Testosterone cyclohexylmethylcarbonate. Lontanyl*
$C_{27}H_{40}O_4$ 428.611
$[\alpha]_D^{20}$ +83 (c, 0.6 in EtOH). Log P 6.74 (uncertain value) (calc).

17-Propanoyl: [57-85-2] *17-(1-Oxopropoxy)androst-4-en-3-one, 9CI*. ***Testosterone propionate, BAN, USAN***. *Agrovirin. Propionyltestosterone. Synandrol. NSC 9166. Many other names*
$C_{22}H_{32}O_3$ 344.493
Stout prisms (EtOH aq.). Mp 118-122°. $[\alpha]_D^{25}$ +90 (dioxan). Log P 4.69 (uncertain value) (calc).

▶ LD_{50} (rat, orl) 1000 mg/kg. Exp. neoplastic agent. Human (male and female) and exp. reprod. effects. XA3115000

17-(2-Methylpropanoyl): [1169-49-9] ***Testosterone isobutyrate***. *Agovirin-Depot. Perandren M. Testocryst. Virex-cryst*
$C_{23}H_{34}O_3$ 358.52
Cryst. (Me_2CO aq.). Mp 134-136°. Log P 5 (uncertain value) (calc).

17-(3-Cyclopentylpropanoyl): [58-20-8] ***Testosterone cypionate***. *Testosterone cyclopentylpropionate. Many other names*
$C_{27}H_{40}O_3$ 412.611
Mp 101-102°. $[\alpha]_D^{25}$ +87 ($CHCl_3$). Log P 6.79 (uncertain value) (calc).

▶ Exp. reprod. effects. XA3066000

17-(3-Cyclohexylpropanoyl): [2034-94-8] ***Testosterone cyclohexylpropionate***. *Andromar. Femolone. Telipex Retard*
$C_{28}H_{42}O_3$ 426.638
Mp 74.5-76°. $[\alpha]_D^{25}$ +74.9 (dioxan). Log P 7.34 (uncertain value) (calc).

17-(4-Methylpentanoyl): [15262-86-9] ***Testosterone isocaproate, BAN***. *Testosterone 4-methylvalerate*
$C_{25}H_{38}O_3$ 386.573
Mp 82-84.5°. $[\alpha]_D^{25}$ +82.3 (dioxan). Log P 6.15 (uncertain value) (calc).

17-Heptanoyl: [315-37-7] ***Testosterone enanthate, BAN, USAN***. *Testosterone heptanoate. Testostroval. Delatestryl. NSC 17591. Many other names*
$C_{26}H_{40}O_3$ 400.6
Mp 36-37.5°. Log P 6.81 (uncertain value) (calc).

▶ LD_{50} (rat, ipr) 2000 mg/kg. Human and exp. reprod. effects. Exp. teratogen. XA3080000

17-Heptanoyl, 3-benziloylhydrazone: [18625-33-7] ***Testosterone enanthate benziloylhydrazone***
$C_{40}H_{52}N_2O_4$ 624.862
Mp 108-110°. $[\alpha]_D$ +156 (EtOH).

17-Decanoyl: [5721-91-5] ***Testosterone decanoate, BAN***
$C_{29}H_{46}O_3$ 442.681
Cryst. (MeOH). Mp 55-57°. Log P 8.4 (uncertain value) (calc).

17-Undecanoyl: [5949-44-0] ***Testosterone undecanoate, BAN***. *Andriol. Androxon. Panteston. Restandol. Undestor*
$C_{30}H_{48}O_3$ 456.707
Log P 8.93 (uncertain value) (calc).

▶ XA3119700

17-(3-Oxododecanoyl): [5874-98-6] *17-[(1,3-Dioxododecyl)oxy]androst-4-en-3-one, 9CI*. ***Testosterone ketolaurate, INN, USAN***. *Testosterone caprinoylacetate. Androdurin. Testosid-Depot*
$C_{31}H_{48}O_4$ 484.718
Log P 8.02 (uncertain value) (calc).

17-Phenylacetyl: [5704-03-0] ***Testosterone phenylacetate***
$C_{27}H_{34}O_3$ 406.564
Stout prisms. Mp 126.5-127.5°. $[\alpha]_D^{25}$ +87 (dioxan). Log P 5.8 (uncertain value) (calc).

17-(Phenylpropanoyl): [1255-49-8] ***Testosterone phenylpropionate, BAN***. *Testosterone hydrocinnamate*
$C_{28}H_{36}O_3$ 420.591
Mp 116-117°. $[\alpha]_D^{25}$ +86.8 (dioxan). Log

P 6.11 (uncertain value) (calc).

►XA3105000

17-(4-Hexyloxyphenyl)propanoyl: [4838-37-3] ***Testosterone hexyloxyphenylpropionate***. *Andradurin*
$C_{34}H_{48}O_4$ 520.751
Mp 59-60°. $[\alpha]_D$ +76 (dioxan). Log P 8.68 (uncertain value) (calc).

17-(2-Furoyl): [60895-85-4] ***Testosterone furoate***. *Furotest*
$C_{24}H_{30}O_4$ 382.499
Mp 221°. $[\alpha]_D^{27}$ +170.5 (c, 1 in EtOH). Log P 5.27 (uncertain value) (calc).

17-Nicotinoyl: [668-56-4] ***Testosterone nicotinate***. *Bolfortan. Linobol. WD 53*
$C_{25}H_{31}NO_3$ 393.525
Log P 4.75 (uncertain value) (calc).

17-Trimethylsilyl ether: [5055-42-5] *17β-[(Trimethylsilyl)oxy]androst-4-en-3-one, 9CI*. ***Silandrone, INN, USAN***. *NSC 95147. SC 16148*
$C_{22}H_{36}O_2Si$ 360.611
Cryst. (hexane). Mp 133-135°. $[\alpha]_D^{25}$ +69 (c, 1 in $CHCl_3$).

17-Phosphate: [1242-14-4] ***Testosterone phosphate***. *Telipex aquosum*
$C_{19}H_{29}O_5P$ 368.409
Cryst. (MeOH aq.). Mp 139-142°. $[\alpha]_D^{20}$ +75 ($CHCl_3$/MeOH).

O-*Sulfate:* [651-45-6]

[6614-81-9]
Mp 215° (as Na salt). $[\alpha]_D^{25}$ +74.5 (c, 1 in H_2O).

O-*Glucopyranosiduronate:* [1180-25-2]
$C_{25}H_{36}O_8$ 464.555
Mp 182-183.5°. $[\alpha]_D^{23}$ +31.7 (EtOH).

(8α,9β,10α,13α,14β,17α)-*form* [86335-11-7]
Mp 152-153.5°. $[\alpha]_D^{26}$ -112 (c, 2.501 in $CHCl_3$). Enantiomer of 17β-form.

(8α,10α,17β)-*form* [4860-75-7]
Cryst. (diisopropyl ether). Mp 156-157°. $[\alpha]_D^{23}$ +108 (c, 0.5 in $CHCl_3$).

(8α,17β)-*form*
Cryst. (hexane/Me_2CO). Mp 182-184°. $[\alpha]_D$ +134 (c, 0.034 in dioxan).

Ac:
Cryst. (hexane). Mp 143-146°.

(8α,13α,14β,17α)-*form* [28336-24-5]
Mp 154-156°. $[\alpha]_D$ +141 (dioxan). Enantiomer of 9β,10α,17β-form.

(9β,10α,13α,17α)-*form* [79732-28-8]
Cryst. (Et_2O). Mp 116-118°. $[\alpha]_D$ -70 (c, 0.1 in dioxan).

(9β,10α,17α)-*form* [4069-18-5]
Mp 217-219°.

(9β,10α,17β)-*form* [571-41-5] ***Retrotestosterone***
Cryst. (Et_2O). Mp 155-156°. $[\alpha]_D^{23}$ -154 ($CHCl_3$).

►BV8396600

Ac: [4069-00-5]
Cryst. (diisopropyl ether/petrol). Mp 113-114.5°.

(9β,17β)-*form* [897-03-0]
Cryst. (MeOH/hexane). Mp 117-120°. $[\alpha]_D^{25}$ +107 ($CHCl_3$).

(10α,17β)-*form* [604-39-7]
Cryst. (Et_2O/petrol). Mp 144-144.5°. $[\alpha]_D$ -208 (c, 0.73 in $CHCl_3$).

Ac: [2201-72-1]
Cryst. (CH_2Cl_2/petrol). Mp 139-140°. $[\alpha]_D$ -222 (c, 0.67 in $CHcl_3$).

(13α,17α)-*form* [4593-60-6]
Rods (Et_2O/hexane). Mp 129.5-131°. $[\alpha]_D^{20}$ +48.9 (c, 1.35 in EtOH).

Ac:
Cryst. (Me_2CO aq.). Mp 103.5-104.5°. $[\alpha]_D$ +55 (c, 1 in dioxan).

(13α,17β)-*form* [4593-59-3]
Needles (Et_2O/hexane). Mp 162.5-164.5°. $[\alpha]_D^{20}$ +90.5 (c, 1 in EtOH).

Ac:
Cryst. (hexane). Mp 136-137.5°. $[\alpha]_D$ +89 (c, 1 in dioxan).

(±)-(17β)-*form* [68833-09-0]
Cryst. (Me_2CO). Mp 167-169°.

(±)-(8α,17β)-*form* [1423-92-3]
Cryst. (Me_2CO/hexane). Mp 172-173.5°.

(±)-(13α,17β)-*form*
Platelets (EtOAc). Mp 167.5-168°.

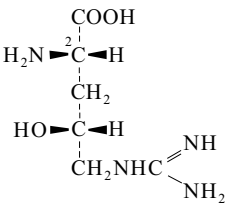
[1159-27-9, 4069-10-7, 6891-35-6, 14958-66-8, 14958-67-9]

Ruzicka, L. *et al., Helv. Chim. Acta*, 1936, **19**, 99; 842; 1141
Mooradian, A. *et al., J.A.C.S.*, 1949, **71**, 3372 (*furoate*)
Holden, G.W. *et al., J.A.C.S.*, 1949, **71**, 3844 (*O-sulfate*)
Rosenkranz, G. *et al., J.A.C.S.*, 1950, **72**, 4077 (*hexahydrobenzoate*)
Ott, A.C. *et al., J. Clin. Endocrinol. Metab.*, 1952, **12**, 3; 15 (*cypionate*)
Dekanski, J. *et al., Br. J. Pharmacol.*, 1953, **8**, 271 (*phenylpropionate*)
Ger. Pat., 1953, 896 805; *CA*, **52**, 10229e (*cypionate*)
U.K. Pat., 1954, 719 402; *CA*, 1938, **50**, 719 402 (*phenylpropionate*)
Voss, H.E. *et al., Arzneim.-Forsch.*, 1955, **5**, 208; 211 (*ketolaurate*)
Djerassi, C. *et al., J.O.C.*, 1955, **21**, 1056 (*8α17β-form, synth, uv, ir*)
Levis, S. *et al., Arch. Int. Pharmacodyn. Ther.*, 1957, **112**, 150 (*furoate*)
Gould, D. *et al., J.A.C.S.*, 1957, **79**, 4472 (*esters*)
Djerassi, C. *et al., Tetrahedron*, 1957, **1**, 22 (*8α17β-form, synth, uv, ir*)
U.K. Pat., 1957, 776 830; *CA*, **52**, 466 (*isocaproate*)
Shoolery, J.N. *et al., J.A.C.S.*, 1958, **80**, 5121 (*17β-form, pmr*)
Bots, J.P.L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 1010 (*synth, uv, ir*)
U.S. Pat., 1958, 2 842 567; *CA*, **53**, 456 (*ketolaurate*)
Wotiz, H.H. *et al., J.A.C.S.*, 1959, **81**, 1704-1708 (*O-glucopyranosiduronate*)
U.S. Pat., 1959, 2 904 562; *CA*, **54**, 3529 (*hexyloxyphenylpropionate*)
Johnson, W.S. *et al., J.A.C.S.*, 1960, **82**, 3409 (*synth, uv, ir*)
Westerhof, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1960, **79**, 794 (*9β10α17β-form, synth, uv, ir*)
Weichsel, H. *et al., Monatsh. Chem.*, 1961, **92**, 667 (*nicotinate*)
Westerhof, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1961, **80**, 1048 (*8α10α17β-form, synth, uv, ir*)
Borrevang, P. *et al., Acta Chem. Scand.*, 1962, **16**, 883 (*Cloxotestosterone*)
Fr. Pat., 1962, M1215; *CA*, **58**, 566 (*hexahydrobenzylcarbonate*)
Wender, R. *et al., Helv. Chim. Acta*, 1962, **45**, 2420 (*10α17β-form, synth, uv, ir, ord*)
Chinn, L.J. *et al., J.O.C.*, 1962, **27**, 54 (*synth*)
Birmingham, M.K. *et al., Steroids*, 1963, **1**, 463 (*ir*)
Alvarez, F. *et al., Steroids*, 1963, **2**, 393 (*17α-form, synth, uv, ir*)
U.K. Pat., 1963, 920 750; *CA*, **61**, 3172 (*Cloxotestosterone*)
Korenman, S.G. *et al., J. Biol. Chem.*, 1964, **239**, 1004 (*isol*)
Gleason, C.H. *et al., J. Med. Chem.*, 1964, **7**, 573 (*hydrazone*)
Knox, L.H. *et al., J.O.C.*, 1964, **29**, 2187 (*pmr*)
Westerhof, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1964, **83**, 169 (*9β17β-form, synth*)
Banerjee, D.K. *et al., Tetrahedron*, 1964, **20**, 2487 (*(±)-8α17β-form, synth*)
Leibetseder, J. *et al., Arzneim.-Forsch.*, 1965, **15**, 474 (*nicotinate*)
Ginsig, R. *et al., J.A.C.S.*, 1965, **87**, 4629 (*10α17β-form, synth*)
Chinn, L.J. *et al., J.O.C.*, 1965, **30**, 4165 (*synth, pmr*)
Halkes, S.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 889 (*pmr*)
Chang, E. *et al., J. Med. Chem.*, 1966, **9**, 433 (*Silandrone*)
Joseph, J.P. *et al., Steroids*, 1966, **7**, 557-587 (*O-sulfate*)
Vulfson, N.S. *et al., Tet. Lett.*, 1966, 3879 (*10α17β-form, ms*)
Overhänsli, W.E. *et al., Helv. Chim. Acta*, 1967, **50**, 53 (*cryst struct*)
Fr. Pat., 1968, 1 519 393; *CA*, **71**, 3577r (*9β10α17β-form, synth*)
Krubiner, A.M. *et al., J.O.C.*, 1968, **33**, 3548 (*9β10α17β-form, synth, uv*)
Nambara, T. *et al., Chem. Pharm. Bull.*, 1969, **17**, 1782 (*13α17α-form, 13α17β-form, synth*)
Fried, J. *et al., J.A.C.S.*, 1970, **92**, 4136 (*8α13α14β17α-form, synth*)
Saucy, G. *et al., Helv. Chim. Acta*, 1971, **54**, 2517 (*synth*)
Grant, J.K. *et al., Pfizer Med. Monogr.*, 1971, **6**, 193 (*rev*)
Weeks, C.M. *et al., Cryst. Struct. Commun.*, 1972, **1**, 79 (*Silandrone*)
Isaacs, N.W. *et al., J.C.S. Perkin 2*, 1972, 2335 (*cryst struct*)
Roberts, P.J. *et al., J.C.S. Perkin 2*, 1973, 1978 (*cryst struct*)
Goncharova, N.M. *et al., Khim.-Farm. Zh.*, 1973, **7**, 27 (*esters*)
Zborucki, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1973, **47**, 2247 (*esters*)
Florey, K. *et al., Anal. Profiles Drug Subst.*, 1975, **4**, 452 (*rev, enanthate*)
Brooks, R.V. *et al., Clin. Endocrinol. Metab.*, 1975, **4**, 503 (*rev*)
Hanson, J.R. *et al., J.C.S. Perkin 1*, 1975, 1956 (*cryst struct*)
Eder, U. *et al., Chem. Ber.*, 1976, **109**, 2954 (*synth, 8α10α17β-form*)
Quilliam, M.A. *et al., Steroids*, 1977, **29**, 579 (*Silandrone*)
Banerjee, D.K. *et al., Proc. Indian Acad. Sci., Sect. A*, 1978, **87A**, 239 (*(±)-17β-form, synth*)
IARC Monog., 1979, **21**, 519 (*tox, rev*)
Highet, R.J. *et al., Steroids*, 1980, **35**, 119 (*17β-form, cmr*)
Rizvi, S.Q.A. *et al., J.O.C.*, 1981, **46**, 1127 (*cmr*)
Chakrabarti, P. *et al., Steroids*, 1981, **37**, 269 (*(±)-8α17β-form, cryst struct*)
Lissel, M. *et al., Synth. Commun.*, 1981, **11**, 545 (*Silandrone*)
Müller, M. *et al., Tetrahedron, Suppl.*, 1981, 257 (*synth, uv, ir, pmr*)
Ramirez, F. *et al., J.O.C.*, 1983, **48**, 1417 (*phosphate*)
Aristoff, P.A. *et al., J.O.C.*, 1985, **50**, 1765 (*17β-form, ir, pmr, cmr, synth*)
Herz, J.E. *et al., Steroids*, 1985, **46**, 947 (*isobutyrate*)
Ihara, M. *et al., J.C.S. Perkin 1*, 1986, 117 (*synth*)

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 5458; 6726; 7474; 7475 (*synonyms*)
Fujiwara, H. *et al., J.C.S. Perkin 2*, 1990, 97 (*cmr*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567 (*pmr*)
Signoret, J.P. *et al., J. Steroid Biochem.*, 1991, **39**, 639 (*biochem*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1196
Böcskei, Z. *et al., Acta Cryst. C*, 1996, **52**, 2899 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBF500; TBG000; TBF600; TBF750

4-Hydroxyarginine, 9CI H-341

2-Amino-5-guanidino-4-hydroxypentanoic acid. γ-Hydroxyarginine



(2S,4R)-form

$C_6H_{14}N_4O_3$ 190.202

(2*S*,4*R*)-*form* [61370-10-3]
L-erythro-*form*
Occurs in the sea-cucumber (*Polycheira rufescens*) and in lentil seeds (*Lens culinaris*). Cryst. (EtOH aq.) (as hydrochloride). Mp 190-191° dec. (hydrochloride). $[\alpha]_D^{18}$ +6.3 (c, 2 in 5*M* HCl) (hydrochloride).

Lactone:
$C_6H_{12}N_4O_2$ 172.186
Needles + $1H_2O$ (EtOH aq.) (as dihydrochloride). Mp 158° (dihydrochloride).

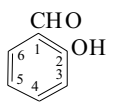
(±)-*form*
Hygroscopic powder. Mp 184-188°. Mixt. of diastereoisomers.

Bell, E.A. *et al., Biochem. J.*, 1965, **97**, 104 (*occur*)
Sulser, H. *et al., Lebensm.-Wiss. Technol.*, 1974, **7**, 327 (*synth, config*)
Mizusaki, K. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 470 (*synth*)
Bell, E.A. *et al., Phytochemistry*, 1999, **50**, 1201-1204 (*isol, pmr, cmr, cryst struct, abs config*)

2-Hydroxybenzaldehyde, 9CI H-342

[90-02-8]

[28777-87-9]
Salicylaldehyde, 8CI. FEMA 3004



$C_7H_6O_2$ 122.123
Present in cinnamon (*Cinnamomum versum*). Flavouring ingredient. Oil. d_4^{20} 1.17. Fp 0.7. Bp 197° Bp_{18} 86°. pK_{a1} 8.37 (25°). Steam-volatile..

► Fl. p. 78°. LD_{50} (rat, orl) 520 mg/kg; LD_{50} (rat, skn) 600 mg/kg. Exp. reprod. and teratogenic effects. VN5250000

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [14907-56-3] ***Spiraein***†
$C_{18}H_{24}O_{11}$ 416.381
Isol. from *Filipendula ulmaria* (meadowsweet). Needles +$1H_2O$ (EtOH). Mp 230-231°. $[\alpha]_D$ -57.9 (c, 1.22 in H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 105D; 106A; 106B; 925A; 961C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 934B; 934C; **3**, 492C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1285B; 1285C (*ir*)
Koepfli, J.M. *et al., J.A.C.S.*, 1932, **54**, 2412 (*isol*)
Sah, P.P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1950, **69**, 1545 (*synth*)
Thieme, H. *et al., Pharmazie*, 1965, **20**, 113; *CA*, **66**, 26602k (*Spiraein*)
Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1825 (*uv*)
Smith, W.B. *et al., Org. Magn. Reson.*, 1976, **8**, 205 (*cmr*)
Gassmann, P.G. *et al., J.A.C.S.*, 1978, **100**, 7611 (*synth, ir*)
Casiraghi, G. *et al., J.C.S. Perkin 1*, 1978, 318 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 70 (*rev*)
Aldred, R. *et al., J.C.S. Perkin 1*, 1994, 1823 (*synth, pmr*)
Bu, X.R. *et al., Synth. Commun.*, 1994, **24**, 1757 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 723
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2485-2486
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SAG000; SAG500

4-Hydroxybenzaldehyde H-343

[123-08-0]

[28777-87-9]
p-*Formylphenol*

$C_7H_6O_2$ 122.123
Occurs naturally combined in many glycosides. Constit. of vanillin. Isol. in free state from opium poppy (*Papaver somniferum*). Needles (H_2O). Mp 115-116°. pK_a 7.62 (25°, H_2O). λ_{max} 221 (ε 12000); 284 (ε 14800); 291 (MeOH) (Berdy). λ_{max} 220 (ε 14800); 280 (ε 18700); 330 (ε 6600) (EtOH) (Berdy).

► CU6475000

O-*(4-O-Acetyl-α-L-rhamnopyranoside):*
[159733-92-3]
$C_{15}H_{18}O_7$ 310.303
Isol. from *Moringa oleifera* (horseradish tree).

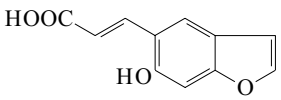
Et ether: [10031-82-0] *4-Ethoxybenzaldehyde. FEMA 2413*
$C_9H_{10}O_2$ 150.177
Present in black tea. Flavouring ingredient. Liq. with a sweet floral odour and taste. Mp 13-14°. Bp 249° Bp_{20} 140°.

► Skin irritant. LD_{50} (rat, orl) 2100 mg/kg. CU6100000

[60221-52-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 111C; 111D; 112A; 132B; 132C; 314B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 941B; 941C; 942A; 943A; 975B; 975C; 1291C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1290D; 1291A; 1291B; 1291C; 1311B; 1311C; 1382B (*ir*)
Gattermann, L. *et al., Ber.*, 1898, **31**, 1765
Gattermann, L. *et al., Annalen*, 1907, **357**, 313
Magnusen, L.B. *et al., J.A.C.S.*, 1963, **85**, 1711
Beistel, D.W. *et al., J. Phys. Chem.*, 1976, **80**, 2023 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 70 (*rev*)
Noller, K. *et al., Chem. Ber.*, 1988, **121**, 1609 (*ethers, synth, ir, pmr, cmr, ms*)
Faizi, S. *et al., J.C.S. Perkin 1*, 1994, 3035-3040 (*4-Ac α-L-rhamnopyranoside*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 211 (*Et ether*)
Harapanhalli, R.S. *et al., J. Med. Chem.*, 1996, **39**, 4804-4809 (*Et ether, synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 936-937 (*Et ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EEL500; FOF000; PMY500

3-(6-Hydroxy-5-benzofuranyl)-2-propenoic acid H-344



$C_{11}H_8O_4$ 204.182
The 1999 ref. is confusing about nomenclature of the geom. isomers, and reuses the name Isopsoralic acid to refer to regioisomer rather than the *Z*-form of psoralic acid.

(*E*)-*form*
Furocoumaric acid. ***Psoralic acid***
Mp 221°.

O-*β-D-Glucopyranoside:*
Mp 244°. $[\alpha]_D^{20}$ -80 (H_2O).

Me ether:
Mp 222°.

(*Z*)-*form* *Furocoumarinic acid.* ***Isopsoralic acid***†
Free acid cyclises to Psoralen, P-557.

O-*β-D-Glucopyranoside:*
$C_{17}H_{18}O_9$ 366.324
Reported from *Ficus carica* (fig). Mp 125°. $[\alpha]_D^{20}$ -61.3 (H_2O).

Me ether:
Mp 166°.

Stoll, A. *et al., Helv. Chim. Acta*, 1950, **33**, 1637-1647 (*isol, struct*)
Yarosh, E.A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 521; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 497 (*isol*)
Hamed, A.I. *et al., Phytochemistry*, 1999, **50**, 887-890 (*isol, uv, ir, pmr, cmr, ms*)

2-Hydroxybenzoic acid, 9CI H-345

[69-72-7]

[29656-58-4]
Salicylic acid. Many other names



$C_7H_6O_3$ 138.123
Preservative, fungicide (superseded), prohibited in milk and wine. Needles (H_2O). Sol. MeOH, Et_2O; fairly sol. H_2O, C_6H_6; poorly sol. hexane. Mp 159°. Bp_{20} 211°. pK_{a1} 2.98; pK_{a2} 13.6 (25°). Log P 2.19 (calc). Steam volatile. Subl. *in vacuo* λ_{max} 234 ; 302 (MeOH) (Berdy).

▶ Fl. p. 157°, autoignition temp. 540°. Mild skin irritant. May cause dermatitis. Severe eye irritant. LD_{50} (rat, orl) 891 mg/kg.; LD_{50} (mus, ivn) 500 mg/kg. Exp. reprod. and teratogenic effects. VO0525000

O-*β-D-Glucopyranoside:* [10366-91-3] *Salicylic acid β-D-glucoside*
$C_{13}H_{16}O_8$ 300.265
Constit. of various plant spp. e.g. white mustard seed (*Sinapis alba*), bell pepper (*Capsicum annuum*) and leaves of thyme, rosemary, basil and sweet marjoram. Cryst. + $1H_2O$ (EtOH) (as Na salt). Mp 162-165° (Na salt). $[\alpha]_D^{30}$ -30.4 (H_2O).

O-*β-D-Glucopyranoside, Me ester:* [10019-60-0]
$C_{14}H_{18}O_8$ 314.291
Constit. of purple passion fruit (*Passiflora edulis*) and other *Passiflora* spp.. Cryst. (EtOH). Mp 106-108°. $[\alpha]_D$ -67.7 (c, 0.9 in H_2O).

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], Me ester:*
$C_{20}H_{28}O_{12}$ 460.434
Constit. of the fruit of purple passion fruit (*Passiflora edulis*).

Et ester: [118-61-6] *Ethyl 2-hydroxybenzoate. Ethyl salicylate. Mesotol. Sal ethyl. Salstan. FEMA 2458*
$C_9H_{10}O_3$ 166.176
Present in feijoa fruit, raspberry, tomato, various spirits, red wine, mountain papaya and cape gooseberry. Flavouring agent. Liq. with wintergreen odour. Mp 1.3°. Bp 231-235°. pK_{a1} 9.92 (25°, 0.1*M* KCl). Log P 2.97 (calc).

▶ Fl. p. 107°. Skin irritant. LD_{50} (rat, orl) 1320 mg/kg. VO3000000

Butyl ester: [2052-14-4] *Butyl 2-hydroxybenzoate. Butyl salicylate. FEMA 3650*
$C_{11}H_{14}O_3$ 194.23
Present in mountain papaya (*Carica pubescens*). Flavouring agent. Liq. with rough herbaceous chemical odour. Mp 6°. Bp 270-271° Bp_{12} 131°.

▶ VO2000000

2-Methylpropyl ester: [87-19-4] *2-Methylpropyl 2-hydroxybenzoate. Isobutyl salicylate. FEMA 2213*
$C_{11}H_{14}O_3$ 194.23
Flavouring agent with orchid/wintergreen odour and bitter taste. LIq. d^{25} 1.07. Mp -6°. Bp 259° Bp_{20} 142-143°. n_D^{25} 1.5075.

Pentyl ester: [2050-08-0] *Pentyl 2-hydroxybenzoate. Amyl salicylate. Isoamyl salicylate*
$C_{12}H_{16}O_3$ 208.257
Flavouring agent.

▶ VO5425000

3-Methylbutyl ester: [87-20-7] *3-Methylbutyl 2-hydroxybenzoate. Isoamyl salicylate. Tressane. Trefle. Orchidee. Trefol. FEMA 2084*
$C_{12}H_{16}O_3$ 208.257
Isol. from fruit aromas. Also present in rum and black tea. Flavouring agent. Liq. with sweet strawberry-like odour. d_4^{15} 1.1. Bp 273° $Bp_{15.2}$ 151-152°. n_D^{20} 1.5065. The commercial material appears to be referred to as isoamyl or amyl salicylate indiscriminately.

▶ VO4375000

Benzyl ester: [118-58-1] *Benzyl salicylate. FEMA 2151*
$C_{14}H_{12}O_3$ 228.247
Isol. from essential oils e.g. *Dianthus caryophyllus, Populus, Primula* spp. Fixative in perfumes and flavourings. Oil or cryst. with weakly sweet odour and currant-like taste. d_4^{20} 1.18. Mp 23.4°. Bp_{10} 186-188°. n_D^{20} 1.5805.

▶ VO1750000

2-Methylphenyl ester: [617-01-6] *2-Methylphenyl 2-hydroxybenzoate.* o-*Tolyl salicylate. FEMA 3734*
$C_{14}H_{12}O_3$ 228.247
Flavouring ingredient. Semisolid to solid.

4-tert-*Butylphenyl ester:* [87-18-3]
$C_{17}H_{18}O_3$ 270.327
Migration residue from food packaging. Cryst. (EtOH). Mp 65-66°.

[63-36-5, 578-36-9, 824-35-1, 18917-95-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 188B; 188C; 273C; 295D; 296A; 383B; 444B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1065B; 1065C; 1251B; 1252A; 1414C; 1511A; 1512A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1323D; 1324A; 1363C; 1364A; 1408B; 1408D (*ir*)
Van Allen, J.A. *et al., J.A.C.S.*, 1947, **69**, 2913 (*synth*)
Urbanski, T. *et al., Nature (London)*, 1950, **166**, 267 (*biol activity*)
Org. Synth., Coll. Vol., 4, 1963, 178 (*tert-butylphenyl ester*)
Smith, M.J.H. *et al., The Salicylates: a Critical Biographical Review*, Wiley, London, 1967,
Shendrikar, A.D. *et al., Talanta*, 1969, **16**, 51 (*use, deriv*)
Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1825 (*uv*)
East Ger. Pat., 1972, 91 052; *CA*, **78**, 29465b (*Benzyl salicylate*)
Scott, K.N. *et al., J.A.C.S.*, 1972, **94**, 8564 (*cmr*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Kochetkova, S.K. *et al., Zh. Anal. Khim.*, 1976, **31**, 44 (*detn, Zr*)
Levy, G. *et al., Drug Metab. Rev.*, 1979, **9**, 1 (*rev, metab*)
Goldsmith, L.A. *et al., Int. J. Dermatol.*, 1979, **18**, 32 (*rev, pharmacol*)
Langade, A.D. *et al., Anal. Chem.*, 1980, **52**, 2031 (*detn, Sc*)
Krom, M.D. *et al., Analyst (London)*, 1980, **105**, 305 (*detn, NH_3*)
Babhair, S.A. *et al., Anal. Profiles Drug Subst.*, 1984, **13**, 521 (*rev*)
Brune, K. *et al., Arzneim.-Forsch.*, 1984, **34**, 1060 (*rev, pharmacol*)
Khadikar, P.V. *et al., Spectrochim. Acta A*, 1986, **42**, 755 (*ir, thermodynamics*)
Klicke, S. *et al., Phytochemistry*, 1988, **27**, 2177 (*occur, glucoside*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **21**, 601 (*rev*)
Vane, J.R. *et al., Aspirin and Other Salicylates*, Chapman and Hall, 1992, (*book*)
Grynkiewicz, G. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1993, **63**, 1251-1254 (*glucoside, synth*)
Abounassif, M.A. *et al., Anal. Profiles Drug Subst.*, 1994, **23**, 421 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 397; 653; 763 (*esters*)
Raskin, I. *et al., Plant Horm. (2nd edn.)*, 1995, 188 (*rev*)
Liu, J.H. *et al., J. Chromatogr., B: Biomed. Appl.*, 1996, **675**, 61 (*hplc*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 29; 48; 51; 96; 1093
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 165; 276; 354; 1040; 1434; 1460; 2168-2169; 2816-2817 (*esters, use, occur*)
Chassagne, D. *et al., J. Agric. Food Chem.*, 1997, **45**, 2685-2689 (*Me ester glycosides*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1099
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BFJ750; CMG000; EEM000; IME000; SAH000; SAJ000; SAL000; SAK000; SAI000; BSL250; SAH500; SAL500,SJO000

3-Hydroxybenzoic acid, 9CI H-346

[99-06-9]

[29656-58-4]

$C_7H_6O_3$ 138.123
Present in fruits. Isol. from *Citrus paradisi* (grapefruit). Needles (H_2O). Sol. H_2O, hot EtOH. Mp 202°. pK_a 5.72 (25°, 50% EtOH aq.). pK_{a1} 3.96; pK_{a2} 9.61 (20°, 0.1*M* KCl).

▶ LD_{50} (mus, orl) 2000 mg/kg. Exp. teratogenic effects (feto-embryotoxic). DH1924980

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 192B; 237D; 296B; 296C; 447A; 1401D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1071A; 1252B; 1252C; 1515A; 1515B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1364C; 1364D; 1410D; 1411A (*ir*)
Woodruff, E.H. *et al., J.A.C.S.*, 1944, **66**, 1799 (*synth*)
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2059 (*uv*)
Exner, O. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 1371; Scott, K.N. *et al., J.A.C.S.*, 1971, **36**, 8564 (*ir*)
Benoit, F. *et al., Org. Mass Spectrom.*, 1973, **7**, 295 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **20**, 516 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HJI100

4-Hydroxybenzoic acid, 9CI, 8CI H-347

[99-96-7]

[29656-58-4]
p-*Salicylic acid. Catalpinic acid (obsol.)*

$C_7H_6O_3$ 138.123
Isol. from many plants, free and combined. Alkyl esters of 4-hydroxybenzoic acid (see below) are used as food and cosmetic preservatives, mainly in their Na salt form, which makes them more water soluble. They are active at low concentrations and more pH-independent than the commonly used Benzoic acid, B-31 and 2,4-Hexadienoic acid, H-172. The taste is more detectable than for those preservatives. Effectiveness increases with chain length of the alcohol, but for some microorganisms this reduces cell permeability and thus counteracts the increased efficiency. Prisms (xylene/EtOH), cryst. + $1H_2O$ (EtOH aq. or Me_2CO/EtOH). Sl. sol. H_2O. Mp 213-214°. pK_{a1} 4.67; pK_{a2} 9.37 (25°,50% EtOH aq.). λ_{max} 222 ; 290 ; 310 (MeOH) (Berdy). λ_{max} 255 (ϵ 11300) (H_2O) (Berdy). λ_{max} 207 ; 255 (HCl) (Berdy).

▶ Fl. p. 157°, autoignition temp. 540°. LD_{50} (mus, orl) 2200 mg/kg. Eye irritant, skin irritant by prolonged or repeated exposure. DH1925000

[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranosyl] ester: [223261-31-2]
$C_{18}H_{24}O_{12}$ 432.38
Occurs in sage. Oil. $[\alpha]_D^{23}$ -32.7 (c, 0.04 in MeOH).

Me ester: [99-76-3] *Methyl 4-hydroxybenzoate.* ***Methylparaben****. Methyl parasept. Nipagin M. Tegosept M. E218. E219 (Na salt). FEMA 2710*
$C_8H_8O_3$ 152.149
Antimicrobial agent, preservative, flavouring agent. Constit. of cloudberry, yellow passion fruit, white wine, botrytised wine and Bourbon vanilla. Needles (EtOH aq.). Mp 131° (127-129°). Bp 270-280° dec.. Log P 1.98 (calc). Used as Na salt.

▶ Fl. p. 96/101°, autoignition temp. 454°. Allergen. DH2450000

Et ester: [120-47-8] ***Ethylparaben, INN, USAN****. Ethyl 4-hydroxybenzoate. Ethyl butex. Ethyl chemosept. Ethyl parasept. Mekkings E. Mycocten. Nipagin A. Solbrol A. Tegosept E. E214. E215 (Na salt)*
$C_9H_{10}O_3$ 166.176
Antimicrobial agent, preservative. Present in red wine, white wine and sake. Cryst. Mp 116°. Bp 297-298° dec.. pK_{a1} 8.5 (25°). Log P 2.51 (calc). Used as Na salt.

▶ Fl. p. 107°. Allergen. DH2190000

Propyl ester: [94-13-3] *Propyl 4-hydroxybenzoate.* ***Propylparaben, USAN****. Chemocide PK. Nipasol. Solbrol P. Propyl parasept. E216. E217 (Na salt). FEMA 2951*
$C_{10}H_{12}O_3$ 180.203
Antimicrobial agent, preservative, flavouring agent. Mp 96-97°. Log P 3.04 (calc).

▶ DH2800000

Butyl ester: [94-26-8] *Butyl 4-hydroxybenzoate.* ***Butylparaben****. Butoben. Butyl chemosept. Butyl parasept. Tegosept B. FEMA 2203*
$C_{11}H_{14}O_3$ 194.23
Preservative and flavouring agent. Mp 68-69°. Log P 3.57 (calc).

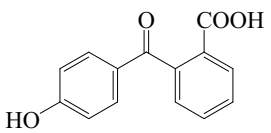
▶ Fl. p. >113°. DH1980000

[456-23-5, 5026-62-0, 35285-69-9]

Struve, A. *et al., J. Prakt. Chem.*, 1895, **52**, 239 (*synth, hydrazide*)
De Cat, A. *et al., Bull. Soc. Chim. Belg.*, 1965, **74**, 270
Kaemmerer, H. *et al., Spectrochim. Acta A*, 1968, **24**, 2059 (*uv*)
Scott, K.N. *et al., J. Magn. Reson.*, 1970, **2**, 361 (*pmr*)
Scott, K.N. *et al., J.A.C.S.*, 1972, **94**, 8564 (*cmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 889 (*occur*)
Benoit, F. *et al., Org. Mass Spectrom.*, 1973, **7**, 295 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 812; **20**, 500 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 863; 1186; 1560 (*synonyms, esters*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HJL000; HJL500
Davidson, P.M. *et al., Antimicrobials in Foods*, 2nd edn., (Eds. Davidson, P.M. *et al*), M. Dekker, 1993, 263 (*parabens, rev*)
Bairati, C. *et al., Clin. Chim. Acta*, 1994, **224**, 147 (*parabens, pharmacol*)
Fukahori, M. *et al., Chem. Pharm. Bull.*, 1996, **14**, 1609 (*activity, parabens*)
Akhtar, M.J. *et al., J. Pharm. Biomed. Anal.*, 1996, **14**, 1609 (*hplc, parabens*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1135
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 343; 1030; 1779; 2364 (*parabens, use, occur*)

4′-Hydroxybenzophenone-2-carboxylic acid H-348

[85-57-4]
2-(4-Hydroxybenzoyl)benzoic acid, 9CI



$C_{14}H_{10}O_4$ 242.231
Leaflets (H_2O). Mp 213°.

▶ DH1950000

Phenylhydrazone:
Needles (EtOH aq.). Mp 267-268°.

Me ester: [21147-23-9]
$C_{15}H_{12}O_4$ 256.257
Cryst. (MeOH). Mp 134°.

Et ester: [65133-93-9]
$C_{16}H_{14}O_4$ 270.284
Needles (H_2O). Mp 114-115°.

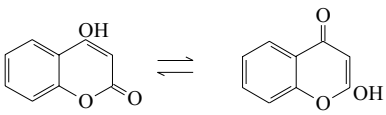
Me ether: [1151-15-1] *4′-Methoxybenzophenone-2-carboxylic acid. (4-Methoxybenzoyl)benzoic acid*
$C_{15}H_{12}O_4$ 256.257
Used in Germany during the 1950s as an artificial sweetener. Sweetness 150 x sucrose. Leaflets (H_2O). Mp 148° (122-123°).

Me ether, Me ester: [5449-71-8]
$C_{16}H_{14}O_4$ 270.284
Cryst. (MeOH). Mp 81-81.5°.

Kipfer, H. *et al., Ber.*, 1905, **38**, 2490
Meyer, H. *et al., Monatsh. Chem.*, 1909, **30**, 481
Ullmann, F. *et al., Ber.*, 1919, **52**, 2098
Orndorff, W.R. *et al., J.A.C.S.*, 1922, **44**, 1518 (*esters*)
Buu-Hoi, Ng.Ph. *et al., Bull. Soc. Chim. Fr.*, 1944, **11**, 410
Hubacher, M.H. *et al., J.A.C.S.*, 1946, **68**, 718
Ghiaci, M. *et al., Org. Prep. Proced. Int.*, 1996, **28**, 609 (*Me ether*)

4-Hydroxy-2*H*-1-benzopyran-2-one, 9CI H-349

[1076-38-6]
4-Hydroxycoumarin. 2-Hydroxy-4H-1-benzopyran-4-one. 2-Hydroxychromone. Benzotetronic acid. 2H-1-Benzopyran-2,4(3H)-dione



$C_9H_6O_3$ 162.145
Tautomeric in soln. Dioxo tautomer also theoretically possible.Needles (H_2O). V. sol. EtOH, Et_2O, hot H_2O. Mp 206° Mp 232-233°. λ_{max} 200 (ϵ 18000); 265 (ϵ 11100) (EtOH/HCl) (Derep). λ_{max} 226 (ϵ 10600); 262 (ϵ 11900) (EtOH) (Derep).

▶ LD_{50} (mus, orl) 2000 mg/kg. DJ3100000

2-Oxo-*form*

4-(2-Propenyl) ether: [31005-07-9] ***Setarin***
$C_{12}H_{10}O_3$ 202.209
Isol. from *Setaria italica* (foxtail millet). Cryst. Mp 104-105°.

[4438-85-1]

Jain, N. *et al., Phytochemistry*, 1991, **30**, 3826-3827 (*Setarin*)

5-Hydroxy-2*H*-1-benzopyran-2-one, 9CI H-350

[6093-67-0]
5-Hydroxycoumarin

$C_9H_6O_3$ 162.145
Cryst. (H_2O). Mp 244-247° (220-222°).

5-O-β-D-Glucopyranoside: ***Mahaleboside***
$C_{15}H_{16}O_8$ 324.287
Constit. of *Prunus mahaleb* (mahaleb cherry). Cryst. Mp 268°. $[\alpha]_D$ -36 (Py).

Ac:
$C_{11}H_8O_4$ 204.182
Mp 88-89° (86-88°).

Me ether: [51559-36-5] *5-Methoxy-2H-1-benzopyran-2-one. 5-Methoxycoumarin*
$C_{10}H_8O_3$ 176.171
Mp 85-87°.

Shah, H.A. *et al., J.C.S.*, 1938, 1832 (*synth, deriv*)
Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 594 (*isol*)
Das Gupta, A.K. *et al., J.C.S.(C)*, 1969, 29 (*synth*)
Dreyer, D.L. *et al., Tetrahedron*, 1975, **31**, 287 (*isol*)
Sadavongvivad, C. *et al., Phytochemistry*, 1977, **16**, 1451 (*isol*)
Joseph-Nathan, P. *et al., J. Het. Chem.*, 1984, **21**, 1141 (*pmr, deriv*)

Dubuffet, T. *et al., Synth. Commun.*, 1999, **29**, 929-936 (*synth, Me ether*)
Cerqueira, N.M.F.S.A. *et al., Helv. Chim. Acta*, 2002, **85**, 442-450 (*synth, pmr*)

7-Hydroxy-2*H*-1-benzopyran-2-one, 9CI H-351

[93-35-6]
7-Hydroxycoumarin. ***Umbelliferone***. *Hydrangin*. *Skimmetin*

$C_9H_6O_3$ 162.145
Occurs widely in plants including *Angelica* spp. Phytoalexin of infected sweet potato. Cryst. (toluene), needles (H_2O), yellow cryst. (EtOH aq.). Sol. EtOH; sl. sol. hot H_2O or Et_2O; mod. sol. Me_2CO. Mp 230-232° (223-224°, 227-228°). pK_{a1} 7.7. Log P 1.61 (calc). Also occurs as terpenoid ethers, e.g. Marmin, M-77 λ_{max} 244 (ε 3650); 257 (ε 2700); 322 (ε 17800); 328 (ε 18600) (MeOH) (Berdy). λ_{max} 377 (NaOH) (Berdy).

▶ GN6820000

Glycoside: ***Gummosinin***
$C_{24}H_{30}O_4$ 382.499
Isol. from galbanum (*Ferula gummosa*). Mp 163-165°. $[\alpha]_D$ -28 ($CHCl_3$).

Me ether: [531-59-9] *7-Methoxy-2*H*-1-benzopyran-2-one, 9CI*. *7-Methoxycoumarin*. ***Herniarin***. *Umbelliferone methyl ether*. *Ayapanin*
$C_{10}H_8O_3$ 176.171
Present in *Prunus mahaleb* (mahaleb cherry). Leaflets (H_2O or MeOH). Mp 117-118°. λ_{max} 247 (ε 2240); 320 (ε 14125) (MeOH) (Berdy).

▶ DJ3100380

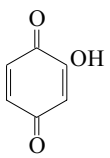
O-*(5-Formyl-3-methyl-2-pentenyl)*(E-): [15334-19-7] *4-Methyl-6-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-4-hexenal, 9CI*. ***Marminal***
$C_{16}H_{16}O_4$ 272.3
Constit. of the roots of *Aegle marmelos* (bael). Prisms (EtOAc/hexane). Mp 104.6° (101-102°).

[80368-70-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 323A; 323C; 325B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1312C; 1313C; 1315C (*nmr*)
Sethna, S. *et al., Org. React. (N.Y.)*, 1953, **7**, 20 (*synth*)
Sen, K. *et al., J.O.C.*, 1959, **24**, 316 (*synth, uv*)
Barnes, C.J. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
das Gupta, A.K. *et al., J.C.S.(C)*, 1969, 29 (*synth*)
Hata, K. *et al., Chem. Pharm. Bull.*, 1971, **19**, 640 (*isol*)
Lassak, E.V. *et al., Aust. J. Chem.*, 1972, **25**, 2491 (*derivs*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1320; 132; 1321 (*occur*)
González, A.G. *et al., An. Quim.*, 1973, **69**, 1013 (*pmr*)
Günther, H. *et al., Org. Magn. Reson.*, 1975, **7**, 339 (*cmr, deriv*)
Brown, D. *et al., Phytochemistry*, 1975, **14**, 1083 (*isol*)
Cussans, N.J. *et al., Tetrahedron*, 1975, **31**, 2719 (*cmr*)
Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, (*ind*)
Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, 1978, **35**, 200 (*rev*)
Hardt, T.J. *et al., Diss. Abstr. Int., B*, 1982, **43**, 1445 (*pharmacol*)
Ritschel, W.A. *et al., Arzneim.-Forsch.*, 1983, **33**, 836 (*metab*)
Joseph-Nathan, P. *et al., J. Het. Chem.*, 1984, **21**, 1141 (*pmr, deriv*)
Ueno, K. *et al., Acta Cryst. C*, 1985, **41**, 1786 (*cryst struct*)
Abu-Eittah, R.H. *et al., Can. J. Chem.*, 1985, **63**, 1173 (*uv*)
Talapatra, B. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 1122 (*synth*)
Gray, A.I. *et al., Phytochemistry*, 1987, **26**, 257 (*deriv*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 375 (*rev, tox, Me ether*)
Ishii, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 3100 (*synth, deriv*)
Yang, X. *et al., J. Chin. Pharm. Sci.*, 1996, **5**, 68-73 (*Marminal*)

Hydroxy-1,4-benzoquinone H-352

[2474-72-8]
2-Hydroxy-2,5-cyclohexadiene-1,4-dione, 9CI. *Hydroxyquinone*



$C_6H_4O_3$ 124.096
Yellow plates (petrol). Mp 130-140° Mp 124° dec. Darkens on exp. to air. Negligible tautomerism to 4-Hydroxy-1,2-benzoquinone.

Me ether: [2880-58-2] *2-Methoxy-1,4-benzoquinone*
$C_7H_6O_3$ 138.123
Isol. from fruits of *Diospyros kaki* (Japanese persimmon). Yellow needles (H_2O). Mp 145°. λ_{max} 248 (ε 10470); 343 (ε 1100) (hexane) (Berdy).

Me ether, 4-oxime: [17576-99-7]
$C_7H_7NO_3$ 153.137
Mp 176-177°.

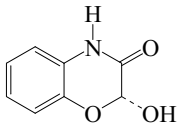
▶ LD_{50} (mus, ipr) 120 mg/kg. GU5675000

Et ether: [51767-58-9] *Ethoxy-1,4-benzoquinone*
$C_8H_8O_3$ 152.149
Yellow needles. Mp 119-120°.

Jacobson, P. *et al., Annalen*, 1909, **369**, 1 (*deriv*)
Willstätter, R. *et al., Ber.*, 1911, **44**, 2171 (*synth*)
Gomberg, M. *et al., J.A.C.S.*, 1916, **38**, 1577 (*deriv*)
Fieser, L.F. *et al., J.A.C.S.*, 1928, **50**, 439 (*tautom*)
Flaig, W. *et al., Annalen*, 1959, **626**, 215 (*ir*)
Deorhra, D.S. *et al., J. Indian Chem. Soc.*, 1965, **42**, 315 (*synth, deriv*)
Blatchly, J.M. *et al., J.C.S.(C)*, 1969, 1353 (*pmr*)
Hayashi, H. *et al., Agric. Biol. Chem.*, 1979, **43**, 113 (*isol, deriv*)
Pratt, D.V. *et al., J.O.C.*, 1987, **52**, 5053 (*deriv, synth, pmr, ir, ms*)
Keegstra, E.M.D. *et al., Chem. Comm.*, 1994, 1633 (*cryst struct, deriv*)

2-Hydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, 9CI H-353

[27779-92-6]
Blepharigenin. *HBOA*



(R)-form

$C_8H_7NO_3$ 165.148

(R)-form
Constit. of juvenile wheat (*Triticum aestivum*). Yellow needles. Mp 207°.

O-*β-D-Glucopyranoside:* [27625-86-1] ***Blepharin***. *HBOA-Glc*
$C_{14}H_{17}NO_8$ 327.29
Glycoside from seedlings of rye and sweet corn (*Zea mays*). Mp 226-227°. $[\alpha]_D$ +127.3 (H_2O).

O-*Ac:* [23520-35-6]
$C_{10}H_9NO_4$ 207.185
Cryst. (MeOH). Mp 177°.

O-*Benzoyl:*
$C_{15}H_{11}NO_4$ 269.256
Cryst. (MeOH/EtOAc). Mp 207°.

Me ether: [27392-93-4] *2-Methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, 9CI*
$C_9H_9NO_3$ 179.175
Cryst. (MeOH aq.). Mp 168-171°.

Me ether, N-*Me:2-Methoxy-4-methyl-2*H*-1,4-benzoxazin-3(4*H*)-one*
$C_{10}H_{11}NO_3$ 193.202
Cryst. (MeOH aq.). Mp 71°. Bp_1 180-185°.

N-*Hydroxy:* [17359-54-5] *2,4-Dihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one. DIBOA*
$C_8H_7NO_4$ 181.148
Isol. from seedlings of rye and sweet corn (*Zea mays*). Cryst. (Et_2O/cyclohexane). Mp 152°.

▶ DM3850000

N-*Hydroxy, 2-Me ether:* [55574-10-2] *4-Hydroxy-2-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, 9CI*
$C_9H_9NO_4$ 195.174
Cryst. Mp 136-138°.

(S)-form

N-*Hydroxy, 2-*O-*β-D-glucopyranoside:* [155835-54-4]

[22260-47-5, 157241-60-6] *DIBOA-Glc*. *GDIMBOA*
$C_{14}H_{17}NO_9$ 343.29
Isol. from seedlings of rye (*Secale cereale*), sweet corn (*Zea mays*) and seeds of *Acanthus mollis*. Cryst. Mp 186.5-187°. $[\alpha]_D^{24}$ +106 (c, 1 in H_2O). λ_{max} 254 (ε 8300); 281 (ε 6380) (prob. MeOH) (Derep).

7-Chloro, O-*β-D-glucopyranoside:*
$C_{14}H_{16}ClNO_8$ 361.735
Amorph. powder. $[\alpha]_D^{26}$ +198 (c, 0.33 in DMSO).

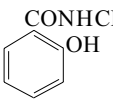
7-Chloro, N-*hydroxy,* O-*β-D-glucopyranoside:7-Cl-DIBOA-Glc*
$C_{14}H_{16}ClNO_9$ 377.734
Amorph. powder. $[\alpha]_D^{22}$ +18.6 (c, 0.86 in DMSO).

Lal, J.B. *et al., J. Indian Chem. Soc.*, 1940, **17**, 269 (*isol, deriv*)

Virtanen, A.L. *et al., Acta Chem. Scand.*, 1960, **14**, 499; 502; 504 (*synth, uv*)
Chatterjee, A. *et al., Chem. Ind. (London)*, 1969, 328 (*synth*)
Hofman, J. *et al., Eur. J. Biochem.*, 1969, **8**, 109-112 (*HBOA-Glc*)
Tipton, C.L. *et al., Phytochemistry*, 1973, **12**, 347 (*biosynth*)
Wilson, A.S. *et al., Cryst. Struct. Commun.*, 1982, **11**, 809-813 (*DIBOA, cryst struct*)
Wolf, R.B. *et al., J. Nat. Prod.*, 1985, **48**, 59-63 (*DIBOA-Glc*)
Atkinson, J. *et al., J.O.C.*, 1991, **56**, 1788 (*synth, pmr, ms, uv, ir*)
Tietze, L.F. *et al., Synthesis*, 1991, 1118 (*synth, pmr, abs config*)
Sicker, D. *et al., Synthesis*, 1993, 771 (*synth*)
Hartenstein, H. *et al., Phytochemistry*, 1994, **35**, 827-828 (*DIBOA-Glc, isol, abs config*)
Bravo, H.R. *et al., J. Agric. Food Chem.*, 1996, **44**, 1569 (*DIBOA, activity*)
Kamperdick, C. *et al., Pharmazie*, 1997, **52**, 965-966 (*isol, pmr, cmr*)
Tays, K. *et al., Synth. Commun.*, 1998, **28**, 903-912 (*N-hydroxy*)
Tanabe, J. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1614-1617 (*isol, biosynth*)
Baumeler, A. *et al., Phytochemistry*, 2000, **53**, 213-222 (*isol, pmr*)
Kanchanapoom, T. *et al., Phytochemistry*, 2001, **58**, 637-640; 811-817 (*7-chloro derivs*)

N-(2-Hydroxybenzoyl)glycine, 9CI H-354

[487-54-7]
o-*Hydroxyhippuric acid, 8CI. Salicyloylaminoacetic acid. Salicyloylglycine. Salicyluric acid. 2-Hydroxybenzamidoacetic acid*



$C_9H_9NO_4$ 195.174
Constit. of milk. Needles (H_2O or EtOH/C_6H_6). Mp 170-172°.

▶ LD_{50} (rat, scu) 3000 mg/kg. MR8160000

Et ester: [5853-89-4]
$C_{11}H_{13}NO_4$ 223.228
Needles (H_2O or Et_2O). Mp 98-99°.

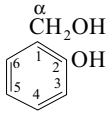
Ac: [5853-85-0]
$C_{11}H_{11}NO_5$ 237.212
Mp 147-149°.

Et ether:
$C_{11}H_{13}NO_4$ 223.228
Mp 176°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1407B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 377C (*ir*)
Bondi, S. *et al., Z. Physiol. Chem.*, 1907, **52**, 170
Fischer, E. *et al., Ber.*, 1909, **42**, 215
Schroeter, G. *et al., Ber.*, 1919, **52**, 2224
Mazzotta, D. *et al., Farmaco, Ed. Sci.*, 1975, **30**, 399
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SAN200

2-Hydroxybenzyl alcohol H-355

[90-01-7]
2-Hydroxybenzenemethanol, 9CI. ***Salicyl alcohol, USAN.*** *α,2-Dihydroxytoluene.* o-*Hydroxymethylphenol. Diathesin. Salicain†. Saligenin. Saligenol. Salicinol*



$C_7H_8O_2$ 124.139
Needles or plates (H_2O or Et_2O). d^{25} 1.16. Mp 87°. pK_{a1} 9.84 (25°). Log P 0.44 (calc). Sublimes at 100°.

▶ Exp. reprod. and teratogenic effects. DO6430000

α-Et ether: [20920-83-6] *2-(Ethoxymethyl)phenol, 9CI. FEMA 3485*
$C_9H_{12}O_2$ 152.193
Flavouring agent. Bp_{20} 111-113° Bp_2 79-82°. n_D^{20} 1.5197.

[29034-41-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1128B; 1128C; 1128D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 342A; 342B; 342C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1053C; 1053D (*ir*)
Shannon, J.S. *et al., Aust. J. Chem.*, 1962, **15**, 265 (*ms*)
Hansch, C. *et al., J. Med. Chem.*, 1970, **13**, 957 (*props*)
Yoon, N.M. *et al., J.O.C.*, 1973, **38**, 2786 (*synth, pmr*)
Nagata, W. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2867 (*synth*)
Kagawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2191 (*occur, pharmacol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 212 (*α-Et ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 937-938 (*α-Et ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HMK100

3-Hydroxybenzyl alcohol H-356

[620-24-6]
3-Hydroxybenzenemethanol, 9CI. α,3-Dihydroxytoluene. m-*Hydroxymethylphenol*

$C_7H_8O_2$ 124.139
Cryst. (C_6H_6). Mp 73°.

α-O-β-D-Glucopyranoside: [143995-98-6]
$C_{13}H_{18}O_7$ 286.281
Constit. of *Sambucus nigra* (elderberry). Oil.

[1515-82-8, 35480-26-3]

D'Abrosca, B. *et al., Phytochemistry*, 2001, **58**, 1073-1081 (*α-glucoside*)

4-Hydroxybenzyl alcohol, 8CI H-357

[623-05-2]
4-Hydroxybenzenemethanol, 9CI. α,4-Dihydroxytoluene. p-*Hydroxymethylphenol. Gastrodigenin*

$C_7H_8O_2$ 124.139
Constit. of muskmelon (*Cucurbita moschata*). Prisms or needles (H_2O). Mp 124.5-125.5°. pK_{a1} 9.73 (25°).

4-Me ether: [105-13-5] *4-Methoxybenzyl alcohol. Anisyl alcohol. FEMA 2099*
$C_8H_{10}O_2$ 138.166
Isol. from vanilla, aniseed oil, sweet osmanthus (*Osmanthus fragrans*) flowers and tarragon (*Artemisia dracunculus*). Used in flower perfumes and flavourings. Liq. with flowery, sweet odour and fruity peach flavour. d_{25}^{25} 1.11. Mp 24-25° (45°). Bp 259° Bp_{12} 135-136°. n_D^{25} 1.5420.

▶ Skin irritant. LD_{50} (rat, orl) 1200 mg/kg. Fl. p. >107°. DO8925000

4-Me ether, O-*β-D-glucopyranoside:* [81381-72-8] *4-Methoxybenzyl glucoside.* p-*Anisyl glucoside*
$C_{14}H_{20}O_7$ 300.308
Present in fennel and marrow (flowers). Needles (EtOAc). Mp 137-138°. $[\alpha]_D^{21}$ -51.1 (c, 1.2 in MeOH).

4-Me ether, α-O-(2-O-sulfo-β-D-glucopyranoside):
$C_{14}H_{20}O_{10}S$ 380.372
Found in fennel. Needles (MeOH) (as Na salt). Mp 149-151° (Na salt). $[\alpha]_D^{21}$ -34.6 (c, 0.8 in MeOH) (Na salt).

4-Me ether, formyl: [122-91-8] *4-Methoxybenzyl formate. Anisyl formate. FEMA 2101*
$C_9H_{10}O_3$ 166.176
Used extensively in food flavouring. Liq. with a strawberry taste. d 0.14. Bp 100°.

4-Me ether, Ac: [104-21-2] *Anisyl acetate. FEMA 2098*
$C_{10}H_{12}O_3$ 180.203
Found in fruits, Bourbon vanilla and Tahiti vanilla. Used in flavour industry. Liq. with floral fruit-like odour and pungent, sweet taste. Bp 270° Bp_{12} 135-136°.

4-Me ether, propanoyl: [7549-33-9] *4-Methoxybenzyl propanoate. Anisyl propionate. FEMA 2102*
$C_{11}H_{14}O_3$ 194.23
Flavouring agent with a fruity taste. $d^{15.5}$ 1.08. Bp 277°. n_D^{20} 1.5490.

4-Me ether, butanoyl: [6963-56-0] *4-Methoxybenzyl butanoate. Anisyl butyrate. FEMA 2100*
$C_{12}H_{16}O_3$ 208.257
Flavouring agent. Liq. Bp 270°.

4-Me ether, phenylacetyl: [102-17-0] *4-Methoxybenzyl phenylacetate. Anisyl phenylacetate. FEMA 3740*
$C_{16}H_{16}O_3$ 256.301
Flavouring agent for honey flavours. Liq. d^{25} 1.13. Bp 370°. n_D^{20} 1.5589.

α-Et ether: [57726-26-8] *4-(Ethoxymethyl)phenol*
$C_9H_{12}O_2$ 152.193
Constit. of *Vanilla fragrans* (vanilla). Yellowish oil.

α-Butyl ether: [57726-27-9] *4-(Butoxymethyl)phenol*
$C_{11}H_{16}O_2$ 180.246
Constit. of the leaves and stems of *Vanilla fragrans* (vanilla). Yellowish oil.

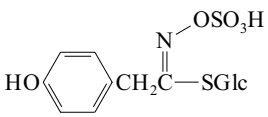
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1135B; 1135C; 1136A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 352B; 352C; 353B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1059C; 1059D (*ir*)
Späth, E. *et al., Monatsh. Chem.*, 1914, **35**, 319 (*synth*)
Carothers, W.H. *et al., J.A.C.S.*, 1924, **46**, 1675 (*synth*)

Shannon, J.S. *et al., Aust. J. Chem.*, 1962, **15**, 265 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 825 (*rev, tox, anisyl alcohol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1976, **14**, 683-685; 1980, **18**, 651 (*butanoate, formate, phenylacetate, rev*)
Torii, S. *et al., J.O.C.*, 1979, **44**, 3305-3310 (*4-Ethoxymethylphenol, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MED500
Hilborn, J.W. *et al., J.A.C.S.*, 1994, **116**, 3337 (*synth, uv, pmr, cmr, ir, ms, 4-Methoxybenzyl acetate, Anisyl acetate*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 45-48 (*derivs*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 179-184 (*derivs, occur, use*)
Sun, R. *et al., J. Agric. Food Chem.*, 2001, **49**, 5161-5164 (*4-Butoxymethylphenol, 4-Ethoxymethylphenol, isol*)

4-Hydroxybenzyl glucosinolate H-358

[19253-84-0]

[20643-28-1]
1-Thio-β-D-glucopyranose 1-[4-hydroxy-N-(sulfooxy)benzeneethanimidate]. ***Glucosinalbin***. *Glucosinalbate*



$C_{14}H_{19}NO_{10}S_2$ 425.437
Isol. from *Brassica* seeds. Prisms (EtOH)(as tetramethylammonium salt). Mp 191-192° (tetramethylammonium salt). $[\alpha]_D^{24}$ -20 (c, 2 in H_2O).

Salt with Sinapine, S-111: [20196-67-2]
Sinalbine. *Sinapinyl glucosinalbate*
Isol. from mustard seed (*Sinapis alba*) and other crucifers. Cryst. + $5H_2O$. Mp 83-84° (hydrate) Mp 139° (anhyd.). $[\alpha]_D$ -8.23 (H_2O). Also see Sinapine, S-111.

4-O-α-L-Rhamnopyranoside: [74542-19-1]
4-O-α-L-Rhamnopyranosylglucosinalbin
$C_{20}H_{29}NO_{14}S_2$ 571.579
Constit. of *Moringa oleifera* (horseradish tree) and *Moringa peregrina*. $[\alpha]_D$ -47 (c, 1 in H_2O).

4-(4-O-Acetyl-α-L-rhamnopyranoside):
$C_{22}H_{31}NO_{15}S_2$ 613.617
Constit. of *Moringa oleifera* (horseradish tree) and *Moringa peregrina*.

4-Me ether: [499-27-4]

[21290-06-2] *4-Methoxybenzyl glucosinolate.* ***Glucoaubrietin***
$C_{15}H_{21}NO_{10}S_2$ 439.464
Prisms (EtOH aq.)(as tetramethylammonium salt). Mp 187-189° (tetramethylammonium salt). $[\alpha]_D^{27}$ -21 (c, 2 in H_2O).

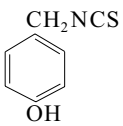
4-Me ether, tetra-Ac: [21412-37-3]
Needles (EtOH) (as K salt). Mp 187-190° (173-174°) (K salt). $[\alpha]_D^{27}$ -7 (c, 0.93 in H_2O).

[16411-05-5, 27299-07-6]

Harrison, K. *et al., Biochem. J.*, 1932, **26**, 88 (*Sinalbine, use*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1956, **10**, 26; 1968, **22**, 2 (*isol, deriv*)
Ettlinger, M.G. *et al., J.A.C.S.*, 1956, **78**, 4172 (*struct*)
Kindl, H. *et al., Monatsh. Chem.*, 1964, **95**, 439; 1965, **96**, 527; 1969, **100**, 1773 (*biosynth*)
Benn, M.H. *et al., Can. J. Chem.*, 1965, **43**, 1 (*synth*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, (*Sinalbine, use*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*pmr, cmr*)
Gueyrard, D. *et al., Tet. Lett.*, 2000, **41**, 8307-8309 (*4-rhamnoside*)
Fahey, J.W. *et al., Phytochemistry*, 2001, **56**, 5-51 (*rev, occur*)

4-Hydroxybenzyl isothiocyanate H-359

[2086-86-4]
4-(Isothiocyanatomethyl)phenol, 9CI



C_8H_7NOS 165.215
Obt. from white mustard seeds (*Sinapis alba*). Formed from 4-Hydroxybenzyl glucosinolate, H-358. Long needles (petrol at -10°). Mp 42°. Unstable.

O-α-L-Rhamnopyranoside: [73255-40-0]
$C_{14}H_{17}NO_5S$ 311.358
Constit. of seeds and other parts of *Moringa oleifera* (horseradish tree), *Moringa peregrina* and *Moringa stenopetala*. Cryst. Sol. H_2O. Mp 74°. λ_{max} 221 (H_2O). λ_{max} 221 (NaOH) (Berdy).

O-(4-O-Acetyl-α-L-rhamnopyranoside): [73255-41-1]
$C_{16}H_{19}NO_6S$ 353.395
Constit. of seeds of *Moringa oleifera* (horseradish tree) and *Moringa peregrina*.

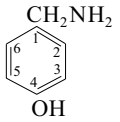
Me ether: [3694-57-3] *1-(Isothiocyanatomethyl)-4-methoxybenzene, 9CI. 4-Methoxybenzyl isothiocyanate*
C_9H_9NOS 179.242
Constit. of *Tropaeolum tuberosum* (anu). Liq. Poorly sol. hexane. d^{20} 1.09. $Bp_{0.5}$ 122°. n_D^{25} 1.5935.

[53690-04-3, 53690-07-6]

Salkowski, H. *et al., Ber.*, 1889, **22**, 2137 (*isol*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1954, **8**, 598; 1956, **10**, 26; 1963, **17**, 2143 (*isol, synth, ms, deriv*)
Barothy, J. *et al., Chem. Ind. (London)*, 1965, 308-309 (*isol, synth*)
Migrab, S. *et al., Phytochemistry*, 1977, **16**, 1719 (*Me ether*)
Kjaer, A. *et al., Phytochemistry*, 1979, **18**, 1485-1487 (*rhamnosides*)
Eilert, U. *et al., Planta Med.*, 1981, **42**, 55-61 (*rhamnoside*)

4-Hydroxybenzylamine H-360

[696-60-6]
4-(Aminomethyl)phenol, 9CI. α-Amino-p-cresol

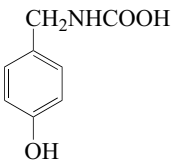


C_7H_9NO 123.154
Isol. from seeds of *Sinapis alba* (white mustard). Plates + $1H_2O$ (H_2O). Mp 114-115° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1288D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 610A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1172D (*ir*)
Salkowski, H. *et al., Ber.*, 1889, **22**, 2137
Tiffeneau, M. *et al., Bull. Soc. Chim. Fr.*, 1911, **9**, 819
Witkop, B. *et al., J.A.C.S.*, 1954, **76**, 5589
Larsen, P.O. *et al., Biochim. Biophys. Acta*, 1965, **107**, 134 (*isol, uv*)
Olsen, O. *et al., Phytochemistry*, 1980, **19**, 1783 (*isol, pmr, cmr*)
Larsen, P.O. *et al., Phytochemistry*, 1984, **23**, 895 (*isol*)
Eur. Pat., 1990, 354 297, (*Mitsui*); *CA*, **113**, 59234j

(4-Hydroxybenzyl)carbamic acid H-361

[(4-Hydroxyphenyl)methyl]carbamic acid. (4-Hydroxybenzyl)aminoformic acid



$C_8H_9NO_3$ 167.164

Benzyl ester: [75383-60-7]
$C_{15}H_{15}NO_3$ 257.288
Cryst. (C_6H_6). Mp 90.5-91° dec.

O-α-L-Rhamnopyranoside, Et ester: [208346-80-9]
$C_{16}H_{23}NO_7$ 341.36
Isol. from seed pods of *Moringa oleifera* (horseradish tree). λ_{max} 202 ; 222 ; 252 (MeOH).

O-(4-O-Acetyl-α-L-rhamnopyranoside), Me ester: [163812-19-9] ***Niazicinin A***
$C_{17}H_{23}NO_8$ 369.371
Constit. of *Moringa oleifera* (horseradish tree). λ_{max} 200 ; 223 ; 271 (MeOH).

O-(Tri-O-acetyl-α-L-rhamnopyranoside), Me ester: [163812-18-8]
$C_{21}H_{27}NO_{10}$ 453.445
Constit. of *Moringa oleifera* (horseradish tree). Isol. as two conformational (rotational) isomers λ_{max} 201 ; 222 ; 247 (MeOH).

O-(4-O-Acetyl-α-L-rhamnopyranoside), Et ester (1): [159768-73-7] ***Niazimin A***
$C_{18}H_{25}NO_8$ 383.397
Constit. of *Moringa oleifera* (horseradish tree). Plates ($CHCl_3$/MeOH). Mp 168-170°.

O-(4-O-Acetyl-α-L-rhamnopyranoside), Et ester (2): ***Niazimin B***
$C_{18}H_{25}NO_8$ 383.397
Constit. of *Moringa oleifera* (horserad-

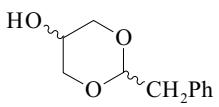
ish tree). Needles ($CHCl_3$/MeOH). Mp 182-184°. Conformational isomer of Niazimin A, differing in the orientation of the NH proton with respect to the carbonyl group.

O-*(Tri-O-acetyl-α-L-rhamnopyranoside), Et ester:* [159733-93-4]
$C_{22}H_{29}NO_{10}$ 467.472
Constit. of *Moringa oleifera* (horseradish tree). λ_{max} 203 ; 222 ; 246 (MeOH).

Nakano, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2212-2216 (*synth, benzyl ester*)
Faizi, S. *et al., J.C.S. Perkin 1*, 1994, 3035-3040 (*Niazimin A, Niazimin B*)
Faizi, S. *et al., Phytochemistry*, 1995, **38**, 957-963 (*isol, uv, pmr, cmr, derivs*)
Leuck, M. *et al., Carbohydr. Res.*, 1998, **312**, 33-44 (*synth*)
Faizi, S. *et al., Planta Med.*, 1998, **64**, 225-228 (*Et ester rhamnoside*)

5-Hydroxy-2-benzyl-1,3-dioxane H-362

[4740-79-8]
2-(Phenylmethyl)-1,3-dioxan-5-ol, 9CI. Phenylacetaldehyde glyceryl acetal. Acetal CD



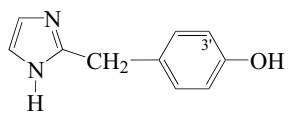
$C_{11}H_{14}O_3$ 194.23
Mixt. with 2-Benzyl-5-hydroxymethyl-1,3-dioxolane, B-57 is used as a flavouring ingredient. No phys. props. reported.

[29895-73-6]

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 829; *CA*, **91**, 198689b
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2180-2181

2-(4-Hydroxybenzyl)imidazole H-363

4-(1H-Imidazol-2-ylmethyl)phenol. ***Semilepidine A***



$C_{10}H_{10}N_2O$ 174.202
Powder (CH_2Cl_2/MeOH). Mp 164-166°. Artifact.

O-*β-D-Galactopyranoside:* ***Semilepidinoside A***
$C_{16}H_{20}N_2O_6$ 336.344
Alkaloid from the seeds of *Lepidium sativum* (garden cress). Amorph. powder. Mp 188-190° dec.

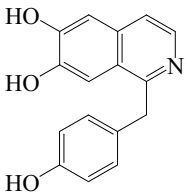
3′-Methoxy:2-(4-Hydroxy-3-methoxybenzyl)imidazole. Semilepidine B
$C_{11}H_{12}N_2O_2$ 204.228
Powder (CH_2Cl_2/MeOH). Mp 187-190°. Artifact.

3′-Methoxy, O-*β-D-galactopyranoside:* ***Semilepidinoside B***
$C_{17}H_{22}N_2O_7$ 366.37
Alkaloid from the seeds of *Lepidium sativum* (garden cress). Amorph. powder. Mp 212-215° dec.

Maier, U.H. *et al., Phytochemistry*, 1998, **49**, 1791-1795 (*isol, pmr, cmr, ms*)

1-(4-Hydroxybenzyl)-6,7-isoquinolinediol H-364

6,7-Dihydroxy-1-(4-hydroxybenzyl)isoquinoline



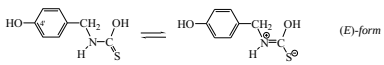
$C_{16}H_{13}NO_3$ 267.284

6-Me ether: [64069-53-0] *7-Hydroxy-1-(4-hydroxybenzyl)-6-methoxyisoquinoline.* ***Juzirine***
$C_{17}H_{15}NO_3$ 281.31
Alkaloid from the leaves of *Zizyphus jujuba* (Chinese date). Cryst. (Me_2CO). Mp 203-205°.

Coomes, R.M. *et al., J.O.C.*, 1973, **38**, 3701-3704 (*synth*)
Ziyaev, R. *et al., Khim. Prir. Soedin.*, 1977, **13**, 239; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 204 (*Juzirine*)
Marsaioli, A.J. *et al., Phytochemistry*, 1978, **17**, 1655-1658 (*cmr*)

(4-Hydroxybenzyl)thiocarbamic acid H-365

[(4-Hydroxyphenyl)methyl]carbamothioic acid. (4-Hydroxybenzyl)aminothioformic acid



(E)-form

$C_8H_9NO_2S$ 183.231
Known as naturally-occurring *O*-alkyl esters, the *E*- and *Z*-isomers of which are separately isolable.

4′-O-α-L-Rhamnopyranoside, O-*Me ester (E-):* [148152-07-2] ***Niazinin A***
$C_{15}H_{21}NO_6S$ 343.4
Constit. of the horseradish tree (*Moringa oleifera*, Moringaceae). λ_{max} 200 ; 224 ; 245 (MeOH).

4′-O-α-L-Rhamnopyranoside, O-*Me ester (Z-):* [147821-47-4] ***Niazinin B***
$C_{15}H_{21}NO_6S$ 343.4
Constit. of *Moringa oleifera* (horseradish tree) (Moringaceae). λ_{max} 200 ; 224 ; 245 (MeOH).

4′-O-α-L-Rhamnopyranoside, O-*Et ester (E-):* [147821-49-6] ***Niazimicin A***
$C_{16}H_{23}NO_6S$ 357.427
Constit. of *Moringa oleifera* (horseradish tree) (Moringaceae). $[\alpha]_D^{25}$ -96.8 (c, 0.5 in $CHCl_3$). λ_{max} 200 ; 223 ; 246 (MeOH).

4′-O-(4-O-Acetyl-α-L-rhamnopyranoside), O-*Me ester (E-):* [159768-74-8] ***Niazicin A***
$C_{17}H_{23}NO_7S$ 385.437
Constit. of *Moringa oleifera* (horseradish tree). λ_{max} 201 ; 223 ; 245 (MeOH).

4′-O-(4-O-Acetyl-α-L-rhamnopyranoside), O-*Me ester (Z-):* ***Niazicin B***
$C_{17}H_{23}NO_7S$ 385.437
Constit. of *Moringa oleifera* (horseradish tree). λ_{max} 201 ; 223 ; 245 (MeOH).

4′-O-(4-O-Acetyl-α-L-rhamnopyranoside), O-*Et ester (E-):* [147821-51-0] ***Niaziminin A***
$C_{18}H_{25}NO_7S$ 399.464
Constit. of *Moringa oleifera* (horseradish tree) (Moringaceae). Cryst. ($CHCl_3$/MeOH). Mp 168-170°. λ_{max} 195 ; 201 ; 222 ; 246 (MeOH).

4′-O-(4-O-Acetyl-α-L-rhamnopyranoside), O-*Et ester (Z-):* [147921-21-9] ***Niaziminin B***
$C_{18}H_{25}NO_7S$ 399.464
Constit. of *Moringa oleifera* (horseradish tree) (Moringaceae).

4′-O-(Tri-O-acetyl-α-L-rhamnopyranoside), O-*Me ester (E-):* [147821-48-5]
$C_{21}H_{27}NO_9S$ 469.512
Constit. of *Moringa oleifera* (horseradish tree) (Moringaceae). λ_{max} 201 ; 222 ; 247 (MeOH).

4′-O-(Tri-O-acetyl-α-L-rhamnopyranoside), O-*Et ester (Z-):*
$C_{21}H_{27}NO_9S$ 469.512
Constit. of *Moringa oleifera* (horseradish tree) (Moringaceae). λ_{max} 200 ; 221 ; 248 (MeOH).

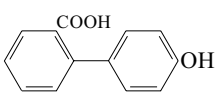
4′-O-(Tri-O-acetyl-α-L-rhamnopyranoside), O-*Et ester:* [147821-50-9]
$C_{22}H_{29}NO_9S$ 483.538
Constit. of *Moringa oleifera* (horseradish tree) (Moringaceae). λ_{max} 203 ; 221 ; 246 (MeOH).

O-*α-L-Rhamnopyranoside, Et ester (Z-):* ***Niazimicin B***
$C_{16}H_{23}NO_6S$ 357.427
Constit. of *Moringa oleifera* (horseradish tree).

Faizi, S. *et al., J.C.S. Perkin 1*, 1992, 3237-3241; 1994, 3035-3040 (*Niazinins, Niaziminins, Niazimicin, Niazicins*)
Faizi, S. *et al., Phytochemistry*, 1995, **38**, 957-963 (*isol, uv, pmr, cmr*)
Leuck, M. *et al., Carbohydr. Res.*, 1998, **312**, 33-44 (*synth, bibl*)
Murakami, A. *et al., Planta Med.*, 1998, **64**, 319-323 (*isol, activity*)

4′-Hydroxy-2-biphenylcarboxylic acid, 8CI H-366

[67526-82-3]
2-(4-Hydroxyphenyl)benzoic acid



$C_{13}H_{10}O_3$ 214.22
Constit. of *Trifolium repens* (white clover). Pale yellow cryst. (H_2O). Mp 206.5°.

Me ester: [170304-68-4]
$C_{14}H_{12}O_3$ 228.247
Grey powder. Mp 105°.

Nitrile: [137863-68-4] *2-Cyano-4′-hydroxybiphenyl*
$C_{13}H_9NO$ 195.22

Cryst. Mp 177-178°.

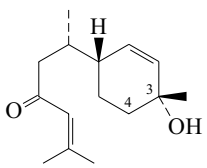
Me ether: [18110-71-9] *4′-Methoxy-2-biphenylcarboxylic acid*
$C_{14}H_{12}O_3$ 228.247
Cryst. (EtOH aq.). Mp 146-148°.

Me ether, Me ester: [17103-25-2]
$C_{15}H_{14}O_3$ 242.274
Cryst. (EtOAc). Mp 132-134°.

Me ether, nitrile: [125610-78-8] *2-Cyano-4′-methoxybiphenyl*
$C_{14}H_{11}NO$ 209.247
Cryst. Mp 155-157°.

Drapala, T. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1960, **34**, 1371-1380; 1972, **46**, 9-13 (*synth, uv*)
Hey, D.H. *et al., J.C.S.*, 1961, 232-238 (*synth*)
Brown, P.M. *et al., J.C.S.(C)*, 1968, 842-848 (*Me ether*)
Glover, S.A. *et al., J.C.S. Perkin 1*, 1981, 842-848 (*synth*)
Ghosal, S. *et al., J. Chem. Res., Synop.*, 1988, 196-197 (*isol, uv, ir, pmr*)
Sain, B. *et al., J.O.C.*, 1990, **55**, 2545-2546 (*Me ether nitrile, synth, pmr*)
Kim, K.S. *et al., J. Med. Chem.*, 1993, **36**, 2335-2342 (*nitrile, synth, pmr, cmr*)
Estenne, G. *et al., Org. Prep. Proced. Int.*, 1995, **27**, 500-503 (*synth, Me ester, ir, pmr*)
Matsuhira, A. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1870-1874 (*Me ether, synth, pmr*)

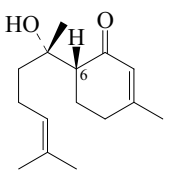
3-Hydroxy-1,10-bisaboladien-9-one H-367



$C_{15}H_{24}O_2$ 236.353
Constit. of *Curcuma longa* (turmeric). Viscous oil. $[\alpha]_D$ +51 (c, 0.22 in MeOH).

Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201 (*isol, pmr, cmr*)

7-Hydroxy-2,10-bisaboladien-1-one H-368



(6*R*,7*S*)-*form*

$C_{15}H_{24}O_2$ 236.353

(6*R*,7*S*)-*form* [110715-85-0]
Epihernandulcin
Oil. $[\alpha]_D^{20}$ -180.6 (c, 1.03 in $CHCl_3$). λ_{max} 236 (log ϵ 4.12) (EtOH).

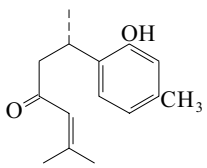
(6*S*,7*S*)-*form* [95602-94-1]
Hernandulcin
Constit. of *Lippia dulcis* leaves and flowers. Natural sweetener more than 1000 times sweeter than sucrose. $[\alpha]_D^{25}$ +109 (c, 0.11 in EtOH). λ_{max} 236 (log ϵ 4.11) (EtOH).

► GW7251000

Compadre, C.M. *et al., Science (Washington, D.C.)*, 1985, **227**, 417 (*struct*)
Mori, K. *et al., Tetrahedron*, 1986, **42**, 5895 (*synth*)
Kaneda, N. *et al., J. Nat. Prod.*, 1992, **55**, 1136 (*isol, pmr, cmr*)
Souto-Bachiller, F.A. *et al., Phytochemistry*, 1997, **44**, 1077 (*isol, uv, ir, ms*)
Kim, J.H. *et al., Tet. Lett.*, 2002, **43**, 4721-4722 (*synth*)

1-Hydroxy-1,3,5,10-bisabolatetraen-9-one H-369

[131651-38-2]
Turmeronol B

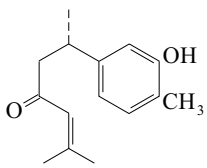


$C_{15}H_{20}O_2$ 232.322
Constit. of turmeric (*Curcuma longa*). Oil. $[\alpha]_D^{23}$ +79 (c, 0.1 in $CHCl_3$). λ_{max} 235 (ϵ 11000); 276 (ϵ 2650) (MeOH) (Derep).

Imai, S. *et al., Agric. Biol. Chem.*, 1990, **54**, 2367 (*isol, pmr, cmr*)
Sharma, M.L. *et al., Tet. Lett.*, 1996, **37**, 2275 (*synth*)

2-Hydroxy-1,3,5,10-bisabolatetraen-9-one H-370

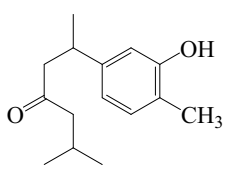
[131651-37-1]
Turmeronol A



$C_{15}H_{20}O_2$ 232.322
Constit. of turmeric (*Curcuma longa*). Oil. $[\alpha]_D^{23}$ +63 (c, 0.1 in $CHCl_3$). λ_{max} 235 (ϵ 11000); 276 (ϵ 2650) (MeOH) (Derep).

Imai, S. *et al., Agric. Biol. Chem.*, 1990, **54**, 2367-2371 (*isol, pmr, cmr*)
Kitahara, T. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1137 (*synth*)

2-Hydroxy-1,3,5-bisabolatrien-9-one H-371



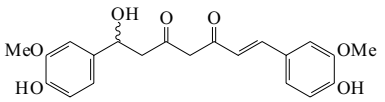
$C_{15}H_{22}O_2$ 234.338

(ξ)-*form*
Constit. of *Curcuma longa* (turmeric).

Jayaprakasha, G.K. *et al., Z. Naturforsch., C*, 2001, **56**, 40-44

7-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-1-heptene-3,5-dione, 9CI H-372

[112494-43-6]

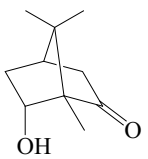


$C_{21}H_{22}O_7$ 386.401
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Yellow powder. Mp 92-96° (84-88°). $[\alpha]_D$ +12.2 (c, 0.06 in EtOH).

Uehara, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3298 (*isol*)
Masuda, T. *et al., Phytochemistry*, 1992, **31**, 3645 (*isol, pmr*)

6-Hydroxy-2-bornanone H-373

6-Hydroxycamphor



$C_{10}H_{16}O_2$ 168.235

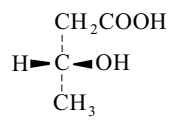
(1*R*,4*R*,6*S*)-*form*

O-*β*-D-*Glucopyranoside:* [155551-16-9]
$C_{16}H_{26}O_7$ 330.377
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -8 (c, 0.2 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 805-808 (*isol, pmr, cmr*)

3-Hydroxybutanoic acid, 9CI H-374

[300-85-6]



(*R*)-*form*

$C_4H_8O_3$ 104.105

(*R*)-*form* [625-72-9]
V. hygroscopic cryst. V. sol. H_2O, EtOH; insol. C_6H_6. Mp 49-50° (44-46°). $[\alpha]_D$ -24.7 (c, 5 in H_2O). $[\alpha]_D^{16}$ -24.9.

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside], butyl ester:*
$C_{19}H_{34}O_{12}$ 454.47
Isol. from Cape gooseberry *Physalis peruviana*. Needles (as hexa-Ac). Mp 104-106° (hexa-Ac). $[\alpha]_D^{22}$ -2.1 (c, 0.29 in MeOH) (hexa-Ac).

(*S*)-*form* [6168-83-8]
$[\alpha]_D$ +10.3 (c, 6 in H_2O).

Et ester, O-*β*-D-*glucopyranoside:*
$C_{12}H_{22}O_8$ 294.301
Constit. of the fruit of mountain papaya *Carica pubescens*.

Butyl ester, O-*β*-D-*glucopyranoside:*
$C_{14}H_{26}O_8$ 322.355
Constit. of the fruit of mountain papaya *Carica pubescens*.

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside], butyl ester:*
Isol. from Cape gooseberry (*Physalis peruviana*). Cryst. (as hexa-Ac). Mp 101-103° (hexa-Ac). $[\alpha]_D^{20}$ +1.8 (c, 0.23 in MeOH).

(±)-*form* [625-71-8]
Hygroscopic syrup. Bp_{13} 130° (lit. gives a pressure range). pK_a 4.29. Steam-volatile.

Et ester: [35608-64-1]

[5405-41-4] *FEMA 3428*
Flavouring ingredient. d^{25} 1.01. Bp_8 72-74° Bp 184-185°. n_D^{20} 1.4200.

[5864-66-4, 25654-45-9, 29435-48-1, 35054-79-6, 127604-16-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 518B; 549A; 660D; 661A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 854C; 1036A; 1036B; 1036C; 1037A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 715B; 715C; 716A (*ir*)
Wislicenus, J. *et al., Annalen*, 1869, **149**, 205 (*synth*)
Levene, P.A. *et al., J. Biol. Chem.*, 1926, **68**, 418 (*abs config*)
Forsyth, W.G.C. *et al., Nature (London)*, 1958, **182**, 800 (*isol*)
Ottaway, J.H. *et al., Biochem. J.*, 1962, **84**, 11 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 238 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 994-995 (*Et ester*)

1-Hydroxy-2-butanone, 9CI H-375

[5077-67-8]
2-Oxo-1-butanol. Ethyl hydroxymethyl ketone. FEMA 3173

$H_3CCH_2COCH_2OH$

$C_4H_8O_2$ 88.106
Constit. of coffee and various edible mushrooms. Flavouring ingredient. Liq. Misc. H_2O, EtOH, Et_2O. Bp 160°.

Oxime:
$C_4H_9NO_2$ 103.121
Cryst. ($CHCl_3$). Mp 60-61°.

Phenylhydrazone:
Yellow oil. Bp_{18} 170°.

Semicarbazone:
Cryst. (EtOH). Spar. sol. H_2O. Mp 87° Mp 136-138° (dimorph.).

Formyl:
$C_5H_8O_3$ 116.116
Bp 176-178°.

Formyl, semicarbazone:
Cryst. ($CHCl_3$). Mp 115°.

Ac: [1575-57-1]
$C_6H_{10}O_3$ 130.143
Bp_{14} 79°.

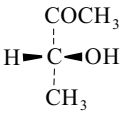
►EL8800000

Me ether:1-Methoxy-2-butanone
$C_5H_{10}O_2$ 102.133
Bp_{729} 130-131°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 654B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 507A (*ir*)
Kling, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1905, **140**, 1345
Knipe, A.C. *et al., J.O.C.*, 1973, **38**, 3429 (*synth*)
Ueno, Y. *et al., Tet. Lett.*, 1976, 4597 (*synth*)

3-Hydroxy-2-butanone, 9CI, 8CI H-376

[513-86-0]
Acetoin. Dimethylketol. Methylacetylcarbinol. 1-Hydroxyethyl methyl ketone. Acetylmethylcarbinol. FEMA 2008



(R)-form

$C_4H_8O_2$ 88.106
Constit. of beer, wine, fresh or cooked apple, fresh or cooked leek, corn, honey, cocoa, butter, cheeses, roasted coffee and other foodstuffs. Flavouring ingredient..

►EL8790000

(R)-form [53584-56-8]
Constit. of butter and produced by many microorganisms. Bp 142.7-143.2° Bp_{20} 49.2°. $[\alpha]_D^{20}$ -58 (neat).

(±)-*form* [52217-02-4]
Misc. H_2O, sol. EtOH. Mp -72° Mp 15°. Bp 148° Bp_{11} 36-37°.

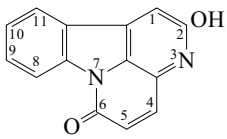
Ac: [4906-24-5] *FEMA 3526*
$C_6H_{10}O_3$ 130.143
Present in pineapple, paw paw, arctic bramble, red wine, cocoa and roast chicken. Flavouring ingredient. Bp 169-173°.

Butanoyl: [84642-61-5] *1-Methyl-2-oxopropyl butyrate. FEMA 3332*
$C_8H_{14}O_3$ 158.197
Flavouring ingredient.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 420C (*ir*)
Fulmer, E.I. *et al., J.A.C.S.*, 1943, **65**, 1427 (*synth*)
Blom, R.H. *et al., J.A.C.S.*, 1945, **67**, 494 (*config*)
Frearson, M.J. *et al., J.C.S.(C)*, 1968, 2909 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 441 (*occur*)
Knipe, A.C. *et al., J.O.C.*, 1973, **38**, 3429 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 509 (*rev, tox*)
Crout, D.H.G. *et al., J.C.S. Perkin 1*, 1983, 2435 (*synth*)
Lee, L.G. *et al., J.O.C.*, 1986, **51**, 25 (*synth, R-form*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ABB500
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 74 (*butanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 18; 32; 312-313 (*occur, props, Ac, butanoyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

2-Hydroxycanthin-6-one H-377

2-Hydroxy-6H-indolo[3,2,1-de][1,5]-naphthyridin-6-one, 9CI



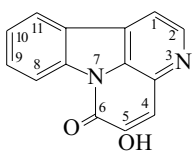
$C_{14}H_8N_2O_2$ 236.229
Amorph. solid.

Me ether: [116353-93-6] *2-Methoxy-6H-indolo[3,2,1-de][1,5]naphthyridin-6-one, 9CI.* ***2-Methoxycanthin-6-one***
$C_{15}H_{10}N_2O_2$ 250.256
Alkaloid from stem wood of *Quassia amara* (Surinam quassia). Pale yellow powder (MeOH/$CHCl_3$). Mp 262-264°.

Crespi-Perellino, N. *et al., J. Nat. Prod.*, 1986, **49**, 1010 (*isol, uv, pmr, ms, struct*)
Njar, V.C.O. *et al., Planta Med.*, 1993, **59**, 259 (*2-Methoxycanthin-6-one*)

5-Hydroxycanthin-6-one H-378

[64118-73-6]
5-Hydroxy-6H-indolo[3,2,1-de][1,5]-naphthyridin-6-one, 9CI



$C_{14}H_8N_2O_2$ 236.229
Orange-yellow platelets (MeOH). Sol. MeOH, $CHCl_3$. Mp 259-261° dec.

Ac:
Needles (C_6H_6). Mp 231.5-232°.

Me ether: [15071-56-4] ***5-Methoxycanthin-6-one****. 5-Methoxy-6H-indolo[3,2,1-de][1,5]naphthyridin-6-one, 9CI*
$C_{15}H_{10}N_2O_2$ 250.256
Alkaloid from the wood of *Picrasma excelsa* (Jamaican quassiawood). Pale-yellow needles (MeOH, $CHCl_3$/MeOH or EtOH/CH_2Cl_2). Mp 243-244° (237-238°) dec. Log P 2.35 (uncertain value) (calc).

Me ether, hydrochloride:
Needles (MeOH). Mp 205-208°.

Me ether, hydrobromide:
Cryst. (MeOH aq.). Mp 210°.

Me ether, picrate:
Yellow needles (MeOH). Mp 244-246°.

Me ether, methiodide:
Orange-red needles (H_2O). Mp 308-309°.

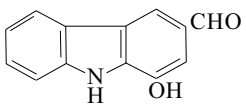
O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [159194-91-9] ***Bruceolline B****. Bruceacanthinoside*
$C_{26}H_{28}N_2O_{12}$ 560.513
Pale yellow amorph. powder. Mp 192-194°. $[\alpha]_D^{23}$ -41 (c, 1 in Py). $[\alpha]_D^{25}$ -64.4 (c, 0.45 in DMSO).

Haynes, H.F. *et al., Aust. J. Sci. Res., Ser. A*, 1952, **5**, 387 (*isol*)
Nelson, E.R. *et al., Aust. J. Sci. Res., Ser. A*, 1952, **5**, 563 (*uv, struct, synth*)

Bartlett, M.F. *et al., J.A.C.S.*, 1960, **82**, 5941 (*synth*)
Awad, A.T. *et al., J. Pharm. Sci.*, 1967, **56**, 279 (*isol*)
Della Casa, D. *et al., J.C.S.(C)*, 1967, 2155 (*isol, uv, ir, pmr*)
Lassak, E.V. *et al., Phytochemistry*, 1977, **16**, 1126 (*isol, synth, uv, ms, struct*)
Cordell, G.A. *et al., J. Nat. Prod.*, 1978, **41**, 166 (*isol, uv, ir, pmr, ms*)
Wagner, H. *et al., Planta Med.*, 1979, **36**, 113 (*isol*)
Forgacs, P. *et al., Planta Med.*, 1982, **46**, 187 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1416 (*Bruceacanthinoside*)
Ouyang, Y. *et al., Phytochemistry*, 1994, **36**, 1543 (*Bruceolline B*)

1-Hydroxy-9*H*-carbazole-3-carboxaldehyde H-379

3-Formyl-1-hydroxycarbazole. ***Demethylmurrayanine***



$C_{13}H_9NO_2$ 211.22
Plates ($CHCl_3$). Mp 237-239°.

Me ether: [723-97-7] *1-Methoxy-9H-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-1-methoxycarbazole.* ***Murrayanine***
$C_{14}H_{11}NO_2$ 225.246
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Needles (C_6H_6/petrol). Sol. MeOH, C_6H_6; poorly sol. hexane. Mp 168-170° Mp 219° dec. (synthetic). $Bp_{0.05}$ 110-115° subl.. λ_{max} 239 (ϵ 29510); 247 (ϵ 19950); 274 (ϵ 36310); 289 (ϵ 36300) (MeOH) (Berdy).

Me ether, picrate:
Fine orange needles (C_6H_6/petrol). Mp 198-200° dec.

Me ether, oxime:
$C_{14}H_{12}N_2O_2$ 240.261
Needles (C_6H_6/petrol). Mp 155-156°.

Me ether, N-*Me:*
$C_{15}H_{13}NO_2$ 239.273
Cream-coloured needles (C_6H_6/petrol). Mp 150.5-151.5°.

Das, K.C. *et al., Experientia*, 1965, **21**, 340 (*activity*)
Chakraborty, D.P. *et al., Tetrahedron*, 1965, **21**, 681 (*isol, uv, ir, pmr, struct*)
Crum, J.D. *et al., Chem. Comm.*, 1966, 417 (*synth, uv, ir, pmr*)
Chakraborty, D.P. *et al., J.O.C.*, 1968, **33**, 1265 (*synth, uv, ir*)
Bhattracharyya, P. *et al., Phytochemistry*, 1973, **12**, 1831 (*isol, uv, ir*)
Ngadjui, B.T. *et al., Phytochemistry*, 1989, **28**, 1517 (*isol, uv, ir, pmr, cmr, ms, struct*)
Knölker, H.-J. *et al., Tetrahedron*, 1993, **49**, 11221 (*synth*)
Bringmann, G. *et al., Planta Med.*, 1998, **64**, 54-57 (*synth, pmr, cmr*)
Bringmann, G. *et al., Synthesis*, 1998, 1501-1505 (*synth, Me ether, cmr*)

6-Hydroxy-9*H*-carbazole-3-carboxaldehyde H-380

3-Formyl-6-hydroxycarbazole

$C_{13}H_9NO_2$ 211.22

Me ether: [107816-72-8] *6-Methoxy-9H-carbazole-3-carboxaldehyde. 8-Methoxy-2-carbazolecarboxaldehyde (obsol.). 3-Formyl-6-methoxycarbazole*
$C_{14}H_{11}NO_2$ 225.246
Alkaloid from the roots of *Clausena lansium* (wampee). Prisms (Me_2CO/hexane). Mp 135-136°.

Hewlins, M.J.E. *et al., J. Chem. Res., Synop.*, 1986, 292

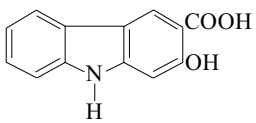
8-Hydroxy-9*H*-carbazole-3-carboxaldehyde H-381

$C_{13}H_9NO_2$ 211.22

Me ether: [87264-45-7] *8-Methoxy-9H-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-8-methoxycarbazole. 6-Formyl-1-methoxycarbazole.* ***Mukolidine***
$C_{14}H_{11}NO_2$ 225.246
Minor alkaloid from roots of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6). Mp 152-155°.

Roy, S. *et al., J. Indian Chem. Soc.*, 1982, **59**, 1369 (*Mukolidine*)

2-Hydroxy-9*H*-carbazole-3-carboxylic acid, 9CI H-382



$C_{13}H_9NO_3$ 227.219

Me ester: [24949-00-6] ***Mukonidine****. 2-Hydroxy-3-carbomethoxycarbazole*
$C_{14}H_{11}NO_3$ 241.246
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6/$CHCl_3$). Mp 245°. Doubts have been expressed as to the correctness of this struct.; see below.

Me ether, Me ester: [14501-65-6] O-*Methylmukonidine. 2-Methoxy-3-carbomethoxycarbazole.* ***Clausine L***
$C_{15}H_{13}NO_3$ 255.273
Alkaloid from stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6/$CHCl_3$). Plates (Me_2CO). Mp 133-135°. Methylmukonidine and Clausine L not compared. Phys. data are not identical.

3-Aldehyde: [20323-67-5] *2-Hydroxy-9H-carbazole-3-carboxaldehyde, 9CI. 2-Hydroxy-3-formylcarbazole.* ***Mukonal***
$C_{13}H_9NO_2$ 211.22
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6/$CHCl_3$). Mp 238°.

3-Aldehyde, O-*Ac:*
Cryst. (C_6H_6). Mp 210°.

3-Aldehyde, Me ether: [51971-08-5] *2-Methoxy-9H-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-2-methoxycarbazole.* ***Glycosinine****.* O-*Methylmukonal*
$C_{14}H_{11}NO_2$ 225.246
Mp 189-189.5° (185°).

Joshi, B.S. *et al., Chem. Ind. (London)*, 1968, 685 (*synth, uv, ir, pmr, Mukonal*)
Bhagwanth, M.R.R. *et al., Indian J. Chem.*, 1969, **7**, 1065 (*synth, Mukonal*)
Chakraborty, D.P. *et al., J. Indian Chem. Soc.*, 1978, **55**, 1114 (*isol, uv, ir, ms, struct, synth, Mukonidine*)
Bhattacharyya, P. *et al., Phytochemistry*, 1984, **23**, 471 (*isol, uv, ir, pmr, cmr, ms, Mukonal*)
Ruangrungsi, N. *et al., J. Nat. Prod.*, 1990, **53**, 946 (*O-Methylmukonal*)
Wu, T.S. *et al., Phytochemistry*, 1993, **32**, 449 (*Clausine L, Glycosinine*)
Bhattacharyya, P. *et al., Phytochemistry*, 1994, **35**, 1085 (*O-Methylmukonidine*)
Knölker, H.J. *et al., Synlett*, 1996, 737 (*synth, Mukonal, O-Methylmukonal*)
Knölker, H.J. *et al., Tet. Lett.*, 1997, **38**, 533 (*synth, Mukonidine*)

6-Hydroxy-9*H*-carbazole-3-carboxylic acid H-383

8-Hydroxy-2-carbazolecarboxylic acid (obsol.)

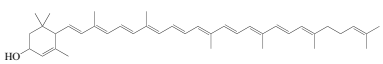
$C_{13}H_9NO_3$ 227.219

Me ether, Me ester: [132922-58-8] ***Methyl 6-methoxy-9H-carbazole-3-carboxylate****. Methyl 8-methoxy-2-carbazolecarboxylate (obsol.)*
$C_{15}H_{13}NO_3$ 255.273
Alkaloid from the roots of *Clausena lansium* (wampee). Prisms (Et_2O/hexane). Mp 147-149°.

Hewlins, M.J.E. *et al., J. Chem. Res., Synop.*, 1986, 292 (*synth*)
Li, W.-S. *et al., Phytochemistry*, 1991, **30**, 343 (*isol*)

3-Hydroxy-δ-carotene H-384

[75324-12-8]
ϵ,ψ-Caroten-3-ol. 3-Hydroxy-α-zeacarotene. Monol 487

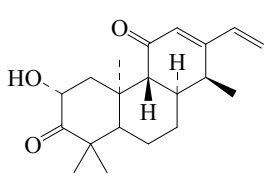


$C_{40}H_{56}O$ 552.882
Very poorly identified and characterised. Isol. from ripe tomatoes, comfrey and kale. λ_{max} 428 ; 455 ; 487 (petrol).

[119105-23-6]

Curl, A.L. *et al., J. Food Sci.*, 1961, **26**, 106
Shimizu, T. *et al., Sagami Joshi Daigaku Kiyo*, 1979, **43**, 235
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 86

2-Hydroxy-12,15-cassadiene-3,11-dione H-385

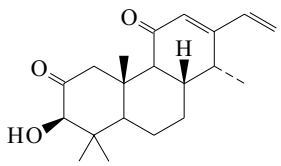


$C_{20}H_{28}O_3$ 316.439
(ent-2β)-*form* [166547-21-3]
Phytocassane A
Phytoalexin from *Oryza sativa* (rice). Gum. λ_{max} 268 (MeOH) (Berdy).

Koga, J. *et al., Tetrahedron*, 1995, **51**, 7907 (*isol, pmr, cmr*)

Yojima, A. *et al., Tet. Lett.*, 2000, **41**, 351-354 (*abs config*)

3-Hydroxy-12,15-cassadiene-2,11-dione H-386



$C_{20}H_{28}O_3$ 316.439

3β-*form* [166547-24-6]

Phytocassane D

Phytoalexin from *Oryza sativa*. Gum. λ_{max} 268 (MeOH) (Berdy).

Koga, J. *et al., Tetrahedron*, 1995, **51**, 7907 (*isol, pmr, cmr*)

Yajima, A. *et al., Eur. J. Org. Chem.*, 2000, 4079-4091 (*synth*)

4-Hydroxycitrulline H-387

[3618-90-4]

N^5-*Carbamoyl-4-hydroxyornithine, 8CI. 2-Amino-4-hydroxy-5-ureidopentanoic acid*

$H_2NCONHCH_2CH(OH)CH_2CH(NH_2)$-COOH

$C_6H_{13}N_3O_4$ 191.186

Isol. from *Vicia faba*. Mp 195° (185-187°). $[\alpha]_D^{25}$ +8 (c, 1 in 2*M* HCl). The nat. prod. is an L-form but the rel. config. has not been detd..

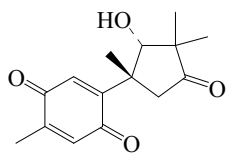
Bell, E.A. *et al., Biochem. J.*, 1965, **97**, 104

Inatomi, H. *et al., CA*, 1970, **72**, 18541y (*isol*)

8-Hydroxy-2,5-cuparadiene-1,4,10-trione H-388

[359701-29-4]

Enokipodin D

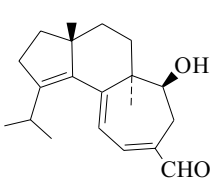


$C_{15}H_{18}O_4$ 262.305

Constit. of *Flammulina velutipes* (velvet shank). Yellow powder. Mp 116-117°. $[\alpha]_D^{24}$ +130 (c, 0.1 in MeOH). λ_{max} 254 (log ϵ 3.83) (MeOH).

Ishikawa, N.K. *et al., J. Nat. Prod.*, 2001, **64**, 932-934 (*isol, pmr, cmr*)

14-Hydroxy-3,5(10),11-cyathatrien-15-al H-389



$C_{20}H_{28}O_2$ 300.44

14β-*form* [70117-00-9]

Allocyathin B2

Yellow syrup. $[\alpha]_D^{25}$ +87.1 (c, 0.95 in MeOH). λ_{max} 201 (ϵ 7700); 338 (ϵ 17000) (MeOH) (Berdy). λ_{max} 266 (ϵ 5150); 325 (ϵ 12100) (hexane) (Berdy).

14-O-β-D-Xylopyranoside: ***Erinacine A***

$C_{25}H_{36}O_6$ 432.556

Metab. of *Hericium erinaceum* (lions mane). Cryst. Sol. MeOH, Me_2CO, EtOAc, $CHCl_3$; fairly sol. EtOH; poorly sol. H_2O. Mp 74-76°. $[\alpha]_D$ +216 (c, 0.28 in MeOH). λ_{max} 201 (ϵ 10500); 339 (ϵ 11300) (MeOH) (Berdy). λ_{max} 201 (ϵ 6100); 338 (ϵ 12000) (EtOH) (Berdy).

Ayer, W.A. *et al., Can. J. Chem.*, 1979, **57**, 3332

Kawagisha, H. *et al., Tet. Lett.*, 1994, **35**, 1569 (*Erinacine A*)

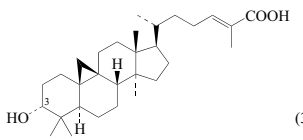
Snider, B.B. *et al., J.A.C.S.*, 1996, **118**, 7644 (*synth*)

Tori, M. *et al., J.O.C.*, 1998, **63**, 306-313 (*synth*)

Snider, B.B. *et al., J.O.C.*, 1998, **63**, 4732-4740 (*synth*)

Kenmoku, H. *et al., Tet. Lett.*, 2000, **41**, 4389-4393 (*synth*)

3-Hydroxycycloart-24-en-26-oic acid H-390



(3α,24*E*)-*form*

$C_{30}H_{48}O_3$ 456.707

(3α,24*E*)-*form* [13878-92-7]

Isomangiferolic acid

Constit. of *Mangifera indica* (mango). Cryst. (EtOH). Mp 168-170°. $[\alpha]_D$ +29 (c, 1 in $CHCl_3$).

26-Aldehyde: ***3-Hydroxycycloart-24-en-26-al***

$C_{30}H_{48}O_2$ 440.708

Gum. $[\alpha]_D$ +10.6 (c, 1 in $CHCl_3$).

(3β,24*E*)-*form* [4184-34-3] ***Mangiferolic acid***

Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 181-183°. $[\alpha]_D$ +49 ($CHCl_3$).

3-Ac: [206197-08-2] ***3-Acetylmangiferolic acid***

$C_{32}H_{50}O_4$ 498.745

Cryst. (EtOAc/petrol). Mp 180-182°.

(3β,24*Z*)-*form* [55511-17-6] ***Schizandrolic acid***. *Shisandrolic acid*

Cryst. (MeOH). Mp 165°. $[\alpha]_D$ +28.5 (c, 0.58 in $CHCl_3$).

Corsano, S. *et al., Tet. Lett.*, 1965, 2377 (*isol*)

Corsano, S. *et al., Ann. Chim. (Rome)*, 1967, **57**, 508 (*isol*)

Cheung, H.T. *et al., Aust. J. Chem.*, 1972, **25**, 2003 (*isol*)

Takahashi, K. *et al., Chem. Pharm. Bull.*, 1975, **23**, 538 (*synth, pmr*)

Takahashi, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2000 (*Schizondrolic acid*)

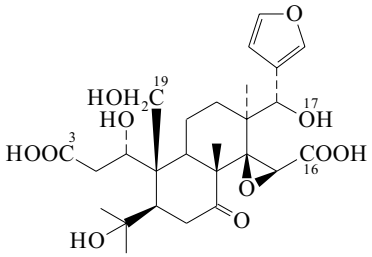
Singh, C. *et al., Tetrahedron*, 1977, **33**, 817 (*synth*)

Januário, A.H. *et al., Phytochemistry*, 1992, **31**, 1251 (*aldehyde, isol, pmr, cmr*)

Sy, L.-K. *et al., Phytochemistry*, 1997, **44**, 1099 (*cmr*)

Huang, P. *et al., Yaoxue Xuebao*, 1997, **32**, 704-707 (*3-Acetylmangiferolic acid*)

19-Hydroxydeacetylnomilinic acid H-391



$C_{26}H_{36}O_{11}$ 524.564

17-O-β-D-Glucopyranoside: ***19-Hydroxydeacetylnomilinic acid 17-β-D-glucopyranoside***

$C_{32}H_{46}O_{16}$ 686.706

Isol. from *Citrus aurantium* (Seville orange). The name 19-hydroxydeacetylnomilinic acid 17-*O*-β-D-glucopyranoside is strictly a misnomer; Nomilinic acid is a 16→17 lactone (see Nomilinic acid, N-76).

3,19-Lactone, 17-O-β-D-glucopyranoside: ***Ichangic acid 17-β-D-glucopyranoside***

$C_{32}H_{44}O_{15}$ 668.691

Constit. of *Citrus aurantium* (Seville orange). The name of this glycoside is also strictly a misnomer as Ichangic acid is a 16 → 17 lactone (see Ichangin, I-2).

Bennett, R.D. *et al., Phytochemistry*, 1991, **30**, 3803 (*isol, pmr, cmr*)

10-Hydroxy-2,8-decadiene-4,6-diynoic acid H-392

10-Hydroxymatricaric acid

$HOCH_2CH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCOOH$

$C_{10}H_8O_3$ 176.171

Isol. as an (*E,Z*)-mixt. from the fungus *Camarophyllus virgineus* (snowy waxcap).

(*E*,*E*)-*form* [51193-98-7]

Constit. of *Fistulina hepatica*.

(*Z*,*Z*)-*form*

Me ester: [65367-59-1]

Isol. from *Camarophyllus virgineus* (snowy waxcap). Mp 38.5-40.5°. λ_{max} 233 ; 246 ; 258 ; 294 ; 310 ; 330 (MeOH).

[62000-93-5, 65367-67-1, 106111-45-9]

Farrell, I.W. *et al., J.C.S. Perkin 1*, 1973, 2642; 1977, 1886 (*isol, struct, synth, ir, uv, pmr, ms*)

Ichihara, K. *et al., Agric. Biol. Chem.*, 1976, **40**, 353 (*isol, struct, uv, ir, ms, pmr*)

Kobayashi, A. *et al., Agric. Biol. Chem.*, 1976, **40**, 2257 (*synth, ir, uv, ms, pmr*)

Davies, D.G. *et al., J.C.S. Perkin 1*, 1978, 1602 (*isol, struct, ir, uv, ms, pmr*)

Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1519; 1980, **19**, 2655; 1981, **20**, 1907 (*epoxide, isol, struct, esters, ms, pmr, ir, uv*)

Rose, A.F. *et al., Phytochemistry*, 1980, **19**, 563 (*epoxide, isol, struct, activity, ir, uv, pmr, ms*)

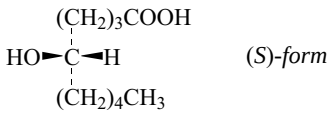
Huneck, S. *et al., Pharmazie*, 1986, **41**, 673 (*isol*)

Rehder, V.L.G. *et al., J. Nat. Prod.*, 1990, **53**, 692 (*isol, cmr*)

Grandjean, D. *et al., Tet. Lett.*, 1992, **33**, 5355 (*synth, epoxide*)

5-Hydroxydecanoic acid H-393

[624-00-0]
5-Hydroxycapric acid



(S)-form

$C_{10}H_{20}O_3$ 188.266

(*S*)-*form* [134625-01-7]
Solid (as Na salt). Mp 161-162.5° (Na salt). $[\alpha]_D^{25}$ -2.3 (c, 1.43 in MeOH).

(±)-*form* [160820-15-5]
Amide:
$C_{10}H_{21}NO_2$ 187.281
Cryst. Mp 75-77°.

Lactone: See Tetrahydro-6-pentyl-2*H*-pyran-2-one, T-116

(ξ)-*form*
Present as triglycerides in milk/butter fat. The glycerol monoester is a synthetic butter-like flavour ingredient.

Wyatt, C.J. *et al., Lipids*, 1967, **2**, 208 (*ms, glc*)
U.S. Pat., 1971, 3 622 605; *CA*, **72**, 42828t (*glycerol monoester*)
Eur. Pat., 1991, 410 446; *CA*, **115**, 28705a (*S-form, synth, ir, pmr*)
Taylor, S.K. *et al., Synth. Commun.*, 2001, **31**, 2391-2397 (*amide*)

6-Hydroxydecanoic acid, 9CI H-394

[16899-10-8]
$H_3C(CH_2)_3CH(OH)(CH_2)_4COOH$
$C_{10}H_{20}O_3$ 188.266

Lactone: [5579-78-2] *7-Butyl-2-oxepanone, 9CI, 8CI. 6-Butylhexanolide. ϵ-Decalactone. 6-Decanolide. FEMA 3613*
$C_{10}H_{18}O_2$ 170.251
Food flavour ingredient. Not reported in nature. Pale yellow liq. with sweet, creamy odour. $Bp_{1.3}$ 96°. n_D^{20} 1.4601.

Netherlands Pat., 1962, 100 368; *CA*, **60**, 2783c (*synth, lactone*)
Japan. Pat., 1974, 74 85 276; *CA*, **82**, 71817a (*use*)
Lercker, G. *et al., Lipids*, 1981, **16**, 912 (*anal*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 383 (*lactone, props, use*)

9-Hydroxydecanoic acid, 9CI H-395

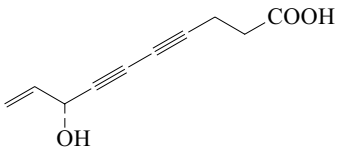
[1422-27-1]

$C_{10}H_{20}O_3$ 188.266
Present in *Agaricus campestris* (field mushroom).

Moore, B.P. *et al., Aust. J. Chem.*, 1976, **29**, 1365 (*isol*)
Gerlach, H. *et al., Helv. Chim. Acta*, 1978, **61**, 1226 (*synth, ir, pmr, ms*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1982, **30**, 89 (*glc, ms*)
Voss, G. *et al., Helv. Chim. Acta*, 1983, **66**, 2294 (*synth*)
Clarke, M.J. *et al., J. Liq. Chromatogr.*, 1986, **9**, 1711 (*hplc*)
Bantra, M. *et al., J.O.C.*, 1991, **56**, 5132 (*synth*)
Nagumo, S. *et al., Tetrahedron*, 1992, **48**, 8667 (*synth*)
Hamada, T. *et al., Synlett*, 1995, 407 (*synth*)

8-Hydroxy-9-decene-4,6-diynoic acid H-396

[151852-49-2]
Helianthenic acid B



$C_{10}H_{10}O_3$ 178.187

(*R*)-*form*
O-*β*-D-*Glucopyranoside, Me ester:* [142449-83-0]
$C_{17}H_{22}O_8$ 354.356
Constit. of *Helianthus tuberosus* (Jerusalem artichoke). Oil. $[\alpha]_D^{22}$ -50 (c, 0.08 in MeOH).

Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1253; 1492

10-Hydroxy-2-decene-4,6-diynoic acid, 9CI H-397

$HOH_2CCH_2CH_2C{\equiv}CC{\equiv}CCH{=}CHCOOH$
$C_{10}H_{10}O_3$ 178.187

(*E*)-*form*
Food lipid. Plates (EtOH aq.). Mp 154.5-156°.

Me ester:
$C_{11}H_{12}O_3$ 192.214
Oil.

Bu'Lock, J.D. *et al., J.C.S.*, 1957, 1607 (*isol, struct, synth, uv*)

10-Hydroxy-8-decene-4,6-diynoic acid H-398

Helianthenic acid F
$HOCH_2CH{=}CHC{\equiv}CC{\equiv}CCH_2CH_2COOH$
$C_{10}H_{10}O_3$ 178.187

(*E*)-*form* [54541-69-4]
(*Z*)-*form* [51193-97-6]
Constit. of *Fistulina hepatica* (beefsteak fungus).

Me ester, O-*β*-D-*glucopyranoside:*
$C_{17}H_{22}O_8$ 354.356
Constit. of *Helianthus tuberosus* (Jerusalem artichoke). Amorph. solid. $[\alpha]_D^{23}$ -16 (c, 0.16 in MeOH).

Farrell, I.W. *et al., J.C.S. Perkin 1*, 1973, 2642 (*isol*)
Ahmed, M. *et al., J.C.S. Perkin 1*, 1974, 1981 (*isol*)
Kobayashi, A. *et al., Agric. Biol. Chem.*, 1975, **39**, 2247 (*synth*)
Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1492 (*isol, deriv*)

10-Hydroxy-8-decenoic acid H-399

[79728-54-4]
$HOCH_2CH{=}CH(CH_2)_6COOH$
$C_{10}H_{18}O_3$ 186.25

(*E*)-*form* [106541-97-3]
Isol. from the injured fruit bodies of *Cantharellus tubaeformis* (funnel chanterelle).
► LD_{50} (mus, ipr) 50 mg/kg.

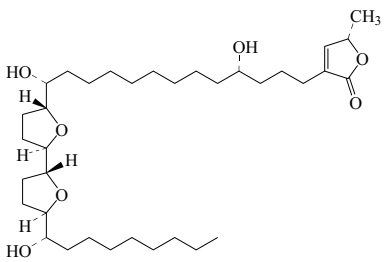
Me ester: [67803-47-8]
$C_{11}H_{20}O_3$ 200.277
$Bp_{0.04}$ 115°.

Ac, Me ester: [67803-46-7]
$C_{13}H_{22}O_4$ 242.314
$Bp_{0.13}$ 115°.

[69152-90-5]

Ranganathan, D. *et al., Tetrahedron*, 1980, **36**, 1869 (*synth*)
Baker, S.R. *et al., Tet. Lett.*, 1983, **24**, 4469 (*synth*)
Pang, Z. *et al., Acta Chem. Scand.*, 1992, **46**, 301; 1994, **48**, 408 (*isol, synth, ir, pmr, cmr*)

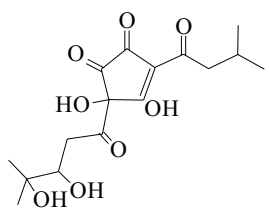
6-Hydroxydesacetyluvaricin (incorr.) H-400



$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona glabra* (pond apple). Solid. $[\alpha]_D^{25}$ +7.8 ($CHCl_3$). The name given in the lit. is incorrect; Desacetyluvaricin is a C_{37} compd. λ_{max} 217 (log ϵ 3.81) (MeOH).

Liu, X. *et al., Nat. Prod. Lett.*, 2000, **14**, 255-263

3-Hydroxy-3-(3,4-dihydroxy-4-methylpentanoyl)-5-(3-methylbutyl)-1,2,4-cyclopentanetrione H-401

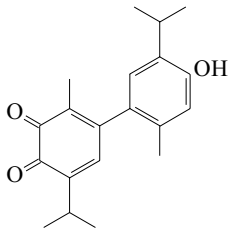


$C_{16}H_{22}O_8$ 342.345
Autoxidn. prod. of Humulone, H-317 present in hops. Pale yellow cryst. (MeOH aq.). Mp 83-87°.

Ashurst, P.R. *et al., J.C.S.(C)*, 1966, 675

4′-Hydroxy-5,5′-diisopropyl-2,2′-dimethyl-3,4-biphenylquinone H-402

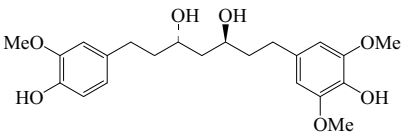
[120866-13-9]
4-(4-Hydroxy-5-isopropyl-2-methylphenyl)-6-isopropyl-3-methyl-3,5-cyclohexadiene-1,2-dione



$C_{20}H_{24}O_3$ 312.408
Constit. of the leaves of thyme (*Thymus vulgaris*). Shows antioxidant activity. Dark red cryst. (EtOAc/hexane). Mp 174-175° (170°). $[\alpha]_D^{25}$ -11.6 (c, 0.14 in $CHCl_3$).

Nakatani, N. *et al., Agric. Biol. Chem.*, 1989, **53**, 1375 (*isol, pmr, cmr*)
Miura, Y. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 1159 (*synth, ir, pmr*)

1-(4-Hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-3,5-heptanediol, 9CI H-403

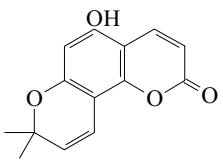


$C_{22}H_{30}O_7$ 406.475
(3*S*,5*S*)-*form* [145888-84-2]
Constit. of the dried rhizomes of *Zingiber officinale* (ginger).

Yamahara, J. *et al., Yakugaku Zasshi*, 1992, **112**, 645 (*isol, abs config*)

5-Hydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, 9CI H-404

5-Hydroxyseselin



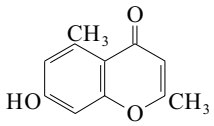
$C_{14}H_{12}O_4$ 244.246
Needles (EtOAc). Mp 210-213°.

Me ether: [31525-76-5] *5-Methoxyseselin*
$C_{15}H_{14}O_4$ 258.273
Consit. of *Citrus grandis* (pummelo). Prisms (Et_2O). Mp 162-164°.

Wu, T.S. *et al., Phytochemistry*, 1983, **22**, 1493 (*deriv*)
Murray, R.D.H. *et al., Tetrahedron*, 1984, **40**, 3129 (*synth*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3805 (*isol*)

7-Hydroxy-2,5-dimethyl-4*H*-1-benzopyran-4-one, 9CI H-405

[38412-47-4]
7-Hydroxy-2,5-dimethylchromone



$C_{11}H_{10}O_3$ 190.198
Constit. of *Rheum* sp. (rhubarb). Cryst. (CH_2Cl_2/MeOH or Me_2CO). Mp 258-260°.

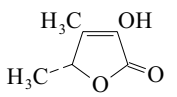
Ac: [41607-29-8]
$C_{13}H_{12}O_4$ 232.235
Needles (Et_2O). Mp 117°.

Me ether: [41607-30-1] *7-Methoxy-2,5-dimethyl-4*H*-1-benzopyran-4-one. 7-Methoxy-2,5-dimethylchromone*
$C_{12}H_{12}O_3$ 204.225
Yellow cryst.($CHCl_3$). Mp 115-117°.

Kimura, Y. *et al., Planta Med.*, 1983, **48**, 164 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3493 (*isol, cmr, pmr, ir*)
Bringmann, G. *et al., Annalen*, 1985, 765 (*synth, pmr*)
Gramatica, P. *et al., Heterocycles*, 1986, **24**, 743 (*synth*)
Ayer, W.A. *et al., Can. J. Chem.*, 1990, **68**, 2085 (*isol, pmr*)
Lee, C.-K. *et al., J. Chin. Chem. Soc. (Taipei)*, 2001, **48**, 1053-1058 (*Me ether, isol, uv, pmr*)

3-Hydroxy-4,5-dimethyl-2(5*H*)-furanone, 9CI H-406

[87021-36-1]
2-Hydroxy-3,4-dimethyl-2-buten-1,4-olide. Sotolone

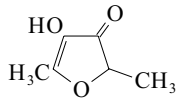

(*R*)-*form*

$C_6H_8O_3$ 128.127
Key flavour compd. found in raw cane sugar, aged sake, coffee, fenugreek, lovage and wines.
(*R*)-*form* [87068-70-0]
$[\alpha]_D^{23.5}$ -6.5 (c, 1.15 in Et_2O).
(*S*)-*form* [87068-69-7]
$[\alpha]_D^{23.5}$ +7.1 (c, 1.55 in Et_2O).
(±)-*form*
$Bp_{0.5}$ 87-88°. n_D^{20} 1.4295.

Sulser, H. *et al., Z. Lebensm.-Unters. -Forsch.*, 1972, **148**, 215 (*synth*)
Rödel, W. *et al., Nahrung*, 1974, **18**, 133 (*synth*)
Takahashi, K. *et al., Agric. Biol. Chem.*, 1976, **40**, 325 (*isol*)
Okada, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 1071 (*synth*)
Fronza, G. *et al., Tet. Lett.*, 1992, **33**, 5625 (*synth*)
Blank, I. *et al., J. Agric. Food Chem.*, 1996, **44**, 1851-1856 (*occur*)

4-Hydroxy-2,5-dimethyl-3(2*H*)-furanone, 9CI H-407

[3658-77-3]
Furaneol. *Alletone. Pineapple ketone. COE 536. FEMA 3174*



$C_6H_8O_3$ 128.127
▶ LU3990000
(±)-*form*
Flavouring agent. Cryst. (petrol) with fruity-caramel or burnt-pineapple odour. Mp 77-78°. Subl.1 85 (bath).

4-O-β-D-Glucopyranoside: [121063-56-7]
$C_{12}H_{18}O_8$ 290.269
Constit. of strawberry juice. Oil. $[\alpha]_D^{20}$ -50.

4-O-(6-O-Malonyl-β-D-glucopyranoside):
$C_{15}H_{20}O_{11}$ 376.316
Constit. of strawberries. λ_{max} 275 (no solvent reported).

Ac: [4166-20-5] *4-Acetoxy-2,5-dimethyl-3(2H)furanone. Furaneol acetate. FEMA 3797*
$C_8H_{10}O_4$ 170.165
Used in meaty and caramel-type flavours. Oil. d 1.17. Bp 243°.

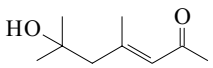
Me ether: [4077-47-8] *4-Methoxy-2,5-dimethyl-3(2*H*)-furanone. O-Methylfuraneol. **Mesifurane**. FEMA 3664*
$C_7H_{10}O_3$ 142.154
Constit. of various fruits incl. raspberry, strawberry, mango, pineapple, blackberry and cape gooseberry. Flavouring agent. Oil with burnt caramel odour. $Bp_{0.3}$ 61-63°.
(ξ)-*form*
Volatile flavour and aroma component of many foods and food products e.g. pineapple, mango, strawberry, cooked beef, roasted nuts, popcorn, shoyu, malt, etc..

[131222-81-6, 131222-82-7]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 19C (*nmr*)
Rodin, J.O. *et al., J. Food Sci.*, 1965, **30**, 280 (*isol, ir, uv, pmr*)
Henry, D.W. *et al., J.O.C.*, 1966, **31**, 2391 (*synth, ir, pmr, uv*)
Re, L. *et al., Helv. Chim. Acta*, 1973, **56**, 1882 (*synth*)
Büchi, G. *et al., J.O.C.*, 1973, **38**, 123 (*synth, pmr*)
Hunter, G.L.K. *et al., J. Food Sci.*, 1974, **39**, 900 (*occur*)
Mills, F.D. *et al., J. Agric. Food Chem.*, 1978, **26**, 894 (*synth, ms*)
Wong, C.H. *et al., J.O.C.*, 1983, **48**, 3493 (*synth, pmr*)
Briggs, M.A. *et al., J.C.S. Perkin 1*, 1985, 795 (*synth*)
Mayerl, F. *et al., Phytochemistry*, 1989, **28**, 631 (*isol, deriv, synth*)
Mazenod, F. *et al., Chimia*, 1992, **46**, 403 (*synth*)
Inokuchi, T. *et al., J.O.C.*, 1992, **57**, 5023 (*synth*)
Farine, J.-P. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 2026 (*isol, ir, ms*)
Roscher, R. *et al., Phytochemistry*, 1996, **43**, 155 (*6-malonylglucoside*)
Zabetakis, I. *et al., Spec. Publ. - R. Soc. Chem.*, 1996, **197**, 90-93 (*biosynth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 861; 1369; 1371 (*use, occur, Me ether*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 17 (*use, Ac*)

6-Hydroxy-4,6-dimethyl-3-hepten-2-one H-408

[83348-17-8]

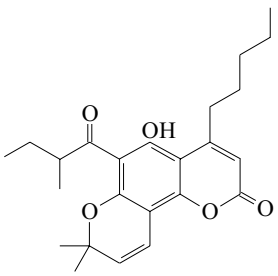


$C_9H_{16}O_2$ 156.224
Found in red and green bell peppers *Capsicum annuum* var. *angulosum*. No phys. props. reported.

Kimura, K. *et al., CA*, 1982, **97**, 159552 (*isol*)
Grote, R. *et al., Annalen*, 1990, 525 (*isol, pmr, cmr*)

5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, 9CI H-409

[39036-48-1]
Mammea C/AB cyclo D

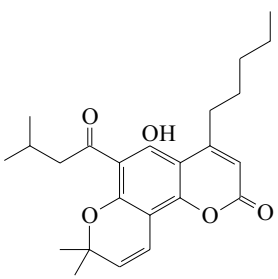


$C_{24}H_{30}O_5$ 398.498
Isol. from *Mammea americana* (mamey).

Games, D.E. *et al., Tetrahedron*, 1972, 3187

5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, 9CI H-410

[39036-47-0]

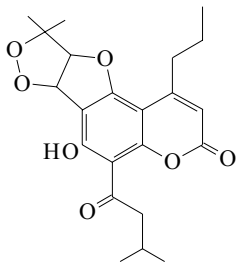


$C_{24}H_{30}O_5$ 398.498
Isol. from *Mammea americana* (mamey).

Games, D.E. *et al., Tet. Lett.*, 1972, 3187

6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3*H*,9*H*-[1,2]-dioxolo[3′,4′:4,5]furo[2,3-*f*][1]benzopyran-3-one, 9CI H-411

[30390-08-0]



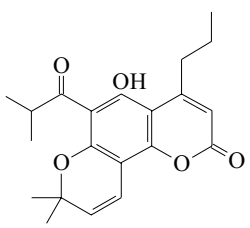
$C_{22}H_{26}O_7$ 402.443
A cyclic peroxide related to Cyclomammein, C-483. Isol. from *Mammea americana* (mamey). An oxidn. prod. of Mammein. Mp 181-182°.

[30390-09-1]

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2241
Finnegan, R.A. *et al., J. Pharm. Sci.*, 1972, **61**, 1603 (*isol, ir, uv, pmr*)

5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, 9CI H-412

[34107-36-3]
Mammea B/AD cyclo D

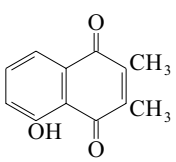


$C_{21}H_{24}O_5$ 356.418
Isol. from *Mammea americana* (mamey).

Games, D.E. *et al., Tet. Lett.*, 1972, 3187-3190 (*isol*)

5-Hydroxy-2,3-dimethyl-1,4-naphthoquinone H-413

[80596-51-6]
3-Methylplumbagin



$C_{12}H_{10}O_3$ 202.209
Constit. of *Juglans regia* (walnut) and *Juglans nigra* (black walnut). Orange needles (hexane). Mp 120-121°. λ_{max} 241 (ε 7762); 287 (ε 13490); 429 (ε 4900) (MeOH) (Berdy).

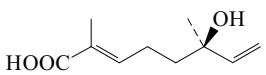
Ac:
$C_{14}H_{12}O_4$ 244.246
Orange cryst. ($CHCl_3$/hexane). Mp 111-114°.

Me ether: [90013-25-5] *5-Methoxy-2,3-dimethyl-1,4-naphthoquinone*
$C_{13}H_{12}O_3$ 216.236
Yellow needles. Mp 144-145°.

Gunaherath, G.M.K.B. *et al., J.C.S. Perkin 1*, 1988, 407-410 (*Me ether*)
Binder, R.G. *et al., Phytochemistry*, 1989, **28**, 2799-2801 (*isol, pmr, ms*)
Bansal, V. *et al., Synth. Commun.*, 1995, **25**, 1669-1675 (*synth*)
Higa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1189-1193 (*isol, cmr*)
Takeya, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 209-219 (*synth, ir, pmr*)

6-Hydroxy-2,6-dimethyl-2,7-octadienoic acid H-414

[28420-25-9]
Linalolic acid. *Linalool-1-oic acid*



(*R,E*)-*form*

$C_{10}H_{16}O_3$ 184.235

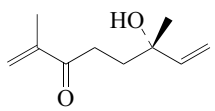
(ξ,*E*)-*form*
Oil. $[\alpha]_D$ -12 (c, 0.5 in $CHCl_3$).

β-D-Glucopyranosyl ester: [191548-38-6]
$C_{16}H_{26}O_8$ 346.377
Present in Riesling wine. No phys. props. reported.

[34935-27-8, 67711-07-3, 121843-29-6]

Konoshima, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2617
Carda, M. *et al., Tetrahedron*, 1995, **51**, 2755 (*synth*)
Bonnlander, B. *et al., J. Agric. Food Chem.*, 1998, **46**, 1474-1478 (*glucopyranosyl ester*)

6-Hydroxy-2,6-dimethyl-1,7-octadien-3-one H-415



$C_{10}H_{16}O_2$ 168.235

(*S*)-*form*
O-*β-D-Glucopyranoside:* [179983-86-9]
Portuloside A
$C_{16}H_{26}O_7$ 330.377
Constit. of *Portulaca oleracea* (purslane). Oil. $[\alpha]_D^{26}$ -19.6 (c, 0.5 in $CHCl_3$).

Sakai, N. *et al., Phytochemistry*, 1996, **42**, 1625-1628 (*isol, pmr, cmr, synth*)

6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one H-416

[64661-54-7]

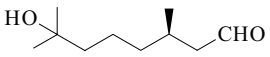
$C_{10}H_{16}O_2$ 168.235
Constit. of *Citrus junos* (yuzu). Oil. $Bp_{0.7}$ 69-70°.

2,3-Dihydro: 6-Hydroxy-2,6-dimethyl-7-octen-4-one, H-420

Kitahara, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 897 (*isol*)

7-Hydroxy-3,7-dimethyloctanal, 9CI, 8CI H-417

[107-75-5]
Hydroxycitronellal. Phixia. Citronellal hydrate. FEMA 2583



(*R*)-*form*

$C_{10}H_{20}O_2$ 172.267
Occurs in essential oils.
►Skin irritant. Fl. p. >100°. RG7850000
(*R*)-*form* [34212-48-1]
Oil. Bp_5 116°. $[\alpha]_D^{20}$ +10.
(*S*)-*form* [34212-53-8]
Oil. $Bp_{0.05}$ 110°. $[\alpha]_D^{20}$ -9.
(±)-*form* [123238-75-5]
Flavouring ingredient. Liq. with fine, flowery odour. Bp_1 94-96°. n_D^{20} 1.4488. Coml. prod. may be opt. active or racemic.

Di-Me acetal: [141-92-4] *8,8-Dimethoxy-2,6-dimethyl-2-octanol. Hydroxydihydrocitronellal dimethyl acetal. FEMA 2585*
$C_{12}H_{26}O_3$ 218.336
Flavouring ingredient. Liq. with weak flowery odour. Bp_{12} 131°. n_D^{20} 1.4419. Alkali-stable.
►RG7900000

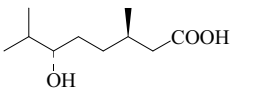
Di-Et acetal: [7779-94-4] *8,8-Diethoxy-2,6-dimethyl-2-octanol, 9CI. FEMA 2584*
$C_{14}H_{30}O_3$ 246.389
Used in citrus fruit flavouring. Liq. with a delicate, green-floral taste and almost no odour. d 0.92. Bp 260°.

Me ether: [3613-30-7] *3,7-Dimethyl-7-methoxyoctanal. Methoxydihydrocitronellal*
$C_{11}H_{22}O_2$ 186.294
Liq. with fresh blossom odour. $Bp_{0.45}$ 60°. n_D^{25} 1.4380.
►RG7890000

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 361A (*deriv*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 470C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 569B (*ir, deriv*)
Skoriantez, W. *et al., Helv. Chim. Acta*, 1971, **54**, 1797 (*synth, ir, pmr, ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 921 (*rev, tox*)
Ishino, R. *et al., J.O.C.*, 1974, **39**, 108 (*synth*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Fischli, A. *et al., Helv. Chim. Acta*, 1978, **61**, 2560 (*synth, ir, pmr, ms*)
Wang, D.J. *et al., CA*, 1980, **92**, 124929d (*occur*)
Tani, K. *et al., J.A.C.S.*, 1984, **106**, 5208
Blakeway, J.M. *et al., Int. J. Cosmet. Sci.*, 1987, **9**, 203 (*di-Et acetal*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CMS850
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 358-359
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1362-1364
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ; DSM800

6-Hydroxy-3,7-dimethyloctanoic acid, 9CI H-418

[57429-74-0]



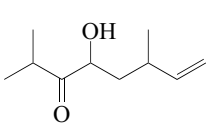
(3*R*,6*S*)-*form*

$C_{10}H_{20}O_3$ 188.266
(3*R*,6*S*)-*form* [84465-67-8] Characterised spectroscopically.
Me ester: [146512-80-3]
$C_{11}H_{22}O_3$ 202.293
$[\alpha]_D^{25}$ -15.5 (c, 1.3 in $CHCl_3$).
Ac:
$C_{12}H_{22}O_4$ 230.303
$Bp_{0.3}$ 168° bath.
Lactone: [68330-67-6]
[68330-68-7, 130981-75-8, 130981-76-9] *4-Methyl-7-(1-methylethyl)-2-oxepanone, 9CI. 7-Isopropyl-4-methyl-2-oxepanone*
$C_{10}H_{18}O_2$ 170.251
Cryst. (hexane). Mp 46-48°. $Bp_{0.6}$ 68-72°. $[\alpha]_D^{25}$ -22 (c, 2 in $CHCl_3$).
(3*S*,6*R*)-*form*
Lactone: [133267-37-5]
Mp 49°. Bp_4 109°. $[\alpha]_D^{25}$ +19.2.
(3ξ,6ξ)-*form*
Lactone: [499-54-7] *FEMA 3355*
Flavouring ingredient with maple syrup-brown sugar odour. Isol. from *Mentha piperita* (peppermint) rhizomes. Low melting solid. Stereochem. not specified by FEMA.

Shono, T. *et al., Tet. Lett.*, 1974, 1295-1298 (*lactone, synth*)
Shankaran, K. *et al., Indian J. Chem., Sect. B*, 1979, **18**, 507-509; 1982, **21**, 542-544 (*3R,6S-form, synth, ir, pmr*)
Jakovac, I.J. *et al., J.O.C.*, 1979, **44**, 2165-2168 (*lactone, synth*)
Croteau, R. *et al., Plant Physiol.*, 1984, **76**, 647-653 (*lactone, isol*)
Daniewski, A.R. *et al., Annalen*, 1992, 965-973 (*lactone, synth, pmr, cmr*)
Daniewski, A.R. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1992, **66**, 1985-1997 (*3R,6S-form, lactone, Me ester*)
Morin-Fox, M.L. *et al., Tet. Lett.*, 1992, **33**, 5699-5700 (*lactone, synth*)
Adams, T.B. *et al., Food Chem. Toxicol.*, 1998, **36**, 249-278 (*tox, rev*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 816-817 (*lactone, use*)

4-Hydroxy-2,6-dimethyl-7-octen-3-one H-419

[211303-26-3]



$C_{10}H_{18}O_2$ 170.251
Constit. of *Tagetes minuta* (Mexican marigold). $[\alpha]_D^{18}$ +35.5 (c, 1 in $CHCl_3$).

Garg, S.N. *et al., Phytochemistry*, 1998, **48**, 395-396 (*isol, pmr, cmr*)

6-Hydroxy-2,6-dimethyl-7-octen-4-one H-420

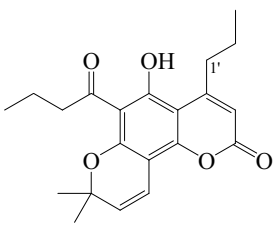
[71547-63-2]
Tagetonol

$C_{10}H_{18}O_2$ 170.251
(+)-*form* [23007-34-3]
Isol. from the essential oil of yuzu (*Citrus junos*). Liq. Bp_4 72-74°. $[\alpha]_D^{15}$ +4.8 (c, 3 in CCl_4).
Semicarbazone: [24048-53-1]
Needles (EtOH). Mp 145.5-146.5°.
(±)-*form* [51298-71-6]
Liq. Bp_6 85-90° (lit. gives a pressure range).

Yoshida, T. *et al., Agric. Biol. Chem.*, 1969, **33**, 343 (*isol, pmr, struct*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 562 (*synth*)
Park, O.S. *et al., Synth. Commun.*, 1977, **7**, 345 (*synth*)
Kitahara, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 897 (*isol, synth*)
Ahmad, A. *et al., Fitoterapia*, 1988, **59**, 413 (*isol*)

5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]-dipyran-2-one H-421

[34107-35-2]
Mammea BlAC cyclo D

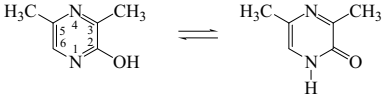


$C_{21}H_{24}O_5$ 356.418
Isol. from *Mammea americana* (mamey).

Games, D.E. *et al., Tet. Lett.*, 1972, 3187-3190 (*isol*)

2-Hydroxy-3,5-dimethylpyrazine, 9CI H-422

[60187-00-0]
3,5-Dimethyl-2(1H)-pyrazinone, 9CI. 3,5-Dimethyl-2-pyrazinol



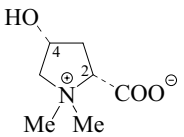
$C_6H_8N_2O$ 124.142
NH-Form predominates. Cryst. (EtOH). Mp 149.5-151°.
***OH*-form**
Me ether: [92508-08-2] *2-Methoxy-3,5-dimethylpyrimidine, 9CI*
$C_7H_{10}N_2O$ 138.169
Microbiol. prod. causing objectionable odour in foods. Liq. with unpleasant musty odour.

Klein, B. *et al., J.O.C.*, 1964, **29**, 2623 (*synth*)
Macdonald, J.C. *et al., Tetrahedron*, 1976, **32**, 655 (*pmr, cmr*)

Ohta, A. *et al., J. Het. Chem.*, 1983, **20**, 311 (*synth*)
Mottram, D.S. *et al., Chem. Ind. (London)*, 1984, 448 (*Me ether, isol, synth, ms*)
Leitner, H. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1990, **12**, 151; *CA*, **113**, 3275f (*Me ether, isol*)

4-Hydroxy-1,1-dimethylpyrrolidinium-2-carboxylate H-423

[105869-44-1]
2-Carboxy-4-hydroxy-1,1-dimethylpyrrolidinium hydroxide inner salt, 9CI. 4-Hydroxyproline betaine



(2*R*,4*R*)-*form*

$C_7H_{13}NO_3$ 159.185

(2*R*,4*R*)-*form* [515-24-2]
Combretin A
Mp 253-257° dec. $[\alpha]_D^{20}$ +37.5 (c, 2.4 in H_2O). Identity not certain.

Hydrochloride:
Needles or prisms (EtOH). Mp 232° dec.

(2*S*,4*R*)-*form* [174851-67-3] ***Turicine***
Constit. of *Canavalia ensiformis* (jack bean). Needles or prisms + $1H_2O$ (EtOH aq.). V. sol. H_2O. Mp 260° (249°) dec. (anhyd.). $[\alpha]_D$ +36.3 (H_2O).

Hydrochloride:
Needles or plates (EtOH). $[\alpha]_D$ +25.7 (H_2O). Dec. at 224°.

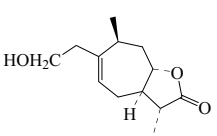
(2*S*,4*S*)-*form* [515-25-3] ***Betonicine***. *Achillein*
Present in *Achillea millefolium* (yarrow). Prisms (EtOH). Mp 252° dec. (244-245°). $[\alpha]_D^{15}$ -36.6 (H_2O).

(2*RS*,4*RS*)-*form* *Combretin B*
Mp 248-249° dec. $[\alpha]_D^{20}$ 0 (c, 2.7 in H_2O). Identity not certain.

[101198-81-6, 119303-01-4]

Schulze, E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1911, **76**, 258; 1912, **79**, 236 (*isol*)
Goodson, J.A. *et al., J.C.S.*, 1919, **115**, 923 (*isol*)
Paudler, W.W. *et al., Chem. Ind. (London)*, 1963, 1693 (*isol, struct*)
Mandava, N. *et al., Annalen*, 1970, **741**, 167 (*pmr, config*)
Ogan, A.U. *et al., Planta Med.*, 1972, **21**, 210 (*Combretins*)
Musich, J.A. *et al., J.O.C.*, 1977, **42**, 139 (*synth*)
Blunden, G. *et al., Magn. Reson. Chem.*, 1986, **24**, 965-971 (*pmr, cmr*)
Jones, G.P. *et al., Acta Cryst. C*, 1988, **44**, 2208 (*cryst struct*)

3-Hydroxy-4,15-dinor-1(5)-xanthen-12,8-olide H-424



(8α,10β,11α)-*form*

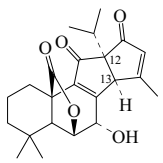
$C_{13}H_{20}O_3$ 224.299

(8α,10β,11α)-*form* [225518-67-2]
Diversifolide
Oil.

(8α,10β,11β)-*form* [342372-61-6]
Constit. of *Helianthus annuus* (sunflower). Oil.

Kuo, Y.-H. *et al., Chem. Pharm. Bull.*, 1999, **47**, 428-429 (*Diversifolide*)
Ohno, S. *et al., Phytochemistry*, 2001, **56**, 577-581 (*Helianthus annuus constit*)

7-Hydroxy-11,16-dioxo-8,14-apianadien-22,6-olide H-425



(6β,7α,12α,13α)-*form*

$C_{23}H_{28}O_5$ 384.471

(6β,7α,12α,13α)-*form* [403613-18-3]
Isol. from sage. Amorph. solid. λ_{max} 216 (log ε 4.3) (EtOH).

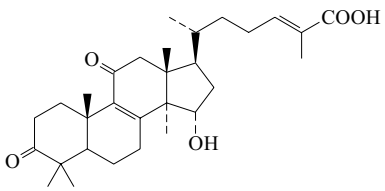
(6β,7α,12β,13β)-*form* [403613-16-1]
Isol. from sage. Amorph. solid. Mp 245°. λ_{max} 211 (log ε 4.09) (EtOH).

Me ether: [178180-06-8] *7-Methoxy-11,16-dioxo-8,14-apianadien-22,6-olide*
$C_{24}H_{30}O_5$ 398.498

(6β,7β,12β,13β)-*form* [403613-17-2]
Isol. from sage. Amorph. solid. λ_{max} 215 (log ε 3.99) (EtOH).

Luis, J.G. *et al., Tet. Lett.*, 1996, **37**, 4213-4216 (*Me ether*)
Miura, K. *et al., Phytochemistry*, 2001, **58**, 1171-1175 (*isol, pmr, cmr*)

15-Hydroxy-3,11-dioxo-8,24-lanostadien-26-oic acid H-426

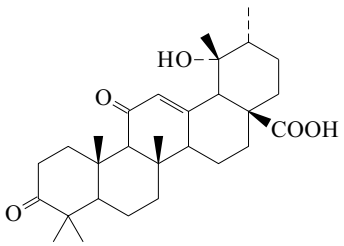


$C_{30}H_{44}O_5$ 484.675

(15α,24*E*)-*form* [114567-50-9]
Ganolucidic acid E
Metab. of *Ganoderma lucidum* (reishi). Syrup (as Me ester). $[\alpha]_D^{24}$ +154 (c, 0.1 in MeOH) (Me ester).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 367 (*isol, pmr, cmr*)

19-Hydroxy-3,11-dioxo-12-ursen-28-oic acid H-427



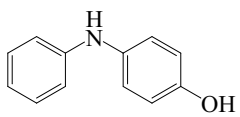
$C_{30}H_{44}O_5$ 484.675

19α-*form*
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Cryst. (CH_2Cl_2/Me_2CO). Mp 285-287°. $[\alpha]_D^{22}$ +42 (c, 0.21 in MeOH).

Cheng, D.-L. *et al., Phytochemistry*, 1992, **31**, 1317 (*isol, pmr, cmr*)

4-Hydroxydiphenylamine H-428

[122-37-2]
4-(Phenylamino)phenol, 9CI. 4-Hydroxy-N-phenylaniline. p-*Anilinophenol*



$C_{12}H_{11}NO$ 185.225
Metabolite of Diphenylamine, D-945 in stored apples. Leaflets (H_2O). Mp 73°. Bp_{12} 215-216°.

▶ Severe eye irritant. LD_{50} (rat, orl) 1220 mg/kg. SJ6950000

O,N-*Di-Ac:*
$C_{16}H_{15}NO_3$ 269.299
Prisms (C_6H_6/petrol).

Me ether: [1208-86-2] *4-Methoxy-N-phenylaniline, 9CI. 4-Methoxydiphenylamine.* N-*Phenyl*-p-*anisidine*
$C_{13}H_{13}NO$ 199.252
Prisms (EtOH). Mp 105°. Bp_{12} 195°.

Willstätter, R. *et al., Ber.*, 1909, **42**, 4138 (*synth*)
Gumprecht, D.L. *et al., J. Chromatogr.*, 1968, **37**, 268 (*chromatog*)
Tsuno, Y. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1519 (*nmr*)
Kasai, M. *et al., Tetrahedron*, 1973, **29**, 267 (*ir, pmr*)
Kim-Kang, H. *et al., J. Agric. Food Chem.*, 1998, **46**, 707-717 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOT000

μ-Hydroxydiphenyldimercury(1+) H-429

Bis(phenylmercuri)oxonium ion
$[(PhHg)_2OH]^{\oplus}$
$C_{12}H_{11}Hg_2O^{\oplus}$ 572.398
Pharmaceutical and agricultural fungicide, now superseded.

Nitrate: [8003-05-2] *Basic phenylmercury nitrate*
$C_{12}H_{11}Hg_2NO_4$ 634.403
Cryst. (EtOH). Spar. sol. H_2O, org. solvs. Mp 188° dec. (177-180°).

► LD_{50} (rat, scu) 56 mg/kg. OW8575000

Perchlorate:Basic phenylmercury perchlorate
$C_{12}H_{11}ClHg_2O_5$ 671.849
Solid. Mp 196-198° dec.

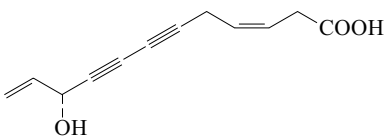
Tetrafluoroborate, monohydrate: [108389-59-9] *Basic phenylmercury tetrafluoroborate*
$C_{12}H_{13}BF_4Hg_2O_2$ 677.218
Cryst. (Me_2CO). Mp 170° dec.

[77090-26-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1149B (*ir*)
Grave, T.B. *et al., J. Am. Pharm. Assoc.*, 1936, **25**, 752 (*nitrate*)
Kuivila, H.G. *et al., J.A.C.S.*, 1962, **84**, 377
Barlow, L.R. *et al., J.C.S.(A)*, 1968, 1609 (*synth*)
Dutta, R.L. *et al., J. Inorg. Nucl. Chem.*, 1981, **43**, 1533 (*ir*)
Nicholson, B.K. *et al., J. Organomet. Chem.*, 1986, **306**, 139 (*synth, pmr, Hg-199 nmr, ir, cryst struct, hydrated BF_4 salt*)
Pesticide Manual, 9th edn., 1991, No. 9600
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1138
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MDH500

10-Hydroxy-3,11-dodecadiene-6,8-diynoic acid H-430

Helianthenic acid A



$C_{12}H_{12}O_3$ 204.225

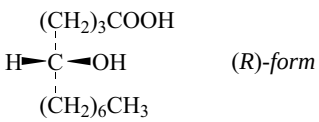
(3*Z*,10*R*)-*form* [152340-28-8]

O-*β*-D-*Glucopyranoside, Me ester:* [152230-54-1]
$C_{19}H_{24}O_8$ 380.394
Constit. of *Helianthus tuberosus* (Jerusalem artichoke). Oil. $[\alpha]_D^{22}$ -10 (c, 0.12 in MeOH).

[142449-82-9]

Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1253; 1492

5-Hydroxydodecanoic acid H-431



(*R*)-*form*

$C_{12}H_{24}O_3$ 216.32Readily forms lactone.

(*R*)-*form* [42550-36-7]
Solid. $[\alpha]_D^{20}$ -8.2 (c, 3.3 in 1*M* NaOH) (Na salt).

(±)-*form*

Amide:
$C_{12}H_{25}NO_2$ 215.335
Cryst. (EtOAc). Mp 88-90°.

Lactone See: 6-Heptyltetrahydro-2*H*-pyran-2-one, H-124

(ξ)-*form* [7779-95-5]
Present as triglycerides in milk and butterfat.

Wyatt, C.J. *et al., Lipids*, 1967, **2**, 208-211 (*occur*)
Egmont, M.R. *et al., Biochim. Biophys. Acta*, 1973, **316**, 1-7 (*R-form, synth*)
Taylor, S.K. *et al., Synth. Commun.*, 2001, **31**, 2391-2397 (*amide*)

6-Hydroxydodecanoic acid H-432

[35875-13-9]
$H_3C(CH_2)_5CH(OH)(CH_2)_4COOH$
$C_{12}H_{24}O_3$ 216.32

(±)-*form* [152752-06-2]

Et ester:
$C_{14}H_{28}O_3$ 244.373
d_4^{20} 0.95. Bp_9 148-150°. n_D^{20} 1.4451.

Lactone: [142285-19-6]

[16429-21-3, 156316-99-3, 156317-02-1] *7-Hexyl-2-oxepanone, 9CI, 8CI. ϵ-Dodecalactone. FEMA 3610*
$C_{12}H_{22}O_2$ 198.305
Food flavouring ingredient for candies, dairy products and soft drinks. Liq. with sweet fruity, celery odour. $Bp_{1.8}$ 130°. n_D^{20} 1.4627.

Netherlands Pat., 1962, 100 368; *CA*, **60**, 2783d (*lactone, synth, use*)
Kameoka, H. *et al., Nippon Kagaku Zasshi*, 1965, **86**, 429-439; *CA*, **65**, 615e (*Et ester, lactone*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*lactone, tox*)
Carling, R.W. *et al., J.C.S. Perkin 1*, 1992, 83-94 (*lactone, synth, pmr, cmr*)
Fellous, R. *et al., Tetrahedron: Asymmetry*, 1994, **5**, 343-346 (*lactone, resoln*)
Adams, T.B. *et al., Food Chem. Toxicol.*, 1998, **36**, 249-278 (*lactone, tox*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 494 (*lactone*)

12-Hydroxy-9-dodecenoic acid H-433

[79894-08-9]
$HOH_2CCH_2CH{=}CH(CH_2)_7COOH$
$C_{12}H_{22}O_3$ 214.304

(*Z*)-*form* [79894-09-0]
Syrup.

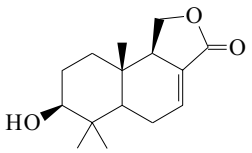
Me ester: [65715-78-8]
$C_{13}H_{24}O_3$ 228.331
Oil. $Bp_{0.25}$ 139-142°.

Lactone: [79894-05-6]

[79894-06-7] *Oxacyclotridec-10-en-2-one, 9CI. 9-Dodecen-12-olide.* ***Yuzu lactone***
$C_{12}H_{20}O_2$ 196.289
Constit. of *Citrus junos* (yuzu). Oil.

Kajiwara, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 1793 (*synth*)
Kuchin, A.V. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1989, **308**, 384 (*synth*)
Doss, R.P. *et al., Phytochemistry*, 1989, **28**, 3311-3315 (*isol, lactone*)
Suzuki, Y. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2049 (*isol, pmr, cmr*)
Rodefeld, L. *et al., Tetrahedron*, 1998, **54**, 5893-5898 (*lactone*)

3-Hydroxy-7-drimen-12,11-olide H-434



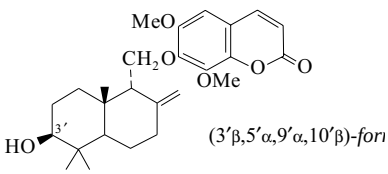
$C_{15}H_{22}O_3$ 250.337

3β-*form*
3β-Hydroxycinnamolide
Constit. of *Marasmius oreades* (fairy ring mushroom). Cryst. Mp 164.5-167°. $[\alpha]_D$ -22.6 (c, 0.42 in MeOH).

Ac:3β-Acetoxy-7-drimen-12,11-olide. ***3β-Acetoxycinnamolide***
$C_{17}H_{24}O_4$ 292.374
Prisms (EtOAc/petrol). Mp 153-155°. $[\alpha]_D$ +7 (c, 3 in $CHCl_3$).

Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371 (*isol, pmr, cmr*)
Kioy, D. *et al., Phytochemistry*, 1990, **29**, 3535 (*isol, pmr, cmr*)
Ayer, W.A. *et al., J. Nat. Prod.*, 1992, **55**, 1454 (*isol, pmr, cmr*)

7-*O*-(3-Hydroxy-8(12)-drimen-11-yl)isofraxidin H-435



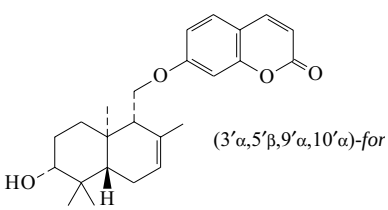
(3′β,5′α,9′α,10′β)-*form*

$C_{26}H_{34}O_6$ 442.551

(3′β,5′β,9′β,10′α)-*form* [81729-14-8]
Pectachol
Constit. of *Artemisia abrotanum* (southernwood) leaves. Cryst. (Et_2O). Mp 113-115°. $[\alpha]_D^{21}$ -18 (c, 0.7 in Me_2CO).

Greger, H. *et al., J. Nat. Prod.*, 1982, **45**, 455 (*Pectachol*)

O-(3-Hydroxy-7-drimen-11-yl)umbelliferone H-436



(3′α,5′β,9′α,10′α)-*form*

$C_{24}H_{30}O_4$ 382.499

(3′α,5′β,9′α,10′α)-*form* [51020-36-1]
Feselol. *Moschatol*
Cryst. (Et_2O). Mp 116.5-117.5°. $[\alpha]_D^{20}$ -98.5 (c, 0.22 in EtOH).

O-*Angeloyl:Feselol angelate*
$C_{29}H_{36}O_5$ 464.6
Cryst. Mp 66-68°. $[\alpha]_D^{22}$ -35.8 ($CHCl_3$).

(3′β,5′α,9′α,10′β)-*form* [60132-70-9] ***Feropolidin***

Cryst. Mp 154-156°. $[\alpha]_D^{20}$ +154 (c, 1 in $CHCl_3$).

(3′β,5′β,9′α,10′α)-*form* [60018-29-3] ***Mogoltacin***
Cryst. Mp 155-156°. $[\alpha]_D^{23}$ -55 (c, 1 in $CHCl_3$).

(3′β,5′α,9′β,10′β)-*form* [41743-46-8] ***Conferol***
Mp 137-138°. $[\alpha]_D^{20}$ -84.2 (EtOH).

Ac: ***Conferol acetate***
$C_{26}H_{32}O_5$ 424.536
Cryst. Mp 160°. $[\alpha]_D^{20}$ -42.4 ($CHCl_3$).

3′-Ketone: [41743-47-9] ***Conferone***
$C_{24}H_{28}O_4$ 380.483
Isol. from *Ferula* spp.. Mp 142-142.5°. $[\alpha]_D^{20}$ -51 (c, 1.3 in EtOH).

(3′α,5′α,9′ξ,10′β)-*form*
Constit. of *Ferula galbaniflua* (galbanum). Cryst. Mp 71-72°.

(3′β,5′α,9′ξ,10′β)-*form*
Constit. of *Ferula galbaniflua* (galbanum). Cryst. Mp 52-53°.

Vandyshev, V.V. *et al., Khim. Prir. Soedin.*, 1972, **8**, 669; 670; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 653; 654 (*isol, ir, uv, pmr, Conferone, Conferol*)

Kir'yalov, N.P. *et al., Khim. Prir. Soedin.*, 1973, **9**, 425; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 395 (*Feselol*)

Kadyrov, A.Sh. *et al., Khim. Prir. Soedin.*, 1974, **10**, 400; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 401 (*Feselol*)

Khasanov, T.K. *et al., Khim. Prir. Soedin.*, 1976, **12**, 91 (*Feropolidin*)

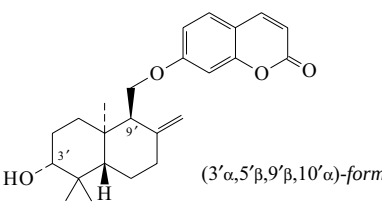
Khasanov, T.K. *et al., Khim. Prir. Soedin.*, 1976, **12**, 95 (*Mogoltacin*)

Nabiev, A.A. *et al., Khim. Prir. Soedin.*, 1978, **14**, 517; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 441 (*Feselol*)

Saidkhodzhaev, A.I. *et al., Khim. Prir. Soedin.*, 1978, **14**, 707; 799; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 601; 681 (*configs*)

Graf, E. *et al., Planta Med.*, 1985, 428 (*isol*)

O-(3-Hydroxy-8(12)-drimen-11-yl)umbelliferone H-437



(3′α,5′β,9′β,10′α)-*form*

$C_{24}H_{30}O_4$ 382.499

(3′α,5′β,9′β,10′α)-*form* [511-33-1] ***Farnesiferol A***. *Isobadrakemin*. *Mogoltadin*
Constit. of *Ferula assa-foetida* (asafoetida) and other *Ferula* spp.. Prismatic needles (EtOH). Mp 155-155.5°. $[\alpha]_D$ -55 (c, 0.71 in $CHCl_3$).

(3′β,5′β,9′β,10′α)-*form* [51819-92-2] ***Gummosin***
From *Ferula gummosa* (galbanum). Mp 176-177°. $[\alpha]_D$ -54 ($CHCl_3$).

Caglioti, L. *et al., Helv. Chim. Acta*, 1958, **41**, 2278

v. Tamelen, E.E. *et al., Chem. Comm.*, 1966, 413 (*synth*)

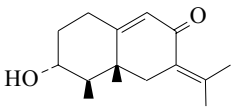
Perel'son, M.E. *et al., Khim. Prir. Soedin.*, 1975, **11**, 244; 1976, **12**, 442; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 246; 1976, **12**, 389 (*nmr, config*)

Terent'ev, P.B. *et al., Khim. Prir. Soedin.*, 1977, **13**, 207; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 178 (*ms*)

Pinar, M. *et al., Phytochemistry*, 1977, **16**, 1987 (*isol, deriv*)

van Tamelen, E.E. *et al., Bioorg. Chem.*, 1982, **11**, 171 (*synth*)

3-Hydroxy-7(11),9-eremophiladien-8-one H-438



$C_{15}H_{22}O_2$ 234.338

3α-*form* [469-67-0] ***Isopetasol***
Cryst. (EtOAc/Et_2O). Mp 126-127° (123.5-125°). $[\alpha]_D$ +113 (c, 0.9 in $CHCl_3$). Artifact of dec. of.

3-O-β-D-Glucopyranoside: [69809-29-6] ***Isopetasoside***
$C_{21}H_{32}O_7$ 396.48
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{20}$ +7.3 (c, 2.2 in EtOH).

Stoll, A. *et al., Experientia*, 1956, **12**, 360 (*isol*)

Brooks, C.J.W. *et al., Tetrahedron*, 1969, **25**, 2865 (*synth*)

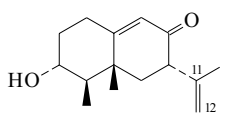
Toropkina, R.Ya. *et al., Khim. Prir. Soedin.*, 1972, **8**, 650; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 622 (*isol*)

Yamada, K. *et al., Phytochemistry*, 1978, **17**, 1667 (*Isopetasoside*)

Sugama, K. *et al., Phytochemistry*, 1983, **22**, 1619 (*Isopetasol*)

Witschel, M.C. *et al., Synthesis*, 1997, 107 (*synth, ir, pmr, cmr, ms*)

3-Hydroxy-9,11-eremophiladien-8-one H-439



(3α,7α)-*form*

$C_{15}H_{22}O_2$ 234.338

(3α,7α)-*form* [64236-38-0] ***Petasol***. *Sencathenone*
Viscous yellow oil. $[\alpha]_D$ +124 (c, 0.74 in $CHCl_3$).

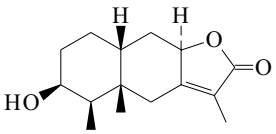
O-*(3-Methylsulfinyl-2Z-propenoyl):* ***Eremopetasin sulfoxide***
$C_{19}H_{26}O_4S$ 350.478
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{24}$ +17 (c, 0.3 in EtOH).

Brooks, C.J.W. *et al., Phytochemistry*, 1972, **11**, 3235 (*biosynth*)

Tori, M. *et al., Phytochemistry*, 1988, **47**, 401-409 (*cmr, Eremopetasin sulfoxide*)

Witschel, M.C. *et al., Tet. Lett.*, 1995, **36**, 3325 (*synth*)

3-Hydroxy-7(11)-eremophilen-12,8-olide H-440



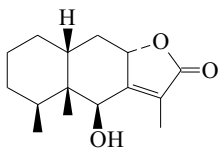
$C_{15}H_{22}O_3$ 250.337

(3β,8β)-*form* [158848-23-8]
Constit. of *Petasites japonicus* (sweet coltsfoot). Needles (Et_2O/EtOAc). Mp 168-169°. $[\alpha]_D^{22}$ -136 (c, 0.3 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1944 (*isol, pmr, cmr*)

6-Hydroxy-7(11)-eremophilen-12,8-olide H-441

6-Hydroxyeremophilenolide

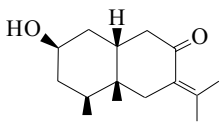


$C_{15}H_{22}O_3$ 250.337

(6β,8α)-*form* [10250-03-0]
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (Et_2O). Mp 208°. $[\alpha]_D$ +205.8 (c, 1 in $CHCl_3$).

Moriyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3196

2-Hydroxy-7(11)-eremophilen-8-one H-442

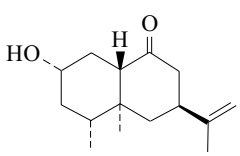


$C_{15}H_{24}O_2$ 236.353
Cryst.

(2β,4β,5β,10β*H*)-*form*
O-*(3-Methylthio-2Z-propenoyl):* [36031-35-3] **S-*Japonin***
$C_{19}H_{28}O_3S$ 336.494
Constit. of leaves of *Petasites japonicus*. Mp 116.5-117°. $[\alpha]_D^{24}$ +7 (c, 1.01 in $CHCl_3$).

Naya, K. *et al., Chem. Lett.*, 1972, 241

2-Hydroxy-11-eremophilen-9-one H-443



$C_{15}H_{24}O_2$ 236.353

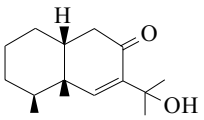
(2α,4α,5α,7β,10β)-*form* [74299-59-5] ***Rishitinone***
Constit. of diseased potato tubers.

Cryst. Mp 72-75°. $[\alpha]_D$ +10.1.

Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2478 (*isol, struct*)
Bohlmann, F. *et al., Annalen*, 1983, 2042 (*synth*)

11-Hydroxy-6-eremophilen-8-one H-444

[35124-22-2]
Petasitolone

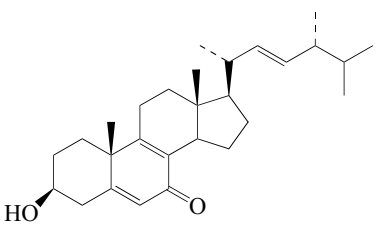


$C_{15}H_{24}O_2$ 236.353
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $Bp_{0.15}$ 92°. $[\alpha]_D^{24}$ +16.7 (c, 0.99 in MeOH).

Naya, K. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 3165
Liu, H.-J. *et al., Can. J. Chem.*, 1984, **62**, 2676 (*synth*)

3-Hydroxyergosta-5,8,22-trien-7-one H-445

3-Hydroxy-24-methylcholesta-5,8,22-trien-7-one

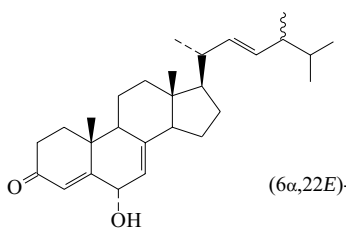


$C_{28}H_{42}O_2$ 410.639
(3β,22*E*,24*R*)-*form* [200942-18-3]
Constit. of *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{24}$ -28.3 (c, 0.1 in $CHCl_3$). λ_{max} 246 (log ϵ 4) (MeOH).

Ishizuka, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1756-1760 (*isol, pmr, cmr*)

6-Hydroxy-4,7,22-ergostatrien-3-one, 9CI H-446

6-Hydroxy-24-methyl-4,7,22-cholestatrien-3-one



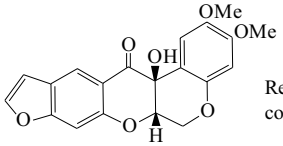
(6α,22*E*)-*form*

$C_{28}H_{42}O_2$ 410.639
(6α,22*E*)-*form* [114020-59-6]
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ -36 (c, 0.1 in EtOH).
(6β,22*E*)-*form* [68378-35-8]
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ -20 (c, 0.1 in EtOH).

Malorni, A. *et al., Nouv. J. Chim.*, 1978, **2**, 351 (*synth*)
Nichitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 211 (*isol*)

12*a*-Hydroxyerosone H-447

[66322-32-5]
6a,13a-Dihydro-13a-hydroxy-2,3-dimethoxy[1]benzopyrano[3,4-b]furo[3,2-g][1]benzopyran-13(6H)-one, 9CI



Relative configuration

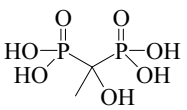
$C_{20}H_{16}O_7$ 368.342
Constit. of *Pachyrrhizus erosus* (yam bean). Needles ($CHCl_3$/petrol). Mp 282-283° dec. $[\alpha]_D$ +170.4 ($CHCl_3$).

Me ether: [61419-05-4] ***Neobanone***. *12a-Methoxyerosone*
$C_{21}H_{18}O_7$ 382.369
Yellow oil. $[\alpha]_D$ +61.

Oberholzer, M.E. *et al., Phytochemistry*, 1976, **15**, 1283 (*Neobanone*)
Kalia, A.J. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 1084 (*isol*)

1-Hydroxy-1,1-ethanediphosphonic acid H-448

[2809-21-4]
(1-Hydroxyethylidene)bisphosphonic acid, 9CI. ***Etidronic acid, BAN, INN, USAN***. *HEBP. Etidronate. Ksidifon. Xidiphone. Dequest 2010. Dequest 2015*



$C_2H_8O_7P_2$ 206.028
Food contaminant arising from its use as a boiler water additive for prepn. of steam used in food processing. Component of antimicrobial washes for poultry carcasses and fruit. Syrup, cryst. + $1H_2O$ (AcOH aq.). Sol. H_2O, EtOH, MeOH. Mp 105°. pK_{a1} 1.7; pK_{a2} 2.47; pK_{a3} 7.28; pK_{a4} 10.29; pK_{a5} 11.13 (25°,H_2O). Log P -2.54 (uncertain value) (calc). Thermally stable up to 125° at up to pH 1.6; between pH 8.5-11.5, thermally stable up to 195°.
▶ LD_{50} (mus, orl) 1800 mg/kg. Exp. reprod. and teratogenic effects. SZ8562100

Di-Na salt: [7414-83-7] *Calcimux. Didronel. Difosfen. Diphos†. Diphosphonat. Etidon. HEDSPA. Sodium etidronate. Etidronate disodium, USAN*
The name Diphos is also used for 1,2-Bis(diphenylphosphino)ethane.
▶ LD_{50} (rat, orl) 1340 mg/kg. Exp. reprod. and teratogenic effects. JL5950000

Tri-Na salt: [2666-14-0]
▶ LD_{50} (rat, orl) 1280 mg/kg. JL6650000

Tc complex: See Technetium etidronate in *The Combined Chemical Dictionary.*

Tetra-Me ester: [15207-88-2] *Tetramethyl (1-hydroxyethylidene)bisphosphonate*
$C_6H_{16}O_7P_2$ 262.136
Cryst. (C_6H_6/hexane). Mp 68-71°.

Tetra-Et ester: [20427-93-4] *Tetraethyl (1-hydroxyethylidene)bisphosphonate*
$C_{10}H_{24}O_7P_2$ 318.243
Liq. which isomerises on distn.

[3794-83-0, 70675-24-0]

Přibil, R. *et al., Talanta*, 1967, **14**, 591 (*use*)
Kasparek, F. *et al., Monatsh. Chem.*, 1968, **99**, 2016 (*synth*)
Nicholson, D.A. *et al., J.O.C.*, 1970, **35**, 3149; 1971, **36**, 3843 (*ester, synth, P-31 nmr*)
Strates, B.S. *et al., Biochim. Biophys. Acta*, 1971, **244**, 121 (*pharmacol*)
Wiers, B.H. *et al., Inorg. Chem.*, 1971, **10**, 2581 (*salts*)
Blaser, B. *et al., Z. Anorg. Allg. Chem.*, 1971, **381**, 247 (*synth, props, P-31 nmr*)
Michael, W.R. *et al., Toxicol. Appl. Pharmacol.*, 1972, **21**, 503 (*metab*)
Maier, L. *et al., Helv. Chim. Acta*, 1973, **56**, 1257 (*ester, synth, pmr, P-31 nmr, props*)
Bikhman, B.I. *et al., Zh. Neorg. Khim.*, 1973, **18**, 2406; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 1273 (*ir, salts*)
Collins, A.J. *et al., J. Appl. Chem. Biotechnol.*, 1977, **27**, 651 (*props, salts*)
De Angelis, L. *et al., Drugs of Today (Barcelona)*, 1978, **14**, 101 (*rev, pharmacol*)
Barnett, B.L. *et al., Acta Cryst. B*, 1979, **35**, 1212 (*cryst struct*)
Worms, K.H. *et al., Z. Anorg. Allg. Chem.*, 1979, **457**, 209 (*synth*)
Motekaitis, R.J. *et al., Inorg. Chem.*, 1980, **19**, 1646 (*props, complexes*)
Rizhalla, E.N. *et al., Talanta*, 1980, **27**, 715 (*complexes*)
Goeva, L.V. *et al., Radiokhimiya*, 1982, **22**, 591; *Sov. Radiochem. (Engl. Transl.)*, 1982, **22**, 489 (*props*)
Fonong, T. *et al., Anal. Chem.*, 1983, **55**, 1089 (*props*)
Van der Pol, H.J. *et al., Pharm. Weekbl.*, 1983, **118**, 330 (*anal, props*)
Perfil'ev, V.A. *et al., Zh. Anal. Khim.*, 1984, **39**, 2133 (*detn, V*)
Afonin, E.G. *et al., Zh. Obshch. Khim.*, 1987, **57**, 538; 1989, **59**, 317; *J. Gen. Chem. USSR (Engl. Transl.)*, 1987, **57**, 469; 1989, **59**, 273 (*acid, salts, ir*)
Fleisch, H. *et al., Bisphosphonates and Tumor Osteolysis*, (Brunner, K.W. *et al*, ed.), Springer-Verlag, Berlin, 1989, 1 (*rev*)
Harris, R.H. *et al., J.C.S. Faraday 1*, 1989, **85**, 1409 (*P-31 nmr*)
Harris, R.H. *et al., Z. Naturforsch., B*, 1989, **44**, 1407 (*cmr, P-31 nmr*)
Shkol'nikova, L.M. *et al., Kristallografiya*, 1991, **36**, 77; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1991, **36**, 40 (*cryst structs*)
Kashina, N.A. *et al., Zh. Obshch. Khim.*, 1992, **62**, 1567; *J. Gen. Chem. USSR (Engl. Transl.)*, 1992, **62**, 1284 (*props*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 658
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1371-1372
Osvath, R. *et al., Food Chem. News*, 2001, **43(32)**, 11 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXD400; TEE250; TNL750; HKS780

2-Hydroxy-1-ethanesulfonic acid, 9CI, 8CI H-449

[107-36-8]
2-Sulfoethyl alcohol. Isethionic acid
$HOCH_2CH_2SO_3H$

$C_2H_6O_4S$ 126.133
Syrup. Misc. H_2O, EtOH.

► Eye, skin and mucous membrane irritant. LD_{50} (mus, ipr) 50 mg/kg. KI7700000

Na salt: [1562-00-1]
Mp 191-194°.

NH_4 salt: [57267-78-4]
Hygroscopic. Mp 139-141°.

► KI7750000

O-*Sulfate:* See Ethionic acid in *The Combined Chemical Dictionary.*

Chloride: [78303-70-5]
$C_2H_5ClO_3S$ 144.578
Syrup. n_D^{25} 1.4902.

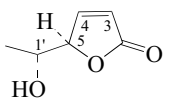
Ac, chloride: [78303-71-6]
$C_4H_7ClO_4S$ 186.616
Bp_{14} 130-132°.

Et ether:2-Ethoxy-1-ethanesulfonic acid
$C_4H_{10}O_4S$ 154.187
Syrup. d^{21} 1.36.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **1**, 1432A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **1**, 889A; 889B (*ir*)
Aschütz, R. *et al., Annalen*, 1918, **415**, 89 (*synth*)
Goldberg, A.A. *et al., J.C.S.* , 1942, 716
Challenger, F. *et al., Biochem. J.* , 1970, **117**, 65p (*occur*)
Wooton, D.L. *et al., J.O.C.* , 1974, **39**, 2112 (*synth*)
Hoskin, F.C.G. *et al., Arch. Biochem. Biophys.* , 1977, **180**, 583 (*biosynth*)
King, J.F. *et al., Can. J. Chem.* , 1983, **61**, 1583 (*chloride*)
Barrow, K.D. *et al., Phytochemistry*, 1993, **34**, 1429 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANL100; HKI500

5-(1-Hydroxyethyl)-2(5*H*)-furanone H-450

5-Hydroxy-2-hexen-4-olide. 2,3,6-Trideoxyhex-3-enono-1,4-lactone



(1'*R*,5*R*)-form

$C_6H_8O_3$ 128.127

(1′*R*,5*R*)-*form*
D-threo-*form*

O-*β*-D-*Glucopyranoside:*
$C_{12}H_{18}O_8$ 290.269
Glass. λ_{max} 275 (ε 800) (H_2O).

(1′*R*,5*S*)-*form* D-erythro-*form*

O-*β*-D-*Glucopyranoside:*
Glass.

3,4-Dihydro: [89195-92-6]
Oil. $Bp_{0.3}$ 110-115°. $[\alpha]_D^{20}$ +9.1 (c, 4.6 in $CHCl_3$).

(1′*S*,5*R*)-*form* [54621-96-4] L-erythro-*form*
Constit. of akaboshi zenmai (*Osmunda japonica*) fronds. Oil. $[\alpha]_D$ +112.4.

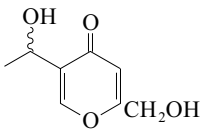
3,4-Dihydro: [54656-51-8] *Dihydro-5-(1-hydroxyethyl)-2(3*H*)-furanone. 5-Hydroxy-4-hexanolide. 2,3,6-Trideoxy-1,4-hexonolactone. Sherry lactone*
$C_6H_{10}O_3$ 130.143
Constit. of akaboshi zenmai (*Osmunda japonica*) fronds. Also isol. from sherry (stereochem. unspecified). Oil. $Bp_{0.2}$ 106-110°. $[\alpha]_D$ -12. $[\alpha]_D^{20}$ -8.7 (c, 4 in $CHCl_3$).

[105814-63-9]

Hollenbeak, K.H. *et al., Tetrahedron*, 1974, **30**, 2307 (*synth*)
Numata, A. *et al., Chem. Pharm. Bull.* , 1984, **32**, 2815 (*isol*)
Lundt, I. *et al., Synthesis*, 1986, 1052 (*dihydro, synth, cmr*)
Buchanan, M.S. *et al., Phytochemistry*, 1995, **40**, 1251 (*isol, pmr, cmr*)
Perry, N.B. *et al., Phytochemistry*, 1996, **42**, 453 (*glucosides*)

5-(1-Hydroxyethyl)-2-(hydroxymethyl)-4*H*-pyran-4-one H-451

[131123-57-4]
Herierin IV

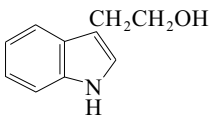


$C_8H_{10}O_4$ 170.165
Constit. of *Hericium erinaceum* (lions mane).

Qian, F. *et al., CA* , 1991, **114**, 20976g (*isol, pmr*)

3-(2-Hydroxyethyl)indole H-452

[526-55-6]
1H-Indole-3-ethanol, 9CI. Tryptophol. 2-(3-Indolyl)ethanol



$C_{10}H_{11}NO$ 161.203
Prisms (C_6H_6/petrol); plates (Et_2O/petrol). Sol. most org. solvs.; spar. sol. H_2O, petrol. Mp 59°. Bp_2 174°. Red. soln. in warm conc. H_2SO_4.

► LD_{50} (mus, ipr) 351 mg/kg. KL3685000

Picrate:
Red needles (H_2O). Mp 100-101°.

O-*Ac:* [13137-14-9]
$C_{12}H_{13}NO_2$ 203.24
Oil.

N-*Benzoyl:*
$C_{17}H_{15}NO_2$ 265.311
Yellow prisms and plates (petrol). Mp 76°.

O-*β*-D-*Galactopyranoside:* [95088-52-1]
Tryptophol galactoside
$C_{16}H_{21}NO_6$ 323.345

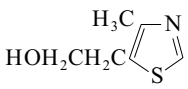
O-*β*-D-*Glucopyranoside:* [40883-44-1]
Tryptophol glucoside
$C_{16}H_{21}NO_6$ 323.345

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [149817-65-2]
$C_{21}H_{29}NO_{10}$ 455.461
Isol. from *Lycium chinense* (Chinese boxthorn). Pale yellow powder. $[\alpha]_D^{20}$ -32.7 (c, 0.4 in MeOH).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **3**, 130A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **2**, 659B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1502A (*ir*)
Ehrlich, F. *et al., Ber.* , 1912, **45**, 884
Jackson, R.W. *et al., J. Biol. Chem.* , 1930, **88**, 659
Oddo, B. *et al., Gazz. Chim. Ital.* , 1937, **69**, 10
Snyder, H.R. *et al., J.A.C.S.* , 1948, **70**, 3770
Fish, M.S. *et al., J.A.C.S.* , 1959, **78**, 3668
Nogrady, T. *et al., Can. J. Chem.* , 1964, **42**, 485
Narayanan, T.K. *et al., Antimicrob. Agents Chemother.* , 1976, **9**, 375 (*isol, props*)
Magnus, V. *et al., Carbohydr. Res.* , 1979, **76**, 261 (*synth, glucoside*)
Lacan, G. *et al., Plant Physiol.* , 1984, **76**, 889; 1985, **78**, 447 (*glucoside, galactoside*)
Ayer, W.A. *et al., Can. J. Chem.* , 1986, **64**, 904 (*isol*)
Yahara, S. *et al., Chem. Pharm. Bull.* , 1993, **41**, 703 (*xylosylglucoside*)
Novák, L. *et al., Annalen*, 1995, 1877 (*Ac*)
Böhlendorf, B. *et al., Annalen*, 1996, 49 (*isol, ir, pmr, cmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICS000

5-(2-Hydroxyethyl)-4-methylthiazole H-453

[137-00-8]
4-Methyl-5-thiazoleethanol, 9CI. 2-(4-Methyl-5-thiazolyl)ethanol. FEMA 3204



C_6H_9NOS 143.209
Flavour ingredient. Present in cooked beef, beer, spirits, cocoa, roast peanut, porcini (*Boletus edulis*) and malt. Oil with nut-like odour on extreme dilution. Bp_{10} 142-145° Bp_3 127-129°. n_D^{20} 1.5470.

N-*Me:* [16311-69-6]
$C_7H_{12}NOS^{\oplus}$ 158.244
Mp 88-89° (as iodide). Light-sensitive. CAS no. refers to iodide.

Ac: [656-53-1] *FEMA 3205*
$C_8H_{11}NO_2S$ 185.246
Flavour ingredient. Mp 131°. Bp_4 123°.

Benzoyl: [31299-77-1]
$C_{13}H_{13}NO_2S$ 247.317
Mp 192°. Bp_4 185°.

Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **2**, 643C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **3**, 111B; 116B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1493D; 1495B (*ir*)
Buchman, E.R. *et al., J.A.C.S.* , 1936, **58**, 1803 (*deriv*)
U.K. Pat. , 1951, 641 426; *CA* , **45**, 2509
Takeda, Y. *et al., Yakugaku Zasshi*, 1951, **71**, 84; *CA* , **45**, 9532
Dornow, A. *et al., Chem. Ber.* , 1953, **86**, 1404
U.S. Pat. , 1954, 2 654 760; *CA* , **48**, 12810
Miyatake, K. *et al., Yakugaku Zasshi*, 1955, **75**, 1054; *CA* , **50**, 5633
Thiel, M. *et al., Annalen*, 1958, **619**, 161
Rubtsov, I.A. *et al., CA* , 1970, **73**, 56015
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1862; 1863 (*occur, props*)

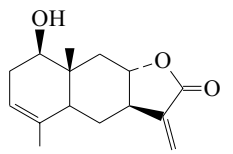
(2-Hydroxyethyl)trimethylarsonium(1+) H-454

[39895-81-3]
Arsenocholine
$[Me_3AsCH_2CH_2OH]^{\oplus}$
$C_5H_{14}AsO^{\oplus}$ 165.087
Claimed isolation from marine crustacea (prawns). Nat. occurrence doubtful. Largely excreted unchanged within 3d when administered orally to small mammals. Main metab. is Arsenobetaine, A-420.

[115195-61-4]

Kunz, H. *et al., Annalen*, 1973, 2001 (*synth*)
Bollino, N.R. *et al., ACS Symp. Ser.*, 1978, **82**, 116
Norin, H. *et al., Chemosphere*, 1982, **11**, 287 (*isol, pmr, ms*)
Hedlund, B. *et al., J. Neurochem.*, 1982, **39**, 871
Marafante, E. *et al., Sci. Total Environ.*, 1984, **34**, 223 (*metab*)
Irgolic, K.J. *et al., Appl. Organomet. Chem.*, 1987, **1**, 403 (*synth, pmr, cmr*)
Siu, K.W. *et al., Rapid Commun. Mass Spectrom.*, 1988, **2**, 69 (*ms*)
Kostick, A. *et al., Acta Cryst. C*, 1989, **45**, 1306 (*synth, pmr, cmr, cryst struct*)
Cullen, W.R. *et al., Appl. Organomet. Chem.*, 1989, **3**, 401
Momplaisir, G.M. *et al., J. Agric. Food Chem.*, 1991, **39**, 1448 (*synth, hplc*)
Francesconi, K.A. *et al., Appl. Organomet. Chem.*, 1992, **6**, 247 (*formn, isol*)
Edmonds, J.S. *et al., Nat. Prod. Rep.*, 1993, **10**, 421 (*rev*)
Minhas, R. *et al., Adv. Organomet. Chem.*, 1998, **12**, 635-641 (*synth, pmr, cmr, ms*)

1-Hydroxy-3,11(13)-eudesmadien-12,8-olide H-455



(1β,8α)-*form*

$C_{15}H_{20}O_3$ 248.321

(1β,8α)-*form*
8-Epiisoivangustin
Constit. of *Inula helenium* (elecampane). Cryst. (Et_2O/petrol). Mp 135.5°. $[\alpha]_D^{24}$ -50.4 (c, 0.48 in $CHCl_3$).

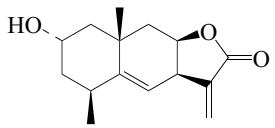
1-(2-Methylpropanoyl): [111625-65-1]
Subcordatolide E
$C_{19}H_{26}O_4$ 318.412
Gum.

(1β,8β)-*form* [68852-09-5]
Isoivangustin. *Grandulin*
Cryst. Mp 141°. $[\alpha]_D^{24}$ +120.8 (c, 0.26 in $CHCl_3$). Grandulin and Isoivangustin have not been compared but the props. of Grandulin (no stereochem. assigned, Mp. 130°; $[\alpha]_D$ +125) are similar to those of Isoivangustin.

[29702-22-5]

Nikonova, L.P. *et al., Khim. Prir. Soedin.*, 1970, **6**, 133; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 128 (*Grandulin*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172 (*8-Epiisoivangustin*)
Nagasampagi, B.A. *et al., Phytochemistry*, 1981, **20**, 2034 (*Isoivangustin*)
Ober, A.G. *et al., J. Nat. Prod.*, 1987, **50**, 604 (*Subcordatolide E*)

2-Hydroxy-5,11(13)-eudesmadien-12,8-olide H-456



$C_{15}H_{20}O_3$ 248.321

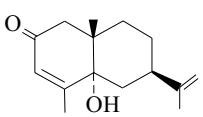
(2α,4β)-*form* [68776-45-4]
2α-Hydroxyalantolactone
Constit. of *Inula helenium* (elecampane). Oil. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. $[\alpha]_D^{24}$ +60.7 (c, 1 in $CHCl_3$). λ_{max} 211 (ε 8200) (MeOH) (Berdy).

2-Ketone: [68776-46-5] *2-Oxo-5,11(13)-eudesmadien-12,8-olide*
$C_{15}H_{18}O_3$ 246.305
Constit. of *Inula helenium* (elecampane). Cryst. (Et_2O). Mp 152-153°. $[\alpha]_D^{24}$ +301.3 (c, 1.3 in $CHCl_3$).

5α,6α-Epoxide:5,6-Epoxy-2-hydroxy-11(13)-eudesmen-12,8-olide. ***5,6-Epoxy-2-hydroxyalantolactone***
$C_{15}H_{20}O_4$ 264.321
Amorph. powder (EtOH). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 198-200° dec. λ_{max} 213 (ε 9800) (EtOH).

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172 (*isol, pmr*)
Al-Yahya, M.A. *et al., J. Nat. Prod.*, 1988, **51**, 621-624 (*epoxide*)

5-Hydroxy-3,11-eudesmadien-2-one H-457



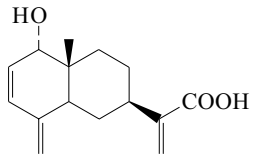
$C_{15}H_{22}O_2$ 234.338

5α-*form* [24405-56-9]
α-Rotunol
Constit. of tubers of nut grass, *Cyperus rotundus*. Cryst. (Et_2O). Mp 87.5-88.5°.

5β-*form* [24405-57-0]
β-Rotunol
Constit. of tubers of nut grass, *Cyperus rotundus*. Cryst. (Et_2O). Mp 118-119°. $[\alpha]_D$ +44.8 (c, 5.8 in $CHCl_3$).

Hikino, H. *et al., Tetrahedron*, 1971, **27**, 4831 (*isol, struct*)
Murai, A. *et al., J.A.C.S.*, 1978, **100**, 7751 (*synth*)
Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1195 (*synth*)

1-Hydroxy-2,4(18),11(13)-eudesmatrien-12-oic acid H-458

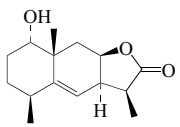


$C_{15}H_{20}O_3$ 248.321

1α-*form* [135594-81-9]
Constit. of *Artemisia vulgaris* (mugwort). Gum. $[\alpha]_D$ +85 (c, 0.3 in $CHCl_3$).

Marco, J.A. *et al., Phytochemistry*, 1991, **30**, 2403 (*isol, pmr, cmr*)

1-Hydroxy-5-eudesmen-12,8-olide H-459



(1α,4β,8β,11α*H*)-*form*

$C_{15}H_{22}O_3$ 250.337

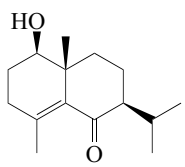
(1α,4β,8β,11α*H*)-*form*
1α-Hydroxy-11α,13-dihydroalantolactone

(1β,4β,8β,11α*H*)-*form*
1β-Hydroxy-11α,13-dihydroalantolactone

11,13-Didehydro: [68776-47-6] *1-Hydroxy-5,11(13)-eudesmadien-12,8-olide.* ***1β-Hydroxyalantolactone***
$C_{15}H_{20}O_3$ 248.321
Constit. of *Inula helenium* (elecampane). Oil.

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172 (*1-Hydroxyalantolactone*)
Öksüz, S. *et al., Phytochemistry*, 1997, **46**, 1131-1134 (*isol, pmr, cmr, cryst struct*)

1-Hydroxy-4-eudesmen-6-one H-460

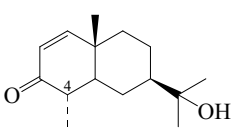


$C_{15}H_{24}O_2$ 236.353

1β-*form* [62311-70-0]
Acorusnol
Constit. of *Acorus calamus* (sweet flag). Oil. λ_{max} 247 (ε 8810) (MeOH).

Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175-1182 (*isol, pmr, cmr*)

11-Hydroxy-1-eudesmen-3-one H-461



4α-*form*

$C_{15}H_{24}O_2$ 236.353

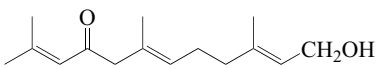
4α-form
4-Epiaubergenone
Cryst. Mp 105-107°. $[\alpha]_D$ -53.5.

4β-*form* [69427-35-6]
***Aubergenone**. Mangeudesmenone*
Found in diseased eggplant (*Solanum melongena*) and from the stem bark of *Mangifera indica* (mango). Oil. $[\alpha]_D$ -4 ($CHCl_3$). λ_{max} 229 (ϵ 5800) (MeOH) (Berdy). λ_{max} 228 (ϵ 5700) (EtOH) (Berdy).

Stoessl, A. *et al., Can. J. Chem.*, 1975, **53**, 3351 (*isol*)
Kelly, R.B. *et al., Can. J. Chem.*, 1978, **56**, 2508 (*synth, struct*)
Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1191 (*synth*)
Gulge, R. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 605 (*synth*)
Sharma, S.K. *et al., J. Indian Chem. Soc.*, 1995, **72**, 339-342 (*Mangeudesmenone*)

1-Hydroxy-2,6,10-farnesatrien-9-one H-462

*12-Hydroxy-2,6,10-trimethyl-2,6,10-dodecatrien-4-one. **9-Oxofarnesol***



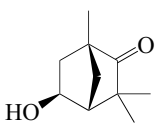
$C_{15}H_{24}O_2$ 236.353

(2*E*,6*E*)-*form* [79421-76-4]
Stress metab. of *Ipomoea batatas* (sweet potato).

Ac: [75911-00-1]
$C_{17}H_{26}O_3$ 278.391
Oil.

Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 841-844 (*Ac*)
Burka, L.T. *et al., Phytochemistry*, 1981, **20**, 647-652 (*isol, synth, pmr, ms, cmr*)

5-Hydroxyfenchone H-463

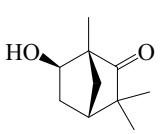


$C_{10}H_{16}O_2$ 168.235

(1*R*,4*R*,5*S*)-*form*
O-β-D-*Glucopyranoside:* [155960-75-1]
$C_{16}H_{26}O_7$ 330.377
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{26}$ -6.2 (c, 0.8 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

6-Hydroxyfenchone H-464

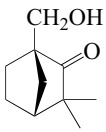


$C_{10}H_{16}O_2$ 168.235

(1*R*,4*S*,6*R*)-*form*
O-β-D-*Glucopyranoside:* [155960-76-2]
$C_{16}H_{26}O_7$ 330.377
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{21}$ -44 (c, 1.1 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

10-Hydroxyfenchone H-465



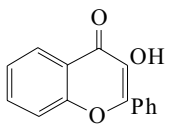
$C_{10}H_{16}O_2$ 168.235

(1*S*,4*R*)-*form*
O-β-D-*Glucopyranoside:* [217960-75-3]
$C_{16}H_{26}O_7$ 330.377
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 91-92°. $[\alpha]_D^{21}$ -1.8 (c, 1.1 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1599-1602 (*isol, pmr, cmr*)

3-Hydroxyflavone, 8CI H-466

[577-85-5]
*3-Hydroxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI. Flavonol. 3,4-Flavandione. 3-Hydroxy-2-phenylchromone*



$C_{15}H_{10}O_3$ 238.242
Constit. of cabbage. Pale yellow needles (EtOH aq.). Sol. EtOH, alkalis; sl. sol. H_2O. Mp 170°.

► LK8650000

Ac:
Mp 110-111°.

Me ether: [7245-02-5] *3-Methoxy-2-phenyl-4*H*-1-benzopyran-4-one. 3-Methoxy-2-phenylchromone. 3-Methoxyflavone*
Mp 114°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 918A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 95B (*ir*)
v. Kostenecki, S. *et al., Ber.*, 1904, **37**, 2819
Oyamada, T. *et al., Anal. Chem.*, 1934, **55**, 1256
Alford, W.C. *et al., Anal. Chem.*, 1951, **23**, 1149 (*detn, Zr*)
Bognar, P. *et al., Annalen*, 1966, **693**, 225
Smith, M.A. *et al., J. Het. Chem.*, 1968, **5**, 425
Ramakrishnan, V.T. *et al., J.O.C.*, 1970, **35**, 2898 (*synth*)
Sommer, L. *et al., Mikrochim. Acta*, 1970, 1181 (*detn, Zr*)
Filer, T.D. *et al., Anal. Chem.*, 1971, **43**, 469; 1753 (*detn, Zr*)
Jose, C.I. *et al., Spectrochim. Acta A*, 1974, **30**, 1199 (*ir*)
Pelter, A. *et al., J.C.S. Perkin 1*, 1981, 3182 (*cmr*)
Moriarty, R.M. *et al., J. Het. Chem.*, 1985, **22**, 583 (*synth*)
Costa, A.M. *et al., J.C.S. Perkin 1*, 1985, 799 (*synth, pmr*)
Cabrera-Martin, C. *et al., Anal. Chim. Acta*, 1986, **183**, 263 (*detn, Cr*)
Etter, M.C. *et al., J. Mol. Struct.*, 1986, **144**, 155 (*cryst struct*)
Rao, T.S. *et al., Heterocycles*, 1987, **26**, 2117 (*synth*)
Wallet, J.C. *et al., Acta Cryst. C*, 1988, **44**, 357 (*cryst struct, deriv*)
Wallet, J.C. *et al., Org. Magn. Reson.*, 1990, 28; 557 (*O-17 nmr*)

5-Hydroxyflavone H-467

[491-78-1]
*5-Hydroxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI. 5-Hydroxy-2-phenylchromone.* ***Primuletin***

$C_{15}H_{10}O_3$ 238.242
Yellow cryst. (EtOAc). Sol. EtOH, MeOH. Mp 159° (156-157°).

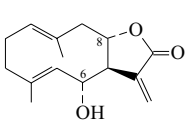
Me ether: [42079-78-7] *5-Methoxyflavone*
$C_{16}H_{12}O_3$ 252.269
Cryst. (petrol). Mp 133° (131°).

Et ether: [162787-72-6] *5-Ethoxyflavone*
$C_{17}H_{14}O_3$ 266.296
Cryst. Mp 111-113°.

O-β-D-*Glucopyranoside:* [71802-04-5]
$C_{21}H_{20}O_8$ 400.384
Constit. of *Medicago sativa*.

Simonis, H. *et al., Ber.*, 1926, **59**, 2914-2919 (*Me ether, synth*)
Sugasawa, S. *et al., J.C.S.*, 1934, 1483-1484 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1941, **24**, 297-298 (*isol*)
Looker, J.H. *et al., J.O.C.*, 1962, **27**, 381-389 (*synth, ir*)
Dev, B. *et al., Fresenius' Z. Anal. Chem.*, 1963, **196**, 178-182 (*detn, U*)
Naik, G.N. *et al., Indian J. Chem.*, 1966, **4**, 273-274 (*pmr*)
Wollenweber, E. *et al., Biochem. Physiol. Pflanz.*, 1974, **166**, 419-424 (*isol*)
Tyukavkina, N.A. *et al., Khim. Prir. Soedin.*, 1975, **11**, 583-587; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 613-616 (*ir, uv*)
Ternai, B. *et al., Tetrahedron*, 1976, **32**, 565-569 (*cmr*)
Volynets, A.P. *et al., CA*, 1979, **91**, 171654 (*glucopyranoside, isol*)
Saxena, S. *et al., Synthesis*, 1985, 697 (*synth*)
Shoja, M. *et al., Acta Cryst. C*, 1990, **46**, 517-519 (*cryst struct*)
Ares, J.J. *et al., J.O.C.*, 1993, **58**, 7903-7905 (*Me ether, !synth*)
Silva, A.M.S. *et al., Tet. Lett.*, 1994, **35**, 5899-5901 (*synth, cmr*)
Ares, J.J. *et al., J. Med. Chem.*, 1995, **38**, 4937-4943 (*Et ether*)

6-Hydroxy-1(10),4,11(13)-germacratrien-12,8-olide H-468



(1(10)*E*,4*E*,6α,8α)-*for*

$C_{15}H_{20}O_3$ 248.321

(1(10)*E*,4*E*,6α,8α)-*form* [35001-24-2]
***Desacetyllaurenobiolide**. Deacetyllaurenobiolide. Chamissellin*
Constit. of *Artemisia* spp.. Gum. $[\alpha]_D$ +34.5 (c, 1.6 in $CHCl_3$).

Ac: [35001-25-3] ***Laurenobiolide***
$C_{17}H_{22}O_4$ 290.358

Constit. of *Laurus nobilis* (bay laurel). Cryst. (Et_2O/hexane). Mp 101-103°. $[\alpha]_D$ +17.1 (EtOH).

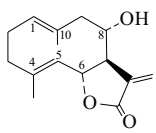
11α,13-Dihydro: ***6-Hydroxy-1(10),4-germacradien-12,8-olide***
$C_{15}H_{22}O_3$ 250.337

(1(10)*E*,4*E*,6β,8α)-*form* [93236-19-2]
6-Epidesacetyllaurenobiolide. *6-Epideacetyllaurenobiolide*
Cryst. ($CHCl_3$/petrol). Mp 117-118°. λ_{max} 205 (ϵ 13045) (MeOH).

Tada, H. *et al., Chem. Comm.*, 1971, 1391 (*struct*)
Shafizadeh, F. *et al., Phytochemistry*, 1973, **12**, 857 (*isol*)
Tada, H. *et al., Chem. Pharm. Bull.*, 1976, **24**, 667 (*isol*)
Tori, K. *et al., Tet. Lett.*, 1976, 387 (*cmr*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1169 (*isol*)
Quijano, L. *et al., Phytochemistry*, 1984, **23**, 1971 (*isol*)
Jakupovic, J. *et al., Phytochemistry*, 1992, **32**, 863 (*isol*)

8-Hydroxy-1(10),4,11(13)-germacratrien-12,6-olide H-469

[5988-66-9]



(1(10)*E*,4*E*,6α,8α)-*form*

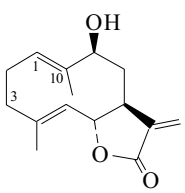
$C_{15}H_{20}O_3$ 248.321
Log P 1.5 (calc).

(1(10)*E*,4*E*,6α,8α)-*form*

11β,13-Dihydro, Ac: ***Acetylbalchanolide***
$C_{17}H_{24}O_4$ 292.374
Constit. of yarrow (*Achillea millefolium*). Cryst. (diisopropyl ether). Mp 125°. $[\alpha]_D^{20}$ +128.1 (c, 3.8 in $CHCl_3$).

Hochmannová, J. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1826 (*Balchanolide*)
Herout, V. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 2612 (*Balchanolide*)
Doskotch, R.W. *et al., J.O.C.*, 1970, **35**, 1928 (*Balchanolide, Tulipinolide*)
Brozdz, B. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1546 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 471-474 (*isol*)
Herz, W. *et al., J.O.C.*, 1979, **44**, 2784 (*isol*)
Gao, F. *et al., Phytochemistry*, 1986, **25**, 1231 (*isol*)
Okunade, A.L. *et al., Phytochemistry*, 1994, **35**, 191 (*isol, pmr, cmr, cryst struct*)

9-Hydroxy-1(10),4,11(13)-germacratrien-12,6-olide H-470



$C_{15}H_{20}O_3$ 248.321

(1(10)*E*,4*E*,6α,9β)-*form* [68715-67-3]
Haageanolide. *9β-Hydroxycostunolide*
Amorph. powder or oil. $[\alpha]_D$ +38.6 (c, 1 in $CHCl_3$).

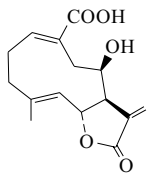
O-*(2-Methylpropanoyl):*
$C_{19}H_{26}O_4$ 318.412
Constit. of *Inula helenium* (elecampane). Cryst. (Et_2O/petrol). Mp 154°. $[\alpha]_D^{24}$ +104.8 (c, 0.48 in $CHCl_3$).

O-*(2-Methylbutanoyl):*
$C_{20}H_{28}O_4$ 332.439
Constit. of *Inula helenium* (elecampane). Oil.

O-*(3-Methylbutanoyl):*
$C_{20}H_{28}O_4$ 332.439
Constit. of *Inula helenium* (elecampane). Oil.

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172; 1982, **21**, 1166; 1357 (*derivs*)

8-Hydroxy-1(10),4,11(13)-germacratrien-12,6-olid-14-oic acid H-471



(1(10)*E*,4*E*,6α,8β)-*form*

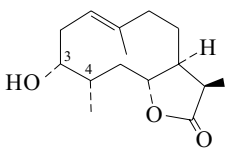
$C_{15}H_{18}O_5$ 278.304

(1(10)*E*,4*E*,6α,8β)-*form*

8-Angeloyl, Me ester: ***Sonchifolin***
$C_{21}H_{26}O_6$ 374.433
Constit. of *Smallanthus sonchifolius* (yacon). Oil. $[\alpha]_D^{25}$ +33 (c, 4.1 in $CHCl_3$). λ_{max} 219 (ϵ 10800) (MeOH) (Berdy).

Inoue, A. *et al., Phytochemistry*, 1995, **39**, 845 (*Sonchifolin*)

3-Hydroxy-1(10)-germacren-12,6-olide H-472



$C_{15}H_{24}O_3$ 252.353

(1(10)*E*,3α,4β*H*,6α,11α*H*)-*form* [17909-94-3]
Hydroxypelenolide
Constit. of *Artemisia absinthium* (wormwood). Cryst. Mp 108° (98°). $[\alpha]_D$ -41.

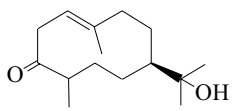
3-Ketone: [17909-92-1] *3-Oxo-1(10)-germacren-12,6-olide.* ***Ketopelenolide a***. *Oxopelenolide a*
$C_{15}H_{22}O_3$ 250.337
From *Artemisia absinthium* (wormwood). Cryst. Mp 114°.

(1(10)*E*,4α*H*,6α,11α*H*)-*form*

3-Ketone: ***Ketopelenolide b***. *Oxopelenolide b. Dihydroargolide*
$C_{15}H_{22}O_3$ 250.337
From *Artemisia absinthium* (wormwood). Cryst. Mp 172°. $[\alpha]_D^{22}$ +45 (c, 0.43 in $CHCl_3$).

Suchý, M. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 3917
Bates, R.B. *et al., J.O.C.*, 1970, **35**, 3960
Wang, W.Z. *et al., Phytochemistry*, 1994, **37**, 1347 (*Ketopelenolide b, pmr, cmr*)
Adekenov, S.M. *et al., Fitoterapia*, 1995, **66**, 142 (*Dihydroargolide, pmr*)
Edil'baeva, T.T. *et al., Khim. Prir. Soedin.*, 1999, **35**, 481-483; *Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 430-432 (*Ketoplenolide B, cryst struct*)

11-Hydroxy-1(10)-germacren-3-one H-473



$C_{15}H_{26}O_2$ 238.369

1(10)*E*-*form* [99957-12-7]
Germacrenone
Constit. of *Carissa edulis* (agam). Oil. $[\alpha]_D^{20}$ +173.2 (c, 1.1 in $CHCl_3$).

Achenbach, H. *et al., Phytochemistry*, 1985, **24**, 2325

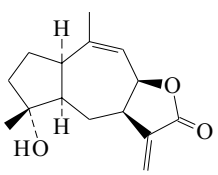
4-Hydroxyglutamine, 9CI H-474

$H_2NCOCH(OH)CH_2CH(NH_2)COOH$
$C_5H_{10}N_2O_4$ 162.145

L-*form*
Present in *Hemerocallis fulva* (day lily). Cryst. (H_2O, EtOH or Me_2CO). Mp 163-164°.

Brandner, G. *et al., Acta Chem. Scand.*, 1963, **17**, 2563 (*isol, synth*)
Kruger, G.J. *et al., J. S. Afr. Chem. Inst.*, 1976, **29**, 24
Lorenz, P. *et al., Phytochemistry*, 1999, **52**, 63-66 (*synth, pmr, cmr, occur*)

4-Hydroxy-9,11(13)-guaiadien-12,8-olide H-475

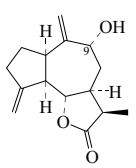


$C_{15}H_{20}O_3$ 248.321

(1α,4β,5α,8α)-*form*
4-Epiisoinuviscolide
Constit. of *Inula helenium* (elecampane). Cryst. Mp 147°. $[\alpha]_D^{24}$ -112.9 (c, 1.8 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1165-1172; 1985, **24**, 1315-1318 (*4-Epiisoinuviscolide, arabinosides*)

9-Hydroxy-4(15),10(14)-guaiadien-12,6-olide H-476



(1α,5α,6α,9α,11α*H*)-*form*

$C_{15}H_{20}O_3$ 248.321

(1α,5α,6α,9α,11α*H*)-*form* [152442-52-9]
Annuolide E
Constit. of *Helianthus annuus* (sunflower). Oil.

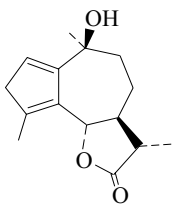
(1α,5α,6α,9α,11β*H*)-*form* [152442-51-8]
Annuolide D
Constit. of *Helianthus annuus* (sunflower). Oil.

9-O-β-D-Glucopyranoside: [106009-45-4]

[170384-77-7] ***Scorzoside***
$C_{21}H_{30}O_8$ 410.463
Constit. of *Scorzonera hispanica* (scorzonera). Cryst. (MeOH). Mp 95-97°. $[\alpha]_D^{20}$ -39 (c, 0.23 in MeOH).

Bryanskii, O.V. *et al., Khim. Prir. Soedin.*, 1992, **38**, 640; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 556 (*isol, pmr, cmr*)
Macias, F.A. *et al., Phytochemistry*, 1993, **34**, 669-674 (*Annuolides*)

10-Hydroxy-1,3-guaiadien-12,6-olide H-477

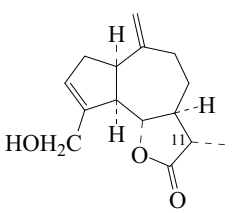


$C_{15}H_{20}O_3$ 248.321

(6α,10β,11α)-*form* [24399-20-0]
Artabsin. *Prochamazulenogenin*
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOH). Mp 133-135°. $[\alpha]_D^{20}$ -49.

Herout, V. *et al., Coll. Czech. Chem. Comm.*, 1953, **18**, 854 (*isol*)
Vokač, K. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1346 (*struct*)

15-Hydroxy-3,10(14)-guaiadien-12,6-olide H-478



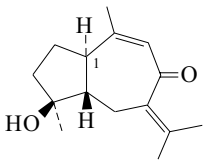
$C_{15}H_{20}O_3$ 248.321

(1α,5α,6α,11β*H*)-*form* [152442-50-7]
Annuolide B
Constit. of *Helianthus annuus* (sunflower). Oil.

11,13-Didehydro: [152442-48-3] *15-Hydroxy-3,10(14),11(13)-guaiatrien-12,6-olide.* ***Annuolide A***
$C_{15}H_{18}O_3$ 246.305
Constit. of *Helianthus annuus* (sunflower). Oil.

Macias, F.A. *et al., Phytochemistry*, 1993, **34**, 669-674; 1996, **43**, 1205-1215

4-Hydroxy-7(11),9-guaiadien-8-one H-479



(1α,4β,5β)-*form*

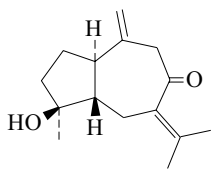
$C_{15}H_{22}O_2$ 234.338

(1α,4β,5β)-*form* [21698-40-8]
Procurcumenol
Constit. of the dried rhizomes of *Curcuma zedoaria* (zedoary) and *Curcuma longa* (turmeric). Oil. $[\alpha]_D$ +140.9 (c, 10.5 in $CHCl_3$). Struct. revised in 1986.

(1β,4β,5β)-*form* [127214-97-5]
1-Epiprocurcumenol
Oil. $[\alpha]_D$ -20.5 (c, 0.3 in MeOH).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1605-1607; 1977, **25**, 6 (*isol*)
Yoshihara, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 434 (*struct*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 55 (*Epiprocurcumenol*)
Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201 (*isol, pmr, cmr*)

4-Hydroxy-7(11),10(14)-guaiadien-8-one H-480



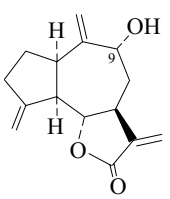
$C_{15}H_{22}O_2$ 234.338

(1α,4β,5β)-*form*
Minor constit. of oil of *Curcuma zedoaria* (zedoary). Needles (Et_2O/hexane). Mp 96-98°. $[\alpha]_D^{18}$ -44 ($CHCl_3$).

(1β,4β,5β)-*form*
Isoprocurcumenol
Needles (hexane). Mp 99.5-100.5°. $[\alpha]_D$ -62.5 (c, 0.2 in MeOH).

Yoshihara, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 434 (*cryst struct*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 55 (*Isoprocurcumenol*)

9-Hydroxy-4(15),10(14),11(13)-guaiatrien-12,6-olide H-481



$C_{15}H_{18}O_3$ 246.305

(1α,5α,6α,9α)-*form* [152442-49-4]
Annuolide C. *9-Hydroxycyclocostunolide*
Constit. of *Helianthus annuus* (sunflower). Oil.

Macias, F.A. *et al., Phytochemistry*, 1993, **34**, 669-674; 1996, **43**, 1205-1215 (*Annuolide C*)

1-Hydroxy-2,5,12,15-heneicosatetraen-4-one H-482

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_5CH{=}CHCOCH{=}CHCH_2OH$

$C_{21}H_{34}O_2$ 318.498

(2*E*,5*E*,12*Z*,15*Z*)-*form*
Constit. of avocado (*Persea americana*). Oil.

5,6-Dihydro:1-Hydroxy-2,12,15-heneicosatrien-4-one
$C_{21}H_{36}O_2$ 320.514
Constit. of avocado (*Persea americana*). Oil.

Paramashivappa, R. *et al., J. Agric. Food Chem.*, 2001, **49**, 2548-2551

5-Hydroxy-14,16-hentriacontanedione H-483

[38971-64-1]
$H_3C(CH_2)_{14}COCH_2CO(CH_2)_8CH(OH)(CH_2)_3CH_3$
$C_{31}H_{60}O_3$ 480.813
Constit. of *Avena sativa* (oats).

Dierickx, P.J. *et al., Phytochemistry*, 1972, **11**, 2654-2655 (*isol*)
Tulloch, A.P. *et al., Lipids*, 1973, **8**, 617-622 (*isol*)
Tulloch, A.P. *et al., Phytochemistry*, 1985, **24**, 131-137 (*cmr*)

8-Hydroxy-14,16-hentriacontanedione H-484

[10368-07-7]
$H_3C(CH_2)_{14}COCH_2CO(CH_2)_5CH(OH)(CH_2)_6CH_3$
$C_{31}H_{60}O_3$ 480.813
Isol. from leaf-surface wax of wheat *Triticum compactum* var. Little Club. Mp 69.5-70.5°. Obt. as a mixt. with the 9-hydroxy compd.

Tulloch, A.P. *et al., Can. J. Chem.*, 1969, **47**, 3119 (*isol, uv, pmr*)
Tulloch, A.P. *et al., Phytochemistry*, 1985, **24**, 131-137 (*cmr*)

25-Hydroxy-14,16-hentriacontanedione H-485

[52262-75-6]
$H_3C(CH_2)_5CH(OH)(CH_2)_8COCH_2CO(CH_2)_{12}CH_3$
$C_{31}H_{60}O_3$ 480.813

(*S*)-*form* [33256-70-1]
Constit. of the leaf wax of durum wheat.

Tulloch, A.P. *et al., Phytochemistry*, 1971, **10**, 871-876; 1983, **22**, 1605-1613; 1985, **24**, 131-137 (*isol, pmr, ms, cmr*)

10-Hydroxy-16-hentriacontanone H-486

[87264-34-4]
10-Hydroxypalmitone
$H_3C(CH_2)_8CH(OH)(CH_2)_5CO(CH_2)_{14}CH_3$
$C_{31}H_{62}O_2$ 466.83

Flavouring ingredient. Isol. from leaf wax of the famine food *Santalum album* (sandalwood). Plates (Me_2CO). Mp 96-97°.

Ac:
Mp 39.5-40°.

Oxime:
Mp 63.4-63.6°.

Chibnall, A.C. *et al., Biochem. J.*, 1937, **31**, 1981 (*isol, struct, synth*)
Talapatra, B. *et al., J. Indian Chem. Soc.*, 1982, **59**, 1364 (*isol*)

1-Hydroxy-9-heptadecene-4,6-diyn-3-one, 9CI H-487

$H_3C(CH_2)_6CH{=}CHCH_2C{\equiv}CC{\equiv}CCOCH_2CH_2OH$

$C_{17}H_{24}O_2$ 260.375

(*Z*)-*form* [13894-95-6]
Oil.

9ξ,10ξ-Epoxide: [155519-47-4] *9,10-Epoxy-1-hydroxy-4,6-heptadecadiyn-3-one.* ***Panaquinquecol 7***. *PQ 7*
$C_{17}H_{24}O_3$ 276.375
Constit. of *Panax quinquefolium* (American ginseng). Oil. $[\alpha]_D$ -74.1 (c, 0.5 in $CHCl_3$).

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 3552 (*isol, uv, ir, pmr*)
Fujimoto, Y. *et al., Phytochemistry*, 1994, **35**, 1255 (*epoxide*)

7-Hydroxyhexadecanedioic acid H-488

[38076-53-8]
7-Hydroxythapsic acid

$HOOC(CH_2)_8CH(OH)(CH_2)_5COOH$

$C_{16}H_{30}O_5$ 302.41

(ξ)-*form*
Constit. of various plant cutins incl. Indian wood apple (*Limonia acidissima*) and tomato.

Hunneman, D.H. *et al., Phytochemistry*, 1972, **11**, 1989-2001 (*isol*)
Pearce, R.B. *et al., Physiol. Plant Pathol.*, 1984, **24**, 71-81 (*isol*)
Hu, Z. *et al., Lipids*, 1988, **23**, 679-681 (*isol*)
Das, S. *et al., Phytochemistry*, 1989, **28**, 509-511 (*isol*)

8-Hydroxyhexadecanedioic acid H-489

[38076-48-1]
8-Hydroxythapsic acid

$HOOC(CH_2)_7CH(OH)(CH_2)_6COOH$

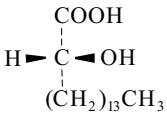
$C_{16}H_{30}O_5$ 302.41

(ξ)-*form*
Constit. of various plant cutins incl. Indian wood apple (*Limonia acidissima*) and tomato.

Hunneman, D.H. *et al., Phytochemistry*, 1972, **11**, 1989-2001 (*isol*)
Franich, R.A. *et al., Phytochemistry*, 1982, **21**, 2687-2689 (*isol*)
Pearce, R.B. *et al., Physiol. Plant Pathol.*, 1984, **24**, 71-81 (*isol*)
Hu, Z. *et al., Lipids*, 1988, **23**, 679-681 (*isol*)
Das, S. *et al., Phytochemistry*, 1989, **28**, 509-511 (*isol*)

2-Hydroxyhexadecanoic acid, 9CI H-490

[764-67-0]
2-Hydroxypalmitic acid


(*R*)-*form*

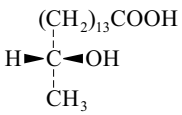
$C_{16}H_{32}O_3$ 272.427

(*R*)-*form* [16452-51-0]
Occurs in wool fat, which is used as a chewing gum softener. Mp 93.3-93.6°. $[\alpha]_D$ -3.2 ($CHCl_3$).

Horn, D.H.S. *et al., J.C.S.*, 1954, 1460 (*isol*)

15-Hydroxyhexadecanoic acid H-491

15-Hydroxypalmitic acid


(*R*)-*form*

$C_{16}H_{32}O_3$ 272.427

(*R*)-*form*

Lactone: [69297-56-9] *15-Hexadecanolide. 16-Methyloxacyclohexadecan-2-one, 9CI*
$C_{16}H_{30}O_2$ 254.412
Constit. of Galbanum absolute (from *Ferula galbaniflua* and *Ferula rubicaulis*). $[\alpha]_D^{25}$ -18.2 (c, 1.2 in hexane).

(*S*)-*form*

Lactone: [129214-00-2]
Oil. $Bp_{0.05}$ 110-115°. $[\alpha]_D^{25}$ +18.7 (c, 1 in hexane).

(±)-*form*

Lactone:
$Bp_{0.06}$ 130°.

Becker, J. *et al., Helv. Chim. Acta*, 1971, **54**, 2889 (*synth*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1978, **61**, 2671 (*isol, synth*)
Kostova, K. *et al., Helv. Chim. Acta*, 1984, **67**, 1713 (*synth, pmr, cmr*)
Stanchev, S. *et al., Helv. Chim. Acta*, 1989, **72**, 1052 (*synth, abs config, bibl*)
Bestmann, H.J. *et al., Synthesis*, 1994, 1257 (*15-Hexadecanolide, synth, pmr, cmr*)
Kuwahara, S. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1261-1263 (*15-Hexadecanolide, synth, ir, pmr*)
Nada, Y. *et al., Heterocycles*, 1998, **48**, 5-10 (*15-Hexadecanolide, synth*)

16-Hydroxy-6-hexadecenoic acid H-492

[4444-16-0]
Δ^6-Isoambrettolic acid

$HOCH_2(CH_2)_8CH{=}CH(CH_2)_4COOH$

$C_{16}H_{30}O_3$ 270.411
Cryst. (C_6H_6). Mp 77-77.5°.

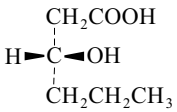
Formyl:
$C_{17}H_{30}O_4$ 298.422
Cryst. (pentane). Mp 53-54°.

Lactone: [7779-50-2] *Oxacycloheptadec-7-en-2-one. 6-Hexadecen-1,16-olide. Δ^6-Ambrettolide. FEMA 2555*
$C_{16}H_{28}O_2$ 252.396
Flavouring ingredient. Liq. with very strong musk-like odour. Mp 28.5°. Bp_2 170° Bp_{16} 185-190°.

Collaud, C. *et al., Helv. Chim. Acta*, 1943, **26**, 849 (*synth*)
Baudart, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1945, **221**, 205-206 (*lactone, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 326 (*lactone, props, use*)
Eur. Pat., 1999, 908455; *CA*, **130**, 301 508s (*lactone, props, use*)
Gaworski, C.L. *et al., Toxicology*, 1999, **139**, 1-17 (*lactone, tox*)

3-Hydroxyhexanoic acid, 9CI, 8CI H-493

[10191-24-9]
3-Hydroxycaproic acid


(*R*)-*form*

$C_6H_{12}O_3$ 132.159

(*R*)-*form* [77877-35-1]
Cryst. (petrol). Mp 41-41.6°. $[\alpha]_D^{24}$ -27.9 ($CHCl_3$).

Me ester: [109053-86-3]
$C_7H_{14}O_3$ 146.186
$[\alpha]_D$ -27.1 ($CHCl_3$).

(±)-*form*
V. sol. H_2O. Mp 13°.

Me ester: [21188-58-9]

[127593-19-5] *FEMA 3508*
Flavouring ingredient. Oil with a fruity aroma.

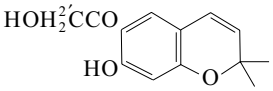
Et ester: [2305-25-1] *FEMA 3545*
$C_8H_{16}O_3$ 160.213
Food flavourant. Present in cognac, Scotch whisky, orange juice and peel, grapefruit, pineapple, purple passion fruit and other fruits. Liq. with fruity odour. Bp_{12} 95-98°.

[66997-60-2]

Baker, C.F. *et al., Annalen*, 1894, **283**, 124 (*synth*)
Lemieux, R.U. *et al., Can. J. Chem.*, 1951, **29**, 678 (*abs config*)
Serck-Hanssen, K. *et al., Ark. Kemi*, 1956, **10**, 136 (*abs config*)
Vuitel, L. *et al., Helv. Chim. Acta*, 1974, **57**, 1713 (*nmr*)
Ketelaar, P.E.F. *et al., Tet. Lett.*, 1985, **26**, 4665 (*synth*)
Burk, M.J. *et al., J.A.C.S.*, 1993, **115**, 10125 (*synth, pmr*)
Yan, T.-H. *et al., J.O.C.*, 1994, **59**, 8187; 1995, **60**, 3301 (*synth, ir, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 241; 514 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 996-997; 1781-1782 (*esters*)
Amantini, D. *et al., J.O.C.*, 2001, **66**, 4463-4467 (*Me ester*)

7-Hydroxy-6-hydroxyacetyl-2,2-dimethyl-2*H*-benzopyran H-494

[69790-24-5]
Desacetylripariochromene B



$C_{13}H_{14}O_4$ 234.251
Oil.

2′-Ac: [27045-16-5] ***Ripariochromene B***
$C_{15}H_{16}O_5$ 276.288
Cryst. Mp 146-147°.

2′-(2-Methylpropanoyl): [27045-17-6] ***Ripariochromene C***
Cryst. Mp 109-110°.

2′-Me ether: [22037-34-9] *7-Hydroxy-6-(methoxyacetyl)-2,2-dimethyl-2*H*-1-benzopyran*
$C_{14}H_{16}O_4$ 248.278
Constit. of *Madia sativa* (Chile tarweed). Mp 88-89°.

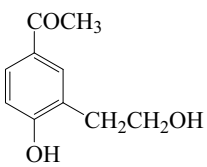
7-Me ether: [69790-25-6] *6-(Hydroxyacetyl)-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran*
$C_{14}H_{16}O_4$ 248.278
Cryst. (Et_2O/petrol). Mp 138°.

7-Me ether, 2′-Ac: [79307-02-1] *6-(Acetoxyacetyl)-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran*
$C_{16}H_{18}O_5$ 290.315
Oil.

Tsukayama, M. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 459
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1677-1678; 1981, **20**, 743 (*isol, ir, pmr*)
Ahluwalia, V.K. *et al., Synthesis*, 1981, 526 (*synth, pmr*)

4-Hydroxy-3-(2-hydroxyethyl)acetophenone H-495

1-[4-Hydroxy-3-(2-hydroxyethyl)phenyl]ethanone, 9CI



$C_{10}H_{12}O_3$ 180.203

4-O-β-D-Glucopyranoside:
$C_{16}H_{22}O_8$ 342.345
Constit. of *Helichrysum italicum* (curry plant). Mp 177°. $[\alpha]_D$ +1 (c, 0.1 in MeOH). λ_{max} 230 ; 246 ; 286 (MeOH).
Sala, A. *et al., J. Nat. Prod.*, 2001, **64**, 1360-1362

5-Hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-phenyl-3-heptanone, 9CI H-496

[79559-61-8]



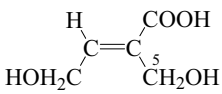
$C_{20}H_{24}O_4$ 328.407
Isol. from *Alpinia officinarum* (lesser galangal).

5-Me ether: [83161-95-9] *7-(4-Hydroxy-3-methoxyphenyl)-5-methoxy-1-phenyl-3-heptanone, 9CI*
$C_{21}H_{26}O_4$ 342.434
From *Alpinia officinarum* (lesser galangal). Oil. Probably an artifact.

5-Ketone: [83161-94-8] *1-(4-Hydroxy-3-methoxyphenyl)-7-phenyl-3,5-heptanedione, 9CI*
$C_{20}H_{22}O_4$ 326.391
From *Alpinia officinarum* (lesser galangal). Oil.

Inoue, T. *et al., Yakugaku Zasshi*, 1978, **98**, 1255 (*isol*)
Kiuchi, F. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2279 (*isol*)

4-Hydroxy-2-(hydroxymethyl)-2-butenoic acid, 9CI H-497



(*E*)-*form*

$C_5H_8O_4$ 132.116

(*E*)-*form*

5-O-E-Cinnamoyl, Me ester: [54118-68-2]
$C_{15}H_{16}O_5$ 276.288
Oil. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 217 (ϵ 27800); 222 (ϵ 22800); 278 (ϵ 22900) (EtOH).

(*Z*)-*form* [111833-91-1]

Nitrile, 4-O-β-D-glucopyranoside: [71933-54-5] *4-(β-D-Glucopyranosyloxy)-2-(hydroxymethyl)-2-butenenitrile, 9CI. **Sarmentosin**†. Nigrumin*
$C_{11}H_{17}NO_7$ 275.258
Isol. from *Ribes nigrum* (blackcurrant). $[\alpha]_D^{24}$ -18 (c, 0.3 in MeOH). Has (*E*)-config..

5-O-(3,4,5-Trihydroxybenzoyl), nitrile, 4-O-β-D-glucopyranoside: [168433-87-2] ***Rhodiocyanoside B***
$C_{18}H_{21}NO_{11}$ 427.364
Powder. $[\alpha]_D$ -12.2 (MeOH). Has (*E*)-config. (change of Cahn-Ingold priorities) λ_{max} 217 (log ϵ 4.48); 279 (log ϵ 3.99) (MeOH).

*5-O-(4-Hydroxy-*E*-cinnamoyl), nitrile, 4-O-β-D-glucopyranoside:* ***5-O-p-Coumaroylnigrumin***
$C_{20}H_{23}NO_9$ 421.403
Constit. of the seeds of *Ribes nigrum* (blackcurrant). Powder. Has (*E*)-config. (change of Cahn-Ingold priorities).

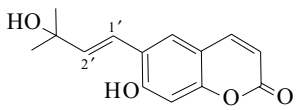
*5-O-(4-Hydroxy-3-methoxy-*E*-cinnamoyl), nitrile, 4-O-β-D-glucopyranoside:* ***5-O-Feruloylnigrumin***
$C_{21}H_{25}NO_{10}$ 451.429
Constit. of the seeds of *Ribes nigrum* (blackcurrant). Has (*E*)-config. (change of Cahn-Ingold priorities).

2,3-Epoxide, nitrile, 4-O-β-D-glucopyranoside: [81907-02-0] ***Epoxysarmentosin***. *Sarmentosin epoxide*
$C_{11}H_{17}NO_8$ 291.257
Hygroscopic powder.

[77459-99-5, 111833-90-0]

Kobayashi, A. *et al., Agric. Biol. Chem.*, 1974, **38**, 1997-2000 (*5-cinnamoyl Me ester*)
Gu, Y.-X. *et al., CA*, 1981, **94**, 183828j (*cryst struct, Sarmentosin*)
Nahrstedt, A. *et al., Phytochemistry*, 1982, **21**, 107 (*epoxide*)
Alen, R. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 76 (*synth, ms*)
Chu, G. *et al., Bioorg. Med. Chem. Lett.*, 1993, **3**, 1343 (*synth, Sarmentosin*)
Nishida, R. *et al., Phytochemistry*, 1994, **36**, 37 (*isol*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1245-1247 (*Rhodiocyanoside B*)
Lu, Y. *et al., Phytochemistry*, 2002, **59**, 465-468 (*Nigrumins*)

7-Hydroxy-6-(3-hydroxy-3-methyl-1-butenyl)-2*H*-1-benzopyran-2-one, 9CI H-498



$C_{14}H_{14}O_4$ 246.262

(*E*)-*form* [62949-89-7]
Platelets (Me_2CO/C_6H_6). Mp 159-160°.

7-Me ether: [18529-47-0] ***(E)-Suberenol***
$C_{15}H_{16}O_4$ 260.289
Isol. from *Limonia acidissima* (wood apple) and *Citrus nobilis* (king orange). V. pale yellow prisms (MeOH). Mp 173°.

1′,2′-Dihydro, 7-Me ether: [81892-79-7] ***Dihydrosuberenol***
$C_{15}H_{18}O_4$ 262.305
Isol. from *Limonia acidissima* (wood apple). Mp 105°.

Di-Me ether: [117597-80-5] ***(E)-Methylsuberenol***
$C_{16}H_{18}O_4$ 274.316
Oil.

7-Me, 3′-Et ether: [86682-61-3] ***Ethylsuberenol***
$C_{17}H_{20}O_4$ 288.343
Constit. of *Citrus sinensis* (orange). Mp 154-155°.

(*Z*)-*form* [62949-90-0]
Platelets (Me_2CO/C_6H_6). Mp 139-140.5°.

7-Me ether: [114032-20-1] ***(Z)-Suberenol***
$C_{15}H_{16}O_4$ 260.289
Oil.

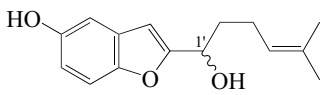
Di-Me ether: [117597-81-6] ***(Z)-Methylsuberenol***
$C_{16}H_{18}O_4$ 274.316
Oil.

[38409-30-2]

Guise, G.B. *et al., Aust. J. Chem.*, 1967, **20**, 2429 (*Suberenol*)
Shibata, S. *et al., Phytochemistry*, 1977, **16**, 291 (*isol, struct*)
Reisch, J. *et al., Planta Med.*, (Suppl.), 1980, 56 (*Suberenol*)
Burke, B.A. *et al., Heterocycles*, 1981, **16**, 897 (*Suberenol*)
Ghosh, P. *et al., Phytochemistry*, 1982, **21**, 240 (*Dihydrosuberenol*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1983, **31**, 901 (*Ethylsuberenol*)
Ju-ichi, M. *et al., Heterocycles*, 1988, **27**, 1451 (*Methylsuberenols*)
Reisch, J. *et al., Annalen*, 1990, 931 (*synth, ir, pmr, cmr, ms*)

5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran H-499

[197971-79-2]
5-Hydroxy-α-(4-methyl-3-pentenyl)-2-benzofuranmethanol, 9CI



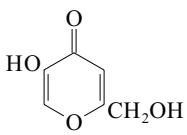
$C_{15}H_{18}O_3$ 246.305
Constit. of a fungus obtained from wintergreen (*Gaultheria procumbens*). Yellow-brown solid. λ_{max} 208 (ϵ 21000); 250 (ϵ 12000); 296 (ϵ 3800) (MeOH).

1′-Ketone: [197971-78-1] *5-Hydroxy-2-(5-methyl-1-oxo-4-hexenyl)benzofuran. 1-(5-Hydroxy-2-benzofuranyl)-5-methyl-4-hexen-1-one*
$C_{15}H_{16}O_3$ 244.29
Constit. of a fungus obtained from wintergreen (*Gaultheria procumbens*). Yellow-brown solid. Mp 56-57°. λ_{max} 204 (ϵ 22000); 218 (ϵ 15000); 292 (ϵ 22000); 336 (sh) (ϵ 6300) (MeOH).

Findlay, J.A. *et al., J. Nat. Prod.*, 1997, **60**, 1214-1215 (*isol, uv, pmr, cmr*)

5-Hydroxy-2-(hydroxymethyl)-4*H*-pyran-4-one, 9CI H-500

[501-30-4]
Kojic acid



$C_6H_6O_4$ 142.111
Synthetic intermed. for prodn. of food additives. Cryst. (H_2O). Sol. H_2O, AcOH; fairly sol. Py, EtOAc, $CHCl_3$, Et_2O; poorly sol. C_6H_6. Mp 161° (152°). λ_{max} 227 (ϵ 20700); 313 (ϵ 5250) (MeOH/KOH) (Derep). λ_{max} 269 (ϵ 7820) (MeOH) (Derep). λ_{max} 217 (ϵ 18200); 269 (ϵ 8320) (MeOH) (Berdy). λ_{max} 319 (ϵ 6020) (MeOH/NaOH) (Berdy).

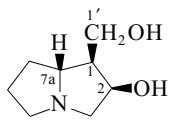
► LD_{50} (mus, ipr) 250 mg/kg. UQ0875000

1′-O-β-D-Glucopyranoside: [149056-78-0]
$C_{12}H_{16}O_9$ 304.253
Sol. H_2O.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 457B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 724C (*nmr*)
Yabuta, T. *et al., J.C.S.*, 1924, **125**, 575 (*struct*)
Beélik, A. *et al., Adv. Carbohydr. Chem.*, 1956, **11**, 145 (*rev*)
Becker, H.D. *et al., Acta Chem. Scand.*, 1962, **16**, 78 (*synth*)
Satyanarayana, D. *et al., Chemist-Analyst*, 1965, **54**, 4 (*detn, V*)
Sommer, L. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 1288 (*detn, U*)
Lichtenthaler, F.W. *et al., Angew. Chem., Int. Ed.*, 1969, **8**, 978
Kingsbury, C.A. *et al., J.O.C.*, 1976, **41**, 2777 (*pmr*)
Bajpai, P. *et al., J. Sci. Ind. Res.*, 1982, **41**, 185 (*rev*)
Lokaj, J. *et al., Acta Cryst. C*, 1991, **47**, 193 (*cryst struct*)
Japan. Pat., 1993, 93 221 846; *CA*, **120**, 14652x (*glucoside*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 759
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HLH500

2-Hydroxy-1-hydroxymethylpyrrolizidine H-501

Hexahydro-2-hydroxy-1H-pyrrolizine-1-methanol, 9CI



(1*S*,2*R*,7a*R*)-*form*

$C_8H_{15}NO_2$ 157.212
(1*S*,2*R*,7a*S*)-*form* [70494-70-1]
(1β,2β,7aα)-form. Petasinecine
Mp 132-134°.

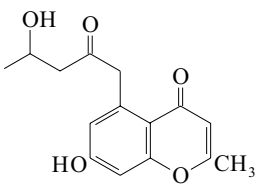
O^2*-Angeloyl:* [70474-33-8] ***Petasinine***
$C_{13}H_{21}NO_3$ 239.314
Alkaloid from *Petasites japonicus* (sweet coltsfoot). Amorph. powder. $[\alpha]_D^{25}$ +16 (c, 2.5 in EtOH).

O^2*-Angeloyl,* $O^{1'}$*-[α-L-rhamnopyranosyl-(→4)-4-hydroxycinnamoyl]:* [70474-34-9] ***Petasinoside***
$C_{28}H_{37}NO_9$ 531.602
Alkaloid from flower stalks of *Petasites japonicus* (sweet coltsfoot). Amorph. powder. $[\alpha]_D^{25}$ -38 (c, 1.1 in EtOH).

Aasen, A.J. *et al., J.O.C.*, 1969, **34**, 4143 (*struct, synth, pmr*)
Yamada, K. *et al., Tet. Lett.*, 1978, 4543 (*isol, pmr, struct, Petasinine, Petasinoside*)
Ma, D. *et al., J.C.S. Perkin 1*, 1999, 1703-1707 (*synth*)

7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone H-502

[128701-06-4]



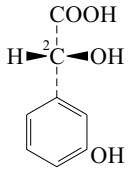
$C_{15}H_{16}O_5$ 276.288
Needles (C_6H_6/Me_2CO). Mp 173-175°. $[\alpha]_D^{19}$ +14.5 (c, 0.29 in MeOH).

7-O-β-D-Glucopyranoside: [128701-05-3]
$C_{21}H_{26}O_{10}$ 438.43
Constit. of Chinese rhubarb (*Rheum* sp.). Needles (H_2O). Mp 219-221°. $[\alpha]_D^{19}$ -49.1 (c, 0.43 in MeOH).

Kashiwada, Y. *et al., Phytochemistry*, 1990, **29**, 1007 (*isol, pmr, cmr*)

2-Hydroxy-2-(3-hydroxyphenyl)acetic acid H-503

[17119-15-2]
α,3-Dihydroxybenzeneacetic acid, 9CI. m-*Hydroxymandelic acid, 8CI. α,3-Dihydroxyphenylacetic acid. 3-Hydroxyphenylglycollic acid. α,3-Dihydroxy-α-toluic acid*



(*R*)-*form*

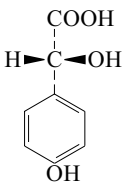
$C_8H_8O_4$ 168.149
(*R*)-*form* [17513-99-4]
Nitrile, 2-O-(6-O-acetyl-β-D-glucopyranoside):6″-O-Acetylholocalin
$C_{16}H_{19}NO_8$ 353.328
Constit. of *Sambucus nigra* (elderberry). $[\alpha]_D$ -47 (c, 0.2 in EtOH). Possible artifact λ_{max} 278 (EtOH).

[19988-46-6]

Greca, M.D. *et al., Nat. Prod. Lett.*, 2000, **14**, 175-182 (*Holocalin, 6″-Acetylholocalin*)

2-Hydroxy-2-(4-hydroxyphenyl)acetic acid H-504

[1198-84-1]
α,4-Dihydroxybenzeneacetic acid, 9CI. p-*Hydroxymandelic acid, 8CI. α,4-Dihydroxyphenylacetic acid. 4-Hydroxyphenylglycollic acid. α,4-Dihydroxy-α-toluic acid.* ***Pisolithin B***



(*R*)-*form*

$C_8H_8O_4$ 168.149
(*R*)-*form* [13244-78-5]
Cryst. + ½H_2O (H_2O). Mp 102-103° (anhyd.). $[\alpha]_D$ -144.4 (H_2O). Readily isomerises during isoln. λ_{max} 228 ; 274 (HCl) (Berdy). λ_{max} 248 (NaOH) (Berdy).

Nitrile, 2-O-β-D-glucopyranoside: [21401-21-8] ***Taxiphyllin***. *Phyllanthin*†. *Phyllanthoside*†
Cyanogenic glucoside of *Macadamia ternifolia*. Cryst. (EtOH/C_6H_6). Mp 168-169° Mp 176°. $[\alpha]_D^{20}$ -66.7 (c, 0.37 in EtOH). Pharmacol. active isomer. Diastereoisomeric, not enantiomeric, with Dhurrin (see below) λ_{max} 216 (ϵ 17780); 222 (ϵ 15490); 277 (ϵ 21880) (MeOH) (Derep).

(*S*)-*form* [13244-75-2]
Plates + $1H_2O$ (H_2O). Mp 114-115°. $[\alpha]_D$ +154.7 (c, 1.36 in H_2O).

Nitrile, 2-O-β-D-glucopyranoside: [499-20-7] ***Dhurrin***
Cyanogenic glucoside isol. from *Sorghum vulgare* (sorghum). Cryst. + $1H_2O$ (H_2O); cryst. + 1EtOH (EtOH). Sol. MeOH, H_2O. Mp 165°. λ_{max} 228 (ϵ 13000) (MeOH) (Berdy).

Nitrile, 2-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Dhurrin 6′-gluco-***

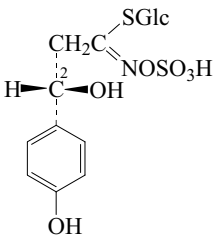
side
$C_{20}H_{27}NO_{12}$ 473.433
Constit. of *Sorghum bicolor* (sorghum).

[59845-69-1, 68758-69-0, 69322-01-6, 69322-02-7, 70013-61-5, 78689-25-5, 79694-14-7, 82492-24-8, 82492-25-9, 82503-24-0]

Pratesi, P. *et al., Farmaco, Ed. Sci.*, 1955, **10**, 563
Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1964, **259**, 665 (*Taxiphyllin*)
Towers, G.H.N. *et al., Tetrahedron*, 1964, **20**, 71 (*Taxiphyllin, isol, uv, ir, pmr*)
Mao, C.H. *et al., Phytochemistry*, 1965, **4**, 297 (*Taxiphyllin, struct*)
Selmar, D. *et al., Phytochemistry*, 1996, **43**, 569 (*Dhurrin 6′-glycoside*)

2-Hydroxy-2-(4-hydroxyphenyl)ethyl glucosinolate H-505

*1-Thio-β-D-glucopyranose 1-[β,4-dihydroxy-*N*-(sulfooxy)benzenepropanimidate], 9CI*



(2*R*)-*form*

$C_{15}H_{21}NO_{11}S_2$ 455.463

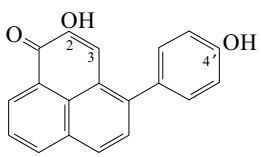
(2*R*)-*form*
Constit. of *Barbarea vulgaris* ssp. *arcuata*.

(2*S*)-*form*
Constit. of *Barbarea vulgaris* ssp. *arcuata* and *Barbarea orthoceras*.

Agerbirk, N. *et al., Phytochemistry*, 2001, **58**, 91-100 (*isol, pmr*)

2-Hydroxy-4-(4-hydroxyphenyl)-1*H*-phenalen-1-one H-506

[149184-19-0]
Irenolone



$C_{19}H_{12}O_3$ 288.302
Isol. from *Musa paradisiaca* (banana). Red needles ($CHCl_3$/MeOH). Mp 285°. λ_{max} 225 (sh) (ϵ 12600); 271 (ϵ 15800); 325 (ϵ 6310); 350 (ϵ 7940); 390 (ϵ 3980) (MeOH) (Derep). λ_{max} 271 (ϵ 15900); 325 (ϵ 6350); 350 (ϵ 3000); 390 (ϵ 4000) (MeOH) (Berdy).

4′-Me ether: [159853-36-8] ***2-Hydroxy-4-(4-methoxyphenyl)-1H-phenalen-1-one***
$C_{20}H_{14}O_3$ 302.329
Constit. of the rhizomes of *Musa acuminata* (dwarf banana). Bright red needles. Mp 222-223°. λ_{max} 272 ; 313 ; 337 ; 388 (EtOH) (Berdy).

*3′-Hydroxy:4-(3,4-Dihydroxyphenyl)-2-hydroxy-1*H*-phenalen-1-one*
$C_{19}H_{12}O_4$ 304.301
Isol. from *Musa acuminata* (dwarf banana). Orange powder. λ_{max} 243 (ϵ 13000); 283 (ϵ 11000); 328 (ϵ 4000); 338 (ϵ 4000); 440 (ϵ 4300) (MeOH).

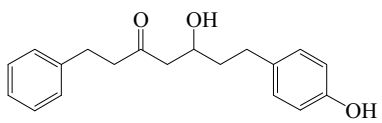
4′-Deoxy: [250606-32-7] *2-Hydroxy-4-phenyl-1*H*-phenalen-1-one, 9CI.* ***4′-Deoxyirenolone***
$C_{19}H_{12}O_2$ 272.303
Red solid. λ_{max} 232 ; 236 ; 262 ; 275 (EtOH).

3-Methoxy, 2-Me ether: ***2,3-Dimethoxy-4-(4-hydroxyphenyl)-1H-phenalen-1-one***
$C_{21}H_{16}O_4$ 332.355
Yellow cryst. (CH_2Cl_2). Mp 184-186°. λ_{max} 243 ; 342 ; 362 (MeOH).

Luis, J.G. *et al., J.O.C.*, 1993, **58**, 4306 (*isol, pmr, cmr*)
Luis, J.G. *et al., Tetrahedron*, 1994, **50**, 10963 (*ethers*)
Hoelscher, D. *et al., Phytochemistry*, 1997, **45**, 87 (*deriv*)
Kamo, T *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 95-101 (*isol, uv, pmr, ms*)
Luis, J.G. *et al., Nat. Prod. Lett.*, 1999, **13**, 299-304; 2000, **14**, 147-152 (*4′-Deoxyirenolone*)

5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone H-507

[83161-96-0]



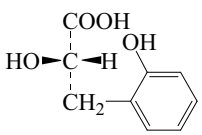
$C_{19}H_{22}O_3$ 298.381
From *Alpinia officinarum* (lesser galangal). Oil. $[\alpha]_D^{30}$ -13.3 (c, 1.04 in $CHCl_3$).

O^5*-Me:* [100667-53-6] *7-(4-Hydroxyphenyl)-5-methoxy-1-phenyl-3-heptanone*
$C_{20}H_{24}O_3$ 312.408
Constit. of *Alpinia officinarum* (lesser galangal). Needles. Mp 68-70°.

Itokawa, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4889 (*Me ether*)

2-Hydroxy-3-(2-hydroxyphenyl)propanoic acid H-508

[6803-09-4]
α,2-Dihydroxybenzenepropanoic acid, 9CI. 3-(2-Hydroxyphenyl)lactic acid



(*S*)-*form*

$C_9H_{10}O_4$ 182.176

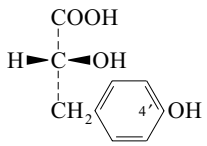
(*S*)-*form*
Constit. of the pollen of *Crocus sativus* (saffron). Powder (as Na salt). $[\alpha]_D$ +59 (c, 0.08 in MeOH). $[\alpha]_D$ +77 (c, 0.07 in MeOH) (Na salt). λ_{max} 253 ; 258 ; 264 (MeOH) (Na salt).

(±)-*form*
Constit. of the fruit of *Prunus cerasus* (cherry). Powder. Dec. at 241° (as Na salt) λ_{max} 218 (log ϵ 3.04); 253 (log ϵ 3.42); 289 (log ϵ 3.66) (MeOH).

Shaw, K.N.F. *et al., J.O.C.*, 1956, **21**, 601-604 (*synth*)
Wang, H. *et al., J. Nat. Prod.*, 1999, **62**, 86-88 (*isol, uv, pmr, cmr*)
Li, C.-Y. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1305-1309 (*S-form, isol, pmr, cmr*)

2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid H-509

[306-23-0]
α,4-Dihydroxybenzenepropanoic acid, 9CI. 3-(4-Hydroxyphenyl)lactic acid, 8CI



$C_9H_{10}O_4$ 182.176
► Tumorigenic. OD5500000

(*R*)-*form* [89919-57-3]
Mp 169-170° (164-165°). $[\alpha]_D^{26}$ -19.6 (c, 1.3 in H_2O).

(*S*)-*form* [23508-35-2]

(±)-*form* [6482-98-0]
Cryst. Mp 147.5-149° (139-140°).

4′-Me ether: [28030-15-1] *2-Hydroxy-3-(4-methoxyphenyl)propanoic acid*
$C_{10}H_{12}O_4$ 196.202
Constit. of wheat, rye (*Secale cereale*), and barley (*Hordeum vulgore*). Cryst. ($CHCl_3$/petrol or EtOAc/petrol). Mp 104-105° (88°).

4′-Me ether, amide: [105955-69-9]
$C_{10}H_{13}NO_3$ 195.218
Cryst. ($CHCl_3$/petrol). Mp 145°.

Di-Me ether: [87387-83-5] *2-Methoxy-3-(4-methoxyphenyl)propanoic acid*
$C_{11}H_{14}O_4$ 210.229
Constit. of barley, rye and wheat grains, prob. in an enantiomeric form.

4′-Me ether, Me ester: [55301-58-1]
$C_{11}H_{14}O_4$ 210.229
Oil. $Bp_{0.1}$ 35°.

Di-Me ether, Me ester:
$C_{12}H_{16}O_4$ 224.256
Oil. $Bp_{0.5}$ 120°.

(ξ)-*form*
Constit. of wheat grains and various other plants.

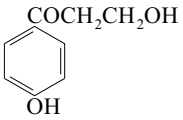
Holden, J.T. *et al., J. Biol. Chem.*, 1951, **191**, 559 (*synth*)
Bubl, E.C. *et al., J.A.C.S.*, 1951, **73**, 4972 (*synth*)
Buckle, A.L.J. *et al., J.C.S.*, 1954, 3981 (*synth*)
Matsuura, T. *et al., J.A.C.S.*, 1959, **81**, 871 (*synth*)
Stoessl, A. *et al., Biochem. Biophys. Res. Commun.*, 1969, **35**, 186 (*isol, synth*)
Rauschenbach, M.O. *et al., Cancer Res.*, 1975, **35**, 577 (*tox*)
Danifshefsky, S. *et al., J.A.C.S.*, 1979, **101**, 7013 (*synth, pmr*)
Lohaus, E. *et al., Z. Naturforsch., C*, 1983, **38**, 524 (*occur*)
Maurya, R. *et al., J. Nat. Prod.*, 1984, **47**, 179 (*isol*)
Gowal, H. *et al., Helv. Chim. Acta*, 1985, **68**, 2132 (*synth*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1624-1626 (*isol, uv, ir, pmr*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HNG700

3-Hydroxy-1-(4-hydroxyphenyl)-1-propanone, 9CI H-510

[53170-93-7]

*3,4′-Dihydroxypropiophenone. 4-(3-Hydroxypropionyl)phenol. 2-(*p*-Hydroxybenzoyl)ethanol. 2-(Hydroxyethyl) 4-hydroxyphenyl ketone*



$C_9H_{10}O_3$ 166.176

Constit. of *Carissa edulis* (agam). Pale yellow prisms (Me_2CO). Mp 142-143°.

Dibenzoyl:

Cryst. (Me_2CO aq.). Mp 157°.

3-O-β-D-Glucopyranoside: [53170-92-6]

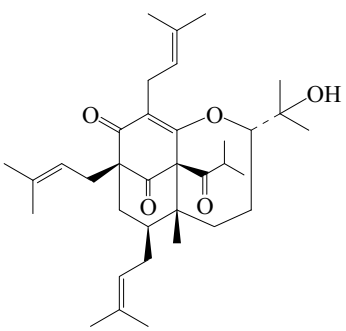
$C_{15}H_{20}O_8$ 328.318

Needles (MeOH). Mp 158-163°. $[\alpha]_D^{23}$ -20.4 (c, 1 in MeOH).

Zigeuner, G. *et al., Monatsh. Chem.*, 1949, **80**, 801 (*synth*)
Tschesche, R. *et al., Phytochemistry*, 1974, **13**, 518 (*isol, glucoside*)
Achenbach, H. *et al., Phytochemistry*, 1983, **22**, 749 (*isol*)
Tsai, W.Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 1991, **38**, 61 (*isol*)
Mori, K. *et al., Annalen*, 1992, 485 (*synth, pmr, cmr*)

8-Hydroxyhyperforin 8,1-hemiacetal H-511

[262857-89-6]



$C_{35}H_{52}O_5$ 552.793

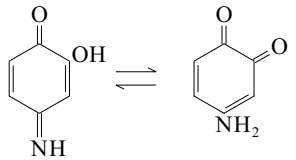
Constit. of *Hypericum perforatum* (St. John's Wort). Viscous oil. $[\alpha]_D^{20}$ +34 (c, 1 in $CHCl_3$). λ_{max} 270 (log ϵ 3.21); 380 (log ϵ 1.66) ($CHCl_3$).

Verotta, L. *et al., J. Nat. Prod.*, 2000, **63**, 412-415

2-Hydroxy-4-imino-2,5-cyclohexadienone H-512

[74331-93-4]

2-Hydroxy-1,4-benzoquinone-4-imine. 4-Amino-3,5-cyclohexadiene-1,2-dione. 490 Quinone



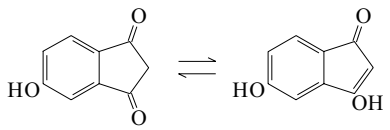
$C_6H_5NO_2$ 123.111

Unstable except at high dilutions. Prob. exists as 4-amino tautomer. Red pigment found in the sporulating gill tissue of the mushroom *Agaricus bisporus* (button mushroom). λ_{max} 490 (no solvent reported).

Bockelheide, K. *et al., J. Biol. Chem.*, 1980, **255**, 4766

5-Hydroxy-1,3-indanedione H-513

*3,5-Dihydroxy-1*H*-inden-1-one*



$C_9H_6O_3$ 162.145

Enol-*form*

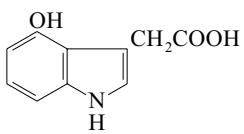
Di-Me ether: [149665-18-9] *3,5-Dimethoxy-1*H*-inden-1-one.* ***Coixinden A***

$C_{11}H_{10}O_3$ 190.198

Constit. of *Coix lacrima-jobi* var. *mayuen*. Cryst. Mp 183° dec.

Ishiguro, Y. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 866 (*isol*)

4-Hydroxy-1*H*-indole-3-acetic acid H-514



$C_{10}H_9NO_3$ 191.186

Nitrile: [118573-52-7] *4-Hydroxy-1*H*-indole-3-acetonitrile. 3-(Cyanomethyl)-4-hydroxyindole*

$C_{10}H_8N_2O$ 172.186

Present in rapeseed and in cooked *Brassica* vegetables as a glucosinolate dec. product. Formed from 4-Hydroxyindol-3-ylmethyl glucosinolate, H-517. Identified by ms.

Nitrile, O-*β-D-glucopyranoside:* [229483-41-4] ***Capparilloside A***

$C_{16}H_{18}N_2O_6$ 334.328

Constit. of the fruit of *Capparis spinosa* (caper). Amorph. $[\alpha]_D^{20}$ -58.8 (c, 0.4 in MeOH). λ_{max} 267 ; 278 ; 289 (MeOH).

Nitrile, O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [229483-42-5] ***Capparilloside B***

$C_{22}H_{28}N_2O_{11}$ 496.47

Constit. of the fruit of *Capparis spinosa* (caper). Amorph. $[\alpha]_D^{20}$ -23.7 (c, 0.3 in MeOH). λ_{max} 272 ; 279 ; 289 (MeOH).

Me ether, nitrile: [4837-74-5] *4-Methoxy-1*H*-indole-3-acetonitrile. 3-(Cyanomethyl)-4-methoxyindole*

$C_{11}H_{10}N_2O$ 186.213

Prisms ($CHCl_3$/hexane). Mp 145-146°.

Nomoto, M. *et al., Agric. Biol. Chem.*, 1970, **34**, 1590-1592 (*isol*)
Slominski, B.A. *et al., J. Chromatogr.*, 1988, **454**, 285-291 (*occur*)
Yamada, F. *et al., Heterocycles*, 1993, **36**, 2783-2804 (*synth*)
Calis, I. *et al., Phytochemistry*, 1999, **50**, 1205-1208 (*Capparilosides*)
Somei, M. *et al., Heterocycles*, 2000, **53**, 1573-1578 (*Capparilloside A, synth*)

6-Hydroxy-1*H*-indole-3-acetic acid H-515

[31031-05-7]

$C_{10}H_9NO_3$ 191.186

No phys. props. reported.

Amide: [192184-73-9] *6-Hydroxy-1*H*-indole-3-acetamide*

$C_{10}H_{10}N_2O_2$ 190.201

Alkaloid from the edible mushroom *Agrocybe cylindracea*. Powder. λ_{max} 224 (ϵ 9870); 274 (ϵ 1690); 295 (ϵ 2360) (MeOH).

Nitrile, O-*β-D-glucopyranoside:*

$C_{16}H_{18}N_2O_6$ 334.328

Mp 240-242°.

Me ether: [103986-22-7] *6-Methoxy-1*H*-indole-3-acetic acid*

$C_{11}H_{11}NO_3$ 205.213

Cryst. (H_2O). Mp 163-164° (dec.).

Me ether, nitrile: [23084-35-7] *6-Methoxy-1*H*-indole-3-acetonitrile. 3-(Cyanomethyl)-6-methoxyindole*

$C_{11}H_{10}N_2O$ 186.213

Needles (EtOH). Mp 113-114°.

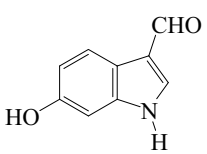
[116621-16-0]

Findlay, S.P. *et al., J.O.C.*, 1948, **13**, 560 (*deriv, synth*)
Toyota, M. *et al., J.C.S. Perkin 1*, 1992, 547-552 (*synth*)
Shinada, T. *et al., Tet. Lett.*, 1996, **37**, 7099-7102 (*synth*)
Kim, W.-G. *et al., J. Nat. Prod.*, 1997, **60**, 721 (*amide, isol, uv, ir, pmr, cmr, ms*)
Li, B. *et al., Yaoxue Xuebao*, 2000, **35**, 508-510 (*nitrile, glucoside*)

6-Hydroxy-1*H*-indole-3-carboxaldehyde H-516

[192184-71-7]

3-Formyl-6-hydroxyindole



$C_9H_7NO_2$ 161.16

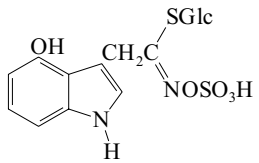
Alkaloid from the edible mushroom *Agrocybe cylindracea*. Powder. λ_{max} 220 (ϵ 3950); 235 (ϵ 3500); 276 (ϵ 2730); 300 (ϵ 1820) (MeOH).

Kim, W.G. *et al., J. Nat. Prod.*, 1997, **60**, 721-723 (*isol, uv, pmr, cmr, ms*)

4-Hydroxyindol-3-ylmethyl glucosinolate H-517

[83327-20-2]

1-Thio-β-D-glucopyranose 1-[4-hydroxy-N-(sulfooxy)-1H-indole-3-ethanimidate], 9CI. ***4-Hydroxyglucobrassicin***



$C_{16}H_{20}N_2O_{10}S_2$ 464.473

Formulated as the 5-hydroxy isomer by Goetz *et al*. λ_{max} 267, 284, 293 nm (MeOH). Readily oxidises in the presence of air and light.

Me ether: [83327-21-3] *4-Methoxyindol-3-ylmethyl glucosinolate.* ***4-Methoxyglucobrassicin***

$C_{17}H_{22}N_2O_{10}S_2$ 478.5

Gummy solid. λ_{max} 267, 282, 292 nm (MeOH).

[87592-99-2, 87593-00-8, 96828-26-1, 96828-27-2]

Truscott, R.J.W. *et al., Biochem. Biophys. Res. Commun.*, 1982, **107**, 1258; 1368 (*isol, struct*)

Truscott, R.J.W. *et al., J. Sci. Food Agric.*, 1983, **34**, 247 (*isol*)

Goetz, J.K. *et al., Phytochemistry*, 1983, **22**, 905 (*isol*)

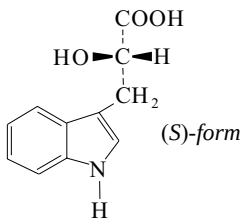
Hanley, A.P. *et al., Phytochemistry*, 1985, **24**, 598 (*isol, struct*)

2-Hydroxy-3-(3-indolyl)propanoic acid H-518

[1821-52-9]

[101312-07-6]

α-Hydroxy-1H-indole-3-propanoic acid, 9CI. 3-(3-Indolyl)lactic acid



(*S*)-*form*

$C_{11}H_{11}NO_3$ 205.213

(*S*)-*form* [7417-65-4]

Cryst. (Et_2O/petrol). Mp 100-101° (99°). $[\alpha]_D^{20}$ -5.36 (H_2O).

N-*Me:α-Hydroxy-1-methyl-1H-indole-3-propanoic acid. 2-Hydroxy-3-(1-methylindolyl)propanoic acid*

$C_{12}H_{13}NO_3$ 219.24

Constit. of the skins of peanuts (*Arachis hypogaea*). Needles (MeOH). Mp 216° dec. $[\alpha]_D^{25}$ +32.2 (c, 0.13 in MeOH).

Me ether:α-Methoxy-1H-indole-3-propanoic acid. 2-Methoxy-3-(3-indolyl)propanoic acid

$C_{12}H_{13}NO_3$ 219.24

Constit. of the skins of peanuts (*Arachis hypogaea*). Needles (MeOH). Mp 252° dec. $[\alpha]_D^{25}$ +22.2 (c, 0.1 in MeOH).

(±)-*form* [832-97-3]

Mp 144-145°.

(ξ)-*form*

Et ester, O-*β-D-glucopyranoside:* [143884-93-9]

$C_{19}H_{25}NO_8$ 395.408

Isol. from grapes (Riesling wine).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 669B (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 140C (*nmr*)

Ehrlich, F. *et al., Ber.*, 1911, **44**, 888

Bauguess, L.C. *et al., J. Biol. Chem.*, 1934, **104**, 679

Ratusky, J. *et al., Chem. Listy*, 1957, **51**, 109; *CA*, **51**, 13843 (*synth*)

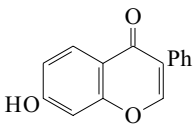
Marinos, V.A. *et al., Phytochemistry*, 1992, **31**, 2755-2759; 4399 (*isol*)

Lou, H. *et al., Planta Med.*, 2001, **67**, 345-349 (*N-Me, Me ether*)

7-Hydroxyisoflavone, 8CI H-519

[13057-72-2]

7-Hydroxy-3-phenyl-4H-1-benzopyran-4-one, 9CI



$C_{15}H_{10}O_3$ 238.242

Leaflets (EtOH). Mp 215° (209-210°).

H_2SO_4 → sky-blue fluor..

▶ DJ3100255Launched 1989

Isopropyl ether: [35212-22-7] *7-Isopropoxyisoflavone.* ***Ipriflavone, INN****. Osten. Yambolap. FL113*

$C_{18}H_{16}O_3$ 280.323

Feed additive, catabolic agent. Cryst. (Me_2CO). Mp 115-117°.

▶ DJ3100500

Ger. Pat., 1971, 2 125 245; *CA*, **76**, 72407e (*Ipriflavone*)

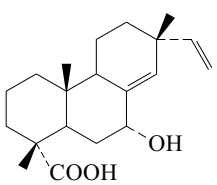
Feuer, L. *et al., Arzneim.-Forsch.*, 1981, **31**, 953-958 (*Ipriflavone, pharmacol*)

Yamazaki, I. *et al., Life Sci.*, 1986, **38**, 951-958 (*Ipriflavone, pharmacol*)

Böcskei, Z. *et al., Acta Cryst. C*, 1996, **52**, 1022-1024 (*Ipriflavone, cryst struct*)

Varga, M. *et al., Eur. J. Org. Chem.*, 2001, 3911-3920 (*Ipriflavone, props*)

7-Hydroxy-8(14),15-isopimaradien-18-oic acid H-520



$C_{20}H_{30}O_3$ 318.455

7α-*form*

Constit. of *Juniperus communis* (juniper). Oil (as Me ester). $[\alpha]_D$ -41 (c, 0.84 in $CHCl_3$) (Me ester).

Ac:

$C_{22}H_{32}O_4$ 360.492

Cryst. Mp 160-163°. $[\alpha]_D^{20}$ -11.29 (c, 0.177 in $CHCl_3$).

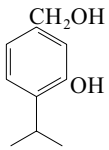
De Pasacual, J. *et al., Phytochemistry*, 1980, **19**, 1153 (*isol*)

Esquivel, B. *et al., Planta Med.*, 1989, **55**, 62 (*isol, pmr, cmr*)

3-Hydroxy-4-isopropylbenzyl alcohol, 8CI H-521

[77311-68-3]

3-Hydroxy-4-(1-methylethyl)benzenemethanol, 9CI. 5-(Hydroxymethyl)-2-isopropylphenol. p-*Mentha-1,3,5-triene-3,7-diol.* p-*Cymene-3,7-diol. 7-Hydroxythymol*



$C_{10}H_{14}O_2$ 166.219

3-O-β-D-Glucopyranoside: [359875-75-5]

$C_{16}H_{24}O_7$ 328.361

Constit. of fruit of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{25}$ -60 (c, 1.9 in MeOH).

Bis(2-methylpropanoyl):

$C_{18}H_{26}O_4$ 306.401

Oil. $Bp_{0.005}$ 120°.

3-Me ether: [66498-33-7] *4-Isopropyl-3-methoxybenzyl alcohol. 3-Methoxy-4-(1-methylethyl)benzenemethanol, 9CI. 3-Methoxy-*p*-cymen-7-ol, 8CI. 3-Methoxy-*p*-mentha-1,3,5-trien-7-ol*

$C_{11}H_{16}O_2$ 180.246

Oil. $Bp_{0.5}$ 94°.

3-Me ether, 7-O-(2-methylpropanoyl): [33280-65-8]

$C_{15}H_{22}O_3$ 250.337

Oil.

3-Me ether, 7-O-(3-methylbutanoyl): [33280-66-9]

$C_{16}H_{24}O_3$ 264.364

Oil.

Bohlmann, F. *et al., Chem. Ber.*, 1969, **102**, 864

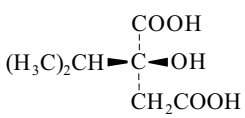
Shtacher, G. *et al., Tetrahedron*, 1971, **27**, 1343 (*derivs*)

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*3-glucoside*)

2-Hydroxy-2-isopropylbutanedioic acid H-522

[3237-44-3]

2-Hydroxy-2-(1-methylethyl)butanedioic acid, 9CI. 2-Isopropylmalic acid, 8CI. 2-Hydroxy-2-isopropylsuccinic acid. β-Carboxy-β-hydroxyisocaproic acid



(*S*)-*form*

$C_7H_{12}O_5$ 176.169

Conflicting assignments of abs. config. Cryst. struct. determination gives (*S*) for the natural (-)-form but other work gives (*R*).

(-)-*form* [49601-06-1]

Prod. by various bacteria and yeast, and from sweet corn (*Zea mays*). Mp 171-173°. $[\alpha]_D^{20}$ -20 (c, 2.5 in MeOH).

Bis(4-β-D-glucopyranosyloxybenzyl) ester: [90139-13-2]
$C_{33}H_{44}O_{17}$ 712.7
Amorph. powder (MeOH/$CHCl_3$). Mp 109-111°. $[\alpha]_D^{20}$ -44.2 (c, 1.27 in MeOH).

(±)-*form* [123164-17-0]
Cryst. (EtOAc/petrol). Mp 145-147°. Bp_{10} 118-120°.

Bis(4-O-β-D-glucopyranosyloxybenzyl) ester:
$C_{33}H_{44}O_{17}$ 712.7

1-Amide:2-Hydroxy-2-isopropylsuccinamic acid
$C_7H_{13}NO_4$ 175.184
Cryst. (EtOAc). Mp 156-157°.

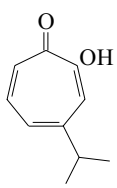
Diamide:2-Hydroxy-2-isopropylsuccinamide
$C_7H_{14}N_2O_3$ 174.199
Cryst. (H_2O). Mp 195-197°.

[43119-99-9, 49601-06-1]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **1**, 812A (*nmr*)
Yamashita, M. *et al., J.O.C.*, 1958, **23**, 835 (*synth, derivs*)
Calvo, J.M. *et al., Biochemistry*, 1962, **1**, 1157 (*synth, props*)
Martin, W.R. *et al., Biochim. Biophys. Acta*, 1962, **62**, 165 (*isol, synth, resoln*)
Sai, T. *et al., Agric. Biol. Chem.*, 1968, **32**, 522 (*isol*)
Cole, F.E. *et al., Biochemistry*, 1973, **12**, 3346 (*abs config, cryst struct*)
Brandange, S. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 153 (*abs config*)
Edgar, J.A. *et al., Tet. Lett.*, 1980, **21**, 2657 (*synth*)
Schloss, J.V. *et al., Methods Enzymol.*, 1988, **166**, 92 (*synth*)
Yi-Ming, L. *et al., Planta Med.*, 1993, **59**, 363 (*isol, ester*)
Li, Y.M. *et al., Yaoxue Xuebao*, 1993, **28**, 766 (*glucosyloxybenzyl ester*)

2-Hydroxy-4(6)-isopropyl-2,4,6-cycloheptatrien-1-one H-523

[499-44-5]
2-Hydroxy-4(6)-(1-methylethyl)-2,4,6-cycloheptatrien-1-one, 9CI. 4(6)-Isopropyltropolone. ***β-Thujaplicin****. Hinokitiol*



$C_{10}H_{12}O_2$ 164.204
Tautomeric with the 2-oxo-1-hydroxy struct. (equivalent to 6-isopropyl). Occurs in *Juniperus communis* (juniper). Cryst. (petrol). Mp 52-52.5°. pK_{a1} 6.72 (25°, I 2.0).
► LD_{50} (mus, ipr) 85 mg/kg. GU4200000

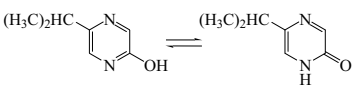
Cu complex:
Mp 177°.

*1-O-β-D-Glucopyranoside:****Cupressotropolone A***
$C_{16}H_{22}O_7$ 326.346Derived from the 2-oxo tautomer
λ_{max} 240 ; 330 (MeOH) (Berdy).

Anderson, A.B. *et al., Acta Chem. Scand.*, 1948, **2**, 644 (*isol, struct*)
Tanaka, K. *et al., Tetrahedron*, 1971, **27**, 4889 (*synth*)
Derry, J.E. *et al., J.C.S. Perkin 2*, 1972, 694 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 573 (*occur*)
Noyori, R. *et al., J.O.C.*, 1975, **40**, 806 (*synth*)
Tamura, Y. *et al., Tet. Lett.*, 1977, 4075 (*synth*)
Neumann, M. *et al., Tet. Lett.*, 1978, 5033 (*synth*)
Miyashita, M. *et al., J.O.C.*, 1987, **52**, 2602 (*synth*)
Banwell, M.G. *et al., Aust. J. Chem.*, 1991, **44**, 705 (*synth*)
Ohishi, H. *et al., Acta Cryst. C*, 1994, **50**, 587 (*cryst struct, bibl*)
Madar, Z. *et al., Phytochemistry*, 1995, **38**, 351 (*Cupressotropolone A*)
Ono, M. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1653-1659 (*prodn*)
Yoshihiko, I. *et al., Biol. Pharm. Bull.*, 1999, **22**, 990-993 (*activity*)
Yamaguchi, T. *et al., J. Wood Sci.*, 1999, **45**, 170-173; *CA*, **131**, 127604 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IRR000

2-Hydroxy-5-isopropylpyrazine H-524

5-(1-Methylethyl)-2(1H)-pyrazinone. 5-Isopropyl-2-pyrazinol



$C_7H_{10}N_2O$ 138.169

OH-form

Me ether:

[56891-99-7, 68039-46-3] *2-Isopropyl-5-methoxypyrazine*
$C_8H_{12}N_2O$ 152.196
Flavouring ingredient. Reported in asparagus, cabbage, peas, carrot, cucumber, lettuce, onion, potato, bell pepper, ginger, white wine, coffee, peanut, beans, beetroot, parsnip and dill. Component of FEMA 3358 together with its regioisomers. See also H-526. Not characterised except as isomeric mixt.

Stofberg, J. *et al., Perfum. Flavor.*, 1984, **9**, 53-56; 58-59; 62; 65-72; 76-83 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1052-1053 (*use, occur*)

2-Hydroxy-6-isopropylpyrazine H-525

6-(1-Methylethyl)-2(1H)-pyrazinone. 6-Isopropyl-2-pyrazinol
$C_7H_{10}N_2O$ 138.169

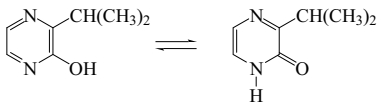
OH-form

Me ether:2-Isopropyl-6-methoxypyrazine
$C_8H_{12}N_2O$ 152.196
Flavouring ingredient. Reported in asparagus, cabbage, peas, carrot, cucumber, lettuce, onion, potato, bell pepper, ginger, white wine, coffee, peanut, beans, beetroot, parsnip and dill. Component of FEMA 3358 together with its regioisomers. Not characterised except as isomeric mixt..

Stofberg, J. *et al., Perfum. Flavor.*, 1984, **9**, 53-56; 58-59; 62; 65-72; 76-83 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1052-1053 (*occur, use*)

3-Hydroxy-2-isopropylpyrazine H-526

2-Hydroxy-3-(1-methylethyl)pyrazine, 9CI. 3-(1-Methylethyl)-2(1H)-pyrazinone



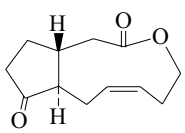
$C_7H_{10}N_2O$ 138.169

OH-form

Me ether: [25773-40-4] *2-Isopropyl-3-methoxypyrazine*
$C_8H_{12}N_2O$ 152.196
Occurs in petitgrain and galbanum oil. Perfumery and flavouring ingredient. Associated with musty/earthy aromas of marine fish, cheeses, drinking water and a wide range of vegetables. Component of FEMA 3358.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 842B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **3**, 404B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1560C (*ir*)
Parliment, T.H. *et al., J. Agric. Food Chem.*, 1972, **20**, 682-684 (*struct*)
Bramwell, A.F. *et al., J.C.S. Perkin 1*, 1972, 2004-2007 (*synth*)
Bramwell, A.F. *et al., Tetrahedron*, 1973, **29**, 3939-3942 (*pmr*)
Calabretta, P.J. *et al., Cosmet. Perfum.*, 1975, **90**, 74; 76; 79-80; *CA*, **83**, 183292c (*synth, props*)
Murray, K.E. *et al., J. Sci. Food Agric.*, 1975, **26**, 973-986; *CA*, **84**, 29266u (*occur*)
Gerber, N.N. *et al., Dev. Ind. Microbiol.*, 1978, **20**, 225-238; *CA*, **91**, 206932t (*isol, rev*)
Karahadian, C. *et al., J. Agric. Food Chem.*, 1985, **33**, 339-343 (*isol*)
McInver, R.C. *et al., ACS Symp. Ser.*, 1986, **317**, 266 (*isol*)
Maga, J.A. *et al., Food Res. Int.*, 1987, **3**, 269-284 (*occur, rev*)
Arnoldi, A. *et al., Heterocycles*, 1988, **27**, 2875-2882 (*ms*)
Leete, E. *et al., Spec. Publ. - R. Soc. Chem.*, 1992, **95**, 75 (*rev, biosynth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1052-1053 (*FEMA 3358*)

5′-Hydroxyjasmonic acid lactone H-527

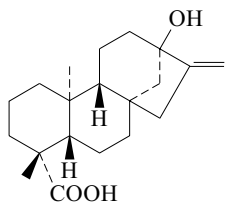


$C_{12}H_{16}O_3$ 208.257

Constit. of *Jasminum grandiflorum* (royal jasmine). Cryst. Mp 104°. $[\alpha]_D^{20}$ -260 (c, 3 in EtOH).

Demole, E. *et al., Helv. Chim. Acta*, 1964, **47**, 1152

13-Hydroxy-16-kauren-19-oic acid H-528



$C_{20}H_{30}O_3$ 318.455

***ent*-form** [471-80-7]
Steviol
Isol. from *Cucurbita maxima*. Cryst. (MeOH). Mp 215°. $[\alpha]_D$ -94.7 (EtOH).

▶ NZ8176000

13-O-*β*-D-*Glucopyranoside:* ***13*-O-*Glucosyl-steviol***
$C_{26}H_{40}O_8$ 480.597Sweet taste.

13-O-*β*-D-*Glucopyranoside, β*-D-*glucopyranosyl ester:* [64849-39-4] ***Rubusoside***
$C_{32}H_{50}O_{13}$ 642.739
Prisms (MeOH aq.). Mp 178-181°. $[\alpha]_D^{18}$ -40.3 (c, 0.8 in MeOH). Sweet taste.

13-O-*β*-D-*Glucopyranoside, 19*-O-*[3,4-dihydroxycinnamoyl-(→6)-β*-D-*glucopyranosyl] ester:* [142543-25-7] ***Suavioside D_2***
$C_{41}H_{56}O_{16}$ 804.884
Amorph. powder. $[\alpha]_D^{25}$ -43.4 (c, 0.5 in MeOH). Bitter taste.

13-O-*[4-Hydroxycinnamoyl-(→6)-β*-D-*glucopyranoside], β*-D-*glucopyranosyl ester:* [142543-23-5] ***Suavioside C_1***
$C_{41}H_{56}O_{15}$ 788.884
Amorph. powder. $[\alpha]_D^{25}$ -47.4 (c, 0.39 in MeOH). Bitter taste.

13-O-*[3,4-Dihydroxycinnamoyl-(→6)-β*-D-*glucopyranoside], β*-D-*glucopyranosyl ester:* [142543-24-6] ***Suavioside D_1***
$C_{41}H_{56}O_{16}$ 804.884
Amorph. powder. $[\alpha]_D^{25}$ -46.5 (c, 1.03 in MeOH). Tasteless.

13-O-*[β*-D-*Glucopyranosyl-(1→2)-α*-D-*glycopyranoside], β*-D-*glucopyranosyl ester:* [57817-89-7] ***Stevioside***. *Eupatorin*†. *Rebaudin*. *Stevin*†. *Steviosin*
$C_{38}H_{60}O_{18}$ 804.881
Constit. of *Stevia rebaudiana* (stevia). Sweetening agent which is 300 times sweeter than sucrose. *Stevia rebaudiana* is extensively cultivated in Japan, and Stevioside is a permitted sweetener in that country. Cryst. (dioxan/MeOH). Mp 238-239°. $[\alpha]_D$ -39.3 (c, 5.7 in H_2O). Log P -3.12 (uncertain value) (calc).

▶ NZ8175000

13-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [41093-60-1] ***Steviobioside***
$C_{32}H_{50}O_{13}$ 642.739
Present in *Stevia rebaudiana* (stevia) extracts.

13-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], [β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranosyl] ester:* [63279-14-1] ***Rebaudioside E***
$C_{44}H_{70}O_{23}$ 967.023
Constit. of *Stevia rebaudiana* (stevia). Cryst. (MeOH). Mp 205-207°. $[\alpha]_D^{25}$ -34.2 (MeOH).

13-O-*[α*-L-*Rhamnopyranosyl-(1→2)-β*-D-*glucopyranoside], β*-D-*glucopyranosyl ester:* [64432-06-0] ***Dulcoside A***
$C_{38}H_{60}O_{17}$ 788.882
Present in *Stevia rebaudiana* (stevia) extracts. Cryst. + $2H_2O$ (MeOH). Mp 193-195°. $[\alpha]_D$ -46.7 (c, 0.45 in MeOH). Sweet taste.

13-O-*[β*-D-*Glucopyranosyl-(1→2)-[β*-D-*glucopyranosyl-(1→3)]-β*-D-*glucopyranoside], [β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranosyl] ester:* [63279-13-0] ***Rebaudioside D***
$C_{50}H_{80}O_{28}$ 1129.165
Constit. of *Stevia rebaudiana* (stevia). Cryst. (EtOH). Mp 283-286°. $[\alpha]_D^{25}$ -22.7 (MeOH).

13-O-*[β*-D-*Glucopyranosyl-(1→2)-[β*-D-*glucopyranosyl-(1→3)]-β*-D-*glucopyranoside]:* [58543-17-2] ***Rebaudioside B***. *Stevioside A_4*
$C_{38}H_{60}O_{18}$ 804.881
Constit. of *Stevia rebaudiana* (stevia). Cryst. Mp 193-195°. $[\alpha]_D^{24}$ -45.4 (MeOH).

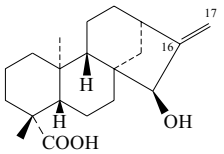
13-O-*[β*-D-*Glucopyranosyl-(1→2)-[β*-D-*glucopyranosyl-(1→3)]-β*-D-*glucopyranoside], β*-D-*glucopyranosyl ester:* [58543-16-1] ***Rebaudioside A***. *Stevioside A_3*
$C_{44}H_{70}O_{23}$ 967.023
Constit. of *Stevia rebaudiana* (stevia). Cryst. Mp 242-244°. $[\alpha]_D^{24}$ -20.8 (MeOH).

13-O-*[α*-L-*Rhamnopyranosyl-(1→2)-[β*-D-*glucopyranosyl-(1→3)]-β*-glucopyranoside], β*-D-*glucopyranosyl ester:* [63550-99-2] ***Rebaudioside C***. *Dulcoside B*
$C_{44}H_{70}O_{22}$ 951.024
Constit. of *Stevia rebaudiana* (stevia). Cryst. Mp 215-217°. $[\alpha]_D^{25}$ -29.9 (MeOH).

[77-05-4, 29584-19-8]

Cook, I.F. *et al., Tet. Lett.*, 1970, 4091-4093 (*synth*)
Mori, K. *et al., Tetrahedron*, 1972, **28**, 3217-3226 (*synth*)
Kohda, H. *et al., Phytochemistry*, 1976, **15**, 981-983 (*Stevioside, Rebaudioside A, Rehbaudioside B, Steviobioside*)
Yamasaki, K. *et al., Tet. Lett.*, 1976, 1005-1008 (*cmr*)
Sakamoto, I. *et al., Chem. Pharm. Bull.*, 1977, **25**, 3437-3439 (*Rebaudiosides*)
Kobayashi, M. *et al., Phytochemistry*, 1977, **16**, 1405-1408 (*Dulcosides*)
Ziegler, F.E. *et al., Tetrahedron*, 1977, **33**, 373-380 (*synth*)
Ogawa, T. *et al., Tetrahedron*, 1980, **36**, 2641-2648 (*Stevioside*)
Tanaka, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 2165-2166 (*Rubusoside*)
DuBois, G.E. *et al., J. Med. Chem.*, 1981, **24**, 1269-1271 (*use*)
Crammer, B. *et al., Chem. Br.*, 1986, **22**, 915-918 (*rev*)
Ohtani, K. *et al., Phytochemistry*, 1992, **31**, 1553-1559 (*Suaviosides*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1049
Hanson, J.R. *et al., Nat. Prod. Rep.*, 1993, **10**, 301-309 (*rev, Stevioside*)
Subrahmanyan, C. *et al., Phytochemistry*, 1999, **51**, 83-90 (*Steviol, cmr*)
Totté, N. *et al., Tet. Lett.*, 2000, **41**, 6407-6410 (*biosynth*)

15-Hydroxy-16-kauren-19-oic acid H-529



(*ent*-15α)-*form*

$C_{20}H_{30}O_3$ 318.455

(*ent*-15α)-*form* [6619-95-0]
Cryst. (MeOH aq.). Sol. MeOH, C_6H_6, bases; poorly sol. H_2O, acids. Mp 209-210°. $[\alpha]_D^{20}$ -107 (c, 1.1 in EtOH).

β-D-*Glucopyranosyl ester:* [60129-63-7] ***Paniculoside I***
$C_{26}H_{40}O_8$ 480.597
Cryst. (MeOH aq.). Mp 134-136°. $[\alpha]_D^{23}$ -69.9 (c, 0.21 in MeOH).

β-D-*Allopyranosyl ester:* [125107-42-8]
$C_{26}H_{40}O_8$ 480.597

15-O-*α*-L-*Arabinopyranoside:* [147103-78-4] ***Rufusoside A***
$C_{25}H_{38}O_7$ 450.571
Prisms (MeOH). Mp 157-158°. $[\alpha]_D^{18}$ -84.2 (c, 1 in MeOH).

15-O-*α*-L-*Arabinopyranoside, β*-D-*glucopyranosyl ester:* [147103-79-5] ***Rufusoside B***
$C_{31}H_{48}O_{12}$ 612.713
Needles (MeOH). Mp 180-182°. $[\alpha]_D^{18}$ -75.5 (c, 1 in MeOH).

O-*β*-D-*Glucopyranoside, β*-D-*glucopyranosyl ester:* [65606-29-3] ***Paniculoside V***. *Crispioside A*
$C_{32}H_{50}O_{13}$ 642.739
Cryst. (C_6H_6/EtOAc). Mp 170-172.5°. $[\alpha]_D^{23}$ +61 (c, 0.2 in MeOH).

Glycoside: [66139-42-2] ***Doronicoside D***
$C_{42}H_{66}O_{21}$ 906.971
Cryst. (MeOH aq.). Mp 110-118°. $[\alpha]_D$ -36.3 (c, 1.129 in MeOH). Contains D-Xyl, L-Ara and 2 D-Mann.

Ac: [6619-97-2] ***Xylopic acid***
$C_{22}H_{32}O_4$ 360.492
Cryst. (EtOAc). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 259-260°. $[\alpha]_D$ -144 (c, 1.2 in $CHCl_3$).

Angeloyl: [77399-93-0]
$C_{25}H_{36}O_4$ 400.557
Gum. Sol. MeOH, bases, C_6H_6; poorly sol. H_2O, hexane. Not obt. pure.

Tigloyl: [77399-94-1]
$C_{25}H_{36}O_4$ 400.557
Gum. Not obt. pure.

3-Methyl-2-butenoyl: [77355-68-1]
$C_{25}H_{36}O_4$ 400.557
Gum. Not obt. pure.

16ξ,17-Epoxide, 15-tigloyl: [79435-56-6]

$C_{25}H_{36}O_5$ 416.556
Gum (as Me ester). $[\alpha]_D^{24}$ -49.3 (c, 0.8 in $CHCl_3$) (Me ester).

15-Ketone, 19-alcohol, 19-Ac: [250353-18-5]
$C_{22}H_{32}O_3$ 344.493
$[\alpha]_D^{20}$ -76 ($CHCl_3$).

15-Ketone, 19-aldehyde: [250353-19-6] ***15-Oxo-16-kauren-19-al***
$C_{20}H_{28}O_2$ 300.44
$[\alpha]_D^{20}$ -98 ($CHCl_3$).

(*ent*-15β)-*form* [22338-69-8] ***Grandiflorolic acid***
Constit. of *Aralia cordata* (udo). Cryst. Mp 216-218°.

Ac: [22343-40-4]
$C_{22}H_{32}O_4$ 360.492
Cryst. Mp 173-174°. $[\alpha]_D^{20}$ -84.9.

2-Methylpropanoyl: [67664-91-9]
$C_{24}H_{36}O_4$ 388.546

2-Methylbutanoyl: [90041-98-8]
$C_{25}H_{38}O_4$ 402.573
Not obt. pure.

3-Methylbutanoyl: [32381-02-5]
$C_{25}H_{38}O_4$ 402.573
Cryst. Mp 169-170°. $[\alpha]_D$ -74.5 ($CHCl_3$).

2-Methylpropenoyl: [78853-03-9]
$C_{24}H_{34}O_4$ 386.53
Gum (as Me ester). $[\alpha]_D^{24}$ -60.3 (c, 1.7 in $CHCl_3$) (Me ester).

Angeloyl: [32381-03-6]
$C_{25}H_{36}O_4$ 400.557
Cryst. Mp 193-195°.

Tigloyl: [53586-31-5]
$C_{25}H_{36}O_4$ 400.557

3-Methyl-2-butenoyl: [53586-30-4]
$C_{25}H_{36}O_4$ 400.557

Cinnamoyl: [65513-87-3] ***Cinnamoylgrandifloric acid***
$C_{29}H_{36}O_4$ 448.601
Cryst. (hexane). Mp 211-213°. $[\alpha]_D^{22}$ +70.

Benzoyl: [67664-92-0]
$C_{27}H_{34}O_4$ 422.563
Oil (as Me ester).

2,3-Epoxy-2-methylbutanoyl: [88664-25-9] ***Epoxyangeloxygrandifloric acid***
$C_{25}H_{36}O_5$ 416.556
Gum (as Me ester).

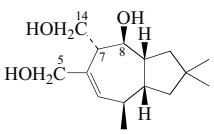
2,3-Dihydroxy-2-methylbutanoyl: [93888-83-6]
$C_{25}H_{38}O_6$ 434.572

16α,17-Epoxide, 15-angeloyl: [63898-23-7] ***Perymenic acid***
$C_{25}H_{36}O_5$ 416.556
Oil (as Me ester). Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. $[\alpha]_D^{24}$ -54 (c, 1.28 in $CHCl_3$) (Me ester).

15-Ketone: [6620-00-4] **ent-*15-Oxo-16-kauren-19-oic acid***
$C_{20}H_{28}O_3$ 316.439
Isol. from *Chrysobalanus icaco*. Tablets (C_6H_6/hexane). Mp 211-213°. $[\alpha]_D^{20}$ -169 (c, 1.19 in MeOH). Log P 3.71 (uncertain value) (calc).

Cannon, J.R. *et al., Aust. J. Chem.*, 1966, **19**, 861
Ekong, D.E.U. *et al., J.C.S.(C)*, 1968, 311 (*derivs*)
Brieskorn, C.H. *et al., Chem. Ber.*, 1969, **102**, 2621 (*struct*)
Pakrashi, S.C. *et al., Indian J. Chem.*, 1971, **9**, 84 (*isol*)
Yamasaki, K. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2895 (*Paniculosides*)
Alieva, Sh.A. *et al., Khim. Prir. Soedin.*, 1977, **13**, 658; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 546 (*Doronicoside D*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 786; 1978, **17**, 483; 1980, **19**, 2655; 1981, **20**, 522; 751 (*derivs*)
Vichnewski, W. *et al., Phytochemistry*, 1977, **16**, 2028 (*Cinnamoylgrandifloric acid*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1957-1960 (*Cinnamoylgrandifloric acid, pmr*)
Panizo, F.M. *et al., An. Quim.*, 1979, **75**, 428 (*isol*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 657 (*15-Oxo-16-kauren-19-oic acid*)
Herz, W. *et al., Phytochemistry*, 1983, **22**, 2021 (*Epoxyangeloxygrandifloric acid*)
Hutchison, M. *et al., J.C.S. Perkin 1*, 1984, 2363 (*cmr*)
Zdero, C. *et al., Phytochemistry*, 1989, **28**, 2745 (*allosyl ester*)
Abdel-Mogib, M. *et al., Phytochemistry*, 1990, **29**, 2581
Gustafson, K.R. *et al., Tetrahedron*, 1991, **47**, 4547 (*15-Oxo-16-kauren-19-oic acid*)
Cheng, D.-L. *et al., Phytochemistry*, 1993, **32**, 151-153 (*Rufusosides*)
Barrero, A.F. *et al., Fitoterapia*, 1998, **69**, 83-84 (*pmr, cmr*)
Flegel, M. *et al., Z. Naturforsch., C*, 1999, **54**, 481-487 (*Blepharidophyllum densifolium isolates*)
Velikova, M. *et al., Fitoterapia*, 2000, **71**, 693-696 (*3-methylbutanoyl, pmr, cmr*)

8-Hydroxy-4(6)-lactarene-5,14-diol H-530



(3β,7α,8β)-*form*

$C_{15}H_{26}O_3$ 254.369
Constit. of *Lactarius piperatus*. λ_{max} 232 (ϵ 9300) (EtOH) (Berdy).

(3β,7α,8β)-*form*

5-Aldehyde: [124673-24-1] ***7-Epipiperalol***
$C_{15}H_{24}O_3$ 252.353
Oil. $[\alpha]_D^{24}$ -62 (c, 2 in $CHCl_3$). λ_{max} 231 (log ϵ 3.67) (EtOH).

(3β,7β,8β)-*form* [118918-26-6] ***8-Epipipertriol***
Cryst. Mp 108-114°. $[\alpha]_D^{20}$ -36.6 (c, 1 in $CHCl_3$).

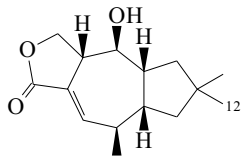
5-Aldehyde: [100288-35-5] *8,14-Dihydroxy-4(6)-lactaren-5-al.* ***Piperalol***
$C_{15}H_{24}O_3$ 252.353
Constit. of *Lactarius piperatus*. Pungent oil. $[\alpha]_D^{23}$ +57 (c, 4.3 in Et_2O). λ_{max} 238 (ϵ 9400) (EtOH) (Berdy).

5,14-Dialdehyde: [100288-36-6] *8-Hydroxy-4(6)-lactarene-5,14-dial.* ***Piperdial***
$C_{15}H_{22}O_3$ 250.337
Constit. of *Lactarius piperatus*. Pungent oil. $[\alpha]_D^{23}$ +77 (c, 0.8 in Et_2O).

Sterner, O. *et al., Tet. Lett.*, 1985, **26**, 3163 (*Piperdial, Piperalol*)
Daniewski, W.M. *et al., Phytochemistry*, 1988, **27**, 3315 (*8-Epipipertriol*)
Sterner, O. *et al., Acta Chem. Scand.*, 1989, **43**, 694 (*7-Epipiperalol*)

8-Hydroxy-4(6)-lactaren-5,14-olide H-531

3a,4,4a,5,6,7,7a,8-Octahydro-4-hydroxy-6,6,8-trimethylazuleno[5.6-c]furan-1(3H)-one, 9CI



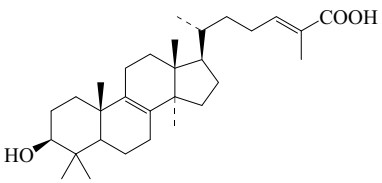
$C_{15}H_{22}O_3$ 250.337
λ_{max} 247 (MeOH) (Berdy).

(3β,7β*H*,8β)-*form* [62860-40-6] ***Blennin A***. *Lactarorufin N*
Constit. of *Lactarius blennius* (slimy milk cap). Oil. $[\alpha]_D^{20}$ +49.9 ($CHCl_3$).

12-Hydroxy: [72776-44-4] *8,12-Dihydroxy-4(6)-lactaren-5,14-olide.* ***12-Hydroxyblennin A***. *15-Hydroxyblennin A*
$C_{15}H_{22}O_4$ 266.336
Cryst. Mp 144°. Tentative stereochem. C-11 config. not detd..

Vidari, G. *et al., Phytochemistry*, 1976, **15**, 1953 (*isol*)
Widén, K.G. *et al., Phytochemistry*, 1979, **18**, 1226 (*12-Hydroxyblennin A*)
De Bernardi, M. *et al., Phytochemistry*, 1980, **19**, 99 (*isol*)
Daniewski, W.M. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1981, **55**, 1247 (*isol*)
Daniewski, W.M. *et al., Tetrahedron*, 1984, **40**, 2757 (*pmr, cmr, abs config*)

3-Hydroxylanosta-8,24-dien-26-oic acid H-532



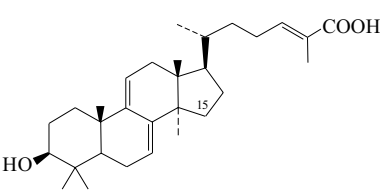
$C_{30}H_{48}O_3$ 456.707

(3β,24*E*)-*form* [86420-19-1] ***Ganoderic acid Z***
Isol. from *Ganoderma lucidum* (reishi). λ_{max} 215 (ϵ 12500) (MeOH).

Me ester:
Cryst. Mp 123-125°. $[\alpha]_D$ +56.

Toth, J.O. *et al., J. Chem. Res., Miniprint*, 1983, 2722 (*isol, pmr*)
Toth, J.O. *et al., Tet. Lett.*, 1983, **24**, 1081

3-Hydroxylanosta-7,9(11),24-trien-26-oic acid H-533



$C_{30}H_{46}O_3$ 454.692

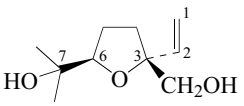
(3β,24*E*)-*form* [86377-52-8]

Ganoderic acid Y
Constit. of *Ganoderma lucidum* (reishi). Sol. EtOH. λ_{max} 222 ; 235 ; 244 ; 252 (EtOH) (Berdy).

Me ester:
Cryst. Mp 139-141°. $[\alpha]_D$ +53.

Toth, J.O. *et al., Tet. Lett.*, 1983, **24**, 1081

10-Hydroxylinalyl oxide H-534



(3*R**,6*R**)-*form*

$C_{10}H_{18}O_3$ 186.25

(3*R*,6*R*)-*form*
trans-*form*

7-O-*β*-D-*Glucopyranoside:* [219814-36-5]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{21}$ -13.8 (c, 0.9 in MeOH).

1,2-Dihydro, 1,2-dihydroxy, 7-O-*β*-D-*glucopyranoside:* [219814-37-6] ***1,2,10-Trihydroxydihydro*-trans-*linalyl oxide 7*-O-*β*-D-*glucopyranoside***
$C_{16}H_{30}O_{10}$ 382.407
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ +0.5 (c, 0.2 in MeOH).

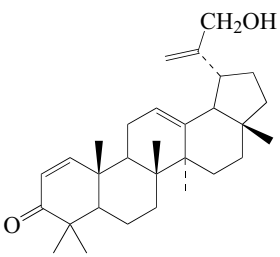
(3*R*,6*S*)-*form*
cis-*form*

7-O-*β*-D-*Glucopyranoside:* [219814-34-3]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{25}$ -3.5 (c, 0.2 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1748-1751 (*isol, pmr, cmr*)

30-Hydroxy-1,12,20(29)-lupatrien-3-one H-535

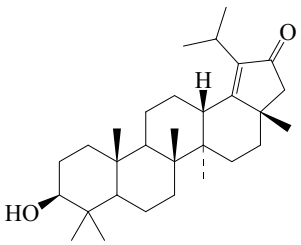
[152369-65-8]
Manglupenone



$C_{30}H_{44}O_2$ 436.676
Constit. of the stem bark of *Mangifera indica* var. Dusehri.

Sharma, S.K. *et al., Indian Drugs*, 1993, **30**, 446; *CA*, **120**, 73344w

3-Hydroxy-18-lupen-21-one H-536



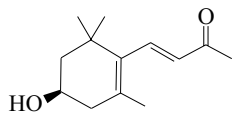
$C_{30}H_{48}O_2$ 440.708

3β-*form* [29367-66-6]
Constit. of *Taraxacum officinale* (dandelion).

Kisiel, W. *et al., Pol. J. Chem. (Rocz. Chem.)*, 2000, **74**, 281-283; *CA*, **132**, 191798t (*isol, pmr, cmr*)

3-Hydroxy-5,7-megastigmadien-9-one H-537

3-Hydroxy-β-ionone



$C_{13}H_{20}O_2$ 208.3

(3*R*,7*E*)-*form*
3-Hydroxy-β-ionone
Isol. from *Phaseolus vulgaris* (kidney bean). Oil. $[\alpha]_D^{22}$ -140.5 (c, 0.1 in $CHCl_3$). λ_{max} 221 ; 290 (EtOH).

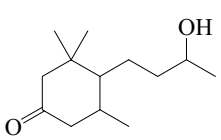
2-Methylpropanoyl: [37704-28-2] ***Quiesone***
$C_{17}H_{26}O_3$ 278.391
Oil. λ_{max} 220 ; 290 (MeOH) (Berdy).

7α,8α-Epoxide, 3-O-*β*-D-*glucopyranoside:* [108906-51-0] ***Icariside B₂***
$C_{19}H_{30}O_8$ 386.441
Needles (MeOH/EtOAc). Mp 172.5-174°. $[\alpha]_D^{25}$ -102.1 (c, 0.97 in MeOH).

Leppik, R.A. *et al., Phytochemistry*, 1972, **11**, 2055 (*isol*)
Mori, K. *et al., Agric. Biol. Chem.*, 1973, **37**, 2899 (*synth*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1109 (*Icariside B₂*)
Kato-Noguchi, H. *et al., Phytochemistry*, 1993, **33**, 553 (*isol, pmr, cmr*)
Suchy, V. *et al., Coll. Czech. Chem. Comm.*, 1995, **60**, 1380 (*Icariside B₂, pmr, cmr*)

9-Hydroxymegastigman-2-one H-538

[128660-70-8]
4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone

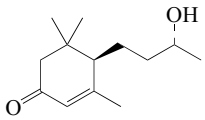


$C_{13}H_{24}O_2$ 212.331
Tentatively identified in oak used in wine and spirit maturation.

Sefton, M.A. *et al., J. Agric. Food Chem.*, 1990, **38**, 2045-2049

9-Hydroxy-4-megastigmen-3-one H-539

4-(3-Hydroxybutyl)-3,5,5-trimethyl-2-cyclohexenone



(6*R*,9*R*)-*form*

$C_{13}H_{22}O_2$ 210.316

(6*R*,9*R*)-*form* [36151-02-7]
Blumenol C
Gum. $[\alpha]_D$ +54 ($CHCl_3$). $[\alpha]_D^{22}$ +112.5 (c, 0.52 in $CHCl_3$).

O-*β*-D-*Glucopyranoside:* [62512-23-6] *Blumenol C glucoside*
$C_{19}H_{32}O_7$ 372.458
Isol. from wine grape *Vitis vinifera*. Amorph. powder. $[\alpha]_D^{22}$ +46.8 (c, 0.63 in MeOH). λ_{max} 240 (log ϵ 3.98) (MeOH).

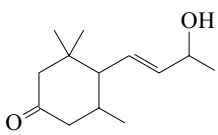
O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [177261-68-6]
$C_{24}H_{40}O_{11}$ 504.573
Constit. of quince (*Cydonia vulgaris*) leaves.

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [177261-67-5]
$C_{25}H_{42}O_{11}$ 518.6
Constit. of quince (*Cydonia vulgaris*) leaves.

Miyase, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2475-2484 (*Blumenol C glucoside*)
Roscher, R. *et al., J. Agric. Food Chem.*, 1993, **41**, 1452-1457 (*Blumenol glucoside*)
De Tommasi, N. *et al., J. Agric. Food Chem.*, 1996, **44**, 1676-1681 (*Cydonia glucosides*)

9-Hydroxy-7-megastigmen-3-one H-540

[52210-16-9]
4,5-Dihydro-3-oxo-α-ionone



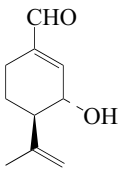
$C_{13}H_{22}O_2$ 210.316

O-*β*-D-*Glucopyranoside:*
$C_{19}H_{32}O_7$ 372.458
Isol. from wine grape *Vitis vinifera* Riesling leaves as a major vine leaf constit. Potential precursor of quince aroma volatiles (megastigma-6,8-dien-3-ones).

Sefton, M.A. *et al., J. Agric. Food Chem.*, 1990, **38**, 2045
Roscher, R. *et al., J. Agric. Food Chem.*, 1993, **41**, 1452

3-Hydroxy-*p*-mentha-1,8-dien-7-al H-541

[182937-26-4]

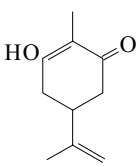


$C_{10}H_{14}O_2$ 166.219
Constit. of *Perilla frutescens* (perilla). Cryst. Mp 51-53°. $[\alpha]_D$ +120 (c, 0.064 in EtOH).

Tada, M. *et al., Phytochemistry*, 1996, **43**, 803-804 (*isol, pmr, cmr*)

2-Hydroxy-*p*-mentha-1,8-dien-6-one H-542

[51200-86-3]
3-Hydroxy-2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one. 6-Hydroxycarvone. p-*Menth-8-ene-2,6-dione*

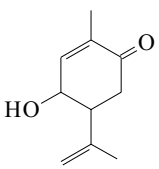


$C_{10}H_{14}O_2$ 166.219
Enolised β-diketone. Isol. from spearmint oil.

Tsuneya, T. *et al., Koryo*, 1973, 23 (*synth, isol*)

5-Hydroxy-*p*-mentha-6,8-dien-2-one H-543

[56423-48-4]
4-Hydroxy-2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one, 9CI

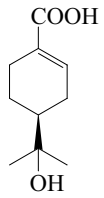


$C_{10}H_{14}O_2$ 166.219
Isol. from spearmint oil.

Canova, L. *et al., Ann. Acad. Bras. Ci&eenc.*, 1972, **44**, 273 (*isol*)

8-Hydroxy-*p*-menth-1-en-7-oic acid H-544

[76509-35-8]
4-(1-Hydroxy-1-methylethyl)-1-cyclohexene-1-carboxylic acid, 9CI. 4-(1-Hydroxyisopropyl)-1-cyclohexene-1-carboxylic acid. ***Oleuropeic acid***



(*S*)-*form*

$C_{10}H_{16}O_3$ 184.235

(*S*)-*form* [5027-76-9]
Aglycone from *Olea europaea* (olive). Cryst. Mp 162-165°. $[\alpha]_D^{28}$ -116.6 (c, 0.3 in MeOH).

β-D-Glucopyranos-1-yl ester:
$C_{16}H_{26}O_8$ 346.377

β-D-Glucopyranos-6-yl ester:
$C_{16}H_{26}O_8$ 346.377

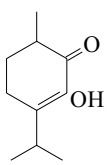
[3,4,5-Trihydroxybenzoyl-(→1)-β-D-glucopyranos-6-yl] ester: [241130-84-7] ***Eucaglobulin***
$C_{23}H_{30}O_{12}$ 498.483
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Amorph. light brown powder.

(±)-*form* [33746-68-8]
Cryst. (Et_2O/hexane). Mp 152-154°.

Panizzi, L. *et al., Gazz. Chim. Ital.*, 1965, **95**, 1279 (*struct*)
Drabdina, A.A. *et al., Zh. Obshch. Khim.*, 1971, **41**, 1412; *CA*, **75**, 88770h (*synth*)
Manns, D. *et al., Planta Med.*, 1994, **60**, 467 (*glycosyl ester, pmr, cmr*)
Hou, A.J. *et al., Chin. Chem. Lett.*, 1998, **9**, 541-543 (*Eucaglobulin*)

3-Hydroxy-*p*-menth-3-en-2-one H-545

[54783-36-7]
2-Hydroxy-6-methyl-3-(1-methylethyl)-2-cyclohexen-1-one, 9CI. ***ψ-Diosphenol****. Pseudodiosphenol*

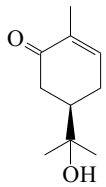


$C_{10}H_{16}O_2$ 168.235
Constit. of *Agathosma betulina* leaf oil (buchu). Cryst. (hexane). Mp 34.5°. Bp_5 93-98°.

Kaiser, R. *et al., J. Agric. Food Chem.*, 1975, **23**, 943 (*isol*)
Ohashi, M. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 2292 (*synth, ir, pmr*)
Utaka, M. *et al., Chem. Lett.*, 1980, 779-780 (*synth*)
Schneider, D.F. *et al., Synth. Commun.*, 2002, **32**, 1285-1292 (*synth, pmr, cmr*)
Schneider, D.F. *et al., Tetrahedron*, 2002, **58**, 5307-5315 (*synth*)

8-Hydroxy-*p*-menth-6-en-2-one H-546

[7712-46-1]
*5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one, 9CI. 8-Hydroxy-*p*-menth-1-en-6-one. Carvone hydrate. 8-Hydroxycarvotanacetone.* ***Aralone***



(*R*)-*form*

$C_{10}H_{16}O_2$ 168.235

(*R*)-*form* [34182-03-1]
Cryst. (Et_2O). Mp 42°. $[\alpha]_D^{25}$ -42 (EtOH).

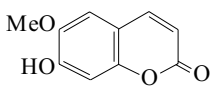
Ac: [56691-69-1]

[87578-93-6]
$C_{12}H_{18}O_3$ 210.272
Constit. of cardamom oil.

Ding, D. *et al., CA*, 1983, **99**, 43303n (*acetate, isol*)
Maurer, B. *et al., Chem. Ind. (London)*, 1988, 587-591 (*acetate, isol*)

7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, 9CI H-547

[92-61-5]
7-Hydroxy-6-methoxycoumarin. ***Scopoletin****. Aesculetin 6-methyl ether. Chrysatropic acid. Gelseminic acid. β-Methylaesculetin. Buxuletin. Escopoletin. Scopoletol. Baogongteng B*



$C_{10}H_8O_4$ 192.171
Isol. from *Angelica acutiloba* (Dong Dang Gui). Needles or prisms (EtOH). Sol. MeOH, C_6H_6. Mp 204°. Log P 1.33 (calc). Reduces Fehling's and Tollen's reagents λ_{max} 229 (ε 13800); 252 (ε 9120); 260 (sh) (ε 8710); 297 (ε 9550); 344 (ε 13500) (MeOH) (Derep). λ_{max} 230 ; 255 ; 295 ; 345 (MeOH) (Berdy). λ_{max} 228 (ε 23000); 254 (ε 7600); 297 (ε 8700); 345 (ε 20500) (EtOH) (Berdy).

▶ LD_{50} (rat, orl) 3800 mg/kg. GN6930000

Ac: [56795-51-8] *7-Acetoxy-6-methoxycoumarin*
$C_{12}H_{10}O_5$ 234.208
Constit. of *Sterculia urens* (karaya gum). Mp 177°.

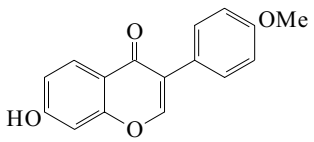
[13544-37-1, 73435-97-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 324B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1314B (*nmr*)
Seka, R. *et al., Ber.*, 1931, **64**, 909
Head, F.G.H. *et al., J.C.S.*, 1931, 1241 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1328; 1329 (*occur*)
González, A.G. *et al., An. Quim.*, 1973, **69**, 1013 (*pmr*)
Andrianova, V.B. *et al., Khim. Prir. Soedin.*, 1975, **11**, 89; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 91 (*Scopoletin, isol*)
Tanaka, S. *et al., Arzneim.-Forsch.*, 1977, **27**, 2039 (*isol*)
Herath, W.H.M. *et al., Phytochemistry*, 1978, **17**, 1007 (*isol*)
Ishibura, N. *et al., Z. Naturforsch., C*, 1979, **34**, 628

Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, (*occur, rev*)
Abu-Eittah, R.H. *et al., Can. J. Chem.*, 1985, **63**, 1173 (*uv*)
Koul, S.K. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 574 (*synth*)
Udovin, A.D. *et al., Khim. Prir. Soedin.*, 1987, **23**, 796; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 660 (*cmr*)
Wollenweber, E. *et al., Fitoterapia*, 1989, **60**, 460 (*isol, derivs*)
Mizuno, M. *et al., Phytochemistry*, 1992, **31**, 717 (*deriv*)
Hauer, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1995, **328**, 737 (*synth*)

7-Hydroxy-4′-methoxyisoflavone H-548

[485-72-3]
*7-Hydroxy-3-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Formononetin****. Formoonenetin. Biochanin B. Neochanin. Pratol*



$C_{16}H_{12}O_4$ 268.268
Widespread isoflavone found in soy beans (*Glycine max*), red clover (*Trifolium pratense* and chick peas (*Cicer arietinum*). Potential nutriceutical. Colourless or pale yellow needles (EtOH). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 265-266° (257-258°). λ_{max} 250 (ϵ 27400); 300 (ϵ 12240) (MeOH) (Berdy). λ_{max} 249 (ϵ 25120); 298 (ϵ 11200) (EtOH) (Berdy). λ_{max} 258 ; 340 (MeOH/NaOH) (Berdy).

*7-*O*-β-D-Glucopyranoside:* [486-62-4]
Ononin†. *Ononoside*
$C_{22}H_{22}O_9$ 430.41
Widely distributed in the Leguminosae subfamily Papilionoideae, e.g. in *Medicago sativa* (alfalfa) and *Trifolium* spp.. Needles (dioxan aq.). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 218-219°. λ_{max} 250 (MeOH) (Berdy).

*7-*O*-(2,6-Di-*O*-acetyl-β-D-glucopyranoside):* ***2″,6″-Di-O-acetylononin***
$C_{26}H_{26}O_{11}$ 514.485
Constit. of soybeans, *Glycine max*. Amorph. yellow powder. $[\alpha]_D^{25}$ +9.3 (c, 0.55 in MeOH). λ_{max} 238 (log ϵ 4.12); 272 (log ϵ 4.48) (MeOH).

*7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside):* [34232-16-1]
$C_{25}H_{24}O_{12}$ 516.457
Isol. from leaves of *Trifolium pratense* (red clover). Needles + ½H_2O (MeOH).

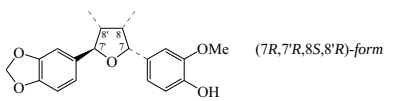
*7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), Me ester:* [34232-18-3]
$C_{26}H_{26}O_{12}$ 530.484
Isol. from leaves of *Trifolium pratense* (red clover). Needles (MeOH). Mp 198°.

*7-*O*-[4-Hydroxybenzoyl-(→2)-β-D-glucopyranoside]:* [122130-27-2] *Formononetin 7-(2-*p*-hydroxybenzoylglucoside)*
$C_{29}H_{26}O_{11}$ 550.518
Isol. from *Trifolium repens* (white clover).

Bose, J.L. *et al., J. Sci. Ind. Res., Sect. B*, 1951, **10**, 291 (*isol, struct*)
Bradbury, R.B. *et al., J.C.S.*, 1951, 3447 (*isol*)
Baker, W. *et al., J.C.S.*, 1953, 1852 (*synth*)
Cooke, R.G. *et al., Aust. J. Chem.*, 1964, **17**, 379 (*isol, struct*)
Lebreton, P. *et al., Phytochemistry*, 1967, **6**, 1675 (*isol*)
Benn, M.H. *et al., Can. J. Chem.*, 1970, **48**, 1624 (*isol*)
Beck, A.B. *et al., Aust. J. Chem.*, 1971, **24**, 1509 (*malonyl derivs*)
Braz Filho, R. *et al., J. Nat. Prod.*, 1977, **40**, 236 (*isol*)
Jha, H.C. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 102 (*synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Al-Ani, H.A.M. *et al., J.C.S. Perkin 1*, 1984, 2831 (*biosynth*)
Elgamal, M.H.A. *et al., J. Prakt. Chem.*, 1986, **328**, 893 (*ms*)
Murthy, M.S.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 225 (*cmr*)
Pivovarenko, V.G. *et al., Khim. Prir. Soedin.*, 1989, **25**, 639; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 542 (*synth*)
Khan, I.A. *et al., J. Nat. Prod.*, 2000, **63**, 1414-1416 (*activity*)
Balasubramanian, S. *et al., Synth. Commun.*, 2000, **30**, 469-484 (*synth, pmr*)
Hosny, M. *et al., J. Nat. Prod.*, 2002, **65**, 805-813 (*2″,6″-Diacetylononin*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 6th edn., Van Nostrand Reinhold*, 1984, 736

4-Hydroxy-3-methoxy-3′,4′-methylenedioxy-7,7′-epoxylignan H-549

4-[5-(1,3-Benzodioxol-5-yl)tetrahydro-3,4-dimethyl-2-furanyl]-2-methoxyphenol, 9CI. Tetrahydro-2-(4-hydroxy-3-methoxyphenyl)-5-(3,4-methylenedioxyphenyl)-3,4-dimethylfuran



(7*R*,7′*R*,8*S*,8′*R*)-*form*

$C_{20}H_{22}O_5$ 342.391

(7*R*,7′*R*,8*S*,8′*R*)-*form* [79120-60-8] ***Zuonin C****. Zuihonin C*

Me ether: [61989-57-9] ***Machilusin***
$C_{21}H_{24}O_5$ 356.418
Plates. Mp 121-122°. $[\alpha]_D$ -130.6 ($CHCl_3$). Probable stereochem. Could be the (7*R*,7′*R*,8*R*,8′*S*) isomer (i.e. with aryl groups interchanged).

(7*R*,7′*S*,8*S*,8′*R*)-*form*

Me ether: [155835-53-3]
Oil. $[\alpha]_D$ -39 (c, 0.002 in MeOH).

(7*R*,7′*S*,8*S*,8′*S*)-*form* [55890-25-0] ***Austrobailignan 7***
Constit. of mace (*Myristica fragrans*). Pale yellow gum. $Bp_{0.02}$ 130°. $[\alpha]_D^{25}$ +12 (c, 2.9 in $CHCl_3$).

Ac: [55730-99-9]
Mp 81-82°.

Me ether: [19950-67-5] *3,4-Dimethoxy-3′,4′-methylenedioxy-7,7′-epoxylignan.* ***Calopiptin***
$C_{21}H_{24}O_5$ 356.418
Cryst. (C_6H_6 or petrol). Mp 95.5°. $[\alpha]_D^{14}$ +28 (c, 2 in $CHCl_3$).

(7*S*,7′*S*,8*R*,8′*S*)-*form* [78919-28-5] ***Chicanine***
Prisms ($CHCl_3$/hexane). Mp 122-124°. $[\alpha]_D^{31}$ +118.8 (c, 4.57 in $CHCl_3$).

(7*S*,7′*S*,8*S*,8′*S*)-*form* ***Talaumidin***
Viscous gum or oil. $[\alpha]_D^{20}$ -90.2 (c, 0.01 in $CHCl_3$). $[\alpha]_D$ -17.9 (c, 0.1 in $CHCl_3$). λ_{max} 233 (log ϵ 4); 283 (log ϵ 3.7) (MeOH).

(7*R,7′*R**,8*R**,8′*R**)-*form***

Me ether: [158569-73-4]
Visc. oil. $[\alpha]_D^{24}$ -41.7 (c, 0.15 in $CHCl_3$). Relative config. only.

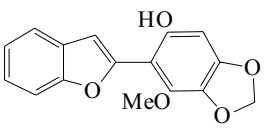
(7*R,7′*S**,8*R**,8′*S**)-*form*** [114488-90-3] ***Machilin F****. Fragransin E_1. 3-Epiaustrobailignan 7*
Constit. of mace (*Myristica fragrans*). Oil. Abs. config. unknown (quasi-meso).

Me ether: [114422-19-4] ***Machilin G***
$C_{21}H_{24}O_5$ 356.418
Oil. $[\alpha]_D^{24}$ +3.9 (c, 0.3 in $CHCl_3$). Abs. config. unknown (quasi-meso). The *P. schmidtii* isolate had -ve opt. rotn..

McAlpine, J.B. *et al., Aust. J. Chem.*, 1968, **21**, 2095 (*Calopiptin*)
Murphy, S.T. *et al., Aust. J. Chem.*, 1975, **28**, 81 (*isol, struct*)
Liu, S.-J. *et al., Can. J. Chem.*, 1981, **59**, 1680 (*Chicanine*)
Urzua, A. *et al., Phytochemistry*, 1987, **26**, 1509 (*Zuonin C*)
Hada, S. *et al., Phytochemistry*, 1988, **27**, 563 (*Fragransin E_1*)
Shimomura, H. *et al., Phytochemistry*, 1988, **27**, 634 (*deriv*)
Tyagi, O.D. *et al., Phytochemistry*, 1993, **32**, 445 (*(-)-Machilin G*)
Urzua, A. *et al., Phytochemistry*, 1993, **34**, 874 (*isol*)
Gonzalez-Coloma, A. *et al., Phytochemistry*, 1994, **35**, 607 (*isol*)
Prasad, A.K. *et al., Tetrahedron*, 1994, **50**, 10579 (*isol, deriv*)
De Almeida Blumenthal, E.E. *et al., Phytochemistry*, 1997, **46**, 745-749 (*isol, pmr, cmr*)
Vieira, L.M. *et al., Phytochemistry*, 1998, **48**, 1079-1081 (*Talaumidin*)

2-(6-Hydroxy-2-methoxy-3,4-methylenedioxyphenyl)benzofuran H-550

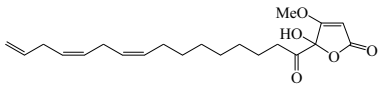
[90996-89-7]
6-(2-Benzofuranyl)-7-methoxy-1,3-benzodioxol-5-ol, 9CI. 2-Benzofuranyl-3-methoxy-4,5-methylenedioxyphenol



$C_{16}H_{12}O_5$ 284.268
Found in baker's yeast. Slender needles (petrol). Mp 118°.

Meisinger, M.A.P. *et al., J.A.C.S.*, 1959, **81**, 4979-4982; 4983-4989 (*isol, synth, struct*)
McKittrick, B.A. *et al., J.C.S. Perkin 1*, 1984, 709-712 (*synth, pmr*)
Jinno, S. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 1029-1032 (*synth*)
Jinno, S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1276-1283 (*synth, activity*)

5-Hydroxy-4-methoxy-5-(1-oxo-9,12,15-hexadecatrienyl)-2(5*H*)-furanone H-551

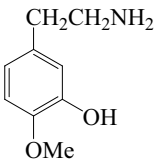


$C_{21}H_{30}O_5$ 362.465
Constit. of etiolated seedlings of *Sorghum bicolor* (sorghum). λ_{max} 224 (ϵ 8900); 268 (sh) (ϵ 200) (EtOH).

Suzuki, Y. *et al., Phytochemistry*, 1998, **47**, 997-1001

3-Hydroxy-4-methoxyphenethylamine H-552

[3213-30-7]
5-(2-Aminoethyl)-2-methoxyphenol



$C_9H_{13}NO_2$ 167.207Identified chromatographically.

Hydrochloride: [645-33-0]
Needles (MeOH/EtOAc). Mp 206.5-207°.

N-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl):* [78510-20-0] **N-trans-*Feruloyl-4*-O-*methyldopamine***
$C_{19}H_{21}NO_5$ 343.379
Alkaloid from roots of the pseudocereal *Chenopodium album* (lambsquarters). Oil.

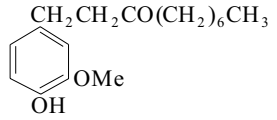
N-*Me:* [35266-68-3] *3-Hydroxy-4-methoxy*-N-*methylphenethylamine*
$C_{10}H_{15}NO_2$ 181.234

N,N,N-*Tri-Me:* [6882-07-1] *3-Hydroxy-4-methoxy*-N,N,N-*trimethylbenzeneethanaminium*. ***Salicifoline***
$C_{12}H_{20}NO_2^{\oplus}$ 210.295
Mp 260-261° dec. (as chloride).

Ramirez, F.A. *et al., J.A.C.S.*, 1950, **72**, 2781-2782 (*synth*)
Tomita, M. *et al., Yakugaku Zasshi*, 1952, **72**, 197; 727; 760; 1256; *CA*, **47**, 1627; 12288; 12409; **48**, 2639 (*Salicifoline*)
Nakano, T. *et al., Pharm. Bull.*, 1954, **2**, 321; 1956, **4**, 409 (*Salicifoline*)
Yang, T.H. *et al., Yakugaku Zasshi*, 1962, **82**, 811; *CA*, **58**, 7991 (*Salicifoline*)
Agurell, S. *et al., J. Nat. Prod.*, 1971, **34**, 183-187 (*isol, struct*)
Kohno, M *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 1252-1254 (*synth, ir, pmr*)
Horio, T. *et al., Phytochemistry*, 1993, **33**, 807 (*N-Feruloyl-4-methyldopamine*)
Clement, B.A. *et al., Phytochemistry*, 1998, **49**, 1377-1380 (*isol*)

1-(4-Hydroxy-3-methoxyphenyl)-3-decanone H-553

[27113-22-0]
2-Methoxy-4-(3-oxodecyl)phenol. [6]-Paradol



$C_{17}H_{26}O_3$ 278.391
From grains of paradise (*Amomum melegueta*) and ginger (*Zingiber officinale*). Cryst. (hexane at -30°). Mp 27-29° Mp 31-32°.

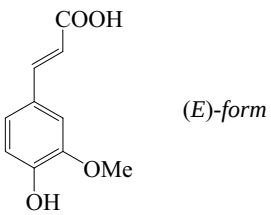
► HE0758000

Benzoyl:
Mp 63-64°.

Connell, D.W. *et al., Aust. J. Chem.*, 1970, **23**, 369 (*isol, ir, ms, uv*)
Locksley, H.D. *et al., J.C.S. Perkin 1*, 1972, 3001 (*ms, pmr, synth*)

3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid, 9CI H-554

[1135-24-6]
4-Hydroxy-3-methoxycinnamic acid, 8CI. ***Ferulic acid***. *Caffeic acid 3-methyl ether*



(*E*)-*form*

$C_{10}H_{10}O_4$ 194.187
Log P 1.27 (calc).

► UD3365500

(*E*)-*form* [537-98-4]
Widely distributed in plants, first isol. from *Ferula foetida* (asafoetida). Antioxidant used to inhibit oxidn. of fats, pastry products, etc. Antifungal agent used to prevent fruit spoilage. Orthorhombic needles (H_2O). Sol. MeOH, EtOAc; fairly sol. H_2O, Et_2O; poorly sol. C_6H_6, hexane. Mp 174°. Undergoes $SOCl_2$-activated polycondensation λ_{max} 236 ; 322 (EtOH) (Berdy).

► Exp. reprod. effects. GD9275000

Na salt: [24276-84-4] *Sodium ferulate. FEMA 3812*
Flavouring ingredient with a sweet clovery, phenolic odour. Light yellow powder.

[α-L-Arabinofuranosyl-(1→3)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl] ester:
$C_{27}H_{38}O_{18}$ 650.586
Constit. of soybean molasses (*Glycine* sp.). Amorph. powder. $[\alpha]_D^{25}$ -23.8 (c, 0.52 in MeOH). λ_{max} 227 (log ϵ 3.9); 275 (log ϵ 4.15) (MeOH).

Hexadecyl ester: [158306-36-6]

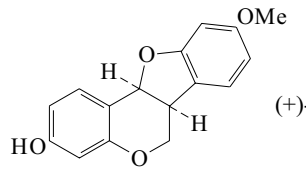
[64190-80-3] *Hexadecyl (*E*)-ferulate*
$C_{26}H_{42}O_4$ 418.615
Isol. from *Ipomoea batatas* (sweet potato).

[115374-26-0]

Achenbach, H. *et al., Z. Naturforsch., C*, 1986, **41**, 164 (*esters*)
Mizuno, M. *et al., Phytochemistry*, 1990, **29**, 2663 (*Hexadecyl ferulate*)
Hosny, M. *et al., J. Nat. Prod.*, 1999, **62**, 853-858 (*arabinosylglucosylglucosyl ester*)
Faulds, C. *et al., Chem. Br.*, May, 2000, 48-50 (*rev, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1640 (*Na salt*)

3-Hydroxy-9-methoxypterocarpan H-555

6a,11a-Dihydro-9-methoxy-6H-benzofuro[3,2-c][1]benzopyran-3-ol, 9CI. ***Medicarpin***. *Demethylhomopterocarpin*



(+)-*form*

$C_{16}H_{14}O_4$ 270.284

(-)-*form* [32383-76-9]
Mp 127.5-128.5°. $[\alpha]_D^{22}$ -226 ($CHCl_3$). λ_{max} 207 (ϵ 72443); 282 (ϵ 9332); 287 (ϵ 100300); 310 (ϵ 2400) (MeOH) (Berdy). λ_{max} 280 ; 285 (EtOH) (Berdy).

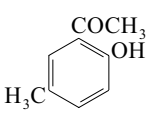
O-*β-D-Glucopyranoside:* [52766-70-8] ***Medicocarpin***
$C_{22}H_{24}O_9$ 432.426
Isol. from roots of *Medicago sativa* (alfalfa) and *Trifolium repens* (white clover). Mp 270-272°. $[\alpha]_D^{23}$ -149 (c, 0.9 in Py). $[\alpha]_D^{20}$ -44.5 (c, 0.05 in MeOH). λ_{max} 287 (ϵ 10253) (dioxane).

3-O-(6-O-Malonyl-β-D-glucopyranoside): [131653-24-2] ***Medicarpin 3-O-(6′-malonylglucoside)***
$C_{25}H_{26}O_{12}$ 518.473
Isol. from *Medicago sativa* (alfalfa). Assignment to the (-)-form assumed here.

Sakagami, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1031-1034 (*Medicocarpin*)
Haznagy, A. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1978, **311**, 318-323 (*Medicocarpin*)
Antus, S. *et al., Chem. Ber.*, 1979, **112**, 480-483 (*Medicocarpin, synth*)
Fraishtat, P.D. *et al., Bioorg. Khim.*, 1980, **6**, 1722 (*glucoside*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1-266 (*rev, occur*)
Kessmann, H. *et al., Plant Physiol.*, 1990, **94**, 227-232 (*6′-Malonylglucoside*)
Kirmizigül, S. *et al., J. Nat. Prod.*, 1997, **60**, 378-381 (*Medicocarpin*)

2′-Hydroxy-5′-methylacetophenone H-556

[1450-72-2]
1-(2-Hydroxy-5-methylphenyl)ethanone, 9CI. 2-Acetyl-p-*cresol. Methyl 6-hydroxy*-m-*tolyl ketone*



$C_9H_{10}O_2$ 150.177
Flavouring for coffee. Prisms (petrol or MeOH aq.). Mp 50°. Bp_{20} 120-125°.

Oxime: [3973-90-8]

$C_9H_{11}NO_2$ 165.191
Needles (EtOH). Mp 145°.

2,4-Dinitrophenylhydrazone: [22020-96-8]
Mp 273-273.5°.

Semicarbazone: [51040-40-5]
$C_{10}H_{13}N_3O_2$ 207.232
Needles (EtOH). Mp 212°.

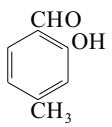
Thiosemicarbazone: [51089-88-4]
$C_{10}H_{13}N_3OS$ 223.298
Yellow cryst. (AcOH).

Me ether: [20628-07-3] *2′-Methoxy-5′-methylacetophenone*
$C_{10}H_{12}O_2$ 164.204
Bp 254° Bp_{11} 132°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 858B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 41D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1259D (*ir*)
Rosenmund, K.W. *et al., Annalen*, 1928, **460**, 56
Yoshino, T. *et al., CA*, 1963, **59**, 7416 (*synth*)
Bonsall, C. *et al., J.C.S.(C)*, 1967, 1836 (*ir, uv, nmr*)
Patel, M.C. *et al., J. Indian Chem. Soc.*, 1973, **50**, 560 (*thiosemicarbazone, use*)
Epshtein, L.M. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1974, 1710
Basinski, W. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1974, **48**, 2217 (*synth*)
Manku, G.S. *et al., Curr. Sci.*, 1976, **45**, 294 (*semicarbazone, use*)

2-Hydroxy-4-methylbenzaldehyde H-557

[698-27-1]
*2-Hydroxy-*p*-tolualdehyde.* m-*Cresol-6-aldehyde. 4-Methylsalicylaldehyde. 2,4-Cresotaldehyde. 2-Formyl-5-methylphenol.* m-*Homosalicylaldehyde. FEMA 3697*



$C_8H_8O_2$ 136.15
Flavouring ingredient. Needles (H_2O or EtOH). Mp 60-61°. Bp_{726} 219-221°. Steam-volatile.

Oxime:4-Methylsalicylaldoxime
$C_8H_9NO_2$ 151.165
Plates (EtOH aq.). Sol. EtOH, Et_2O, $CHCl_3$, hot H_2O. Mp 108.5-109°.

Semicarbazone: [54825-10-4] *2-[(2-Hydroxy-4-methylphenyl)methylene]hydrazinecarboxamide, 9CI*
$C_9H_{11}N_3O_2$ 193.205
Cryst. (EtOH). Sol. EtOH, DMF. Mp 268°.

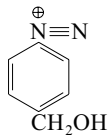
2,4-Dinitrophenylhydrazone: [973-82-0]
Mp 266-267°.

Me ether: [57415-35-7] *2-Methoxy-4-methylbenzaldehyde*
$C_9H_{10}O_2$ 150.177
Needles. Mp 42-43°. Bp_{720} 263-264°. Steam-volatile.

Anselmino, O. *et al., Ber.*, 1917, **50**, 395
Duff, J.C. *et al., J.C.S.*, 1941, 547
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **3**, 255 (*synth, use*)
Gross, H. *et al., Chem. Ber.*, 1963, **96**, 308
Casnati, G. *et al., Tet. Lett.*, 1965, 243 (*synth*)
Morishige, K. *et al., Anal. Chim. Acta*, 1974, **73**, 245 (*synth, detn, Sc*)
Bruce, J.M. *et al., J.C.S. Perkin 1*, 1974, **2**, 288 (*synth*)
Deguchi, M. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1985, **34**, 640; *CA*, **104**, 61168y (*synth, detn, Ga*)
Hauser, F.M. *et al., Synthesis*, 1987, 723 (*deriv, synth, ir, pmr, ms*)
Glennon, R.A. *et al., J. Med. Chem.*, 1992, **35**, 734 (*Me ether, synth, pmr*)
Bu, X.R. *et al., Synth. Commun.*, 1994, **24**, 1757 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 365
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1375-1376

4-(Hydroxymethyl)benzenediazonium(1+), 9CI H-558

[78246-53-4]



$C_7H_7N_2O^{\oplus}$ 135.145
Constit. of the basal stalk of the common edible mushroom *Agaricus bisporus*.

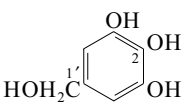
▶ Mutagenic and carcinogenic.

[109835-10-1, 112177-79-4]

Levenberg, B. *et al., Biochim. Biophys. Acta*, 1962, **63**, 212 (*detn*)
Gannett, P.M. *et al., Tet. Lett.*, 1987, **28**, 1015 (*tox, bibl*)

5-(Hydroxymethyl)-1,2,3-benzenetriol H-559

[68325-64-4]
α,3,4,5-Tetrahydroxytoluene. 3,4,5-Trihydroxybenzyl alcohol. Gallyl alcohol



$C_7H_8O_4$ 156.138
Unstable, readily polymerises.

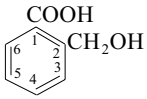
1,3-Di-Me ether, 2-O-β-D-glucopyranoside: [64121-98-8] ***Di-O-methylcrenatin***
$C_{15}H_{22}O_9$ 346.333
Constit. of fennel (*Foeniculum vulgare*). Needles (EtOH or MeOH). Mp 175-177° (164-165°). $[\alpha]_D^{20}$ -22.2 (c, 1.6 in MeOH).

[119188-79-3]

Cuendet, M. *et al., Helv. Chim. Acta*, 1997, **80**, 1144-1152 (*Dimethylcrenatin*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1587-1590 (*1,3-di-Me 2-glucoside*)

2-(Hydroxymethyl)benzoic acid, 9CI H-560

[612-20-4]
*α-Hydroxy-*o*-toluic acid, 8CI. Benzyl alcohol 2-carboxylic acid. 2-Carboxybenzyl alcohol*

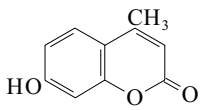


$C_8H_8O_3$ 152.149
Isol. from watercress. Needles (H_2O). Mp 127-128°. pK_a 3.8 (25°).

Gilman, H. *et al., J.A.C.S.*, 1940, **62**, 977-979 (*synth*)
Davey, W. *et al., J.O.C.*, 1961, **26**, 3699-3705 (*synth*)
Sofowora, E.A. *et al., Lloydia*, 1975, **38**, 169-171 (*isol*)
Spence, R.-M.M. *et al., Phytochemistry*, 1983, **22**, 2521-2523 (*isol*)

7-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one, 9CI H-561

[90-33-5]
7-Hydroxy-4-methylcoumarin. 4-Methylumbelliferone. Coumarin 4. ***Hymecromone, INN, JAN, USAN****. Cantabiline. BMU. Pilot 447. Hymechromone. Many other names*



$C_{10}H_8O_3$ 176.171
Needles (EtOH). Sol. EtOH, bases, AcOH. Mp 194-195°. pK_a 7.8 (25°). Log P 2.11 (calc). Phototautomerises.

▶ LD_{50} (rat, ipr) 2550 mg/kg. Exp. reprod. and teratogenic effects. GN7000000

Ac: [2747-05-9]
$C_{12}H_{10}O_4$ 218.209
Isol. from fenugreek (*Trigonella foenum-graecum*). Cryst. Mp 153-154° (150-151°).

Et ether: [87-05-8] *7-Ethoxy-4-methyl-2*H*-1-benzopyran-2-one. 7-Ethoxy-4-methylcoumarin. Maraniol. Madescol. Ethoxy resocyanin*
$C_{12}H_{12}O_3$ 204.225
Used in nut food flavouring. Needles with sweet, nutty taste. Mp 114° (95°).

[5980-33-6, 103764-33-6, 116523-82-1]

U.S. Pat., 1933, 1 934 361; *CA*, **28**, 578 (*Et ether*)
Bhardwaj, D.K. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 94 (*isol, Ac*)
Deshmukh, J.G. *et al., J. Indian Chem. Soc.*, 1986, **63**, 442 (*Et ether, synth*)

7-Hydroxy-6-methyl-2*H*-1-benzopyran-2-one, 9CI H-562

[53811-56-6]
7-Hydroxy-6-methylcoumarin. 6-Methylumbelliferone

$C_{10}H_8O_3$ 176.171
Constit. of *Trachyspermum roxburghianum* (Bishop's weed). Cubes (EtOH aq.). Mp 247-248°.

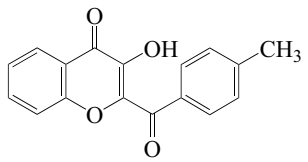
Ac:
$C_{12}H_{10}O_4$ 218.209
Needles (C_6H_6). Mp 147-148°.

*Me ether:7-Methoxy-6-methyl-2*H*-1-benzopyran-2-one. 7-Methoxy-6-methylcoumarin*
$C_{11}H_{10}O_3$ 190.198
Constit. of *Trachyspermum roxburghianum* (Bishop's weed). Plates (MeOH). Mp 135-137°.

Bell, J.C. *et al., J.C.S.*, 1936, 1828 (*synth*)
Bandopadhyay, M. *et al., Indian J. Chem.*, 1974, **12**, 295 (*synth*)
Sharma, B.R. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 85 (*isol*)
Mali, R.S. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 759 (*synth*)

3-Hydroxy-2-(4-methylbenzoyl)-4*H*-1-benzopyran-4-one, 9CI H-563

[173866-78-9]
3-Hydroxy-2-(4-methylbenzoyl)chromone



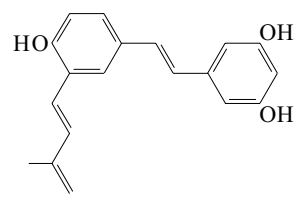
$C_{17}H_{12}O_4$ 280.279
Constit. of the roots of *Mangifera indica* (mango).

Me ether: [173866-79-0] *3-Methoxy-2-(4-methylbenzoyl)-4*H*-1-benzopyran-4-one. 3-Methoxy-2-(4-methylbenzoyl)chromone*
$C_{18}H_{14}O_4$ 294.306
Constit. of the roots of *Mangifera indica* (mango).

Khan, M.A. *et al., Fitoterapia*, 1995, **66**, 423-424 (*isol, struct*)

1-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]-2-(3,5-dihydroxyphenyl)ethylene H-564

5-[2-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]ethenyl]-1,3-benzenediol. 3′,4,5′-Trihydroxy-3-isopentadienylstilbene

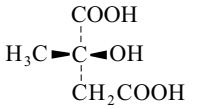


$C_{19}H_{18}O_3$ 294.349
(*E*)-*form*
Constit. of *Arachis hypogaea* (peanuts). λ_{max} 298 (ε 22000) (MeOH) (Berdy). λ_{max} 296 (EtOH) (Berdy). λ_{max} 341 (MeOH-NaOH) (Berdy).

Cooksey, C.J. *et al., Phytochemistry*, 1988, **27**, 1015

2-Hydroxy-2-methylbutanedioic acid H-565

[2306-22-1]
2-Hydroxy-2-methylsuccinic acid. Citramalic acid. 2-Methylmalic acid



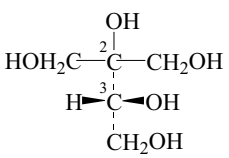
(*R*)-*form*

$C_5H_8O_5$ 148.115
(*R*)-*form* [6236-10-8]
Constit. of apple peel. $[\alpha]_D$ -30. Referred to as the L-form but this is ambiguous.
Di-Me ester: [81426-68-8]
$C_7H_{12}O_5$ 176.169
Liq. $Bp_{0.15}$ 90° (bath). $[\alpha]_D^{20}$ -27 (c, 1.1 in $CHCl_3$) (>97% ee).
1-Me ester, 4-nitrile: [141562-85-8] *Methyl-3-cyano-2-hydroxy-2-methylpropanoate*
$C_6H_9NO_3$ 143.142
Liq. $Bp_{0.25}$ 120° (bath). $[\alpha]_D^{20}$ +8.5 (c, 1.8 in $CHCl_3$) (>97% ee).
(*S*)-*form* [6236-09-5]
Cryst. (EtOAc/petrol). Mp 112-115°. $[\alpha]_D^{22}$ +23.6 (c, 3 in H_2O).
Di-Me ester: [38574-61-7]
$[\alpha]_D^{21}$ +26.4 (c, 4.22 in $CHCl_3$).
(±)-*form* [597-44-4]
Cryst. (EtOAc/petrol). Mp 119°.
[81426-68-8]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 811C (*nmr*)
Hulme, A.C. *et al., Biochim. Biophys. Acta*, 1954, **11**, 36 (*isol*)
Biochem. Prep., 1962, **9**, 25 (*synth*)
Stadler, P.A. *et al., Helv. Chim. Acta*, 1963, **46**, 2300 (*abs config*)
Brandänge, S. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 153
Spencer, H.K. *et al., J.O.C.*, 1975, **40**, 217 (*synth, pmr, ir*)
Behr, D. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 309 (*cd*)
Wilkes, J.B. *et al., J.O.C.*, 1980, **45**, 247 (*synth*)
Brandi, A. *et al., Synthesis*, 1982, 719
Stevens, R.W. *et al., Chem. Lett.*, 1983, 1799
Seebach, D. *et al., Tetrahedron*, 1984, **40**, 1313 (*synth*)
Staring, E.G.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1986, **105**, 374 (*synth*)
Frye, S.V. *et al., Diss. Abstr. Int., B*, 1988, **48**, 2649 (*synth*)
Kabuto, K. *et al., Chem. Lett.*, 1989, 385 (*pmr, abs config*)
Whitesell, J.K. *et al., J.O.C.*, 1989, **54**, 2258 (*synth*)
Yang, S. *et al., Synthesis*, 1992, 365 (*synth*)
Eck, R. *et al., Tetrahedron*, 1994, **50**, 13641-13654 (*synth, R-form, S-form*)

2-(Hydroxymethyl)-1,2,3,4-butanetetrol, 9CI H-566

[89615-91-8]
*2-C-(Hydroxymethyl)-*glycero*-tetritol. 3-C-(Hydroxymethyl)erythritol. 3-C-(Hydroxymethyl)threitol. Apiitol*



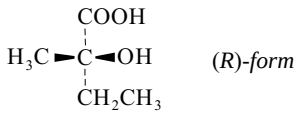
(*R*)-*form*

$C_5H_{12}O_5$ 152.147
Numbering reverses if named as a deoxytetritol. C-2 is not a chiral centre.
(*R*)-*form* [217975-02-5]
L-*form*
Constit. of the fruit of *Foeniculum vulgare* (fennel). Syrup. $[\alpha]_D^{25}$ +4.4 (c, 0.5 in MeOH).
(*S*)-*form* [10592-17-3]
D-*form*
Syrup.
2,3-Isopropylidene:
$C_8H_{16}O_5$ 192.211
Cryst. ($CHCl_3$). Mp 86-88°. $[\alpha]_D^{20}$ 0 (c, 1.2 in MeOH).
2,3-Isopropylidene, tribenzoyl:
$C_{29}H_{28}O_8$ 504.535
Mp 102-104°.

Witczak, Z.J. *et al., Carbohydr. Res.*, 1984, **133**, 235 (*synth, pmr, cmr*)
Kindel, P.K. *et al., Carbohydr. Res.*, 1990, **199**, 55 (*acetal derivs*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1583-1586 (*isol*)

2-Hydroxy-2-methylbutanoic acid, 9CI H-567

[3739-30-8]
Ethylmethylglycollic acid. 2-Ethyllactic acid



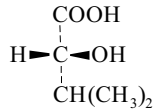
(*R*)-*form*

$C_5H_{10}O_3$ 118.132
(*R*)-*form* [37505-02-5]
Mp 73.5-74.5°. $[\alpha]_D^{24}$ -8.9 (c, 3.0 in $CHCl_3$).
Nitrile, O-*β*-D-*glucopyranoside:* [534-67-8] ***Lotaustralin***
$C_{11}H_{19}NO_6$ 261.274
Glycoside from *Trifolium repens* (white clover) and other plants. Needles (EtOAc). Mp 139°. $[\alpha]_D^{20}$ -26.4 (H_2O).
Nitrile, O-*[β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [72229-42-6] ***Neolinustatin***
$C_{17}H_{29}NO_{11}$ 423.416
Isol. from flaxseed meal. Cryst. (EtOH). Mp 190-192°. $[\alpha]_D^{25}$ -37 (c, 0.37 in H_2O).
Nitrile, O-*[β*-D-*apiofuranosyl-(1→6)-β*-D-*glucopyranoside]:* [170033-25-7]
$C_{16}H_{27}NO_{10}$ 393.39
Constit. of the roots of *Manihot esculenta* (cassava). Probable abs. config..
(*S*)-*form* [37505-07-0]
Mp 74-75°. $[\alpha]_D^{25}$ +9.1 (c, 1.6 in $CHCl_3$).
Nitrile, O-*β*-D-*glucopyranoside:* [55758-42-4] ***Epilotaustralin***
$C_{11}H_{19}NO_6$ 261.274
Isol. from *Triticum monococcum* (wheat).

Finnemore, H. *et al., J. Soc. Chem. Ind., London*, 1938, **57**, 162-169 (*Lotaustralin*)
Butler, G.W. *et al., Phytochemistry*, 1965, **4**, 127-131 (*Lotaustralin*)
Smith, C.R. *et al., J.O.C.*, 1980, **45**, 507-510 (*Neolinustatin*)
Pitsch, C. *et al., Planta Med.*, 1984, **50**, 388-390 (*Epilotaustralin*)
Olafsdottir, E.S. *et al., Phytochemistry*, 1988, **28**, 127-132 (*Epilotaustralin*)
Prawat, H. *et al., Phytochemistry*, 1995, **40**, 1167-1173 (*nitrile apiosylglucoside*)

2-Hydroxy-3-methylbutanoic acid, 9CI H-568

[4026-18-0]
2-Hydroxyisovaleric acid. 3-Hydroxy-3,3-dimethylpropanoic acid



(*R*)-*form*

$C_5H_{10}O_3$ 118.132

(*R*)-*form* [17407-56-6]
Mp 67-68° (63-65°). $[\alpha]_D^{25}$ -19.3 (c, 0.90 in $CHCl_3$).

3-Methylbutanoyl:
$C_{10}H_{18}O_4$ 202.25
Isol. from roots of *Valeriana officinalis* (valerian). Bp_{35} 136°. $[\alpha]_D$ +4.83. n_D^{19} 1.4368.

[14487-24-2, 15344-34-0, 21632-23-5, 69798-62-5, 90244-32-9, 106533-49-7, 106533-50-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 518D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 808C; 809A (*nmr*)
Fischer, E. *et al., Ber.*, 1908, **31**, 2897 (*synth*)
Cionga, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1935, **201**, 1152-1154 (*3-methylbutanoyl, isol*)
Bartlett, P.D. *et al., J. Biol. Chem.*, 1937, **118**, 503-511 (*synth*)
Cook, A.H. *et al., J.C.S.*, 1949, 1022-1028 (*S-form, synth*)
Baker, C.G. *et al., J.A.C.S.*, 1951, **73**, 1336 (*abs config*)
Vining, L.C. *et al., Can. J. Chem.*, 1957, **35**, 1109 (*abs config*)
Vigneron, J.P. *et al., Tetrahedron*, 1977, **33**, 507 (*synth*)
Kim, H.-O. *et al., J.O.C.*, 1987, **52**, 4531 (*synth*)
Li, W.R. *et al., J.A.C.S.*, 1990, **112**, 7659 (*synth, ir, pmr*)

3-Hydroxy-3-methylbutanoic acid, 9CI H-569

[625-08-1]
3-Hydroxy-3-methylbutyric acid, 8CI. 3-Hydroxyisovaleric acid
$(H_3C)_2C(OH)CH_2COOH$
$C_5H_{10}O_3$ 118.132
Oil. Sol. H_2O. Bp_{12} 162°. pK_a 4.43. Mp < -32°.

Me ester: [6149-45-7]
$C_6H_{12}O_3$ 132.159
Oil. Bp_{10} 70-71°.

Nitrile: [13635-04-6] *1-Cyano-2-methyl-2-propanol*
C_5H_9NO 99.132
Oil. Spar. sol. H_2O. Mp -12°. Bp 210-212° Bp_{30} 130-132°.

Nitrile, O-*β*-D-*glucopyranoside:* [126050-09-7] ***Epidermin***†
$C_{11}H_{19}NO_6$ 261.274
Constit. of barley (*Hordeum vulgare*).

Ac, nitrile:
$C_7H_{11}NO_2$ 141.169
Oil. Bp 198-200°.

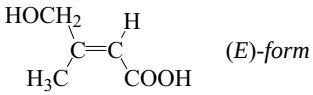
Phenylurethane:
Mp 129-130°.

[18267-36-2]

Coffman, D.D.V. *et al., J.A.C.S.*, 1958, **80**, 2882 (*synth*)
Rathka, M.W. *et al., J.A.C.S.*, 1970, **90**, 3222 (*synth*)
Vuitel, L. *et al., Synthesis*, 1972, 608 (*synth*)
Pourmohseni, H. *et al., Phytochemistry*, 1993, **33**, 295-297 (*Epidermin*)
Sekine, M. *et al., J.O.C.*, 1996, **61**, 4087 (*nitrile, synth, pmr, cmr*)
Lechtenberg, M. *et al., Phytochemistry*, 1996, **41**, 779-785 (*Epidermin*)

4-Hydroxy-3-methyl-2-butenoic acid, 9CI H-570

4-Hydroxy-3-methylcrotonic acid



(*E*)-*form*

$C_5H_8O_3$ 116.116

(*E*)-*form* [44647-19-0]
Needles (C_6H_6). Mp 112-113° (108-110°).

Me ester: [13866-57-4]
$C_6H_{10}O_3$ 130.143
Bp_1 30-50°.

Nitrile: [120696-93-7]

[13931-34-5] *4-Hydroxy-3-methyl-2-butenenitrile. 3-Cyano-2-methyl-2-propen-1-ol*
C_5H_7NO 97.116
Yellow liq. Bp_1 70° $Bp_{0.001}$ 75-77°. Presumably an error in Bp pressure reported by Schmidt or Jordis.

Ac: [21622-85-5]
$C_7H_{10}O_4$ 158.154
Bp_{12} 154-155°.

Ac, nitrile: [13931-33-4]
$C_7H_9NO_2$ 139.154
$Bp_{0.08}$ 60°.

(*Z*)-*form*

O-*β*-D-*Glucopyranoside, nitrile:* [160551-60-0]

[126050-10-0] ***Osmaronin***
$C_{11}H_{17}NO_6$ 259.258
Constit. of the leaves of *Hordeum vulgare* (barley). Config. of product from *Hordeum* sp. not stated.

O-*Tetradecanoyl, nitrile:3-Methyl-4-tetradecanoyloxy-2-butenenitrile*
$C_{19}H_{33}NO_2$ 307.475
Mp 49-51°.

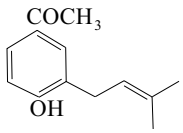
O-*(14Z-Eicosenoyl), nitrile:4-(14Z-Eicosenoyloxy)-3-methyl-2-butenenitrile*
$C_{25}H_{43}NO_2$ 389.62

*2S,3*R-*Epoxide,* O-*β*-D-*glucopyranoside, nitrile:* [160492-57-9] ***Osmaronin epoxide***
$C_{11}H_{17}NO_7$ 275.258Incorrect config. given in paper.

Nechvatal, A. *et al., J.C.S.(C)*, 1968, 185 (*synth*)
Larcheveque, M. *et al., Synthesis*, 1983, 297-300 (*nitrile*)
Bourguignon, J.-J. *et al., J. Med. Chem.*, 1988, **31**, 893 (*synth, pmr*)
Pourmohseni, H. *et al., Phytochemistry*, 1993, **33**, 295-297 (*Osmaronin*)
Lechtenberg, M. *et al., Phytochemistry*, 1994, **37**, 1039-1043; 1996, **41**, 779-785 (*Osmaronin, Osmaronin epoxide*)
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, Ac, pmr*)
Jordis, U. *et al., Org. Prep. Proced. Int.*, 1997, **29**, 549-560 (*nitrile*)
Akita, H. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 2429-2439 (*Osmaronin, synth*)
Yang, X. *et al., Yaoxue Xuebao*, 2000, **35**, 279-283 (*isol, nitrile, esters*)

4-Hydroxy-3-(3-methyl-2-butenyl)acetophenone H-571

[26932-05-8]
1-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]ethanone, 9CI. 4-Acetyl-2-prenylphenol. 4′-Hydroxy-3′-prenylacetophenone



$C_{13}H_{16}O_2$ 204.268
Constit. of roots of *Polymnia sonchifolia* (yacon). Cryst. (Et_2O/petrol). Mp 93-94°. λ_{max} 245 (ϵ); 334 (ϵ) (MeOH/NaOMe) (Derep). λ_{max} 226 (ϵ 14800); 279 (ϵ 13000) (MeOH) (Derep).

O-*β*-D-*Glucopyranoside:*
$C_{19}H_{26}O_7$ 366.41
Constit. of *Helichrysum italicum* (curry plant). Mp 160°. $[\alpha]_D$ -45 (c, 0.1 in MeOH). λ_{max} 221 ; 226 (MeOH).

Me ether: [26931-99-7] *4′-Methoxy-3′-prenylacetophenone*
$C_{14}H_{18}O_2$ 218.295
Oil. $Bp_{0.05}$ 90°.

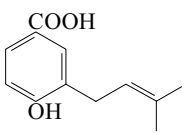
3″-Hydroxy, 2″,3″-dihydro: [81944-40-3] *4-Hydroxy-3-(3-hydroxy-3-methylbutyl)acetophenone*
$C_{13}H_{18}O_3$ 222.283
Needles (C_6H_6). Mp 100-102°.

4″-Hydroxy: See 4-Hydroxy-3-(4-hydroxy-3-methyl-2-butenyl)acetophenone in *The Combined Chemical Dictionary.*

Bohlmann, F. *et al., Chem. Ber.*, 1970, **103**, 90; 1972, **105**, 863 (*isol, struct, synth*)
De Pascual Teresa, J. *et al., Phytochemistry*, 1980, **19**, 2781; 1981, **20**, 2417 (*isol, uv, ir, pmr*)
Loyola, L.A. *et al., Phytochemistry*, 1985, **24**, 1600-1602 (*isol, dihydrohydroxy deriv*)
Sudalai, A. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 760-761 (*synth, ir, pmr, deriv*)
Takasugi, M. *et al., Phytochemistry*, 1996, **43**, 1019 (*isol, uv, ir, pmr, cmr, ms*)
Sala, A. *et al., J. Nat. Prod.*, 2001, **64**, 1360-1362 (*glucoside*)

4-Hydroxy-3-(3-methyl-2-butenyl)benzoic acid, 9CI H-572

[1138-41-6]
4-Hydroxy-3-prenylbenzoic acid. 3-(3,3-Dimethylallyl)-4-hydroxybenzoic acid



$C_{12}H_{14}O_3$ 206.241
Cryst. Mp 100°. λ_{max} 256 (ϵ 36500)

(MeOH) (Berdy). λ_{max} 286 (ϵ 60700) (MeOH/NaOH) (Berdy).

O-*β-D-Glucopyranoside:*
$C_{18}H_{24}O_8$ 368.383
Constit. of almond hulls (*Prunus amygdalus*). Amorph. solid.

Me ester: [101511-34-6]
$C_{13}H_{16}O_3$ 220.268
Cryst. Mp 86-87°.

Et ester: [1145-42-2]
$C_{14}H_{18}O_3$ 234.294
Cryst. Mp 76-77°. Artifact.

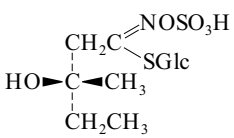
2′,3′-Dihydro, 2′,3′-dihydroxy, Me ester: [117176-70-2]
$C_{13}H_{18}O_5$ 254.282
Constit. of the famine food *Pandanus odoratissimus*. Needles. Mp 143-144°. $[\alpha]_D^{25}$ +12 (c, 0.4 in EtOH). λ_{max} 220 (sh) ; 259 ; 290 (sh) (no solvent reported).

Δ3′-Isomer, 2′-hydroxy, Me ester: [108544-66-7]
$C_{13}H_{16}O_4$ 236.267
Powder. Mp 124-126°. λ_{max} 217 (log ϵ 3.7); 251 (log ϵ 3.6) (MeOH).

Hinman, J.W. *et al., J.A.C.S.*, 1957, **79**, 3789 (*synth*)
Tanino, H. *et al., Tetrahedron*, 1969, **25**, 3033 (*synth*)
Shima, K. *et al., Yakugaku Zasshi*, 1972, **92**, 1410 (*isol, synth, uv, pmr*)
Diaz, D. *et al., Phytochemistry*, 1987, **26**, 809-811 (*isol, deriv*)
Arriaga-Giner, F.J. *et al., Z. Naturforsch., C*, 1988, **43**, 337-340 (*deriv*)
Abraham, W.F. *et al., Phytochemistry*, 1990, **29**, 2641 (*isol*)
Venkatasubbaiah, P. *et al., J. Nat. Prod.*, 1991, **54**, 1293 (*isol, pmr, cmr*)
Orjala, J. *et al., Planta Med.*, 1993, **59**, 546-551 (*isol, ester*)
Pereda-Miranda, R. *et al., J. Nat. Prod.*, 1997, **60**, 282 (*esters, isol, pmr, cmr, ms*)
Terreaux, C. *et al., Phytochemistry*, 1998, **49**, 461-464 (*isol, deriv*)
Jong, T.-T. *et al., Phytochemistry*, 1998, **49**, 2145-2148 (*isol, deriv*)
Sang, S. *et al., J. Agric. Food Chem.*, 2002, **50**, 607-609 (*glucoside*)

2-Hydroxy-2-methylbutyl glucosinolate H-573

[36286-64-3]
*1-Thio-β-D-glucopyranose 1-[3-hydroxy-3-methyl-*N*-(sulfooxy)pentanimidate], 9CI.* ***Glucocleomin***

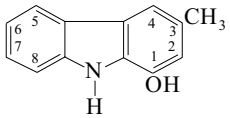


$C_{12}H_{23}NO_{10}S_2$ 405.446
Isol. from capers (*Capparis spinosa* and *Capparis ovata*).

Kjaer, A. *et al., Acta Chem. Scand.*, 1962, **16**, 591; 1963, **17**, 279 (*isol, struct, abs config*)
Ahmed, Z.F. *et al., Phytochemistry*, 1972, **11**, 251 (*isol*)

1-Hydroxy-3-methyl-9*H*-carbazole H-574

[14960-81-7]
*3-Methyl-9*H*-carbazol-1-ol*



$C_{13}H_{11}NO$ 197.236
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (EtOH aq.). Mp 157-158°.

Me ether: [4532-33-6] *1-Methoxy-3-methyl-9*H*-carbazole, 9CI.* ***Murrayafoline A***
$C_{14}H_{13}NO$ 211.263
Plates (hexane). Mp 52-54°.

Me ether, picrate:
Brown needles (C_6H_6). Mp 188-190°.

Chakraborty, D.P. *et al., J.O.C.*, 1968, **33**, 1265 (*synth*)
Wu, T.-S. *et al., Heterocycles*, 1983, **20**, 1267 (*occur, pmr*)
Furukawa, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4132 (*isol, uv, ir, pmr, cmr, ms*)
Martin, T. *et al., J.C.S. Perkin 1*, 1988, 235 (*synth, uv, ir, pmr, ms*)
Knölker, H.-J. *et al., Tetrahedron*, 1993, **49**, 11221 (*synth*)
Bhattacharyya, P. *et al., Phytochemistry*, 1994, **35**, 1085 (*isol, uv, ir, pmr, cmr, struct*)
Murakami, Y. *et al., Heterocycles*, 1998, **49**, 127-132 (*Murrayafoline A, synth*)
Bringmann, G. *et al., Synthesis*, 1998, 1501-1505 (*synth, Me ether, ir, pmr, cmr, ms*)
Itoigawa, M. *et al., J. Nat. Prod.*, 2000, **63**, 893-897 (*Murrayafoline A, activity*)

2-Hydroxy-3-methyl-9*H*-carbazole H-575

[24224-30-4]
*3-Methyl-9*H*-carbazol-2-ol, 9CI*

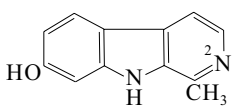
$C_{13}H_{11}NO$ 197.236
Alkaloid from the roots of *Murraya koenigii* (curryleaf tree). Mp 245-246°.

Me ether: [24224-28-0] ***2-Methoxy-3-methyl-9*H*-carbazole***
$C_{14}H_{13}NO$ 211.263
Alkaloid from the seeds of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6 or C_6H_6/petrol). Mp 225° (218°).

Chakraborty, D.P. *et al., Chem. Ind. (London)*, 1969, 1662 (*synth, uv, ir*)
Bhattacharyya, P. *et al., Chem. Ind. (London)*, 1986, 246 (*isol, uv, ir, pmr, cmr*)
Knölker, H. *et al., J. Indian Chem. Soc.*, 1994, **71**, 345 (*synth, 2-Methoxy-3-methylcarbazole*)
Wu, T.-S. *et al., Phytochemistry*, 1996, **43**, 133-140 (*isol*)
Knölker, H.J. *et al., Synlett*, 1996, 737 (*synth*)

7-Hydroxy-1-methyl-β-carboline H-576

[487-03-6]
*1-Methyl-9*H*-pyrido[3,4-*b*]indol-7-ol, 9CI.* ***Harmol****. 7-Hydroxyharman*



$C_{12}H_{10}N_2O$ 198.224
Alkaloid from *Elaeagnus angustifolia* (Russian olive) and *Passiflora incarnata* (maypops). Sol. $CHCl_3$, Me_2CO, bases; poorly sol. H_2O. Mp 304-307°. λ_{max} 210 ; 240 ; 300 ; 325 (MeOH) (Berdy).

O-*Ac:* [257938-78-6]
$C_{14}H_{12}N_2O_2$ 240.261
Needles (EtOH). Mp 155°.

1,2,3,4-Tetrahydro: [17952-75-9] ***Tetrahydroharmol****. 2,3,4,9-Tetrahydro-1-methyl-1*H*-pyrido[3,4-*b*]indol-7-ol, 8CI. 1,2,3,4-Tetrahydro-7-hydroxy-1-methyl-β-carboline*
$C_{12}H_{14}N_2O$ 202.255
Alkaloid from *Elaeagnus angustifolia* (Russian olive). Mp 254-255°.

1,2,3,4-Tetrahydro, N^2,O-*di-Ac:* [28090-84-8]
$C_{16}H_{18}N_2O_3$ 286.33
Cryst. (EtOAc). Mp 202°.

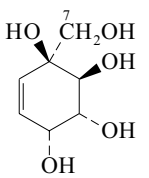
1,2,3,4-Tetrahydro, N^2*-Me:*N^b***-Methyltetrahydroharmol***
$C_{13}H_{16}N_2O$ 216.282
Alkaloid from *Elaeagnus angustifolia* (Russian olive). Cryst. (EtOH). Mp 268-270°. Racemic.

[28090-85-9]

Borkowski, B. *et al., CA*, 1960, **54**, 15844e (*isol*)
Lutomski, J. *et al., CA*, 1960, **54**, 16751f; 1961, **55**, 21479a (*isol*)
Ayer, W.A. *et al., Can. J. Chem.*, 1970, **48**, 1980-1984 (*Tetrahydroharmol*)
Ribas, I. *et al., CA*, 1972, **77**, 123811n (*isol*)
Allen, J.R.F. *et al., Phytochemistry*, 1980, **19**, 1573-1582 (*rev, bibl*)
Salm, R.F. *et al., Phytochemistry*, 1998, **49**, 887-892 (*isol*)
Ponce, M.A. *et al., J. Het. Chem.*, 2001, **38**, 1071-1082 (*O-Ac*)

1-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol H-577

1-Hydroxymethylconduritol



(1*S*,2*S*,3*R*,4*R*)-*form*

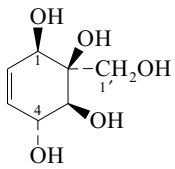
$C_7H_{12}O_5$ 176.169

(1*S*,2*S*,3*R*,4*R*)-*form*
1-Hydroxymethylconduritol E
4,7-Dibenzoyl: [134476-91-8] ***Piperenol B***
$C_{21}H_{20}O_7$ 384.385
Isol. from *Piper cubeba* (cubeb pepper). Semi-solid. $[\alpha]_D$ +50 (c, 1 in MeOH).

Ogawa, S. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 505; 1161; 1990, **63**, 1549 (*synth, derivs*)
Ogawa, S. *et al., Carbohydr. Res.*, 1986, **156**, 273 (*synth, derivs*)
Liang, G.Y. *et al., Phytochemistry*, 1988, **27**, 3857 (*isol, derivs*)
Taneja, S.C. *et al., Phytochemistry*, 1991, **30**, 871 (*Piperenol B*)

2-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol H-578

1,2,3,6-Tetrahydroxy-4-cyclohexene-1-methanol



(1*R*,2*R*,3*S*,4*R*)-*form*

$C_7H_{12}O_5$ 176.169

Numbering systems vary.

(1*R*,2*S*,3*R*,4*S*)-*form*

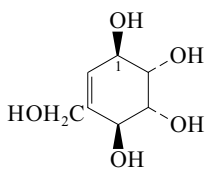
1′,4-Dibenzoyl: [113532-12-0] ***(+)-Zeylenol***. *Uvaribonol B*
$C_{21}H_{20}O_7$ 384.385
Constit. of *Piper cubeba* (cubeb pepper). Needles (EtOAc). Mp 132-133°. $[\alpha]_D$ +113.5. λ_{max} 228 (ϵ 26900); 274 (ϵ 1910); 281 (ϵ 1380) (EtOH) (Derep).

Jolad, S.D. *et al., J.O.C.*, 1981, **46**, 4267 (*struct, Zeylenol*)
Schulte, G.R. *et al., Tet. Lett.*, 1982, **23**, 289; 4299 (*abs config, Zeylenol, Ferrudiol*)
Tuntiwachwuttikul, P. *et al., Aust. J. Chem.*, 1987, **40**, 2049 (*isol, Zeylenol*)
Pancharoen, O. *et al., Phytochemistry*, 1989, **28**, 1143; 1996, **43**, 305 (*isol, synth*)
Pan, X.-P. *et al., Yaoxue Xuebao*, 1998, **33**, 275-281 (*Uvaribonols*)
Hiroya, K. *et al., Chem. Comm.*, 1999, 2197-2198 (*synth, Uvarigranol G, Zeylenol*)

5-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol, 9CI H-579

[53839-04-6]

3,4,5,6-Tetrahydroxy-1-cyclohexene-1-methanol. ***Rosevionol***



(1*R*,2*S*,3*R*,4*S*)-*form*

$C_7H_{12}O_5$ 176.169

(1*R*,2*S*,3*R*,4*S*)-*form*

1′,3-Dibenzoyl: [134476-89-4] ***Piperenol A***
$C_{21}H_{20}O_7$ 384.385
Isol. from *Piper cubeba* (cubeb pepper). Cryst. (EtOAc/hexane). Mp 48-49°. $[\alpha]_D$ +14.6 (c, 0.5 in MeOH).

1′,3-Dibenzoyl, 1,2,4-tri-Ac: [134476-92-9] ***Piperenol A triacetate***
$C_{27}H_{26}O_{10}$ 510.496
Constit. of *Piper cubeba* (cubeb pepper). Cryst. Mp 118-119°. $[\alpha]_D^{25}$ +17.5 (c, 1.1 in $CHCl_3$).

(1*S*,2*R*,3*S*,4*R*)-*form*

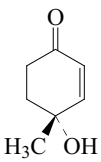
1′-Benzoyl, 1,2,3,4-tetra-Ac: [174819-31-9] ***Piperenol C***
$C_{22}H_{24}O_{10}$ 448.426
Constit. of *Piper cubeba* (cubeb pepper). Semi-solid. $[\alpha]_D^{25}$ -40 (c, 0.2 in $CHCl_3$). C-3 incorrectly assigned (*R*)-config. in ref..

Japan. Pat., 1974, 74 54587; *CA*, **81**, 150300j (*isol*)
Taneja, S.C. *et al., Phytochemistry*, 1991, **30**, 871-874 (*Piperenol A*)
Koul, J.L. *et al., Phytochemistry*, 1996, **41**, 1097-1099 (*Piperenol A tri-Ac, Piperenol C*)
Mehta, G. *et al., Tet. Lett.*, 2000, **41**, 3509-3512 (*synth, struct*)

4-Hydroxy-4-methyl-2-cyclohexen-1-one H-580

[70150-56-0]

[123285-72-3]



(*R*)-*form*

$C_7H_{10}O_2$ 126.155

(*R*)-*form* [73041-86-8]
$[\alpha]_D$ +43 (c, 0.82 in EtOH).

4-Hydroperoxide: [263844-51-5] ***4-Hydroperoxy-4-methyl-2-cyclohexen-1-one***
$C_7H_{10}O_3$ 142.154
Oil. $[\alpha]_D^{20}$ -100 (c, 0.05 in $CHCl_3$).

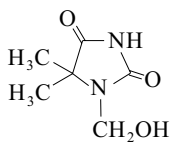
(ξ)-*form*
Constit. of *Nigella sativa* (black cumin) and peppermint oil (*Mentha piperita*).

Takahashi, K. *et al., Agric. Biol. Chem.*, 1980, **44**, 1535-1543 (*isol, synth*)
Bueno, A.B. *et al., Tet. Lett.*, 1995, **36**, 3737-3740 (*synth*)
Buchanan, M.S. *et al., J. Indian Chem. Soc.*, 1998, **75**, 613-615
Becker, H. *et al., Z. Naturforsch., C*, 1999, **54**, 997-1004 (*hydroperoxide*)

1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione, 9CI H-581

[116-25-6]

1-(Hydroxymethyl)-5,5-dimethylhydantoin, 8CI. Monomethyloldimethylhydantoin. Methylol dimethylhydantoin. MDMH



$C_6H_{10}N_2O_3$ 158.157

FDA approved for use as an adjuvant in the bleaching of food-contact recycled paper and board used in food packaging. Cryst. Sol. H_2O. Mp 110-117° (100°).

▶ Irritant.

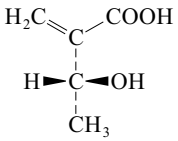
[16228-00-5, 27636-82-4]

Higuchi, S. *et al., J. Am. Pharm. Assoc.*, 1959, **48**, 557 (*synth*)
U.S. Pat., 1960, 2 995 538; *CA*, **55**, 26308b (*synth, use*)
Wilson, C.H. *et al., CA*, 1977, **87**, 189289m (*detn, use*)
Romanian Pat., 1980, 72 413; *CA*, **96**, 199694q (*synth*)
Eur. Pat., 1983, 91 740; *CA*, **100**, 25948m (*use*)
Japan. Pat., 1985, 60 231 736; *CA*, **104**, 187749 (*use*)
Katritzky, A.R. *et al., Magn. Reson. Chem.*, 1988, **26**, 129 (*cmr*)
Food Chem. News, 2002, **43(47)**, 20 (*use*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 736; 840

3-Hydroxy-2-methylenebutanoic acid, 9CI H-582

[27977-20-4]

2-(1-Hydroxyethyl)propenoic acid. 2-(1-Hydroxyethyl)acrylic acid



(*R*)-*form*

$C_5H_8O_3$ 116.116

(ξ)-*form* No mention of abs. config. of isolated esters.

Butyl ester: [22141-40-8]
$C_9H_{16}O_3$ 172.224
Constit. of the oil of *Anthemis nobilis* (Roman chamomile).

2-Methylpropyl ester: [80758-68-5]
$C_9H_{16}O_3$ 172.224
Constit. of the oil of *Anthemis nobilis* (Roman chamomile).

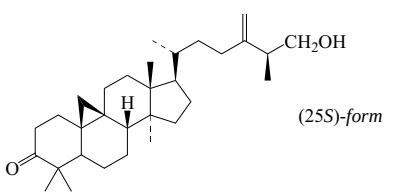
2-Methylbutyl ester: [80758-69-6]
$C_{10}H_{18}O_3$ 186.25
Constit. of the oil of *Anthemis nobilis* (Roman chamomile).

3-Methylbutyl ester: [80758-72-1]
$C_{10}H_{18}O_3$ 186.25
Constit. of the oil of *Anthemis nobilis* (Roman chamomile).

[106060-25-7]

Loeffler, A. *et al., Helv. Chim. Acta*, 1970, **53**, 383-403 (*synth*)
Goldberg, O. *et al., Helv. Chim. Acta*, 1976, **59**, 1904-1910 (*synth, ester*)
Klimes, I. *et al., Helv. Chim. Acta*, 1981, **64**, 2338-2349 (*isol, ester*)
Hoffmann, H.M.R. *et al., Angew. Chem., Int. Ed.*, 1983, **22**, 795-796 (*synth*)
Drewes, S.E. *et al., Synth. Commun.*, 1985, **15**, 1067-1074 (*synth*)
Huot, J.-F. *et al., Chem. Lett.*, 1991, 1599-1602 (*synth*)
Kita, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 12-20 (*synth, ir, pmr*)

26-Hydroxy-24-methylenecycloartan-3-one H-583



(25*S*)-*form*

$C_{31}H_{50}O_2$ 454.735

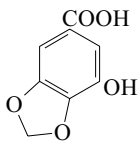
(25*S*)-*form* [232266-06-7]
Constit. of *Mangifera indica* (mango). Needles ($CHCl_3$/MeOH). Mp 145-146°. $[\alpha]_D^{30}$ +175 (c, 0.6 in $CHCl_3$).

(25ξ)-*form* [178117-39-0]
Amorph. solid. Mp 138-140°. $[\alpha]_D$ +18.7 (c, 0.05 in $CHCl_3$).

Pupo, M.T. *et al., Phytochemistry*, 1996, **42**, 795 (*isol, pmr, cmr*)
Anjaneyulu, V *et al., Phytochemistry*, 1999, **50**, 1229-1236 (*isol, pmr, cmr*)

3-Hydroxy-4,5-methylenedioxybenzoic acid H-584

7-Hydroxy-1,3-benzodioxole-5-carboxylic acid



$C_8H_6O_5$ 182.132

Me ether: [526-34-1] *3-Methoxy-4,5-methylenedioxybenzoic acid. 5-Methoxypiperonylic acid. Myristicic acid. Myristicin acid*
$C_9H_8O_5$ 196.159
Isol. from seeds of *Apium graveolens*. Needles (MeOH). Mp 212°.

Me ether, Me ester: [22934-58-3]
$C_{10}H_{10}O_5$ 210.186
Cryst. (EtOAc/2-propanol). Mp 91°. Bp_2 138°.

Me ether, chloride: [76015-47-9]
$C_9H_7ClO_4$ 214.605
Needles (C_6H_6/petrol). Mp 105°. Bp_{20} 189-190°.

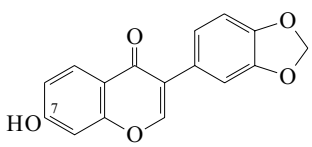
Me ether, amide:
$C_9H_9NO_4$ 195.174
Needles + $1H_2O$ (H_2O). Mp 184°.

Me ether, nitrile: [6443-68-1] *3-Methoxy-4,5-methylenedioxybenzonitrile, 8CI*
$C_9H_7NO_3$ 177.159
Cryst. (MeOH). Mp 154-155°.

Salway, A.H. *et al., J.C.S.*, 1909, **95**, 1161; 1911, **99**, 268 (*synth*)
Baker, W. *et al., J.C.S.*, 1932, 1283 (*synth*)
Seshadri, T.R. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1950, **32**, 25 (*synth*)
Dallacker, F. *et al., Monatsh. Chem.*, 1960, **91**, 1089; 1103; 1969, **100**, 560 (*synth*)
Garg, G.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 658; 1979, **18**, 352 (*isol*)
Dallacker, F. *et al., Z. Naturforsch., C*, 1978, **33**, 465 (*synth*)
Baba, K. *et al., CA*, 1984, **101**, 97724 (*isol*)
Barrero, A.F. *et al., Phytochemistry*, 1994, **37**, 1351 (*isol, deriv*)

7-Hydroxy-3′,4′-methylenedioxyisoflavone H-585

[90-29-9]
*3-(1,3-Benzodioxol-5-yl)-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI.* ***Pseudobaptigenin****. ψ-Baptigenin*



$C_{16}H_{10}O_5$ 282.252
Isol. from *Pisum sativum* (pea) and *Trifolium pratense* (red clover). Mp 296-298°.

O-*β*-D-*Glucopyranoside:* [63347-43-3]
Rothindin
$C_{22}H_{20}O_{10}$ 444.394
Isol. from *Trifolium pratense* (red clover). Needles (MeOH). Mp 236-237°. $[\alpha]_D^{32}$ -37.5 (Py).

Schmidt, O. *et al., Monatsh. Chem.*, 1929, **53**, 454 (*isol, struct*)
Baker, W. *et al., J.C.S.*, 1953, 1582 (*synth*)
Bevan, C.W.L. *et al., J.C.S.(C)*, 1966, 509 (*pmr*)
Dhoubhadel, S.P. *et al., Indian J. Chem., Sect. B*, 1975, **52**, 440 (*synth*)
Nair, A.G.R. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 801 (*Rothindin*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Murthy, M.S.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 225 (*cmr*)
Schuda, P.F. *et al., J.O.C.*, 1987, **52**, 1972 (*synth*)
Khan, I.A. *et al., J. Nat. Prod.*, 2000, **63**, 1414-1416 (*activity*)
Wang, Y. *et al., Synth. Commun.*, 2001, **31**, 3423-3427 (*Rothindin, synth*)

1-Hydroxy-3-methylene-2-pentanone H-586

3-Ethyl-1-hydroxy-3-buten-2-one
$H_2C{=}C(CH_2CH_3)COCH_2OH$
$C_6H_{10}O_2$ 114.144

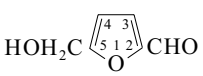
Me ether: [55956-45-1] *1-Methoxy-3-methylene-2-pentanone. 3-Ethyl-1-methoxy-3-buten-2-one*
$C_7H_{12}O_2$ 128.171
Constit. of *Actinidia chinensis* (kiwi fruit), *Phaseolus lunatus* (butter bean) and *Jasminum sambac* (Arabian Jasmine).

Liu, S.H. *et al., J. Agric. Food Chem.*, 1989, **37**, 496 (*isol*)
Tatsuka, K. *et al., J. Agric. Food Chem.*, 1990, **38**, 2176 (*isol*)

5-Hydroxymethyl-2-furancarboxaldehyde, 9CI H-587

[67-47-0]

[25376-49-2]
5-Hydroxymethylfurfural. 2-Formyl-5-hydroxymethylfuran



$C_6H_6O_3$ 126.112
Obtainable from various carbohydrates. Present in tomatoes, tobacco oil etc. Constit. of numerous plant spp.. Used as an index of heat treatment and deterioration in food such as tomato paste, honey and fruit juices. Also an indicator of adulteration with acid-converted invert sugars. Needles. Mp 35-35.5° (31.5°). $Bp_{0.02}$ 110°. n_D^{18} 1.5627.
► Exp. tumorigen. LT7031100

Oxime: [37110-03-5]
$C_6H_7NO_3$ 141.126
Cryst. Mp 108° (*E*-) Mp 77-78° (*Z*-).

Phenylhydrazone:
Cryst. Mp 140°.

Semicarbazone:
Cryst. Mp 192° (166-167°).

O-*β*-D-*Glucopyranoside:* [135213-82-0]
$C_{12}H_{16}O_8$ 288.254
Prisms (Me_2CO). Mp 96°. $[\alpha]_D^{20}$ +131 (c, 1 in MeOH).

O-*β*-D-*Glucopyranoside, 2,4-dinitrophenylhydrazone:*
Orange cryst. (EtOAc). Mp 186°. $[\alpha]_D^{20}$ +80.8 (c, 1 in DMSO).

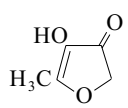
Ac: [10551-58-3]
$C_8H_8O_4$ 168.149
Cryst. (MeOH/petrol). Mp 55-56° (33°).

2-Hydroxyphenyl ether:5-[(2-Hydroxyphenoxy)methyl]-2-furancarboxaldehyde. 5-(2-Hydroxyphenoxymethyl)furfural
$C_{12}H_{10}O_4$ 218.209
Mp 102-103°. λ_{max} 278 (log ϵ 3.52) (MeOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 584B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 26A (*nmr*)
Teunissen, H.P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1930, **49**, 784 (*bibl*)
Haworth, W.N. *et al., J.C.S.*, 1944, 667 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 919
Fukuzumi, T. *et al., Holzforschung*, 1966, **20**, 51; *CA*, **65**, 9158e (*Ac, ir*)
Harris, D.W. *et al., J.O.C.*, 1974, **39**, 724 (*synth*)
Hearn, M.T.W. *et al., Aust. J. Chem.*, 1976, **29**, 107 (*cmr*)
Gaset, A. *et al., Inf. Chim.*, 1981, **212**, 179; **214**, 203 (*revs*)
Fayet, C. *et al., Carbohydr. Res.*, 1983, **122**, 59 (*synth*)
El Hajj, T. *et al., Bull. Soc. Chim. Fr.*, 1987, 855 (*synth, pmr, ms*)
Kulkarni, A.D. *et al., J. Sci. Ind. Res.*, 1989, **47**, 335 (*rev*)
Antal, M.J. *et al., Carbohydr. Res.*, 1990, **199**, 91 (*formn from sugars*)
Lichtenthaler, F.W. *et al., Annalen*, 1993, 967 (*glucoside*)
Shimizu, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1469 (*isol, props*)
Cottier, L. *et al., Synthesis*, 1995, 303 (*Ac*)
Theobald, A. *et al., J. Agric. Food Chem.*, 1998, **46**, 1850-1854 (*anal, hplc*)
Kuo, Y.-H. *et al., J. Nat. Prod.*, 2002, **65**, 1165-1167 (*2-hydroxyphenyl ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ORG000

4-Hydroxy-5-methyl-3(2*H*)-furanone, 9CI H-588

[19322-27-1]
Norfuraneol



$C_5H_6O_3$ 114.101
Isol. from oil of figs and from guava. Beef flavouring ingredient. Cryst. (Et_2O/petrol). Mp 126.6-127.5° (dec.).

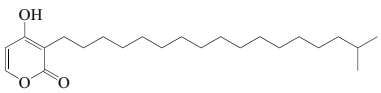
O-*β*-D-*Glucopyranoside:* [166990-08-5]
Psydrin
$C_{11}H_{16}O_8$ 276.243
$[\alpha]_D^{20}$ -66.2 (c, 0.1 in MeOH).

Peer, H.G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1968, **87**, 1011-1016; 1017-1020 (*synth, ir, pmr, ms*)
Re, L. *et al., Helv. Chim. Acta*, 1973, **56**, 1882-1894 (*synth, ir, pmr, ms*)

Hicks, K.B. *et al., J. Agric. Food Chem.*, 1975, **23**, 957-960; *CA*, **83**, 164458v
Ger. Pat., 1978, 2 812 713; *CA*, **90**, 38775c (*synth*)
Shono, T. *et al., J.O.C.*, 1983, **48**, 5126-5128 (*synth*)
Idstein, H. *et al., J. Agric. Food Chem.*, 1985, **33**, 138 (*isol*)
Farine, J.P. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 2026 (*isol, ir, ms*)
Boo, Y.-C. *et al., CA*, 1995, **122**, 101677u (*isol*)
Nahrstedt, A. *et al., Phytochemistry*, 1995, **39**, 375 (*Psydrin*)
Comte, G. *et al., Phytochemistry*, 1996, **41**, 1329 (*Psydrin*)

4-Hydroxy-3-(16-methylheptadecyl)-2*H*-pyran-2-one, 9CI H-589

[203300-23-6]



$C_{23}H_{40}O_3$ 364.567
Constit. of *Centella asiatica* (Asiatic pennywort). Solid. Mp 82°. λ_{max} 268 (MeOH).

Srivastava, R. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 963-964 (*isol, uv, ir, pmr, cmr, ms*)

3-(Hydroxymethyl)-2-heptanone, 9CI H-590

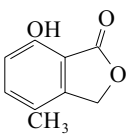
[65405-68-7]
$H_3CCOCH(CH_2OH)(CH_2)_3CH_3$
$C_8H_{16}O_2$ 144.213

(±)-*form*
Food additive. Bp_{25} 169-175°.

Ramaswami, S. *et al., J.O.C.*, 1964, **29**, 2245-2248 (*synth, ir*)

7-Hydroxy-4-methyl-1(3*H*)-isobenzofuranone H-591

[62596-59-2]
7-Hydroxy-4-methylphthalide



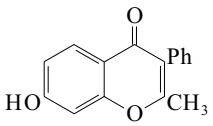
$C_9H_8O_3$ 164.16
Cryst. (C_6H_6). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 123-125° Mp 167°. λ_{max} 228 (ε 6200); 243 (ε 6650); 305 (ε 4600) (EtOH).

O-*[β-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [170473-74-2]
$C_{20}H_{26}O_{12}$ 458.418
Constit. of the bark of *Quillaja saponaria* (soap-bark tree). Cryst. $[\alpha]_D^{20}$ +88.5 (c, 0.3 in H_2O). Incorrect anomer of arabinosyl moiety named in CA.

Asaoka, M. *et al., Chem. Lett.*, 1977, 167-170 (*synth*)
Sawai, K. *et al., Agric. Biol. Chem.*, 1984, **48**, 3151-3152 (*isol, uv, ir, pmr, cmr*)
Steinbeck, C. *et al., Phytochemistry*, 1995, **40**, 1313 (*glycoside*)

7-Hydroxy-2-methylisoflavone H-592

[2859-88-3]
*7-Hydroxy-2-methyl-3-phenyl-4*H*-1-benzopyran-4-one, 9CI*



$C_{16}H_{12}O_3$ 252.269
Isol. from roots of *Glycyrrhiza glabra* (licorice). Mp 240°.

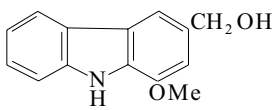
Ac: [3211-63-0]
$C_{18}H_{14}O_4$ 294.306
Isol. from *Glycyrrhiza glabra* (licorice). Mp 161-162°.

Me ether: [19725-44-1] *7-Methoxy-2-methylisoflavone*
$C_{17}H_{14}O_3$ 266.296
Isol. from *Glycyrrhiza glabra* (licorice). Mp 142-143°.

Woods, L.L. *et al., CA*, 1965, **62**, 6454f (*synth*)
Bhardwaj, D.K. *et al., Phytochemistry*, 1976, **15**, 352-353 (*isol*)

3-Hydroxymethyl-1-methoxycarbazole H-593

[3909-78-2]
*1-Methoxy-9*H*-carbazole-3-methanol, 9CI.* ***Koenoline***



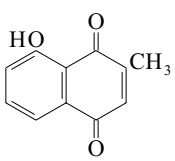
$C_{14}H_{13}NO_2$ 227.262
Alkaloid from the root bark of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6/petrol). Mp 142° (130°). Partially converted to Murrayanine (see 1-Hydroxy-9*H*-carbazole-3-carboxaldehyde, H-379) on standing at r.t..

O-*Ac:*
Cryst. (Py aq.). Mp 110°.

Chakraborty, D.P. *et al., Tetrahedron*, 1965, **21**, 681 (*synth*)
Fiebig, M. *et al., Phytochemistry*, 1985, **24**, 3041 (*isol, uv, ir, pmr, cmr, ms*)
Knölker, H.-J. *et al., Tetrahedron*, 1993, **49**, 11221 (*synth*)
Bringmann, G. *et al., Synthesis*, 1998, 1501-1505 (*synth, ms*)

8-Hydroxy-2-methyl-1,4-naphthoquinone H-594

[14777-17-4]
8-Hydroxy-2-methyl-1,4-naphthalenedione, 9CI. ***Isoplumbagin***



$C_{11}H_8O_3$ 188.182
Constit. of *Juglans regia* (walnut) and *Juglans nigra* (black walnut). Orange cryst. Mp 67-68°.

Me ether: [22273-29-6] *8-Methoxy-2-methyl-1,4-naphthoquinone*
$C_{12}H_{10}O_3$ 202.209
Mp 133-135°.

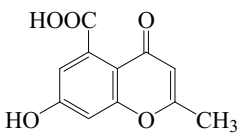
Hiranuma, H. *et al., J.O.C.*, 1982, **47**, 5083-5088 (*Me ether, synth, ir, pmr*)
Laatsch, H. *et al., Annalen*, 1984, 319-339 (*synth, ir, pmr*)
Binder, R.G. *et al., Phytochemistry*, 1989, **28**, 2799-2801 (*isol, pmr, ms*)
Gupta, S. *et al., Phytochemistry*, 1993, **33**, 723-724 (*isol, pmr, cmr*)

3-(Hydroxymethyl)-2-octanone, 9CI H-595

[59191-78-5]
FEMA 3292
$H_3C(CH_2)_4CH(CH_2OH)COCH_3$
$C_9H_{18}O_2$ 158.24
Flavouring ingredient. Liq. with musty herbaceous, sweet, sl. earthy odour. d_{13}^{13} 0.93. Bp_{14} 128°.

Dubois, J.E. *et al., Ann. Chim. (Paris)*, 1951, **6**, 406-486 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 367 (*use*)

7-Hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-carboxylic acid H-596



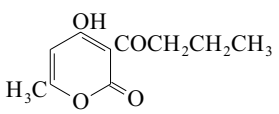
$C_{11}H_8O_5$ 220.181
Constit. of *Rheum* sp..

7-O-β-D-Glucopyranoside:
$C_{17}H_{18}O_{10}$ 382.323
Constit. of *Rheum* sp..

Traditional Chinese Medicines, (ed. Milne, G.A.), Ashgate, 1999, 883; 884

4-Hydroxy-6-methyl-3-(1-oxobutyl)-2*H*-pyran-2-one, 9CI H-597

[22073-85-4]



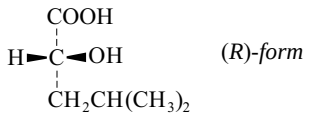
$C_{10}H_{12}O_4$ 196.202
Constit. of *Pogostemon cablin* (patchouli). Cryst. (MeOH). Mp 57-59°.

Marcus, E. *et al., J. Het. Chem.*, 1969, **6**, 13 (*synth*)
Caputo, O. *et al., Gazz. Chim. Ital.*, 1977, **107**, 455 (*synth*)
De Rijke, D. *et al., Phytochemistry*, 1978, **17**, 1664 (*isol*)
Suzuki, T. *et al., Appl. Entomol. Zool.*, 1993, **28**, 108 (*isol*)

2-Hydroxy-4-methylpentanoic acid, 9CI H-598

[498-36-2]

2-Hydroxy-4-methylvaleric acid, 8CI. Leucic acid. Leucinic acid



(*R*)-*form*

$C_6H_{12}O_3$ 132.159

(±)-*form* [10303-64-7]
Mp 76-77°.

Me ester: [40348-72-9] *FEMA 3706*
$C_7H_{14}O_3$ 146.186
Flavouring ingredient. Liq. Bp_{10} 72°. n_D^{20} 1.4250.

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 514 (*Me ester*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1782 (*Me ester*)

4-Hydroxy-4-methyl-2-pentanone, 9CI H-599

[123-42-2]

Diacetone alcohol. Acetonyldimethylcarbinol. Pyranton A

$(H_3C)_2C(OH)CH_2COCH_3$

$C_6H_{12}O_2$ 116.16

Isol. from the arctic bramble *Rubus arcticus*. Oil. Sol. H_2O. Mp -44°. Bp 164° Bp_{11} 63-64°.

▶ Skin, mucous membrane and severe eye irritant. Inhalation causes headache, nausea, eye and pulmonary effects. Exp. hepatotoxic. Flammable, fl. p. 55/59/64°, autoignition temp. 603/643°. OES: long-term 50 ppm; short-term 75 ppm.
SA9100000

Oxime: [17918-67-1]
$C_6H_{13}NO_2$ 131.174
Mp 104-105° (58.5°).

2,4-Dinitrophenylhydrazone: [95122-53-5]
Mp 198-199°.

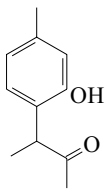
Me ether: [107-70-0] *4-Methoxy-4-methyl-2-pentanone. Pentoxone*
$C_7H_{14}O_2$ 130.186
Bp_{22} 95° Bp_{10} 48°.

▶ SA9185000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 655B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 421C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 507D (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 199 (*synth*)
Lorette, N.B. *et al., J.O.C.*, 1958, **23**, 937 (*Me ether*)
Epstein, W. *et al., Experientia*, 1964, **20**, 390 (*isol*)
Nourse, J.G. *et al., J.A.C.S.*, 1975, **97**, 4584 (*cmr*)
Lechevallier, A. *et al., Tetrahedron*, 1983, **39**, 3317 (*Me ether*)
March, R.E. *et al., Can. J. Chem.*, 1988, **66**, 591 (*ms*)
Sato, S. *et al., J. Organomet. Chem.*, 1988, **352**, 223 (*Me ether*)
Coleman, W.M. *et al., Appl. Spectrosc.*, 1989, **43**, 305 (*ir*)
Grote, R. *et al., Annalen*, 1990, 525 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DBF750; MEX250
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 702

3-(2-Hydroxy-4-methylphenyl)-2-butanone, 9CI H-600

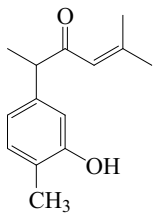
[83810-64-4]



$C_{11}H_{14}O_2$ 178.23
Constit. of peppermint oil. Cryst. (EtOH). Mp 67-68°.

Sukari, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 1249

2-(3-Hydroxy-4-methylphenyl)-5-methyl-4-hexen-3-one H-601

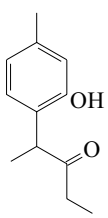


$C_{14}H_{18}O_2$ 218.295
Constit. of the oil of turmeric (*Curcuma longa*).

Jayaprakasha, G.K. *et al., Z. Naturforsch., C*, 2001, **56**, 40-44

2-(2-Hydroxy-4-methylphenyl)-3-pentanone, 9CI H-602

[86843-15-4]

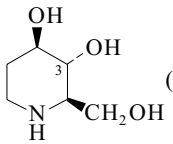


$C_{12}H_{16}O_2$ 192.257
Constit. of peppermint oil. Cryst. (EtOH). Mp 71-72°.

Sakurai, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 1249

2-(Hydroxymethyl)-3,4-piperidinediol, 9CI H-603

3,4-Dihydroxy-2-(hydroxymethyl)piperidine. 3,4-Dihydroxy-2-piperidinemethanol. 1,2,5-Trideoxy-1,5-iminohexitol



(2*R*,3*R*,4*R*)-*form*

$C_6H_{13}NO_3$ 147.174

Care needed with numbering; if named as an iminosugar the numbering is different.

(2*R*,3*R*,4*R*)-*form* [53185-12-9]
Fagomine
Alkaloid from buckwheat seeds (*Fagopyrum esculentum*). Needles (MeOH/EtOH). Mp 186-188°. $[\alpha]_D^{11}$ +23 (c, 1 in H_2O). $[\alpha]_D^{11}$ +37 (c, 1 in 0.1*M* HCl).

Hydrochloride:
Mp 176-177°.

*3-O-β-D-Glucopyranosyl:**3-O-β-D-Glucopyranosylfagomine***
$C_{12}H_{23}NO_8$ 309.316
Cryst. (MeOH/EtOH/Me_2CO). Mp 232-233° dec. $[\alpha]_D^{20}$ -3.1 (c, 1.2 in H_2O). Can also be named as 4-glucopyranosylfagomine (confusion with 4-isomer below).

*4-O-β-D-Glucopyranosyl:**4-O-β-D-Glucopyranosylfagomine***
$C_{12}H_{23}NO_8$ 309.316
$[\alpha]_D$ -18.2 (c, 0.48 in H_2O). Can also be numbered as the 3-isomer (see above).

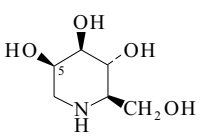
(2*R*,3*R*,4*S*)-*form*
***4-Epifagomine**. 3-Epifagomine*
Alkaloid from roots of *Morus alba* (white mulberry). Powder. $[\alpha]_D$ +69 (c, 0.5 in H_2O). Numbering systems vary.

(2*R*,3*S*,4*S*)-*form*
3,4-Diepifagomine
$[\alpha]_D$ -8.7 (c, 0.3 in H_2O).

Koyama, M. *et al., Agric. Biol. Chem.*, 1974, **38**, 1111 (*ir, pmr, ms, struct*)
Evans, S.V. *et al., Tet. Lett.*, 1985, **26**, 1465 (*deriv*)
Fleet, G.W.J. *et al., Tet. Lett.*, 1985, **26**, 1469 (*abs config, synth*)
Molyneux, R.J. *et al., J. Nat. Prod.*, 1988, **51**, 1198-1206 (*isol*)
Asano, N. *et al., Carbohydr. Res.*, 1994, **259**, 243 (*3-Epifagomine*)
Kato, A. *et al., J. Nat. Prod.*, 1997, **60**, 312-314 (*glucoside, diepimer*)
Schneider, C. *et al., Eur. J. Org. Chem.*, 1998, 1155-1159 (*synth*)

2-(Hydroxymethyl)-3,4,5-piperidinetriol, 12CI H-604

3,4,5-Trihydroxy-2-piperidinemethanol. 3,4,5-Trihydroxy-2-hydroxymethylpiperidine. 1,5-Dideoxy-1,5-iminohexitol



(2*R*,3*R*,4*R*,5*R*)-*form*

$C_6H_{13}NO_4$ 163.173
CAS name was changed for 12CI period. Different numbering systems depending on whether named as a piperidine or as an iminosugar.

(2*R*,3*R*,4*R*,5*S*)-*form* [19130-96-2]
*1,5-Dideoxy-1,5-imino-D-glucitol, 9CI. **Moranoline**. 1-Deoxynojirimycin. S-GI. Antibiotic S-GI*
Alkaloid from *Morus* spp.. Cryst. (MeOH). Mp 206° (195-197°). $[\alpha]_D^{22}$ +44.7 (c, 1 in H_2O). pK_a 6.6. Log P -2.85 (calc).

5-O-*α-D-Galactopyranoside:* [155168-05-1]
2-O-α-D-Galactopyranosyl-1-deoxynojirimycin
$C_{12}H_{23}NO_9$ 325.315
From *Morus alba* (white mulberry). Powder. $[\alpha]_D$ +118.8 (c, 0.1 in H_2O).

N-*Me:* [69567-10-8] *1,5-Dideoxy-1,5-(methylimino)-D-glucitol, 9CI*. **N-*Methyl-1-deoxynojirimycin***. N-*Methylmoranoline*
$C_7H_{15}NO_4$ 177.2
Alkaloid from *Morus alba* (white mulberry). Cryst. (EtOH). Mp 141-142°. $[\alpha]_D^{24}$ +15.5 (H_2O).

Yoshikuni, Y. *et al., Agric. Biol. Chem.*, 1988, **52**, 121 (*Moranoline, pharmacol*)
Ermert, P. *et al., Helv. Chim. Acta*, 1991, **74**, 2043 (*Moranoline, synth*)
Behling, J. *et al., Synth. Commun.*, 1991, **21**, 1383 (*Moranoline, synth*)
Asano, N. *et al., Carbohydr. Res.*, 1994, **253**, 235; **259**, 243 (*N-Methyl-1-deoxynojirimycin, 2-O-α-D-Galactopyranosyl-1-deoxynojirimycin*)
Hughes, A.B. *et al., Nat. Prod. Rep.*, 1994, **11**, 135 (*rev, Moranoline*)
Ikota, N. *et al., Heterocycles*, 1997, **46**, 637-643 (*synth, Moraniline*)

2-Hydroxy-2-methylpropanoic acid, 9CI H-605

[594-61-6]
2-Methyllactic acid, 8CI. 2-Hydroxyisobutyric acid. Acetonic acid
$(H_3C)_2C(OH)COOH$
$C_4H_8O_3$ 104.105
Hygroscopic prisms (Et_2O). Sol. H_2O; spar. sol. C_6H_6. Mp 79°. Bp 212° Bp_{12} 114°.

Nitrile, O-*β-D-glucopyranoside:* [554-35-8]
2-(β-D-Glucopyranosyloxy)-2-methylpropanenitrile, 9CI. ***Linamarin***. *Phaseolunatin. Manihotoxin*
$C_{10}H_{17}NO_6$ 247.247
Occurs in manioc (*Manihot utilissimus*), flax (*Linum usitatissimum*), *Phaseolus lunatus* (butter bean), *Trifolium repens* (white clover) and other plants. First isol in 1830. Needles. Mp 143-144°. $[\alpha]_D$ -28.5 (c, 3.86 in H_2O).
▶ Exp. teratogen. TZ4850000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 518C; 662A; 852D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 807C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 716C (*ir*)
Hepworth, H. *et al., J.C.S.*, 1919, 1207 (*synth*)
Rule, H.G. *et al., J.C.S.*, 1930, 2319 (*synth*)
Butler, G.W. *et al., Phytochemistry*, 1965, **4**, 127 (*Linamarin*)
Gayhema, W.P.J. *et al., Cryst. Struct. Commun.*, 1978, **7**, 463 (*cryst struct*)
Malik, B.K. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 76 (*Linamarin*)
Hirata, K. *et al., CA*, 1990, **114**, 162500n (*Linamarin, anal*)
Olafsdottir, E.S. *et al., Phytochemistry*, 1992, **31**, 4129 (*biosynth*)
Nakajima, N. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 453-458 (*Linamarin, synth, pmr, cmr*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 295 (*nitrile*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GFC100; MLC750

2-Hydroxy-2-methylpropyl glucosinolate H-606

[28463-28-7]
1-Thio-β-D-glucopyranose 1-[3-hydroxy-3-methyl-N-*(sulfooxy)butanimidate]*. ***Glucoconringiin***
$(H_3C)_2C(OH)CH_2C(SGlc)=NOSO_3H$
$C_{11}H_{21}NO_{10}S_2$ 391.42
Isol. from *Conringia orientalis* (hare's ear mustard). Needles (EtOH aq.) (as K salt). Mp 168° dec. (K salt). $[\alpha]_D^{21}$ -10.87 (c, 3.68 in H_2O).

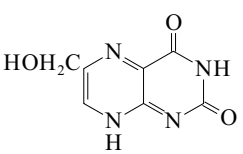
Tetra-Ac:
Needles (EtOH aq.) (as K salt). Mp 152° dec. (K salt). $[\alpha]_D^{24}$ -5.3 (c, 5.3 in H_2O).

[73519-00-3]

Kjaer, A. *et al., Acta Chem. Scand.*, 1956, **10**, 432 (*isol*)
Gmelin, R. *et al., Acta Chem. Scand.*, 1959, **13**, 1718 (*isol*)
Gmelin, R. *et al., Phytochemistry*, 1970, **9**, 599 (*isol*)
Underhill, E.W. *et al., Phytochemistry*, 1972, **11**, 2085 (*biosynth*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)

6-(Hydroxymethyl)-2,4(1*H*,3*H*)-pteridinedione H-607

[10129-99-4]
6-Hydroxymethyllumazine, 8CI

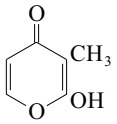


$C_7H_6N_4O_3$ 194.149
Isol. from leaves of spinach *Spinacia oleracea*. Mp 260-262° dec.

Sugiura, K. *et al., CA*, 1966, **65**, 15375; 20508 (*isol, uv, synth, struct*)

2-Hydroxy-3-methyl-4*H*-pyran-4-one H-608

[61892-88-4]



$C_6H_6O_3$ 126.112
Solid.

O-*(6*E*-Cinnamoyl-β-D-glucopyranoside):*
[84888-58-4]
$C_{21}H_{22}O_9$ 418.399
Constit. of the shoots of *Silene vulgaris* (bladder campion). Plates (MeOH). Mp 163-163.7°. $[\alpha]_D^{22}$ -96.8 (c, 1.37 in MeOH).

Schlotzhauer, W.S. *et al., J. Agric. Food Chem.*, 1978, **26**, 1277 (*occur*)
Borris, R.P. *et al., Helv. Chim. Acta*, 1982, **65**, 2481 (*synth, pmr, cmr, isol, deriv*)
Liu, X. *et al., CA*, 1994, **121**, 104077p (*isol*)

3-Hydroxy-2-methyl-4*H*-pyran-4-one, 9CI H-609

[118-71-8]
3-Hydroxy-2-methyl-γ-pyrone. ***Maltol***. *Laricin†. Laricinic acid. Larixinic acid. Veltol. FEMA 2656*

$C_6H_6O_3$ 126.112
Found in chicory, roasted malt, breads, milk, heated butter, uncured smoked pork, cocoa, coffee, roasted barley, roasted peanuts, roasted filbert, soybean etc. Flavour enhancer and flavouring agent. Needles or prisms (toluene or $CHCl_3$) with odour of caramel/butterscotch. Mod. sol. H_2O; sol. EtOH. Mp 161-162°. λ_{max} 318 (MeOH) (Berdy). λ_{max} 274 (ϵ 8400) (HCl) (Berdy). λ_{max} 317 (ϵ 7300) (NaOH) (Berdy).
▶ Skin irritant. LD_{50} (rat, orl) 2330 mg/kg. UQ1050000

O-*[4-Carboxy-3-hydroxy-3-methylbutanoyl-(→6)-β-D-glucopyranoside]:* ***Licoagroside B***
$C_{18}H_{24}O_{12}$ 432.38
Isol. from hairy root cultures of *Glycyrrhiza glabra* (licorice). Powder. $[\alpha]_D^{24}$ -61.4 (c, 0.6 in MeOH). λ_{max} 210 (log ϵ 4.04); 254 (log ϵ 4.07) (MeOH).

Propanoyl: [68555-63-5] *Maltol propionate. FEMA 3941*
$C_9H_{10}O_4$ 182.176
Flavouring agent.

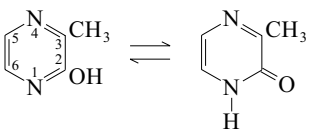
[65416-14-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 457A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 724A (*nmr*)
Spielman, M.A. *et al., J.A.C.S.*, 1947, **69**, 2908 (*synth*)
Shimizu, Y. *et al., Agric. Biol. Chem.*, 1970, **34**, 845 (*isol, ir, ms*)
Food Chemicals Codex, 2nd Ed., 1972, 487 (*anal*)
Chawla, R.K. *et al., J.O.C.*, 1974, **39**, 3281 (*synth, ir, pmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 841 (*rev, tox*)
Torri, S. *et al., Chem. Lett.*, 1976, 495 (*synth*)

Shono, T. *et al., Tet. Lett.*, 1976, 1363 (*synth*)
Tanaka, N. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1015 (*isol*)
Arnarp, J. *et al., Acta Chem. Scand.*, 1990, **44**, 916 (*ms*)
Geordiadis, M. *et al., Org. Prep. Proced. Int.*, 1992, **24**, 95 (***synth***)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 440
Burgess, J. *et al., Acta Cryst. C*, 1996, **52**, 2917 (*cryst struct*)
Atta-ur-Rahman, *et al., J. Nat. Prod.*, 1997, **60**, 472 (*isol, cryst struct*)
Li, W. *et al., Phytochemistry*, 2000, **55**, 447-456 (*Licoagroside B*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAO350

2-Hydroxy-3-methylpyrazine H-610

[19838-07-4]
3-Methyl-2(1H)-pyrazinone, 9CI. 3-Methylpyrazinol, 8CI



$C_5H_6N_2O$ 110.115
Cryst. (EtOAc). Mp 151-152°.

OH-form

Me ether:

[2847-30-5] *2-Methoxy-3-methylpyrazine*
$C_6H_8N_2O$ 124.142
Reported in sherry and krill. Flavouring ingredient, esp. for coffee. Main component (75%) of FEMA 3183, a mixt. with its regioisomers. Liq. Bp_{60} 87°.

Et ether: [32737-14-7] *2-Ethoxy-3-methylpyrazine*
$C_7H_{10}N_2O$ 138.169
Flavouring ingredient with roast chocolate flavour. Component of FEMA 3569, a mixt. with its regioisomers. Bp_{48} 88-90°.

Et ether, 4-oxide:
$C_7H_{10}N_2O_2$ 154.168
Cryst. (EtOH). Mp 121-122.5°.

Karmus, G. *et al., J.A.C.S.*, 1952, **74**, 1580 (*synth*)
Hirschberg, A. *et al., J.O.C.*, 1961, **26**, 2356-2360 (*Et ether, synth*)
Klein, B. *et al., J.O.C.*, 1964, **29**, 2623-2626 (*Et ether, Et ether N-oxide*)
Fr. Pat., 1965, 1 391 212; *CA*, **62**, 16270g (*FEMA 3183*)
Kolor, M.G. *et al., Org. Mass Spectrom.*, 1971, **5**, 959-966 (*Me ether, ms*)
Nakel, G.M. *et al., J. Agric. Food Chem.*, 1972, **20**, 682-684 (*Me ether, struct*)
Bramwell, A.F. *et al., Tetrahedron*, 1972, **28**, 4155-4170; 1973, **29**, 3939 (*synth, pmr*)
Parliment, T.H. *et al., J. Agric. Food Chem.*, 1973, **21**, 714-716 (*synth*)
Calabretta, P.J. *et al., Cosmet. Perfum.*, 1975, **90**, 74; 76; 79-80 (*Me ether, synth, use*)
Macdonald, J.C. *et al., Tetrahedron*, 1976, **32**, 655 (*pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1057-1058; *Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press*, 1995, 1118 (*FEMA 3569, FEMA 3183*)

2-Hydroxy-5-methylpyrazine H-611

5-Methyl-2(1H)-pyrazinone, 9CI. 5-Methylpyrazinol, 8CI

$C_5H_6N_2O$ 110.115

OH-form [20721-17-9]
Cryst. Mp 68-69° Mp 126-128°.

Me ether: [2882-22-6] *2-Methoxy-5-methylpyrazine*
$C_6H_8N_2O$ 124.142
Nut-like flavouring ingredient. Component of FEMA 3183, together with its regioisomers. See also information given under 2-Methoxy-3-methylpyrazine, H-610.

Et ether: [67845-34-5] *2-Ethoxy-5-methylpyrazine*
$C_7H_{10}N_2O$ 138.169
Flavouring ingredient with roast, chocolate odour. Component of FEMA 3183, together with its regioisomers. See also further information given under 2-Ethoxy-3-methylpyrazine, H-610.

Karmus, G. *et al., J.A.C.S.*, 1952, **74**, 1580-1584 (*synth*)
Koelsch, C.F. *et al., J.O.C.*, 1958, **23**, 1603-1606 (*synth*)
Bramwell, A.F. *et al., Tetrahedron*, 1972, **28**, 4155-4170 (*Me ether, synth, pmr*)
Macdonald, J.C. *et al., Tetrahedron*, 1976, **32**, 655-660 (*pmr, cmr*)

2-Hydroxy-6-methylpyrazine H-612

[20721-18-0]
6-Methyl-2(1H)-pyrazinone, 9CI. 6-Methylpyrazinol, 8CI

$C_5H_6N_2O$ 110.115
Cryst. (H_2O). Mp 250-251°.

OH-form

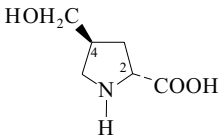
Me ether: [2882-21-5] *2-Methoxy-6-methylpyrazine*
$C_6H_8N_2O$ 124.142
Nut-like flavouring ingredient. Component of FEMA 3183, together with its regioisomers. Constit. of botrytised grape must. Bp_{45} 80°. See also information given under 2-Methoxy-3-methylpyrazine, H-610.

Et ether: [53163-97-6] *2-Ethoxy-6-methylpyrazine*
$C_7H_{10}N_2O$ 138.169
Flavouring ingredient with roast taste and pineapple odour. Component of FEMA 3569, together with its regioisomers. See also further information given under 2-Ethoxy-3-methylpyrazine, H-610.

Karmus, G. *et al., J.A.C.S.*, 1952, **74**, 1580-1584 (*synth*)
Bramwell, A.F. *et al., Tetrahedron*, 1972, **28**, 4155-4170 (*Me ether, synth, pmr*)
U.S. Pat., 1974, 3 803 331; *CA*, **81**, 62394n (*Et ether, synth, use*)
Macdonald, J.C. *et al., Tetrahedron*, 1976, **32**, 655-660 (*pmr, cmr*)
Shimuzu, J. *et al., Agric. Biol. Chem.*, 1982, **46**, 1339-1344 (*Me ether, occur, grape*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1057; *Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press*, 1995, **4**, 1118 (*FEMA 3183, FEMA 3569*)

4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid H-613

[3850-38-2]
4-(Hydroxymethyl)proline, 9CI



(2*R*,4*S*)-*form*

$C_6H_{11}NO_3$ 145.158

(2*R*,4*S*)-*form* [36149-81-2]
D-trans-*form*
Constit. of the seeds of *Eriobotrya japonica* (loquat). Mp 227.5-229°.

(2*S*,4*S*)-*form* [2370-39-0]
L-cis-*form*
Constit. of apples and loquat. Mp 257-258° dec. $[\alpha]_D^{19.5}$ -75.6 (H_2O).

N-*Benzyloxycarbonyl:*
$C_{14}H_{17}NO_5$ 279.292
Mp 115.5-116.5°. $[\alpha]_D^{23}$ -48.5.

Lactone:
$C_6H_9NO_2$ 127.143
Mp 94.5-95.5°.

(2*S*,4*R*)-*form* L-trans-*form*
Mp 227.5-229°. $[\alpha]_{590}$ -48 (H_2O).

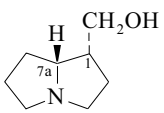
N-*Benzyloxycarbonyl:*
Oil.

(2*RS*,4*RS*)-*form* (±)-cis-*form*
Mp 220-221° dec.

Abraham, R.J. *et al., Nature (London)*, 1961, **192**, 1150 (*pmr, conformn*)
Kenner, G.W. *et al., J.C.S.*, 1965, 3850 (*synth*)
Welter, A. *et al., Phytochemistry*, 1978, **17**, 131 (*occur, isol*)

1-Hydroxymethylpyrrolizidine H-614

Hexahydro-1H-pyrrolizine-1-methanol, 9CI



(1*R*,7*aR*)-*form*

$C_8H_{15}NO$ 141.213

Only simple esters are included here. Many others have individual entries.pK_a 10.83 (26°).

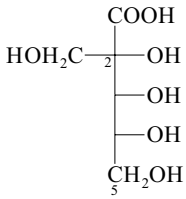
(1*R*,7*aR*)-*form* [488-06-2]
Lindelofidine. *(+)-Isoretronecanol*
Oil or cryst. Mp 40-41°. Bp_2 116-117°. $[\alpha]_D^{23}$ +72 (c, 1 in EtOH).

O-*[β-D-Glucopyranosyl-(→4)-4-hydroxy-*E*-cinnamoyl]:* ***Thesinine 4′-O-glucoside***
$C_{23}H_{31}NO_8$ 449.5
Alkaloid from the seeds of *Borago officinalis* (borago). Amorph. solid. $[\alpha]_D^{20}$ -22.8 (c, 2 in DMSO). λ_{max} 204 (log ε 4.15); 225 (log ε 4.06); 297 (log ε 4.28); 305 (log ε 4.29) (MeOH).

Herrmann, M. *et al., Phytochemistry*, 2002, **60**, 399-402 (*Thesinine, Thesinine 4′-glucoside*)

2-*C*-(Hydroxymethyl)ribonic acid, 9CI H-615

2-Carboxyarabinitol. Hamamelonic acid



D-*form*

$C_6H_{12}O_7$ 196.157

D-*form* [469-09-0]
Needles (MeOH aq.) (as NH_4 salt). Mp 152° (NH_4 salt). $[\alpha]_D$ -3.9 (c, 10 in H_2O).

5-O-Phosphate: [112160-91-5]
$C_6H_{13}O_{10}P$ 276.136
Isol. from the leaves of *Phaseolus vulgaris* (kidney bean).

L-*form*
Needles (MeOH aq.) (as NH_4 salt). Mp 151-152° (NH_4 salt). $[\alpha]_D$ +4.8 (c, 1.2 in 1*M* NH_4OH).

γ-Lactone:
$C_6H_{10}O_6$ 178.141
Plates (MeCN/$CHCl_3$). Mp 88-89°. $[\alpha]_D$ -74 (c, 2.1 in H_2O).

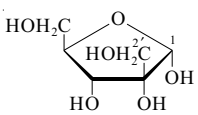
γ-Lactone, tetra-Ac:
$C_{14}H_{18}O_{10}$ 346.29
Cryst. (EtOH). Mp 103-104°. $[\alpha]_D$ -102 (c, 1.6 in $CHCl_3$).

[98587-21-4, 122907-93-1]

Ferrier, R.J. *et al., J.C.S.*, 1962, 3544 (*synth*)
Burton, J.S. *et al., J.C.S.*, 1965, 3433 (*synth*)
Thanbichler, A. *et al., Z. Naturforsch., B*, 1971, **26**, 912 (*synth*)
Gutteridge, S. *et al., Biochem. J.*, 1989, **260**, 711 (*synth*)
Beck, E. *et al., Plant Physiol.*, 1989, **90**, 13 (*pmr, cmr*)
Moore, B.D. *et al., Phytochemistry*, 1993, **34**, 703 (*occur*)

2-*C*-Hydroxymethylribose H-616

Hamamelose



α-D-Furanose-*form*

$C_6H_{12}O_6$ 180.157

D-Furanose-*form*

5-O-(3,4,5-Trihydroxybenzoyl): [90275-97-1] *5-O-Galloylhamamelofuranose*
$C_{13}H_{16}O_{10}$ 332.263
Isol. from *Castanea crenata* (Japanese chestnut). Amorph. powder. $[\alpha]_D^{19}$ +19.9 (c, 1.0 in H_2O). Exists as an equilibrated mixt. of α- and β-anomers.

1,2′-Bis(3,4,5-trihydroxybenzoyl): [90275-98-2] *1,2′-Di-O-galloylhamamelofuranose*
$C_{20}H_{20}O_{14}$ 484.37
Isol. from the bark of *Castanea crenata* (Japanese chestnut). Needles + H_2O (H_2O). Mp 216°. $[\alpha]_D^{27}$ -26.1 (c, 1.0 in Me_2CO aq.). The configuration of the anomeric centre unknown.

1,2′,5-Tris(3,4,5-trihydroxybenzoyl): [90275-99-3] *1,2′,5-Tri-O-galloylhamamelofuranose*
$C_{27}H_{24}O_{18}$ 636.476
Isol. from the bark of *Castanea crenata* (Japanese chestnut). Needles + $^3/_2H_2O$ (H_2O). Mp 230°. $[\alpha]_D^{20}$ -60 (c, 0.9 in Me_2CO aq.). Config. of the anomeric centre unknown.

2,2′,5-Tris(3,4,5-trihydroxybenzoyl): [91573-80-7] *2,2′,5-Tri-O-galloylhamamelofuranose.* ***Kurigalin***
$C_{27}H_{24}O_{18}$ 636.476
A gallotannin isol. from the bark of *Castanea crenata* (Japanese chestnut). Amorph. powder + $2^1/_2H_2O$. $[\alpha]_D^{21}$ +26.3 (c, 1.30 in H_2O). Exists as an equilibrated mixt. of α- and β-anomers.

2′,3,5-Tris(3,4,5-trihydroxybenzoyl): [86588-94-5] *2′,3,5-Tri-O-galloylhamamelofuranose.* ***3-O-Galloylhamamelitannin***
$C_{27}H_{24}O_{18}$ 636.476
Isol. from *Castanea crenata* (Japanese chestnut), *Sanguisorba officinalis* (burnet bloodwort). Needles +H_2O (H_2O). Mp 209-210°. $[\alpha]_D^{23}$ +38.8 (c, 0.79 in Me_2CO aq.). Exists as an equilibrated mixt. of α- and β-anomers.

1,2′,3,5-Tetrakis(3,4,5-trihydroxybenzoyl): [90276-00-9] *1,2′,3,5-Tetra-O-galloylhamamelofuranose*
$C_{34}H_{28}O_{22}$ 788.582
Isol. from the bark of *Castanea crenata* (Japanese chestnut). Needles + $^3/_2H_2O$ (H_2O). Mp 290°. $[\alpha]_D^{22}$ -47.7 (c, 0.45 in Me_2CO aq.). Config. of the anomeric centre unknown.

β-D-Furanose-*form*

2′,5-Bis(3,4,5-trihydroxybenzoyl): [469-32-9] *2′,5-Digalloylhamamelofuranose.* ***Hamamelitannin***
$C_{20}H_{20}O_{14}$ 484.37
Isol. from *Castanea sativa* (sweet chestnut). Prisms or needles + $^1/_2H_2O$ (H_2O). Mp 146-147°. $[\alpha]_D^{19}$ +33 (c, 1.24 in H_2O).

Mayer, W. *et al., Annalen*, 1965, **688**, 232 (*struct, Hamamelitannin*)
Overend, W.G. *et al., J.C.S.*, 1965, 3446 (*D-form, synth*)
Ezekiel, A.D. *et al., Carbohydr. Res.*, 1969, **11**, 233 (*synth, Hamamelitannin*)
Paulsen, H. *et al., Chem. Ber.*, 1972, **105**, 1978 (*D-form, synth*)
Gilck, H. *et al., Carbohydr. Res.*, 1975, **39**, 160 (*D-form, isol*)
Ozawa, T. *et al., Agric. Biol. Chem.*, 1984, **48**, 1411 (*Kurigalin*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1984, **32**, 483 (*gallates*)
Haberland, C. *et al., Phytochemistry*, 1994, **60**, 464 (*gallates*)
Hartisch, C. *et al., Phytochemistry*, 1996, **42**, 191 (*gallates*)
Hricoviniová-Bílicová, Z. *et al., Carbohydr. Res.*, 1999, **319**, 38-46 (*D-form, synth*)

2-Hydroxy-22-methyltetracosanoic acid H-617

[52900-16-0]

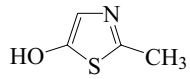
$H_3CCH_2CH(CH_3)CH_2(CH_2)_{18}CH(OH)COOH$

$C_{25}H_{50}O_3$ 398.668
Found in lanolin wool fat. No phys. props. reported.

Fawaz, F. *et al., Ann. Pharm. Fr.*, 1974, **32**, 59 (*occur*)
Carballeira, N.M. *et al., Lipids*, 1992, **27**, 681 (*isol*)

5-Hydroxy-2-methylthiazole H-618

2-Methyl-5-thiazolol



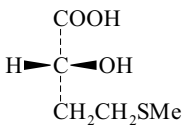
C_4H_5NOS 115.156

Me ether: [38205-64-0] *5-Methoxy-2-methylthiazole, 9CI. FEMA 3192*
C_5H_7NOS 129.182
Flavouring ingredient. Liq. with cabbage-sulfurous odour. $Bp_{0.5}$ 33°.

Ger. Pat., 1972, 2 152 557; *CA*, **77**, 88488p (*Me ether, use*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264-269 (*Me ether, synth, ms, props*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 523 (*Me ether, use*)

2-Hydroxy-4-(methylthio)butanoic acid H-619

[583-91-5]
α-Hydroxy-γ-methylmercaptobutyric acid. Desmeninol, INN. Alimet



(*R*)-*form*

$C_5H_{10}O_3S$ 150.198
▶ ET4731500

(*R*)-*form* [39638-34-1]

[71597-88-1]
Oil; cryst. (EtOAc/petrol)(as dicyclohexylamine salt). Mp 127-129° (dicyclohexylamine salt). $[\alpha]_D^{25}$ +22.2 (c, 1 in EtOH).

(*S*)-*form* [48042-96-2]
Cryst. (as dicyclohexylamine salt). Mp 128-129° (dicyclohexylamine salt). $[\alpha]_D$ -22.5 (c, 1 in EtOH).

Et ester:
$C_7H_{14}O_3S$ 178.252
$[\alpha]_D$ +20.5 (c, 1.12 in MeOH).

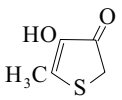
(±)-*form* [120-91-2]
Animal and poultry feed additive.
Cryst. (as Zn salt). Mp 250° (Zn salt).

[71597-86-9]

Akobe, K. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1936, **244**, 14 (*synth*)
Kleeman, A. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 797 (*synth*)
Merck Index, 11th edn., 1989, No. 5897 (*use, bibl*)
Urban, F.J. *et al., J.O.C.*, 1990, **55**, 3670 (*synth, pmr*)

4-Hydroxy-5-methyl-3(2*H*)-thiophenone, 9CI, 8CI H-620

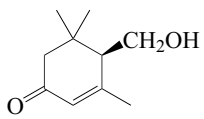
[26494-09-7]



$C_5H_6O_2S$ 130.167
Roasted meat-like flavour component. Cryst. (C_6H_6 under N_2). Polymerises on contact with air.

Mortensen, J.Z. *et al., Tetrahedron*, 1971, **27**, 3839 (*synth, props*)
Hincelin, O. *et al., Food Chem.*, 1992, **44**, 381-389 (*occur*)

4-(Hydroxymethyl)-3,5,5-trimethyl-2-cyclohexen-1-one H-621



(*R*)-*form*

$C_{10}H_{16}O_2$ 168.235

(R)-form

O-*β*-D-*Glucopyranoside:* [214125-03-8]
Jasminoside A
$C_{16}H_{26}O_7$ 330.377
Amorph. powder. $[\alpha]_D$ -33 (c, 0.06 in MeOH). λ_{max} 236 (log ϵ 3.75) (MeOH).

(S)-form

O-*β*-D-*Glucopyranoside:* [189148-81-0]
Epijasminoside A
Constit. of saffron (*Crocus sativus*). Amorph. powder. $[\alpha]_D$ -91.4 (c, 0.35 in MeOH). λ_{max} 236 (log ϵ 3.95) (MeOH).

Straubinger, M. *et al., J. Agric. Food Chem.*, 1997, **45**, 1678-1681 (*isol, glucoside*)
Machida, K. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1295-1300 (*isol, pmr, cmr*)

28-Hydroxy-6-methyl-5-tritriacontanone, 9CI H-622

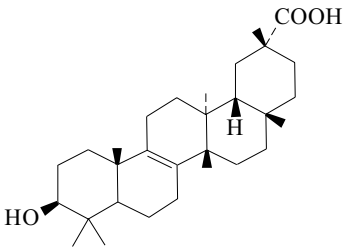
[239091-54-4]

$H_3C(CH_2)_4CH(OH)(CH_2)_{21}CH(CH_3)$-$CO(CH_2)_3CH_3$

$C_{34}H_{68}O_2$ 508.91
Constit. of the fruit of the famine food (*Momordica dioica*).

Ali, M. *et al., Indian J. Pharm. Sci.*, 1998, **60**, 287-289

3-Hydroxy-8-multifloren-29-oic acid H-623



$C_{30}H_{48}O_3$ 456.707

3β-*form* [24480-45-3]
Bryonolic acid
Constit. of *Sandoricum indicum* (santol). Cryst. (EtOAc). Mp 300-303°. $[\alpha]_D$ +24 (c, 2.53 in Py).

Ac: [24480-46-4]
$C_{32}H_{50}O_4$ 498.745

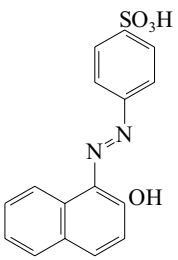
3-Ketone: [24480-44-2] *3-Oxo-8-multifloren-29-oic acid.* ***Bryonomic acid***
$C_{30}H_{46}O_3$ 454.692
Constit. of *Sandoricum indicum* (santol). Cryst. (Me_2CO/MeOH). Mp 244-245°. $[\alpha]_D$ +37.6 (c, 8.0 in $CHCl_3$).

Sim, K.Y. *et al., Phytochemistry*, 1972, **11**, 3341
Cattel, L. *et al., Planta Med.*, 1981, **41**, 328-336 (*occur, Ac*)
Kamisako, W. *et al., Org. Magn. Reson.*, 1984, **22**, 93 (*cmr*)
Kamisako, W. *et al., Magn. Reson. Chem.*, 1987, **25**, 848 (*cmr*)
Cho, H.J. *et al., Phytochemistry*, 1992, **31**, 3893 (*occur*)
Tabata, M. *et al., J. Nat. Prod.*, 1993, **56**, 165 (*isol, use*)
Cho, H.J. *et al., Phytochemistry*, 1993, **33**, 1407 (*biosynth*)
Kosela, S. *et al., Phytochemistry*, 1995, **38**, 691 (*Bryononic acid, pmr, cmr, cryst struct*)
Akiyama, K. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 762-769 (*isol, pmr, cmr, ms*)

4-[(2-Hydroxy-1-naphthalenyl)azo]benzenesulfonic acid, 9CI H-624

[573-89-7]

[633-96-5]
1-(4-Sulfophenylazo)-2-naphthol. C.I. 15510 Acid orange 7. C.I. 15510 Pigment orange 17. Acid orange A. Orange II. Mandarin G. Wool orange A. DFC Orange 4. Acid orange II. Acid orange 7. Tropaeolin OOO

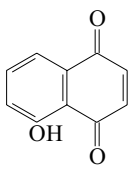


$C_{16}H_{12}N_2O_4S$ 328.348
Mainly used as the Na salt, to which some of the names apply. Food dye. Banned by the FDA for food use. Orange needles + $5H_2O$ (H_2O)(as Na salt). Sol H_2O, EtOH.

Sigma-Aldrich Library of Stains, Dyes and Indicators, 541
Ruggli, P. *et al., Helv. Chim. Acta*, 1924, **7**, 496 (*synth*)
Org. Synth., 1943, 36 (*synth*)
Popa, G. *et al., Zh. Anal. Khim.*, 1959, **14**, 322 (*use*)
Hseu, T.M. *et al., J. Chin. Chem. Soc. (Taipei)*, 1971, **18**, 203 (*detn, Co*)
Nursten, H.E. *et al., J. Soc. Dyers Colour.*, 1973, **89**, 49 (*purifn*)
Bell, S. *et al., J. Assoc. Off. Anal. Chem.*, 1975, **58**, 717 (*anal*)
Kawase, J. *et al., Analyst (London)*, 1979, **104**, 750 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2656n
Merck Index, 11th edn., 1989, No. 6813

5-Hydroxy-1,4-naphthoquinone H-625

[481-39-0]
5-Hydroxy-1,4-naphthalenedione, 9CI. ***Juglone****. Nucin. Regianin. PD7. Antibiotic PD7. CI 75500. C.I. Natural Brown 7*



$C_{10}H_6O_3$ 174.156
Occurs in *Juglans* spp. and pecan nuts (*Carya illinoensis*). Yellow needles (C_6H_6/petrol). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 155°. Log P 1.52 (calc). Sublimes. Steam-volatile λ_{max} 282 ; 350 ; 533 (MeOH/NaOH) (Berdy). λ_{max} 251 (ϵ 14300); 337 (ϵ 1200); 415 (sh) (ϵ 3600); 429 (ϵ 3800) ($CHCl_3$). λ_{max} 245 (ϵ 12880); 340 (sh) (ϵ 1130); 407 (sh) (ϵ 3550); 422 (ϵ 3630) (MeOH).

▶ LD_{50} (mus, orl) 2.5 mg/kg; LD_{50} (mus, ipr) 25 mg/kg. Exp. neoplastic agent. QJ5775000

O-*β*-D-*Glucopyranoside:* [22427-35-6]
$C_{16}H_{16}O_8$ 336.298
Isol. from pecan nuts. Yellow powder.

1-Monoxime:
$C_{10}H_7NO_3$ 189.17
Red needles (EtOH aq.). Mp 187-187.5°.

4-Monoxime:
$C_{10}H_7NO_3$ 189.17
Mp 203°.

Ac: [5196-28-1]
$C_{12}H_8O_4$ 216.193
Yellow plates (EtOH). Mp 154-155°.

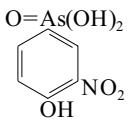
Me ether: [4923-61-9] *5-Methoxy-1,4-naphthoquinone*
$C_{11}H_8O_3$ 188.182
Red solid (EtOH). Mp 186-187°.

2,3-Dihydro: [6312-53-4] *2,3-Dihydro-5-hydroxy-1,4-naphthoquinone.* ***β-Hydrojuglone***
$C_{10}H_8O_3$ 176.171
Greenish-yellow needles ($CHCl_3$). Mp 96-97°. Oxid. to Juglone on standing.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 85C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 80B (*ir*)
Singh, I. *et al., Tetrahedron*, 1968, **24**, 6053-6073 (*uv*)
Cradwick, P.D. *et al., Acta Cryst. B*, 1971, **27**, 1468-1470 (*cryst struct*)
Moir, M. *et al., Phytochemistry*, 1973, **12**, 1351-1353 (*2,3-dihydro, isol*)
Torssell, K. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 353-357 (*synth*)
Hanson, R.W. *et al., J. Chem. Educ.*, 1976, **53**, 400 (*synth, props*)
Kobayashi, M. *et al., Tet. Lett.*, 1976, 619-620 (*cmr*)
Grundmann, C. *et al., Synthesis*, 1977, 644-645 (*synth, bibl*)
Hedin, P.A. *et al., J. Agric. Food Chem.*, 1980, **28**, 340-342 (*glucoside*)
Farina, F. *et al., Synthesis*, 1985, 781-784 (*synth*)
Barret, R. *et al., Synth. Commun.*, 1990, **20**, 2907-2912 (*synth*)
Masquelin, T. *et al., Synthesis*, 1995, 780-786 (*Me ether, synth, ir, pmr, ms*)
Contant, P. *et al., Synthesis*, 1999, 821-828 (*Me ether*)
Munday, R. *et al., Planta Med.*, 2000, **66**, 399-402 (*activity*)
Villemin, D. *et al., Synth. Commun.*, 2002, **32**, 1501-1515 (*synth, uv, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, WAT000

(4-Hydroxy-3-nitrophenyl)arsonic acid, 9CI H-626

[121-19-7]
(4-Hydroxy-3-nitrobenzene)arsonic acid. ***Roxarsone, BAN, INN, USAN.*** *Ren-O-sal. Ristat. NSC 2101*



$C_6H_6AsNO_6$ 263.038

Interatomic distances: As–C 191, C–N 147, C–O 136, As–O 167-173 pm. Used to control enteric infections in chicken and to improve growth and feed efficiency. FDA approved additive for chicken, turkey and swine feeds. Pale yellow needles or plates (H_2O). Spar. sol. hot H_2O; insol. Et_2O, EtOAc; v. sol. MeOH, EtOH, Me_2CO. Mp 300°. Log P -0.23 (calc). Puffs up and deflagrates on heating.

▶ LD_{50} (rat, orl) 155 mg/kg. Exp. neurotoxic and nephrotoxic props.. CY5250000

Dimethylamine salt: [83340-35-6]
Cryst. (EtOH/Me_2CO). Mp 156-157°.

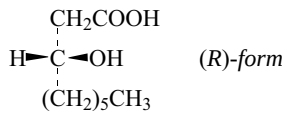
O-*(4-Methylbenzenesulfonyl):*
$C_{13}H_{12}AsNO_8S$ 417.227
Cryst. (MeOH aq.). Mp 171°.

[54599-05-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1142D (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 1019C (*nmr*)
Benda, L. *et al., Ber.*, 1911, **44**, 3445; 3449 (*synth*)
Izmailskii, V.A. *et al., Khim.-Farm. Promst.*, 1933, 317; *CA*, **28**, 3721 (*synth*)
Pressman, D. *et al., J.A.C.S.*, 1943, **65**, 540 (*synth, pKa*)
Patrovsky, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1727 (*detn, Ta*)
Kyrs, M. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 747 (*detn, Zr*)
Chatterjee, A. *et al., Acta Cryst. B*, 1977, **33**, 3593 (*cryst struct*)
Tsentovskii, V.M. *et al., Zh. Obshch. Khim.*, 1982, **52**, 1567; *J. Gen. Chem. USSR (Engl. Transl.)*, 1982, **52**, 1383 (*deriv*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13220
Cullen, W.R. *et al., Appl. Organomet. Chem.*, 1988, **2**, 1 (*hplc*)
Merck Index, 11th edn., 1989, No. 8251
Abdo, K.M. *et al., Toxicol. Lett.*, 1989, **45**, 55
Nuttall, R.H. *et al., Acta Cryst. C*, 1995, **51**, 2342 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HMY000

3-Hydroxynonanoic acid, 9CI H-627

[40165-87-5]
3-Hydroxypelargonic acid



(R)-form

$C_9H_{18}O_3$ 174.239

(R)-form [33796-87-1]
Me ester: [28941-56-2]
$C_{10}H_{20}O_3$ 188.266
Oil. $[\alpha]_D^{20}$ -5.5 (neat).

(S)-form [45023-83-4]
Mp 47-48° Mp 58-59°. $[\alpha]_D^{25}$ +3.3 (c, 12.9 in $CHCl_3$).

Me ester: [66997-65-7]
$[\alpha]_D^{23}$ -1 (c, 1.97 in $CHCl_3$).

Me ether, Me ester:
$C_{11}H_{22}O_3$ 202.293
$[\alpha]_D^{23}$ -0.07 (c, 5.00 in $CHCl_3$).

(±)-*form* [88930-09-0]
Isol. from milk. Mp 61°.

Et ester: [26257-80-7]
$C_{11}H_{22}O_3$ 202.293
Oil. Bp_{13} 145°.

Hydrazide: [33824-92-9]
$C_9H_{20}N_2O_2$ 188.269
Mp 111-112°.

Harding, V.J. *et al., J.C.S.*, 1910, **97**, 299 (*synth*)
Kuhn, M. *et al., Ber.*, 1938, **71**, 1119 (*synth*)
Meyers, A.I. *et al., Tet. Lett.*, 1974, 1333 (*synth*)
Sugimura, T. *et al., Bull. Chem. Soc. Jpn.*, 2002, **75**, 355-363 (*R-form, Me ester*)

5-Hydroxynonanoic acid, 9CI H-628

$H_3C(CH_2)_3CH(OH)CH_2CH_2CH_2COOH$

$C_9H_{18}O_3$ 174.239

(±)-*form*

Hydrazide: [16425-12-0]
$C_9H_{20}N_2O_2$ 188.269
Mp 84.6-85.4°.

Lactone: [3301-94-8] *6-Butyltetrahydro-2H-pyran-2-one, 9CI. FEMA 3356*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient. Oil with a mild nut-like odour and a fatty creamy taste. Prac. insol. H_2O, sol. EtOH. d^{20} 0.99. Bp_{11} 137-138°. n_D^{20} 1.4562.

Rosemund, K.W. *et al., Chem. Ber.*, 1961, **94**, 2401; 2406 (*synth*)
Lardelli, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 481 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 367 (*lactone*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1379-1380 (*lactone*)

1-Hydroxy-3-nonanone, 9CI H-629

[67801-46-1]
$H_3C(CH_2)_5COCH_2CH_2OH$
$C_9H_{18}O_2$ 158.24
Bp_{15} 113°. $n_D^{22.5}$ 1.4280.

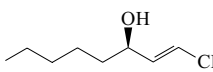
Ac: [7779-54-6]
$C_{11}H_{20}O_3$ 200.277
Flavouring ingredient. Removed from the GRAS list (formerly FEMA 2566). Oily liq. with herbaceous, fruity odour. $Bp_{0.4}$ 100-101°. $n_D^{22.5}$ 1.4340.

Koulkes, M. *et al., Bull. Soc. Chim. Fr.*, 1957, 127-129 (*synth, Ac*)
Cavicchioli, S. *et al., J.O.C.*, 1984, **49**, 1246-1251 (*synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1978 (*Ac*)

4-Hydroxy-2-nonenal H-630

[29343-52-0]

[75899-68-2]



(2*E*,4*R*)-*form*

$C_9H_{16}O_2$ 156.224
Constit. of beef and pork. Lipid peroxidation product.

(2E,4R)-form [119008-08-1]
$[\alpha]_D^{25}$ -46 (c, 0.45 in $CHCl_3$) (95% op).

(2E,4S)-form [119008-09-2]
$[\alpha]_D^{25}$ +47.7 (c, 0.69 in $CHCl_3$) (95% op).

Ac:
$C_{11}H_{18}O_3$ 198.261
Oil. $[\alpha]_D^{25}$ +12.7 ($CHCl_3$).

Di-Et acetal: [158930-55-3] *1,1-Diethoxy-2-nonen-4-ol*
$C_{13}H_{26}O_3$ 230.347
$[\alpha]_D^{22}$ +11.3 (c, 0.36 in CH_2Cl_2).

(±)-(*E*)-*form* [128946-65-6]

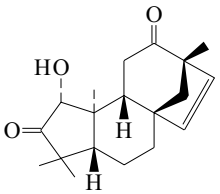
[18286-49-2]
Oil. Sol. $CHCl_3$, hexane; poorly sol. H_2O. $Bp_{0.4}$ 84-87°. λ_{max} 217 (ε 12000) (MeOH) (Berdy). λ_{max} 225 (ε 11000) (MeOH) (Berdy).

[123620-46-2, 156619-59-9, 156619-64-6]

Esterbauer, H. *et al., Monatsh. Chem.*, 1967, **98**, 1884; 1994 (*synth*)
Paul, V.J. *et al., Tet. Lett.*, 1980, **21**, 3327 (*isol*)
Ball, J.R. *et al., J. Biol. Phys.*, 1986, **14**, 127 (*conformn*)
Gree, R. *et al., Tet. Lett.*, 1986, **27**, 4983 (*synth*)
De Montarby, L. *et al., Bull. Soc. Chim. Fr.*, 1989, 419 (*synth, pmr, cmr*)
Gardner, H.W. *et al., Lipids*, 1992, **27**, 686 (*synth*)
Yu, L. *et al., Chem. Comm.*, 1993, 232 (*synth*)
Allevi, P. *et al., J.O.C.*, 1993, **58**, 5000 (*isol, ms*)
Bringmann, G. *et al., Tetrahedron*, 1994, **50**, 10245 (*synth*)

Allevi, P. *et al., Tetrahedron: Asymmetry*, 1994, **5**, 13 (*synth*)
Sakai, T. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1379 (*occur*)
Matsushita, Y. *et al., Tet. Lett.*, 1995, **36**, 1879 (*synth*)
Chandra, A. *et al., Lipids*, 1997, **32**, 779-782 (*synth*)

1-Hydroxy-3-nor-15-beyerene-2,12-dione H-631

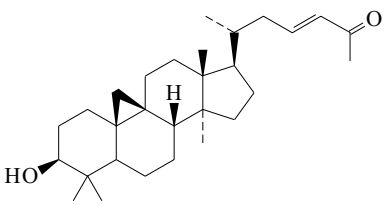


$C_{19}H_{26}O_3$ 302.413

(*ent*-1β)-*form* [119642-80-7]
Yucalexin B 11
Constit. of cassava roots (*Manihot esculenta*).

Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769

3-Hydroxy-27-norcycloart-23-en-25-one H-632



$C_{29}H_{46}O_2$ 426.681

Error in structure diag. in ref..

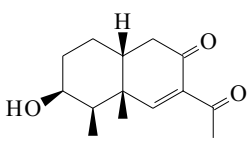
(3β,23*E*)-*form* [132943-49-8]
Constit. of *Garcinia mangostana* (mangosteen). Mp 142-143°. $[\alpha]_D^{27}$ +32.5 (c, 0.24 in MeOH).

23,24-Dihydro: [348608-17-3] ***3-Hydroxy-27-norcycloartan-25-one***
$C_{29}H_{48}O_2$ 428.697
Cryst. Mp 127-129°. $[\alpha]_D^{25}$ +38 (c, 0.3 in $CHCl_3$).

3-Ketone, 23,24-dihydro: ***27-Norcycloartane-3,25-dione***
$C_{29}H_{46}O_2$ 426.681
$[\alpha]_D^{20}$ +23 (c, 0.15 in $CHCl_3$).

Parveen, M. *et al., Phytochemistry*, 1991, **30**, 361 (*isol, pmr, ms*)
Cabrera, G.M. *et al., Phytochemistry*, 1997, **45**, 1019-1021 (*isol, pmr, cmr*)
Chiang, Y.-M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 581-583 (*23,24-dihydro*)

3-Hydroxy-13-nor-6-eremophilene-8,11-dione H-633

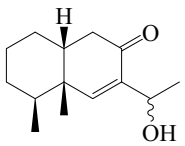


$C_{14}H_{20}O_3$ 236.31

3β-*form* [163135-94-2]
Eremopetasidione
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{28}$ -43.2 (c, 0.3 in $CHCl_3$).

Yaoita, Y. *et al., Phytochemistry*, 1994, **37**, 1765 (*isol, pmr, cmr*)
Hsu, D.-S. *et al., Org. Lett.*, 2001, **3**, 263-265 (*synth*)

11-Hydroxy-13-nor-6-eremophilen-8-one H-634



$C_{14}H_{22}O_2$

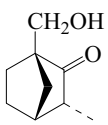
(10β*H*,11ξ)-*form* [348615-40-7]
Constit. of *Petasites japonicus* ssp. *giganteus* (Japanese butterbur). Oil. $[\alpha]_D^{29}$ +12.4 (c, 1, in $CHCl_3$). λ_{max} 230 (EtOH).

11-Ketone: [348119-85-7] *13-Nor-6-eremophilene-8,11-dione*
$C_{14}H_{20}O_2$ 220.311
Constit. of *Petasites japonicus* ssp. *giganteus* (Japanese butterbur). Yellow oil. $[\alpha]_D$ -19.4 (c, 0.34 in $CHCl_3$). λ_{max} 227 (EtOH).

Goto, Y. *et al., Phytochemistry*, 2001, **57**, 109-113 (*isol, pmr, cmr*)

10-Hydroxy-8-nor-2-fenchanone H-635

10-Hydroxy-8-norfenchone

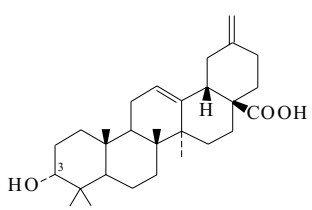


$C_9H_{14}O_2$ 154.208

O-β-D-*Glucopyranoside:* [240495-82-3]
$C_{15}H_{24}O_7$ 316.35
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -7.7 (c, 0.1 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 805-808 (*isol, pmr, cmr*)

3-Hydroxy-30-nor-12,20(29)-oleanadien-28-oic acid H-636



3α-*form*

$C_{29}H_{44}O_3$ 440.665

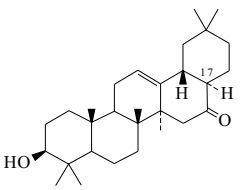
3β-*form* [104777-60-8]
Akebonoic acid
Cryst. ($CHCl_3$/MeOH) (as Me ester). Mp 152-155° (Me ester). $[\alpha]_D^{24}$ +127.7 (c, 0.658 in $CHCl_3$) (Me ester).

3-O-[(2-Carboxy-1-carboxymethoxy-2-hydroxyethyl)-(→3)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [178535-52-9] ***Betavulgaroside VIII***
$C_{46}H_{68}O_{20}$ 941.031
Constit. of *Beta vulgaris* (sugar beet). Cryst. ($CHCl_3$/MeOH). Mp 215-217°. $[\alpha]_D^{30}$ +64.3 (c, 0.1 in MeOH).

3-O-[β-D-Xylopyranosyl-(1→3)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [219805-92-2] ***Betavulgaroside X***
$C_{46}H_{70}O_{18}$ 911.048
Constit. of *Beta vulgaris* (sugar beet). Cryst. ($CHCl_3$/MeOH). Mp 211-213°. $[\alpha]_D^{26}$ +46.9 (c, 0.1 in MeOH).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1758-1763 (*Betavulgarosides VIII and X*)

3-Hydroxy-28-nor-12-oleanen-16-one H-637



(3β,17α)-*form*

$C_{29}H_{46}O_2$ 426.681

(3β,17α)-*form*
Auriculatone

(3β,17β)-*form* [71545-19-2]
Maragenin I
Cryst. (EtOAc). Mp 218-220°.

Ac:
Cryst. Mp 215-217°.

3-O-β-D-Glucuronopyranoside: [204332-94-5] ***Auriculatusaponin A***
$C_{35}H_{54}O_8$ 602.807
Amorph. powder. Mp 219-221°. $[\alpha]_D^{21}$ -14.5 (c, 0.107 in MeOH).

17,18-Didehydro: [71545-20-5] *3-Hydroxy-28-nor-12,17-oleanadien-16-one.* ***Maragenin II***
$C_{29}H_{44}O_2$ 424.665
Mp 215-217° (as 3-Ac).

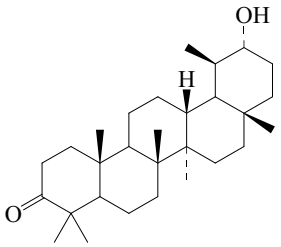
17,18-Didehydro, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [380303-68-4] ***Camellioside C***
$C_{53}H_{82}O_{23}$ 1087.217
Constit. of *Camellia japonica*. Cryst. (MeOH aq.). Mp 224-227°. $[\alpha]_D^{26}$ -15.8 (c, 0.1 in MeOH).

12,13-Dihydro, 17,18-didehydro: [71545-21-6] *3-Hydroxy-28-nor-17-oleanen-16-one.* ***Maragenin III***
$C_{29}H_{46}O_2$ 426.681
Cryst. (As 3-Ac). Mp 216-218° (3-Ac).

Hylands, P.J. *et al., Tetrahedron*, 1979, **35**, 417 (*Maragenins*)
Rowan, D.D. *et al., Phytochemistry*, 1984, **23**, 639 (*cmr*)

Gao, C.-W. *et al., CA*, 1994, **121**, 297129p (*Auriculatone, cryst struct*)
Wang, C.Z. *et al., Planta Med.*, 1998, **64**, 50-53 (*Auriculatusaponin A*)
Yoshikawa, M. *et al., Heterocycles*, 2001, 1653-1657 (*Camellioside C*)

20-Hydroxy-30-norursan-3-one H-638



$C_{29}H_{48}O_2$ 428.697

20α-*form* [259144-62-2]
Mangiferdesmethylursanone
Constit. of the root bark of *Mangifera indica* (mango). Cryst. (MeOH). Mp 228-229°. λ_{max} 242 (log ε 2.1) (MeOH).

Gupta, J. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1093-1098

28-Hydroxy-7-octacosanone H-639

[138416-85-0]

$HOCH_2(CH_2)_{20}CO(CH_2)_5CH_3$

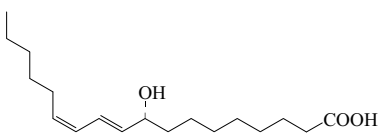
$C_{28}H_{56}O_2$ 424.749

Constit. of the seeds of *Musa balbisiana*.

Ali, M. *et al., Orient. J. Chem.*, 1991, **7**, 167-169

9-Hydroxy-10,12-octadecadienoic acid, 9CI H-640

[15514-85-9]



(9*R*,10*E*,12*Z*)-*form*

$C_{18}H_{32}O_3$ 296.449

(9*R*,10*E*,12*Z*)-*form* [10075-11-3]

(9*S*,10*E*,12*E*)-*form* [6114-34-7]
β-Dimorphecolic acid
Cryst. (Me_2CO). Mp 36-37°. $[\alpha]_D^{25}$ +15.2 (c, 5.2 in MeOH).

Me ester:
$C_{19}H_{34}O_3$ 310.476
$[\alpha]_D^{25}$ +5 (c, 5.0 in $CHCl_3$).

9-Ketone: See 9-Oxo-10,12-octadecadienoic acid in *The Combined Chemical Dictionary.*

(9*S*,10*E*,12*Z*)-*form*
α-Dimorphecolic acid
Present in plant and animal lipids as autoxidn. or lipoxygenase oxidn. prod. of linoleic acid. $[\alpha]_{400}$ +1.5 (c, 1.6 in hexane).

Me ester:
$[\alpha]_{540}^{20}$ +4.2 (c, 4.17 in EtOH).

9-Ketone: See 9-Oxo-10,12-octadecadienoic acid in *The Combined Chemical Dictionary.*

Smith, C.R. *et al., J.A.C.S.*, 1960, **82**, 1417
Applewhite, T.H. *et al., Chem. Comm.*, 1965, 255 (*abs config*)
Powell, R.C. *et al., J.O.C.*, 1967, **32**, 1442
Chan, H.W.S. *et al., Lipids*, 1977, **12**, 99 (*synth*)
Sessa, D.J. *et al., Lipids*, 1977, **12**, 613 (*isol, uv, ir, pmr, ms*)
Tsuboi, S. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2050 (*synth*)
Rao, A.V.R. *et al., Tetrahedron*, 1986, **42**, 4523 (*synth, ir, pmr*)
Kuehn, H. *et al., Eur. J. Biochem.*, 1989, **186**, 155-162 (*isol, ketone*)
Kraus, R. *et al., Annalen*, 1991, 335 (*isol, synth, bibl*)
Murakami, N. *et al., Lipids*, 1992, **27**, 776-778 (*isol*)
Tassignon, P. *et al., Chem. Phys. Lipids*, 1994, **71**, 187 (*isol*)
Ley, S.V. *et al., Chem. Comm.*, 1995, 1751 (*synth*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1656-1662 (*isol, ketone*)
Martini, D. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 1489 (*synth*)
Kuklev, D.V. *et al., Chem. Phys. Lipids*, 1997, **85**, 125-134 (*synth, uv, ir, pmr, cmr*)
Ley, S.V. *et al., J.C.S. Perkin 1*, 1997, 1125 (*synth, ir, pmr*)

12-Hydroxy-8,10-octadecadienoic acid H-641

[170171-31-0]

$H_3C(CH_2)_5CH(OH)CH{=}CHCH{=}CH(CH_2)_6COOH$

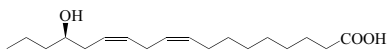
$C_{18}H_{32}O_3$ 296.449

Constit. of the seeds of *Elaeagnus angustifolia* (Russian olive).

Goncharova, N.P. *et al., Khim. Prir. Soedin.*, 1994, **30**, 715 (*isol*)

15-Hydroxy-9,12-octadecadienoic acid H-642

[36479-79-5]



$C_{18}H_{32}O_3$ 296.449

(9*Z*,12*Z*,15*R*)-*form* [177931-23-6]
15-Hydroxylinoleic acid. ***Avenoleic acid***
Constit. of oat seeds (*Avena sativa*). Oil.

[52222-88-5]

Hamberg, M. *et al., Phytochemistry*, 1996, **42**, 729-732 (*isol, pmr, ms*)
Hamberg, M. *et al., Adv. Exp. Med. Biol.*, 1997, **433**, 69-72 (*isol*)
Hamberg, M. *et al., Lipids*, 1998, **33**, 355-363 (*isol*)

10-Hydroxyoctadecanoic acid, 9CI H-643

10-Hydroxystearic acid. Rosilic acid
$H_3C(CH_2)_7CH(OH)(CH_2)_8COOH$

$C_{18}H_{36}O_3$ 300.481

(±)-*form*
Mp 84°.

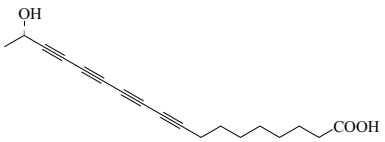
Me ester:
$C_{19}H_{38}O_3$ 314.507
Mp 54.1-54.2°. Bp_4 212-216°.

(ξ)-*form*
Constit. of leaf cutins of rosemary.

Bergström, S. *et al., Acta Chem. Scand.*, 1952, **6**, 1157 (*synth*)
Fischmeister, I. *et al., Ark. Kemi*, 1967, **27**, 127 (*ir*)
Rohwedder, K.W. *et al., Lipids*, 1971, **6**, 906 (*ms*)
Brieskorn, C.H. *et al., Phytochemistry*, 1971, **10**, 3195
Tulloch, A.P. *et al., Org. Magn. Reson.*, 1978, **11**, 109 (*cmr*)

17-Hydroxy-9,11,13,15-octadecatetraynoic acid H-644

Minquartynoic acid



$C_{18}H_{20}O_3$ 284.354

(*S*)-*form* [123154-43-8]
Grey-yellow needles (CH_2Cl_2). Isol. from *Coula edulis*. Cryst. ($CHCl_3$). Mp 97°. $[\alpha]_D$ -37.6 (c, 0.1 in MeOH). λ_{max} 208 (ε 42700); 217 (ε 91200); 227 (ε 214000); 239 (ε 288000) (MeOH).

*15,16-Dihydro(*E*-):17-Hydroxy-15-octadecene-9,11,13-triynoic acid.* ***15,16-Dihydrominquartynoic acid***
$C_{18}H_{22}O_3$ 286.37
Amorph. powder. $[\alpha]_D$ -12.8 (c, 0.05 in MeOH). λ_{max} 206 (log ε 4.58); 212 (log ε 4.62); 231 (log ε 4.8); 243 (log ε 4.92); 258 (log ε 3.81); 273 (log ε 3.92); 290 (log ε 4.12); 309 (log ε 4.21); 330 (log ε 4.07) (MeOH).

Marles, R.J. *et al., J. Nat. Prod.*, 1989, **52**, 261-266 (*isol, struct, pmr, cmr, ir, uv, ms*)
Rasmussen, H.B. *et al., J. Nat. Prod.*, 2000, **63**, 1295-1296 (*abs config*)
Ito, A. *et al., J. Nat. Prod.*, 2001, **64**, 246-248 (*isol, pmr, abs config*)
Rashid, M.A. *et al., Nat. Prod. Lett.*, 2001, **15**, 21-26 (*abs config*)
Gung, B.W. *et al., Org. Lett.*, 2002, **4**, 2517-2519 (*synth*)

2-Hydroxy-9,12,15-octadecatrienoic acid H-645

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_6CH(OH)COOH$

$C_{18}H_{30}O_3$ 294.433

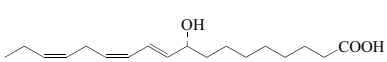
(*R*)-(*all-Z*)-*form*
2-Hydroxylinolenic acid
Constit. of *Thymus vulgaris* (thyme) seed oil. $[\alpha]_{400}$ -24.3 (c, 0.16 in $CHCl_3$).

Smith, C.R. *et al., Lipids*, 1969, **4**, 9 (*isol, struct, ord*)
Bohannon, M.B. *et al., Lipids*, 1975, **10**, 703 (*isol, ms, ir, nmr*)

9-Hydroxy-10,12,15-octadecatrienoic acid H-646

[21402-68-6]

[51197-09-2, 166735-07-5]



$C_{18}H_{30}O_3$ 294.433

(9*R*,10*E*,12*Z*,15*Z*)-*form* [133397-71-4]

9-Ketone: [125559-74-2] *9-Oxo-10,12,15-octadecatrienoic acid*
$C_{18}H_{28}O_3$ 292.417

(9*S*,10*E*,12*Z*,15*Z*)-*form* [89886-42-0]
Constit. of *Artocarpus communis* (breadfruit). $[\alpha]_D$ +5.3 (c, 0.5 in $CHCl_3$). λ_{max} 236 (EtOH).

(9*RS*,10*E*,12*Z*,15*Z*)-*form* [115511-52-9]

[115476-07-8]
Oil (as Me ester).

Rao, A.V. *et al., Tetrahedron*, 1987, **43**, 4385-4394 (*synth*)
Pollio, A. *et al., Biochim. Biophys. Acta*, 1988, **963**, 53-60 (*isol*)
Kuehn, H. *et al., Eur. J. Biochem.*, 1989, **186**, 155-162 (*isol*)
Zdero, C. *et al., Phytochemistry*, 1990, **29**, 2247-2252 (*isol*)
Aliotta, G. *et al., J. Chem. Ecol.*, 1991, **17**, 2223-2234 (*isol*)
Kato, T. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 373-375 (*synth*)
Murakami, N. *et al., Lipids*, 1992, **27**, 776-778 (*isol*)
Hamberg, M. *et al., J.C.S. Perkin 1*, 1993, 3065-3072 (*synth*)
Gianfrani, C. *et al., Experientia*, 1995, **51**, 48-56 (*isol*)
McLean, S. *et al., Magn. Reson. Chem.*, 1996, **34**, 719-722 (*isol, pmr, cmr*)
Dong, M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 882-886 (*isol*)

16-Hydroxy-9,12,14-octadecatrienoic acid, 9CI H-647

$C_{18}H_{30}O_3$ 294.433

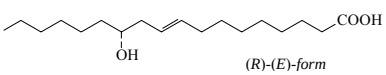
(9*Z*,12*Z*,14*E*)-*form* [81325-65-7]

[89886-41-9, 99530-29-7, 115511-51-8]
Isol. from the resistant cultivar of rice (*Oryza sativa*).

Kato, T. *et al., Chem. Lett.*, 1984, 409-412 (*isol*)
Rama Rao, A.V. *et al., Tetrahedron*, 1987, **43**, 4385-4394 (*synth*)

12-Hydroxy-9-octadecenoic acid, 9CI H-648

[7431-95-0]



(*R*)-(*E*)-*form*

$C_{18}H_{34}O_3$ 298.465

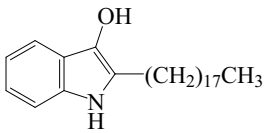
(*R*,*Z*)-*form* [141-22-0]
Ricinoleic acid. *12-Hydroxyoleic acid. Ricinusoleic acid. Ricinic acid. Ricinolic acid*
Occurs in castor oil and other oils e.g. grape and ergot (*Claviceps purpurea*). Viscous liq. Insol. H_2O; sol. most org. solvs. Mp 5.5°. Bp_{10} 245°. $[\alpha]_D^{22}$ +6.67 (c, 5 in Me_2CO). $[\alpha]_D^{26}$ +7.15 (c, 5 in Me_2CO). n_D^{20} 1.4697.
► VJ3150000

[35732-94-6, 127062-51-5, 127062-52-6, 238761-41-6]

James, A.T. *et al., Biochem. J.*, 1965, **95**, 448 (*biosynth*)
Applewhite, T.H. *et al., J.O.C.*, 1967, **32**, 1173 (*abs config*)
Suzuki, O. *et al., Yakugaku Zasshi*, 1970, **19**, 140 (*pmr*)
Chakrabarti, P. *et al., Biochemistry*, 1975, **14**, 5021 (*synth*)
Ariga, T. *et al., Chem. Phys. Lipids*, 1977, **19**, 14 (*ms*)
Rakoff, H. *et al., Lipids*, 1979, **14**, 81 (*cmr*)
McGhie, J.F. *et al., Chem. Ind. (London)*, 1982, 719-720 (*synth*)
Steliou, K. *et al., J.A.C.S.*, 1983, **105**, 7130 (*synth, pmr, cmr, ms*)
Yamada, H. *et al., Chem. Lett.*, 1989, 1775-1776 (*R,E-form, R,Z-form, lactones, synth*)
Fuerstner, A. *et al., J.A.C.S.*, 1997, **119**, 9130-9136 (*synth*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1468 (*Na ricinoleate*)
Nagarajan, M. *et al., Synth. Commun.*, 1999, **29**, 2467-2475 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RJP000

3-Hydroxy-2-octadecylindole H-649

*1,2-Dihydro-2-octadecyl-3*H*-indol-3-one. 2-Octadecyl-1*H*-indol-3-ol.* ***Fistulosin***



$C_{26}H_{43}NO$ 385.632

Tautomeric with oxo form. Alkaloid from the roots of *Allium fistulosum* (Welsh onion). Cryst. Mp 80-83°. λ_{max} 220 ; 237 ; 252 ; 277 ; 302 (EtOH).

Phay, N. *et al., Phytochemistry*, 1999, **52**, 271-274 (*isol, uv, ir, pmr, cmr*)

8-Hydroxy-5,6-octadienoic acid H-650

$HOCH_2CH{=}C{=}CH(CH_2)_3COOH$

$C_8H_{12}O_3$ 156.181

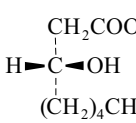
Present in the glycerides of *Sapium sebiferum* (Chinese tallowtree) in an enantiomeric form.

Me ester: [38818-76-7]
$C_9H_{14}O_3$ 170.208
Oil. λ_{max} 219 (ε 1200); 244 (ε 710) (EtOH) (Berdy).

Sprecher, H.W. *et al., Biochemistry*, 1965, **4**, 1856 (*isol, ord*)
Ohigashi, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 1399 (*isol, uv, ir, pmr*)
Heimermann, W.H. *et al., Phytochemistry*, 1972, **11**, 799 (*isol*)
Back, T.G. *et al., Tet. Lett.*, 1992, **33**, 4725 (*synth*)
Harusawa, S. *et al., Tetrahedron*, 1995, **51**, 6475-6494 (*synth, bibl*)

3-Hydroxyoctanoic acid, 9CI H-651

[14292-27-4]
3-Hydroxycaprylic acid



(*R*)-*form*

$C_8H_{16}O_3$ 160.213

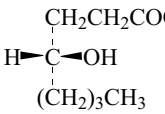
(*R*)-*form* [44987-72-6]
Found in milk, strawberries and pineapple concentrate. $[\alpha]_D^{24}$ -21 (c, 1.9 in $CHCl_3$).

(ξ)-*form*
Et ester, O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{22}H_{40}O_{13}$ 512.55
Isol. from Cape gooseberry (*Physalis peruviana*). Gum (as hepta-Ac). $[\alpha]_D^{22}$ -4.6 (c, 0.087 in MeOH).

Lemieux, R.U. *et al., Can. J. Chem.*, 1951, **29**, 678 (*synth*)
Schildknecht, H. *et al., Angew. Chem., Int. Ed.*, 1971, **10**, 124 (*isol*)
Kuwajima, I. *et al., Tet. Lett.*, 1976, 2253 (*synth*)
Tahara, S. *et al., Agric. Biol. Chem.*, 1978, **42**, 879 (*synth*)
Ketelaar, P.E.F. *et al., Tet. Lett.*, 1985, **26**, 4665 (*synth*)
Mayorga, H. *et al., Phytochemistry*, 2002, **59**, 439-445 (*Physalis glycoside*)

4-Hydroxyoctanoic acid, 9CI H-652

[7779-55-7]



(*R*)-*form*

$C_8H_{16}O_3$ 160.213

Free acid immediately lactonises.

(*R*)-*form*
Et ester: [107736-67-4]
$C_{10}H_{20}O_3$ 188.266
Liq.

Lactone: [107797-24-0] *5-Butyldihydro-2(3*H*)-furanone, 9CI. 4-Octanolide. 4-Butyl-γ-butyrolactone*
$C_8H_{14}O_2$ 142.197
Liq. with coconut-like odour. $Bp_{1.3}$ 116-117°. $[\alpha]_D$ +56.2.

(±)-*form*
Amide:
$C_8H_{17}NO_2$ 159.228
Cryst. Mp 84-86°.

Methylamide:
$C_9H_{19}NO_2$ 173.255
Cryst. (EtOAc/hexane). Mp 51-53°.

Hydrazide: [24535-12-4]
$C_8H_{18}N_2O_2$ 174.242
Cryst. Mp 79-80°.

Nitrile: [154870-36-7] *4-Hydroxyoctanenitrile. 1-Cyano-3-heptanol*
$C_8H_{15}NO$ 141.213
$Bp_{2.5}$ 95° (kugelrohr). Was resolved.

Lactone: [104-50-7] *FEMA 2796*
Present in apricots, peaches and other fruits. Flavouring ingredient. Liq. with a strong fruity odour and a very sweet taste. Bp_{20} 132-133° $Bp_{5.5}$ 102-105°.
► Mod. skin irritant. LU3562000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 698D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1129B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 750D (*ir*)
Sadtler Standard Infrared Spectra, No. 20213, (*lactone*)

Sadtler Standard NMR Spectra, Nos. 2500; 2362 (*lactone, pmr, cmr*)
Terai, Y. *et al., Bull. Chem. Soc. Jpn.*, 1956, **29**, 822 (*lactone, hydrazide*)
Schmidt, U. *et al., Annalen*, 1963, **666**, 201 (*synth*)
McFadden, W.H. *et al., Anal. Chem.*, 1965, **37**, 89 (*lactone, ms*)
Sedavkina, V. *et al., CA*, 1976, **84**, 30362 (*synth*)
Thijs, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1986, **105**, 332 (*ester*)
Takagi, Y. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 2949 (*nitrile*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 609 (*lactone*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2002-2003 (*lactone*)
Taylor, S.K. *et al., Synth. Commun.*, 1998, **28**, 1691-1701; 2001, **31**, 2391-2397 (*nitrile, amide, methylamide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OCE000

5-Hydroxyoctanoic acid, 9CI, 8CI H-653

[17369-50-5]

$H_3CCH_2CH_2CH(OH)CH_2CH_2CH_2$-COOH

$C_8H_{16}O_3$ 160.213

(±)-*form*

Lactonises on dist..

Hydrazide: [16425-11-9]
$C_8H_{18}N_2O_2$ 174.242
Cryst. Mp 97-98°.

Lactone: See Tetrahydro-6-propyl-2*H*-pyran-2-one, T-122

Honkanenea, E. *et al., Acta Chem. Scand.*, 1965, **19**, 370 (*synth, ms*)
McFadden, W.H. *et al., Anal. Chem.*, 1965, **37**, 89 (*ms*)
Wyatt, C.J. *et al., Lipids*, 1967, **2**, 208 (*isol*)
Lardelli, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 481 (*synth*)

1-Hydroxy-3-octanone, 9CI H-654

[7786-52-9]
FEMA 2804

$H_3C(CH_2)_4COCH_2CH_2OH$

$C_8H_{16}O_2$ 144.213
Flavouring ingredient. Oil with a fruity, herbaceous, spicy odour. $Bp_{8.5}$ 94.6°.

O-*β-D-Glucopyranoside:* [194919-40-9] *1-(β-D-Glucopyranosyloxy)-3-octanone*
$C_{14}H_{26}O_7$ 306.355
Constit. of the fruit of *Carica pubescens* (mountain papaya).

Ac: [6085-30-9]
$C_{10}H_{18}O_3$ 186.25
Bp_{12} 121°.

Koulkes, M. *et al., Bull. Soc. Chim. Fr.*, 1957, 127-129 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 616
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2015
Krajewski, D. *et al., Phytochemistry*, 1997, **45**, 1627-1631 (*synth, isol, pmr, cmr, deriv, ms*)
Miyashita, M. *et al., Tetrahedron*, 1997, **53**, 12469-12486 (*synth, ir, pmr*)

5-Hydroxy-4-octanone, 9CI H-655

[496-77-5]
Butyroin. FEMA 2587

$H_3CCH_2CH_2CH(OH)COCH_2CH_2CH_3$

$C_8H_{16}O_2$ 144.213

(±)-*form* [116296-89-0]
Flavouring agent. Oil with sweet buttery/nut-like odour and sweet, oily taste. d^{20} 0.92. Bp 180-190° Bp_4 62-63°. n_D^{20} 1.4290.

Oxime:
$C_8H_{17}NO_2$ 159.228
Oil. Bp_{10} 143°.

Ac:
$C_{10}H_{18}O_3$ 186.25
Oil. Bp_7 90-92°.

[86838-18-8, 116214-05-2]

Org. Synth., Coll. Vol., 2, 1943, 114-116 (*synth*)
Stetter, H. *et al., Synthesis*, 1976, 733-735 (*synth*)
Srinivason, N.S. *et al., Synthesis*, 1979, 520-521 (*synth, ir, pmr, ms*)
Tamao, K. *et al., Tet. Lett.*, 1986, **27**, 65-68 (*synth*)
Org. Synth., Coll. Vol., 7, 1990, 95-99 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 368
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1380

8-Hydroxy-2,4,6-octatriynoic acid H-656

$HOCH_2C{\equiv}CC{\equiv}CC{\equiv}CCOOH$

$C_8H_4O_3$ 148.118

Amide: [544-44-5] *8-Hydroxy-2,4,6-octatriynamide.* ***Agrocybin***
$C_8H_5NO_2$ 147.133
From *Marasmius oreades* (fairy ring mushroom). Cryst. (EtOH aq.). Sol. MeOH, EtOH, Me_2CO, Et_2O; fairly sol. H_2O; poorly sol. hexane. Mp 130-140° dec. λ_{max} 216 (ε 67600); 224 (ε 87000); 269 (ε 1740); 286 (ε 2400); 304 (ε 3020); 325 (ε 1950) (MeOH) (Berdy).
► Causes dermatitis. LD_{50} (mus, ivn) 6 mg/kg. RH2100000

Jones, E.R.H. *et al., J.C.S.*, 1953, 3719
Bu'Lock, J.D. *et al., Chem. Ind. (London)*, 1954, 990 (*struct*)
Ashworth, P.J. *et al., J.C.S.*, 1958, 950 (*synth, ir*)
Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371 (*isol*)

8-Hydroxy-2-octene-4,6-diynoic acid, 9CI H-657

$HOCH_2C{\equiv}CC{\equiv}CCH{=}CHCOOH$

$C_8H_6O_3$ 150.134

(*E*)-*form* [65367-65-9]
Metab. of *Camarophyllus virgineus* (snowy wax cap).

Me ester:
$C_9H_8O_3$ 164.16
Mp 80-82°.

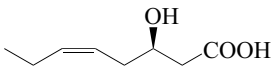
(*Z*)-*form* [65367-62-6]

Me ester:
Mp 49-50°.

Schnell, A. *et al., J.C.S. Perkin 1*, 1977, 1886 (*isol, synth*)

3-Hydroxy-5-octenoic acid H-658

[146935-47-9]



(3*R*,5*Z*)-*form*

$C_8H_{14}O_3$ 158.197

(3*R*,5*Z*)-*form*

Et ester: [182510-22-1]
$C_{10}H_{18}O_3$ 186.25
Constit. of apple juice.

(3*S*,5*E*)-*form*

Me ester: [163955-02-0]
$C_9H_{16}O_3$ 172.224
Oil. Bp_2 135°. $[\alpha]_D$ +18 (c, 1 in $CHCl_3$) (>99% ee).

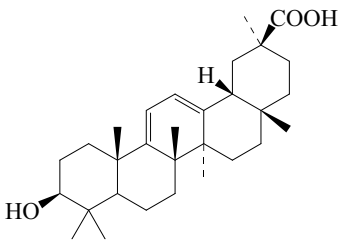
(±)-(*E*)-*form*

Et ester:
Oil.

[71677-19-5, 71677-20-8, 77234-15-2, 77234-21-0]

Genet, J.P. *et al., Tetrahedron: Asymmetry*, 1994, **5**, 675; 1995, **6**, 1989 (*synth, ester*)
Beuerle, T. *et al., Phytochemistry*, 1996, **43**, 145 (*isol, synth*)
Fleming, F.F. *et al., J.O.C.*, 1999, **64**, 8568-8575 (*Et ester*)

3-Hydroxy-9(11),12-oleanadien-30-oic acid H-659



$C_{30}H_{46}O_3$ 454.692

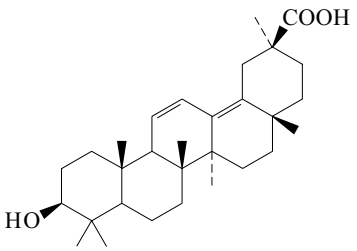
3β-*form* [14884-88-9]
9(11)-Dehydroglycyrrhetic acid
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice) and from licorice root (*Glycyrrhiza glabra*).

Ac:
$C_{32}H_{48}O_4$ 496.729
Mp 232-234°.

3-Ketone: [270907-27-2] ***3-Oxo-9(11),12-oleanadien-30-oic acid***
$C_{30}H_{44}O_3$ 452.676
Powder. Mp 259°. $[\alpha]_D^{25}$ +200 (c, 0.11 in $CHCl_3$). λ_{max} 210 (log ε 3.98); 235 (log ε 2.85) (MeOH).

Canonica, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 769
Kir'yalov, N.P. *et al., Khim. Prir. Soedin.*, 1974, **10**, 102; *Chem. Nat. Compd. (Engl. Transl.)*, 112 (*isol*)
Muhammad, I. *et al., J. Nat. Prod.*, 2000, **63**, 605-610 (*3-ketone*)

3-Hydroxy-11,13(18)-oleanadien-30-oic acid H-660



$C_{30}H_{46}O_3$ 454.692

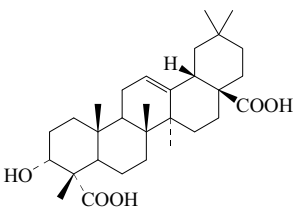
3β-*form* [17991-81-0]
Glypallidifloric acid
Occurs in roots of *Glycyrrhiza uralensis* (Chinese licorice) (isol. as Me ester). Cryst. (Me_2CO). Mp 308-312° dec. (synthetic).

3-O-[β-D-Glucuronopyranosyl(1→2)-β-D-glucuronate]: [118525-49-8]

[120711-08-2] ***Licoricesaponin C2***
$C_{42}H_{62}O_{15}$ 806.943
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice). Trihydrate. Mp 249-251°. $[\alpha]_D^{21}$ -120 (MeOH).

Canonica, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 769-786 (*isol,synth*)
Kir'yalov, N.P. *et al., Khim. Prir. Soedin.*, 1974, **10**, 102; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 112 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3710-3713 (*Licoricesaponin C2*)
Kan, Y. *et al., Fitoterapia*, 1994, **65**, 91 (*isol*)

3-Hydroxy-12-oleanene-23,28-dioic acid H-661



3α-*form*

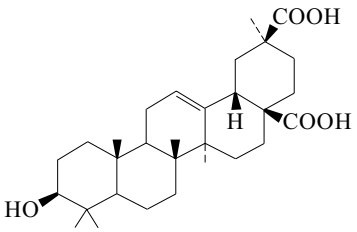
$C_{30}H_{46}O_5$ 486.69

3β-*form* [5143-05-5]
Gypsogenic acid. *Astrantiagenin J. Gypsogeninic acid*
Cryst. (MeOH aq.). Mp 370°. $[\alpha]_D$ +90 (c, 1.11 in dioxan).

3-O-β-D-Glucopyranoside, 28-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [82793-04-2] ***Azukisaponin IV***
$C_{48}H_{76}O_{20}$ 973.116
Isol. from *Vigna angularis* (azuki bean). Fine cryst. + $2H_2O$ (MeOH). Mp 235-237°. $[\alpha]_D^{25}$ -1.8 (c, 1.1 in MeOH).

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 674 (*Azukisaponins*)

3-Hydroxy-12-oleanene-28,30-dioic acid H-662



$C_{30}H_{46}O_5$ 486.69

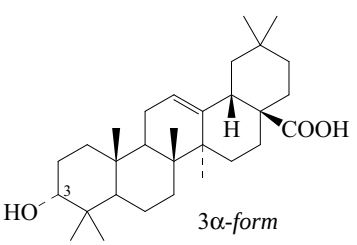
3β-*form* [18671-48-2]
Spergulagenic acid
Cryst. (MeOH). Mp 347-350° dec. $[\alpha]_D^{26.5}$ +121.2 (Py).

3-O-β-D-Glucuronopyranoside, 28-O-β-D-glucopyranosyl ester, 30-Me ester: [145826-48-8] ***Talinumoside I***
$C_{43}H_{66}O_{16}$ 838.985
Constit. of *Talinum triangulare* (waterleaf). Powder. $[\alpha]_D$ +57.5 (c, 0.8 in Py).

3-O-[α-L-Arabinopyranosyl-(1→3)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester, 30-Me ester: [359775-97-6]
$C_{48}H_{74}O_{20}$ 971.101
Constit. of *Chenopodium quinoa* (quinoa) seeds. Powder. $[\alpha]_D$ +2.3 (c, 0.003 in MeOH).

Kohda, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2557 (*Talinumoside I*)
Nielsen, S.E. *et al., Phytochemistry*, 1995, **39**, 625 (*derivs*)
Dini, I. *et al., J. Agric. Food Chem.*, 2001, **49**, 3976-3981 (*Chenopodium quinoa saponin*)

3-Hydroxy-12-oleanen-28-oic acid H-663



3α-*form*

$C_{30}H_{48}O_3$ 456.707

Many glycosides of Oleanolic acid are known. See also Oleanolic acid 3-glycosides, O-147 and Oleanolic acid bisdesmosides, O-146.

3α-*form* [25499-90-5]
3-Epioleanolic acid
Isol. from sage *Salvia officinalis* and other plants. Needles (MeOH). Mp 297-299°. $[\alpha]_D^{20}$ +68 (c, 1.66 in $CHCl_3$).

3β-*form* [508-02-1]
Oleanolic acid. *Oleanol. Caryophyllin. Swertiaic acid. Sugarbeet acid. Guagenin. Momorgenin. Taraligenin. Panaxsapogenin. Araligenin. Taragenin. Viscic acid†. Mistletoe sapogenin. Oleanic acid. Astrantiagenin C. Giganteumgenin C. Virgaureagenin B. Gledigenin 1*
Occurs as glycosides in cloves (*Syzygium aromaticum*), sugar beet (*Beta vulgaris*), olive leaves, etc. Very widely distributed aglycone. Cryst. (EtOH). Mp 306-308°. $[\alpha]_D^{12}$ +79.5 ($CHCl_3$). Log P 8.59 (uncertain value) (calc).

▶ RK0177965

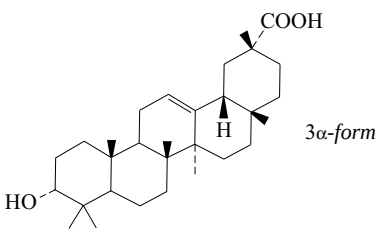
3-Hexadecanoyl: [19833-14-8]
$C_{46}H_{78}O_4$ 695.12
Isol. from the famine food *Madhuca longifolia*. Mp 145°.

3-(4-Methoxycinnamoyl)(Z-), Me ester: [189140-50-9]
$C_{41}H_{58}O_5$ 630.906
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. Mp 208-209°.

[39316-91-1, 70620-39-2]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 595B (*nmr*)
Bischoff, B. *et al., Helv. Chim. Acta*, 1949, **32**, 1911-1921 (*struct, ir*)
Huneck, S. *et al., Tetrahedron*, 1963, **19**, 479-482 (*3α-form*)
Savoir, R. *et al., Bull. Soc. Chim. Belg.*, 1967, **76**, 335-367 (*pmr*)
Renwick, J.D. *et al., J.C.S.(C)*, 1969, 2544-2549 (*cd, ord*)
Tori, K. *et al., Tet. Lett.*, 1974, 4227-4230 (*cmr*)
Seo, S. *et al., Chem. Comm.*, 1975, 270-271 (*biosynth, cmr*)
Roques, R. *et al., Acta Cryst. B*, 1978, **34**, 2367-2370 (*cryst struct, Ac*)
Seo, S. *et al., Chem. Comm.*, 1986, 1141-1143 (*biosynth*)
Corey, E.J. *et al., J.A.C.S.*, 1993, **115**, 8873-8874 (*synth*)
Santos, G.G. *et al., Phytochemistry*, 1997, **44**, 1309-1312 (*methoxycinnamoyl Me ester*)
Higa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1189-1193 (*activity*)
Kashiwada, Y. *et al., J. Nat. Prod.*, 1998, **61**, 1090-1095 (*anti-HIV activity*)
Santos, M.H. *et al., Rev. Bras. Cienc. Farm.*, 1999, **35**, 297-301; *CA*, **133**, 220085m (*activity*)
Konoike, T. *et al., Tetrahedron*, 1999, **55**, 14901-14914 (*synth*)

3-Hydroxy-12-oleanen-29-oic acid H-664



3α-*form*

$C_{30}H_{48}O_3$ 456.707

3α-*form* [6894-46-8]
Katonic acid
Constit. of *Sandoricum koetjape* (santol). Cryst. (MeOH). Mp 285-287° (275-278°). $[\alpha]_D$ +47 (c, 1 in $CHCl_3$).

Me ester: [103881-95-4]
Mp 190-192°.

3-O-[α-L-Rhamnopyranosyl-(1→2)[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranosyl-(1→2)-β-D-glucuronopyranoside], 29-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl] ester: [107110-04-3]

$C_{66}H_{106}O_{32}$ 1411.544
Constit. of *Cyamopsis tetragonoloba* (guar).

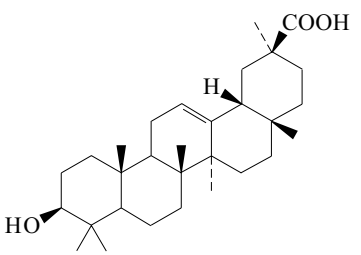
3-Benzoyl, Me ester:
$C_{38}H_{54}O_4$ 574.842
Cryst. Mp 280-282°.

3-Ketone: [76094-29-6] *3-Oxo-12-oleanen-29-oic acid.* ***Katononic acid***
$C_{30}H_{46}O_3$ 454.692
Constit. of *Sandoricum koetjape* (santol). Cryst. ($CHCl_3$/MeOH). Mp 246-249°.

3β-*form* [76035-62-6]
3-Epikatonic acid
Constit. of *Cyamopsis tetragonoloba* (guar). Cryst. ($CHCl_3$/MeOH). Mp 283-284°. $[\alpha]_D^{23}$ +61.

King, F.E. *et al., J.C.S.*, 1960, 4738 (*isol*)
Coxon, D.T. *et al., Phytochemistry*, 1980, **19**, 1247
Gaul, K.L. *et al., Aust. J. Chem.*, 1985, **38**, 1371 (*isol*)
Curi, C.L. *et al., Phytochemistry*, 1986, **25**, 2675 (*deriv*)
De Sousa, J.R. *et al., Phytochemistry*, 1990, **29**, 3259 (*Katononic acid*)
Kaneda, N. *et al., J. Nat. Prod.*, 1992, **55**, 654 (*isol, pmr, cmr*)
Mukherjee, K.S. *et al., Phytochemistry*, 1995, **38**, 1273 (*deriv*)
Nakano, K. *et al., Phytochemistry*, 1997, **45**, 293 (*cmr*)
Filho, S.A.V. *et al., Acta Horticult.*, 1999, **501**, 199 (*isol, activity*)
Sun, D.-A. *et al., J. Nat. Prod.*, 1999, **62**, 1110-1113 (*activity*)
Silva, G.D.F. *et al., Magn. Reson. Chem.*, 2002, **40**, 366-370 (*3-Epikatonic acid, pmr, cmr, cryst struct*)

3-Hydroxy-12-oleanen-30-oic acid H-665



$C_{30}H_{48}O_3$ 456.707

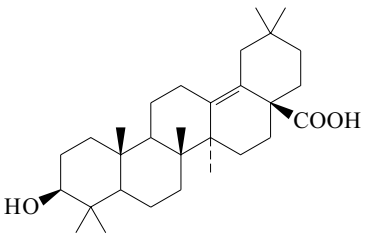
3β-*form* [564-16-9]
11-Deoxoglycyrrhetinic acid
Isol. from roots of *Glycyrrhiza glabra* (licorice). Cryst. (AcOH). Mp 330°. $[\alpha]_D$ +148 (c, 0.473 in $CHCl_3$).

3-O-[β-D-Glucuronopyranosyl(1→2)-β-D-glucuronate]: [118536-86-0] ***Licoricesaponin B2***. *Deoxoglycyrrhizin*
$C_{42}H_{64}O_{15}$ 808.959
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice). Monohydrate. Mp 209-210°. $[\alpha]_D^{19}$ +54 (MeOH).

3-Ketone: ***3-Oxo-12-oleanen-30-oic acid***
$C_{30}H_{46}O_3$ 454.692
Needles (MeOH). Mp 270-272°. $[\alpha]_D^{22}$ +110 (c, 0.06 in $CHCl_3$).

Canonica, L. *et al., Gazz. Chim. Ital.*, 1966, **96**, 833 (*isol, struct*)
Chakrabarti, P. *et al., J. Indian Chem. Soc.*, 1969, **46**, 626 (*synth*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3710 (*Licoricesaponin B2*)
Nick, A. *et al., Phytochemistry*, 1995, **40**, 1691 (*isol, pmr, cmr*)
Pellegata, R. *et al., Org. Prep. Proced. Int.*, 1999, **31**, 181-187 (*synth*)

3-Hydroxy-13(18)-oleanen-28-oic acid H-666



$C_{30}H_{48}O_3$ 456.707

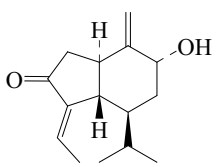
3β-*form* [6713-26-4]

Ac, Me ester:
$C_{33}H_{52}O_4$ 512.771
Isol. from leaves of *Olea europaea* (olive). Mp 237-239°. $[\alpha]_D$ -65 (c, 1 in $CHCl_3$).

3-O-[β-D-Xylopyranosyl-(1→3)-β-D-glucuronopyranoside]: ***Scoparianoside C***
$C_{41}H_{64}O_{13}$ 764.949
Cryst. ($CHCl_3$/MeOH). Mp 207-209°. $[\alpha]_D^{27}$ -7.7 (c, 0.3 in MeOH).

Caputo, R. *et al., Phytochemistry*, 1974, **13**, 2825 (*isol*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1300-1305 (*Scoparianoside C*)

9-Hydroxy-4,10(14)-oplopadien-3-one H-667



(4*E*,9α)-*form*

$C_{15}H_{22}O_2$ 234.338

(4*E*,9α)-*form*

*9-(3-Methyl-2*E*-pentenoyl):* [237407-01-1]
$C_{21}H_{30}O_3$ 330.466
Constit. of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D^{25}$ -33.3 (c, 0.03 in $CHCl_3$). λ_{max} 225 (log ϵ 4) (MeOH).

(4*Z*,9α)-*form*

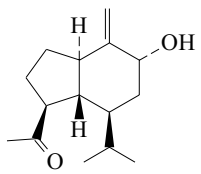
9-Angeloyl: [237407-00-0]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D^{28}$ -104.5 (c, 0.07 in $CHCl_3$). λ_{max} 224 (log ϵ 4.1) (MeOH).

9-(3-Methyl-2-butenoyl): [237406-99-4]
$C_{20}H_{28}O_3$ 316.439
Constit. of *Tussilago farfara* (coltsfoot). Oil. $[\alpha]_D^{27}$ -97.6 (c, 0.04 in $CHCl_3$). λ_{max} 223 (log ϵ 4.3) (MeOH).

*9-(3-Methyl-2*E*-pentenoyl):* [110042-38-1]
Tussilagonone
$C_{21}H_{30}O_3$ 330.466
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{23}$ -50.3 (c, 0.2 in $CHCl_3$).

Shi, W. *et al., Chin. Chem. Lett.*, 1995, **6**, 585-586 (*isol, pmr, cmr*)
Shi, W. *et al., J. Chin. Pharm. Sci.*, 1996, **5**, 63-67; *CA*, **126**, 314812d (*isol, pmr, cmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 705-707 (*isol, pmr, cmr*)

9-Hydroxy-10(14)-oplopen-4-one H-668



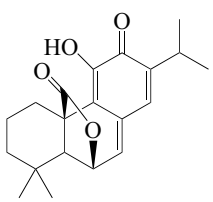
$C_{15}H_{24}O_2$ 236.353

9α-*form* [147545-38-8]
Tuberonone
Constit. of *Solanum tuberosum* (potato). $[\alpha]_D^{20}$ -33.1 (c, 0.048 in MeOH).

9β-*form* [152242-36-9]
Oil. $[\alpha]_D$ -11.5 (c, 0.9 in $CHCl_3$).

Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1890 (*isol, pmr, cmr*)
Marco, J.A. *et al., Phytochemistry*, 1993, **34**, 1061 (*isol, pmr, cmr*)

11-Hydroxy-12-oxo-7,9(11),13-abietatrien-20,6-olide H-669

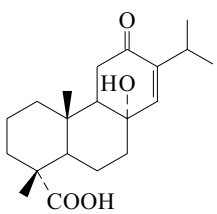


$C_{20}H_{24}O_4$ 328.407

6β-*form* [194472-90-7]
Sagequinone methide A
Constit. of *Salvia officinalis* (sage). Yellow cryst. Mp 145-147°. $[\alpha]_D^{25}$ -80.7 (c, 0.29 in $CHCl_3$).

Tada, M. *et al., Phytochemistry*, 1997, **45**, 1475-1477 (*isol, pmr, cmr*)

8-Hydroxy-12-oxo-13-abieten-18-oic acid H-670



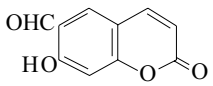
$C_{20}H_{30}O_4$ 334.455

8α-*form* [130252-62-9]
Constit. of *Pinus sylvestris* (Scotch pine).

Buratti, L. *et al., Phytochemistry*, 1990, **29**, 2708 (*isol, pmr, ms*)

7-Hydroxy-2-oxo-2*H*-1-benzopyran-6-carboxaldehyde, 9CI H-671

*6-Formyl-7-hydroxycoumarin. 6-Formyl-7-hydroxy-2*H*-1-benzopyran-2-one.* ***6-Formylumbelliferone***



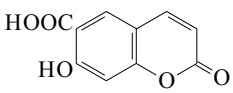
$C_{10}H_6O_4$ 190.155
Constit. of *Citrus medica* (citron). Oil.

Me ether: [4444-74-0] *7-Methoxy-2-oxo-2*H*-1-benzopyran-6-carboxaldehyde. 6-Formyl-7-methoxy-2*H*-1-benzopyran-2-one. 6-Formyl-7-methoxycoumarin.* ***Angelical****. Crenulatin*†
$C_{11}H_8O_4$ 204.182
Cryst. (EtOAc). Mp 256-257°. Prob. artifact λ_{max} 256 (ϵ 14800); 308 (ϵ 7400); 331 (ϵ 7750) (EtOH) (Berdy).

Guise, G.B. *et al., Aust. J. Chem.*, 1967, **20**, 2429 (*Angelical*)
Basa, S.C. *et al., Aust. J. Chem.*, 1975, **28**, 1159 (*Angelical*)
Talapatra, S.K. *et al., Phytochemistry*, 1975, **14**, 836 (*Angelical*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3805 (*6-Formylumbelliferone*)
Paradkar, M.V. *et al., J. Chem. Res., Synop.*, 1995, 262 (*synth, Angelical, pmr*)

7-Hydroxy-2-oxo-2*H*-1-benzopyran-6-carboxylic acid, 9CI H-672

[833-52-3]
7-Hydroxycoumarin-6-carboxylic acid. Umbelliferone-6-carboxylic acid



$C_{10}H_6O_5$ 206.154
Cryst. Mp 258-259° dec.

Me ester: [52591-14-7] ***Peuruthenicin****. Officinalin*
Cream coloured needles (MeOH). Mp 196-197°. The structs. of Officinalin and its esters were questioned in 1977.

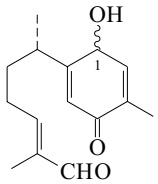
Ac, Me ester: [61467-57-0] *Officinalin acetate*
$C_{13}H_{10}O_6$ 262.218
Cryst. (C_6H_6/petrol). Mp 193.5-195°.

2-Methylpropanoyl, Me ester: [61467-56-9] *Officinalin isobutyrate*
$C_{15}H_{14}O_6$ 290.272
Cryst. (C_6H_6/petrol). Mp 118.5-120°.

Me ether: [52525-63-0] *7-Methoxycoumarin-6-carboxylic acid.* ***Buntansin A***
$C_{11}H_8O_5$ 220.181
Constit. of *Citrus grandis* (pummelo). Granules (Me_2CO). Mp 237-239° (216-217°).

Soine, T.O. *et al., J. Pharm. Sci.*, 1973, **63**, 1879 (*isol, synth, ir, pmr*)
Gonzalez, A.G. *et al., An. Quim.*, 1976, **72**, 60 (*isol*)
Ahluwalia, V.K. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 423 (*synth*)
Gonzalez, A.G. *et al., An. Quim.*, 1978, **74**, 637-640 (*isol*)
Macias, F.A. *et al., Magn. Reson. Chem.*, 1989, **27**, 892-904 (*cmr*)
Huang, S.-C. *et al., Phytochemistry*, 1989, **28**, 3574 (*isol, pmr*)

1-Hydroxy-4-oxo-2,5,10-bisabolatrien-12-al H-673



(*E*)-*form*

$C_{15}H_{20}O_3$ 248.321

(*E*)-*form*
Glandulone C
Constit. of *Helianthus annuus* (sunflower). Brown oil. $[\alpha]_D^{25}$ +23.6 (c, 0.12 in MeOH). λ_{max} 230 ; 292 (MeOH) (Berdy).

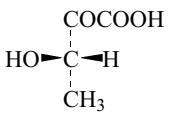
1-Ketone:1,4-Dioxo-2,5,10-bisabolatrien-12-al. ***Glandulone A***
$C_{15}H_{18}O_3$ 246.305
Constit. of *Helianthus annuus* (sunflower). Brown oil. $[\alpha]_D^{25}$ +142.5 (c, 0.12 in MeOH). λ_{max} 232 ; 262 (MeOH) (Berdy).

(*Z*)-*form*
1-Ketone:
$C_{15}H_{18}O_3$ 246.305
Pale yellow oil. $[\alpha]_D$ -115.3 (c, 0.93 in $CHCl_3$).

Spring, O. *et al., Phytochemistry*, 1992, **31**, 1541 (*isol, pmr*)
Mendoza, G.V. *et al., J. Nat. Prod.*, 1993, **56**, 2073 (*isol, pmr, cmr, synth*)

3-Hydroxy-2-oxobutanoic acid H-674

[1944-42-9]



(*S*)-*form*

$C_4H_6O_4$ 118.089

(*S*)-*form*
Me ether, Me ester:
$C_6H_{10}O_4$ 146.143
Oil. $[\alpha]_D^{25}$ -7.7 (c, 2.0 in $CHCl_3$).

Benzyl ether, Me ester:
$C_{12}H_{14}O_4$ 222.24
Viscous oil. $[\alpha]_D^{24}$ -6.9 (c, 1.0 in $CHCl_3$).

(±)-*form*
Et ester, phenylhydrazone:
Prisms. Mp 93-94°.

(ξ)-*form*
Isol. from fruits of cowberry (*Vaccinium vitis-idaea*). Component of cheese aroma.

[68862-42-0]

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1955, **9**, 188 (*isol*)
Bowman, R.E. *et al., J.C.S.*, 1957, 1583 (*synth, deriv*)
Harding, J.R. *et al., J.C.S. Perkin 1*, 2000, 3406-3416 (*S-form, Me ether Me ester, benzyl ether Me ester, synth, pmr, ir, ms*)

4-Hydroxy-2-oxobutanoic acid H-675

[22136-38-5]
γ-Hydroxy-α-ketobutyric acid
$HOCH_2CH_2COCOOH$
$C_4H_6O_4$ 118.089
Isol. from fruits of *Vaccinium vitis-idaea* (cowberry) and from *Vaccinium oxycoccus* (small cranberry). Unstable, stabilised in frozen soln. at neutral pH.

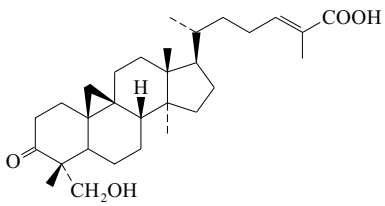
2,4-Dinitrophenylhydrazone: [22136-40-9]
Long yellow needles (EtOH). Mp 238-239°.

Lactone: See Dihydro-2,3-furandione in *The Combined Chemical Dictionary.*

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1955, **9**, 188 (*isol*)
Lane, A.S. *et al., Biochemistry*, 1969, **8**, 2958 (*synth, ir, uv*)

28-Hydroxy-3-oxocycloart-24-en-26-oic acid H-676

28-Hydroxy-3-oxo-9,19-cyclolanost-24-en-26-oic acid

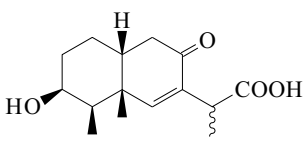


$C_{30}H_{46}O_4$ 470.691

(24*E*)-*form* [155511-27-6]
28-Hydroxymangiferonic acid
Constit. of *Mangifera indica* (mango). Cryst. (C_6H_6). Mp 182-183°. $[\alpha]_D^{26}$ +42 (c, 1.2 in $CHCl_3$). Incorrectly named as 29-Hydroxymangiferonic acid in ref..

Anjaneyulu, V. *et al., Phytochemistry*, 1994, **35**, 1301 (*isol, pmr, cmr*)

3-Hydroxy-8-oxo-6-eremophilen-12-oic acid H-677

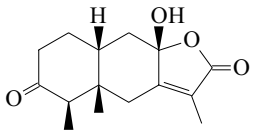


$C_{15}H_{22}O_4$ 266.336

(3β,11ξ)-*form*
Me ester: [64964-00-7]
$C_{16}H_{24}O_4$ 280.363
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{24}$ -9.3 (c, 0.2 in MeOH).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1738-1743 (*isol, pmr, cmr*)

8-Hydroxy-3-oxo-7(11)-eremophilen-12,8-olide H-678

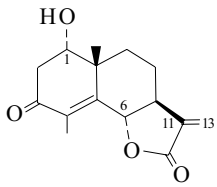


$C_{15}H_{20}O_4$ 264.321

(8βOH,10β)-*form* [171422-92-7]
Constit. of *Petasites japonicus* (sweet coltsfoot). Needles (EtOAc). Mp 204-206°. $[\alpha]_D^{27}$ +48.4 (c, 0.1 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1738 (*isol, pmr, cmr*)

1-Hydroxy-3-oxo-4,11(13)-eudesmadien-12,6-olide H-679



(1α,6α)-*form*

$C_{15}H_{18}O_4$ 262.305

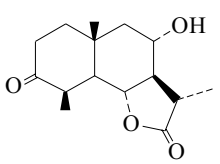
(1α,6α)-*form* [27740-15-4]
Ludovicin C
Cryst. (Et_2O/CH_2Cl_2). Mp 193-195°. $[\alpha]_D^{25}$ +95 ($CHCl_3$). λ_{max} 208 (ε 13700); 243 (ε 15200) (EtOH) (Berdy).

11,13-Dihydro: See 1,3-Dihydroxy-4-eudesmen-12,6-olide, D-459

(1β,6α)-*form* [64929-15-3]
Armexifolin. *1-Epiludovicin C*
Isol. from *Tanacetum vulgare* (tansy). Cryst. Mp 201-203°.

Lee, K.H. *et al., Phytochemistry*, 1970, **9**, 403 (*isol*)
Serkerov, S. *et al., Khim. Prir. Soedin.*, 1979, **15**, 488; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 424
Ognyanov, I. *et al., Planta Med.*, 1983, **48**, 181 (*isol*)
Mata, R. *et al., Phytochemistry*, 1984, **23**, 1665 (*isol*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)
Suzuki, T. *et al., Heterocycles*, 2001, **54**, 865-870 (*synth*)

8-Hydroxy-3-oxo-12,6-eudesmanolide H-680

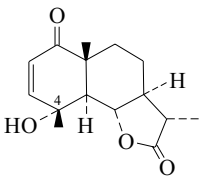


$C_{15}H_{22}O_4$ 266.336

(4β,6α,8α,11α)-*form* [38412-44-1]
Arabsin
Constit. of *Artemisia absinthium* (wormwood). Cryst. (C_6H_6). Mp 188-189°. $[\alpha]_D^{23}$ +89 (c, 2.71 in EtOH).

Akhmedov, I.S. *et al., Khim. Prir. Soedin.*, 1972, **8**, 245; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 245

4-Hydroxy-1-oxo-2-eudesmen-12,6-olide H-681



(4α,6α,11α)-*form*

$C_{15}H_{20}O_4$ 264.321

(4α,6α,11α)-*form* [3162-56-9]
Vulgarin. *Barrelin. Judaicin. Tauremisin A. Tauresmin*
Constit. of *Artemisia vulgaris* (mugwort). Cryst. (EtOH). Mp 174-175°. $[\alpha]_{Hg}^{27}$ +48.7 (c, 3.86 in $CHCl_3$).
► LE3170000

4-Hydroperoxide: [72505-77-2] ***4α-Hydroperoxydesoxyvulgarin***. *Peroxyvulgarin*
$C_{15}H_{20}O_5$ 280.32
Gum, needles (Me_2CO/Et_2O). Mp 170-171°. $[\alpha]_D$ -44 (c, 0.1 in MeOH).

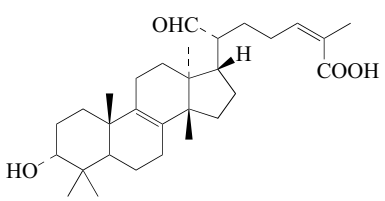
11,13-Didehydro: See 1,4-Dihydroxy-2,11(13)-eudesmadien-12,6-olide in *The Combined Chemical Dictionary.*

(4β,6α,11α)-*form* [66289-87-0]
4-Epivulgarin
Cryst. (C_6H_6/hexane)(also descr. as gum). Mp 192-194°. $[\alpha]_D$ +77.5 (c, 5.7 in $CHCl_3$).

[5091-07-6]

Geissman, T.A. *et al., J.O.C.*, 1962, **27**, 1855 (*isol, struct*)
González, G. *et al., J.C.S. Perkin 1*, 1978, 1243 (*synth*)
Ando, M. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 2737 (*synth*)
Gonzalez, A.G. *et al., Phytochemistry*, 1983, **22**, 1509 (*isol*)
Metwally, M.A. *et al., Phytochemistry*, 1985, **24**, 1103 (*derivs*)
Abagaz, B. *et al., Tetrahedron*, 1986, **42**, 6003 (*cryst struct*)
Arias, J.M. *et al., J.C.S. Perkin 1*, 1987, 471 (*synth*)
Al-Said, M.S. *et al., Phytochemistry*, 1989, **28**, 107 (*synth*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **43**, 4761 (*synth, rev*)
Glasl, S. *et al., Phytochemistry*, 1995, **38**, 159 (*Tauresmin, pmr, cmr*)

3-Hydroxy-21-oxoeupha-8,24-dien-26-oic acid H-682



$C_{30}H_{46}O_4$ 470.691

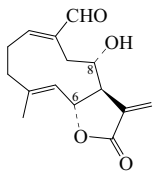
(3α,20*R*,24*Z*)-*form* [195204-05-8]
Constit. of *Schinus molle* (California peppertree). Constit. of *Schinus molle* (California peppertree).

(3α,20*S*,24*Z*)-*form*
3-Hydroxy-21-oxotirucalla-8,24-dien-26-oic acid
Constit. of *Schinus molle* (California peppertree).

Olafsson, K. *et al., Planta Med.*, 1997, **63**, 352-355 (*isol, pmr, cmr*)

8-Hydroxy-14-oxo-1(10),4,11(13)-germacratrien-12,6-olide H-683

8-Hydroxy-14-oxoacanthospermolide



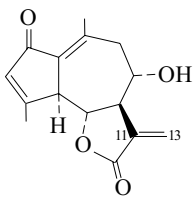
(1(10)*E*,4*E*,6α,8α)-*form*

$C_{15}H_{18}O_4$ 262.305

(1(10)*E*,4*E*,6α,8β)-*form*
Angeloyl:
$C_{20}H_{24}O_5$ 344.407
Constit. of *Helianthus annuus* (sunflower).

Macías, F.A. *et al., Phytochemistry*, 1996, **43**, 1205 (*angeloyl*)

8-Hydroxy-2-oxo-1(10),3,11(13)-guaiatrien-12,6-olide H-684



(5α,6α,8α)-*form*

$C_{15}H_{16}O_4$ 260.289

(5α,6α,8α)-*form* [74635-52-2]
11,13-Dehydrodesacetylmatricarin. ***14-Deoxylactucin***
Cryst. (EtOAc). Mp 224-226° (215-217°).

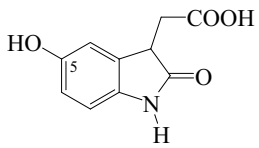
11β,13-Dihydro, Ac: [5989-43-5] ***Matricarin***. *Artilesin A*
$C_{17}H_{20}O_5$ 304.342
Constit. of *Matricaria chamomilla* (German chamomile). Cryst. (C_6H_6/petrol). Mp 193-195°. $[\alpha]_D^{23}$ +23.5 (c, 0.65 in $CHCl_3$).

[35879-92-6]

White, E.H. *et al., Tet. Lett.*, 1963, 137-140 (*Achillea lanulosa constit*)
Parvez, M. *et al., Acta Cryst. E*, 2002, **58**, o324-o325 (*Matricarin, cryst struct*)

5-Hydroxy-2-oxo-1*H*-indole-3-acetic acid, 9CI H-685

*5-Hydroxyoxindole-3-acetic acid. 2,5-Dihydroxy-1*H*-indole-3-acetic acid*

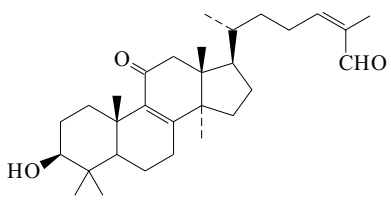


$C_{10}H_9NO_4$ 207.185

Me ester:
$C_{11}H_{11}NO_4$ 221.212
Isol. from rice bran. Amorph. powder.

Kinashi, H. *et al., Agric. Biol. Chem.*, 1976, **40**, 2465

3-Hydroxy-11-oxolanosta-8,24-dien-26-al H-686

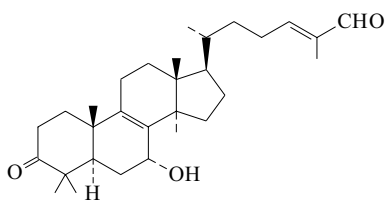


$C_{30}H_{46}O_3$ 454.692

3β-*form* [126313-85-7]
Metab. of *Ganoderma lucidum* (reishi). Needles (MeOH). Mp 131-133°. $[\alpha]_D^{20}$ +248.4 (c, 0.095 in $CHCl_3$).

Lin, C.-N. *et al., Phytochemistry*, 1990, **29**, 673 (*isol, pmr, cmr*)

7-Hydroxy-3-oxolanosta-8,24-dien-26-al H-687



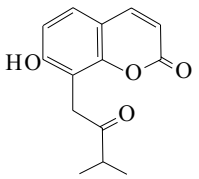
$C_{30}H_{46}O_3$ 454.692

(7α,24*E*)-*form* [114020-55-2]
Ganoderal B
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ +94 (c, 0.1 in EtOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 211

7-Hydroxy-8-(3-methyl-2-oxobutyl)-2*H*-1-benzopyran-2-one H-688

7-Hydroxy-8-(3-methyl-2-oxobutyl)coumarin



$C_{14}H_{14}O_4$ 246.262

Me ether: [1088-17-1] ***Isomeranzin***. *Isomerancin. Isoauraptene*
$C_{15}H_{16}O_4$ 260.289
Cryst. (pentane). Mp 60-62°. The name Isoauraptene (given in CAS) is misleading.

O-*(3-Methyl-2-butenyl):* [72545-59-6] ***Anisocoumarin E***
$C_{19}H_{22}O_4$ 314.38
Yellow oil. λ_{max} 247 (sh) (ϵ 4570); 259 (ϵ 4900); 324 (ϵ 11200) (EtOH) (Derep).

O-*(2,3-Dihydroxy-3-methylbutyl):* [81445-98-9] ***Triphasiol***
$C_{19}H_{24}O_6$ 348.395
Constit. of *Triphasia trifolia* (limeberry). Cryst. ($CHCl_3$/petrol). Mp 85°.

O-*(2,3-Epoxy-3-methylbutyl):* [59176-65-7] ***Isoponcimarin***
$C_{19}H_{22}O_5$ 330.38
Cryst. (hexane). Mp 85°. $[\alpha]_{465}^{20}$ -6.94 (c, 3.75 in $CHCl_3$).

O-*(3-Chloro-2-hydroxy-3-methylbutyl):* [157230-20-1] ***3″-Chloro-3″-deoxytriphasiol***
$C_{19}H_{23}ClO_5$ 366.84
Constit. of *Triphasia trifolia* (limeberry). Amorph.

Atkinson, E. *et al., Phytochemistry*, 1974, **13**, 853-855 (*Isomeranzin*)
Guiotto, A. *et al., Phytochemistry*, 1976, **15**, 348; 1977, **16**, 1257-1260 (*Isoponcimarin*)
De Silva, L.B. *et al., Phytochemistry*, 1981, **20**, 2776-2778 (*Triphasiol*)
Ngadjui, B.T. *et al., J. Nat. Prod.*, 1989, **52**, 243 (*Anisocoumarin E*)
Abaul, J. *et al., J. Nat. Prod.*, 1994, **57**, 846 (*3″-Chloro-3″-deoxytriphasiol*)

9-Hydroxy-16-oxo-10,12,14-octadecatrienoic acid H-689

$H_3CCH_2COCH{=}CHCH{=}CHCH{=}CHCH(OH)(CH_2)_7COOH$

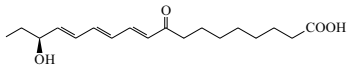
$C_{18}H_{28}O_4$ 308.417

(9*S*,10*E*,12*E*,14*E*)-*form*
Corchorifatty acid A
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{26}$ +13 (c, 0.4 in Me_2CO). Isol. as a partial racemate of 60% op λ_{max} 310 (log ϵ 4.6) (MeOH).

(10*E*,12*Z*,14*E*)-(+)-*form*
Corchorifatty acid C
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{24}$ +12.9 (c, 0.2 in Me_2CO). λ_{max} 311 (log ϵ 4.4) (MeOH).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1008-1014 (*isol, uv, ir, pmr, cmr, ms*)

16-Hydroxy-9-oxo-10,12,14-octadecatrienoic acid H-690



$C_{18}H_{28}O_4$ 308.417

(10*E*,12*E*,14*E*,16*S*)-*form*
Corchorifatty acid B
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{28}$ +17.3 (c, 0.2 in Me_2CO). λ_{max} 309 (log ϵ 4.3) (MeOH).

Me ester: [147383-00-4]
$C_{19}H_{30}O_4$ 322.444
Oil. $[\alpha]_D^{25}$ +19 (c, 0.25 in Me_2CO).

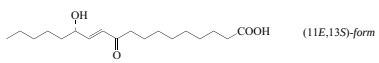
(10*E*,12*Z*,14*E*,16*S*)-*form* *Corchorifatty acid D*
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{26}$ +19.7 (c, 0.04 in Me_2CO). λ_{max} 311 (log ϵ 4.3) (MeOH).

(10*E*,12*Z*,14*E*,16*RS*)-*form*
Me ester: [147292-99-7]
Oil.

Bernart, M.W. *et al., Phytochemistry*, 1993, **56**, 245 (*isol, struct*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1008-1014 (*isol, uv, ir, pmr, cmr, ms*)

13-Hydroxy-10-oxo-11-octadecenoic acid H-691

[104840-02-0]



$C_{18}H_{32}O_4$ 312.448

(11*E*,13*S*)-*form*
$[\alpha]_D^{25}$ +15.8 (c, 2 in MeOH).

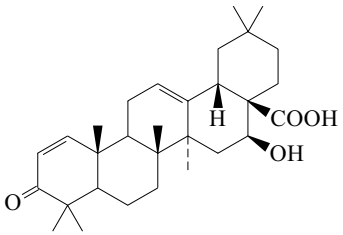
(±)-(*E*)-*form* [28979-44-4]
Isol. from corn. Powder. Sol. DMSO, MeOH, EtOAc; poorly sol. H_2O. Mp 64°. λ_{max} 210 (ϵ 8500) (EtOH) (Berdy).

Lactone:

[159504-60-6, 174690-92-7, 174690-94-9] *14-Pentyloxacyclotetradec-11-ene-2,11-dione. 10-Oxo-11-octadecen-13-olide*
$C_{18}H_{30}O_3$ 294.433
Isol. from corn. Powder. Sol. DMSO, MeOH, EtOAc; poorly sol. H_2O. Mp 52°. λ_{max} 210 (ϵ 7500) (MeOH) (Berdy).

Yabuuchi, S. *et al., Phytochemistry*, 1976, **15**, 387
Kuga, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1020-1021
Hayashi, Y. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1115-1117; 1998, **62**, 1771-1773 (*isol, uv, ir, pmr, cmr, activity*)
Nokami, J. *et al., J.C.S. Perkin 1*, 1997, 2947-2948 (*synth*)
Matsushita, Y. *et al., Tet. Lett.*, 1997, **38**, 6055-6058 (*lactone, synth, config*)

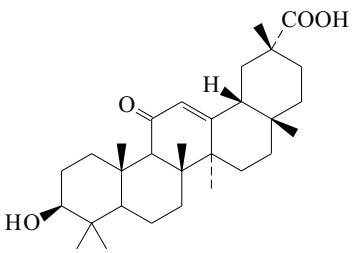
16-Hydroxy-3-oxo-1,12-oleanadien-28-oic acid H-692



$C_{30}H_{44}O_4$ 468.675

16β-*form* [77625-72-0]
Constit. of *Vitis vinifera* (wine grape). Cryst. (MeOH) (as Me ester, Ac). Mp 175-177° (Me ester, Ac).
Brieskorn, C.H. *et al., CA*, 1981, **94**, 188662k (*isol, pmr, cmr*)

3-Hydroxy-11-oxo-12-oleanen-29-oic acid H-693



$C_{30}H_{46}O_4$ 470.691

3β-*form* [10379-72-3]
Liquiritic acid
Isol. from *Glycyrrhiza glabra* (licorice). Cryst. (MeOH). Mp 298-303°. $[\alpha]_D^{20}$ +85 (c, 0.34 in EtOH). Log P 6.25 (calc).

Me ester: [10379-74-5]
Cryst. ($CHCl_3$/pet ether). Mp 223-224°. $[\alpha]_D^{20}$ +71.5 (c, 0.98 in EtOH).

Ac:
Mp 313-316°.

Ac, Me ester: [10379-75-6]
Cryst. (Me_2CO). Mp 245-246°. $[\alpha]_D^{20}$ +58 (c, 0.4 in EtOH).

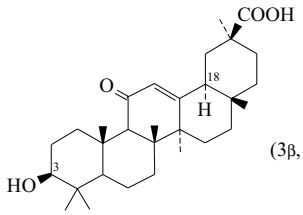
3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: [135815-61-1]
Licoricesaponin H2
$C_{42}H_{62}O_{16}$ 822.942
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Mp 209-210°. $[\alpha]_D^{25}$ +31 (MeOH).

3-O-[6-Butyl-β-D-glucuronopyranosyl-(1→2)-6-ethyl-β-D-glucuronopyranoside]: ***Inflasaponin III***
$C_{48}H_{74}O_{16}$ 907.103

3-O-[6-Butyl-β-D-glucuronopyranosyl-(1→2)-6-butyl-β-D-glucuronopyranoside]: ***Inflasaponin V***
$C_{50}H_{78}O_{16}$ 935.157

Canonica, L. *et al., Gazz. Chim. Ital.*, 1966, **96**, 833 (*isol, struct*)
Wahlberg, I. *et al., Acta Chem. Scand.*, 1971, **25**, 3192 (*ms*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1991, **39**, 244 (*Licoricesaponin H2*)
Zou, K. *et al., CA*, 1994, **121**, 297132j (*Inflasaponins*)
Zou, K. *et al., J. Chin. Pharm. Sci.*, 1994, **3**, 90; *CA*, **122**, 51291r (*Inflasaponins*)

3-Hydroxy-11-oxo-12-oleanen-30-oic acid H-694



(3β,18α)-*form*

$C_{30}H_{46}O_4$ 470.691
Log P 6.25 (calc).

► RK0180000

(3β,18α)-*form* [1449-05-4]
18α-Glycyrrhetic acid. Isoglycyrrhetinic acid. β-Glycyrrhetinic acid. Uralenic acid
Constit. of licorice (*Glycyrrhiza glabra*) root. Cryst. ($CHCl_3$/MeOH). Sol. MeOH, $CHCl_3$; fairly sol. EtOH; poorly sol. H_2O. Mp 330-335°. $[\alpha]_D$ +98. λ_{max} 242 (ε 12200) (MeOH) (Berdy).

► LD_{50} (mus, orl) 560 mg/kg. RK0190000

(3β,18β)-*form* [471-53-4]
Glycyrrhetic acid. *α-Glycyrrhetinic acid. Enoxolone, BAN, INN. Biogastrone acid. Biosone. Glycyrrhetin. Glycyrrhetinic acid. Rhetinic acid. Uralenic acid*
Aglycone from licorice (*Glycyrrhiza glabra*). Cryst. (MeOH). Mp 300-304°. $[\alpha]_D$ +161 ($CHCl_3$). Log P 6.25 (calc). Sweet taste.

► LD_{50} (mus, ivn) 56 mg/kg, inhibits 11β-hydroxysteroid dehydrogenase.

Me ester: [1477-44-7]
$C_{31}H_{48}O_4$ 484.718
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Cryst. (EtOH). Mp 253-255°.

► RK0256000

3-O-β-D-Glucuronopyranoside: [34096-83-8] *Monoglucuronylglycyrrhetinic acid. MGGR*
$C_{36}H_{54}O_{10}$ 646.817
Sweetener *ca.* 940 times sweeter than sucrose.

3-O-[β-D-Glucopyranuronosyl-(1→2)-α-D-glucuronopyranoside], β-D-glucopyranosyl ester: [118325-22-7] ***Licoricesaponin A3***
$C_{48}H_{72}O_{21}$ 985.084
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice). Trihydrate. Mp 196-199°. $[\alpha]_D^{23}$ +69 (MeOH).

3-O-[β-D-Glucuronopyranosyl-(1→3)-β-D-glucuronopyranoside]: [105038-43-5] ***Uralsaponin B***
$C_{42}H_{62}O_{16}$ 822.942
Constit. of *Glycyrrhiza uralensis* (Chinese licorice).

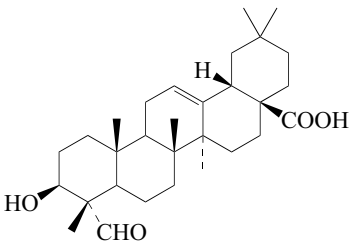
3-Glycoside: ***Glabranin A***
$C_{54}H_{86}O_{23}$ 1103.26
Saponin from roots of licorice (*Glycyrrhiza glabra*). Light brown powder. Mp 160-163°. $[\alpha]_D$ +60 (c, 1 in MeOH). Gives 3-Glu and 1-Rha on hydrol. Said to contain α-D-glucosyl residues.

3-Glycoside(2): ***Glabranin B***
$C_{59}H_{94}O_{27}$ 1235.375
Saponin from licorice (*Glycyrrhiza glabra*). Light-brown powder. Mp 165-167°. $[\alpha]_D$ +72 (c, 1 in MeOH). Gives 3-Glu, 1-Rha and 1-Xyl on hydrol..

30-Alcohol: [14226-18-7] *3,30-Dihydroxy-12-oleanen-11-one.* ***Glycyrrhetol***
$C_{30}H_{48}O_3$ 456.707
Saponin from licorice (*Glycyrrhiza glabra*). Cryst. (MeOH aq.). Mp 252-254°. $[\alpha]_D^{20}$ +87 (c, 1.9 in $CHCl_3$).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1057D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 596A (*nmr*)
Beaton, J.M. *et al., J.C.S.*, 1955, 3126 (*synth*)
Mer, J. *et al., Am. Perfum. Aromat.*, 1959, **74**, 39 (*isol*)
U.K. Pat., 1960, 843 133; *CA*, **55**, 2027i (*Carbenoxolone*)
Witz, P. *et al., Bull. Soc. Chim. Fr.*, 1963, 1101 (*cd*)
Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688 (*ms*)
Murav'ev, I.A. *et al., CA*, 1966, **69**, 44029v (*rev*)
Canonica, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 1347; 1968, **98**, 602 (*Glycyrrhetol*)
Robson, J.M. *et al., Carbenoxolone Sodium, Orig. Pap. Discuss. Group Meet.*, Butterworth, London, 1969, (*rev*)
Wahlberg, I. *et al., Acta Chem. Scand.*, 1971, **25**, 3192 (*ms*)
Varshney, I.P. *et al., Int. J. Crude Drug Res.*, 1983, **21**, 169 (*Glabranins*)
Sandiya, R. *et al., J. Het. Chem.*, 1984, **21**, 845 (*isol*)
Tolstikov, G.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 645; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 605 (*cmr*)
Sakano, K. *et al., Agric. Biol. Chem.*, 1986, **50**, 763 (*deriv*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7889; 8042 (*synonyms*)
Kanaoka, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3264 (*synth*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3710; 1989, **37**, 551 (*Licoricesaponin A3, Araboglycyrrhizin, Apioglycyrrhizin*)
Pandey, H.S. *et al., Planta Med.*, 1992, **58**, 225 (*Glycyrrhetol, isol, ms*)
Mizutani, K. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 554-555 (*MGGR, synth, props*)
Saito, S. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1016 (*synth*)
Zou, K. *et al., J. Chin. Pharm. Sci.*, 1995, **4**, 113; *CA*, **124**, 50610y (*Inflasaponins*)
Mizutani, K. *et al., New Food Ind.*, 1998, **40(3)**, 1-10; *CA*, **128**, 320665r (*MGGR, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GIE000; BGD000; GIEO5O; CBO500

3-Hydroxy-23-oxo-12-olea-nen-28-oic acid H-695



$C_{30}H_{46}O_4$ 470.691

3β-*form* [639-14-5]
Gypsogenin. *Gypsophilasapogenin*. *Albasapogenin*. *Githagenin*. *Astrantiagenin D*
Cryst. (MeOH). Mp 274-276°. $[\alpha]_D$ +91 (EtOH).

► RK0178000

3-O-*β-D-Glucopyranoside:* [32448-19-4] ***Lucyoside K***
$C_{36}H_{56}O_9$ 632.833
Constit. of *Luffa cylindrica* (smooth luffa). Cryst. Mp 230-232°. $[\alpha]_D$ +55.1 (c, 2.2 in MeOH).

3-O-*(6*-O-*Acetyl-β-D-glucopyranoside), 28*-O-*β-D-glucopyranosyl ester:* [100156-32-9] ***Lucyoside M***
$C_{44}H_{68}O_{15}$ 837.012
Isol. from *Luffa cylindrica* (smooth luffa). Amorph. $[\alpha]_D$ +49.8 (c, 0.4 in MeOH).

3-O-*α-D-Glucuronopyranoside:* ***Vaccaroside***
$C_{36}H_{54}O_{10}$ 646.817
Isol. from *Luffa cylindrica* (smooth luffa). Cryst. + $2H_2O$ (EtOH). Mp 204-206°. $[\alpha]_D$ +16.5 (c, 1.75 in EtOH).

3-O-*β-D-Glucuronopyranoside:* [105762-16-1]
$C_{36}H_{54}O_{10}$ 646.817
Constit. of the famine food *Momordica dioica*. Cryst. Mp 238-240°.

3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*[β-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosyl] ester:* [229484-38-2] ***Silenoside A***
$C_{64}H_{100}O_{31}$ 1365.475
Constit. of *Silene vulgaris* (bladder campion). Powder.

3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-fucopyranosyl] ester:* [333333-20-3] ***Goyasaponin I***
$C_{65}H_{102}O_{31}$ 1379.502
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{24}$ -13.5 (c, 0.5 in Py).

3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-fucopyranosyl] ester:* [333333-23-6] ***Goyasaponin II***
$C_{70}H_{110}O_{35}$ 1511.618
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{24}$ -18.5 (c, 1 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [100179-68-8] ***Lucyoside L***
$C_{48}H_{76}O_{19}$ 957.117
Constit. of *Luffa cylindrica* (smooth luffa). Amorph. $[\alpha]_D$ +27.4 (c, 2.1 in MeOH). λ_{max} 238 (ε 33500) (MeOH) (Berdy).

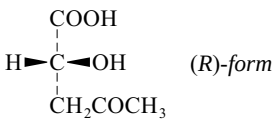
3-O-*[β-D-Galactopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosyl] ester:* [96552-95-3] ***Momordicasaponin I***
$C_{76}H_{120}O_{40}$ 1673.76
Isol. from seeds of *Momordica cochinchinensis* (Chinese cucumber). Powder (MeOH). Mp 241-244° dec. $[\alpha]_D^{19}$ -14.8 (c, 0.7 in 33% MeOH aq.).

[60407-57-0]

Kon, G.A.R. *et al., J.C.S.*, 1940, 617-620 (*isol, bibl*)
Vogel, A. *et al., Helv. Chim. Acta*, 1951, **34**, 2321-2328 (*isol, struct*)
Iwamoto, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 464-478 (*Momordicasaponin I*)
Takemoto, T. *et al., Yakugaku Zasshi*, 1985, **105**, 834; *CA*, **104**, 95321h (*Lucyosides*)
Luo, L. *et al., Acta Physiol. Scand.*, 1998, **33**, 839-842 (*3-glucuronoside*)
Glensk, M. *et al., J. Nat. Prod.*, 1999, **62**, 717-721 (*Silenoside A*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 54-63 (*Goyasaponins*)

2-Hydroxy-4-oxopentanoic acid, 9CI H-696

[54031-97-9]
2-Hydroxy-4-oxovaleric acid. Acetolactic acid. α-Hydroxylevulinic acid. α-Hydroxy-β-acetylpropionic acid



(*R*)-*form*

$C_5H_8O_4$ 132.116
Formed in beer wort fermentation.

(*R*)-*form*
Me ester: [142395-20-8]
$C_6H_{10}O_4$ 146.143
$[\alpha]_D^{24}$ +11.3 (c, 3.22 in Me_2CO) (99% ee).

(*S*)-*form* [150337-72-7]
Me ester: [142395-24-2]
$[\alpha]_D^{24}$ -11.6 (c, 3.35 in Me_2CO) (99% ee).

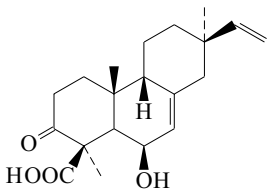
(±)-*form* [142896-50-2]
Cryst. (THF/hexane). Mp 25°.

Me ether, Me ester: [85858-44-2] *Methyl 2-methoxy-4-oxopropanoate*
$C_7H_{12}O_4$ 160.169
Liq. Bp_{12} 100.5°. n_D^{20} 1.4292.

[26453-27-0, 55134-90-2]

Birkofer, L. *et al., Annalen*, 1957, **608**, 7 (*deriv*)
Kiehlmann, E. *et al., Can. J. Chem.*, 1976, **54**, 1998 (*deriv*)
Andersen, S.H. *et al., Acta Chem. Scand., Ser. B*, 1982, **36**, 1 (*synth, pmr*)
Bonadies, F. *et al., Gazz. Chim. Ital.*, 1983, **113**, 421 (*synth*)
Lueoend, R.M. *et al., J.O.C.*, 1992, **57**, 5005 (*synth, pmr, cmr, ms, ir*)
Baraldi, P.G. *et al., Tet. Lett.*, 1992, **33**, 2871 (*synth*)
Casy, G. *et al., Tet. Lett.*, 1992, **33**, 8159 (*synth*)

6-Hydroxy-3-oxo-7,15-pimar-adien-19-oic acid H-697



$C_{20}H_{28}O_4$ 332.439

6β-*form*
19→6 Lactone: [51415-07-7] *3-Oxo-7,15-pimaradien-19,6-olide.* ***Momilactone A***
Constit. of *Oryza sativa* (rice). Cryst. (CH_2Cl_2/EtOH). Mp 235-236° dec. $[\alpha]_D$ -277 ($CHCl_3$). λ_{max} 225 (EtOH) (Berdy).

Kato, T. *et al., J.C.S. Perkin 1*, 1977, 250-254 (*struct*)
Kato, T. *et al., Phytochemistry*, 1977, **16**, 45-48 (*isol*)
Wickham, K.A. *et al., Arch. Biochem. Biophys.*, 1992, **293**, 320-322 (*biosynth*)
Koga, J. *et al., Tetrahedron*, 1995, **51**, 7907 (*cmr*)
Atawong, A. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 566-570 (*biosynth*)
Germain, J. *et al., J.O.C.*, 2002, **67**, 5269-5278 (*synth*)

3-Hydroxy-2-oxopropanoic acid, 9CI H-698

[1113-60-6]
Hydroxypyruvic acid. Aldehydohydroxyacetic acid. Formylhydroxyacetic acid. Formylglycollic acid. FEMA 3843
$HOCH_2COCOOH \Leftrightarrow OHCCH(OH)COOH$
$C_3H_4O_4$ 104.062
Food additive listed in the EAFUS Food Additive Database (Jan 2001). Found in cheeses, beer and cocoa, also in plants and microorganism cultures. Flavouring agent.
Mp 81-82° dec.

4-Nitrophenylhydrazone:
Red solid. Mp 260°.

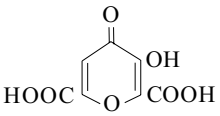
2,4-Dinitrophenylhydrazone:
Mp 112°.

Sprinson, D.B. *et al., J. Biol. Chem.*, 1946, **164**, 417 (*synth*)
Virtanen, A.I. *et al., Acta Chem. Scand.*, 1954, **8**, 1720; 1955, **9**, 188 (*isol*)
Biochem. Prep., 1962, **9**, 86 (*synth*)
Kretovich, V.L. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 471 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 827
Mayorga, H. *et al., Phytochemistry*, 2002, **59**, 439-445 (*Physalis glycosides*)

3-Hydroxy-4-oxo-4*H*-pyran-2,6-dicarboxylic acid, 9CI H-699

[497-59-6]
3-Hydroxy-4-pyrone-2,6-dicarboxylic acid.

Meconic acid. Opium acid. ***Poppy acid***



$C_7H_4O_7$ 200.104

Occurs in opium (*Papaver somniferum*) and other *Papaver* spp.. Cryst. + $3H_2O$ (H_2O), loses $3H_2O$ at 100°. Sol. EtOH, C_6H_6. Mp 270° dec. Subl. 210-215. pK_{a1} 1.83; pK_{a2} 2.11; pK_{a3} 11.3 (30% EtOH μ = 0.1).

Di-Me ester: [58262-33-2]
$C_9H_8O_7$ 228.158
Cryst. (MeOH). Mp 117°.

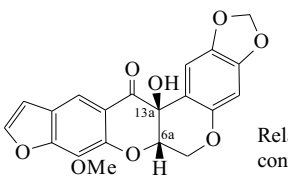
Di-Et ester: [729-63-5]
$C_{11}H_{12}O_7$ 256.212
Cryst. (H_2O). Mp 111.5°. pK_{a1} 4.85.

Ac:
$C_9H_6O_8$ 242.142
Cryst. (H_2O). Mp 218°.

Benzoyl:
$C_{14}H_8O_8$ 304.212
Mp 248°.

Mennel, *et al., J. Prakt. Chem.*, 1882, **26**, 456
Garkusha, G.A. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1946, **16**, 2025
Sommer, L. *et al., Coll. Czech. Chem. Comm.*, 1956, **21**, 1645; 1966, **31**, 1288 (*detn, Fe*)
Goryaev, M.I. *et al., CA*, 1963, **59**, 11419
Garkusha, G.A. *et al., Zh. Obshch. Khim.*, 1963, **33**, 3579; *CA*, **60**, 11969 (*synth*)
Lovell, S. *et al., J.A.C.S.*, 1999, **121**, 7020-7025 (*synth, cryst struct*)

12*a*-Hydroxypachyrrhizone H-700



Relative configuration

$C_{20}H_{14}O_8$ 382.326

The 12*a* position in the trivial name corresponds to 13*a* in CA numbering (illus.).

(+)-*form* [28768-44-7]
Isol. from yam beans (*Pachyrrhizus erosus*). Needles (MeOH/$CHCl_3$). Mp 214°.

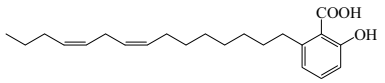
(±)-*form* [28617-73-4]
Cubes (MeOH/$CHCl_3$). Mp 232-234°.

Ac:
Mp 232-233°.

Krishnamurti, M. *et al., Tetrahedron*, 1970, **26**, 3023 (*isol, synth*)
Phrutivorapongkul, A. *et al., Chem. Pharm. Bull.*, 2002, **50**, 534-537 (*isol, pmr, cmr*)

2-Hydroxy-6-(8,11-pentadecadienyl)benzoic acid, 9CI H-701

[18654-17-6]
6-Pentadecadienylsalicylic acid



$C_{22}H_{32}O_3$ 344.493

More recently the term Anacardic acid has been accepted as a more suitable name for 6-alkylsalicylic acids in general.

(*all-E*)-*form*
Cryst. (EtOAc/hexane). Mp 68-69°.

(*all-Z*)-*form* [103904-74-1]
Anacardic acid
Found in cashew nut shell. Mp 25-26°. Log P 8.57 (uncertain value) (calc).

11′,12′-Dihydro: [22910-60-7] *2-Hydroxy-6-(8-pentadecenyl)benzoic acid, 9CI. 6-(8-Pentadecenyl)salicylic acid.* ***Ginkgoic acid****. Ginkgolic acid. Romanicardic acid*
$C_{22}H_{34}O_3$ 346.509
Constit. of *Ginkgo biloba* (ginkgo) and minor constit. of cashew nut shell. Needles by subl. Mp 45.3-48° (42-43°). Log P 9.06 (uncertain value) (calc).

11′,12′-Dihydro, Me ester: [58682-65-8]
Bp_2 230-233°.

8′,9′-Dihydro, $\Delta^{10'}$-isomer: [110202-77-2] *2-Hydroxy-6-(10-pentadecenyl)benzoic acid, 9CI. 6-(10-Pentadecenyl)salicylic acid*
$C_{22}H_{34}O_3$ 346.509
Needles. Mp 45.8-46.2°.

Tetrahydro: See 2-Hydroxy-6-pentadecylbenzoic acid, H-704

14′,15′-Didehydro: [103904-73-0] *2-Hydroxy-6-(8,11,14-pentadecatrienyl)benzoic acid, 9CI*
$C_{22}H_{30}O_3$ 342.477
Minor constit. of cashew nut shell. Geom. isom. not specified.

[25377-74-6]

Paul, V.J. *et al., Nature (London)*, 1954, **174**, 604 (*isol*)
Tyman, J.H.P. *et al., J.O.C.*, 1976, **41**, 894 (*synth*)
Tyman, J.H.P. *et al., Chem. Soc. Rev.*, 1979, **8**, 499-537 (*rev*)
Kubo, I. *et al., Chem. Lett.*, 1987, 1101-1104 (*deriv, isol, pmr*)
Yamigawa, Y. *et al., Tetrahedron*, 1987, **43**, 3387-3394 (*synth, ir, pmr*)
Vanoycke, S. *et al., Bull. Soc. Chim. Belg.*, 1988, **97**, 297-311 (*isol*)
Zehnter, R. *et al., Annalen*, 1995, 2209-2220 (*Anacardic acid, Ginkgoic acid, synth, ir, pmr, cmr*)
Gonzalez, M.J.T.G. *et al., Phytochemistry*, 1996, **43**, 1333-1337 (*isol, deriv, pmr, cmr*)
Fuerstner, A. *et al., J.O.C.*, 1997, **62**, 2332-2336 (*synth*)
Satoh, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1501-1505 (*synth, bibl*)
Satoh, M. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1115-1116; 2001, **49**, 18-22 (*synth*)
Green, I.R. *et al., Synth. Commun.*, 2002, **32**, 947-957 (*all-E form, synth, pmr, cmr*)

6-Hydroxypentadecanedioic acid H-702

[38076-52-7]
$HOOC(CH_2)_8CH(OH)(CH_2)_4COOH$
$C_{15}H_{28}O_5$ 288.383
Constit. of *Gnetum gnemon* (bago).

Hunneman, D.H. *et al., Phytochemistry*, 1972, **11**, 1989-2001 (*isol*)

15-Hydroxypentadecanoic acid H-703

[4617-33-8]
$HOCH_2(CH_2)_{13}COOH$
$C_{15}H_{30}O_3$ 258.4
Mp 82-84°.

Me ester: [76529-42-5]
$C_{16}H_{32}O_3$ 272.427
Solid. Mp 50-51°.

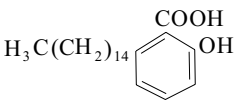
Ac:
$C_{17}H_{32}O_4$ 300.437
Mp 59°.

Lactone: [106-02-5] *Oxacyclohexadecan-2-one, 9CI, 8CI. Pentadecanolide.* ***Exaltolide****. Muskalactone. FEMA 2840*
$C_{15}H_{28}O_2$ 240.385
Constit. of angelica root oil (*Angelica archangelica*). Flavouring agent. Mp 34°
Mp 52-53°. Bp_{15} 176°.

Dhekne, V.V. *et al., J.C.S.*, 1962, 2348 (*lactone*)
Klouwen, M.H. *et al., Parfuem. Kosmet.*, 1962, **43**, 35 (*rev*)
Mathur, H.H. *et al., J.C.S.*, 1963, 3505
McCrae, W. *et al., Tetrahedron*, 1964, **20**, 1773 (*lactone*)
McFadden, W.H. *et al., Anal. Chem.*, 1965, **37**, 89 (*ms, lactone*)
Nozaki, H. *et al., Can. J. Chem.*, 1968, **46**, 3767 (*synth*)
Scott, L.T. *et al., Synthesis*, 1976, 738 (*lactone*)
Narasaka, K. *et al., Chem. Lett.*, 1978, 885 (*lactone*)
Sato, T. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 945 (*synth*)
Subramanian, G.B.V. *et al., Chem. Ind. (London)*, 1985, 379 (*synth*)
Milenkov, B. *et al., Helv. Chim. Acta*, 1987, **70**, 760 (*synth*)
Stanchev, S. *et al., Tet. Lett.*, 1993, **34**, 6107 (*lactone, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 636 (*lactone*)
Jun, L. *et al., Synth. Commun.*, 1995, **25**, 3457 (*synth, ir, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2113-2114 (*lactone*)
Cundy, D.J. *et al., Org. Prep. Proced. Int.*, 2000, **32**, 461-468 (*Me ester*)

2-Hydroxy-6-pentadecylbenzoic acid, 9CI H-704

[16611-84-0]
6-Pentadecylsalicylic acid. (15:0)-Anacardic acid. Cyclogallipharic acid. Hydroginkgolic acid



$C_{22}H_{36}O_3$ 348.525

Synthesised by immature seeds of *Ginkgo biloba* (ginkgo). Needles (petrol). Mp 92.5-93°.

▶ Strong irritant and allergen.

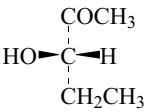
Me ester: [38449-27-3]
Cryst. (pentane). Mp 39-41° (35-37°).

Ac: [79688-42-9]
Needles (petrol). Mp 73-74.5°.

Backer, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1941, **60**, 661-667 (*isol*)
Gellerman, J.L. *et al., Biochim. Biophys. Acta*, 1976, **431**, 16-21 (*biosynth*)
Tyman, J.H.P. *et al., Chem. Soc. Rev.*, 1979, **8**, 499-537 (*rev*)
Zehnter, R. *et al., Annalen*, 1995, 2209-2220 (*synth, Me ester, ir, pmr, cmr*)
Fuerstner, A. *et al., J.O.C.*, 1997, **62**, 2332-2336 (*synth, pmr, cmr, ms*)
Satoh, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1501-1505; 1999, **47**, 1115-1116 (*synth*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 379

3-Hydroxy-2-pentanone, 9CI H-705

[3142-66-3]
2-Oxo-3-pentanol. Acetylethylcarbinol. FEMA 3550


(*S*)-*form*

$C_5H_{10}O_2$ 102.133

(*S*)-*form* [132881-72-2]
$[\alpha]_{578}^{15}$ +52 (c, 7 in $CHCl_3$) (≥ 98% ee).

(±)-*form* [118712-30-4]
Flavouring agent. Present in yoghurt. Liq. d_4^{20} 0.95. Bp 147-148° Bp_{35} 77°. n_D^{20} 1.4350.

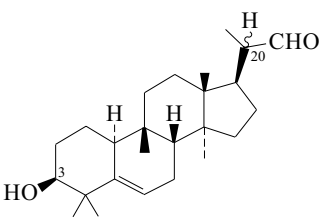
Ac: [20510-66-1]
$C_7H_{12}O_3$ 144.17
Bp_{13} 68-70°.

Me ether:3-Methoxy-2-pentanone
$C_6H_{12}O_2$ 116.16
Bp_{761} 154-155°.

[113919-08-7]

Vénus-Daniloff, E. *et al., Bull. Soc. Chim. Fr.*, 1928, **43**, 582-586 (*synth*)
Bouis, M. *et al., Bull. Soc. Chim. Fr.*, 1932, **51**, 1177-1178 (*synth*)
Singh, M. *et al., J.O.C.*, 1992, **57**, 4263-4270 (*Ac, synth, ir, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 368
Bel-Rhlid, R. *et al., Bull. Soc. Chim. Fr.*, 1996, **133**, 1011-1021 (*synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1381

3-Hydroxy-23,24,25,26,27-pentanorcucurbit-5-en-22-al H-706



$C_{25}H_{40}O_2$ 372.59

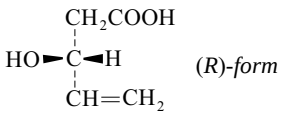
(3β,20ξ)-*form*
Needles (MeOH). Mp 153-159°.

3-O-[β-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [78887-74-8] ***Momordicoside E***
$C_{37}H_{60}O_{12}$ 696.874
Constit. of *Momordica charantia* (bitter melon). Cryst. (MeOH) (as hepta-Ac). Mp 177-183° (hepta-Ac). $[\alpha]_D^{20}$ +0.83 (c, 2.00 in $CHCl_3$) (hepta-Ac).

Miyahara, Y. *et al., Chem. Pharm. Bull.*, 1981, **29**, 1561

3-Hydroxy-4-pentenoic acid, 9CI H-707

[81357-28-0]


(*R*)-*form*

$C_5H_8O_3$ 116.116

(*R*)-*form* [38996-04-2]
Oil or cryst. Mp 41.5-42.5°. $Bp_{0.04}$ 69°. $[\alpha]_D^{17}$ -26 (c, 1 in 95% EtOH) (>99.8% op).

Nitrile: [7451-85-6] *3-Hydroxy-4-pentenenitrile, 9CI. 1-Cyano-3-buten-2-ol. 1-Cyano-2-hydroxy-3-butene*
C_5H_7NO 97.116
Potential neutriceutical. Oil.

Nitrile, 1-naphthylurethane:
Cryst. Mp 89-92°.

(*S*)-*form* [38996-05-3]

Nitrile: [6071-81-4] ***Crambene***
Oil. n_D^{20} 1.4544.
► LD_{50} (rat, scu) 200 mg/kg. Exp. teratogen. SB4500000

Nitrile, 1-naphthylurethane:
Cryst. (C_6H_6/heptane). Mp 93°.

(±)-*form* [38996-03-1]
$Bp_{0.07}$ 74-76°. n_D^{30} 1.4633.

Et ester: [38996-01-9]

[134896-00-7]
$C_7H_{12}O_3$ 144.17
Liq. $Bp_{0.6}$ 57°.

tert-*Butyl ester:* [122763-67-1]

[159787-33-4]
$C_9H_{16}O_3$ 172.224
$Bp_{0.04}$ 35°. n_D^{20} 1.4374.

Nitrile: [27451-36-1]
Bp_{30} 132-133°.
► SB2270000

Nitrile, 1-naphthylurethane:
Mp 112.5-113.5°.

[27451-36-1]

Bissinger, W.E. *et al., J.A.C.S.*, 1947, **69**, 2955-2961 (*nitrile, synth*)
Daxenbichler, M.E. *et al., Biochemistry*, 1966, **5**, 692-697 (*isol, pmr, ord, nitrile*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359-367 (*ms, nitrile*)
Das, N.B. *et al., Tetrahedron*, 1983, **39**, 2247-2253 (*synth, nitrile*)
Graf, S. *et al., Annalen*, 1993, 1091-1098 (*synth, pmr, cmr*)
Org. Synth., Coll. Vol., 9, 1998, 423-435 (*Et ester, synth, ir, pmr*)
Jeffery, E.H. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 169-191
Niedoborski, T.E. *et al., J. Agric. Food Chem.*, 2001, **49**, 3394-3399 (*Crambene, isol, purifn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COP400

2-Hydroxy-4-pentenyl glucosinolate H-708

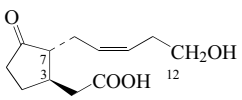
[19764-03-5]
1-Thio-β-D-glucopyranose 1-[3-hydroxy-N-(sulfooxy)-5-hexenimidate], 9CI. ***Gluconapoleiferin***
$H_2C{=}CHCH_2CH(OH)CH_2C(SGlc){=}NOSO_3H$
$C_{12}H_{21}NO_{10}S_2$ 403.431

[107657-50-1]

Tapper, B.A. *et al., Phytochemistry*, 1967, **6**, 749 (*occur*)
Josefsson, E. *et al., Acta Agric. Scand.*, 1968, **18**, 97; *CA*, **69**, 57420r (*isol*)

2-(5-Hydroxy-2-pentenyl)-3-oxocyclopentaneacetic acid H-709

[124649-26-9]


(3*R*,7*R*)-*form*

$C_{12}H_{18}O_4$ 226.272
Similar to Jasmonic acid, J-8.

(3*R*,7*R*)-*form* [140631-27-2]
12-Hydroxyjasmonic acid

O-*Sulfate:* [155408-18-7]
$C_{12}H_{18}O_7S$ 306.336
Amorph. $[\alpha]_D^{20}$ -24 (c, 0.2 in MeOH).

O-*β-D-Glucopyranoside:*
$C_{18}H_{28}O_9$ 388.414
Solid (as K salt).

(3*R*,7*S*)-*form*
Tuberonic acid

O-*β-D-Glucopyranoside:* [124649-25-8]
$C_{18}H_{28}O_9$ 388.414
Isol. from potato leaves (*Solanum tuberosum*). Powder. $[\alpha]_D^{26}$ +96.8 (MeOH).

O-*β-D-Glucopyranoside, Me ester:* [142465-56-3]
$C_{19}H_{30}O_9$ 402.441
Isol. from potato leaves (*Solanum tuberosum*) and Jerusalen artichoke (*Helianthus tuberosus*). Oil. $[\alpha]_D^{22}$ -52.5 (c, 0.08 in EtOH).

(3ξ,7ξ)-*form*

O-*β-D-Glucopyranoside, Et ester:*
$C_{20}H_{32}O_9$ 416.467
Constit. of sage (*Salvia officinalis*). Oil. Config. not confirmed.

[135911-63-6]

Yoshihara, T. *et al., Agric. Biol. Chem.*, 1989, **53**, 2835 (*isol*)
Miersch, O. *et al., Phytochemistry*, 1991, **30**, 4049 (*isol*)
Cui, B. *et al., Chem. Pharm. Bull.*, 1993, **41**, 178 (*glycoside*)
Achenbach, H. *et al., Phytochemistry*, 1994, **35**, 1527 (*sulfate*)
Simko, I. *et al., Phytochemistry*, 1996, **43**, 727 (*glucoside Me ester*)
Kiyota, H. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 2110-2117 (*synth*)
Wang, M. *et al., J. Agric. Food Chem.*, 2000, **48**, 235-238 (*glucoside, Et ester*)

Ueda, M. *et al., Tetrahedron*, 2000, **56**, 8101-8105 (*isol, glucoside*)

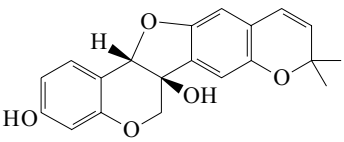
2-Hydroxypentyl glucosinolate H-710

[76265-23-1]
1-Thio-β-D-glucopyranose 1-[3-hydroxy-N-(sulfooxy)hexanimidate], 9CI
$H_3CCH_2CH_2CH(OH)CH_2C(SGlc)=NOSO_3H$
$C_{12}H_{23}NO_{10}S_2$ 405.446
Present in horseradish (*Armoracia lapathifolia*).

Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)

6*a*-Hydroxyphaseollin H-711

[34144-10-0]
*3,3-Dimethyl-3*H,*7*H-*furo[3,2-*c*:5,4-*f*′*]bis[1]benzopyran-6*b,*10(12*bH*)-diol, 9CI*

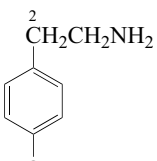


$C_{20}H_{18}O_5$ 338.359
Phytoalexin from soybeans (*Glycine max*) infected by *Phytophthora* sp.. Oil. $[\alpha]_D^{20}$ -207 (EtOAc). λ_{max} 227 (ϵ 26900); 285 (ϵ 8320); 305 (ϵ 2450); 318 (ϵ 1700) (EtOH) (Berdy). λ_{max} 293 (ϵ 13200); 318 (ϵ 3100) (EtOH-NaOH) (Berdy).

Sims, J.J. *et al., Phytochemistry*, 1972, **11**, 827
Burden, R.S. *et al., Phytochemistry*, 1975, **14**, 1389

4-Hydroxyphenethylamine H-712

[51-67-2]
*4-(2-Aminoethyl)phenol, 9CI. 2-(*p*-Hydroxyphenyl)ethylamine.* ***Tyramine****. Tyrosamine*



$C_8H_{11}NO$ 137.181
Present in germinating barley, sawa millet seed hulls, *Pisum sativum, Piper nigrum* (pepper) and in putrefied animal tissues. Also isol. from commercial and household prepared sauerkraut. Mp 164-164.5° (161°). pK_{a1} 9.3; pK_{a2} 10.9 (25°). Log P 0.62 (calc).

▶ LD_{50} (mus, ivn) 229 mg/kg. SJ5950000

N-*Benzoyl:* [41859-54-5] N-*[2-(4-Hydroxyphenyl)ethyl]benzamide, 9CI.* **N-*Benzoyltyramine***
$C_{15}H_{15}NO_2$ 241.289
Alkaloid from seeds of the Mexican apple (*Casimiroa edulis*). Plates (Et_2O). Mp 161-162°.

N-*(4-Hydroxy*-E-*cinnamoyl):* [36417-86-4] **N-p-trans-*Coumaroyltyramine****. N-(*p*-Hydroxyphenyl)ethyl* p*-hydroxycinnamide. Paprazine*
$C_{17}H_{17}NO_3$ 283.326
Constit. of Chinese onion (*Allium chinense*) and broad bean (*Vicia faba*). Cryst. (MeOH). Mp 260-261°.

▶ LD_{50} (mus, ipr) 780 mg/kg.

N-*(4-Hydroxy-*Z*-cinnamoyl):* [111129-11-4] **N-p-cis-*Coumaroyltyramine***
$C_{17}H_{17}NO_3$ 283.326
Constit. of Chinese onion *Allium chinense*. Needles ($CHCl_3$/MeOH). Mp 234-235°.

N-*(3,4-Dihydroxy-*Z*-cinnamoyl):* [219773-48-5] **N-cis-*Caffeoyltyramine***
$C_{17}H_{17}NO_4$ 299.326
Alkaloid from stems of cherimoya (*Annona cherimola*). Yellow oil. λ_{max} 203 (log ϵ 2.43); 220 (sh) (log ϵ 3.36); 280 (log ϵ 2.53); 310 (log ϵ 3.21) (EtOH).

N-*(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* [66648-43-9]

[65646-26-6] **N-trans-*Feruloyltyramine****. Moupinamide*
$C_{18}H_{19}NO_4$ 313.352
Alkaloid from *Piper nigrum*. Cryst.($Me_2CO/CHCl_3$). Mp 144.5-145°.

N-*(4-Hydroxy-3-methoxy-*Z*-cinnamoyl):* [80510-09-4] **N-cis-*Feruloyltyramine***
$C_{18}H_{19}NO_4$ 313.352
Isol. from bell pepper. Pale yellow oil.

N-*[3-(4-Hydroxy-3-methoxyphenyl)propanoyl]:* [184877-32-5] **N-*Dihydroferuloyltyramine***
$C_{18}H_{21}NO_4$ 315.368
Alkaloid from stems of cherimoya (*Annona cherimola*). Amorph. powder. Mp >300° λ_{max} 206 (log ϵ 2.73); 255 (sh) (log ϵ 3.65); 280 (log ϵ 2.34) (EtOH).

N-*Me:* [370-98-9] *4-[2-(Methylamino)ethyl]phenol, 9CI.* **N-*Methyltyramine***
$C_9H_{13}NO$ 151.208
Present in germinating barley roots but not dormant grains. Also present in dormant sawa millet seed hulls, but not hulled seeds. Alkaloid from prosso millet (*Panicum miliaceum*). Mp 130-131° (127-128°).

▶ SL8300000

O-*(3-Methyl-2-butenyl),* N-*tigloyl:* [172837-74-0] N-*[2-(4-Prenyloxyphenyl)ethyl]tiglamide*
$C_{18}H_{25}NO_2$ 287.401
Constit. of *Boronia megastigma* (brown boronia). Cryst. (Et_2O). Mp 69-71°.

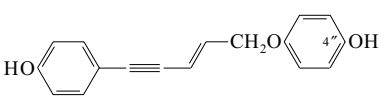
O-*(3-Methyl-2-butenyl),* N-E-*cinnamoyl:* [87596-51-8] N-*[2-[4-[(3-Methyl-2-butenyl)oxy]phenyl]ethyl]-3-phenyl-2-propenamide.* **N-*2-[4-(3,3-Dimethylallyloxy)phenyl]ethylcinnamide***. N-*Cinnamoyl*-p-*prenyloxyphenethylamine*
$C_{22}H_{25}NO_2$ 335.445
Alkaloid from the leaves of *Aegle marmelos* (bael fruit). Cryst. (MeOH). Mp 125-126°.

[20375-37-5, 70185-64-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1289C; 1289D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 612A; 612B (*nmr*)
Barger, G. *et al., J.C.S.*, 1909, **95**, 1127; 1722 (*synth*)
Kincl, F.A. *et al., J.C.S.*, 1956, 4163 (*N-Benzoyltyramine*)
Mann, J.D. *et al., J. Biol. Chem.*, 1963, **238**, 676-681 (*N-Me, isol*)
Kappe, T. *et al., J. Med. Chem.*, 1965, **8**, 368 (*uv*)
Boulton, A.A. *et al., Nature (London)*, 1967, **215**, 132 (*occur*)
Rondest, J. *et al., Bull. Soc. Chim. Fr.*, 1968, 2411-2414 (*N-4-hydroxycinnamoyl*)
Takahashi, T. *et al., Agric. Biol. Chem.*, 1970, **34**, 1256-1258 (*isol, sawa millet*)
Stuart, K.L. *et al., Phytochemistry*, 1971, **10**, 460 (*isol, derivs*)
Milne, G.W. *et al., Anal. Chem.*, 1973, **45**, 1952 (*ms*)
Tamura, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 2682 (*cryst struct*)
Lambert, F. *et al., Org. Magn. Reson.*, 1975, **72**, 66 (*pmr*)
Kruger, T.L. *et al., J.O.C.*, 1977, **42**, 4161 (*derivs, ms*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*rev, occur, derivs*)
Doetsch, P.W. *et al., J. Chromatogr.*, 1980, **189**, 79 (*occur*)
Govindachari, T.R. *et al., Phytochemistry*, 1983, **22**, 755 (*N-cinnamoyl-p-prenyl*)
Xu, L. *et al., Yaoxue Xuebao*, 1984, **19**, 48; *CA*, **101**, 107360y (*Moupinamide*)
Tseng, C.-F. *et al., Chem. Pharm. Bull.*, 1992, **40**, 396-400 (*synth, cinnamic amides*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1992, **31**, 2869-2872 (*Paprazine*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 780
Weyerstahl, P. *et al., Annalen*, 1994, 1043 (*Prenyloxyphenylethyltiglamide*)
Wu, T.-S. *et al., Phytochemistry*, 1994, **36**, 1063 (*N-p-cis-Coumaroyltyramine*)
Posso, O. *et al., Rev. Colomb. Quim.*, 1994, **23**, 53-62; *CA*, **122**, 286624r (*N-Cinnamoyltyramine*)
Wu, Y.-C. *et al., Planta Med.*, 1995, **61**, 146 (*N-Caffeoyltyramine*)
Chen, C.-Y. *et al., Phytochemistry*, 1998, **49**, 1443-1447 (*Annona cherimola amides*)
Kalač, P. *et al., Biologically-active Phytochemicals in Food*, (eds. Pfannhauser, W. *et al*), Royal Society of Chemistry, 2001, 217-220 (*sauerkraut*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TOF750; TOG250

4-[5-(4-Hydroxyphenoxy)-3-penten-1-ynyl]phenol, 9CI H-713

1-(4-Hydroxyphenoxy)-5-(4-hydroxyphenyl)-2-penten-4-yne



$C_{17}H_{14}O_3$ 266.296

(*E*)-*form* [166762-98-7]
Prod. by asparagus (*Asparagus officinalis*) cell cultures. Cryst. (CCl_4/C_6H_6). Mp 182° dec.

4″-Me ether: [166762-97-6] *4-[5-(4-Methoxyphenoxy)-3-penten-1-ynyl]phenol.* ***Asparenyol***
$C_{18}H_{16}O_3$ 280.323
Constit. of cultured cells of asparagus (*Asparagus officinalis*). Cryst. (CCl_4/

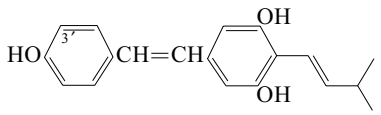
C_6H_6). Mp 140-140.5°.

Di-Me ether: [166762-96-5] *1-Methoxy-4-[5-(4-methoxyphenoxy)-3-penten-1-ynyl]benzene*
$C_{19}H_{18}O_3$ 294.349
Constit. of the cultured cells of asparagus (*Asparagus officinalis*). Cryst. (MeOH). Mp 124-125.5°.

Terada, K. *et al., Chem. Pharm. Bull.*, 1995, **43**, 564 (*isol, uv, ir, pmr, cmr*)

5-[(4-Hydroxyphenyl)ethenyl]-2-(3-methyl-1-butenyl)-1,3-benzenediol H-714

4-(3-Methyl-1-butenyl)-3,4′,5-trihydroxystilbene. 3,4′,5-Trihydroxy-4-



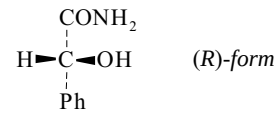
$C_{19}H_{20}O_3$ 296.365
Isol. from ground nuts incubated at 25°. Readily dec..

3′-Hydroxy:4-(3-Methyl-1-butenyl)-3,3′,4′,5-tetrahydroxystilbene
$C_{19}H_{20}O_4$ 312.365
Isol. from ground nuts. Microcryst. solid (MeCN aq.). Dec. in light.

Aguamah, G.E. *et al., Phytochemistry*, 1981, **20**, 1381

2-Hydroxy-2-phenylacetamide H-715

[4410-31-5]
α-Hydroxybenzeneacetamide, 9CI. Mandelamide, 8CI



(*R*)-*form*

$C_8H_9NO_2$ 151.165
(*R*)- and (*S*)-forms confused in early lit..

(*R*)-*form* [24008-62-6]
Plates (C_6H_6). Mp 123-124°. $[\alpha]_D^{20}$ -73 (c, 1.60 in Me_2CO).

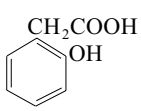
O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Lucuminamide***
$C_{19}H_{27}NO_{11}$ 445.422
Constit. of *Calocarpum sapota* (marmalade plum). Powder.

[65645-88-7]

Takeda, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 697 (*Lucuminamide*)

2-Hydroxyphenylacetic acid H-716

[614-75-5]
2-Hydroxybenzeneacetic acid, 9CI. o-*Hydroxy-α-toluic acid*



$C_8H_8O_3$ 152.149
Needles (Et_2O), prisms ($CHCl_3$). Mp 147-149°.

O-*β-D-Glucopyranoside:*
$C_{14}H_{18}O_8$ 314.291
Constit. of the roots of *Phyllanthus emblica* (emblic). Amorph. tan powder + $1^1/_4H_2O$. $[\alpha]_D^{20}$ -30.5 (c, 0.7 in MeOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 151D; 152B; 430B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1004A; 1005B; 1488C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1320A (*ir*)
Zhang, Y.-J. *et al., J. Nat. Prod.*, 2001, **64**, 870-873 (*glucoside*)

4-Hydroxyphenylacetic acid H-717

[156-38-7]
4-Hydroxybenzeneacetic acid, 9CI. p-*Hydroxy-α-toluic acid*

$C_8H_8O_3$ 152.149
Constit. of sweet clover (*Melilotus officinalis*) and yeast. Needles (H_2O). Sol. EtOH, Et_2O, hot H_2O. Mp 148-150°. pK_a 4.59 (10% EtOH aq.).

▶ AI2680000

Nitrile: [14191-95-8] *4-Hydroxybenzeneacetonitrile. 4-Hydroxybenzyl cyanide. 4-(Cyanomethyl)phenol*
C_8H_7NO 133.149
Isol. from white mustard (*Brassica alba*) as a dec. product of 4-Hydroxybenzyl glucosinolate, H-358. Needles (H_2O). Mp 72°. Bp 330°.

▶ AM0530000

Nitrile, O-*α-L-rhamnopyranoside:* [122001-32-5] ***Niazirin***
$C_{14}H_{17}NO_5$ 279.292
Constit. of the leaves of the horseradish tree (*Moringa oleifera*, Moringaceae).

▶ Mutagen.

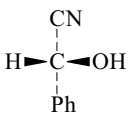
Nitrile, O-*(4-*O*-acetyl-α-L-rhamnopyranoside):* [159397-73-6] ***Niazirinin***
$C_{16}H_{19}NO_6$ 321.329
Constit. of the leaves of the horseradish tree (*Moringa oleifera*, Moringaceae). Needles ($CHCl_3$/MeOH). Mp 183-184°. Struct. originally given as the 3-Ac isomer but revised without comment. 4-Ac is more likely (cf. other *M. oleifera* isolates) λ_{max} 200 ; 222 (MeOH).

Nitrile, O-*(tri-*O*-acetyl-α-L-rhamnopyranoside):*
$C_{20}H_{23}NO_8$ 405.404
Constit. of the leaves of the horseradish tree (*Moringa oleifera*, Moringaceae). Cryst. (EtOAc/petrol). Mp 103° (synthetic). λ_{max} 200 ; 220 ; 278 (MeOH).

Power, F.B. *et al., J.C.S.*, 1912, **101**, 2411-2429 (*isol*)
Cain, J.C. *et al., J.C.S.*, 1913, **103**, 1035-1039 (*Me ether, synth*)
Kindler, K. *et al., Ber.*, 1941, **74**, 315-322 (*Me ether, synth*)
Looker, J.H. *et al., J.O.C.*, 1954, **19**, 784-788 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 576-579 (*Me ether-nitrile, synth*)
Kawakishi, S. *et al., Agric. Biol. Chem.*, 1967, **7**, 823-830 (*isol, synth, nitrile*)
Oehme, G. *et al., Chem. Ber.*, 1967, **100**, 425-437 (*Me ether, synth, ir*)
Hoefnagel, A.J. *et al., J.A.C.S.*, 1973, **95**, 5357-5366 (*pKa*)
Kuchar, M. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 1723-1735 (*Me ester, synth*)
Shapiro, B.L. *et al., J. Phys. Chem. Ref. Data*, 1977, **6**, 919-991 (*pmr*)
Wahlund, K.G. *et al., J. Liq. Chromatogr.*, 1981, **4**, 309-323 (*chromatog*)
Li, S. *et al., CA*, 1984, **100**, 117826y (*isol, nitrile*)
Bodor, N. *et al., J. Med. Chem.*, 1988, **31**, 1651-1656 (*synth*)
Dombrowicz, E. *et al., Pharmazie*, 1991, **46**, 156-157; *CA*, **114**, 225712f (*isol*)
Faizi, S. *et al., J. Nat. Prod.*, 1994, **57**, 1256-1261 (*Niazirin, Niazirinin*)
Faizi, S. *et al., Phytochemistry*, 1995, **38**, 957-963 (*isol, nitrile-rhamnoside*)
Leuck, M. *et al., Carbohydr. Res.*, 1998, **312**, 33-44 (*Niazirin derivs, synth, struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFE250; MFF000

2-Hydroxy-2-phenylacetonitrile H-718

[532-28-5]
α-Hydroxybenzeneacetonitrile, 9CI. Benzaldehyde cyanohydrin. Amygdonitrile. Mandelonitrile



(*R*)-*form*

C_8H_7NO 133.149
Glycosides widespread in (mostly higher) plants as cyanogenic glycosides. Glycosides of both enantiomers and of the racemate occur.

(*R*)-*form* [10020-96-9]
Needles. Mp 28.5-29.5°. $[\alpha]_{Hg}^{25}$ +46.9 (C_6H_6).

▶ Eye irritant. LD_{50} (rat, orl) 116 mg/kg.
OO8400000

O-*β-D-Allopyranoside:* ***Passiedulin***
$C_{14}H_{17}NO_6$ 295.291
Constit. of the leaves and stems of *Passiflora edulis* (passion fruit). $[\alpha]_D^{25}$ -69 (c, 0.24 in MeOH).

O-*β-D-Glucopyranoside:* [99-18-3] ***Prunasin***
$C_{14}H_{17}NO_6$ 295.291
Isol. from kernels of *Prunus* spp., immature fruits of *Passiflora* spp. and leaves of perilla (*Perilla frutescens* var. *acuta*). Needles ($CHCl_3$). Mp 147-148°. $[\alpha]_D$ -29.6 (H_2O).

▶ UL3420000

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [1392-28-5] ***Lucumin***. *Lucuminoside*
$C_{19}H_{25}NO_{10}$ 427.407
Isol. from marmalade plum (*Lucuma mammosa*) seeds. Mp 184-185°. $[\alpha]_D^{20}$ -50.5 (c, 0.4 in H_2O).

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [184002-37-7] *Mandelonitrile rutinoside*
$C_{20}H_{27}NO_{10}$ 441.434
Constit. of the fruit of purple passion fruit (*Passiflora edulis*).

O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [99520-78-2] *Mandelonitrile sophoroside*

$C_{20}H_{27}NO_{11}$ 457.433
Isol. from leaves of perilla (*Perilla frutescens* var. *acuta*). Needles (H_2O). Mp 193-195°. $[\alpha]_D^{22}$ -22.6 (c, 0.14 in MeOH).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [29883-15-6]

[672-72-0] ***Amygdalin***. *Amygdaloside. Glucoprunasin. Mandelonitrile gentiobioside. NSC 15780*
$C_{20}H_{27}NO_{11}$ 457.433
Bitter glycoside of the Rosaceae, found esp. in kernels of cherries, peaches and apricots. Present in cold pressed bitter almond oil from the above sources prior to enzymic hydrolysis and steam distillation for food use. Trihydrate. Poorly sol. Et_2O. Mp 214°. $[\alpha]_D^{25}$ -40.6 (H_2O). Log P -4.18 (uncertain value) (calc).

▶ LD_{50} (rat, orl) 522 mg/kg. Exp. teratogen. OO8450000

(*S*)-*form*

O-*β-D-Allopyranoside:*
Constit. of the leaves and stems of passion fruit (*Passiflora edulis*).

O-*β-D-Glucopyranoside:* [99-19-4] ***Sambunigrin***
$C_{14}H_{17}NO_6$ 295.291
Isol. from leaves of elderberry (*Sambucus nigra*) and from other plants. Needles (EtOAc). Mp 151-152°. $[\alpha]_D$ -76.3 (EtOAc).

O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{19}H_{25}NO_{10}$ 427.407
Constit. of *Sambucus nigra* (elderberry). $[\alpha]_D$ -73 (c, 0.7 in EtOH). λ_{max} 278 (EtOH).

(±)-*form* [613-88-7]
Isol. from peach kernels (*Prunus persica*). Prisms or oil. Mp 21.5-22°.

O-*β-D-Glucopyranoside:* [138-53-4] ***Prulaurasin***
$C_{14}H_{17}NO_6$ 295.291
Isol. from cherry laurel leaves (*Prunus laurocerasus*) and other plants. Needles (EtOAc). Mp 122-123°. $[\alpha]_D$ -53 (H_2O).

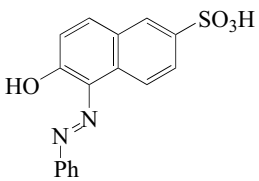
▶ UL3200000

[29883-16-7, 51371-34-7, 60981-47-7, 61091-09-6, 61091-10-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 426B; 426D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1483B; 1484A (*nmr*)
Caldwell, R.J. *et al., J.C.S.*, 1907, **91**, 671 (*Sambunigrin, Prulaurasin*)
Power, F.B. *et al., J.C.S.*, 1909, **95**, 243; 1910, **97**, 1099 (*Prunasin*)
Hawarth, W.N. *et al., J.C.S.*, 1923, 3120; 1924, 1337 (*Amygdalin*)
Jones, M.B. *et al., Science (Washington, D.C.)*, 1961, **134**, 284 (*isol, (±)-form*)
Schwartzmaier, U. *et al., Chem. Ber.*, 1976, **109**, 3250 (*pmr, Amygdalin*)
Turczan, J.W. *et al., J. Assoc. Off. Anal. Chem.*, 1978, **61**, 192; 1979, **62**, 190 (*pmr, derivs*)
Dreifuss, P.A. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 201 (*ms, Amygdalin*)
Huebel, W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1981, **314**, 609 (*cmr*)
Spencer, K.C. *et al., J. Agric. Food Chem.*, 1983, **31**, 794-796 (*Prunasin*)
Aritomi, M. *et al., Phytochemistry*, 1985, **24**, 2438 (*sophoroside*)
Cardona, L. *et al., Phytochemistry*, 1992, **31**, 3507 (*Prunasin, cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1428
Takeda, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 697 (*Lucumin*)
Nakajima, N. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 453-458 (*Prunasin, synth, pmr, cmr*)
Chassagne, D. *et al., Phytochemistry*, 1998, **49**, 757-759 (*rutinoside*)
Greca, M.D. *et al., Nat. Prod. Lett.*, 2000, **14**, 175-182 (*2-apiosylglucoside*)

6-Hydroxy-5-(phenylazo)-2-naphthalenesulfonic acid, 9CI H-719

[23481-33-6]
1-Phenylazo-2-naphthol-6-sulfonic acid. C.I. Acid Orange 12, 8CI. Crocein Orange G. C.I. Food Orange 1. C.I. Pigment Orange 18. C.I. 15970



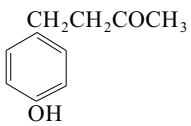
$C_{16}H_{12}N_2O_4S$ 328.348
Strictly the names Acid orange 12, Crocein orange G and Food orange 1 refer to the Na salt.

Na salt: [1934-20-9]
$C_{16}H_{11}N_2NaO_4S$ 350.33
Food pigment. Bright orange powder. λ_{max} 482 (no solvent reported).

Stein, C. *et al., J. Assoc. Off. Agric. Chem.*, 1949, **32**, 672-679 (*synth, uv*)
Colour Index, 3rd edn., 1971, **4**, 4087 (*props, bibl*)
Gaunt, I.F. *et al., Food Cosmet. Toxicol.*, 1971, **9**, 619-630 (*tox*)
Gelbcke, M. *et al., Anal. Lett.*, 1980, **13**, 975-984 (*cmr*)
Oka, H. *et al., J. Chromatogr., A*, 1994, **674**, 301-307 (*detn, tlc, ms*)

4-(4-Hydroxyphenyl)-2-butanone, 9CI H-720

[5471-51-2]
Frambinone. Raspberry ketone. Rheosmine. FEMA 2588



$C_{10}H_{12}O_2$ 164.204
Isol. from raspberries (*Rubus idaeus*), rhubarb (*Rheum* spp.), European cranberry (*Vaccinium oxycoccus*), blackberry, loganberry and redcurrants. Important flavour ingredient. Needles (H_2O) with raspberry odour. Mp 82.5°.

▶ LD_{50} (rat, orl) 1320 mg/kg. EL8925000

Oxime: [58484-75-6]
$C_{10}H_{13}NO_2$ 179.218
Cryst. (C_6H_6). Mp 97.5-100°.

2,4-Dinitrophenylhydrazone:
Red needles (EtOH). Mp 145°.

O-*β-D-Glucopyranoside:* [38963-94-9]
$C_{16}H_{22}O_7$ 326.346
Present in rhubarb and raspberries. Prisms. Mp 110-112°. $[\alpha]_D^{22}$ -52.1 (c, 0.34 in EtOH).

O-*[3,4,5-Trihydroxybenzoyl-(→2)-β-D-glucopyranoside]:* [87075-18-1] ***Isolindleyin***
$C_{23}H_{26}O_{11}$ 478.452
Isol. from commercial rhubarb. Amorph. powder + $1H_2O$. $[\alpha]_D^{20}$ +7.5 (c, 0.88 in Me_2CO).

O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:* [59282-56-3] ***Lindleyin***
$C_{23}H_{26}O_{11}$ 478.452
Isol. from rhubarb. Needles. Mp 210-211° (206-207°). $[\alpha]_D$ +14 (c, 0.38 in Py). $[\alpha]_D$ -18.6 (c, 0.8 in MeOH).

▶ DH9110000

O-*[2,6-Bis(3,4,5-trihydroxybenzoyl)-β-D-glucopyranoside]:* [105274-14-4]
$C_{30}H_{30}O_{15}$ 630.558
Isol. from commercial rhubarb. Off-white amorph. powder + $1\frac{1}{2}H_2O$. $[\alpha]_D^{27}$ -21.2 (c, 0.94 in Me_2CO).

O-*[3,4,5-Trihydroxybenzoyl-(→2)-6-O-cinnamoyl-β-D-glucopyranoside]:* [105274-15-5]
$C_{32}H_{32}O_{12}$ 608.598
Isol. from commercial rhubarb. Needles. Mp 125-127°. $[\alpha]_D^{26}$ -34 (c, 0.98 in Me_2CO).

O-*[3,4,5-Trihydroxybenzoyl-(→6)-2E-cinnamoyl-β-D-glucopyranoside]:*
$C_{32}H_{32}O_{12}$ 608.598
Pale brown solid. $[\alpha]_D^{25}$ -94.9 (c, 0.01 in MeOH). λ_{max} 218 (log ε 4.34); 275 (log ε 3.9) (MeOH).

O-*[4-Hydroxy-E-cinnamoyl-(→6)-[3,4,5-trihydroxybenzoyl-(→2)]-β-D-glucopyranoside]:* [105274-16-6]
$C_{32}H_{32}O_{13}$ 624.597
Isol. from commercial rhubarbs. Needles + $\frac{1}{2}H_2O$. Mp 134-136°. $[\alpha]_D^{26}$ -38.2 (c, 0.73 in Me_2CO).

Ac: [3572-06-3] ***Cuelure***. *FEMA 3652*
$C_{12}H_{14}O_3$ 206.241
Flavour ingredient. Liq. with sweet raspberry, fruity odour. $Bp_{0.06}$ 107.5-109.5°. n_D^{20} 1.5088.

▶ LD_{50} (rat, orl) 3038 mg/kg. EL8950000

Me ether: [104-20-1] *4-(4-Methoxyphenyl)-2-butanone. Anisylacetone. FEMA 2672*
$C_{11}H_{14}O_2$ 178.23
Flavour ingredient. Present in anise (*Pimpinella anisum*). Liq. with raspberry-cherry flavour at low conc. d_4^{22} 1.05. Mp 9-10°. Bp 277° $Bp_{0.025}$ 87-89°.

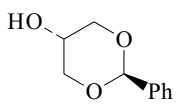
▶ EL9085500

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 5C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 794C; 795B; 1292C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1222A; 1383B (*ir*)
Schinz, H. *et al., Helv. Chim. Acta*, 1957, **40**, 1839; 1961, **44**, 278 (*isol, struct*)
Winter, H. *et al., Helv. Chim. Acta*, 1961, **44**, 2110 (*synth*)
Prasad, D. *et al., J. Indian Chem. Soc.*, 1962, **39**, 735 (*synth*)

Murakami, T. *et al., Tet. Lett.*, 1972, 2965-2968 (*isol, glucoside*)
Chalk, A.J. *et al., J.O.C.*, 1976, **41**, 1206 (*synth*)
Gonzalez, A.G. *et al., Phytochemistry*, 1976, **15**, 344 (*Lindleyin*)
Shimaiskaya, G.V. *et al., CA*, 1978, **89**, 6065; 1982, **96**, 85168 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 781 (*rev, tox*)
Nonaka, G.I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2862 (*Lindleyin, Isolindleyin*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3237 (*glycosides*)
Pabst, A. *et al., Phytochemistry*, 1990, **29**, 3853-3858 (*isol, glucoside*)
Tateiwa, J. *et al., J.O.C.*, 1994, **59**, 5901 (*synth*)
Borejsza-Wysocki, W. *et al., Phytochemistry*, 1994, **35**, 623 (*biosynth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 26; 1382; 1699 (*occur, props*)
Fan, W. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1055-1061 (*isol, pmr, cmr, glycosides*)
Pesticide Manual, 12th edn., 2000, No. 178
Koltunov, K.Yu *et al., Zh. Org. Khim.*, 2001, **37**, 1610-1617; *Russ. J. Org. Chem. (Engl. Transl.)*, 2001, **37**, 1534-1541 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAR500; RBU000

5-Hydroxy-2-phenyl-1,3-dioxane H-721

[1708-40-3]
*2-Phenyl-1,3-dioxan-5-ol, 9CI. 1,3-*O*-Benzylideneglycerol*



(2*RS*,5*RS*)-*form*

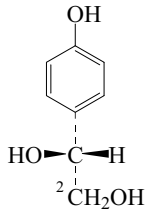
$C_{10}H_{12}O_3$ 180.203
Benzaldehyde glyceryl acetal, comprising this compd. and/or 2-Phenyl-1,3-dioxolane-4-methanol, P-267, is used as a food flavouring agent (FEMA 2129).

[4141-23-5, 26310-31-6]

Hill, H.S. *et al., J.A.C.S.*, 1928, **50**, 2235 (*synth*)
Baggett, N. *et al., J.C.S.*, 1960, 2574 (*synth, ir, conformn*)
Jochims, J.C. *et al., Tet. Lett.*, 1976, **24**, 2065 (*pmr*)
Kobayashi, Y.M. *et al., Chem. Ber.*, 1978, **111**, 3442 (*synth, pmr*)
Juaristi, E. *et al., Tetrahedron*, 1992, **48**, 5941 (*synth, derivs, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 128
Crich, D. *et al., J.A.C.S.*, 1995, **117**, 8757 (*synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 246
Juaristi, E. *et al., J.O.C.*, 1997, **62**, 4029-4035 (*synth, derivs*)

1-(4-Hydroxyphenyl)-1,2-ethanediol H-722

[2380-75-8]
4-(1,2-Dihydroxyethyl)phenol. p-*Hydroxyphenylglycol*



(*R*)-*form*

$C_8H_{10}O_3$ 154.165

(*R*)-*form*

*2-*O*-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* [177795-29-8]
$C_{18}H_{18}O_6$ 330.337
Constit. of *Coriandrum sativum* (coriander).

4′-Me ether: [32345-64-5]
Cryst. Mp 93-95°. $[\alpha]_D$ -35 (c, 1 in EtOH) (98% ee).

(ξ)-*form*

*2-*O*-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* ***Decursidate***
$C_{18}H_{18}O_6$ 330.337
Yellow powder. λ_{max} 325 (MeOH).

4′-Me ether:1-(4-Methoxyphenyl)-1,2-ethanediol
$C_9H_{12}O_3$ 168.192

1-Et ether:β-Ethoxy-4-hydroxybenzeneethanol. 2-Ethoxy-2-(4-hydroxyphenyl)ethanol
$C_{10}H_{14}O_3$ 182.219
Cubic cryst. (Me_2CO). Mp 99-100°. $[\alpha]_D^{22}$ -0.5 (c, 0.56 in Me_2CO). λ_{max} 221 ; 275 (no solvent reported).

(±)-*form*

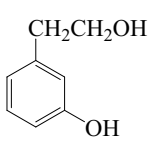
4′-Me ether: [13603-63-9]
Cryst. Mp 79-81°.

[147159-72-6, 147254-29-3, 181272-41-3]

Russell, G.A. *et al., J.A.C.S.*, 1966, **88**, 5498-5504 (*Me ether, synth*)
Ferraboschi, P. *et al., J.C.S. Perkin 1*, 1990, 2469-2474 (*R-form, Me ether, synth, pmr*)
Taniguchi, M. *et al., Phytochemistry*, 1996, **42**, 843-846
Kong, L.Y. *et al., Chin. Chem. Lett.*, 2000, **11**, 315-318 (*Decursidate*)
Roesecke, J. *et al., Phytochemistry*, 2000, **54**, 603-610 (*4′-Me ether*)
Zhou, Y. *et al., Chin. Chem. Lett.*, 2001, **12**, 333-334 (*1-Et ether*)

2-(3-Hydroxyphenyl)ethanol H-723

[13398-94-2]
3-Hydroxybenzeneethanol, 9CI. m-*Hydroxyphenethyl alcohol, 8CI*



$C_8H_{10}O_2$ 138.166
Yellow, highly viscous oil. Bp_4 168-173°.

*1′-*O*-β-D-Glucopyranoside:*
$C_{14}H_{20}O_7$ 300.308
Constit. of *Sambucus nigra* (elderberry).
Oil. λ_{max} 280 (EtOH).

3,5-Dinitrobenzoyl:
Light-yellow needles. Mp 146.5-147°.

3-Me ether: [5020-41-7] *2-(3-Methoxyphenyl)ethanol. 3-Methoxyphenethyl alcohol*
$C_9H_{12}O_2$ 152.193
Bp_{12} 141-143°. n_D^{20} 1.5380.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1164D; 1165A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 406B; 406C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1084B; 1084C (*ir*)
Scheiler, L. *et al., J.A.C.S.*, 1951, **73**, 4045 (*synth*)
Weibel, P.A. *et al., Helv. Chim. Acta*, 1973, **56**, 2460 (*ms*)
D'Abrosca, B. *et al., Phytochemistry*, 2001, **58**, 1073-1081 (*1′-glucoside*)

2-(4-Hydroxyphenyl)ethanol H-724

[501-94-0]
4-Hydroxybenzeneethanol, 9CI. p-*Hydroxyphenethyl alcohol. Tyrosol. Salidrosol*

$C_8H_{10}O_2$ 138.166
Isol. from peanuts. Needles ($CHCl_3$). Sol. H_2O, EtOH, Et_2O, Me_2CO; spar. sol. petrol. Mp 85-86°.

*1-*O*-[4-Hydroxy-*E*-cinnamoyl-(→4)-β-D-glucopyranoside]:* [97457-19-7]

[132697-37-1] ***Osmanthuside A***
$C_{23}H_{26}O_9$ 446.453
Isol. from *Osmanthus fragrans* (sweet osmanthus) leaves. $[\alpha]_D$ -37.5 (c, 0.8 in $CHCl_3$) (as penta-Ac).

*1-*O*-[4-Hydroxy-Z-cinnamoyl-(→4)-β-D-glucopyranoside]:* [97457-21-1] ***Osmanthuside C***
$C_{23}H_{26}O_9$ 446.453
Isol. from *Osmanthus fragrans* (sweet osmanthus). Mp 187-190°.

*1-*O*-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [139742-28-2] ***Crosatoside B***
$C_{20}H_{30}O_{11}$ 446.45
Isol. from the pollen of *Crocus sativus* (saffron).

*1-*O*-[α-L-Rhamnopyranosyl-(1→3)-[4-hydroxy-*E*-cinnamoyl-(→4)]-β-D-glucopyranoside]:* [94492-23-6] ***Osmanthuside B***
$C_{29}H_{36}O_{13}$ 592.596
Isol. from leaves of *Osmanthus fragrans* (sweet osmanthus). Amorph. powder. Mp 80-85° (as hepta-Ac). $[\alpha]_D^{19}$ -82.5 (c, 1.34 in MeOH). $[\alpha]_D^{23}$ -47.4 (c, 1.4 in $CHCl_3$) (hepta-Ac).

*1-*O*-4-Hydroxy-3-methoxycinnamoyl(*E*-):* [84873-15-4] p-*Hydroxyphenethyl* trans-*ferulate*
$C_{18}H_{18}O_5$ 314.337
Constit. of *Oenanthe javanica* (water dropwort). Powder. Mp 165-166°.

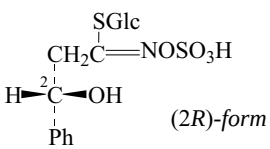
*4′-*O*-(3-Methyl-2-butenyl):* [119417-97-9] *2-[4-(Prenyloxy)phenyl]ethanol.* ***Etrogol***
$C_{13}H_{18}O_2$ 206.284
Isol. from the roots of *Citrus* spp.. Oil.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1166B; 1166D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 409A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1085D; 1086A (*ir*)

Siefken, W. *et al., Annalen*, 1949, **562**, 75-136 (*synth*)
Veer, W.L.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1957, **76**, 810-812 (*isol*)
Cross, B.E. *et al., J.C.S.*, 1963, 2937-2943 (*isol*)
Weibel, P.A. *et al., Helv. Chim. Acta*, 1973, **56**, 2460-2479 (*synth, ms*)
Nakata, H. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4554-4556 (*ferulate*)
Kobayashi, H. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3880
Ayer, W.A. *et al., Can. J. Chem.*, 1986, **64**, 904-909 (*isol, ir, pmr*)
Jimenez, C. *et al., Phytochemistry*, 1987, **26**, 1805; 1988, **27**, 2947
Ito, C. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3292-3295 (*Etrogol*)
Jimenez, C. *et al., J. Nat. Prod.*, 1989, **52**, 408
Sugiyama, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2953 (*Osmanthusides*)
Cano, E. *et al., Planta Med.*, 1990, **56**, 24
Song, C. *et al., Huaxue Xuebao*, 1991, **49**, 917-920; *CA*, **116**, 148197d (*Crosatoside B*)
Yoshikawa, K. *et al., Nat. Med. (Tokyo)*, 1996, **50**, 176; *CA*, **125**, 81942h (*cmr, derivs*)
Kuwayima, H. *et al., Chem. Pharm. Bull.*, 1998, **46**, 581-586 (*synth, pmr*)
Lou, H. *et al., Planta Med.*, 2001, **67**, 345-349 (*isol, pmr, cmr*)

2-Hydroxy-2-phenylethyl glucosinolate H-725

[30688-64-3]
1-Thio-β-D-glucopyranose 1-[β-hydroxy-N-(sulfooxy)benzenepropanimidate]. β-Hydroxyphenethyl glucosinolate. ***Glucobarbarin***



(2*R*)-*form*

$C_{15}H_{21}NO_{10}S_2$ 439.464

(2*R*)-*form*
Constit. of *Barbarea vulgaris* (winter cress).

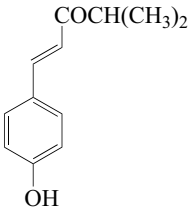
(2*S*)-*form* [37913-31-8]
Constit. of *Barbarea vulgaris* (winter cress).

2-O-α-L-Arabinopyranoside: [80754-95-6]
2-(α-L-Arabinopyranosyloxy)-2-phenylethyl glucosinolate
$C_{20}H_{29}NO_{14}S_2$ 571.579
(*S*)-Config. not certain for this deriv..

[73519-01-4]

Kjaer, A. *et al., Acta Chem. Scand.*, 1957, **11**, 906; 1958, **12**, 1693 (*occur*)
Underhill, E.W. *et al., Phytochemistry*, 1972, **11**, 1973 (*biosynth*)
Olsen, O. *et al., Phytochemistry*, 1981, **30**, 1857 (*arabinoside*)
Agerbirk, N. *et al., Phytochemistry*, 2001, **58**, 91-100 (*isol, pmr*)

1-(4-Hydroxyphenyl)-4-methyl-1-penten-3-one, 9CI H-726



$C_{12}H_{14}O_2$ 190.241
Cryst. (EtOAc/petrol). Mp 81.5-82.5°.
$Bp_{0.03}$ 159-167°.

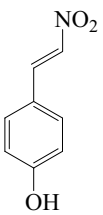
Me ether: [67962-14-5]

[103-13-9] *1-(4-Methoxyphenyl)-4-methyl-1-penten-3-one, 9CI. α,α-Dimethylanisalacetone. Homoethone*
$C_{13}H_{16}O_2$ 204.268
Flavouring ingredient. Liq. with a caramel/fruity odour and sweet taste. Bp_1 135-140°.

Winter, M. *et al., Helv. Chim. Acta*, 1961, **44**, 2110 (*synth*)
Nasipuri, D. *et al., J.C.S. Perkin 1*, 1976, 19 (*Me ether, synth*)
Huang, Y.-Z. *et al., Synthesis*, 1988, 975 (*Me ether, synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1700-1701

1-(4-Hydroxyphenyl)-2-nitroethylene H-727

[3179-08-6]
4-(2-Nitroethenyl)phenol, 9CI. p-*(2-Nitrovinyl)phenol, 8CI. 4-Hydroxy-β-nitrostyrene*



$C_8H_7NO_3$ 165.148

(*E*)-*form*
Fine yellow needles (MeOH aq.). Mp 167-168° (164-165°).
▶ Strongly irritant to mucous membranes.

Ac: [18984-24-2]
$C_{10}H_9NO_4$ 207.185
Yellow needles (EtOH). Mp 163° (158-159°).

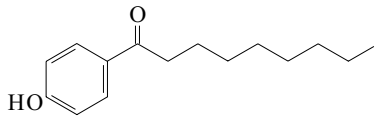
Me ether: [3179-10-0] *1-(4-Methoxyphenyl)-2-nitroethylene. Anisylidenenitromethane*
$C_9H_9NO_3$ 179.175
Used for the control of rice blast disease. Yellow needles (EtOH) or plates (C_6H_6). Mp 88°. Prob. of no significance.

[5576-97-6]

Peterli, S. *et al., Helv. Chim. Acta*, 1992, **75**, 696 (*synth, ir, pmr, cmr, ms*)

1-(4-Hydroxyphenyl)-1-nonanone, 9CI H-728

[14392-69-9]
p-*Hydroxynonanophenone*

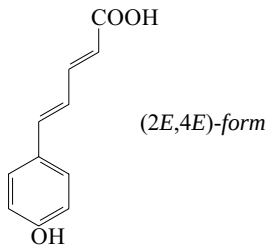


$C_{15}H_{22}O_2$ 234.338
Constit. of *Humulus lupulus* (hops). Oil.

Chandra, A. *et al., Phytochemistry*, 1991, **30**, 495 (*isol, pmr, cmr*)

5-(4-Hydroxyphenyl)-2,4-pentadienoic acid H-729

[56148-66-4]



(2*E*,4*E*)-*form*

$C_{11}H_{10}O_3$ 190.198

(2*E*,4*E*)-*form* [135754-92-6]
Avenalumic acid
Constit. of oats (*Avena sativa*).

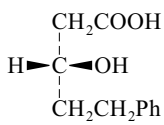
(2*Z*,4*E*)-*form* [99877-60-8]
Psilotic acid
Yellow cryst. (MeOH/EtOH). Mp 165°.

[135754-95-9, 135754-96-0]

Shamsuddin, T. *et al., Phytochemistry*, 1985, **24**, 2458
Collins, F.W. *et al., Cereal Chem.*, 1991, **68**, 184

3-Hydroxy-5-phenylpentanoic acid H-730

[41479-99-6]
β-Hydroxybenzenepentanoic acid, 9CI



(*R*)-*form*

$C_{11}H_{14}O_3$ 194.23

(*R*)-*form* [21080-41-1]
Isol. from the leaves of *Populus balsamifera* (balsam poplar). Mp 129-131°. $[\alpha]_{Hg}^{25}$ -10.4 (c, 2.55 in EtOH).

Me ester: [118133-67-8]
$C_{12}H_{16}O_3$ 208.257
$[\alpha]_D^{23}$ -12.2 (c, 1.16 in $CHCl_3$). $[\alpha]_D^{25}$ +2.4 (c, 0.15 in CH_2Cl_2).

O-*β-D-Glucopyranoside:*
$C_{17}H_{24}O_8$ 356.372
Powder. $[\alpha]_D^{23}$ -7.5 (c, 0.22 in MeOH). The butyl ester was also isol. and deemed to be an artifact λ_{max} 248 ; 252 ; 261 ; 268 (MeOH).

(±)-*form*

Sol. H_2O, spar. sol. C_6H_6. Mp 131°.

Me ester: [129880-16-6]
Oil. $Bp_{0.5}$ 114-116°.

Ac:
$C_{13}H_{16}O_4$ 236.267
Oil. $Bp_{0.09}$ 142°.

(ξ)-*form*

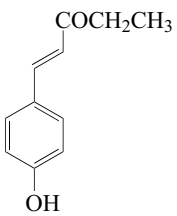
O-*β*-D-*Glucopyranoside:*
Constit. of *Perilla frutescens* (perilla). Powder. $[\alpha]_D^{20}$ -9.5 (c, 0.06 in MeOH). C-3 Config. uncertain, but probably (*R*-) λ_{max} 248 (log ε 2.31); 254 (log ε 2.37); 261 (log ε 2.41); 268 (log ε 2.31) (no solvent reported).

[53376-62-8, 118133-69-0]

Farmer, E.H. *et al., J.C.S.*, 1933, 966 (*synth*)
Linstead, R.P. *et al., J.C.S.*, 1953, 1211 (*synth*)
Pearl, I.A. *et al., Phytochemistry*, 1968, **7**, 1845 (*isol*)
Kuwajima, I. *et al., Tet. Lett.*, 1976, 2253 (*synth, ester*)
Fujisawa, T. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 1273 (*synth, ester*)
Fujita, T. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 732 (*glucoside*)
Rho, H-S. *et al., Synth. Commun.*, 1997, **27**, 3887-3893 (*Me ester*)
Calis, I. *et al., J. Nat. Prod.*, 1999, **62**, 1101-1105 (*glucoside*)
Ganci, W.M. *et al., Chirality*, 2000, **12**, 139-142 (*glucoside, abs config*)

1-(4-Hydroxyphenyl)-1-penten-3-one, 9CI H-731

[126521-57-1]



(*E*)-*form*

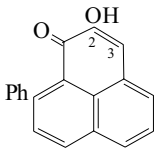
$C_{11}H_{12}O_2$ 176.215
Needles (EtOH). Mp 115°.

Me ether: [104-27-8] *1-(4-Methoxyphenyl)-1-penten-3-one. Ethyl* p-*methoxystyryl ketone. Ethone. FEMA 2673*
$C_{12}H_{14}O_2$ 190.241
Flavouring ingredient. Mp 61.3-61.9°. Bp_{12} 278°.

Inamoto, K. *et al., Bull. Chem. Soc. Jpn.*, 1927, **2**, 51 (*Me ether*)
McGookin, A. *et al., J.C.S.*, 1928, 1170 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17 (Suppl.)**, 863 (*Me ether, rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 462
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1701-1702

2-Hydroxy-9-phenyl-1*H*-phenalen-1-one, 9CI H-732

[56252-32-5]
Anigorufone



$C_{19}H_{12}O_2$ 272.303
Pigment from *Musa acuminata* (dwarf banana). Orange needles (petrol). Mp 123-125°.

Me ether: [56252-05-2] *2-Methoxy-9-phenyl-1*H-*phenalen-1-one*
$C_{20}H_{14}O_2$ 286.329
Isol. from *Musa acuminata* (dwarf banana). Yellow needles (C_6H_6/petrol). Mp 107-109°.

*4-Hydroxy:2,4-Dihydroxy-9-phenyl-1*H-*phenalen-1-one, 9CI.* ***4-Hydroxyanigorufone***
$C_{19}H_{12}O_3$ 288.302
Red cryst. (CH_2Cl_2). Mp 115°. λ_{max} 224 (log ε 3.7); 272 (log ε 3.6); 330 (log ε 1); 448 (log ε 1.5) (MeOH).

4′-Hydroxy: [56252-02-9] *2-Hydroxy-9-(4-hydroxyphenyl)-1*H-*phenalen-1-one.* ***Hydroxyanigorufone.*** *Emenolone*
$C_{19}H_{12}O_3$ 288.302
Pigment from *Musa acuminata* (dwarf banana). Red rosettes (EtOH). Mp 238-242°. Struct. of Emenolone revised in 1995.

*4′-Hydroxy, Me ether:9-(4-Hydroxyphenyl)-2-methoxy-1*H-*phenalen-1-one*
$C_{20}H_{14}O_3$ 302.329
Constit. of *Musa acuminata* (dwarf banana). λ_{max} 237 (ε 9700); 260 (ε 11100); 267 (ε 10900); 308 (ε 2600); 348 (ε 3400); 368 (ε 4600); 404 (ε 4000); 411 (ε 4100) (MeOH).

3′,4′-Dihydroxy: [56252-03-0] *9-(3,4-Dihydroxyphenyl)-2-hydroxy-1*H-*phenalen-1-one.* ***Dihydroxyanigorufone***
$C_{19}H_{12}O_4$ 304.301
Red needles by subl. Mp 215-220° dec.

3,4′-Dihydroxy: [173560-65-1] *2,3-Dihydroxy-9-(4-hydroxyphenyl)-1*H-*phenalen-1-one.* ***Musanolone E***
$C_{19}H_{12}O_4$ 304.301
Constit. of *Musa acuminata* (dwarf banana). Orange solid. Mp 273-276°. λ_{max} 276 ; 362 (EtOH).

*4,4′-Dihydroxy:2,4-Dihydroxy-9-(4-hydroxyphenyl)-1*H-*phenalen-1-one.* ***Thyrsiflorin***
$C_{19}H_{12}O_4$ 304.301
Orange-brown solid. Mp 218-222°.

3′-Methoxy, 4′-hydroxy: [173560-66-2] *2-Hydroxy-9-(4-hydroxy-3-methoxyphenyl)-1*H-*phenalen-1-one.* ***Musanolone F***
$C_{20}H_{14}O_4$ 318.328
Constit. of *Musa acuminata* (dwarf banana). Red solid. Mp 182-183°. λ_{max} 270 ; 324 ; 356 ; 364 (EtOH).

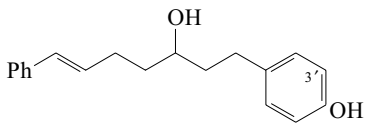
*3′,4′-Dimethoxy, Me ether:9-(3,4-Dimethoxyphenyl)-2-methoxy-1*H-*phenalen-1-one*
$C_{22}H_{18}O_4$ 346.382
Constit. of *Musa acuminata* (dwarf banana). λ_{max} 258 (ε 17000); 270 (ε 16000); 365 (ε 5000); 410 (ε 4600) (MeOH).

[149184-20-3]

Cooke, R.G. *et al., Aust. J. Chem.*, 1975, **28**, 1053; 1978, **31**, 193 (*isol, synth, pmr, ms*)
Dora, G. *et al., Planta Med.*, 1990, **56**, 569 (*Thyrsiflorin*)
Luis, J.G. *et al., Nat. Prod. Lett.*, 1995, **6**, 23
Hölscher, D. *et al., Nat. Prod. Lett.*, 1995, **7**, 177 (*Hydroxyanigorufone, biosynth, pmr, cmr*)
Luis, J.G. *et al., Tetrahedron*, 1995, **51**, 4117 (*Emenolone*)
Luis, J. G. *et al., Phytochemistry*, 1996, **41**, 753 (*Musanolones*)
Binks, R.H. *et al., Phytochemistry*, 1997, **45**, 47 (*isol, uv, pmr*)
Kamo, T. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 95-101 (*isol, uv, pmr, ms*)
Hoelscher, D. *et al., Phytochemistry*, 1999, **50**, 155-161 (*4-Hydroxyanigorufone*)
Schmitt, B. *et al., Phytochemistry*, 1999, **52**, 45-53 (*biosynth*)

1-(4-Hydroxyphenyl)-7-phenyl-6-hepten-3-ol H-733

4-Hydroxy-α-(4-phenyl-3-butenyl)benzenepropanol, 9CI



$C_{19}H_{22}O_2$ 282.382

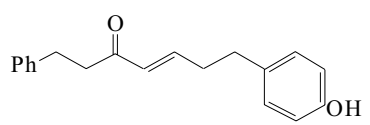
(-)-(*E*)-*form* [158697-54-2]
Constit. of the rhizomes of *Curcuma xanthorrhiza* (Java turmeric). Cryst. ($CHCl_3/C_6H_6$). Mp 94-95°. $[\alpha]_D^{25}$ -66.8 (c, 0.17 in MeOH). λ_{max} 249 (ε 17400); 278 (ε 3900) (MeOH).

3′-Hydroxy: [158697-56-4] *4-(3-Hydroxy-7-phenyl-6-heptenyl)-1,2-benzenediol, 9CI. 1-(3,4-Dihydroxyphenyl)-7-phenyl-6-hepten-3-ol*
$C_{19}H_{22}O_3$ 298.381
Constit. of the rhizomes of *Curcuma xanthorrhiza* (Java turmeric). Cryst. ($CHCl_3/C_6H_6$). Mp 100-102°. $[\alpha]_D^{25}$ +77.3 (c, 0.19 in MeOH). Abs. config. not known - may not be the same as the dihydroxy compd. λ_{max} 249 (ε 14100); 282 (ε 4000) (MeOH).

Suksamrarn, A. *et al., Phytochemistry*, 1994, **36**, 1505-1508 (*isol, uv, ir, pmr, cmr, ms*)

7-(4-Hydroxyphenyl)-1-phenyl-4-hepten-3-one H-734

[100667-52-5]



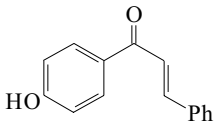
$C_{19}H_{20}O_2$ 280.366
Constit. of rhizomes of *Alpinia officinarum* (lesser galangal). Oil.

Itokawa, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4889

1-(4-Hydroxyphenyl)-3-phenyl-2-propen-1-one, 9CI H-735

[2657-25-2]

4′-Hydroxychalcone, 8CI. p-*Hydroxyphenyl styryl ketone*



$C_{15}H_{12}O_2$ 224.259
Yellow needles (EtOH aq.). Mp 172-173°.

O-*β*-D-*Glucopyranoside:* [82784-43-8]
$C_{21}H_{22}O_7$ 386.401
Mp 191-193°.

Ac: [57558-83-5]
$C_{17}H_{14}O_3$ 266.296
Mp 90°.

Me ether: [22966-19-4]

[959-23-9] *4′-Methoxychalcone*
$C_{16}H_{14}O_2$ 238.285
Reported to occur in *Citrus limon* (lemon) (unsubstantiated). Needles (MeOH). Mp 107°.

[30925-53-2, 38239-52-0, 102692-58-0]

Shriner, R.L. *et al., J.A.C.S.*, 1930, **52**, 2538-2540 (*synth*)
Peyron, L. *et al., C. R. Hebd. Seances Acad. Sci.*, 1963, **257**, 235 (*isol, deriv*)
Wittmann, H. *et al., Monatsh. Chem.*, 1966, **97**, 896-904 (*uv*)
Dinya, Z. *et al., Acta Chim. Acad. Sci. Hung.*, 1972, **73**, 453-467 (*ir*)
Jain, A. *et al., Phytochemistry*, 1982, **21**, 957 (*glycoside*)
Zhengdong, L. *et al., Acta Cryst. C*, 1992, **48**, 751 (*cryst struct, Me ether*)
Sasse, A. *et al., Arch. Pharm. (Weinheim, Ger.)*, 2001, **334**, 45-52 (*synth, pmr*)

3-(4-Hydroxyphenyl)-1-phenyl-2-propen-1-one, 9CI H-736

[20426-12-4]
4-Hydroxychalcone, 8CI. *ω*-p-*Hydroxybenzylideneacetophenone. 4-Hydroxystyryl phenyl ketone*

$C_{15}H_{12}O_2$ 224.259
Constit. of *Glycyrrhiza glabra* (licorice) roots. Yellow cryst. (C_6H_6). Mp 128° Mp 182-183°.

Ac:
$C_{17}H_{14}O_3$ 266.296
Mp 129-131°.

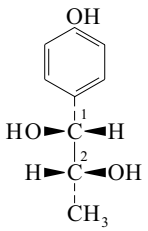
Me ether: [959-33-1] *4-Methoxychalcone. Anisylideneacetophenone.* p-*Methoxystyryl phenyl ketone. Anisalacetophenone*
$C_{16}H_{14}O_2$ 238.285
Yellow needles. Mp 77-78°. Bp_{19} 187.5-188°.

[22252-15-9, 30925-52-1]

Shriner, R.L. *et al., J.A.C.S.*, 1930, **52**, 2538-2540 (*synth*)
Davey, W. *et al., J.C.S.*, 1958, 1230-1236 (*synth, Me ether*)
Wittmann, H. *et al., Monatsh. Chem.*, 1966, **97**, 896-904 (*uv*)
Rabinovich, D. *et al., J.C.S.(B)*, 1970, 6 (*cryst struct, deriv*)
Dinya, Z. *et al., Acta Chim. Acad. Sci. Hung.*, 1972, **73**, 453-467 (*ir*)
Hoton-Dorge, M. *et al., J. Pharm. Belg.*, 1974, **29**, 560; *CA*, **83**, 111099x (*isol*)
Sasse, A. *et al., Arch. Pharm. (Weinheim, Ger.)*, 2001, **334**, 45-52 (*synth, pmr*)

1-(4-Hydroxyphenyl)-1,2-propanediol, 9CI H-737

[22805-45-4]
*1-(*p-*Hydroxyphenyl)propylene glycol*



(1*R*,2*R*)-*form*

$C_9H_{12}O_3$ 168.192

(1*R*,2*S*)-*form*
(+)-erythro-*form*
Cryst. (MeOH). Mp 153-154°. $[\alpha]_D^{25}$ +23.1 (c, 0.6 in MeOH).

*4′-Me ether, 1-*O-*β*-D-*glucopyranoside:* [217973-33-6]
$C_{16}H_{24}O_8$ 344.361
Isol. from *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{26}$ -61 (c, 0.3 in MeOH).

*4′-Me ether, 2-*O-*β*-D-*glucopyranoside:* [217973-39-2]
$C_{16}H_{24}O_8$ 344.361
Isol. from *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -29 (c, 0.3 in MeOH).

(1*S*,2*R*)-*form*
*4′-Me ether, 1-*O-*β*-D-*glucopyranoside:* [217973-29-0]
Isol. from *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{26}$ +13.8 (c, 0.9 in MeOH).

*4′-Me ether, 2-*O-*β*-D-*glucopyranoside:* [217973-45-0]
Isol. from *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 125-127°. $[\alpha]_D^{23}$ -15 (c, 0.5 in MeOH).

(1*S*,2*S*)-*form*
*4′-Me ether, 1-*O-*(4-methoxybenzoyl):* [212516-35-3] ***Verimol B***
$C_{18}H_{20}O_5$ 316.353
Constit. of *Illicium verum* (Chinese star anise). Oil.

(1*R*,2*R*)-*form*
4′-Me ether: [112018-74-3]
Isol. from *Foeniculum vulgare* (fennel) and *Pleurotus pulmonarius*.

*4′-Me ether, 2-*O-*(4-methoxybenzoyl):* [212516-34-2] ***Verimol A***
$C_{18}H_{20}O_5$ 316.353
Constit. of *Illicium verum* (Chinese star anise). Oil.

*4′-Me ether, 1,2-*O-*(4-methoxybenzylidene):* [212516-36-4] *2,4-Bis(4-methoxyphenyl)-5-methyl-1,3-dioxolane.* ***Verimol C***
$C_{18}H_{20}O_4$ 300.354
Constit. of *Illicium verum* (Chinese star anise). Oil. $[\alpha]_D$ +2.1 (c, 0.08 in $CHCl_3$). Partial racemate.

(1*R*,2*S*)-*form*
4′-Me ether: [103687-27-0]
Isol. from *Foeniculum vulgare* (fennel).

(1*RS*,2*RS*)-*form* [28282-82-8]
(±)-threo-*form*
Mp 141-142°.

*4′-*O-*β*-D-*Glucopyranoside:*
$C_{15}H_{22}O_8$ 330.334
Isol. from *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -49 (c, 0.2 in MeOH).

4′-Me ether: [94497-48-0] *1-(4-Methoxyphenyl)-1,2-propanediol.* ***Anethole glycol***
$C_{10}H_{14}O_3$ 182.219
Constit. of *Illicium verum* (Chinese star anise). Prisms (C_6H_6). Mp 67.5-68°. λ_{max} 224 (ϵ 11700); 274 (ϵ 1570); 280 (ϵ 1330) (MeOH).

(1*RS*,2*SR*)-*form* [28282-81-7]
(±)-erythro-*form*
Mp 128.5-129°.

4′-Me ether: [94497-49-1]
Constit. of *Illicium verum* (Chinese star anise). Mp 118-119°. λ_{max} 224 (ϵ 11800); 274 (ϵ 1550); 280 (ϵ 1330) (MeOH).

[111004-04-7, 166735-88-2, 166735-89-3, 166735-90-6]

St. Pfau, A. *et al., Helv. Chim. Acta*, 1939, **22**, 382 (*Me ether, isol*)
Ayer, W.A. *et al., J. Nat. Prod.*, 1993, **56**, 85 (*isol, deriv*)
Stadler, M. *et al., Planta Med.*, 1994, **60**, 128-132 (*Me ether, isol*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 337-342 (*Me ether, isol*)
Nakamura, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1908 (*Me ether, isol*)
Pelter, A. *et al., Tetrahedron*, 1996, **52**, 1085-1094 (*Me ether, synth*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1591-1594 (*Foeniculum vulgare glucosides*)
Sy, L.-K. *et al., J. Nat. Prod.*, 1998, **61**, 987-992 (*Anethole glycol, Verimols*)

3-(4-Hydroxyphenyl)-1,2-propanediol H-738

[22805-47-6]

$C_9H_{12}O_3$ 168.192

(±)-*form* [78472-12-5]
Mp 90-92° (81-82°).

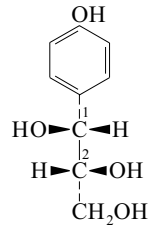
*4′-*O-*β*-D-*Glucopyranoside:*
$C_{15}H_{22}O_8$ 330.334
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{23}$ -57 (c, 0.2 in MeOH).

[28188-87-6]

Yamaguchi, A. *et al., CA*, 1970, **72**, 132209w (*synth*)
Ayer, W.A. *et al., Phytochemistry*, 1980, **19**, 2717-2721 (*isol, ir, pmr*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1591-1594 (*isol, glucoside*)

1-(4-Hydroxyphenyl)-1,2,3-propanetriol, 9CI H-739

[22805-48-7]
1-(4-Hydroxyphenyl)glycerol



(1*R*,2R)-*form*

$C_9H_{12}O_4$ 184.191

Configs. of the naturally occurring glycosides not yet detd..

(1*RS*,2*RS*)-*form* [25743-67-3]
(±)-threo-*form*
Constit. of *Pinus sylvestris* (Scotch pine).

(1*RS*,2*SR*)-*form* [38916-91-5]
(±)-erthyro-*form*
Constit. of *Pinus sylvestris* (Scotch pine). Mp 149-151°.

(1ξ,2ξ)-*form*

2-O-*β*-D-*Glucopyranoside:* [84744-60-5]
$C_{15}H_{22}O_9$ 346.333
Constit. of *Pinus sylvestris* (Scotch pine).

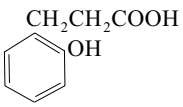
3-O-*β*-D-*Glucopyranoside:* [67151-73-9]
$C_{15}H_{22}O_9$ 346.333
Constit. of *Pinus sylvestris* (Scotch pine).

[25743-67-3]

Lundgren, L.N. *et al., Acta Chem. Scand., Ser. B*, 1982, **36**, 695-699; 1985, **39**, 241-248 (*synth, glucoside, 1RS,2RS-form, isol, bibl*)
Yang, S.-J. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 811-818 (*Taxumaiglucosides*)

3-(2-Hydroxyphenyl)propanoic acid H-740

[495-78-3]
*2-Hydroxybenzenepropanoic acid, 9CI. 3-(*o*-Hydroxyphenyl)propionic acid, 8CI. Melilotic acid.* o*-Hydroxyhydrocinnamic acid. Hydrocoumaric acid*



$C_9H_{10}O_3$ 166.176
Found in *Melilotus alba* (whilte melilot). Cryst. (H_2O). Sol. EtOH, Et_2O; fairly sol. H_2O; poorly sol. hexane. Mp 82-83°. pK_{a1} 4.75 (25°).

O-*β*-D-*Glucopyranoside:* [24696-05-7] ***Dihydromelilotoside***. *Cryptamygin B*
$C_{15}H_{20}O_8$ 328.318
Isol. from Chinese cinnamon. Cryst. (EtOAc) or syrup. Mp 144-145°. λ_{max} 224 (sh) (log ε 4.41); 276 (log ε 3.74) (MeOH).

O-*[β*-D-*Apiofuranosyl-(1→6)-β*-D-*glucopyranoside]:* ***Cryptamygin C***
$C_{20}H_{28}O_{12}$ 460.434
Syrup. λ_{max} 222 (sh) (log ε 4.55); 269 (log ε 3.86) (MeOH).

Et ester: [20921-04-4]
$C_{11}H_{14}O_3$ 194.23
Prisms (Et_2O). Mp 34°.

Amide: [22367-76-6]
$C_9H_{11}NO_2$ 165.191
Needles. Mp 70°.

Nitrile: [59577-13-8] *2-(2-Cyanoethyl)-phenol*
C_9H_9NO 147.176
Bp_1 147-149°.

Lactone: See 3,4-Dihydro-2*H*-1-benzopyran-2-one, D-222

Me ether: [6342-77-4] *3-(2-Methoxyphenyl)propanoic acid. 2-Methoxyhydrocinnamic acid*
$C_{10}H_{12}O_3$ 180.203
Cryst. (petrol). Mp 92°.

Me ether, Me ester: [55001-09-7]
$C_{11}H_{14}O_3$ 194.23
Liq. $d_4^{18.4}$ 1.1. Bp_{754} 274-275° Bp_{12} 142.5-143°.

Me ether, amide: [59734-18-8]
$C_{10}H_{13}NO_2$ 179.218
Needles (EtOH). Mp 111°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 152A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1004C (*nmr*)
Stoermer, R. *et al., Ber.*, 1911, **44**, 637
v. Auwers, *et al., Annalen*, 1918, **415**, 98
Houben, J. *et al., Ber.*, 1926, **59**, 1594
Slotta, K.H. *et al., Ber.*, 1930, **63**, 3036
Holberg, G.A. *et al., Acta Chem. Scand.*, 1955, **9**, 555
Ranarivelo, Y. *et al., Ann. Pharm. Fr.*, 1990, **48**, 273-277 (*Dihydromelilotoside*)
Begum, N.S. *et al., Acta Cryst. C*, 1992, **48**, 1076 (*cryst struct*)
Malakov, P.Y. *et al., Fitoterapia*, 1998, **69**, 552 (*cmr*)
Chan, Y.-Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 2002, **49**, 263-268 (*Cryptamygins B,C*)

3-(4-Hydroxyphenyl)propanoic acid H-741

[501-97-3]
*4-Hydroxybenzenepropanoic acid, 9CI. 3-(*p*-Hydroxyphenyl)propionic acid, 8CI. Dihydro-*p*-coumaric acid.* p*-Hydroxyhydrocinnamic acid. Phloretic acid. Phloretinic acid. HPPA*

$C_9H_{10}O_3$ 166.176
Prisms (Et_2O). Mp 129-130°. pK_a 4.76 (25°).

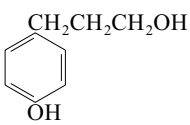
▶ MW5342000

Tridecyl ester: [232262-50-9]
$C_{22}H_{36}O_3$ 348.525
Constit. of *Piper longum* (long pepper).

Das, B. *et al., Boll. Chim. Farm.*, 1998, **137**, 319-320 (*tridecyl ester*)

3-(4-Hydroxyphenyl)-1-propanol H-742

[10210-17-0]
*4-Hydroxybenzenepropanol, 9CI. 4-γ-Hydroxypropylphenol. 4-(3-Hydroxypropyl)-phenol. Dihydro-*p*-coumaroyl alcohol*



$C_9H_{12}O_2$ 152.193
Constit. of *Pinus sylvestris* (Scotch pine). Cryst. (Et_2O/petrol). Mp 55°.

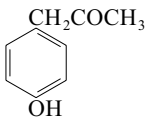
4′-Me ether, 1-O-*(2*-O-*sulfo-β*-D-*glucopyranoside):* [217971-99-8]
$C_{16}H_{24}O_{10}S$ 408.426
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder (as Na salt). $[\alpha]_D$ -25.5 (c, 0.3 in MeOH) (Na salt).

[125092-37-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1167A; 1167B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 409B; 409C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1086B; 1086C (*ir*)
v. Braun, J. *et al., Ber.*, 1912, **45**, 2504-2522 (*synth*)
Perold, G.W. *et al., J.C.S. Perkin 1*, 1972, 2450-2457 (*synth*)
Henley-Smith, P. *et al., J.C.S. Perkin 1*, 1980, 614-622 (*synth*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1587-1590 (*4′-Me, 1-sulfoglucoside*)
Hori, M. *et al., J.O.C.*, 1998, **63**, 889-894 (*synth, pmr*)

1-(4-Hydroxyphenyl)-2-propanone H-743

[770-39-8]
p-*Hydroxyphenylacetone*



$C_9H_{10}O_2$ 150.177
Yellowish oil or cryst. Mp 40°. Bp_{11} 168-170°.

Semicarbazone:
Mp 212°.

Ac:
$C_{11}H_{12}O_3$ 192.214
Yellow oil. Bp 130-145°.

Me ether: [122-84-9] *1-(4-Methoxyphenyl)-2-propanone. Anisylacetone. Anisyl ketone. FEMA 2674*
$C_{10}H_{12}O_2$ 164.204
Isol. from anise oil, fennel oil and oil of star anise fruit (*Illicium verum*). Oil or cryst. with anise-like taste and odour. d_4^{18} 1.07. Mp 46°. Bp 261-265° Bp_{12} 136-138°. n_D^{20} 1.5253.

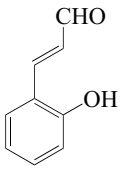
▶ Skin irritant. LD_{50} (rat, orl) 3330 mg/kg.
UC2990000

Me ether, semicarbazone: [7306-38-9]
Mp 183-184° (174°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 5B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 794B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1226A (*ir*)
Tardy, E. *et al., Bull. Soc. Chim. Fr.*, 1897, 660-664; 1902, 990-997 (*Me ether, isol*)
Hoover, E.W. *et al., J.O.C.*, 1947, **12**, 501-505 (*Me ether, synth*)
Jones, D.D. *et al., J.O.C.*, 1967, **32**, 1402-1409 (*synth*)
Bricout, J. *et al., Bull. Soc. Chim. Fr.*, 1974, 1901-1903 (*Me ether, occur*)
Franke, A. *et al., Helv. Chim. Acta*, 1975, **58**, 278-283 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOV875

3-(2-Hydroxyphenyl)-2-propenal, 9CI H-744

[3541-42-2]
o-*Hydroxycinnamaldehyde, 8CI.* o-*Coumaraldehyde. Cumaraldehyde*



$C_9H_8O_2$ 148.161

Data on derivs., which mostly comes from the older lit., presumably refers to the (*E*)-form.

▶ GD6565000

(*E*)-*form* [60125-23-7]
Constit. of the bark of *Cinnamomum cassia* (Chinese cinnamon). Needles (EtOH aq.), or cryst. (Me_2CO/hexane). Mp 131-132° (133°). λ_{max} 214 (ϵ 7000); 285 (ϵ 16000); 337 (ϵ 5000) (MeOH).

Oxime:
$C_9H_9NO_2$ 163.176
Mp 126°.

2,4-Dinitrophenylhydrazone:
Mp 257-259°.

Ac: [33538-94-2]
$C_{11}H_{10}O_3$ 190.198
Mp 81-82°.

▶ UC4900200

Me ether: [1504-74-1] o-*Methoxycinnamaldehyde.* ***Cassiastearoptene****. FEMA 3181*
$C_{10}H_{10}O_2$ 162.188
Flavouring ingredient. Isol. from oils of *Cinnamomum cassia* (Chinese cinnamon). Cryst. (C_6H_6/petrol) with sweet, spicy, warm flavour. Sol. MeOH, Et_2O; fairly sol. H_2O. Mp 45-46°. Bp 295° dec. Bp_{12} 160°.

▶ Skin irritant. LD_{50} (mus, scu) 8670 mg/kg , LD_{50} (mus, orl) 4430 mg/kg. GD6590000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **2**, 929B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1282C (*ir*)
Pauly, H. *et al., Ber.*, 1923, **56**, 603
Chatterjea, J.N. *et al., J. Indian Chem. Soc.*, 1959, **36**, 76
Sakai, T. *et al., Tet. Lett.*, 1963, 1171 (*isol, Me ether*)
Billman, J.H. *et al., J. Pharm. Sci.*, 1971, **60**, 1188
Bellasoued, M. *et al., J.O.C.*, 1993, **58**, 2517 (*synth, pmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 456 (*Me ether*)
Kwon, B.-M. *et al., Planta Med.*, 1996, **62**, 183 (*isol, uv, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1693-1694 (*Me ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MEJ750

3-(4-Hydroxyphenyl)-2-propenal, 9CI H-745

[2538-87-6]
p-*Hydroxycinnamaldehyde, 8CI.* p-*Coumaraldehyde*

$C_9H_8O_2$ 148.161

Some derivs. not specifically assigned as (*E*)- in the lit. but this can be inferred.

(*E*)-*form* [20711-53-9]
Constit. of *Alpinia galanga* (greater galangal) rhizomes and *Cucurbita maxima*. Cryst. (EtOAc). Mp 140° (136-138°).

Semicarbazone:
Mp 224°.

Ac: [157096-53-2]

[58505-83-2]
$C_{11}H_{10}O_3$ 190.198
Yellowish cryst. Mp 77-78°.

Me ether: [24680-50-0]

[1963-36-6] *3-(4-Methoxyphenyl)-2-propenal.* p-*Methoxycinnamaldehyde. FEMA 3567*
$C_{10}H_{10}O_2$ 162.188
Isol. from oil of tarragon (*Artemisia dracunculus*) and other oils. Flavouring ingredient. Yellow needles (EtOH aq.). Mp 58-59°. Bp 277° Bp_{15} 171°.

4′-O-(4-Hydroxy-3-methylbutyl):3-[4-(4-Hydroxy-3-methylbutoxy)phenyl]-2-propenal
$C_{14}H_{18}O_3$ 234.294
Solid. $[\alpha]_D^{24}$ +5.7 (c, 0.1 in MeOH).

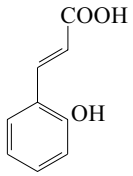
4′-O-[3-(Methoxycarbonyl)butyl]:3-[4-(3-Methoxycarbonylbutyl)phenyl]-2-propenal
$C_{15}H_{18}O_4$ 262.305
Solid. $[\alpha]_D^{24}$ +29.4 (c, 0.07 in MeOH).

*4′-O-(3,7-Dimethyl-2,6-octadienyl)(*E*-):* [194150-49-7] ***Colenemal***
$C_{19}H_{24}O_2$ 284.397
Cryst. Mp 36-38°. λ_{max} 218 ; 232 ; 303 (sh) (Et_2O).

Pauly, H. *et al., Ber.*, 1923, **56**, 603
Friedrich, K. *et al., Chem. Ber.*, 1961, **94**, 838
Aulin-Erdtman, G. *et al., Acta Chem. Scand.*, 1968, **22**, 1187 (*uv*)
Sadler, I.H. *et al., Chem. Comm.*, 1969, 773
Barik, B.R. *et al., Phytochemistry*, 1987, **26**, 2126 (*isol*)
Naidoo, L.A.C. *et al., Phytochemistry*, 1992, **31**, 3929 (*isol, pmr, cmr*)
Bellassoued, M. *et al., J.O.C.*, 1993, **58**, 2517 (*Me ether, synth, pmr, ir*)
Francesch, C. *et al., Synthesis*, 1994, 369 (*acetate*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 457 (*Me ether*)
Hsiao, H.-J. *et al., Phytochemistry*, 1995, **39**, 825; 1996, **41**, 1637 (*4′-O-alkyl derivs*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1694-1695 (*Me ether*)
Brader, G. *et al., Phytochemistry*, 1997, **45**, 1207 (*Colenemal*)
Iliefski, T. *et al., Acta Chem. Scand.*, 1998, **52**, 1177-1182 (*Me ether*)
Stange, R.R. *et al., Phytochemistry*, 1999, **52**, 41-43 (*isol, pmr, cmr*)

3-(2-Hydroxyphenyl)-2-propenoic acid, 9CI H-746

[583-17-5]
o-*Hydroxycinnamic acid, 8CI.* o-*Cumaric acid.* o-*Coumaric acid*



(*E*)-*form*

$C_9H_8O_3$ 164.16
pK_{a1} 3.7 (30°, 1.0*M* LiCl).

(*E*)-*form* [614-60-8]
Occurs in many plants e.g. *Melilotus officinalis* (sweet clover). Needles (H_2O). Sol. EtOH, hot H_2O, Et_2O; insol. CS_2, $CHCl_3$. Mp 207-208° dec. pK_a 4.61. Nonvolatile in steam. Dec. on dist..

▶ LD_{50} (mus, ivn) 180 mg/kg. GD9090000

O-*β*-*D*-*Glucopyranoside:* [618-67-7] ***Melilotoside***
$C_{15}H_{18}O_8$ 326.302
Isol. from *Melilotus alba* (white melilot), *Melilotus altissima* (tall yellow sweet clover) and other plants. Needles (H_2O). Mp 240-241°. $[\alpha]_D$ -60.9 (50% EtOH aq.).

(*Z*)-*form* [495-79-4]
Coumarinic acid
Readily loses H_2O giving coumarin.

O-*β*-*D*-*Glucopyranoside:*
$C_{15}H_{18}O_8$ 326.302
Isol. from *Melilotus alba* (white melilot). Syrup.

[6099-03-2, 69038-81-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 176C; 176D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **2**, 1046A; 1046B (*nmr*)
Tiemann, F. *et al., Ber.*, 1877, **10**, 284 (*synth*)
Fittig, R. *et al., Annalen*, 1883, **216**, 141; 1884, **226**, 351 (*synth*)
Roth, W.A. *et al., Ber.*, 1913, **46**, 260 (*synth*)
Sen, R.N. *et al., J. Indian Chem. Soc.*, 1930, **7**, 247 (*synth*)
Jensen, K.A. *et al., Fresenius' Z. Anal. Chem.*, 1933, **94**, 177 (*use, indicator*)
Dippy, F.J.F. *et al., J.C.S.*, 1938, 357 (*synth*)
Lock, G. *et al., Ber.*, 1939, **72**, 1064 (*deriv*)
Baddar, F.G. *et al., J.C.S.*, 1947, 224 (*synth*)
Narayana, M. *et al., J.O.C.*, 1962, **27**, 4704 (*synth, uv*)
Wheeler, O.H. *et al., J.O.C.*, 1963, **28**, 2015 (*uv*)
Bergman, J. *et al., J.C.S.*, 1964, 2021 (*cryst struct, deriv*)
Hadjoudis, E. *et al., J.C.S. Perkin 2*, 1972, 1060 (*synth, ir*)
Purohit, M.C. *et al., Phytochemistry*, 1993, **32**, 431 (*Melilotoside methyl ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MEJ775

3-(3-Hydroxyphenyl)-2-propenoic acid, 9CI H-747

[588-30-7]

[25429-38-3]
m-*Hydroxycinnamic acid.* m-*Coumaric acid.* m-*Cumaric acid*

$C_9H_8O_3$ 164.16

(*E*)-*form* [14755-02-3]
Present in roots of *Citrus sinensis* (orange), *Citrus limon* (lemon) and *Citrus paradisi* (grapefruit). Prisms

(H_2O). Sol. EtOH, Et_2O, C_6H_6, hot H_2O. Mp 191° (194°). pK_a 4.44.

Me ether, pyrrolidide: [29647-01-6] ***1-(m-Methoxycinnamoyl)pyrrolidine, 8CI***. m-*Methoxycinnamic acid pyrrolidide*
$C_{14}H_{17}NO_2$ 231.294
Alkaloid from the roots of kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Needles (petrol). Mp 90-93°.

[6099-04-3]

Jones, J.I. *et al., J.C.S.*, 1935, 1600 (*synth*)
Dippy, F.J.F. *et al., J.C.S.*, 1938, 357 (*synth*)
Feldman, A.W. *et al., Nature (London)*, 1965, **207**, 985 (*isol*)
Achenbach, H. *et al., Chem. Ber.*, 1970, **103**, 2535 (*Me ether pyrrolidide*)

3-(4-Hydroxyphenyl)-2-propenoic acid, 9CI H-748

[7400-08-0]
p-*Hydroxycinnamic acid, 8CI*. p-*Hydroxyphenylacrylic acid*. **p-*Coumaric acid***. *Naringenic acid*. *Naringeninic acid*. p-*Cumaric acid*

$C_9H_8O_3$ 164.16

▶ LD_{50} (mus, ipr) 657 mg/kg. Exp. reprod. effects. GD9094000

(*E*)-*form* [501-98-4]
Widespread in plants, e.g. peel of black cherry (*Prunus serotina*), lentil seeds and from red clover (*Trifolium pratense*). Found by Bate-Smith in 48% of investigated dicotyledonous and 55% of monocotyledonous spp.. Cryst. + $1H_2O$ (cold H_2O), anhyd. cryst. (hot H_2O). Sol. Et_2O, hot EtOH; spar. sol. C_6H_6; insol. petrol. Mp 210-213°. pK_{a1} 4.64; pK_{a2} 9.45 (25°). $SOCl_2$-activated polycondensation gives the homopolyester with an all-*trans* struct. Polyesters with other hydroxy acids are also known λ_{max} 225 ; 290 ; 310 (MeOH) (Berdy). λ_{max} 223 (ε 14450); 286 (ε 19000) (EtOH) (Berdy).

▶ GD9095000

Octadecyl ester: [72943-88-5] *Octadecyl* E-p-*coumarate*
$C_{27}H_{44}O_3$ 416.643
Constit. of *Ipomoea batatas* (sweet potato). Powder. Mp 99-100°. λ_{max} 203 (log ε 3.97); 228 (log ε 3.85); 311 (log ε 4.12); 424 (log ε 2.68) (MeOH).

O-*β-D-Glucopyranoside:* [117405-49-9] *4-O-β-D-Glucopyranosyl*-p-*coumaric acid*
$C_{15}H_{18}O_8$ 326.302
Constit. of *Brassica* spp. and other plant spp.. Needles (MeOH). Mp 191-192.5°. $[\alpha]_D^{24}$ -72.6 (c, 0.7 in MeOH).

O-*β-D-Glucopyranoside, Me ester:* ***Linocinnamarin***
$C_{16}H_{20}O_8$ 340.329
Glycoside from seeds of *Linum usitatissimum* (flax). Fine needles (MeOH aq.). Mp 167° (anhyd.). $[\alpha]_D^{27}$ -73 (c, 1 in MeOH).

O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{20}H_{26}O_{12}$ 458.418
Constit. of *Salvia officinalis* (sage). λ_{max} 296 (no solvent reported).

Me ether, Me ester: [3901-07-3]

[832-01-9]
$C_{11}H_{12}O_3$ 192.214
Isol. from *Kaempferia galanga* (galangal). Mp 94-95°.

▶ OO3724000

Me ether, Et ester: [24393-56-4]
$C_{12}H_{14}O_3$ 206.241
Major constit. of oil of *Kaempferia galanga* (galangal). Large prisms. Sol. EtOH, $CHCl_3$. Mp 49-50°. Bp_1 132°. λ_{max} 227 ; 308 (MeOH) (Berdy). λ_{max} 273 (ε 21000) (EtOH) (Berdy).

(*Z*)-*form* [4501-31-9]
Cryst. (C_6H_6 or H_2O). Mp 134-134.5° dec. (subl. from 124°).

▶ GD9095100

Octadecyl ester: [72943-89-6] *Octadecyl* Z-p-*coumarate*
$C_{27}H_{44}O_3$ 416.643
Constit. of *Ipomoea batatas* (sweet potato).

O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{20}H_{26}O_{12}$ 458.418
Constit. of *Salvia officinalis* (sage). λ_{max} 282 (no solvent reported).

O-*(3,7-Dimethyl-2,6-octadienyl), Me ester:*
$C_{20}H_{26}O_3$ 314.424
Constit. of *Boronia megastigma* (brown boronia). Wax.

(ξ)-*form*

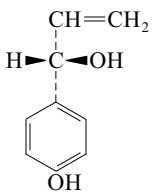
O-*β-D-Glucopyranoside:* [14364-05-7]
$C_{15}H_{18}O_8$ 326.302
Constit. of various fruits and vegetables incl. faba beans (*Vicia faba*) and tomato fruits. Cryst. (H_2O). Config. not determined.

[830-09-1, 1929-30-2, 2979-06-8, 3943-97-3, 7139-64-2, 13080-39-2, 14364-05-7, 117405-48-8, 117405-49-9, 155339-66-5, 155339-67-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 180C; 181A; 440D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1051C; 1506A (*nmr*)
Zincke, T. *et al., Annalen*, 1902, **322**, 224 (*isol*)
Ogawa, S. *et al., Bull. Chem. Soc. Jpn.*, 1927, **2**, 25 (*isol*)
Dippy, F.J.F. *et al., J.C.S.*, 1938, 357 (*synth*)
Klosterman, H.J. *et al., J.A.C.S.*, 1954, **76**, 1229; 1955, **77**, 420 (*Linocinnamarin*)
Bate-Smith, E.C. *et al., Sci. Proc. R. Dublin Soc.*, 1956, **27**, 165 (*occur*)
Bloomfield, J.J. *et al., J.O.C.*, 1961, **26**, 2991 (*synth, uv*)
U.S. Pat., 1963, 3 094 471; *CA*, **60**, 16556 (*isom*)
Cohen, M.D. *et al., J.C.S.*, 1964, 2000 (*cryst struct, deriv*)
Prager, R.H. *et al., Aust. J. Chem.*, 1966, **19**, 451 (*Methyl p-geranyloxycinnamate*)
Utsumi, H. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 426 (*cryst struct*)
Aulin-Erdtman, G. *et al., Acta Chem. Scand.*, 1968, **22**, 1187 (*props, uv*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 951; 953; 955 (*occur*)
Quick, J. *et al., Chem. Comm.*, 1978, 355 (*synth, isom, nmr, deriv*)
Coutrot, P. *et al., Synthesis*, 1978, 128 (*synth*)
Durkee, A.B. *et al., Carbohydr. Res.*, 1979, **77**, 252 (*glucoside*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1177-1179 (*octadecyl esters*)
Achenbach, H. *et al., Z. Naturforsch., C*, 1986, **41**, 164 (*esters*)
Schuster, B. *et al., Z. Naturforsch., C*, 1986, **41**, 511 (*glucoside*)
El-Negoumy, S.I. *et al., CA*, 1987, **107**, 194879q (*isol, lentils*)
Cui, C.-B. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3218 (*glucoside*)
Balde, A.M. *et al., Phytochemistry*, 1991, **30**, 1024-1026 (*octadecyl esters*)
Koetter, U. *et al., Planta Med.*, 1993, **59**, 279 (*esters*)
Weyerstahl, P. *et al., Annalen*, 1994, 1043 (*derivs*)
Lemmich, J. *et al., Phytochemistry*, 1995, **38**, 427 (*glucosides*)
Rasmussen, S. *et al., Phytochemistry*, 1996, **42**, 81 (*cis-glucoside*)
Ueda, M. *et al., Phytochemistry*, 1998, **49**, 633-635 (*glucoside*)
Roesecke, J. *et al., Phytochemistry*, 2000, **54**, 757-762 (*Me ether Me ester*)
Lu, Y. *et al., Phytochemistry*, 2000, **55**, 263-267 (*2-apiosylglucosides*)
Fonseca, F.N. *et al., Phytochemistry*, 2000, **55**, 575-580 (*octadecyl esters*)
Bujak, M. *et al., Acta Cryst. C*, 2002, **58**, o76-o77 (*Me ether Me ester, cryst struct*)

1-(4-Hydroxyphenyl)-2-propen-1-ol H-749

[53580-61-3]
α-Ethenyl-4-hydroxybenzenemethanol, 9CI. *4-(1-Hydroxy-2-propenyl)phenol*. *4-Hydroxy-α-vinylbenzyl alcohol*. *1′-Hydroxychavicol*



(*S*)-*form*

$C_9H_{10}O_2$ 150.177

(*S*)-*form*

Di-Ac: [52946-22-2] ***1′-Acetoxychavicol acetate***. *Galangal acetate*
$C_{13}H_{14}O_4$ 234.251
Constit. of *Alpinia galanga* (greater galangal). Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D^{20}$ -80 (c, 1 in EtOH). λ_{max} 216 (ε 10460); 260 (ε 468) (MeOH) (Berdy).

(±)-*form*

1-Ac: [151986-17-3] ***1′-Acetoxychavicol***
$C_{11}H_{12}O_3$ 192.214
Constit. of *Acorus calamus* (sweet flag).

4′-Ac: [101135-02-8] ***1′-Hydroxychavicol acetate***
$C_{11}H_{12}O_3$ 192.214
Constit. of *Alpinia galanga* (greater galangal).

Di-Ac: [108147-21-3]
$C_{13}H_{14}O_4$ 234.251
Constit. of *Alpinia galanga* (greater galangal).

4′-Me ether: [66821-63-4] *1-(4-Methoxyphenyl)-2-propen-1-ol*. *4-Methoxy-α-vinylbenzyl alcohol*
$C_{10}H_{12}O_2$ 164.204

Liq. $Bp_{0.1}$ 100-101°.

[51410-44-7, 53890-21-4, 108093-86-3]

Mitsui, S. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2377 (*synth*)
McWilliam, D.C. *et al., J.A.C.S.*, 1978, **100**, 6407 (*4′-Me ether*)
Jurd, L. *et al., Tetrahedron*, 1978, **34**, 57 (*4′-Me ether*)
Rajashekkar, B. *et al., J. Biol. Chem.*, 1984, **259**, 6925 (*synth*)
Janssen, A.M. *et al., Planta Med.*, 1985, **51**, 507 (*4′-Ac*)
Kondo, A. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1344 (*synth 1′-Acetoxychavicol acetate*)
Chowdhury, A.K.A. *et al., Pharmazie*, 1993, **48**, 786 (*synth*)
Watanabe, N. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1566 (*di-Ac, isol, pmr, cmr, activity*)
Yang, X. *et al., J. Agric. Food Chem.*, 1999, **47**, 1657-1662 (*1′-Acetoxychavicol acetate, pmr, cmr*)

3-(4-Hydroxyphenyl)-2-propen-1-ol, 9CI H-750

[3690-05-9]
4-(3-Hydroxy-1-propenyl)phenol, 9CI. 4-Hydroxycinnamyl alcohol. p-*Coumaryl alcohol*

$C_9H_{10}O_2$ 150.177

Props. and derivs. appear to belong to the (*E*)-form although this is not explicit in the lit..

(E)-form [20649-40-5]
Prisms. Mp 124° (89.3-90.5°). Acid-sensitive.

Bis(3,5-dinitrobenzoyl):
Needles. Mp 195°.

1-O-*β*-D-*Glucopyranoside:* [19764-35-3] p-*Coumaryl β-D-glucopyranoside.* ***Triandrin***. *Sachaliside 1*
$C_{15}H_{20}O_7$ 312.319
Needles (EtOAc). Mp 177-179° (152-152.5°). $[\alpha]_D^{20}$ -60.5 (c, 1.85 in H_2O). Stereochem. of Triandrin not detd. but prob. (*E*-). Stereochem. of Sachaliside 1 detd. as (*E*-).

4′-O-*β*-D-*Glucopyranoside:* [120442-73-1]

[59092-89-6]
$C_{15}H_{20}O_7$ 312.319
Needles. Mp 171-174°. $[\alpha]_D^{17}$ -57.4 (c, 0.9 in MeOH).

1-O-*[β-D-Glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→3)-[3,4-dihydroxy*-E-*cinnamoyl-(→4)]-β-D-glucopyranoside]:* [80458-55-5] ***Rossicaside B***
$C_{36}H_{46}O_{19}$ 782.748
Needles (H_2O or MeOH aq.). Mp 177-178° dec. $[\alpha]_D^{17}$ -66.6 (c, 1.1 in MeOH).

1-O-*[β-D-Glucopyranosyl-(1→2)-[4-hydroxy*-E-*cinnamoyl-(→6)]-β-D-glucopyranoside]:* [80458-56-6] ***Rossicaside C***
$C_{30}H_{36}O_{14}$ 620.606
Needles + ½H_2O (MeOH). Mp 236-237.5° dec. $[\alpha]_D^{19}$ -18.3 (c, 1.1 in Py).

1-O-*[β-D-Glucopyranosyl-(1→2)-[4-hydroxy*-E-*cinnamoyl-(→4)]-β-D-glucopyranoside]:* [80458-57-7] ***Rossicaside D***
$C_{30}H_{36}O_{14}$ 620.606
Needles + 1½H_2O (MeOH aq.). Mp 198-201.5° dec. $[\alpha]_D^{20}$ -58.3 (c, 0.5 in MeOH).

1-Me ether, 4′-O-*β*-D-*glucopyranoside:*
$C_{16}H_{22}O_7$ 326.346
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder. $[\alpha]_D^{23}$ -60 (c, 0.2 in MeOH).

4′-Me ether: [53484-50-7] *3-(4-Methoxyphenyl)-2-propen-1-ol*
$C_{10}H_{12}O_2$ 164.204
Constit. of *Alpinia galanga* (greater galangal). Cryst. (EtOH aq.). Mp 76°.

► UD5100000

4′-Me ether, 1-O-*β*-D-*glucopyranoside:* [19764-36-4] ***Vimalin***
$C_{16}H_{22}O_7$ 326.346
Cryst. (H_2O). Mp 143-144°. $[\alpha]_D^{20}$ -60.6 (c, 1.9 in MeOH). Stereochem. not explicit but prob. (*E*-).

4′-Me ether, 1-Ac: [53484-54-1] ***Verimol I***
$C_{12}H_{14}O_3$ 206.241
Constit. of *Illicium verum* (Chinese star anise). Oil. Bp_1 98-99°.

4′-Me ether, 1-O-*[2-(angeloyloxymethyl)-2Z-butenoyl]:* [161928-85-4]
$C_{20}H_{24}O_5$ 344.407
Light yellow oil. λ_{max} 213 ; 266 (EtOH).

Di-Me ether: [53484-53-0]

[120507-24-6, 181302-76-1] *1-Methoxy-4-(3-methoxy-1-propenyl)benzene, 9CI. 3-Methoxy-1-(4-methoxyphenyl)-1-propene*
$C_{11}H_{14}O_2$ 178.23

4′-O-*(4-Hydroxy-3-methylbutyl):* [156372-06-4] ***Ailanthoidiol***
$C_{14}H_{20}O_3$ 236.31
Prisms (Et_2O). Mp 77-79°.

4′-O-*(3-Methyl-2-butenyl):* [163634-05-7] ***Evofolin C***
$C_{14}H_{18}O_2$ 218.295
Prisms. Mp 65-67°. λ_{max} 205 (ϵ 21900); 233 (ϵ 3390); 263 (ϵ 17000); 293 (ϵ 2630) (MeOH).

4′-O-*(3-Methyl-2-butenyl), 1-Ac:Evofolin C acetate*
$C_{16}H_{20}O_3$ 260.332
Oil. λ_{max} 218 ; 263 ; 294 (sh) ; 306 (sh) (Et_2O).

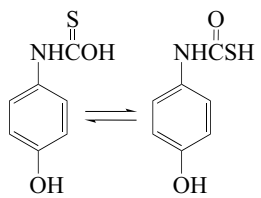
4′-O-*(3,7-Dimethyl-2,6-octadienyl)(*E-*):* [194150-48-6] ***Colenemol***
$C_{19}H_{26}O_2$ 286.413
Oil. λ_{max} 218 ; 263 ; 293 (sh) ; 305 (sh) (Et_2O).

4′-O-*(3,7-Dimethyl-2,6-octadienyl)(*E-*), 1-Ac:*
$C_{21}H_{28}O_3$ 328.45
Oil.

[17581-85-0, 132294-76-9]

Karrer, P. *et al., Helv. Chim. Acta*, 1928, **11**, 1209
Freudenberg, K. *et al., Chem. Ber.*, 1951, **84**, 443 (*synth*)
Marshall, D. *et al., J.C.S.*, 1956, 4082
Thieme, H. *et al., Naturwissenschaften*, 1963, **50**, 571; 1964, **51**, 217
Steglich, W. *et al., Chem. Ber.*, 1978, **111**, 3939 (*synth, pmr*)
Konishi, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2807 (*Rossicasides*)
Nakano, K. *et al., Phytochemistry*, 1989, **28**, 301-303 (*glucoside*)
Mizuno, M. *et al., Heterocycles*, 1990, **31**, 1409 (*Sachaliside 1*)
Quideau, S. *et al., J. Agric. Food Chem.*, 1992, **40**, 1108 (*synth, pmr, cmr*)
Naidoo, L.A.C. *et al., Phytochemistry*, 1992, **31**, 3929 (*Triandrin*)
Sheen, W.-S. *et al., Phytochemistry*, 1994, **36**, 213 (*Ailanthoidiol*)
Francesch, C. *et al., Synthesis*, 1994, 369 (*synth, pmr, cmr, ir, ms*)
Wu, T.-S. *et al., J. Chin. Chem. Soc. (Taipei)*, 1995, **42**, 107 (*Evofolin C*)
Pistelli, L. *et al., J. Nat. Prod.*, 1995, **58**, 112 (*Me ether angeloyloxymethylbutenoyl*)
Farrell, R. *et al., J. Nat. Prod.*, 1996, **59**, 446 (*synth, pmr, cmr*)
Brader, G. *et al., Phytochemistry*, 1997, **45**, 1207-1212 (*Evofolin C, Colenemol*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1587-1590 (*1-Me-4′-glucoside*)
Sy, L.-K. *et al., J. Nat. Prod.*, 1998, **61**, 987-992 (*Verimol I*)
Yenesew, A. *et al., Phytochemistry*, 1998, **47**, 295-300 (*4′-geranyl-1-Ac*)
Daubresse, N. *et al., Synthesis*, 1998, 157-161 (*synth, 4′-glucoside*)
Su, B.-N. *et al., J. Nat. Prod.*, 1999, **62**, 1363-1366 (*Morina chinensis derivs*)

4-Hydroxyphenylthiocarbamic acid H-751



$C_7H_7NO_2S$ 169.204

OH-form

Et ester: [53409-36-2]
$C_9H_{11}NO_2S$ 197.257
Constit. of *Moringa oleifera* (horseradish tree). Mp 94°.

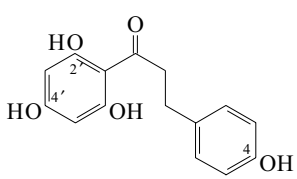
SH-form

Et ester: [121781-94-0]
$C_9H_{11}NO_2S$ 197.257
Mp 98-98.8°.

Nishimura, J. *et al., CA*, 1951, **45**, 5120d (*synth,* O-*ester*)
Abe, Y. *et al., Chem. Express*, 1988, **3**, 727-730 (*synth,* S-*ester*)
Faizi, S. *et al., J. Nat. Prod.*, 1997, **60**, 1317-1321 (*isol,* O-*ester*)

3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone H-752

[60-82-2]
2′,4,4′,6′-Tetrahydroxydihydrochalcone. ***Phloretin***. *Asebogenol. Dihydronarigenin. Phloretol*



$C_{15}H_{14}O_5$ 274.273

Chalcone numbering shown.Needles (EtOH aq.). Sol. MeOH, Me_2CO, bases; poorly sol. H_2O, Et_2O, $CHCl_3$, C_6H_6.

Mp *ca.* ° 262-264 dec. Log P 2.07 (calc).

*2′-*O*-β-*D*-Glucopyranoside:* [60-81-1] ***Phloridzin***. *Phlorrhizin*. *Phlorhizin*. *Phlorizin*. *Phlorizoside*
$C_{21}H_{24}O_{10}$ 436.415
Isol. from apple leaves and bark. Needles. $[\alpha]_D^{18}$ -52.1 (EtOH aq.). Various Mp's, some double, recorded between 108° and 170°.

▶Exp. reprod. effects. UC2080000

*2′-*O*-(6-*O*-Acetyl-β-*D*-glucopyranoside):6′′-*O*-Acetylphloridzin*. *6′′-*O*-Acetylphlorizoside*
$C_{23}H_{26}O_{11}$ 478.452
Powder. Mp 103-107°. $[\alpha]_D^{20}$ -37 (c, 0.5 in MeOH). λ_{max} 223 (log ε 4.3); 284 (log ε 4.2) (MeOH).

*4′-*O*-β-*D*-Glucopyranoside:* [4192-90-9] **p-*Phlorizin***. p-*Phloridzin*. *Trilobatin*
$C_{21}H_{24}O_{10}$ 436.415
Isol. from apple leaves. Pale yellow cryst. (MeOH aq.). Mp 166°. $[\alpha]_D^{20}$ -70 (c, 2 in EtOH).

*2′-*O*-α-*L*-Rhamnopyranoside:* [19253-17-9] ***Glycyphyllin***
$C_{21}H_{24}O_9$ 420.415
Large prisms (H_2O). Mp 175-180° dec. Found only in some chemical races of *S. glycyphylla* and not detected in other *S.* spp..

*2′-*O*-[Xylosyl-(1→?)-β-*D*-glucopyranoside]:*
$C_{26}H_{32}O_{13}$ 552.531
Isol. from apple plants. Complete struct. not detd..

*4′,6′-Di-Ac, 2′-*O*-β-*D*-glucopyranoside:* [145039-89-0] ***Zosterin***
$C_{25}H_{28}O_{12}$ 520.489

2′-Me ether: [111316-17-7] *1-(2,4-Dihydroxy-6-methoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone, 9CI. 2′,4,4′-Trihydroxy-6′-methoxydihydrochalcone*
$C_{16}H_{16}O_5$ 288.299
Needles (EtOH). Mp 195°.

4-Me ether:3-(4-Methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone. ***2′,4′,6′-Trihydroxy-4-methoxydihydrochalcone***
$C_{16}H_{16}O_5$ 288.299
Cryst. (Me_2CO). Mp 202-204°.

*4-Me ether, 2′-*O*-β-*D*-glucopyranoside:*
$C_{22}H_{26}O_{10}$ 450.441

4′-Me ether: [520-42-3] *1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone.* ***Asebogenin***. *Asebotol*. *Lyonigenin*
$C_{16}H_{16}O_5$ 288.299
Cryst. (EtOH). Mp 168°.

*4′-Me ether, 2′-*O*-β-*D*-glucopyranoside:* [11075-15-3] ***Asebotin***. *Asebotoside*. *Lyonotin*
$C_{22}H_{26}O_{10}$ 450.441
Mp 148° (135-136°). $[\alpha]_D^{25}$ -46.2 (EtOH).

2′,4-Di-Me ether: [75679-58-2] *1-(2,4-Dihydroxy-6-methoxyphenyl)-3-(4-methoxyphenyl)-1-propanone. 2′,4′,-Dihydroxy-4,6′-dimethoxydihydrochalcone*
$C_{17}H_{18}O_5$ 302.326
Needles (EtOAc/petrol), cryst. (C_6H_6). Mp 182-184° (175-176°).

2′,4-Di-Me ether, di-Ac:
Mp 92-94°.

2′,4′-Di-Me ether:1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone. 2′,4-Dihydroxy-4′,6′-dimethoxydihydrochalcone
$C_{17}H_{18}O_5$ 302.326
Needles (hexane). Mp 182-184°. λ_{max} 232 (log ε 4.45); 285 (log ε 4.39) (MeOH).

4,4′-Di-Me ether: [35241-54-4] *1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)-1-propanone. 2′,6′-Dihydroxy-4,4′-dimethoxydihydrochalcone.* ***Calomelanone***. *Calomelanen*
$C_{17}H_{18}O_5$ 302.326
Platelets (C_6H_6). Mp 145°.

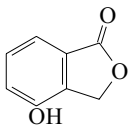
2′,4,4′-Tri-Me ether: [3791-75-1] *1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-(4-methoxyphenyl)-1-propanone, 9CI. 2′-Hydroxy-4,4′,6′-trimethoxydihydrochalcone*
$C_{18}H_{20}O_5$ 316.353
Plates (EtOH). Mp 110-112°.

[7061-54-3]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **2**, 866B (*nmr*)
Eykman, J.F. *et al., Ber.* , 1883, **16**, 2769 (*isol*)
Tamura, K. *et al., Nippon Kagaku Kaishi*, 1936, **57**, 1141 (*synth, Asebogenin*)
Zemplén, R. *et al., Ber.* , 1942, **75**, 645; 1298 (*synth*)
Murakami, S. *et al., Yakugaku Zasshi*, 1955, **75**, 573; 603 (*isol*)
Nilsson, M. *et al., Acta Chem. Scand.* , 1961, **15**, 154 (*Calomelanone*)
Williams, A.H. *et al., J.C.S.* , 1961, 4133 (*p-Phlorizin*)
Batterham, T.J. *et al., Aust. J. Chem.* , 1964, **17**, 428 (*pmr*)
Farkas, L. *et al., Chem. Ber.* , 1965, **98**, 2926 (*synth*)
Williams, A.H. *et al., Phytochemistry*, 1967, **6**, 1583 (*Glycyphyllin*)
King, B. *et al., Phytochemistry*, 1975, **14**, 1448 (*deriv*)
Mancini, S.D. *et al., J. Nat. Prod.* , 1979, **42**, 483 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 885 (*isol*)
Braz Filho, R. *et al., Phytochemistry*, 1980, **19**, 1195 (*derivs*)
Hufford, C.D. *et al., Phytochemistry*, 1980, **19**, 2036 (*cmr*)
Bhardwaj, D.K. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 476 (*2′,4-di-Me ether*)
Hutz, C. *et al., Z. Naturforsch., C*, 1982, **37**, 337 (*isol*)
Mizuno, M. *et al., Phytochemistry*, 1987, **26**, 2071-2074 (*2′-Me ether*)
Garzon, L. *et al., Phytochemistry*, 1987, **26**, 2835 (*4-Me ether*)
Bohm, A. *et al., The Flavonoids: Advances in Research since 1980* , (Ed. Harborne, J.B.), Chapman and Hall, London, 1988, 346 (*rev*)
Yang, Z. *et al., CA* , 1993, **118**, 18925v (*Zosterin*)
Barrero, A.F. *et al., J. Nat. Prod.* , 1997, **60**, 65 (*cmr*)
Silva, D.H.S. *et al., Phytochemistry*, 1997, **46**, 579-582 (*4-Me, 2′-glucoside*)
Silva, D.H.S. *et al., J. Nat. Prod.* , 1999, **62**, 1475-1478 (*2′,4′-di-Me ether*)
Cuendet, M. *et al., Phytochemistry*, 2000, **54**, 871-874 (*6′′-Acetylphloridzin, activity*)
Seidel, V. *et al., Phytochemistry*, 2000, **55**, 439-446 (*2′,4,4′-tri-Me ether*)

4-Hydroxyphthalide, 8CI H-753

[13161-32-5]
*4-Hydroxy-1(3*H*)-isobenzofuranone, 9CI*



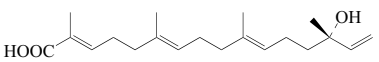
$C_8H_6O_3$ 150.134
Constit. of oats (*Avena sativa*). Cryst. (MeOH). Mp 255-256°.

Ac:
$C_{10}H_8O_4$ 192.171
Cryst. (H_2O). Mp 96-97°.

Me ether: [4792-33-0] *4-Methoxy-1(3*H*)-isobenzofuranone. 4-Methoxyphthalide*
$C_9H_8O_3$ 164.16
Cryst. (H_2O or MeOH aq.). Mp 129°.

Buehler, C.A. *et al., J.A.C.S.* , 1944, **66**, 417-418 (*synth, Ac, Me ether*)
Duncanson, L.A. *et al., J.C.S.* , 1953, 1331-1333 (*ir*)
Eliel, E.L. *et al., J.O.C.* , 1953, **18**, 1679-1688 (*synth*)
Knights, B.A. *et al., Nature (London)* , 1966, **210**, 1261 (*isol, uv, ir, ms*)
Marumo, S. *et al., Agric. Biol. Chem.* , 1968, **32**, 209 (*isol*)
Houbion, J.A. *et al., Org. Prep. Proced. Int.* , 1979, **11**, 27-32 (*Me ether*)
Broom, N.J.P. *et al., J.C.S. Perkin 1* , 1981, 465-470 (*synth, Me ether*)

3-Hydroxy-1,6,10,14-phytatetraen-16-oic acid H-754



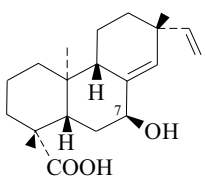
$C_{20}H_{32}O_3$ 320.471

(3*S*,6*E*,10*E*,14*E*)-*form*

*3-*O*-[β-*D*-Glucopyranosyl(1→2)-*D*-glucopyranoside]:* [121924-05-8] ***Capsianoside IV***. *Capsianside IV*
$C_{32}H_{52}O_{13}$ 644.755
Constit. of *Capsicum annuum*. Powder. $[\alpha]_D^{30}$ -8.4 (c, 0.6 in MeOH).

Izumitani, Y. *et al., Chem. Pharm. Bull.* , 1990, **38**, 1299-1307 (*isol, ir, pmr, cmr, ms*)

7-Hydroxy-8(14),15-pimaradien-19-oic acid H-755



(*ent*-7α)-*form*

$C_{20}H_{30}O_3$ 318.455

(ent*-7α)-*form [23807-91-2]
Constit. of *Aralia cordata* (udo). Cryst. Mp 218°. $[\alpha]_D$ -62.8 (Py).

(ent*-7β)-*form [23807-89-8]
Constit. of *Aralia cordata* (udo). Cryst. Mp 292-294° dec. $[\alpha]_D$ -70.4 (Py).

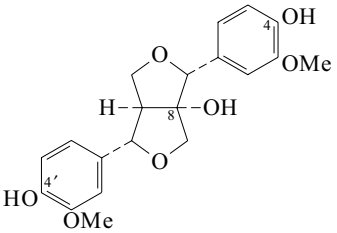
7-Ketone: [23807-90-1] **ent-*7-Oxo-***

8(14),15-pimaradien-19-oic acid
$C_{20}H_{28}O_3$ 316.439
Constit. of *Aralia cordata* (udo). Mp 247-243°.

Mihashi, S. *et al., Tet. Lett.*, 1969, 1683
Chang, L.C. *et al., J. Nat. Prod.*, 2000, **63**, 1235-1238 (*activity*)

8-Hydroxypinoresinol H-756

[81426-17-7]
2,6-Bis(4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo[3.3.0]octan-1-ol. 4,4′,8-Trihydroxy-3,3′-dimethoxy-7,9′:7′,9-diepoxylignan. 1-Hydroxypinoresinol



$C_{20}H_{22}O_7$ 374.39
Lignan numbering shown. Constit. of bark of *Olea europaea* (olive). Cryst. powder. Mp 183-185°. $[\alpha]_D^{15}$ +39 (c, 0.65 in EtOH).

4-O-*β*-D-*Glucopyranoside:*
$C_{26}H_{32}O_{12}$ 536.532
Constit. of *Olea europaea* (olive). Mp 127-129°. $[\alpha]_D^{23}$ -9.3 (c, 0.42 in MeOH).

4′-O-*β*-D-*Glucopyranoside:* [102582-69-4]
$C_{26}H_{32}O_{12}$ 536.532
Amorph. $[\alpha]_D^{18}$ -28.8 (c, 1 in MeOH). λ_{max} 228 ; 278 (MeOH).

8-O-*β*-D-*Glucopyranoside:*
$C_{26}H_{32}O_{12}$ 536.532
Constit. of *Olea europaea* (olive). Amorph. powder. Mp 179-183°. $[\alpha]_D^{23}$ -17.5 (c, 0.38 in EtOH).

4,4′-Di-O-*β*-D-*glucopyranoside:* [112747-99-6]
$C_{32}H_{42}O_{17}$ 698.674

8-Ac: [81426-14-4] *8-Acetoxypinoresinol*
$C_{22}H_{24}O_8$ 416.427
Constit. of *Olea europaea* (olive). Amorph. powder. $[\alpha]_D^{21}$ +31.4 (c, 0.99 in EtOH).

8-Ac, 4-O-*β*-D-*glucopyranoside:*
$C_{28}H_{34}O_{13}$ 578.569
Constit. of bark of *Olea europaea* (olive). Needles. Mp 183.5-185°. $[\alpha]_D^{22}$ +7.9 (c, 1.0 in EtOH).

4′-Me ether: [81426-18-8]
$C_{21}H_{24}O_7$ 388.416
Constit. of *Olea europaea* (olive). Amorph. powder. $[\alpha]_D^{23}$ +37.9 (c, 0.81 in $CHCl_3$).

4′-Me ether, 8-Ac:
$C_{23}H_{26}O_8$ 430.454
Constit. of *Olea europaea* (olive). Amorph. powder. $[\alpha]_D^{23}$ +29.9 (c, 1.14 in $CHCl_3$).

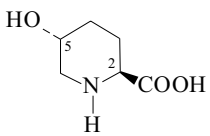
4′-Me ether, 8-Ac, 4-O-*β*-D-*glucopyranoside:*
$C_{29}H_{36}O_{13}$ 592.596
Constit. of *Olea europaea* (olive). Amorph. powder. $[\alpha]_D^{20}$ +9.1 (c, 1.6 in EtOH).

4,4′-Di-Me ether: See Gmelinol in *The Combined Chemical Dictionary.*

Tsukamoto, H. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2730; 4482; 1985, **33**, 1232
Deyama, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 523 (*4-glucosides*)
Deyama, T. *et al., CA*, 1988, **108**, 91694s (*4,4′-diglucoside*)
Macias, F.A. *et al., Acta Cryst. C*, 1992, **48**, 2240 (*cryst struct*)
Joshi, R.K. *et al., Fitoterapia*, 1998, **69**, 275-276 (*pmr, cmr*)
Schumacher, B. *et al., J. Nat. Prod.*, 2002, **65**, 1479-1485 (*4-glucoside, 4′-glucoside, isol, pmr, cmr*)

5-Hydroxy-2-piperidinecarboxylic acid H-757

[13096-31-6]
5-Hydroxypipecolic acid



(2*S*,5*R*)-*form*

$C_6H_{11}NO_3$ 145.158

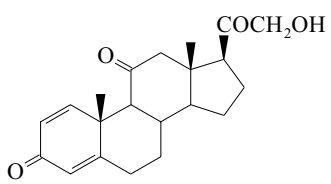
(2*S*,5*R*)-*form* [50439-45-7]
L-trans-*form*
Present in dates (*Phoenix dactylifera*), leaves of *Morus alba* (white mulberry). Mp 235° dec. $[\alpha]_D^{20}$ -23.1 (c, 1 in H_2O).

(2*S*,5*S*)-*form* [63088-78-8]
L-cis-*form*
Present in the leaves of *Morus alba* (white mulberry). Cryst. (EtOH aq.). Mp 230-235° dec. $[\alpha]_D^{22}$ -29.5 (c, 2 in H_2O). $[\alpha]_D^{22}$ -17.3 (6*M* HCl).

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1954, **8**, 1290 (*isol*)
Witkop, B. *et al., J.A.C.S.*, 1957, **79**, 192-197; 1964, **86**, 1844 (*isol, synth*)
Kristensen, I. *et al., Tetrahedron*, 1976, **32**, 2799 (*nmr*)
Hatanaka, S.-I. *et al., Phytochemistry*, 1977, **16**, 1041 (*isol*)
Evans, C.S. *et al., Phytochemistry*, 1978, **17**, 1127 (*isol, occur*)
Callen, R.E.A. *et al., Bull. Soc. Chim. Belg.*, 1982, **91**, 713 (*synth*)
Adams, D.R. *et al., Chem. Comm.*, 1996, 349-350 (*synth*)

21-Hydroxypregna-1,4-diene-3,11,20-trione H-758

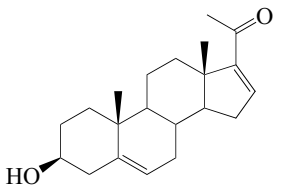
[67067-81-6]



$C_{21}H_{26}O_4$ 342.434
Cryst. Mp 220-220° dec.

Truscott, S. *et al., Steroids*, 1978, **31**, 573

3-Hydroxypregna-5,16-dien-20-one H-759



$C_{21}H_{30}O_2$ 314.467

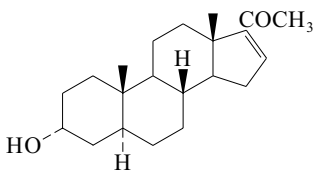
3*β*-*form* [1162-53-4]
Cryst. (Me_2CO). Mp 210-212°. $[\alpha]_D$ -34 (c, 1 in $CHCl_3$/dioxan).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* [312304-02-2]
$C_{45}H_{70}O_{19}$ 915.037
Constit. of *Allium ursinum* (ramsons).

[23549-24-8, 23549-26-0]

Janeczo, L. *et al., Acta Pol. Pharm.*, 2000, **57**, 131-133; *CA*, **134**, 27504q (*Allium ursinum saponin*)

3-Hydroxypregn-16-en-20-one, 9CI H-760



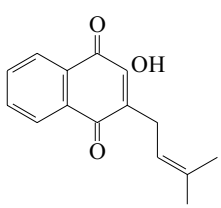
$C_{21}H_{32}O_2$ 316.483

(3β,5α)-*form* [566-61-0]
Isol. from *Lycopersicon esculentum* (tomato). Cryst. (EtOAc). Mp 207-209° (180-183°). $[\alpha]_D^{25}$ +51 (c, 0.530 in $CHCl_3$).

Crabbé, P. *et al., Can. J. Chem.*, 1963, **41**, 156 (*synth, 3β,5α-form*)
Tschesche, R. *et al., Chem. Ber.*, 1965, **98**, 1188 (*synth, 3β,5α-form*)
Jankowski, K. *et al., Steroids*, 1972, **19**, 189 (*pmr, 3β,5α-form*)

2-Hydroxy-3-prenylnaphthoquinone H-761

[84-79-7]
2-Hydroxy-3-(3-methyl-2-butenyl)-1,4-naphthalenedione, 9CI. ***Lapachol****. Greenhartin. Taiguic acid. Tecomin†. Groenhartin. Lapachoic acid. NSC 11905*



$C_{15}H_{14}O_3$ 242.274
Yellow prisms (EtOH or Et_2O). Mp 139-140°. Log P 3.21 (calc). λ_{max} 250 (ε 23400);

275 (ϵ 21400); 325 (ϵ 5130); 395 (ϵ 1700) (EtOH) (Derep).

▶ LD_{50} (mus, orl) 487 mg/kg. QL8750000

Ac:
Yellow prisms (EtOH). Mp 82-83°.

Me ether: [17241-45-1] *2-Methoxy-3-prenylnaphthoquinone*
$C_{16}H_{16}O_3$ 256.301
Yellow cryst. (petrol). Mp 54-55°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 81D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 910A (*nmr*)
Hooker, S.C. *et al., J.A.C.S.*, 1936, **58**, 1181 (*synth, bibl*)
Burnett, A.R. *et al., J.C.S.(C)*, 1967, 2100 (*synth*)
Burnett, A.R. *et al., Chem. Ind. (London)*, 1968, 1771 (*synth*)
Pettit, G.R. *et al., J.C.S.(C)*, 1971, 509 (*synth*)
Jacobsen, N. *et al., Acta Chem. Scand.*, 1973, **27**, 3211 (*synth*)
Rao, K.V. *et al., Cancer Chemother. Rep., Part 2*, 1974, **4**, 11 (*use*)
Da Silveira, J.C. *et al., Phytochemistry*, 1975, **14**, 1829 (*isol*)
Sawnhey, S.S. *et al., Indian J. Chem.*, 1976, **14**, 295 (*use*)
McDonald, I.A. *et al., Aust. J. Chem.*, 1977, **30**, 1727 (*pmr, cmr*)
Sawnhey, S.S. *et al., J. Indian Chem. Soc.*, 1977, **54**, 403 (*use*)
Kapoor, N.K. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 189 (*synth*)
Ghera, E. *et al., J.O.C.*, 1985, **50**, 3355 (*synth*)
Sun, J.S. *et al., Tet. Lett.*, 1998, **39**, 8221-8224 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HLY500

Hydroxypropanedial, 9CI H-762

[497-15-4]
Glucosereductone
$HOCH(CHO)_2$
$C_3H_4O_3$ 88.063
Present in free and conjugated form in botrytised wines. Mp 143° dec.

▶ WW8740000

Eistert, B. *et al., Chem. Ber.*, 1955, **88**, 939 (*synth*)
Guillou, I. *et al., J. Agric. Food Chem.*, 1997, **45**, 3382-3386 (*occur, glc*)

Hydroxypropanedioic acid, 9CI H-763

[80-69-3]
Tartronic acid, 8CI. Hydroxymalonic acid
$HOCH(COOH)_2$
$C_3H_4O_5$ 120.062
Prisms + H_2O (H_2O). Sol. H_2O, EtOH; spar. sol. Et_2O. Mp 141-142° Mp 156-158° (rapid heating). pK_{a1} 2.37; pK_{a2} 4.74 (25°). Sublimes.

2-O-(4-Hydroxycinnamoyl)(E-): [95519-23-6] ***2-O-p-Coumaroyltartronic acid***
$C_{12}H_{10}O_7$ 266.207
Constit. of *Vigna radiata* (mung bean).

2-O-(3,4-Dihydroxycinnamoyl): [102606-75-7] ***2-O-Caffeoyltartronic acid***
$C_{12}H_{10}O_8$ 282.206
Constit. of *Vigna radiata* (mung bean).

2-O-(4-Hydroxy-3-methoxycinnamoyl)(E-): [95519-25-8]
[102606-76-8] ***2-O-Feruloyltartronic acid***
$C_{13}H_{12}O_8$ 296.233
Constit. of *Vigna radiata* (mung bean).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 668B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1051A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 725B (*ir*)
Bak, B. *et al., Annalen*, 1939, **537**, 286 (*synth*)
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Terencio, M.C. *et al., Z. Naturforsch., C*, 1993, **48**, 417 (*Caffeoyltartronic acid*)

2-Hydroxypropanethioic acid H-764

$H_3CCH(OH)COSH \Leftrightarrow H_3CCH(OH)C(=S)OH$
$C_3H_6O_2S$ 106.145

SH-form

O-*Ac*, S-*Me ester:* [74586-09-7]
$C_6H_{10}O_3S$ 162.209
Flavour enhancer, e.g. for strawberry flavour.

O-*Ac*, S-*Ph ester:* [22198-55-6]

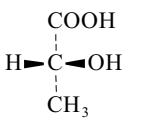
[24144-95-4]
$C_{11}H_{12}O_3S$ 224.28
$Bp_{0.1}$ 98°.

[96965-14-9, 206278-65-1]

Rosnati, V. *et al., Gazz. Chim. Ital.*, 1969, **99**, 152-164 (*Ac S-Ph ester*)
Japan. Pat., 1980, 80 02 264; *CA*, **93**, 112561k (*Ac S-Me ester, use*)

2-Hydroxypropanoic acid, 9CI H-765

[50-21-5]
Lactic acid, 8CI, JAN, USAN. *Chem-Cast. Enyper. Kerlactine. Lactogyn. Lactolavol. Lactovagan. Neostil. Tonsillosan. Variclene. E270. FEMA 2611*



(R)-form

$C_3H_6O_3$ 90.079
Widely distributed in nature as a fermentation product from starch, molasses, potatoes etc. "Natural" lactic acid is produced commercially by fermentation of beet/cane sugar or glucose. No commercial lactic acid is dairy-based. Synthetic lactic acid is a racemic mixture of the L- and D-forms. Among the oldest known preservatives used to preserve milk products and a broad range of traditional fermented vegetables. The modern use of lactic acid as a food additive covers several functions: flavouring, acidity control, preservation. Due to its mild flavour, lactic acid can be used in high concentrations. Also in brewing, manuf. of cheese and confectionery. Log P -0.76 (calc).

▶ Eye and skin irritant. LD_{50} (rat, orl) 3543 mg/kg. Fl. p. >74°. OD2800000

(R)-form [10326-41-7]
D-form
Widely distributed in nature - starch, molasses, potatoes etc.. Prismatic plates; cryst. (diisopropyl ether aq.). Sol. H_2O, EtOH, Et_2O; prac. insol. $CHCl_3$. Mp 26-27° Mp 53°. $[\alpha]_D$ -2.26 (H_2O). pK_a 3.83.

(S)-form [79-33-4]
L-form. Paralactic acid. Sarcolactic acid
Occurs in the juice of muscular tissue, bile etc. Flavour ingredient, food antioxidant. Various esters are also used in flavourings. V. hygroscopic prisms (AcOH or $CHCl_3$). Mp 25-26° Mp 53°. $[\alpha]_D^{15}$ +3.82 (H_2O). pK_a 3.79 (25°).

▶ OD3100000

(±)-form [598-82-3]
Cryst., or colourless or yellowish syrupy liq. Sol. H_2O, EtOH; spar. sol. Et_2O; insol. $CHCl_3$, CS_2, petrol. Volatile in superheated steam.

Na salt: [72-17-3] ***Sodium lactate, JAN, USAN.*** *Gynaegnost. Lacolin. E325*
Emulsifier, flavour-enhancer, humectant, pH control agent, glycerol substitute and other food processing uses. Liq.

K salt: [996-31-6]

[31981-04-1] *Potassium lactate. E326*
pH control agent. One of the least bitter-tasting salts available; finds wide used in the food industry.

Ca salt: [814-80-2] *Calcium lactate, JAN, USAN. E327*
Antioxidant, buffer, dough conditioner, yeast nutrient, firming agent, preservative used in food and beverages and other food uses. Dietary supplement (Ca source). Cryst. + $5H_2O$.

Et ester: [97-64-3]

[2676-33-7] *Ethyl lactate. FEMA 2440*
Present in cabbage, peas, vinegar, bread, roasted chicken, butter, blackberry, pineapple, raspberry and various wines and spirits. Flavouring agent. Liq. Bp 154°.

▶ Fl. p. 46.1°. OD5075000

Butyl ester: [138-22-7]

[126872-21-7] *Butyl lactate. FEMA 2205*
$C_7H_{14}O_3$ 146.186
Flavouring agent. Liq. with a faintly sweet, pleasant odour. d^{20} 0.97. Bp 185-187°. n_D^{20} 1.4210.

▶ OD4025000

Octadecanoyl: [4253-64-9]

[18200-72-1] *1-Carboxyethyl stearate. Stearoyllactic acid*
$C_{21}H_{40}O_4$ 356.545
Emulsifying agent for food products, as Na salt. Solid (Na salt). Extra CAS no. refers to Na salt.

3-Hexenyl ester(Z-): [61931-81-5] cis-*3-Hexenyl lactate. FEMA 3690*
$C_9H_{16}O_3$ 172.224
Found in cognac. Flavouring ingredient. Liq. with a fruity-green odour. Bp_{15} 96-98°. n_D^{20} 1.4451.

[113-21-3, 535-17-1, 867-55-0, 5743-47-5, 26100-51-6, 27848-80-2, 31587-11-8, 34451-19-9, 38939-83-2, 41372-22-9, 58742-64-6, 89673-71-2]

Eder, R. *et al., Pharm. Acta Helv.*, 1931, **6**, 118-123 (*calcium lactate*)
Christensen, E.V. *et al., Arch. Pharm. Chemi*, 1933, **40**, 13 (*sodium lactate*)

Milton, G.M. *et al., Can. J. Chem.*, 1957, **35**, 541 (*use*)
Strelow, F.W. *et al., Talanta*, 1970, **17**, 1 (*cation exchange*)
Holten, C.H. *et al., Lactic Acid*, Verlag Chemie, Weinheim, 1971,
Wood, G.W. *et al., Can. J. Chem.*, 1975, **53**, 3500 (*ms*)
Jankowski, K. *et al., J.O.C.*, 1975, **40**, 960 (*pmr*)
Szyper, M. *et al., Anal. Chim. Acta*, 1976, **85**, 357 (*uv*)
Hayashi, T. *et al., Tet. Lett.*, 1976, 4351 (*synth*)
Waldron, R.W. *et al., Inorg. Chem.*, 1977, **16**, 1220 (*synth*)
Imuta, M. *et al., J.O.C.*, 1978, **43**, 3530-3532 (*Ac Me ester*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 80
Motosugi, K. *et al., Biotechnol. Bioeng.*, 1984, **26**, 805 (*resoln*)
König, W.A. *et al., J. Chromatogr.*, 1984, **301**, 129 (*resoln*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1986, **12**, 226; 1990, **15**, 181 (*use, S-form*)
Sheikh, M.S. *et al., N. Engl. J. Med.*, 1987, **317**, 532 (*Calcium lactate*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, LAG000
Merck Index, 11th edn., 1989, 3773
Al-Shammary, F.J. *et al., Anal. Profiles Drug Subst.*, 1993, **22**, 263 (*rev*)
Yamamoto, T. *et al., Int. J. Clin. Pharmacol., Ther. Toxicol.*, 1993, **31**, 588 (*sodium lactate*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 250-251
Schouten, A. *et al., J. Mol. Struct.*, 1994, **323**, 165 (*cryst struct, conformn*)
Hamalainen, M.H. *et al., J. Nutr.*, 1994, **124**, 874 (*calcium lactate*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 343 (*3-hexenyl ester*)
Tappy, L. *et al., Clin. Physiol.*, 1996, **16**, 393 (*sodium lactate*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1082; 1174; 1176; 1718 (*salts*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 347-348; 1002-1003; 1317; 1530-1533 (*esters, use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1159
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 765
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BRR600; LAG000; LAH000; LAJ000; LAM000; LAQ000

1-Hydroxy-2-propanone, 9CI H-766

[116-09-6]
Hydroxyacetone. Acetol. Acetylcarbinol. Acetonyl alcohol. Pyruvic alcohol. Hydroxymethyl methyl ketone

H_3CCOCH_2OH

$C_3H_6O_2$ 74.079

Present in beer, tobacco and honey. Sol. H_2O. d_{20}^{20} 1.08. Fp -17 approx. Bp 145-146° Bp_{150} 96-97°. n_D^{20} 1.4295. Unstable. Stabilised by MeOH.

► Exp. causes hypersensitivity reactions. Asthma, eye and nose irritation, and urticaria may result. LD_{50} (rat, orl) 2200 mg/kg. UC2800000

Ac: [592-20-1] *Acetoxypropanone. Acetoxyacetone*
$C_5H_8O_3$ 116.116
Maillard product. Sweet-smelling liq. d_{15}^{15} 1.08. Bp 172°. n_D^{11} 1.4197. Hydrol. by H_2O.

[134252-15-6, 134252-16-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 420A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 506D (*ir*)
Perkin, W.H. *et al., J.C.S.*, 1891, **59**, 786 (*synth*)
Hildesheimer, A. *et al., Ber.*, 1910, **43**, 2796 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 5 (*synth*)
Reich, H. *et al., J.O.C.*, 1956, **21**, 68 (*synth*)
Sakae, U. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 1499 (*Ac, synth, pmr*)
Kubasik, N.P. *et al., Biochemistry*, 1972, **11**, 2225 (*synth*)
Wesdemiotsis, C. *et al., Org. Mass Spectrom.*, 1985, **20**, 98 (*ms*)
Griesbaum, K. *et al., Chem. Ber.*, 1990, **123**, 391 (*Ac, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABC000

2-Hydroxypropyl glucosinolate H-767

[76265-21-9]
1-Thio-β-D-glucopyranose 1-[3-hydroxy-N-(sulfooxy)butanimidate], 9CI

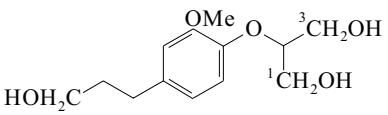
$H_3CCH(OH)CH_2C(SGlc){=}NOSO_3H$

$C_{10}H_{19}NO_{10}S_2$ 377.393

Present in horseradish (*Armoracia lapathifolia*).

Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)
Hogge, L.R. *et al., J. Chromatogr. Sci.*, 1986, **26**, 551 (*occur*)

2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol H-768



$C_{13}H_{20}O_5$ 256.298

Constit. of *Vitis vinifera* cv. Gewurztraminer.

1-O-β-D-Glucopyranoside: [68340-35-2]
$C_{19}H_{30}O_{10}$ 418.44
Constit. of Riesling wine.

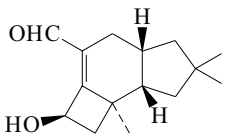
1-O-β-D-Xylopyranoside:
$C_{18}H_{28}O_9$ 388.414
Constit. of Scotch pine (*Pinus sylvestris*) bark. Famine food. $[\alpha]_D$ -39.1 (c, 0.7 in MeOH).

3′′-α-L-Rhamnopyranoside: [138614-65-0] ***Ampelopsisrhamnoside***
$C_{19}H_{30}O_9$ 402.441
Oil. $[\alpha]_D$ -18.1 (c, 0.04 in MeOH).

1-O-[4-Hydroxy-3-methoxybenzoyl-(1→6)-β-D-glucopyranoside]:
$C_{27}H_{36}O_{13}$ 568.574
Syrup. $[\alpha]_D^{13}$ -18.4 (c, 0.2 in MeOH).

Sakakibara, A. *et al., Holzforschung*, 1987, **41**, 1 (*glucoside, isol*)
Inuda, A. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2437 (*Ampelopsisrhamnoside*)
Marinos, V.A. *et al., Phytochemistry*, 1992, **31**, 4307 (*glucoside, isol, ms*)
Kouno, I. *et al., Phytochemistry*, 1993, **32**, 1573 (*isol*)
Pan, H. *et al., Phytochemistry*, 1996, **42**, 1185 (*xyloside*)
Baltenweck-Guyot, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 6178-6182 (*isol, pmr, cmr, ms*)

5-Hydroxy-6-protoilluden-14-al H-769



$C_{15}H_{22}O_2$ 234.338

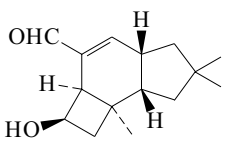
5β-*form*

O-*(2-Hydroxy-4-methoxy-6-methylbenzoyl):* [119516-61-9] ***Armillaribin***
$C_{24}H_{30}O_5$ 398.498
Metab. of *Armillaria mellea* (honey mushroom).

O-*(3-Chloro-6-hydroxy-4-methoxy-2-methylbenzoyl):* [119516-62-0] ***Armillaricin***
$C_{24}H_{29}ClO_5$ 432.943
Metab. of *Armillaria mellea* (honey mushroom). Cryst. (Et_2O/petrol). Mp 190-192°.

Yang, J.S. *et al., Huaxue Xuebao*, 1988, **46**, 1093 (*Armillaribin*)
Yang, J.S. *et al., Planta Med.*, 1989, **55**, 564 (*isol, pmr, cryst struct, Armillaricin*)

5-Hydroxy-7-protoilluden-14-al H-770



$C_{15}H_{22}O_2$ 234.338

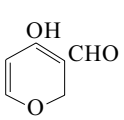
5β-*form*

5-(2,4-Dihydroxy-6-methylbenzoyl): [135247-97-1] ***Armillarivin***
$C_{23}H_{28}O_5$ 384.471
Metab. of *Armillaria mellea* (honey mushroom). Rods (Et_2O/petrol). Mp 159-172°. $[\alpha]_D$ +136.6 (c, 0.465 in $CHCl_3$).

Yang, J.S. *et al., Yaoxue Xuebao*, 1991, **26**, 117; *CA*, **115**, 89082s (*isol, pmr, cmr*)

4-Hydroxy-2*H*-pyran-3-carboxaldehyde, 9CI, 8CI H-771

[26110-68-9]
*3-Formyl-4-hydroxy-2*H*-pyran*



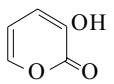
$C_6H_6O_3$ 126.112
Constit. of *Punica granatum* (pomegranate).

2,4-Dinitrophenylhydrazone:
Cryst. (MeOH). Mp 211°.

Koleoso, O.A. *et al., Biochemistry*, 1969, **8**, 4172
Schulte, K.E. *et al., Phytochemistry*, 1972, **11**, 2649

3-Hydroxy-2*H*-pyran-2-one H-772

[496-64-0]
Hydroxycoumalin. 3-Hydroxy-α-pyrone. Isopyromucic acid



$C_5H_4O_3$ 112.085
Component of brandy spirit. Cryst. (petrol). Mp 92°.

Ac:
$C_7H_6O_4$ 154.122
Cryst. (Et_2O). Mp 28° Mp 34-36°.

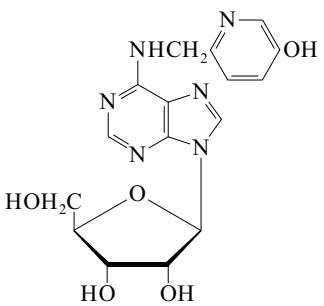
*Me ether:3-Methoxy-2*H*-pyran-2-one*
$C_6H_6O_3$ 126.112
Needles. Mp 60°. Bp 130-135°.

*Et ether:3-Ethoxy-2*H*-pyran-2-one*
$C_7H_8O_3$ 140.138
Mp 52°.

Wiley, R.H. *et al., J.A.C.S.*, 1956, **78**, 2398 (*synth, ir*)
Pirkle, W.H. *et al., J.O.C.*, 1975, **40**, 1617 (*nmr*)
Profitt, J.A. *et al., Synth. Commun.*, 1975, **5**, 457 (*synth*)
Warren, J.D. *et al., J. Het. Chem.*, 1979, **16**, 1617 (*use*)
Middlemiss, D. *et al., Synthesis*, 1979, 987 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 254

N-[(5-Hydroxy-2-pyridinyl)-methyl]adenosine, 9CI H-773

[123369-41-5]
6-(5-Hydroxy-2-pyridinylmethylamino)-9β-ribofuranosylpurine. AMG 1

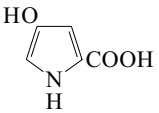


$C_{16}H_{18}N_6O_5$ 374.355
Isol. from *Armillaria mellea* (honey mushroom). Powder. Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. λ_{max} 268 (MeOH) (Berdy). λ_{max} 265 (MeOH-HCl) (Berdy). λ_{max} 264 (MeOH-NaOH) (Berdy).

Watanabe, N. *et al., Planta Med.*, 1990, **56**, 48 (*isol, pmr, cmr, struct*)

4-Hydroxy-1*H*-pyrrole-2-carboxylic acid H-774

Hydroxyminaline



$C_5H_5NO_3$ 127.099
Component of the molecule pectase found in *Penicillium* and *Aspergillus*. Grey-brown amorph. powder which cannot be recryst. or subl. Dec. readily in soln..

Me ether:4-Methoxy-2-pyrrolecarboxylic acid
$C_6H_7NO_3$ 141.126
Cryst. by subl. Mp 179-180°.

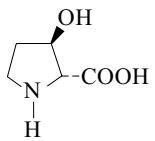
Me ether, Me ester:
$C_7H_9NO_3$ 155.153
Cryst. (MeOH). Mp 85-86°.

Me ether, Et ester:
$C_8H_{11}NO_3$ 169.18
Cryst. (C_6H_6). Mp 55-58°.

Minagawa, T. *et al., Proc. Imp. Acad. (Tokyo)*, 1945, **21**, 33; 37; *CA*, **47**, 151i; 152b (*isol*)
Kuhn, R. *et al., Chem. Ber.*, 1956, **89**, 1423 (*synth, uv*)
Rapoport, H. *et al., J.A.C.S.*, 1962, **84**, 630 (*derivs, synth, uv, ir*)

3-Hydroxy-2-pyrrolidinecarboxylic acid H-775

3-Hydroxyproline, 9CI



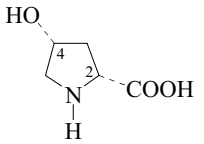
(2*R*,3*R*)-*form*

$C_5H_9NO_3$ 131.131
(2*S*,3*S*)-*form* [4298-08-2]
L-trans-*form*
Constit. of collagen. Cryst. (EtOH aq.). Mp 230-236° (dec.) (232°). $[\alpha]_D^{20}$ -18.8 (c, 0.14 in H_2O).

Sheehan, J.C. *et al., J.A.C.S.*, 1962, **84**, 3980; 1963, **85**, 3863 (*synth*)
Irreverre, F. *et al., J.A.C.S.*, 1963, **85**, 2832 (*synth*)
Gallina, C. *et al., Org. Magn. Reson.*, 1972, **4**, 31 (*pmr*)
Szymanovicz, G. *et al., Biochimie*, 1978, **60**, 499 (*synth*)
Häusler, J. *et al., Annalen*, 1981, 1073 (*synth*)
Cooper, J. *et al., Chem. Comm.*, 1988, 509 (*synth*)
Thaning, M. *et al., Acta Chem. Scand.*, 1989, **43**, 290 (*synth*)
Roemmele, R.C. *et al., J.O.C.*, 1989, **54**, 1866 (*synth*)
Hughes, P. *et al., J.O.C.*, 1989, **54**, 3260 (*synth*)
Cooper, J. *et al., J.C.S. Perkin 1*, 1993, 1313 (*synth, ir, pmr, cmr, ms*)
Mulzer, J. *et al., J.O.C.*, 1996, **61**, 566 (*synth, pmr, cmr, ir, ms*)
Durand, J.-O. *et al., Tet. Lett.*, 1998, **39**, 5743-5746 (*synth*)

4-Hydroxy-2-pyrrolidinecarboxylic acid H-776

4-Hydroxyproline. Oxyproline



(2*R*,4*R*)-*form*

$C_5H_9NO_3$ 131.131
Non-essential amino acid. Not reported as added to food.

(2*S*,4*R*)-*form* [51-35-4]
L-trans-*form*
Constit. of proteins. Mp 274°. $[\alpha]_D^{26}$ -74.6. pK_{a2} 9.73 (25°). Sweet taste.

β-D-Galactopyranosyl ester: [79284-73-4]
$C_{11}H_{19}NO_8$ 293.273
Isol. from hydrolysed wheat endosperm.

O-*β-D-Galactopyranoside:* [80185-44-0]
$C_{11}H_{19}NO_8$ 293.273
Isol. from hydrolysed wheat endosperm.

(2*S*,4*S*)-*form* [618-27-9]
L-allo-*form*. L-cis-*form*
Mp 238-241°. $[\alpha]_D^{18}$ -58.1. Sweet taste.

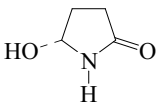
(2*RS*,4*RS*)-*form* [49761-17-3]
DL-allo-*form*. (±)-cis-*form*
Mp 238°.

[67463-44-9, 89771-43-7]

Goodson, J.A. *et al., J.C.S.*, 1919, 923 (*isol, struct, deriv*)
Abraham, R.J. *et al., J.C.S.*, 1964, 3739 (*pmr*)
Koetzle, T.F. *et al., Acta Cryst. B*, 1973, **29**, 231 (*cryst struct*)
Kaneko, T. *et al., Synth. Prod. Util. Amino Acids*, 1974, 123 (*rev*)
Shamala, N. *et al., Acta Cryst. B*, 1976, **32**, 3267 (*cryst struct*)
Ramaswamy, S.G. *et al., J.O.C.*, 1977, **42**, 3440 (*synth*)
Hara, J. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 3871 (*synth*)
Field, L. *et al., J.O.C.*, 1981, **46**, 17114182 (*synth, derivs*)
Strahm, A. *et al., Phytochemistry*, 1981, **20**, 1061 (*galactosyl ester*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13051
Sciuto, S. *et al., Phytochemistry*, 1983, **22**, 2311 (*isol, pmr, cmr, deriv*)
Inigo, R.P.A. *et al., An. Asoc. Quim. Argent.*, 1984, **72**, 1428 (*isol, deriv*)
Figliuolo, R. *et al., Phytochemistry*, 1987, **26**, 3255 (*isol, ir, pmr, cmr, ms, deriv*)
Jones, G.P. *et al., Phytochemistry*, 1987, **26**, 3343 (*isol, deriv*)
Jones, G.P. *et al., Acta Cryst. C*, 1988, **44**, 2208 (*cryst struct, deriv*)
Papaioannon, D. *et al., Acta Chem. Scand.*, 1990, **44**, 243 (*synth, pmr*)
De Martino, G. *et al., J. Het. Chem.*, 1990, **27**, 507 (*synth*)
Burger, K. *et al., Angew. Chem., Int. Ed.*, 1993, **32**, 285 (*synth*)
Matsuoka, T. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1747 (*synth*)
Mehlfuehrer, M. *et al., Chem. Comm.*, 1994, 1291 (*synth*)
Seki, M. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1161 (*synth, pmr, cmr*)
Remuzon, P. *et al., Tetrahedron*, 1996, **52**, 13803-13835 (*2S,4R-form, rev, use in chiral synth*)

5-Hydroxy-2-pyrrolidinone, 9CI H-777

[62312-55-4]
5-Hydroxy-2-pyrrolidone, 8CI



(*R*)-*form*

$C_4H_7NO_2$ 101.105

(*R*)-*form* [168111-92-0]
Amorph. powder. λ_{max} 198 (log ϵ 1.55); 224 (sh) (log ϵ 0.61); 241 (sh) (log ϵ 0.55) (H_2O). λ_{max} 198 (ϵ 35) (MeOH) (Berdy).

(±)-*form*
Cryst. Mp 98-99°.

Me ether:

[63853-74-7] *5-Methoxy-2-pyrrolidinone*
$C_5H_9NO_2$ 115.132
Cryst. (EtOAc/hexane). Mp 59-60.5°.

(ξ)-*form*

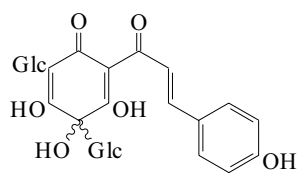
Me ether: [38072-88-7]

[63853-74-7] ***Pterolactam***
$C_5H_9NO_2$ 115.132
Constit. of *Pteridium aquilinum* (bracken fern). Cryst. (petrol). Mp 56-67°. $[\alpha]_D^{25}$ +2 ($CHCl_3$).

De Mayo, P. *et al., Chem. Ind. (London)*, 1962, 1576 (*synth*)
Takatori, K. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1087 (*isol, Me ether*)
Iwasaki, T. *et al., J.O.C.*, 1979, **44**, 1552 (*synth, Me ether*)
Cue, B.W. *et al., Org. Prep. Proced. Int.*, 1979, **11**, 285 (*synth*)
Barco, A. *et al., Synthesis*, 1979, 68 (*synth, ir, pmr*)
Lundgren, D.W. *et al., J. Biol. Chem.*, 1980, **255**, 4481 (*ms*)
Phan, X.T. *et al., J.O.C.*, 1983, **48**, 5164 (*synth, Me ether*)
Farina, F. *et al., Heterocycles*, 1984, **22**, 1733-1739 (*synth*)
Shono, T. *et al., J.O.C.*, 1985, **50**, 3243 (*synth, Me ether*)
Kuhnt, M. *et al., Planta Med.*, 1995, **61**, 227-232 (*isol, uv, pmr, cmr, ms*)
Staubmann, R. *et al., Phytochemistry*, 1999, **50**, 337-338 (*isol, pmr, cmr*)

Hydroxysafflor yellow A H-778

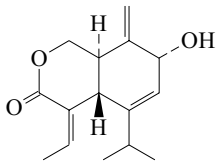
[146087-19-6]



$C_{27}H_{32}O_{16}$ 612.54
Ring-opened form of Safflor Yellow A, S-7. Constit. of the flower petals of *Carthamus tinctorius* (safflower). Yellow powder. $[\alpha]_D$ -54.3 (c, 0.1 in MeOH).

Meselhy, M.R. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1796 (*isol, pmr, cmr*)

9-Hydroxy-2,3-seco-4,7,10(14)-oplopatrien-3,2-olide H-779



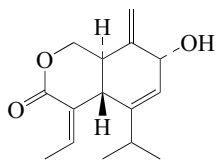
$C_{15}H_{20}O_3$ 248.321

(4*Z*,9α)-*form*

*9-(3-Methyl-2*E*-pentenoyl):* [168482-85-7] ***Neotussilagolactone I***
$C_{21}H_{28}O_4$ 344.45
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{23}$ -37.2 (c, 0.1 in $CHCl_3$).

Shi, W. *et al., Chin. Chem. Lett.*, 1995, **6**, 585-586 (*isol, pmr, cmr*)

9-Hydroxy-2,3-seco-4,7,10(14)-oplopatrien-3,2-olide H-780



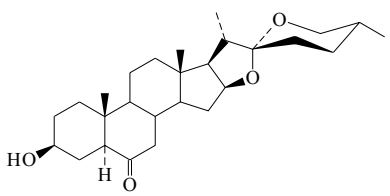
$C_{15}H_{20}O_3$ 248.321

(4*Z*,9α)-*form*

*9-(3-Methyl-2*E*-pentenoyl):* [189389-03-5] ***Neotussilagolactone***
$C_{21}H_{28}O_4$ 344.45
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{23}$ -37.2 (c, 0.1 in $CHCl_3$).

Shi, W. *et al., J. Chin. Pharm. Sci.*, 1996, **5**, 63-67; *CA*, **126**, 314812d (*isol, pmr, cmr*)

3-Hydroxyspirostan-6-one H-781



$C_{27}H_{42}O_4$ 430.626

(3β,5α,25*R*)-*form* [1177-71-5] ***Laxogenin***
Cryst. ($CHCl_3$/MeOH). Mp 202-204°. $[\alpha]_D^{24.5}$ -86.3 (c, 1.05 in $CHCl_3$).

3-O-[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]: [123941-70-8] ***Smilaxin A***
$C_{38}H_{60}O_{13}$ 724.884
Needles (MeOH). Mp 265-266°. $[\alpha]_D^{20}$ -66.7 (c, 0.09 in Py).

3-O-[2-O-Acetyl-α-L-arabinopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{40}H_{62}O_{14}$ 766.921
Constit. of *Allium chinense* (rakkyo). Amorph. solid. $[\alpha]_D$ -36 (c, 0.1 in MeOH).

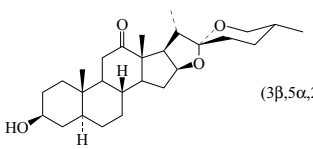
3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [384343-15-1]
$C_{39}H_{62}O_{13}$ 738.911

3-O-[β-D-Glucopyranosyl-(1→4)-[α-L-arabinopyranosyl-(1→6)]-β-D-glucopyranoside]: [143202-92-0] ***Smilaxin B***
$C_{44}H_{70}O_{18}$ 887.026
Needles (MeOH). Mp 270-272°. $[\alpha]_D^{21}$ -20 (c, 0.13 in MeOH).

Ac:
$C_{29}H_{44}O_5$ 472.664
Cryst. ($CHCl_3$/MeOH). Mp 159-162°.

Akahori, A. *et al., Chem. Pharm. Bull.*, 1965, **13**, 545
Chincharadze, D.G. *et al., Khim. Prir. Soedin.*, 1979, **15**, 509; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 442
De Valeri, B. *et al., Phytochemistry*, 1989, **28**, 2509 (*isol, pmr, cmr*)
Woo, M.H. *et al., J. Nat. Prod.*, 1992, **55**, 1129 (*Smilaxins*)
Kuroda, M. *et al., Phytochemistry*, 1995, **40**, 1071 (*isol, pmr, cmr*)
Abbas, F.A. *et al., Bull. Fac. Pharm. (Cairo Univ.)*, 2000, **38**, 147-153; *CA*, **136**, 66915k (*Solanum unguiculatum constit*)
Iglesias-Arteaga, M.A. *et al., J.C.S. Perkin 1*, 2001, 261-266 (*synth*)

3-Hydroxyspirostan-12-one H-782



(3β,5α,25*R*)-*form*

$C_{27}H_{42}O_4$ 430.626

(3β,5α,25*R*)-*form* [467-55-0] ***Hecogenin***. *Hocogenin*
Cryst. (three forms). Poorly sol. hexane. Mp 245° Mp 253° Mp 268°. $[\alpha]_D$ -10 (dioxan).

3-O-β-D-Galactopyranoside: [56857-65-9] ***Agavoside A***. *Agaveside A*
$C_{33}H_{52}O_9$ 592.768
From the famine food *Agave americana*. Amorph.

▶ WH1322700

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-galactopyranoside]: [56857-66-0] ***Agavoside B***. *Agaveside B*
$C_{39}H_{62}O_{14}$ 754.91
From the famine food *Agave americana*. Amorph.

▶ WH1322750

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [56316-35-9] ***Agavasaponin C***. *Agavoside C. Agavesaponin C. Agaveside C*
$C_{45}H_{72}O_{19}$ 917.052
From the famine food *Agave americana*. Cryst. (MeOH). Mp 275°. $[\alpha]_D$ -55 ($CHCl_3$).

▶ WH1322800

3-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [58546-17-1] ***Agavasaponin C′***. *Agavoside C′. Agavesaponin C′. Agaveside C′*
$C_{50}H_{80}O_{23}$ 1049.168
From the famine food *Agave americana*. Mp 200-204°. $[\alpha]_D^{20}$ -54 (c, 1.1 in $CHCl_3$).

► WH1322850

3-O-[α-L-Rhamnopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [58546-18-2] ***Agavasaponin D***. *Agavoside D. Agavesaponin D. Agaveside D*

$C_{56}H_{90}O_{27}$ 1195.311

From the famine food *Agave americana*. Mp 298-300°. $[\alpha]_D^{20}$ -60 (c, 1.33 in MeOH).

► WH1322650

3-O-[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [58546-19-3] ***Agavasaponin E***. *Agavoside E. Agavesaponin E. Agaveside E*

$C_{62}H_{100}O_{31}$ 1341.453

From the famine food *Agave americana*. Amorph. Mp 304-308°. $[\alpha]_D^{20}$ -130 (c, 0.83 in MeOH).

► WH1322600

3-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [58572-18-2] ***Agavoside F***. *Agaveside F*

$C_{68}H_{110}O_{35}$ 1487.596

From the famine food *Agave americana*.

(3β,5β,25*R*)-*form* [38676-82-3] ***Furcogenin***. *Gloriogenin*

Cryst. (MeOH). Mp 188.5-190°. $[\alpha]_D$ +15 (c, 0.22 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→6)]-β-D-glucopyranoside]: [244762-25-2]

$C_{44}H_{70}O_{18}$ 887.026

Constit. of the wild asparagus (*Asparagus africanus*). Needles (MeOH). Mp 206-208°. $[\alpha]_D^{20}$ +52 (c, 0.18 in CH_2Cl_2). λ_{max} 232 (MeOH).

(3β,5β,25ξ)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranoside]: [266998-23-6] ***Schidigerasaponin E1***

$C_{44}H_{70}O_{18}$ 887.026

Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -12.7 (c, 1 in MeOH). Mixt. of C-25 epimers.

Kintya, P.K. *et al., Khim. Prir. Soedin.*, 1975, **11**, 104; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 121 (*Agavasaponins*)

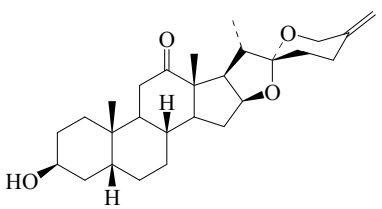
Bodeiko, V.A. *et al., Khim. Prir. Soedin.*, 1975, **11**, 751; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 775 (*Agavasaponins*)

Kintya, P.K. *et al., Tezisy Dokl. Vses. Simp. Bioorg. Khim., 1975*, 1975, 20 (*Agavosides*)

Debella, A. *et al., Phytochemistry*, 1999, **51**, 1069-1075 (*glucosylarabinosylglucoside*)

Miyakoshi, M. *et al., J. Nat. Prod.*, 2000, **63**, 332-338 (*Schidigerasaponin E1*)

3-Hydroxyspirost-25(27)-en-12-one H-783



$C_{27}H_{40}O_4$ 428.611

(3β,5β)-*form* [267003-21-4] ***Schidigeragenin B***

Genin from *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{23}$ +18.1 (c, 1 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranoside]: [266997-32-4] ***Schidigerasaponin B1***

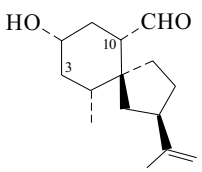
$C_{44}H_{68}O_{18}$ 885.01

Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -10.3 (c, 1.71 in MeOH).

Miyakoshi, M. *et al., J. Nat. Prod.*, 2000, **63**, 332-338 (*isol, pmr, cmr*)

2-Hydroxy-11-spirovetiven-14-al H-784

[35951-50-9] ***Lubimin***



$C_{15}H_{24}O_2$ 236.353

Stress product from potato tubers. $[\alpha]_D^{32}$ +39 (c, 1 in EtOH). Phytoalexin of infected potato tubers.

14-Alcohol: [55784-92-4] *11-Spirovetivene-2,14-diol*. ***Lubiminol***

$C_{15}H_{26}O_2$ 238.369

Isol. from infected potatoes. Cryst. (Et_2O). Mp 129-130°. $[\alpha]_D$ +33.

14-Carboxylic acid: [349106-26-9] *2-Hydroxy-11-spirovetiven-14-oic acid*. ***Lubiminoic acid***

$C_{15}H_{24}O_3$ 252.353

Solid. $[\alpha]_D^{20}$ +24.4 (c, 0.09 in $CHCl_3$).

10-Epimer: [64024-09-5] ***Epilubimin***

$C_{15}H_{24}O_2$ 236.353

Isol. from infected potatoes. Oil. $[\alpha]_D^{20}$ -21 (c, 1.63 in $CHCl_3$).

10-Epimer, 14-carboxylic acid: [349106-27-0] ***Epilubiminoic acid***

$C_{15}H_{24}O_3$ 252.353

Solid. $[\alpha]_D^{20}$ -20 (c, 0.5 in $CHCl_3$).

Hardwiger, L. *et al., Plant Physiol.*, 1971, **47**, 346 (*isol*)

Birnbaum, G.I. *et al., Chem. Comm.*, 1976, 330 (*biosynth*)

Stoessl, A. *et al., Tet. Lett.*, 1976, 3271 (*Lubiminol*)

Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 1217 (*struct*)

Birnbaum, G.I. *et al., Can. J. Chem.*, 1977, **55**, 1619 (*cryst struct*)

Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2424 (*derivs*)

Stoessl, A. *et al., Can. J. Chem.*, 1983, **61**, 1766 (*biosynth*)

Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 2286; 2291 (*synth*)

Coolbear, T. *et al., Phytochemistry*, 1985, **24**, 1963 (*biosynth*)

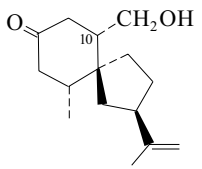
Iwata, C. *et al., Chem. Pharm. Bull.*, 1989, **37**, 866 (*synth*)

Crimmins, M.T. *et al., J.A.C.S.*, 1998, **120**, 1747-1756 (*synth*)

Nagase, H. *et al., Z. Naturforsch., C*, 2001, **56**, 181-187 (*Lubiminoic acid, Epilubiminoic acid*)

14-Hydroxy-11-spirovetiven-2-one H-785

[60077-68-1] ***Isolubimin***



$C_{15}H_{24}O_2$ 236.353

Possible precursor of 2-Hydroxy-11-spirovetiven-14-al, H-784 in infected potato tubers. Oil. $[\alpha]_D$ +34.4 ($CHCl_3$).

10-Epimer: ***Epiisolubimin***

$C_{15}H_{24}O_2$ 236.353

Isol. from infected potatoes. Oil.

[92541-83-8]

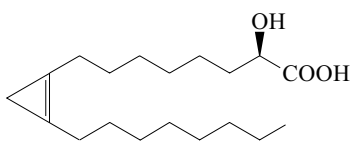
Kalan, E.B. *et al., Phytochemistry*, 1976, **15**, 775 (*isol, struct*)

Stoessl, A. *et al., Can. J. Chem.*, 1978, **56**, 645 (*biosynth*)

Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2424 (*isol, struct*)

2-Hydroxysterculic acid H-786

[18273-00-2] *α-Hydroxy-2-octyl-1-cyclopropene-1-octanoic acid, 8CI. 2-Hydroxy-8-(2-octyl-1-cyclopropenyl)octanoic acid*



$C_{19}H_{34}O_3$ 310.476

(*R*)-*form* [14602-38-1]

Constit. of seed oils of *Pachira aquatica* (Malabar chestnut).

Me ester: [13487-77-9]

$C_{20}H_{36}O_3$ 324.503

Oil. $[\alpha]_{Hg}^{24}$ -5.1 (c, 3 in $CHCl_3$). $[\alpha]_D^{24}$ -10 (c, 0.083 in $CHCl_3$). Ir ν 1740 cm^{-1}.

Morris, L.J. *et al., Chem. Ind. (London)*, 1967, 32

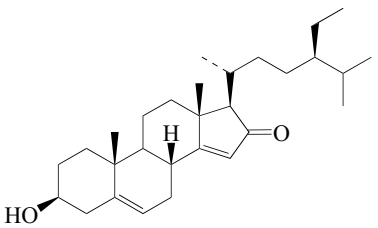
Recourt, J.H. *et al., J. Chromatogr.*, 1967, **30**, 35 (*ms, ir, pmr*)

Nakatani, M. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 3084 (*isol, ir, pmr, cmr, ms, ester, abs config*)

Baird, M.S. *et al., J.C.S. Perkin 1*, 1993, 1547 (*synth*)

3-Hydroxystigmasta-5,14-dien-16-one H-787

24-Ethyl-3-hydroxycholesta-5,14-dien-16-one

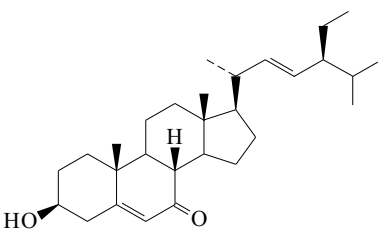


$C_{29}H_{46}O_2$ 426.681

(3β,24*R*)-*form* [189156-41-0]
Momordenol
Constit. of *Momordica charantia* (bitter melon). Needles. Mp 160-161°. $[\alpha]_D^{27}$ -62.9 (c, 0.1 in $CHCl_3$). λ_{max} 275 (EtOH).

Begum, S. *et al., Phytochemistry*, 1997, **44**, 1313-1320 (*isol, pmr, cmr, ms*)

3-Hydroxystigmasta-5,22-dien-7-one H-788



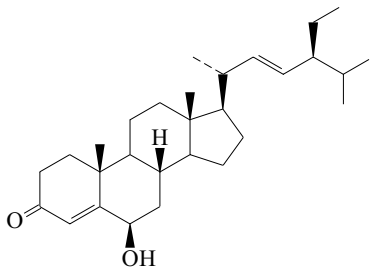
$C_{29}H_{46}O_2$ 426.681

(3β,22*E*)-*form* [36449-99-7]
7-Oxostigmasterol
Isol. from roots of French bean. Needles (MeOH/petrol). Mp 162°.

3-Ac: [33028-07-8]
Flakes (MeOH). Mp 183-185° (189-191°). $[\alpha]_D$ -127 (c, 1 in $CHCl_3$).

Bory, S. *et al., Bull. Soc. Chim. Fr.*, 1971, 1298 (*synth*)
Schroeder, G. *et al., Phytochemistry*, 1980, **19**, 2213 (*isol*)
Tal, D.M. *et al., Steroids*, 1983, **41**, 683
Pearson, A.J. *et al., J.C.S. Perkin 1*, 1985, 267 (*synth*)
Wong, S.M. *et al., J. Nat. Prod.*, 1986, **49**, 330 (*isol*)
Kovganko, N.V. *et al., Khim. Prir. Soedin.*, 1996, **32**, 206-211; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 183-186 (*synth*)

6-Hydroxystigmasta-4,22-dien-3-one H-789



$C_{29}H_{46}O_2$ 426.681

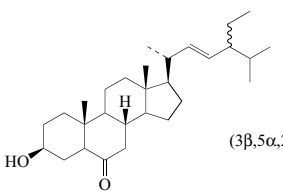
(6β,22*E*)-*form* [36450-01-8]
Constit. of the roots of *Phaseolus vulgaris* (kidney bean) and the stems of *Phoenix dactylifera* (date). Cryst. (EtOH). Mp 210-212°. $[\alpha]_D$ +8 ($CHCl_3$).

Ac: [36450-03-0]
Cryst. (hexane). Mp 107-109°. $[\alpha]_D$ +16 ($CHCl_3$).

Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 223 (*isol*)
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087 (*isol*)
Galagovsky, L.R. *et al., J. Chem. Res., Synop.*, 1990, 366 (*synth, pmr*)
Ayyad, S.N. *et al., Pharmazie*, 2001, **56**, 212-214 (*isol, pmr, cmr*)

3-Hydroxystigmast-22-en-6-one H-790

24-Ethyl-3-hydroxycholest-22-en-6-one



(3β,5α,22*E*,24*R*)-*form*

$C_{29}H_{48}O_2$ 428.697

(3β,5α,22*E*,24ξ)-*form* [135029-95-7]
(5α,22*E*,24*R*)-*form*

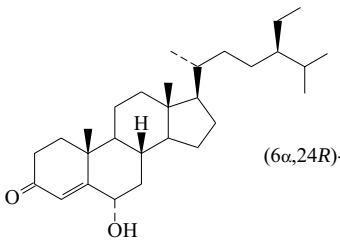
3-Ketone: [88661-99-8]

[138875-86-2] ***Stigmast-22-ene-3,6-dione***
$C_{29}H_{46}O_2$ 426.681
Constit. of *Phoenix dactylifera* (date).

Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087-2088 (*isol, diketone*)
Aliotta, G. *et al., J. Chem. Ecol.*, 1991, **17**, 2223-2234 (*isol, diketone*)
Cabrera, G. *et al., Phytochemistry*, 1991, **30**, 1239 (*isol, pmr, cmr*)

6-Hydroxystigmast-4-en-3-one H-791

[75521-65-2]



(6α,24*R*)-*form*

$C_{29}H_{48}O_2$ 428.697

(6α,24*R*)-*form* [75686-40-7] Possible artifact.
6-Hydroperoxide: ***6-Hydroperoxystigmast-4-en-3-one***
$C_{29}H_{48}O_3$ 444.696

(6α,24*S*)-*form* [125355-20-6]
Procesterol
Cryst. (Me_2CO). Mp 167°. $[\alpha]_D$ +21.5 (c, 0.217 in $CHCl_3$).

(6β,24*R*)-*form* [36450-02-9]
Isol. from various plant spp. incl. roots of French bean (*Phaseolus vulgaris*). Needles (petrol). Mp 213-215°. $[\alpha]_D$ +29 ($CHCl_3$).

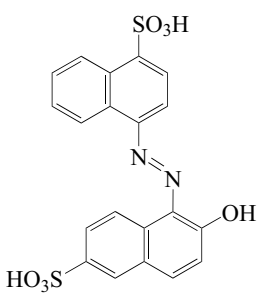
[54963-09-6]

Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 223 (*isol*)
Tunnmann, P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 966 (*isol*)
Hui, W.-H. *et al., J.C.S. Perkin 1*, 1977, 897 (*isol*)
Aringer, L. *et al., Lipids*, 1980, **15**, 563 (*synth*)
Khan, A.Q. *et al., Phytochemistry*, 1989, **28**, 2859 (*isol, pmr, cmr*)
Della Greca, M. *et al., J. Nat. Prod.*, 1990, **53**, 1430 (*isol, pmr, cmr*)
Della Greca, M. *et al., Nat. Prod. Lett.*, 1994, **5**, 7 (*hydroperoxides*)
Arai, Y. *et al., Phytochemistry*, 1998, **48**, 471-474 (*isol, pmr, cmr*)

4-[(2-Hydroxy-6-sulfo-1-naphthalenyl)azo]-1-naphthalenesulfonic acid, 9CI H-792

[25317-26-4]

[2302-96-7]
C.I. Acid Red 13, 8CI. C.I. Food Red 4. C.I. 16045. Fast Red E



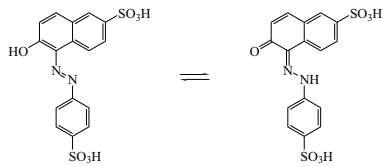
$C_{20}H_{14}N_2O_7S_2$ 458.472
Food dye; banned in the USA in 1976. Normally employed as di-Na salt, to which trade names refer.

[113824-46-7]

Colour Index, 3rd edn., 1971, **4**, 4089 (*props, bibl*)
Nursten, H.E. *et al., J. Soc. Dyers Colour.*, 1973, **89**, 49-53 (*purifn, uv, chromatog*)
Sugiura, T. *et al., J. Chem. Res., Miniprint*, 1980, 2426-2441 (*ms, detn*)
Egginger, R. *et al., Fleischwirtschaft*, 1988, **68**, 41-42 (*detn, tlc*)
Croft, S.N. *et al., J. Soc. Dyers Colour.*, 1992, **108**, 546-551 (*detn*)

6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid, 9CI H-793

[5859-11-0]
*1-(*p*-Sulfophenylazo)-2-naphthol-6-sulfonic acid. C.I. Food Yellow 3, 8CI. Food Yellow No. 5. Sunset Yellow FCF. C.I. 15985. E110. FD and C Yellow No. 6. Many other synonyms*



$C_{16}H_{12}N_2O_7S_2$ 408.412
Exists predominantly as the hydrazone form at pH 7.0. Strictly the trade names refer to the di-Na salt. Yellow food dye used in cereals, bakery products, sweets, snack foods, ice cream, drinks and canned fish. Orange cryst. Sol. H_2O, EtOH.

Di-Na salt: [2783-94-0]
Food dye. Sol. H_2O; v. sl. sol. EtOH.
▶ Genotoxic activity not detected.
QK2450000

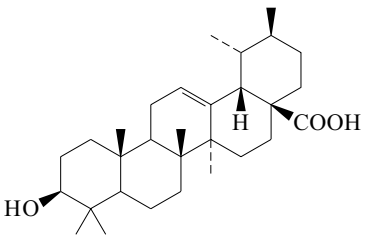
Ba salt:
Deep orange-red, microscopic needles. V. sl. sol. H_2O.

Al salt: [15790-07-5]

[12227-60-0, 39290-75-0, 53026-64-5, 68921-43-7] *C.I. Pigment Yellow 104*
Colour additive for foods.

Stein, C. *et al., J. Assoc. Off. Agric. Chem.*, 1949, **32**, 672 (*synth, uv, anal*)
Berkman, Yu.P. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1956, **106**, 693 (*synth, use*)
Reich, G. *et al., Zh. Anal. Khim.*, 1960, **177**, 274 (*anal*)
Gaunt, I.F. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 1-10 (*tox*)
Marmino, D.M. *et al., J. Assoc. Off. Anal. Chem.*, 1974, **57**, 495 (*pmr*)
Saeva, F.D. *et al., J.A.C.S.*, 1975, **97**, 5631 (*synth*)
Chudy, J. *et al., J. Chromatogr.*, 1978, **154**, 306 (*chromatog*)
Gelbcke, M. *et al., Anal. Lett. Part A:, Sect. A*, 1980, **13**, 975 (*cmr*)
Broadbent, P. *et al., J. Chem. Res., Synop.*, 1980, 160 (*Raman*)
Sugiura, T. *et al., J. Chem. Res., Synop.*, 1980, 164 (*ms, uv*)
Saint-Martin, P. *et al., Analusis*, 1987, **15**, LV (*hplc*)
Young, M. L. *et al., J. Assoc. Off. Anal. Chem.*, 1988, **71**, 458 (*tlc*)
Wever, J. *et al., Environ. Mol. Mutagen.*, 1989, **13**, 271
Mazzola, E.P. *et al., Tetrahedron*, 1996, **52**, 5691-5698 (*cmr, pmr, tautom*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1083-1088 (*Al salt, props, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG150

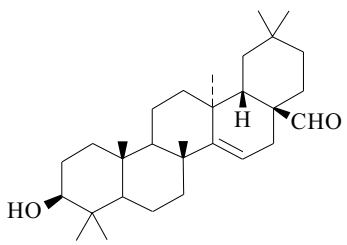
3-Hydroxy-12-taraxasten-28-oic acid H-794



$C_{30}H_{48}O_3$ 456.707
(3β,18β)-*form* [121467-37-6]
Carissic acid
Constit. of *Carissa carandas* (karanda). Cryst. (MeOH). Mp 232°. $[\alpha]_D^{30}$ +86 (EtOH).

Naim, Z. *et al., Pak. J. Sci. Ind. Res.*, 1988, **31**, 753 (*isol*)

3-Hydroxy-14-taraxeren-28-al H-795

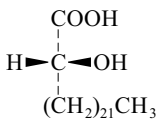


$C_{30}H_{48}O_2$ 440.708
3β-*form*
Myricolal
Constit. of *Myrica gale* (bog myrtle). Cryst. Mp 288°.

Matyukhina, I.G. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1959, **131**, 316

2-Hydroxytetracosanoic acid H-796

[544-57-0]
Cerebronic acid. *α-Hydroxylignoceric acid. Phrenosic acid. Phrenosinic acid*



(*R*)-*form*

$C_{24}H_{48}O_3$ 384.641
Constit. of various glycosphingolipids of wheat, corn and other plant spp..
(*R*)-*form* [26632-11-1]
Isol. from *Polyporus umbellatus* (zhu ling). Cryst. ($CHCl_3$); plates (Me_2CO). Mp 104.5-105.5° (99.5-100°). $[\alpha]_D^{25}$ +3.4 (c, 1.6 in Py).

Me ester:
$C_{25}H_{50}O_3$ 398.668
Mp 64-65°. $[\alpha]_D$ -3.25 (c, 0.92 in $CHCl_3$).

Ac: [127061-75-0]
$C_{26}H_{50}O_4$ 426.679
Cryst. (petrol or MeCN). Mp 81.5-82.5°. $[\alpha]_D^{20}$ +8.46 (c, 1.01 in $CHCl_3$).
(*S*)-*form* [54563-87-0]
Cryst.
(±)-*form* [139237-67-5]
Cryst. (C_6H_6). Mp 99.5-100° (94-95°).

[2433-95-6, 54563-85-8, 54563-86-9, 54563-88-1, 73580-21-9, 132842-33-2, 139237-68-6]

Ashton, R. *et al., J.C.S.*, 1936, 283 (*synth*)
Muller, A. *et al., Ber.*, 1939, **72B**, 615 (*synth*)
Yoshioka, I. *et al., Yakugaku Zasshi*, 1964, **84**, 742 (*isol, deriv*)
Vacheron, H.J. *et al., Phytochemistry*, 1968, **7**, 1645 (*isol*)
Hoshi, M. *et al., J. Biol. Chem.*, 1973, **248**, 4123 (*pharmacol*)
Tatsumi, K. *et al., Arch. Biochem. Biophys.*, 1974, **165**, 656 (*abs config*)
Florentina, N. *et al., Chem. Phys. Lipids*, 1984, **34**, 257 (*synth*)
Koike, K. *et al., Carbohydr. Res.*, 1987, **162**, 237 (*synth*)
Sugiyama, S. *et al., Annalen*, 1990, 1063 (*synth*)
Yamagata, K. *et al., J.C.S. Perkin 1*, 1990, 3355 (*synth*)
Sugai, T. *et al., Tet. Lett.*, 1991, **32**, 7063 (*synth, bibl*)

5-Hydroxytetradecanoic acid H-797

$H_3C(CH_2)_8CH(OH)CH_2CH_2CH_2COOH$
$C_{14}H_{28}O_3$ 244.373
(±)-*form*
Lactone: [2721-22-4] *Tetrahydro-6-nonyl-2*H*-pyran-2-one, 9CI. 5-Tetradecanolide. δ-Tetradecalactone*
$C_{14}H_{26}O_2$ 226.358
Found in coconut oil, butter, cheese, pork fat, tuberose oil, chicken fat, beef fat, milk and others (poss. in an enantiomeric form). Flavouring ingredient. Liq. Mp 14°. Bp_1 148°. n_D^{25} 1.4592.

[92446-06-5]

Allen, R.R. *et al., Chem. Ind. (London)*, 1965, 1560 (*isol, ir*)
Landelli, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 481 (*synth*)
Ijima, J. *et al., Chem. Pharm. Bull.*, 1973, **21**, 215 (*synth*)
Oser, B.L. *et al., Food Technol. (Chicago)*, (2), 1978, **32**, 60; (2), 64; 68 (*rev, tox*)

10-Hydroxytetradecanoic acid, 9CI H-798

[16899-08-4]
10-Hydroxymyristic acid
$H_3C(CH_2)_3CH(OH)(CH_2)_8COOH$
$C_{14}H_{28}O_3$ 244.373
Mp 56-57°. Probably an opt. active form.

Me ester:
$C_{15}H_{30}O_3$ 258.4
Occurs in oat (*Avena sativa*) leaf wax.

Papa, D. *et al., J.O.C.*, 1949, **14**, 723
Michiano, M. *et al., J. Biochem. (Tokyo)*, 1968, **63**, 390 (*synth*)
Tulloch, A.P. *et al., Lipids*, 1973, **8**, 617

14-Hydroxy-5-tetradecene-8,10,12-triynoic acid H-799

$HOCH_2C{\equiv}CC{\equiv}CC{\equiv}CCH_2CH{=}CH(CH_2)_3COOH$

$C_{14}H_{14}O_3$ 230.263

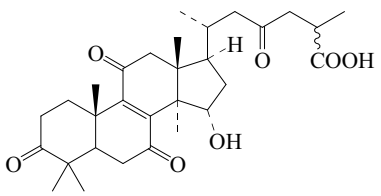
(Z)-form

*4-Hydroxycinnamoyl(*E-*)*: ***Cinnatriacetin A***
$C_{23}H_{20}O_5$ 376.408
Prod. by *Fistulina hepatica* (beefsteak fungus). Pale brown powder. λ_{max} 314 (ϵ 14400) (MeOH).

*4-Hydroxycinnamoyl(*Z-*)*: ***Cinnatriacetin B***
$C_{23}H_{20}O_5$ 376.408
Prod. by *Fistulina hepatica* (beefsteak fungus). Pale brown powder. λ_{max} 314 (ϵ 14100) (MeOH).

Tsuge, N. *et al., J. Antibiot.*, 1999, **52**, 578-581 (*isol, uv, ir, pmr, cmr*)

15-Hydroxy-3,7,11,23-tetraoxolanost-8-en-26-oic acid H-800



$C_{30}H_{42}O_7$ 514.658

(15α,25ξ)-*form* [100440-26-4]
Ganoderic acid J
Metab. of *Ganoderma lucidum* (reishi).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 3637 (*isol, pmr, cmr*)

22-Hydroxy-13-tetratriacontanone H-801

[61774-47-8]
Grewinol

$H_3C(CH_2)_{11}CH(OH)(CH_2)_8$-$CO(CH_2)_{11}CH_3$

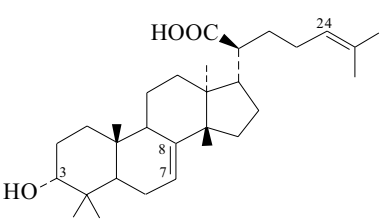
$C_{34}H_{68}O_2$ 508.91
Constit. of the flowers of *Grewia asiatica* (phalsa). Cryst. (MeOH/$CHCl_3$). Mp 81-82°.

Ac:
$C_{36}H_{70}O_3$ 550.947
Cryst. (MeOH). Mp 70-71°.

2,4-Dinitrophenylhydrazone:
Mp 140-141°.

Lakshmi, V. *et al., J. Nat. Prod.*, 1976, **39**, 372 (*isol*)

3-Hydroxytirucalla-7,24-dien-21-oic acid H-802



$C_{30}H_{48}O_3$ 456.707

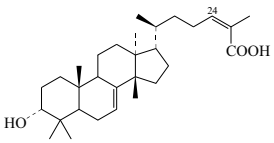
3α-*form* [341035-17-4]
Constit. of elemi resin (from *Canarium* spp.). Flavouring agent.

Me ester:
Cryst. (MeOH aq.). Mp 147-149°. $[\alpha]_D^{20}$ -34 (c, 1.1 in $CHCl_3$).

3-Ketone: [82464-35-5] ***3-Oxotirucalla-7,24-dien-21-oic acid***
$C_{30}H_{46}O_3$ 454.692
Cryst. Mp 250°.

Cotterrell, G.P. *et al., J.C.S.(C)*, 1970, 739
Tessier, A.M. *et al., Planta Med.*, 1982, **44**, 215 (*3-ketone*)
Mora, A.J. *et al., Acta Cryst. C*, 2001, **57**, 638-640 (*cryst struct*)

3-Hydroxytirucalla-7,24-dien-26-oic acid H-803



(3α,24Z)-*form*

$C_{30}H_{48}O_3$ 456.707

(3α,24*Z*)-*form*
3-Epimasticadienolic acid
Isol. from terebinth (*Pistacia terebinthus*). Cryst. (as Me ester). Mp 122-123° (Me ester). $[\alpha]_D$ -44 ($CHCl_3$) (Me ester).

(3β,24*Z*)-*form* [472-30-0]
Masticadienolic acid
Isol. from terebinth (*Pistacia terebinthus*). Cryst. (as Me ester). Mp 122-123° (Me ester). $[\alpha]_D$ -44 ($CHCl_3$) (Me ester).

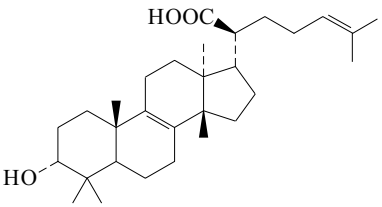
3-Ketone: [514-49-8] *3-Oxotirucalla-7,24-dien-26-oic acid*. ***Masticadienonic acid***. *Terebinthone*
$C_{30}H_{46}O_3$ 454.692
Constit. of *Pistacia* spp.. Cryst. (Et_2O/petrol). Mp 181-183°. $[\alpha]_D$ -76 (c, 1.35 in $CHCl_3$).

(24*E*)-*form*

3-Ketone: [66052-86-6] ***Adenophoric acid***
$C_{30}H_{46}O_3$ 454.692
Cryst. Mp 170-174°. $[\alpha]_D^{22}$ -12.3 (c, 0.292 in $CHCl_3$).

Kier, L.B. *et al., Bull. Soc. Chim. Fr.*, 1963, 911 (*isol*)
Corsano, S. *et al., Tet. Lett.*, 1965, 2377 (*struct*)
Caputo, R. *et al., Gazz. Chim. Ital.*, 1970, **100**, 317 (*Masticadienolic acid, Epimasticadienolic acid*)
Monaca, P. *et al., Phytochemistry*, 1974, **13**, 1992 (*isol*)
Polonsky, J. *et al., Isr. J. Chem.*, 1977, **16**, 16 (*isol, pmr*)
Mulholland, D.A. *et al., Phytochemistry*, 1994, **37**, 1409 (*isol, pmr, cmr*)

3-Hydroxytirucalla-8,24-dien-21-oic acid H-804



$C_{30}H_{48}O_3$ 456.707

3α-*form* [28282-27-1]
α-Elemolic acid. *Elemadienolic acid*
Constit. of elemi resin (from *Canarium* spp.). Flavouring agent. Needles (Me_2CO/EtOH). Mp 220-224°. $[\alpha]_D^{20}$ -15 ($CHCl_3$). $[\alpha]_D$ -25.6 (MeOH).

Me ester:
Cryst. (MeOH). Mp 149-150°. $[\alpha]_D^{20}$ -11 (c, 1 in $CHCl_3$).

3β-*form* [28282-54-4] ***β-Elemolic acid***
Constit. of elemi resin. Flavouring agent. Cryst. (MeOH aq.). Mp 198-201°. $[\alpha]_D$ -6 ($CHCl_3$).

Me ester:
Cryst. (MeOH aq.). Mp 117-118°. $[\alpha]_D^{20}$ -2 (c, 1 in $CHCl_3$).

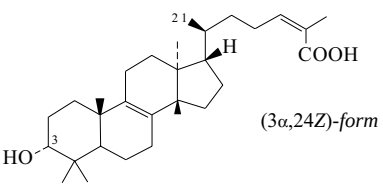
3-Ketone: [28282-25-9] *3-Oxotirucalla-8,24-dien-21-oic acid*. ***β-Elemonic acid***. *Elemadienonic acid*. *δ-Elemic acid*
$C_{30}H_{46}O_3$ 454.692
Constit. of elemi resin. Flavouring agent. Cryst. (MeOH). Mp 224-225°. $[\alpha]_D^{20}$ +31 ($CHCl_3$).

3-Ketone, Me ester:
Cryst. (MeOH). Mp 109-111°. $[\alpha]_D^{20}$ +28 (c, 1 in $CHCl_3$).

Arigoni, D. *et al., Helv. Chim. Acta*, 1955, **38**, 222 (*struct*)
Cotterrell, G.P. *et al., J.C.S.(C)*, 1970, 739 (*isol, struct*)
Hatakeyama, S. *et al., Tet. Lett.*, 1985, **26**, 865 (*synth*)

3-Hydroxytirucalla-8,24-dien-26-oic acid H-805

[31539-03-4]



(3α,24Z)-*form*

$C_{30}H_{48}O_3$ 456.707

(3α,24*Z*)-*form* [31297-68-4]
3-Epiisomasticadienolic acid. *Instipolinacic acid*
Sol. MeOH, C_6H_6; poorly sol. H_2O. The struct. of Instipolinacic acid from *Amphyterygium adstringens* was revised by Watson *et al* but the stereochem. of their proposed struct. is not clear λ_{max} 218 (ϵ 19060) (EtOH) (Berdy).

Me ester:
Cryst. (MeOH). Mp 140-141°. $[\alpha]_D$ -16

(c, 1 in $CHCl_3$).

3-Ketone: [5956-26-3] *3-Oxotirucalla-8,24-dien-26-oic acid*. ***Isomasticadienonic acid***
$C_{30}H_{46}O_3$ 454.692
Constit. of *Schinus molle* (California peppertree). Cryst. (petrol). Mp 166-167°. $[\alpha]_D$ +34 ($CHCl_3$).

3-Ketone, Me ester:
Cryst. (MeOH). Mp 110-111°. $[\alpha]_D$ +35 (c, 1 in $CHCl_3$).

3-Ketone, 21-oxo: [62499-11-0] *3,21-Dioxotirucalla-8,24*E*-dien-26-oic acid*. ***Isomasticadienonalic acid***
$C_{30}H_{44}O_4$ 468.675
Constit. of *Schinus molle* (California peppertree). Cryst. (hexane) (as Me ester). Mp 136-138° (Me ester). $[\alpha]_D$ +40 (c, 0.65 in $CHCl_3$) (Me ester). 20-Config. not detd..

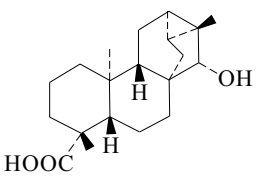
(3β,24*Z*)-*form*
Isomasticadienolic acid

Me ester:
Cryst. (MeOH). Mp 142-143°. $[\alpha]_D$ -11 (c, 1 in $CHCl_3$).

[88424-64-0]

Seaone, E. *et al., J.C.S.*, 1956, 4158 (*isol, struct, deriv*)
Caputo, R. *et al., Gazz. Chim. Ital.*, 1970, **100**, 317 (*isol*)
Lanfredi, A.M.M. *et al., Cryst. Struct. Commun.*, 1975, **4**, 551 (*cryst struct, Isomasticadienonic acid*)
Pozzo-Balbi, T. *et al., Gazz. Chim. Ital.*, 1976, **106**, 785 (*isol*)
Watson, W.H. *et al., Rev. Latinoam. Quim.*, 1987, **18**, 89 (*Instipolinacic acid*)
Olafsson, K. *et al., Planta Med.*, 1997, **63**, 352-355 (*cmr*)

15-Hydroxy-19-trachylobanoic acid H-806



$C_{20}H_{30}O_3$ 318.455

(*ent*-15β)-*form* [83404-76-6]
Occurs in sunflowers. Powder (EtOH). Mp 265-267°.

Me ester: [83508-81-0]
Mp 110-111°. $[\alpha]_D$ -35 (EtOH).

15-Ketone: ***15-Oxo-19-trachylobanoic acid***
$C_{20}H_{28}O_3$ 316.439
Pale yellow gum. $[\alpha]_D$ -83.5 (c, 1.2 in $CHCl_3$).

[90041-99-9, 90042-00-5, 90042-01-6, 90042-05-0, 90042-06-1, 90042-07-2, 99297-49-1]

Ferguson, G. *et al., J. Chem. Res., Synop.*, 1982, 200 (*cryst struct*)
Bohlmann, F. *et al., Annalen*, 1984, 495 (*isol*)
Harrigan, G.G. *et al., Phytochemistry*, 1994, **36**, 109 (*ketone*)
Takahashi, J.A. *et al., Quim. Nova*, 2001, **24**, 616-618 (*isol, pmr, cmr*)

11-Hydroxy-9-triacontanone H-807

[144357-41-5]

$H_3C(CH_2)_{18}CH(OH)CH_2CO(CH_2)_7CH_3$

$C_{30}H_{60}O_2$ 452.803

(+)-*form*
Constit. of the fruit of *Laurus nobilis* (bay laurel). Gum. $[\alpha]_D$ +25 (c, 0.3 in $CHCl_3$).

Garg, S.N. *et al., J. Nat. Prod.*, 1992, **55**, 1315-1319 (*isol*)

11-Hydroxy-9-tridecenoic acid H-808

[105798-56-9]

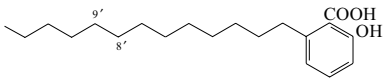
$H_3CCH_2CH(OH)CH{=}CH(CH_2)_7COOH$

$C_{13}H_{24}O_3$ 228.331
Constit. of *Elaeagnus angustifolia* (Russian olive).

Zhmyrko, T.G. *et al., Khim. Prir. Soedin.*, 1986, **22**, 161-168; 1989, **25**, 626-634; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 149-155; 1989, **25**, 529-536 (*isol, ms*)
Goncharova, N.P. *et al., Khim. Prir. Soedin.*, 1994, **30**, 715-719; *Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 661-665 (*isol*)

2-Hydroxy-6-tridecylbenzoic acid, 9CI H-809

[20261-38-5]
6-Tridecylsalicylic acid



$C_{20}H_{32}O_3$ 320.471
Isol. from pistachio shells. Isol. from *Ginkgo biloba* (ginkgo). Plates (hexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 85-86° (73-74°). Log P 8.48 (uncertain value) (calc). λ_{max} 244 ; 308 (MeOH) (Berdy).

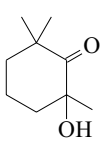
► DH2944000

8′,9′-Didehydro (Z-): [88640-88-4] *2-Hydroxy-6-(8-tridecenyl)benzoic acid. 6-(8-Tridecenyl)salicylic acid*
$C_{20}H_{30}O_3$ 318.455
Isol. from pistachio shells.

Durrani, A.A. *et al., J.C.S. Perkin 1*, 1979, 2069 (*synth*)
Buckle, P.J. *et al., Agents Actions*, 1980, **10**, 361 (*pharmacol*)
Kazlauskas, R. *et al., Aust. J. Chem.*, 1980, **33**, 2097 (*isol, pmr, cmr, ir, ms*)
Yalponi, M. *et al., Phytochemistry*, 1983, **22**, 2263 (*isol, deriv*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3016 (*isol, ms, ir, pmr*)
Zehnter, R. *et al., Annalen*, 1995, 2209 (*synth, ir, pmr, cmr*)

2-Hydroxy-2,6,6-trimethylcyclohexanone H-810

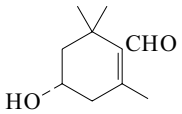
[7500-42-7]



$C_9H_{16}O_2$ 156.224
Constit. of the aroma of black tea.

Muggler-Chavan, F. *et al., Helv. Chim. Acta*, 1969, **52**, 549
Ragoussis, N. *et al., Synthesis*, 1985, 489 (*synth*)
Subbaraju, G.V. *et al., Synthesis*, 1992, 816 (*synth, ir, pmr, cmr, ms*)

4-Hydroxy-2,6,6-trimethyl-1-cyclohexenecarboxaldehyde H-811



$C_{10}H_{16}O_2$ 168.235

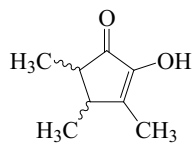
(*R*)-*form*

O-β-D-*Glucopyranoside:* [138-55-6] ***Picrocrocin***. *Safranbitter. Saffronbitter*
$C_{16}H_{26}O_7$ 330.377
Isol. from saffron (stamens of *Crocus sativus*). Food colour and flavouring ingredient. Cryst. (MeOH/$CHCl_3$/Et_2O). Mp 156°. $[\alpha]_D^{20}$ -58 (H_2O). λ_{max} 250 (ε 10100) (MeOH) (Berdy).

Duquenois, P. *et al., Bull. Soc. Pharm. Strasbourg*, 1972, **155**, 149 (*rev*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1973, **56**, 1121 (*struct*)

2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one H-812

[109682-87-3]



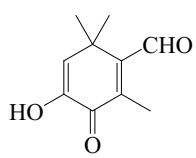
$C_8H_{12}O_2$ 140.182
Aroma constit. of roasted Arabica coffee beans as mixed *cis*- and *trans*- isomers. Flavouring agent. Oil with sweet, burnt odour/taste. $Bp_{0.02}$ 45-48°.

[125476-23-5, 125476-24-6]

Mihara, S. *et al., J. High Resol. Chromatogr.*, 1989, **12**, 763-764 (*glc*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*occur, synth, pmr, cmr, ir, ms*)
U.S. Pat., 1990, 4 892 966; *CA*, **113**, 23189j (*synth, ir, pmr, ms, use*)

4-Hydroxy-2,6,6-trimethyl-3-oxo-1,4-cyclohexadiene-1-carboxaldehyde, 9CI H-813

[35692-95-6]

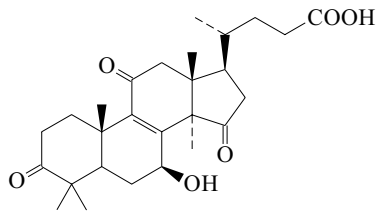


$C_{10}H_{12}O_3$ 180.203
Constit. of saffron, *Crocus sativus*. Yellow solid. Mp 107-108°.

Zarghami, N.S. *et al., Phytochemistry*, 1971, **10**,

2755-2761

7-Hydroxy-25,26,27-trinor-3,11,15-trioxo-8-lanosten-24-oic acid H-814



$C_{27}H_{38}O_6$ 458.594

7β-*form* [95311-94-7]

Lucidenic acid A

Metab. of *Ganoderma lucidum* (reishi). Needles (EtOAc). Mp 194-195°. $[\alpha]_D^{24}$ +173 (c, 0.2 in $CHCl_3$).

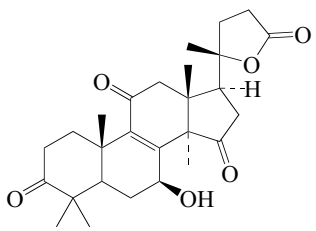
Nishitoba, T. *et al., Agric. Biol. Chem.*, 1984, **48**, 2905; 1985, **49**, 1793 (*isol, pmr, cmr*)

Wu, T.-S. *et al., J. Chin. Chem. Soc. (Taipei)*, 1997, **44**, 157-161 (*isol, pmr, cmr, cryst struct*)

7-Hydroxy-25,26,27-trinor-3,11,15-trioxo-8-lanosten-24,20-olide H-815

[173268-82-1]

Ganolactone A



$C_{27}H_{36}O_6$ 456.578

Mp 294-296°. $[\alpha]_D^{20}$ +6 (c, 0.1 in $CHCl_3$). λ_{max} 256 (log ϵ 3.72) (MeOH).

(7β, 20*S*)-*form*

Lucidenolactone

Metabolite of *Ganoderma lucidum* (reishi). Cryst. (Me_2CO/MeOH). $[\alpha]_D^{23}$ +85.4 (c, 0.024 in $CHCl_3$). Mp>300° λ_{max} 256 (log ϵ 3.72) (MeOH).

Wang, F.S. *et al., Chin. Chem. Lett.*, 1995, **6**, 1049-1050 (*isol, pmr, cmr*)

Wang, F.S. *et al., Yaoxue Xuebao*, 1996, **31**, 200-204 (*isol, pmr, cmr*)

Wu, T.-S. *et al., J. Chin. Chem. Soc. (Taipei)*, 1997, **44**, 157-161 (*isol, pmr, cmr, cryst struct*)

11-Hydroxy-9,15,16-trioxooctadecanoic acid, 9CI H-816

Caprifolonic acid

$H_3CCH_2COCO(CH_2)_3CH(OH)CH_2CO(CH_2)_7COOH$

$C_{18}H_{30}O_6$ 342.431

(-)-*form* [38076-39-0]

Isol. from the seeds of *Sambucus nigra* (elderberry). Viscous yellow oil. d_{24}^{24} 1.05. $[\alpha]_D^{20}$ -32.4 (c, 0.2 in EtOH). n_D^{24} 1.4870.

Gigienova, E. *et al., Khim. Prir. Soedin.*, 1972, **8**, 3; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 1 (*isol, ir, uv, pmr*)

Hydroxytriphenylstannane, 9CI H-817

[76-87-9]

Triphenyltin hydroxide. Fentin hydroxide, BSI. Du-Ter

Ph_3SnOH

$C_{18}H_{16}OSn$ 367.034

Agricultural fungicide for potatoes, sugar beet, pecans and peanuts. White powder. Mod. sol. most org. solvs., v. spar. sol. H_2O. Mp 116-120° dec.

▶ Highly toxic orally. LD_{50} (rat, orl) 171 mg/kg. WH8575000

Ac: [900-95-8] *(Acetyloxy)triphenylstannane. Triphenyltin acetate. Brestan. Fentin acetate*

$C_{20}H_{18}O_2Sn$ 409.071

Nonsystemic fungicide. White cryst. Mp 121-123°.

▶ LD_{50} (rat, orl) 125 mg/kg. WH6650000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 749B; 750A (*nmr*)

U.S. Pat., 1960, 3 140 977; *CA*, **61**, 11273h

Ford, B.F.E. *et al., J. Organomet. Chem.*, 1969, **19**, 23 (*deriv, Mössbauer, ir*)

McFarlane, W. *et al., J. Organomet. Chem.*, 1972, **40**, C17 (*nmr*)

Brown, J.M. *et al., J.C.S. Dalton*, 1972, 338 (*ir, Mössbauer*)

Japan. Pat., 1976, 76 141 847; *CA*, **86**, 171602c (*synth*)

Japan. Pat., 1977, 77 12 149; *CA*, **87**, 39660m (*synth*)

Japan. Pat., 1977, 77 113 950; *CA*, **88**, 37970j (*synth*)

Glidewell, C. *et al., Acta Cryst. B*, 1978, **34**, 129 (*struct*)

Molloy, K.C. *et al., J. Organomet. Chem.*, 1984, **267**, 237 (*deriv, cryst struct, Mössbauer*)

Pesticide Manual, 11th edn., 1997, No. 317

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABX250; HON000

4-Hydroxy-16,18-tritriacontanedione H-818

[97191-41-8]

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_{11}CH(OH)CH_2CH_2CH_3$

$C_{33}H_{64}O_3$ 508.867

Constit. of the leaf waxes of *Eucalyptus globulus* (Tasmanian blue gum).

Osawa, T. *et al., J. Agric. Food Chem.*, 1985, **33**, 777 (*occur*)

18-Hydroxy-16-tritriacontanone H-819

[97191-42-9]

$H_3C(CH_2)_{14}CH(OH)CH_2CO(CH_2)_{14}CH_3$

$C_{33}H_{66}O_2$ 494.883

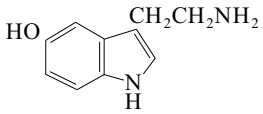
Constit. of the leaf waxes of *Eucalyptus globulus* (Tasmanian blue gum).

Osawa, T. *et al., J. Agric. Food Chem.*, 1985, **33**, 777 (*occur*)

5-Hydroxytryptamine H-820

[50-67-9]

*3-(2-Aminoethyl)-1*H*-indol-5-ol, 9CI. 3-(2-Aminoethyl)-5-hydroxyindole. Anthemovister. Enteramine. Hippophaine. **Serotonin**. Thrombocytin. Thrombotonin. 5HT*



$C_{10}H_{12}N_2O$ 176.218

Isol. from bananas and other fruits. Also from cotton (*Gossypium hirsutum*). pK_{a1} 1; pK_{a2} 4.52; pK_{a3} 15 (20°). Log P 0.61 (calc).

▶ LD_{50} (mus, orl) 60 mg/kg. Exp. reprod. and teratogenic effects. NM2450000

Hydrochloride: [153-98-0]

[21591-86-6]

Sol. H_2O. Mp 167-168°. Light-sensitive. Aq. solns. stable at acid pH.

N^b-*(4-Hydroxy*-E-*cinnamoyl):* [68573-24-0] N^b-p-*Coumaroylserotonin*. ***Ipobscurine A***

$C_{19}H_{18}N_2O_3$ 322.363

Alkaloid from *Carthamus tinctorius* (safflower).

N^b-*(4-Hydroxy*-E-*cinnamoyl),* O-*β-D-glucopyranoside:* [76423-56-8]

$C_{25}H_{28}N_2O_8$ 484.505

Alkaloid from *Carthamus tinctorius* (safflower). Needles. Mp 240-242°. $[\alpha]_D^{25}$ -14.9 (c, 0.7 in MeOH).

N^b-*(4-Hydroxy*-Z-*cinnamoyl):* N^6-cis-p-*Coumaroylserotonin*

$C_{19}H_{18}N_2O_3$ 322.363

Constit. of dried *Amorphophallus konjac* (devil's tongue). Amorph. powder. Mp 205-206°. λ_{max} 277 (log ϵ 4.4) (MeOH aq.).

N^b-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl):* [68573-23-9] N^b-*(*E*)-Feruloylserotonin*. ***Moschamine***

$C_{20}H_{20}N_2O_4$ 352.389

Alkaloid from *Carthamus tinctorius* (safflower). Needles. Mp 115-117°. Isol. with *Z*-isomer as a mixt..

N^b-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl),* O-*β-D-glucopyranoside:*

$C_{26}H_{30}N_2O_9$ 514.531

Alkaloid from *Carthamus tinctorius* (safflower). Needles. Mp 143-145°. $[\alpha]_D^{25}$ -8.8 (c, 1.2 in MeOH).

N^b-*Me:* [1134-01-6]

[15558-50-6] ***5-Hydroxy-N$^{\omega}$-methyltryptamine***. *3-(2-Methylaminoethyl)-1*H*-indol-5-ol, 9CI*

$C_{11}H_{14}N_2O$ 190.244

Isol. from *Citrus unshiu* (satsuma mandarin). Mp 153-156° (as oxalate).

Hamlin, K.E. *et al., J.A.C.S.*, 1951, **73**, 5007 (*synth, uv*)

Speeter, H.E. *et al., J.A.C.S.*, 1951, **73**, 5515 (*synth*)

Asero, B. *et al., Annalen*, 1952, **576**, 69 (*synth, uv*)

Bowden, K. *et al., Nature (London)*, 1954, **174**, 925 (*isol*)

Abramovitch, R.A. *et al., Chem. Ind. (London)*, 1955, 1255 (*synth*)

Stoll, A. *et al., Helv. Chim. Acta*, 1955, **38**, 1452 (*N-Me*)

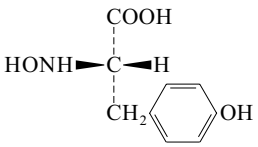
Mathias, A.P. *et al., Nature (London)*, 1957, **180**, 658 (*isol, occur*)

Thewalt, U. *et al., Acta Cryst. B*, 1972, **28**, 82 (*cryst struct*)

Couch, M.W. *et al., Anal. Biochem.*, 1972, **50**, 612 (*ms*)

Biagini, S. *et al., J.C.S. Faraday 2*, 1983, **79**, 491 (*pmr, cmr*)
Borgulya, J. *et al., Synthesis*, 1983, 29 (*deriv*)
Eich, E. *et al., Planta Med.*, 1986, **52**, 523 (*Ipobscurine A*)
Nishida, R. *et al., Experientia*, 1987, **43**, 342 (*5-Hydroxy-N$^{\omega}$-methyltryptamine*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1411
Zhang, H.L. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1910-1914 (*isol, cinnamides*)
Somei, M. *et al., Heterocycles*, 1997, **46**, 91-94 (*synth*)
Sarker, S.D. *et al., Nat. Prod. Lett.*, 1997, **9**, 189-199 (*Moschamines*)
Niwa, T. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 2269-2271 (*N-coumaroylserotonin*)
Somei, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 87-96 (*synth*)

N-Hydroxytyrosine, 9CI H-821



(*S*)-*form*

$C_9H_{11}NO_4$ 197.19

(*S*)-*form* [64448-49-3]
L-form
Biosynthetic intermediate of dhurrin in *Sorghum bicolor* (sorghum).

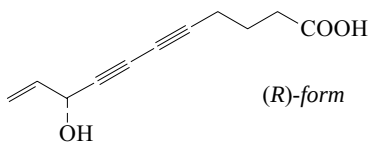
(±)-*form* [63577-99-1]
Cryst. (H_2O). Mp 226-228° dec.

[42429-16-3]

Kaminski, K. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1973, **47**, 653 (*synth*)
Moeller, B.L. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 343 (*synth*)
Moeller, B.L. *et al., J. Biol. Chem.*, 1980, **255**, 3049 (*occur*)
Cutler, A.J. *et al., J. Biol. Chem.*, 1981, **256**, 4253 (*occur*)

9-Hydroxy-10-undecene-5,7-diynoic acid H-822

Helianthenic acid D



(*R*)-*form*

$C_{11}H_{12}O_3$ 192.214

(*R*)-*form* [152340-30-2]

O-*β-D-Glucopyranoside, Me ester:* [152141-44-1]
$C_{18}H_{24}O_8$ 368.383
Constit. of *Helianthus tuberosus* (Jerusalem artichoke). Amorph. solid. $[\alpha]_D^{23}$ -40 (c, 0.03 in MeOH).

Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1492

5-Hydroxy-8-undecenoic acid H-823

H_3CCH_2CH
$=CHCH_2CH_2CH(OH)(CH_2)_3COOH$

$C_{11}H_{20}O_3$ 200.277

(*Z*)-*form*
Spontaneously lactonises.

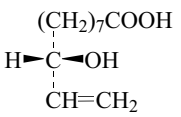
Lactone: [68959-28-4]

[32764-99-1, 259210-34-9] *6-(3-Hexenyl)tetrahydro-2H-pyran-2-one, 9CI, 8CI. FEMA 3758*
$C_{11}H_{18}O_2$ 182.262
Flavouring ingredient. Liq. with milky, buttery note. d_4^{25} 0.98. Bp_{12} 166-166.5°.

Rosenmund, K.W. *et al., Chem. Ber.*, 1961, **94**, 2401-2405 (*synth*)
Watanabe, S. *et al., Yukagaku*, 1980, **29**, 196-198 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 370 (*props, use*)
Adams, T.B. *et al., Food Chem. Toxicol.*, 1998, **36**, 249-278 (*tox*)

9-Hydroxy-10-undecenoic acid H-824

Corchorifatty acid E

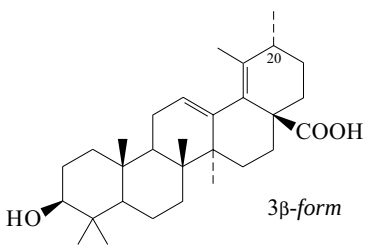


$C_{11}H_{20}O_3$ 200.277

(*S*)-*form*
Constit. of *Corchorus olitorius* (Jew's mallow). Oil. $[\alpha]_D^{24}$ -14.2 (c, 0.7 in $CHCl_3$) (approx. 57% op).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1008-1014 (*isol, ir, pmr, cmr*)

3-Hydroxy-12,18-ursadien-28-oic acid H-825



3β-*form*

$C_{30}H_{46}O_3$ 454.692

3β-*form* [14021-14-8]
Randialic acid B. *18-Dehydroursolic acid. 19-Dehydroursolic acid (incorr.). Vanguerolic acid*
Granular cryst. (MeOH). Mp 256-257°. $[\alpha]_D$ +213. Once thought to be a taraxastane.

3-O-α-L-Arabinopyranoside: [356785-74-5]
$C_{35}H_{54}O_7$ 586.807
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Amorph. solid. $[\alpha]_D^{25}$ +112 (c, 0.1 in MeOH).

3-O-β-D-Xylofuranoside: [85344-31-6] ***Ilexolide A***
$C_{35}H_{54}O_7$ 586.807

3-O-β-D-Xylopyranoside, 28-O-β-D-glucopyranosyl ester: [138995-23-0] ***Ilexsaponin B***
$C_{41}H_{64}O_{12}$ 748.949

3-O-[α-L-Rhamnopyranosyl-(1→?)-α-L-rhamnopyranoside]: ***Knautioside B***
$C_{42}H_{66}O_{11}$ 746.977
Mp 240-244°. $[\alpha]_D$ -13 (Py).

3-O-[D-Glucopyranosyl-(1→?)-L-arabinoside], 28-O-[D-xylosyl-(1→?)-D-glucosyl] ester: ***Knautioside A***
$C_{52}H_{82}O_{21}$ 1043.207
Mp 208-213°. $[\alpha]_D$ -10 (Py).

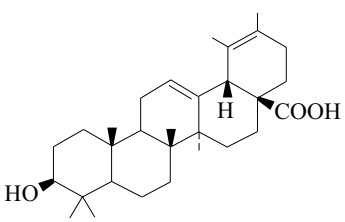
3-O-[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside], 28-O-β-D-glucopyranosyl ester: [354537-14-7] ***Latifoloside K***
$C_{53}H_{84}O_{21}$ 1057.234
Powder. $[\alpha]_D^{25}$ +0.74 (c, 0.78 in MeOH).

Me ester: [14021-15-9]
Mp 165-166°. $[\alpha]_D$ +88.

3-Ketone: [273223-69-1] ***3-Oxo-12,18-ursadien-28-oic acid***
$C_{30}H_{44}O_3$ 452.676
Constit. *Pyrus communis* (pear). Cryst. ($CHCl_3$/MeOH). Mp 90-91°. $[\alpha]_D^{35}$ +165 (c, 0.15 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1962, 5163 (*Vanguerolic acid*)
Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688 (*ms*)
Tandon, J.S. *et al., Indian J. Chem.*, 1966, **4**, 483 (*Randialic acid B*)
Surkova, L.N. *et al., Khim. Prir. Soedin.*, 1975, **11**, 661; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 698 (*Knautiosides*)
Qureshi, M.A. *et al., Planta Med.*, 1977, **32**, 229 (*isol*)
Zhang, S. *et al., CA*, 1984, **100**, 121395z (*cryst struct*)
Zeng, L. *et al., CA*, 1984, **101**, 226825p (*Ilexolide A*)
Ali, M. *et al., Phytochemistry*, 1990, **29**, 3601 (*ketone*)
Jiang, Z. *et al., CA*, 1992, **117**, 44518p (*Ilexsaponin B*)
Younes, M.E. *et al., Egypt. J. Chem.*, 1999, **42**, 573-586; *CA*, **133**, 28459v (*ketone*)
Huang, J. *et al., Chem. Pharm. Bull.*, 2001, **49**, 765-767 (*Latifoloside K*)
Mimaki, Y. *et al., Phytochemistry*, 2001, **57**, 773-779 (*3-arabinopyranoside*)

3-Hydroxy-12,19-ursadien-28-oic acid H-826



$C_{30}H_{46}O_3$ 454.692

3β-*form* [6812-98-2]
Tomentosolic acid. *19-Dehydroursolic acid. Sanguisorbigenin*
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Cryst. (MeOH). Mp 284.5-286° (*in vacuo*). $[\alpha]_D$ +18 (c, 1 in $CHCl_3$). Prob. artifact.

Me ester: [23660-55-1]
Cryst. (MeOH). Mp 205-207°. $[\alpha]_D$ +15 (c, 0.2 in $CHCl_3$).

Ac:
Cryst. ($CHCl_3$/MeOH). Mp 318-323°. $[\alpha]_D$ +6 (c, 0.54 in $CHCl_3$).

3-Ketone:3-Oxo-12,19-ursadien-28-oic

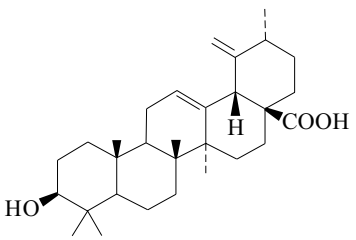
acid. ***Tomentosonic acid***
$C_{30}H_{44}O_3$ 452.676

3-Ketone, Me ester:
Platelets ($CHCl_3$/MeOH). Mp 208-212° dec. $[\alpha]_D$ +45 (c, 0.5 in $CHCl_3$).

[6805-65-8]

Barton, D.H.R. *et al., J.C.S.*, 1962, 5163
Brieskorn, C.H. *et al., Chem. Ber.*, 1967, **100**, 1252

3-Hydroxy-12,19(29)-ursadien-28-oic acid H-827



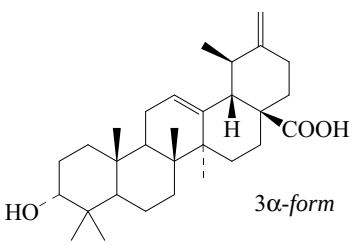
$C_{30}H_{46}O_3$ 454.692

3β-*form* [252189-21-2]
19(29)-Dehydroursolic acid
Cryst. Mp 226-228°. $[\alpha]_D^{22}$ +48 (c, 0.2 in MeOH).

3-O-α-L-Arabinopyranoside, 28-O-β-D-glucopyranosyl ester: [356785-72-3]
$C_{41}H_{64}O_{12}$ 748.949
Constit. of *Sanguisorba officinalis* (burnet bloodwort). Amorph. solid. $[\alpha]_D^{25}$ +12 (c, 0.1 in MeOH).

Brieskorn, C.H. *et al., Tet. Lett.*, 1972, 1515
Deng, J.-Z. *et al., J. Nat. Prod.*, 1999, **62**, 1624-1626 (*isol, pmr, cmr*)
Mimaki, Y. *et al., Phytochemistry*, 2001, **57**, 773-779 (*Sanguisorba officinalis saponin*)

3-Hydroxy-12,20(30)-ursadien-28-oic acid H-828



$C_{30}H_{46}O_3$ 454.692

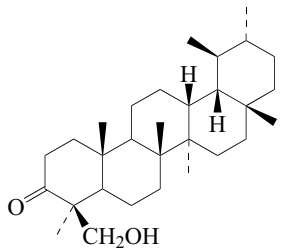
3α-*form* [260541-77-3]
3-Epimicromeric acid

3β-*form* [22477-85-6]
Micromeric acid
Constit. of lavender.

Ac, Me ester:
Mp 181-183°. $[\alpha]_D^{20}$ +127.

Bermejo, J. *et al., Tet. Lett.*, 1967, 4649 (*isol*)
Arteaga, J.M. *et al., An. Quim.*, 1970, **66**, 181 (*isol*)
Miyaichi, Y. *et al., Nat. Med. (Tokyo)*, 1999, **53**, 237-241; *CA*, **132**, 205458w (*3-Epimicromeric acid*)

24-Hydroxy-3-ursanone H-829

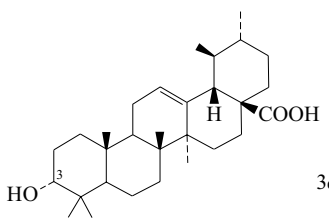


$C_{30}H_{50}O_2$ 442.724

*24-(2-Hydroxy-3*E*-hexen-2-yl) ether:*
[189156-40-9] ***Momordicilin***
$C_{36}H_{60}O_3$ 540.868
Constit. of *Momordica charantia* (bitter melon). Needles. Mp 170-171°. $[\alpha]_D^{27}$ +42 (c, 0.19 in $CHCl_3$). Contains an unusual hemiacetal.

Begum, S. *et al., Phytochemistry*, 1997, **44**, 1313-1320 (*isol, pmr, cmr, ms*)

3-Hydroxy-12-ursen-28-oic acid H-830



$C_{30}H_{48}O_3$ 456.707

3β-*form* [77-52-1]
Ursolic acid. *Micromerol. Formosolic acid. Forucosolic acid. Bungeolic acid. Prunol. Urson. Malol*
Found in wax of apples, pears and other fruits. V. widely distributed in plants. Cryst. (Et_2O). Mp 291°. $[\alpha]_D$ +66 (EtOH). Log P 8.59 (uncertain value) (calc). Identity of Formosolic (?Forucosolic) acid not clear from abstract.

3-O-β-L-Arabinopyranoside: [32180-34-0] ***Sanguisorbin B***
$C_{35}H_{56}O_7$ 588.823
Constit. of burnet bloodwort (*Sanguisorba officinalis*). Cryst. Mp 266-267°.

3-O-β-L-Arabinopyranoside, 28-O-(3-O-acetyl-β-D-glucopyranosyl) ester: [33055-20-8] ***Sanguisorbin E***
$C_{43}H_{68}O_{13}$ 793.002
Constit. of burnet bloodwort (*Sanguisorba officinalis*). Cryst. Mp 190-192°.

3-O-β-D-Glucuronopyranoside, 28-O-β-D-glucopyranosyl ester: [117804-09-8] ***Cynarasaponin C***
$C_{42}H_{66}O_{14}$ 794.975
Constit. of globe artichoke (*Cynara cardunculus*) root. Powder + $1^1/_2H_2O$ (as Me ester). $[\alpha]_D^{21}$ -7.5 (c, 0.93 in MeOH) (Me ester).

3-O-[β-D-Glucopyranosyl-(1→3)-α-L-arabinopyranoside], 28-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [164178-28-3] ***Matesaponin 3***. *Araliasaponin X*
$C_{53}H_{86}O_{22}$ 1075.249
Constit. of maté leaf (*Ilex paraguariensis*). Powder. $[\alpha]_D$ +4.8 (c, 0.46 in Py).

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-xylopyranoside]: [169303-86-0]
$C_{41}H_{66}O_{12}$ 750.965
Constit. of *Majorana hortensis* (sweet majoram). Cryst. (MeOH). Mp 286°. $[\alpha]_D^{25}$ +19.7 (c, 1 in Py).

3-O-[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside], 28-O-β-D-glucopyranosyl ester: [164178-27-2] ***Matesaponin 2***
$C_{53}H_{86}O_{21}$ 1059.25
Constit. of maté leaf (*Ilex paraguariensis*). Powder. $[\alpha]_D^{23}$ +6.7 (c, 0.7 in Py).

3-O-[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside], 28-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [164178-29-4] ***Matesaponin 4***
$C_{59}H_{96}O_{26}$ 1221.392
Constit. of maté leaf (*Ilex paraguariensis*). Powder. $[\alpha]_D^{23}$ -8.8 (c, 1.2 in Py).

3-O-[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside], 28-O-[β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [178330-60-4] ***Matesaponin 5***
$C_{65}H_{106}O_{31}$ 1383.534
Constit. of maté leaf (*Ilex paraguariensis*). Amorph. powder. $[\alpha]_D^{18}$ +1.5 (c, 1.9 in MeOH).

Ac: [7372-30-7] ***Acetylursolic acid***
$C_{32}H_{50}O_4$ 498.745
Isol. from various plants, e.g. *Leptospermum scoparium* (red tea). Cryst. (EtOH aq.). Mp 285°. $[\alpha]_D^{20}$ +71.5 ($CHCl_3$).

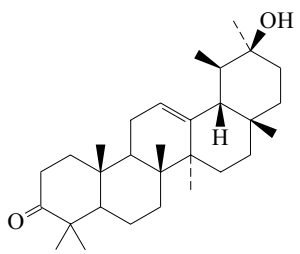
3-Ketone: [6246-46-4] *3-Oxo-12-ursen-28-oic acid*. ***Ursonic acid***
$C_{30}H_{46}O_3$ 454.692
Constit. of dammar resin and blackberry whole plant. Cryst. (MeOH). Mp 270-275° dec. $[\alpha]_D$ +80 (c, 0.9 in $CHCl_3$).

[74984-66-0, 117804-17-8, 117804-18-9, 117804-25-8]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 595A (*nmr*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1945, **28**, 199 (*struct*)
Mills, J.S. *et al., J.C.S.*, 1955, 3132 (*Ursonic acid*)
Huneck, S. *et al., J. Prakt. Chem.*, 1968, **38**, 233 (*ms*)
Bukharov, V.G. *et al., Izv. Akad. Nauk Kaz. SSR, Ser. Khim.*, 1970, 171; 2402 (*Sanguisorbins, Empetroside C*)
Huneck, S. *et al., Phytochemistry*, 1971, **10**, 3279 (*isol*)
Mezzetti, T. *et al., Planta Med.*, 1971, **20**, 244 (*struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2015 (*occur*)
Seo, S. *et al., Chem. Comm.*, 1975, 270; 954 (*biosynth, pmr*)
Seo, S. *et al., Tet. Lett.*, 1975, 7 (*cmr*)
Romeo, G. *et al., Org. Magn. Reson.*, 1977, **9**, 29 (*pmr*)

Yankov, L.K. *et al., CA*, 1980, **93**, 150418b (*Formosolic acid*)
Mukherjee, K.S. *et al., Phytochemistry*, 1982, **21**, 2416 (*isol*)
Johns, S.R. *et al., Aust. J. Chem.*, 1983, **36**, 2537 (*cmr*)
Tomita, Y. *et al., Chem. Comm.*, 1985, 1087 (*biosynth*)
Seo, S. *et al., Chem. Comm.*, 1986, 1141 (*biosynth*)
Poehland, B.L. *et al., J. Nat. Prod.*, 1987, **50**, 706 (*Ursonic acid, pmr, cmr*)
Shimizu, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2466 (*Cynarasaponins*)
Simon, A. *et al., Acta Cryst. C*, 1992, **48**, 726 (*cryst struct*)
Hasanean, H.A. *et al., Pharm. Pharmacol. Lett.*, 1992, **1**, 115 (*isol, pmr, ms*)
Tomita, Y. *et al., Phytochemistry*, 1994, **35**, 121 (*biosynth*)
Sohn, K. *et al., Cancer Lett. (Shannon, Irel.)*, 1995, **94**, 213-218 (*Ursolic acid, activity*)
Yadava, R.N. *et al., Fitoterapia*, 1995, **66**, 185 (*glucosylxyloside*)
Gosmann, G. *et al., J. Nat. Prod.*, 1995, **58**, 438 (*Matesaponins*)
Kraemer, K.H. *et al., Phytochemistry*, 1996, **42**, 1119 (*Matesaponin 5*)
Kashiwada, Y. *et al., J. Nat. Prod.*, 1998, **61**, 1090-1095 (*Ursolic acid, activity*)
Ahn, K.-S. *et al., Planta Med.*, 1998, **64**, 468-470 (*Ursolic acid, activity*)
Byung, S.-M. *et al., Planta Med.*, 1999, **65**, 374-375 (*Ursolic acid, activity*)
Alves, J.S. *et al., Magn. Reson. Chem.*, 2000, **38**, 201-206 (*pmr, cmr*)

20-Hydroxy-12-ursen-3-one H-831

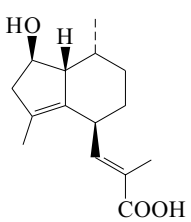


$C_{30}H_{48}O_2$ 440.708

20β-*form* [150148-82-6]
Rofficerone
Constit. of *Rosmarinus officinalis* (rosemary). Amorph. $[\alpha]_D^{20}$ +107.3 (c, 0.4 in $CHCl_3$).

Ganeva, Y. *et al., Planta Med.*, 1993, **59**, 276 (*isol, pmr, cmr*)

2-Hydroxy-4,7(11)-valerenadien-12-oic acid H-832



$C_{15}H_{22}O_3$ 250.337
Cryst. (Et_2O). Mp 169-169.5°.

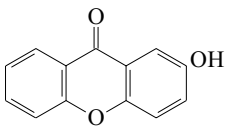
(1β,2β,10α)-*form* [1619-16-5]
Valerenolic acid
Constit. of the roots of *Valeriana officinalis* (valerian). $[\alpha]_D^{20}$ -93.8 (c, 0.79 in EtOH).

Ac: ***Acetylvalerenolic acid***
$C_{17}H_{24}O_4$ 292.374
Constit. of *Valeriana officinalis* (valerian). Oil (as Me ester). $[\alpha]_D^{20}$ -61 (c, 1.75 in EtOH) (Me ester).

Stoll, A. *et al., Annalen*, 1957, **603**, 158 (*isol*)
Birnbaum, G.I. *et al., J.O.C.*, 1978, **43**, 272 (*cryst struct*)

2-Hydroxyxanthone H-833

[1915-98-6]
*2-Hydroxy-9*H*-xanthen-9-one, 9CI*



$C_{13}H_8O_3$ 212.204
Constit. of *Hypericum* spp., *Mammea americana* (mamey). Yellow needles. Mp 241-241.5°.

Ac: [2007-05-8]
$C_{15}H_{10}O_4$ 254.242
Cryst. ($CHCl_3$/hexane). Mp 164.8-165.2°.

Me ether: [1214-20-6] *2-Methoxyxanthone*
$C_{14}H_{10}O_3$ 226.231
Constit. of *Hypericum* spp. and *Mammea americana* (mamey). Cryst. ($CHCl_3/C_6H_6$). Mp 134° (129°).

Scheinmann, F. *et al., Tetrahedron*, 1962, **18**, 853 (*uv*)
Finnegan, R.A. *et al., J. Pharm. Sci.*, 1965, **54**, 633 (*isol, synth*)
Paquette, L.A. *et al., J.O.C.*, 1966, **31**, 1232 (*synth*)
Crombie, L. *et al., Tet. Lett.*, 1966, 145 (*isol, deriv*)
Gottlieb, O.R. *et al., Phytochemistry*, 1970, **9**, 447; 2537 (*uv, isol*)
Steinberg, N.G. *et al., J. Het. Chem.*, 1972, **9**, 1181 (*synth, ms*)
Finnegan, R.A. *et al., J.C.S. Perkin 1*, 1972, 1896 (*isol*)
Mahfouz, N.M.A. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1990, **323**, 163 (*synth*)
Han, Y. *et al., J.O.C.*, 1996, **61**, 6326 (*synth, pmr*)
Gnerre, C. *et al., Helv. Chim. Acta*, 2001, **84**, 552-570 (*synth, ir, pmr, cmr*)

4-Hydroxyxanthone H-834

[14686-63-6]
*4-Hydroxy-9*H*-xanthen-9-one, 9CI*

$C_{13}H_8O_3$ 212.204
From seeds of *Mammea americana* (mamey). Needles (EtOH aq.). Mp 245-246°.

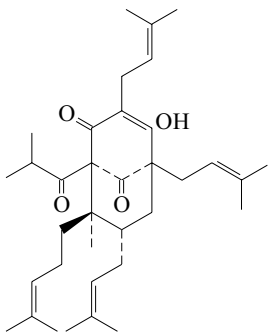
Ac: [87504-15-2]
$C_{15}H_{10}O_4$ 254.242
Cryst. (EtOH aq.). Mp 137-138°.

Me ether: [6702-58-5] *4-Methoxyxanthone*
$C_{14}H_{10}O_3$ 226.231
Needles (EtOH). Mp 173°.

Ullmann, F. *et al., Ber.*, 1905, **38**, 2118 (*synth*)
Finnegan, R.A. *et al., J.C.S. Perkin 1*, 1972, 1896 (*isol*)
Akhtar, Z.M. *et al., Org. Mass Spectrom.*, 1973, **7**, 647 (*ms*)
Mizutani, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1596 (*uv*)
Jojima, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 198 (*synth*)
Cervena, I. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 1307 (*synth*)
Horne, S. *et al., J.O.C.*, 1990, **55**, 4520 (*synth*)
Coelho, P.J. *et al., Helv. Chim. Acta*, 2001, **84**, 552-570 (*synth, pmr*)

Hyperforin H-835

[11079-53-1]

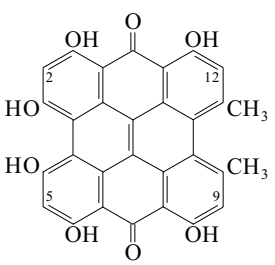


$C_{35}H_{52}O_4$ 536.793
Constit. of *Hypericum perforatum* (St John's Wort). Cryst. Sol. C_6H_6. Mp 79-80°. $[\alpha]_D^{18}$ +41 (EtOH). λ_{max} 278 (ε 8400) (EtOH/HCl) (Derep). λ_{max} 298 (ε 12000) (EtOH/NaOH) (Derep). λ_{max} 278 (ε 8200); 298 (ε 11000) (EtOH) (Berdy).

Gurevich, A.I. *et al., Antibiotiki (Moscow)*, 1971, **16**, 510; *CA*, **75**, 95625 (*isol, props*)
Bystrov, N.S. *et al., Tet. Lett.*, 1975, **16**, 2791
Bystrov, N.S. *et al., Bioorg. Khim.*, 1978, **4**, 791 (*struct*)
Brondz, I. *et al., Tet. Lett.*, 1982, **23**, 1299 (*cryst struct*)
Linde, K. *et al., Br. Med. J.*, 1996, **313**, 253-258 (*clin trial*)
Schempp, C.M. *et al., Lancet*, 1999, **i**, 2129 (*activity*)
Moore, L.B. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 7500-7502 (*pharmacol*)

Hypericin H-836

[548-04-9]
1,3,4,6,8,13-Hexahydroxy-10,11-dimethylphenanthro[1,10,9,8-opqra]perylene-7,14-dione, 9CI. Mycoporphyrin. Hypericum red



$C_{30}H_{16}O_8$ 504.452
The 7,14-dioxo tautomer (illus.) is the stable one. Several other tautomers have been obt. Numbering systems vary. Widespread in *Hypericum* spp. esp. *Hypericum perforatum* (St John's Wort). Solvated blue-black needles. Mp 300° (dec.). Log P 4.55 (calc). Yields cherry-

red soln. with red fluor. in org. bases λ_{max} 290 (ϵ 34000); 340 (ϵ 26000); 465 (ϵ 11500); 600 (ϵ 18500); 640 (ϵ 22500) (DMSO as potassium salt) (Derep). λ_{max} 384 (ϵ 12100); 446 (ϵ 12900); 472 (ϵ 13800); 509 (ϵ 10000); 546 (ϵ 24700); 589 (ϵ 43600) (MeOH as potassium salt) (Derep). λ_{max} 292 (ϵ 34000); 340 (ϵ 26500); 377 (ϵ 12000); 475 (ϵ 13500); 509 (ϵ 10000); 560 (ϵ 24000); 607 (ϵ 44000) (DMSO) (Derep). λ_{max} 508 ; 548 ; 590 (MeOH) (Berdy). λ_{max} 520 ; 559 ; 603 (Py) (Berdy).

Hexabenzoyl:
Yellow leaflets. Mp 304-305° (228°).

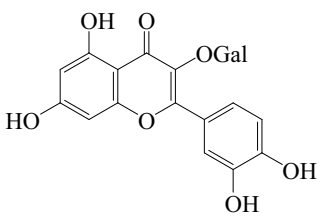
*2,5-Dichloro:**7,7′-**Dichlorohypericin***
$C_{30}H_{14}Cl_2O_8$ 573.341
Purple cryst. (AcOH). Mp 350°.

*2,5,9,12-Tetrachloro:**2,2′,7,7′-**Tetrachlorohypericin***
$C_{30}H_{12}Cl_4O_8$ 642.231
Purple cryst. (AcOH). Mp 350°.

Pace, N. *et al., J.A.C.S.*, 1941, **63**, 2570 (*struct*)
Brockmann, H. *et al., Chem. Ber.*, 1957, **90**, 2302; 1958, **91**, 81; 547 (*synth*)
Banks, H.J. *et al., Aust. J. Chem.*, 1976, **29**, 1509 (*isol*)
Rodewald, G. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 46 (*synth, bibl*)
Duran, N. *et al., Photochem. Photobiol.*, 1986, **43**, 677 (*rev, props*)
Meruelo, D. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1988, **85**, 5230 (*anti-HIV activity*)
Raser, L.N. *et al., Photochem. Photobiol.*, 1992, **56**, 157 (*Raman*)
Falk, H. *et al., Monatsh. Chem.*, 1993, **124**, 339 (*synth*)
Etzlstorfer, C. *et al., Monatsh. Chem.*, 1993, **124**, 923 (*tautom*)
Freeman, D. *et al., Chem. Comm.*, 1994, 891 (*cryst struct, ir*)
Cohen, P.A. *et al., J. Nat. Prod.*, 1995, **58**, 520 (*chloro derivs*)
Wynn, J.L. *et al., J. Phys. Chem.*, 1995, **99**, 4317 (*ir, Raman*)
Gutman, I. *et al., Monatsh. Chem.*, 1998, **129**, 481-486; 1999, **130**, 827 (*tautom*)
Gruszecka-Kowalik, E. *et al., Org. Prep. Proced. Int.*, 2000, **32**, 57-61 (*synth, pmr*)
Skalkos, D. *et al., Tetrahedron*, 2002, **58**, 4925-4929 (*pmr, conformn*)

Hyperin, 8CI H-837

[482-36-0]
3-O-β-D-Galactopyranosyloxy-3′,4′,5,7-tetrahydroxyflavone. Quercetin 3-galactoside. Hyperoside



$C_{21}H_{20}O_{12}$ 464.382
Occurs widely in plants, e.g. in apple peel and *Hypericum perforatum* (St John's wort). Yellow needles (EtOH). Mp 232-233° dec. $[\alpha]_D^{20}$ -83 (c, 0.2 in Py). Log P -2.92 (calc).

▶ DJ3009200

7-O-α-L-Rhamnopyranoside: [38784-81-5]
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Solanum* spp..

2″-Ac:Quercetin 3-(2-acetylgalactoside). ***2″-O-Acetylhyperin***
$C_{23}H_{22}O_{13}$ 506.419
Constit. of *Hypericum perforatum* (St John's wort). $[\alpha]_D^{20}$ -63.4 (c, 0.1 in MeOH).

6″-Ac, 7-O-α-L-rhamnopyranoside: [124027-51-6]
$C_{29}H_{32}O_{17}$ 652.562
Isol. from broad bean (*Vicia faba*) leaves.

6″-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl): [106915-93-9]
$C_{27}H_{28}O_{16}$ 608.509
Isol. from fruits of *Rubus* spp..

6″-O-(3,4-Dihydroxycinnamoyl): [84575-22-4] ***6″-Caffeoylhyperin***
$C_{30}H_{26}O_{15}$ 626.526
Isol. from *Hydrocotyle sibthorpioides* (water pennywort). Yellow needles. Mp 198-200°. $[\alpha]_D^{30}$ -19.5 (c, 0.12 in Py). λ_{max} 257 (27300); 340 (27900) (EtOH).

2″-O-β-D-Apiofuranosyl, 6″-O-α-L-rhamnopyranosyl: [165880-62-6]
$C_{32}H_{38}O_{20}$ 742.64
Constit. of cañihua (*Chenopodium pallidicaule*) flour.

2″-O-β-D-Xylopyranosyl: [83144-69-8]
$C_{26}H_{28}O_{16}$ 596.498
Isol. from horseradish (*Armoracia rusticana*) leaves.

2″-O-β-D-Glucopyranosyl: [95043-15-5]
$C_{27}H_{30}O_{17}$ 626.524
Isol. from pollen of *Corylus avellana* (filbert).

2″-O-[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranosyl], 6″-O-α-L-rhamnopyranosyl:
$C_{39}H_{50}O_{25}$ 918.809
Constit. of the leaves of *Maytenus aquifolium*. λ_{max} 266 ; 350 (MeOH).

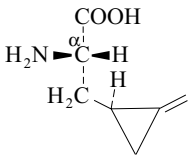
6″-O-[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranosyl]: [134953-93-8]
$C_{33}H_{40}O_{21}$ 772.666
Isol. from *Camellia sinensis* (tea).

[30113-33-8, 56508-10-2, 77133-40-5, 124086-76-6]

Larsen, L.M. *et al., Phytochemistry*, 1982, **21**, 1029 (*2″-xylosyl*)
Shigematsu, N. *et al., Phytochemistry*, 1982, **21**, 2156 (*6″-Caffeoylhyperin*)
Strack, D. *et al., Phytochemistry*, 1984, **23**, 2970 (*2″-glucosyl*)
Wald, B. *et al., Phytochemistry*, 1986, **25**, 2904 (*6-(4-carboxy-3-hydroxy-3-methylbutanoyl)*)
Tomas-Lorente, F. *et al., Phytochemistry*, 1989, **28**, 1993 (*6″-Ac 7-rhamnoside*)
Finger, A. *et al., Phytochemistry*, 1991, **30**, 2057 (*6″-glucosylrhamnosyl*)
Rastrelli, L. *et al., J. Agric. Food Chem.*, 1995, **43**, 2020 (*2″-apiosyl 6″-rhamnosyl*)
Vilegas, W. *et al., J. Agric. Food Chem.*, 1999, **47**, 403-406 (*2″-glucosylrhamnosyl 6-rhamnosyl*)
Datta, B.K. *et al., Fitoterapia*, 2000, **71**, 459-460 (*6″-Caffeoylhyperin*)
Jürgenliemk, G. *et al., Planta Med.*, 2002, **68**, 88-91 (*2″-Acetylhyperin*)

Hypoglycin A H-838

α-Amino-2-methylenecyclopropanepropanoic acid, 9CI. 2-Amino-3-(methylenecyclopropyl)propanoic acid. Hypoglycine



(αS,γS)-*form*

$C_7H_{11}NO_2$ 141.169Log P -2.12 (calc).

(αS,γS)-form [156-56-9]
L-form
Isol. from the unripe fruit of akee apple (*Blighia sapida*). Plates (MeOH aq.). Sol. H_2O. Mp 280-284°. $[\alpha]_D^{26}$ +11 (c, 1.0 in H_2O). $[\alpha]_D$ +49 (c, 1.0 in H_2O at pH2).

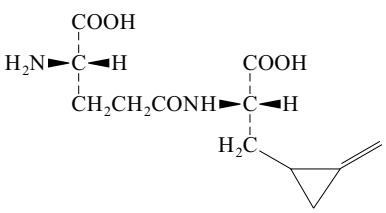
▶ Poisonous by ingestion (gastrointestinal, hypoglycaemic, CNS, death). LD_{50} (rat, orl) 98 mg/kg. Exp. reprod. and teratogenic effects. Suggested antidote glycine. GZ2215000

(αRS,γRS)-form
(±)-form
Leaflets (Me_2CO aq.). Mp 300°.

Hassall, C.H. *et al., Biochem. J.*, 1955, **60**, 334 (*isol*)
Hassall, C.H. *et al., J.C.S.*, 1959, 80 (*struct*)
Black, D.K. *et al., Tet. Lett.*, 1963, 1065 (*synth, abs config*)
Billington, D. *et al., Methods Enzymol.*, 1981, **72**, 610 (*rev*)
Sherratt, H.S.A. *et al., Trends Pharmacol. Sci.*, 1986, **7**, 186 (*tox*)
Stammer, H. *et al., Tetrahedron*, 1990, **46**, 2231 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 12837
Baldwin, J.E. *et al., Tetrahedron*, 1994, **50**, 12015 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MJP500

Hypoglycin B H-839

[502-37-4]
N-γ-Glutamyl-3-(methylenecyclopropyl)alanine, 9CI



$C_{12}H_{18}N_2O_5$ 270.285
Biologically active component of *Blighia sapida* (akee apple). Needles (Me_2CO aq.). Mp 194-195° (189-191°) Mp 200-207° (200-204°) (double Mp). pK_a 9.36. Log P -1.69 (calc).

▶ Exp. reprod. and teratogenic effects. AY6330000

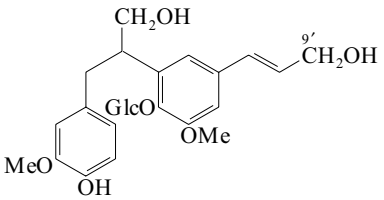
N-(2,4-Dinitrophenyl):
Cryst. ($EtOAc/CHCl_3$). Mp 170-172°.

Phenylthiohydantoin deriv.:
Needles (EtOH aq.). Mp 186-188°.

Hassall, C.H. *et al., J.C.S.*, 1960, 4112 (*struct, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HOW100

Icariside E_5 I-1

[126176-79-2]



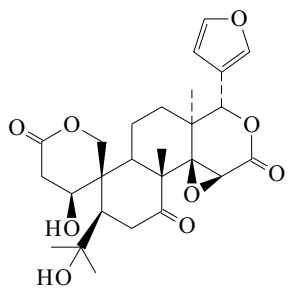
$C_{26}H_{34}O_{11}$ 522.548
Constit. of ripe fruits of *Capsicum annuum* var. *acuminatum*. Amorph. powder. $[\alpha]_D^{22}$ -118.8 (c, 1.04 in MeOH).

9′-Aldehyde: [166604-05-3] ***Ehletianol D***
$C_{26}H_{32}O_{11}$ 520.532
Amorph. powder. $[\alpha]_D^{20}$ -165 (c, 2.5 in MeOH).

Miyase, T. *et al., Phytochemistry*, 1989, **28**, 3483 (*isol, pmr, cmr*)
Yoshikawa, K. *et al., Phytochemistry*, 1995, **39**, 659 (*Ehletianol D*)
Iorizzi, M. *et al., J. Agric. Food Chem.*, 2001, **49**, 2022-2029 (*isol, pmr, cmr*)

Ichangin I-2

[10171-61-6]



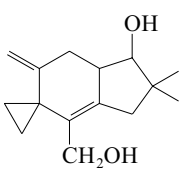
$C_{26}H_{32}O_9$ 488.533
Cryst. (MeOH). Mp 209-212°. $[\alpha]_{600}^{27}$ -78.6 (c, 0.09 in dioxan).

4-O-β-D-Glucopyranoside:
$C_{32}H_{42}O_{14}$ 650.675
Isol. from *Citrus limon* (lemon). Cryst. Mp 268-270° dec. $[\alpha]_D^{20}$ -0.7 (c, 0.72 in MeOH).

Dreyer, D.L. *et al., J.O.C.*, 1966, **31**, 2279
Matsubara, Y. *et al., Agric. Biol. Chem.*, 1990, **54**, 1143 (*deriv*)
Guthrie, N. *et al., ACS Symp. Ser.*, 2000, **758**, 164-174 (*activity*)

2,7(14)-Illudadiene-10,15-diol I-3

[141940-52-5]

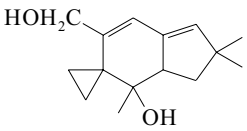


$C_{15}H_{22}O_2$ 234.338
Metab. of *Agrocybe aegerita*.

Stránsky, K. *et al., Coll. Czech. Chem. Comm.*, 1992, **57**, 590 (*isol, pmr, cmr*)

7,9-Illudadiene-3,14-diol I-4

[141940-51-4]



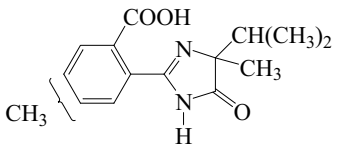
$C_{15}H_{22}O_2$ 234.338
Metab. of *Agrocybe aegerita*.

Stránsky, K. *et al., Coll. Czech. Chem. Comm.*, 1992, **57**, 590 (*isol, pmr, cmr*)

Imazamethabenz, ANSI, BSI, WSSA I-5

[100728-84-5]

[89318-81-0, 89318-82-1]
*2-[4,5-Dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-4(5)-methylbenzoic acid, 9CI. AC 263840. CL 263840*



$C_{15}H_{18}N_2O_3$ 274.319
Mixt. of regioisomers. Herbicidal metabolite of imazamethabenz-methyl. Acetolactate synthase inhibitor.

(±)-*form*
Me ester: [81405-85-8]

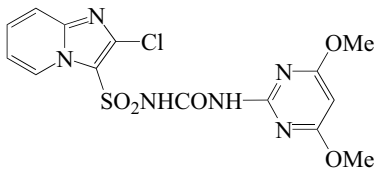
[69969-22-8, 69969-62-6] *Imazamethabenz-methyl. Assert®. AC 222293. Dagger. CL 222293*
$C_{16}H_{20}N_2O_3$ 288.346
Herbicide. Activity and selectivity are due to differential de-esterification to the active parent acid in target and crop species. Used on cereals and sunflowers, esp. against wild oats. Powder. Mp 143-151° (123-130°). pK_{a1} 2.9 (23.5°). Used commercially as a mixt. of 4- and 5-methyl isomers.

▶ LD_{50} (rat, orl) >5000 mg/kg.

Ger. Pat., 1979, 2 833 274; *CA*, **90**, 186949c (*Me ester, synth, activity*)
U.S. Pat., 1980, 4 188 487; *CA*, **104**, 104426a (*Me ester, synth, use*)
Shaner, D.L. *et al., Brighton Crop Prot. Conf. - Weeds*, 1982, 25 (*activity*)
Cardaciotto, S.J. *et al., Org. Mass Spectrom.*, 1987, **22**, 342-347 (*Me ester, ms*)
Rouchaud, J. *et al., Pestic. Biochem. Physiol.*, 1987, **27**, 24-29 (*activity*)
Hedlund, K. *et al., Weeds Weed Control*, 1987, **28**, 1-9 (*Me ester, use*)
Brown, M.A. *et al., Bull. Soc. Chim. Belg.*, 1992, **101**, 959-968 (*props*)
D'Ascenzo, G. *et al., Rapid Commun. Mass Spectrom.*, 1998, **12**, 1359-1365 (*detn, hplc*)
Pesticide Manual, 12th edn., 2000, No. 438

Imazosulfuron, BSI I-6

[122548-33-8]
*2-Chloro-*N*-[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]imidazo[1,2-a]pyridine-3-sulfonamide, 9CI. 1-(2-Chloroimidazo[1.2-a]pyridin-3-ylsulfonyl)-3-(4,6-dimethoxypyrimidin-2-yl) urea. Takeoff. TH 913*



$C_{14}H_{13}ClN_6O_5S$ 412.813
Powder. Mp 183-184° dec. pK_a 4.

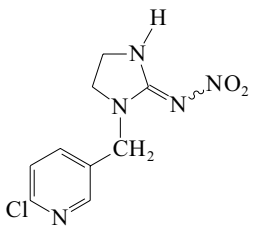
▶ LD_{50} (rat, orl) >5000 mg/kg.

Eur. Pat., 1989, 305 939, (*Takeda*); *CA*, **111**, 134183f (*synth, activity*)
Ishida, Y. *et al., J. Pestic. Sci. (Int. Ed.)*, 1993, **18**, 175-182 (*synth, use*)
Nagase, H. *et al., Agrochem. Jpn.*, 1994, **64**, 15-16 (*activity*)
Ishida, Y. *et al., Nippon Noyaku Gakkaishi*, 1996, **21**, 247-258 (*rev, activity, sar*)
Pesticide Manual, 11th edn., 1997, No. 416

Imidacloprid, BSI I-7

[105827-78-9]

[138261-41-3]
*1-[(6-Chloro-3-pyridinyl)methyl]-4,5-dihydro-*N*-nitro-1*H*-imidazol-2-amine, 9CI. Gaucho. Admire. Confidor*



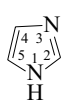
$C_9H_{10}ClN_5O_2$ 255.663
Insecticide. Cryst. Mp 143-144°.

▶ LD_{50} (rat, orl) 410 mg/kg. NJ0560000

Eur. Pat., 1986, 192 060; *CA*, **106**, 28848p (*synth, activity*)
Elbert, A. *et al., Br. Crop Prot. Conf. - Pests Dis., Proc.*, 1990, 21 (*activity*)
Pesticide Manual, 9th edn., 1991, No. 7242
Kagabu, S. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1216-1224 (*uv, ir, pmr, cmr, ms*)
Kagabu, S. *et al., J. Agric. Food Chem.*, 1998, **46**, 276-281 (*cryst struct*)

Imidazole, 9CI, 8CI I-8

[288-32-4]
Glyoxaline. Iminazole. 1,3-Diazole



$C_3H_4N_2$ 68.078
In general, imidazoles show $1H \Leftrightarrow 3H$ tautomerism. 4-Substituted imidazoles are indistinguishable from 5-substituted unless blocked by *N*-substitution. Isol. from the seeds of *Lens culinaris* (lentil). Also present in the seeds of other legumes: *Macrotyloma uniflorum* (horse

gram), *Psophocarpus tetragonolobus* (winged bean), *Vigna radiata* (mung bean). Sol. H_2O, EtOH, Et_2O, Me_2CO. Mp 88-90°. Bp 255°. pK_{a1} 7; pK_{a2} 14.52 (25°,acidic). Sublimes.

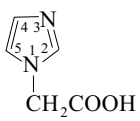
► LD_{50} (mus, orl) 880 mg/kg. NI3325000

[17009-90-4, 36877-68-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 611D; 612A; 619C; 625B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 75B; 75C; 77C; 86B; 88C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1483C (*ir*)
Org. Synth., Coll. Vol., 3, 1955, 471
Bredereck, H. *et al., Chem. Ber.*, 1964, **97**, 827 (*synth*)
Grimmett, M.R. *et al., Adv. Heterocycl. Chem.*, 1970, **12**, 103; 1980, **27**, 241 (*bibl*)
Pugmire, R.J. *et al., J.A.C.S.*, 1975, **95**, 2791 (*pmr, cmr*)
Jäckle, H. *et al., Biopolymers*, 1981, **20**, 65 (*uv*)
Ishii, H. *et al., Mikrochim. Acta*, 1983, **1**, 279
Hayman, A.R. *et al., Phytochemistry*, 1987, **26**, 3247 (*isol, pmr, ms*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2793-2794 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACO250; IAL000

1*H*-Imidazole-1-acetic acid, 9CI I-9

[22884-10-2]



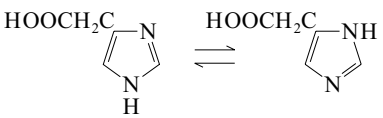
$C_5H_6N_2O_2$ 126.115
Isol. from *Coprinus atramentarius* (common ink cap). Cryst. (MeOH aq.). Mp 268-269° dec.

Et ester: [17450-34-9]
$C_7H_{10}N_2O_2$ 154.168
Mp 50°. Bp_{17} 160°.

Easson, A.P.T. *et al., J.C.S.*, 1932, 1806
List, P.H. *et al., Arzneim.-Forsch.*, 1960, **10**, 34-40 (*isol*)
Birkofer, L. *et al., Chem. Ber.*, 1960, **93**, 2804 (*synth*)
Sunjic, V. *et al., Croat. Chem. Acta*, 1969, **41**, 107-110 (*struct*)

1*H*-Imidazole-4(5)-acetic acid, 9CI I-10

[645-65-8]



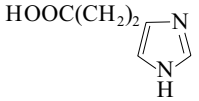
$C_5H_6N_2O_2$ 126.115
Isol. from various fungi, e.g. *Coprinus atramentarius* (common ink cap) and *Phallus impudicus* (common stinkhorn). Cryst. + $1H_2O$. Mp 222° dec.

[4200-48-0, 51718-81-1]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 491D (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 620C (*ir*)
Tabor, H. *et al., J.A.C.S.*, 1955, **77**, 505
Baddiley, J. *et al., J.C.S.*, 1958, 3743
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 260; 777; 1960, **319**, 17; 1962, **295**, 564 (*isol*)
Jones, G.P. *et al., J.C.S. Perkin 2*, 1976, 34 (*cryst struct*)
Okabe, N. *et al., Acta Cryst. C*, 1999, **55**, 1142-1144 (*cryst struct*)

1*H*-Imidazole-4(5)-propanoic acid, 9CI I-11

[1074-59-5]
3-(4-Imidazolyl)propionic acid



$C_6H_8N_2O_2$ 140.141
Isol. from the fungus *Coprinus atramentarius* (common ink cap). Cryst. (1-butanol aq.). Mp 206-208°.

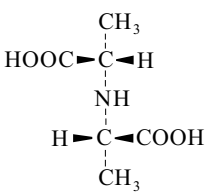
Me ester: [31434-93-2]
$C_7H_{10}N_2O_2$ 154.168
Cryst. (Me_2CO) (as hydrochloride). Mp 106-107° (hydrochloride).

Et ester: [52237-38-4]
$C_8H_{12}N_2O_2$ 168.195
$Bp_{0.05}$ 143-152°.

Windaus, A. *et al., Ber.*, 1910, **43**, 499
Akabori, S. *et al., Ber.*, 1933, **66**, 156
List, P.H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1960, **319**, 17 (*isol*)
Schunack, W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 517

2,2′-Iminobispropanoic acid I-12

[73890-66-1]
N-*(1-Carboxyethyl)alanine, 9CI. 2,2′-Iminodipropionic acid, 8CI. Diethylamine-1,1′-dicarboxylic acid. 1,1′-Dicarboxydiethylamine. Alanopine*



(*S,S*)-*form*

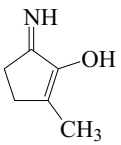
$C_6H_{11}NO_4$ 161.157
(***RS,RS*)-*form*** [19149-54-3]
(±)-form
Found in the squid, *Todarodes pacificus*. Needles (H_2O). Mp 254-255° Mp 234-235° dec.
(***RS,SR*)-*form*** [65621-33-2]
meso-*form*
From scallops (*Patinopecten yessoensis*) and squids (possibly *Todarodes pacificus*). Needles.

[101541-15-5, 103954-11-6]

Karrer, P. *et al., Helv. Chim. Acta*, 1942, **25**, 595 (*synth, resoln*)
Bejaud, M. *et al., Tet. Lett.*, 1975, 2985 (*synth*)
Sato, M. *et al., CA*, 1977, **87**, 181060; 1978, **88**, 84761 (*isol, pmr, ir*)

5-Imino-2-methyl-1-cyclopenten-1-ol, 9CI I-13

[61133-60-6]
2-Hydroxy-3-methyl-2-cyclopentenimine

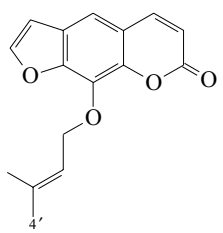


C_6H_9NO 111.143
Maillard product, formed in roast meat aroma model systems. Mp 95.2-96.2°. $Subl._{10}$ 80.

Flamont, I. *et al., Helv. Chim. Acta*, 1976, **59**, 2308-2313 (*synth, ms, pmr, ir*)
Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*isol, ms, pmr, ir*)
Reese, G. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **194**, 417-421 (*formn*)

Imperatorin I-14

[482-44-0]
9-[(3-Methyl-2-butenyl)oxy]-7H-furo[3,2-g][1]benzopyran-7-one, 9CI. 9-(3-Methyl-2-butenyloxy)-7-oxofuro[3,2-g]chromene. ***Pentasalen, BAN.*** *Marmelide. Ammidin. Marmelosin*



$C_{16}H_{14}O_4$ 270.284
Struct. of Marmelide revised in 1984. Present in *Aegle marmelos* (bael fruit) and seeds of *Pastinaca sativa* (parsnip). Mp 102°. Log P 3.8 (calc). λ_{max} 218 (ε 22800); 249 (ε 20600); 301 (ε 10600) (MeOH).

► LD_{50} (mus, ipr) 330 mg/kg. LV1575000

4′-Hydroxy: [65853-14-7] ***Trichoclin***
$C_{16}H_{14}O_5$ 286.284
Cryst. (EtOAc). Mp 123.5-124.5°.

4′-β-D-Glucopyranosyloxy(E-):
$C_{22}H_{24}O_{10}$ 448.426
Amorph. powder. $[\alpha]_D^{22}$ -42.3 (c, 0.5 in MeOH).

4′-β-D-Glucopyranosyloxy(Z-):
Amorph. powder. $[\alpha]_D^{22}$ -46.9 (c, 0.2 in MeOH).

Späth, E. *et al., Ber.*, 1933, **66**, 1137 (*struct*)
Govindachari, T.R. *et al., Tetrahedron*, 1968, **24**, 753 (*isol*)
Basa, S.C. *et al., Chem. Ind. (London)*, 1970, 746 (*isol, uv, ir, nmr*)
Booer, M. *et al., Ghana J. Sci.*, 1970, **10**, 82 (*pharmacol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1377 (*occur*)

Miyakado, M. *et al., Phytochemistry*, 1978, **17**, 143 (*Trichoclin*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, (*occur, tox*)
Murray, R.D.H. *et al., Tetrahedron*, 1984, **40**, 5225 (*struct*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1404-1407 (*4′-glucosyloxy derivs*)
Masuda, T. *et al., Phytochemistry*, 1998, **47**, 13-16 (*isol, uv, pmr, cmr*)
Zhou, P. *et al., Phytochemistry*, 2000, **53**, 689 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IHR300

Incarnatrin I-15

$C_{21}H_{20}O_{12}$ 464.382

Flavonoid glycoside of unknown struct.. Constit. of the flowering tops of *Trifolium incarnatum* (crimson clover). Pale yellow needles + $3H_2O$ (H_2O). Softens at 165°, dec. at 242-245°.

Rogerson, H. *et al., J.C.S.*, 1910, **97**, 1004 (*isol*)

Incarnatyl alcohol I-16

$C_{34}H_{70}O$ 494.926

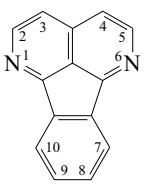
Struct. unknown. Constit. of the flowering tops of *Trifolium incarnatum* (crimson clover). Needles (EtOAc/EtOH). Mp 74-75° (72-74°).

Benzoyl:
Mp 55°.

Rogerson, H. *et al., J.C.S.*, 1910, **97**, 1004 (*isol*)

Indeno[1,2,3-*ij*][2,7]naphthyridine, 9CI I-17

[58786-39-3]
1,6-Diazafluoranthene. ***Eupolauridine.*** *Canangine. EL Base 1*



$C_{14}H_8N_2$ 204.231
Alkaloid from the bark of *Cananga odorata* (ylang ylang). Mp 156-157°.

Hydrochloride:
Orange cryst. (MeOH/Et_2O). Mp 248-249° dec.

N-*Oxide:* [96889-95-1] ***Eupolauridine* N-*oxide***
$C_{14}H_8N_2O$ 220.23
Yellow needles ($CHCl_3$). Mp 186-188°.

N-*Me:1-Methylindeno[1,2,3-*ij*][2,7]-naphthyridinium*
$C_{15}H_{11}N_2^{\oplus}$ 219.265
Red prismatic needles (MeOH)(as iodide). Mp 267-269° dec. (iodide).

*3-Methoxy:****3-Methoxyeupolauridine***
$C_{15}H_{10}N_2O$ 234.257
Yellow needles (petrol). Mp 166-168°.

Bowden, B.F. *et al., Aust. J. Chem.*, 1972, **25**, 2659; 1975, **28**, 2681 (*isol, uv, pmr, ms, struct, synth*)
Leboeuf, M. *et al., Ann. Pharm. Fr.*, 1975, **33**, 43 (*isol*)
Leboeuf, M. *et al., J. Nat. Prod.*, 1976, **39**, 459 (*uv, ir, pmr, ms, struct*)
Waterman, P.G. *et al., Phytochemistry*, 1985, **24**, 523 (*oxide*)
Hufford, C.D. *et al., J. Nat. Prod.*, 1987, **50**, 961-964 (*activity*)
Carroll, A.R. *et al., Aust. J. Chem.*, 1991, **44**, 1615 (*3-Methoxyeupolauridine*)
Tong, T.H. *et al., Synth. Commun.*, 1992, **22**, 1773 (*synth*)

Indicamine I-18

$C_{14}H_{23}NO$ 221.342

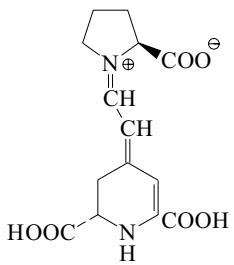
Monoterpene alkaloid. Struct. unknown. Alkaloid from *Plantago psyllium* (African plantain).

Picrate:
Mp 127-128°.

Danilova, A.V. *et al., Zh. Obshch. Khim.*, 1952, **22**, 2237; *CA*, **48**, 691c (*isol*)
Abdusamatov, A. *et al., Khim. Prir. Soedin.*, 1968, **4**, 195; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 168
Karawya, M.S. *et al., U. A. R. J. Pharm. Sci.*, 1971, **12**, 53; *CA*, **78**, 13729e (*isol*)

Indicaxanthin I-19

[2181-75-1]
4-[2-(2-Carboxy-1-pyrrolidinyl)ethenyl]-2,3-dihydro-2,6-pyridinedicarboxylic acid, 9CI

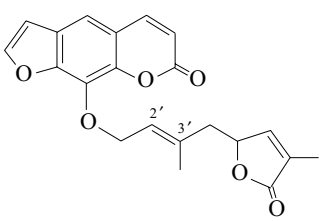


$C_{14}H_{16}N_2O_6$ 308.29
Constit. of the fruits of *Opuntia ficus-indica* (Indian fig). Orange cryst. (H_2O). Mp 160-162° dec. $[\alpha]_D^{20}$ +394 (c, 1 in 0.1*M* phosphate buffer; pH 7). pK_a 3.3. Undergoes rapid E/Z-isomerism in soln..

Piattelli, M. *et al., Tetrahedron*, 1964, **20**, 2325 (*isol, struct, abs config*)
Piattelli, M. *et al., Phytochemistry*, 1965, **4**, 817 (*isol*)
Piattelli, M. *et al., Phytochemistry*, 1972, **11**, 2499 (*biosynth*)
Wyler, H. *et al., Helv. Chim. Acta*, 1984, **67**, 1793 (*pmr*)

Indicolactone I-20

Dehydroindicolactone



$C_{21}H_{18}O_6$ 366.37
Constit. of *Clausena anisata* and *Clausena lansium* (wampee). Viscous mass. $[\alpha]_D^{25}$ +26.3 (c, 2.66 in $CHCl_3$).

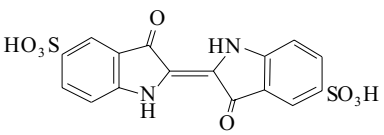
Z-Isomer: [89824-26-0] ***Wampetin***
$C_{21}H_{18}O_6$ 366.37
Isol. from *Clausena wampi* (wampee). Cryst. (EtOAc/Et_2O). Mp 78°. Not correlated with Indicolactone, no abs. config. implied.

2′,3′-Dihydro, 2′,3′-dihydroxy: [68729-09-9] ***Indicolactonediol***
$C_{21}H_{20}O_8$ 400.384
Mp 116-117°. $[\alpha]_D$ +13.3 (c, 2.32 in MeOH).

Prakash, D. *et al., Phytochemistry*, 1978, **17**, 1194 (*Indicolactonediol*)
Kong, Y.C. *et al., Fitoterapia*, 1983, **54**, 47 (*Indicolactone*)
Khan, N.U. *et al., Phytochemistry*, 1983, **22**, 2624 (*Wampetin*)
Lakshmi, V. *et al., Phytochemistry*, 1984, **23**, 2629 (*Indicolatone*)

Indigo-5,5′-disulfonic acid I-21

[483-20-5]
*2-(1,3-Dihydro-3-oxo-5-sulfo-2*H*-indol-2-ylidene)-2,3-dihydro-3-oxo-1*H*-indole-5-sulfonic acid, 9CI. 3,3′-Dioxo[$\Delta^{2,2'}$-biindoline]-5,5′-disulfonate, 8CI. Indigotindisulfonic acid*



$C_{16}H_{10}N_2O_8S_2$ 422.396
Cryst. Sol. H_2O.

Di-Na salt: [860-22-0] ***Indigotin disulfonate sodium, USAN.*** *C.I. Acid blue 74. C.I. Food blue 1. C.I. 73015. Indigo carmine. Soluble indigo blue. Amacid brilliant blue. Carmine blue. Indigotin†. FD and C Blue No. 2. E132*
Colour additive for food. Dark blue solid. Sol. H_2O; sl. sol. EtOH; insol. C_6H_6, $CHCl_3$. Sensitive to light and oxidising agents.
▶ LD_{50} (rat, orl) 2000 mg/kg. DU3000000

Al salt: [16521-38-3]

[12227-85-9, 39290-72-7, 53026-58-7] *C.I. Pigment Blue 63*
Colour additive for food.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1040C (*ir*)
Heymann, B. *et al., Ber.*, 1891, **24**, 1476; 3066 (*synth*)
Vorländer, D. *et al., Ber.*, 1901, **34**, 1860 (*struct*)
Holness, H. *et al., Analyst (London)*, 1942, **67**, 221 (*detn, Ti*)
Welcher, F.J. *et al., Organic Analytical Reagents*, van Nostrand, N.Y., 1947, **4**, 505 (*detn, Cl_2, $NO_3^{\ominus}$, $MnO_4^{\ominus}$*)
Loomis, W.F. *et al., Anal. Chem.*, 1956, **28**, 1347 (*detn, O_2*)
Tandon, J.P. *et al., Fresenius' Z. Anal. Chem.*, 1962, **187**, 410 (*detn, Cr*)
Henze, G. *et al., Fresenius' Z. Anal. Chem.*, 1964, **200**, 434 (*detn, Sn*)
Hooson, J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 177 (*tox*)
Bergshoeff, G. *et al., Analyst (London)*, 1984, **109**, 1165 (*detn, O_3*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1065-1067; 1069-1070 (*Al salt*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 405
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAE100

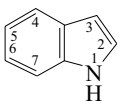
Indocentoic acid I-22

Struct. unknown. Isol. from *Centella asiatica* (Asiatic pennywort). Mp 272°. $[\alpha]_D$ +38.6 (c, 0.015 in Py). Isomeric with Centoic acid, C-177 and expected to have same basic skeleton.

Bhattacharyya, S.C. *et al., J. Indian Chem. Soc.*, 1956, **33**, 893-898 (*isol*)

Indole, 9CI, 8CI I-23

[120-72-9]
1-Benzazole. 2,3-Benzopyrrole. 1-Azaindene. Ketole (obsol.). FEMA 2593



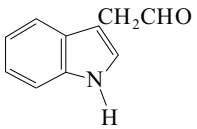
C_8H_7N 117.15
Constit. of several flower oils, esp. of *Jasminum* and *Citrus* spp. (Oleaceae) prod. of bacterial dec. of proteins. Flavouring ingredient. Also present in crispbread, Swiss cheese, Camembert cheese, wine, cocoa, black and green tea, rum, roasted filbert, rice bran, clary sage, raw shrimp and other foodstuffs. Cryst. (H_2O). Sol. EtOH, MeOH, Et_2O; poorly sol. H_2O. Mp 52°. Bp 253-254° Bp_5 122.5-124°. pK_{a1} -2.4; pK_{a2} 16.97 (25°,NH, KOH aq.). λ_{max} 216 ; 270 ; 278 ; 281 ; 295 (MeOH) (Berdy).

▶ LD_{50} (rat, orl) 1000 mg/kg. NL2450000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 653A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 121A; 153B (*nmr*)
Stowe, B.B. *et al., Prog. Chem. Org. Nat. Prod.*, 1959, **17**, 250 (*occur*)
Sawicki, E. *et al., Talanta*, 1963, **10**, 641 (*use*)
Jennings, A.L. *et al., J.O.C.*, 1964, **29**, 2065 (*ms*)
Black, P.J. *et al., Aust. J. Chem.*, 1965, **18**, 353 (*pmr*)
Chignell, D.A. *et al., J. Phys. Chem.*, 1968, **72**, 2934 (*uv*)
Bravo, P. *et al., Gazz. Chim. Ital.*, 1970, **100**, 652 (*synth*)
Parker, R.G. *et al., J.O.C.*, 1970, **35**, 996 (*cmr*)
Sundberg, R.J. *et al., The Chemistry of Indoles*, Academic Press, N.Y., 1970, (*rev*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 925 (*rev, tox*)
Roychowdhury, P. *et al., Acta Cryst. B*, 1975, **31**, 1559 (*cryst struct*)
Lieto, J. *et al., Bull. Soc. Chim. Fr.*, 1976, 1246 (*synth*)
Nakazuki, M. *et al., J.O.C.*, 1976, **41**, 1877 (*synth*)
Ito, Y. *et al., J.A.C.S.*, 1977, **99**, 3532 (*synth*)
Chem. Heterocycl. Compd., (Houlihan, W., Ed.), Parts I-III, Wiley, N.Y., 1978, (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 213 (*rev*)
Robinson, B. *et al., The Fischer Indole Synthesis*, Wiley, 1982, (*book*)
Rahim, S.A. *et al., Microchem. J.*, 1983, **28**, 479 (*use*)
Apps, P.J. *et al., J. Chem. Ecol.*, 1989, **15**, 1681
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1393-1394 (*occur, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICM000

1*H*-Indole-3-acetaldehyde, 9CI I-24

[2591-98-2]
β-Indolylacetaldehyde. 3-(Formylmethyl)indole. Skototenin



$C_{10}H_9NO$ 159.187
Syrup. $Bp_{0.00005}$ 120°.

Oxime: [2776-06-9]

[95394-24-4, 95394-25-5]
$C_{10}H_{10}N_2O$ 174.202
Cryst. ($CHCl_3$). Mp 140-141°. Isol. as a mixt. of *E*/*Z*-isomers.

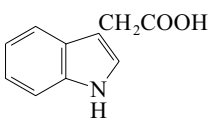
Semicarbazone:
Mp 142-155°.

2,4-Dinitrophenylhydrazone:
Mp 196-202°.

Gordon, S.A. *et al., Arch. Biochem.*, 1949, **43**, 7096
Brown, J.B. *et al., Nature (London)*, 1952, **169**, 335 (*synth, uv, ir*)
Ahmad, A. *et al., Can. J. Chem.*, 1960, **38**, 2523 (*synth, oxime*)
Ihara, M. *et al., Tetrahedron*, 1985, **41**, 2109 (*synth, ir, pmr*)
Schlecht, M.F. *et al., J. Med. Chem.*, 1990, **33**, 386 (*synth*)
Bohlendorf, B. *et al., Annalen*, 1996, 49-53 (*isol, oxime*)

1*H*-Indole-3-acetic acid, 9CI I-25

[87-51-4]
3-Indolylacetic acid. Heteroauxin. Rhizopin. IAA. Rhizipon A



$C_{10}H_9NO_2$ 175.187
Widely distributed in higher plants. Cryst. ($CHCl_3$). Sol. EtOH, Me_2CO; fairly sol. H_2O, $CHCl_3$. Mp 164-165°. pK_{a1} 4.36; pK_{a2} 16.9 (NH). λ_{max} 229 (ϵ 10400); 273 (ϵ 9900); 278 (ϵ 10000); 289 (ϵ 8700) (MeOH) (Berdy).

▶ Exp. reprod. and teratogenic effects. NL3150000

Me ester: [1912-33-0]
$C_{11}H_{11}NO_2$ 189.213
Isol. from immature seeds of beach pea (*Lathyrus maritimus*), *Vicia amurensis*, wild soybean (*Glycine soja*), lobiya (*Vigna catiang* var. *sinensis*) and hyacinth bean (*Dolichos lablab*). Mp 125° (as picrate).

Et ester: [778-82-5]
Mp 44-45°. Bp_1 164-166°.

▶ NL3528000

Chloride: [50720-05-3]
$C_{10}H_8ClNO$ 193.632
Flakes (Et_2O). Mp 63-65°.

Amide: [879-37-8] ***1H-Indole-3-acetamide***
$C_{10}H_{10}N_2O$ 174.202
Isol. from etiolated seedlings of the black gram (*Phaseolus mungo*). Mp 150-151°.

Hydrazide: [5448-47-5]
$C_{10}H_{11}N_3O$ 189.216
Mp 138-139°.

▶ NL3600000

Nitrile: [771-51-7] ***1H-Indole-3-acetonitrile.*** *3-Cyanomethyl-1H-indole*
$C_{10}H_8N_2$ 156.187
Myrosinase-induced hydrolysis product of indole glucosinolates, found in cabbage and other crucifers. Mp 36.5-37°. $Bp_{0.2}$ 157°. Log P 1.55 (calc). Functions by enzymic hydrol. to the acid.

▶ LD_{50} (rat, scu) 255 mg/kg. AM0700000

N-*Methoxy, nitrile:* [30536-48-2] ***1-Methoxy-1H-indole-3-acetonitrile, 9CI***
$C_{11}H_{10}N_2O$ 186.213
Stress metab. from the Japanese radish Daikon (*Raphanus sativus* var. *hortensis*) inoculated with *Pseudomonas cichorii* and from clubroots of Chinese cabbage (*Brassica pekinensis*) infected with *Plasmodiophora brassicae*.

N-*Me:* [1912-48-7]
$C_{11}H_{11}NO_2$ 189.213
Mp 128°. $Bp_{0.1}$ 130-150°.

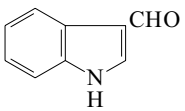
[2338-19-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 667C; 675D; 676D; 678C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 138B; 149A; 154A; 159A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1503C (*ir*)
Henbest, H.B. *et al., J.C.S.*, 1953, 3796 (*isol, nitrile*)
Stowe, B.B. *et al., Prog. Chem. Org. Nat. Prod.*, 1959, **17**, 248 (*bibl*)
Isogai, Y. *et al., Chem. Pharm. Bull.*, 1963, **11**, 1217 (*isol, amide*)
Johnson, H.E. *et al., J.O.C.*, 1963, **28**, 1246
Stefanescu, P. *et al., Rev. Chim. (Bucharest)*, 1969, **20**, 65; *CA*, **69**, 30311 (*synth*)
Nomoto, M. *et al., Agric. Biol. Chem.*, 1970, **34**, 1590 (*isol, 1-Methoxy-3-indoleacetonitrile*)
Abe, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 2259 (*isol, uv, ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 2514; 2515 (*bibl*)
Savorov, N.N. *et al., CA*, 1973, **79**, 146320 (*synth*)
Chandrasekhar, K. *et al., Acta Cryst. B*, 1982, **38**, 2534 (*cryst struct*)
Vekrel, J. *et al., Spectrochim. Acta A*, 1983, **39**, 887 (*ir, pmr, ms*)
Acheson, R.M. *et al., J. Chem. Res., Synop.*, 1984, 101 (*synth, Me ether nitrile*)
Somei, M. *et al., Heterocycles*, 1985, **23**, 1101 (*synth, Me ether nitrile*)
Cardellina, J.H. *et al., J. Nat. Prod.*, 1986, **49**, 1065-1067 (*isol, amide*)
Pfeiffer, D. *et al., Cryst. Res. Technol.*, 1987, **22**, KI (*cryst struct*)
Raucher, S. *et al., J.A.C.S.*, 1987, **109**, 442 (*chloride*)

Morales-Rios, M.S. *et al., Magn. Reson. Chem.*, 1987, **25**, 377 (*cmr*)
Katayama, N. *et al., Plant Cell Physiol.*, 1987, **28**, 383 (*isol, Me ester*)
Wall, M.E. *et al., J. Nat. Prod.*, 1988, **51**, 129 (*isol, nitrile*)
Pesticide Manual, 9th edn., 1991, No. 7260
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A232
Nagarathnam, D. *et al., J. Het. Chem.*, 1992, **29**, 953 (*synth*)
Fukuyama, T. *et al., J.A.C.S.*, 1994, **116**, 3127 (*synth*)
Monde, K. *et al., Phytochemistry*, 1995, **39**, 581 (*isol, 1-Methoxy-3-indoleacetonitrile*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICN000; ICW000

1*H*-Indole-3-carboxaldehyde, 9CI I-26

[487-89-8]
Indole-3-aldehyde. 3-Formylindole



C_9H_7NO 145.16
Found in barley and tomato seedlings and cotton. Mp 180° Mp 197-199°. pK_{a2} 12.36 (25°,NH).

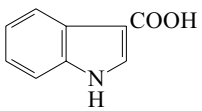
▶ NL5993600

N-*Methoxy:* [67282-55-7] ***1-Methoxy-1H-indole-3-carboxaldehyde, 9CI***. *1-Methoxy-3-formylindole*
$C_{10}H_9NO_2$ 175.187
Stress metab. from the Japanese radish Daikon (*Raphanus sativus* var. *hortensis*) inoculated with *Pseudomonas cichorii*. Prisms + ½H_2O (Et_2O/hexane). Mp 50-51°.

Org. Synth., Coll. Vol., 4, 1963, 539 (*synth*)
Jackson, A.H. *et al., J.C.S.*, 1964, 5510
Bestmann, H.J. *et al., Annalen*, 1968, **718**, 24 (*synth*)
Hart, J.C. *et al., Can. J. Chem.*, 1970, **48**, 177 (*synth*)
Chowdhury, B.K. *et al., Phytochemistry*, 1971, **10**, 481 (*isol, ir, pmr, ms*)
Schneider, E.A. *et al., J. Exp. Bot.*, 1972, **23**, 152 (*occur*)
Wratten, S.J. *et al., Antimicrob. Agents Chemother.*, 1977, **11**, 411 (*isol*)
Oikawa, Y. *et al., J.O.C.*, 1977, **42**, 1213 (*synth*)
Acheson, R.M. *et al., J.C.S. Perkin 1*, 1978, 1117-1125 (*N-methoxy*)
Jo, S. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 2120 (*synth*)
Lahoti, R.J. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 1007 (*synth*)
Komiyama, M. *et al., Makromol. Chem. Rapid Commun.*, 1981, **2**, 757 (*synth*)
Badenoch-Jones, J. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 429 (*isol, ms*)
Okuda, R.K. *et al., Pure Appl. Chem.*, 1982, **54**, 1907 (*isol*)
Moody, C.J. *et al., J.C.S. Perkin 1*, 1984, 2903 (*synth*)
Golubev, S.N. *et al., Zh. Strukt. Khim.*, 1984, **25**, 145; *CA*, **101**, 141424 (*cryst struct*)
Pindur, U. *et al., Annalen*, 1986, 1621 (*synth, ir, pmr, ms*)
Somei, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 677 (*N-methoxy, synth*)
Bano, S. *et al., J. Nat. Prod.*, 1986, **49**, 549 (*isol*)
Evidente, A. *et al., J. Nat. Prod.*, 1986, **49**, 938 (*isol*)
Amat, M. *et al., J.O.C.*, 1994, **59**, 10 (*synth*)
Monde, K. *et al., Phytochemistry*, 1995, **39**, 581 (*isol, 1-Methoxy-3-indolecarboxaldehyde*)

1*H*-Indole-3-carboxylic acid I-27

[771-50-6]
Indole-β-carboxylic acid



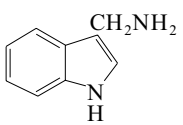
$C_9H_7NO_2$ 161.16
Present in plants, e.g. apple (*Pyrus malus*), garden pea (*Pisum sativum*) and brassicas. Mp 210-218° (198-200°). pK_{a1} 3.87; pK_{a2} 15.59 (25°,NH).

N-*Methoxy, Me ester:* [18377-50-9] ***Methyl 1-methoxy-1H-indole-3-carboxylate***
$C_{11}H_{11}NO_3$ 205.213
Prod. by Japanese horseradish (*Wasabia japonica*). Prisms ($CHCl_3$). Mp 45-46° (40-41°) Mp 40-41°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 138A; 158B (*nmr*)
Kasparek, S. *et al., Can. J. Chem.*, 1966, **40**, 2805 (*synth, derivs*)
Glombitza, K.W. *et al., Planta*, 1966, **69**, 135 (*biosynth*)
Katner, A.S. *et al., Org. Prep. Proced. Int.*, 1970, **2**, 297 (*synth*)
Aldridge, D.C. *et al., J.C.S.(C)*, 1971, 1623 (*isol*)
Abe, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 2259 (*isol, uv, ms*)
Acheson, R.M. *et al., J. Chem. Res., Synop.*, 1984, 101; *J. Chem. Res., Miniprint*, 1984, 1301; 1319 (*N-hydroxy, N-methoxy Me ester, synth*)
Bano, S. *et al., Planta Med.*, 1987, **53**, 117 (*isol, uv, pmr, cmr, ms, esters*)
Baiocchi, L. *et al., J. Het. Chem.*, 1988, **25**, 1905 (*synth*)
Pedras, M.S.C. *et al., Phytochemistry*, 1998, **49**, 1959-1965 (*1-methoxy Me ester*)
Somei, M *et al., Heterocycles*, 2001, **54**, 425-432 (*1-methoxy Me ester synth*)

1*H*-Indole-3-methanamine I-28

[22259-53-6]
3-Indolylmethylamine. 3-(Aminomethyl)indole



$C_9H_{10}N_2$ 146.191
Detected in *Hordeum vulgare* (barley). Cryst. (C_6H_6). Mp 84° Mp 104-107°.

3-N-*Ac:*
$C_{11}H_{12}N_2O$ 188.229
Cryst. (C_6H_6). Mp 133-134°.

N^1-*Me:* [19293-60-8] *1-Methyl-1H-indole-3-methanamine. 3-(Aminomethyl)-1-methylindole.* ***Donaxamine***
$C_{10}H_{12}N_2$ 160.218
Mp 178-179°.

3-N-*Me:3-(Methylaminomethyl)indole.* N-*Norgramine*
$C_{10}H_{12}N_2$ 160.218
Detected in *Hordeum vulgare* (barley).

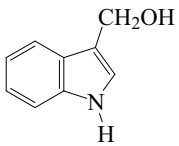
3-N-*Me, picrate:*
Cryst. (EtOH). Mp 176-176.5° dec.

*3*N,*3*N-*Di-Me:* 3-(Dimethylaminomethyl)indole, D-753

Putochin, N. *et al., Ber.*, 1926, **59**, 1987
Mudd, S.H. *et al., Nature (London)*, 1961, **189**, 489 (*N-Norgramine*)
Gower, B.E. *et al., J.A.C.S.*, 1963, **85**, 3683 (*synth*)
Zhalolov, I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2000, **36**, 528-530 (*Donaxamine*)
Kutschy, P. *et al., Tetrahedron*, **54**, 3549-3566 (***synth, 1-Me***)

1*H*-Indole-3-methanol I-29

[700-06-1]
3-Hydroxymethylindole. Indole-3-carbinol



C_9H_9NO 147.176
Produced from glucosinolates in *Brassica* sp. on crushing or cooking. Potential nutriceutical. Platelets (C_6H_6). Mp 89-91° Mp 158°. pK_{a1} 16.5 (25°,NH, KOH aq.). Mp dependent on rate of heating.

▶ Exp. teratogenic effects. NL9483000

N-*Ac:*
$C_{11}H_{11}NO_2$ 189.213
Cryst. (C_6H_6/EtOAc). Mp 137-139°.

O,N-*Di-Ac:*
$C_{13}H_{13}NO_3$ 231.251
Cryst. (EtOH). Mp 89-90°.

N-*Me:* [6965-44-2]
$C_{10}H_{11}NO$ 161.203
Needles. Mp 30°. Bp_5 150-160°.

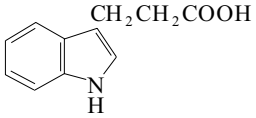
▶ NL9486900

N-*Me, trinitrobenzene complex:*
Cryst. (MeOH). Mp 139-141°.

Mingoia, G. *et al., Gazz. Chim. Ital.*, 1932, **62**, 844 (*synth*)
Ames, D.E. *et al., J.C.S.*, 1956, 1984 (*synth*)
Leete, E. *et al., J.A.C.S.*, 1959, **81**, 6023 (*N-methyl*)
Mattocks, A.R. *et al., J.C.S. Perkin 1*, 1978, 896 (*N-methyl*)
Broadbent, T.A. *et al., Curr. Med. Chem.*, 1998, **5**, 337-352; 469-491 (*rev, pharmacol*)
Jeffery, E.H. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press,, 2001, 169-191
Goyal, R.N. *et al., J.C.S. Perkin 2*, 2001, 618-623 (*props, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICP100

1*H*-Indole-3-propanoic acid I-30

[830-96-6]
3-(3-Indolyl)propionic acid. KG 431B. Antibiotic KG 431B



$C_{11}H_{11}NO_2$ 189.213
Mp 134° (111-112°).
▶ NM1329000

Me ester: [5548-09-4]
$C_{12}H_{13}NO_2$ 203.24
Mp 79-80°.
▶ NM1480000

Cyclohexyl ester: [109897-76-9] ***Indobinine***
$C_{17}H_{21}NO_2$ 271.358
Elongated rods (MeOH). Mp 180-181°.

Benzyl ester: [85612-35-7] ***Indobine***
$C_{18}H_{17}NO_2$ 279.338
Needles (MeOH). Mp 163-164°.

Amide: [5814-93-7] ***1H-Indole-3-propanamide***
$C_{11}H_{12}N_2O$ 188.229
Cryst. (MeOH aq.). Mp 134-136°.

Methylamide: [69397-85-9] **N-*Methyl-1H-indole-3-propanamide***. *3-(3-Indolyl)-N-methylpropanamide*
$C_{12}H_{14}N_2O$ 202.255
Prod. by *Omphalotus olearius* (common chanterelle). Cryst. (CH_2Cl_2/petrol). Mp 97.5-99° (synthetic).

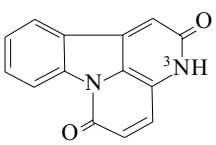
Hydrazide: [20401-90-5]
$C_{11}H_{13}N_3O$ 203.243
Mp 129-130°.

Nitrile: [4414-76-0] *3-(2-Cyanoethyl)indole*
$C_{11}H_{10}N_2$ 170.213
Mp 67-68°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 667D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 138C (*nmr*)
Yamano, T. *et al., CA*, 1963, **58**, 763 (*isol*)
Ghosal, S. *et al., J. Indian Chem. Soc.*, 1964, **41**, 496 (*synth*)
Bowman, R.E. *et al., Chem. Ind. (London)*, 1971, 154 (*synth*)
Siddiqui, S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 279 (*Indobinine*)
Siddiqui, S. *et al., Z. Naturforsch., B*, 1987, **42**, 783 (*Indobine*)
Thompson, A.M. *et al., J. Med. Chem.*, 1994, **37**, 598-609 (*synth, amide*)
Mayer, A. *et al., Nat. Prod. Lett.*, 1997, **10**, 25-32 (*methylamide*)
Okabe, N. *et al., Acta Cryst. C*, 1998, **54**, 386-387 (*cryst struct*)

3*H*-Indolo[3,2,1-*de*][1,5]-naphthyridine-2,6-dione, 9CI I-31

Canthin-2,6-dione



$C_{14}H_8N_2O_2$ 236.229
Yellow microneedles. Mp 290-305°. λ_{max} 227 (ε 27500); 247 (ε 21900); 253 (ε 20400); 291 (ε 9770); 300 (ε 10200); 400 (sh) (ε 8130); 421 (ε 12900); 445 (ε 13800) (MeOH) (Derep).

N^3-*Me:* [82652-21-9] ***3-Methylcanthin-2,6-dione***
$C_{15}H_{10}N_2O_2$ 250.256
Orange-red needles ($CHCl_3$/MeOH). Mp 330°. Strong yellow-green fluor. in soln..

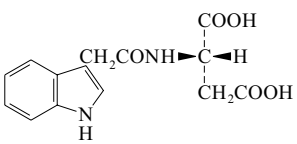
N^3-*Methoxy:* [74991-92-7] ***3-Methoxycanthin-2,6-dione***
$C_{15}H_{10}N_2O_3$ 266.256
Red cryst. (AcOH). Mp 330°. Strong green fluor. in soln. λ_{max} 227 (ε 17400); 232 (sh) (ε 17400); 248 (ε 16600); 253 (sh) (ε 16200); 292 (ε 10200); 302 (ε 10200); 325 (ε 6460); 403 (sh) (ε 9330); 420 (ε 13500) (MeOH) (Derep). λ_{max} 226 (ε 14500); 247 (ε 13500); 290 (ε 4300); 302 (ε 4500); 325 (ε 2700); 422 (ε 7100); 446 (ε 8000) (MeOH) (Berdy).

N^3-*Me, 4-methoxy, 5-hydroxy:* [129724-30-7] ***5-Hydroxy-4-methoxy-3-methyl-2,6-canthinedione***
$C_{16}H_{12}N_2O_4$ 296.282
Alkaloid from the wood of *Quassia amara* (Surinam quassia). Orange-red needles (MeOH). Mp 250-254°.

Giesbrecht, A.M. *et al., Phytochemistry*, 1980, **19**, 313 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1204 (*isol, uv, ir, pmr, ms, struct*)
Arisawa, M. *et al., J. Nat. Prod.*, 1983, **46**, 222 (*isol, uv, ir, pmr, ms, struct*)
Barbetti, P. *et al., Planta Med.*, 1990, **56**, 216 (*5-Hydroxy-4-methoxy-3-methyl-2,6-canthinedione*)

N-(1*H*-Indol-3-ylacetyl)aspartic acid, 9CI I-32

Indole-3-acetylaspartic acid



(*S*)-*form*

$C_{14}H_{14}N_2O_5$ 290.275

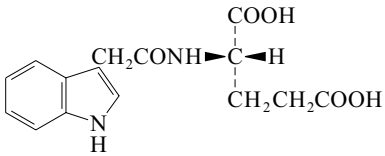
(*S*)-*form* [2456-73-7]
L-*form*
Constit. of many plant spp. incl. soybean *Glycine max*. Metab. of 1*H*-Indole-3-acetic acid, I-25 in plant tissues. Cryst. (EtOH aq.) or pale pink glass. Mp 164.5° dec. $[\alpha]_D^{25}$ +8.5 (c, 0.64 in H_2O).

(±)-*form* [32449-99-3]
Cryst. (H_2O). Mp 190-191° (186-188°).

[53438-36-1, 53667-64-4, 53667-65-5, 80784-13-0, 109736-05-2]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 156A (*nmr*)
Good, N.E. *et al., Can. J. Chem.*, 1956, **34**, 1356 (*synth*)
Weller, L.E. *et al., J.O.C.*, 1958, **23**, 1776 (*synth*)
Suedi, J. *et al., Nature (London)*, 1964, **201**, 1009
Mollan, R.C. *et al., Phytochemistry*, 1972, **11**, 1485 (*synth, uv, ir, pmr*)
Sirokman, F. *et al., Acta Phys. Chem.*, 1974, **20**, 125
Feung, C.-S. *et al., J. Agric. Food Chem.*, 1975, **23**, 1120 (*ms, chromatog*)
Hollenberg, S.M. *et al., J. Agric. Food Chem.*, 1981, **29**, 1173 (*synth, hplc*)
Cohen, J.D. *et al., J. Labelled Compd. Radiopharm.*, 1981, **18**, 1393

N-(1*H*-Indol-3-ylacetyl)glutamic acid, 9CI I-33



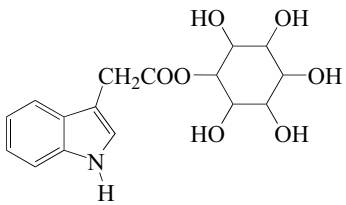
$C_{15}H_{16}N_2O_5$ 304.302

(*S*)-*form* [57105-48-3]
L-*form*
Constit. of various plant spp. incl. soybean (*Glycine max*). Cryst. (EtOH aq.). Mp 162.5° dec. $[\alpha]_D^{27}$ -10.57 (H_2O).

Weller, L.E. *et al., J.O.C.*, 1958, **23**, 1776 (*synth*)
Feung, C.-S. *et al., Agric. Biol. Chem.*, 1975, **23**, 1120 (*ms, chromatog*)
Hollenberg, S.M. *et al., J. Agric. Food Chem.*, 1981, **29**, 1173 (*synth, hplc*)
Epstein, E. *et al., Plant Physiol.*, 1986, **80**, 256 (*isol*)

1*H*-Indol-3-ylacetyl-*myo*-inositol I-34

[73925-84-5]

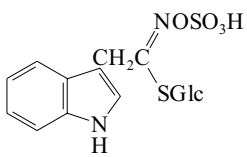


$C_{16}H_{19}NO_7$ 337.329
The inositol residue has the *myo*- config. but the point of attachment is variable (i.e. exact config. is unknown). Present in *Oryza sativa* (rice) and *Zea mays* (corn).

Hall, P.J. *et al., Phytochemistry*, 1980, **19**, 2121

3-Indolylmethyl glucosinolate I-35

[4356-52-9]
Glucobrassicin



$C_{16}H_{20}N_2O_9S_2$ 448.474
Constit. of *Brassica* and *Raphanus* spp., e.g. rape (*Brassica napus* var. *napus*) and Brussels sprouts (*Brassica oleracea* var. *gemmifera*). Mp 149-150° (as Me_4N salt). $[\alpha]_D^{22}$ -13.3 (Me_4N salt).

N-*Ac:* [103951-50-4] *(1-Acetyl-1H-indol-3-yl)methyl glucosinolate.* **N-*Acetylglucobrassicin***
$C_{18}H_{22}N_2O_{10}S_2$ 490.511

N-*Sulfonic acid:* [29702-28-1] *(1-Sulfo-1H-*

indol-3-yl)methyl glucosinolate, 9CI.
Sulfoglucobrassicin
$C_{16}H_{20}N_2O_{12}S_3$ 528.538
Cryst. (EtOH aq.) (as Me_4N salt). Mp 156° dec. (Me_4N salt).

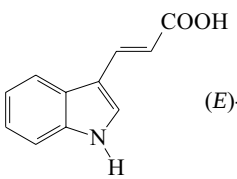
N-*Methoxy:* [5187-84-8] ***Neoglucobrassicin***. N-*Methoxyglucobrassicin*
$C_{17}H_{22}N_2O_{10}S_2$ 478.5
Widespread in *Brassica* spp. and found in the Cruciferae, Tovariaceae, Capparidaceae and Resedaceae. Mp 175° dec. (as brucine salt).

N,*4-Dimethoxy:* ***1,4-Dimethoxyglucobrassicin***
$C_{18}H_{24}N_2O_{11}S_2$ 508.526
Isol. from the roots of *Barbarea vulgaris* ssp. *arcuata*.

Gmelin, R. *et al., Suom. Kemistil. B*, 1961, **34**, 15 (*isol*)
Gmelin, R. *et al., Acta Chem. Scand.*, 1962, **16**, 1378 (*Neoglucobrassicin*)
Gmelin, R. *et al., CA*, 1965, **63**, 5584
Schraudolf, H. *et al., Experientia*, 1965, **21**, 520 (*occur*)
Elliott, M.C. *et al., Phytochemistry*, 1970, **9**, 1629 (*sulfonic acid*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410 (*ms*)
Hanley, A.B. *et al., J. Sci. Food Agric.*, 1983, **34**, 869 (*isol*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*cmr, pmr*)
Schraudolf, H. *et al., Z. Naturforsch., C*, 1986, **41**, 526 (*acetyl*)
Belkhiri, A. *et al., Phytochemistry*, 1990, **29**, 1315 (*isol, uv, pmr*)
Viaud, M.C. *et al., Tet. Lett.*, 1990, **31**, 1417 (*synth*)
Agerbirk, N. *et al., J. Agric. Food Chem.*, 2001, **49**, 1502-1507 (*1,4-Dimethoxyglucobrassicin*)

3-(1*H*-Indol-3-yl)-2-propenoic acid I-36

[1204-06-4]
1H-Indole-3-propenoic acid. 3-(3-Indolyl)acrylic acid



(*E*)-*form*

$C_{11}H_9NO_2$ 187.198
Major auxin from roots of *Lens culinaris* (lentil).

► Exp. carcinogenic data. NL3680000

(E)-form [29953-71-7]
Red-brown cryst. (H_2O or AcOH). Mp 195-196°.

Me ester:
$C_{12}H_{11}NO_2$ 201.224
Cryst. (C_6H_6). Mp 153-154°.

Me ester, N-*Ac:*
$C_{14}H_{13}NO_3$ 243.262
Cryst. (C_6H_6). Mp 179-180°.

Amide:3-(1H-Indol-3-yl)-2-propenamide. ***3-(3-Indolyl)acrylamide***
$C_{11}H_{10}N_2O$ 186.213
Amber cryst. (Me_2CO). Mp 212.8-214.2°. λ_{max} 226 (log ε 1.49); 275 (log ε 1.25); 322 (log ε 1.55) (MeOH). λ_{max} 226 ; 275 ; 322 (MeOH) (Berdy).

Amide, N^b*-formyl:* [142677-08-5] N-*Formyl-3-(1H-indol-3-yl)-2-propenamide, 9CI.* **N-*Formyl-3-indoleacrylamide***
$C_{12}H_{10}N_2O_2$ 214.223
Oil.

7′-Hydroxy: [142677-11-0] *3-(7-Hydroxy-1H-indol-3-yl)-2-propenoic acid, 9CI.* ***7-Hydroxy-3-indoleacrylic acid***
$C_{11}H_9NO_3$ 203.197

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 668B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 139B (*nmr*)
Furst, A. *et al., Arch. Biochem. Biophys.*, 1951, **31**, 190 (*synth*)
Inhoffen, H.H. *et al., Annalen*, 1963, **668**, 108
Rappe, C. *et al., Acta Chem. Scand.*, 1964, **18**, 818 (*config*)
Hofinger, M. *et al., Phytochemistry*, 1970, **9**, 1757 (*isol*)
Palermo, J.A. *et al., Tet. Lett.*, 1992, **33**, 3097 (*Chondria derivs, isol*)
Davyt, D. *et al., J. Nat. Prod.*, 1998, **61**, 1560-1563 (*isol, amide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ICO000

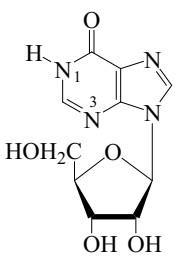
Inhibitory protein I-37

Protein, MW 5.4 kDa. Prod. by *Lactobacillus acidophilus* AC_1. Shows antimicrobial activity.

Mehta, A.M. *et al., Microbios*, 1983, **37**, 37-43 (*isol*)

Inosine, 9CI, INN, JAN I-38

[58-63-9]
1,9-Dihydro-9-β-D-ribofuranosyl-6H-purin-6-one, 9CI. 9-β-D-Ribofuranosylhypoxanthine, 8CI. Hypoxanthine riboside. Hypoxanthosine. Aminosin†. Carnine. Delimmun. Inosie. Oxiamine. Trophicardyl



1*H-form*

$C_{10}H_{12}N_4O_5$ 268.229
Present in meat extracts and sugar beet. Mp 215° dec. $[\alpha]_D^{18}$ -49.2 (c, 0.9 in H_2O). pK_{a1} 1.5; pK_{a2} 8.85; pK_{a3} 12.5 (25°). Log P -3.76 (calc). λ_{max} 249 (ε 12200) (H_2O) (pH 6).

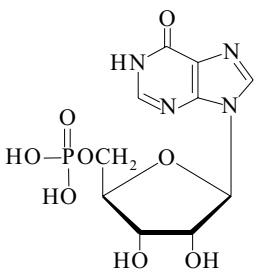
► Probable mutagen. Exp. reprod. effects (very high dose) LD_{50} (mus, ivn) 3000 mg/kg. NM7460000

[35908-31-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 712B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 215C (*nmr*)
Gulland, J.M. *et al., J.C.S.*, 1936, 765 (*struct*)
Hall, R.H. *et al., Biochem. Biophys. Res. Commun.*, 1963, **13**, 394 (*isol, deriv*)
Kinichi, I. *et al., Chem. Pharm. Bull.*, 1966, **14**, 1377 (*synth*)
Munns, A.R.I. *et al., Acta Cryst. B*, 1970, **26**, 1114 (*cryst struct*)
Ger. Pat., 1972, 2038262; *CA*, **76**, 99993e (*synth*)
Chenon, M.T. *et al., J.A.C.S.*, 1975, **97**, 4627 (*cmr*)
Westhof, E. *et al., Z. Naturforsch., C*, 1975, **30**, 131 (*pmr*)
Hawkes, G.E. *et al., J.C.S. Perkin 2*, 1977, 1268 (*N-15 nmr*)
Yamazaki, A. *et al., J. Het. Chem.*, 1978, **15**, 353 (*rev, synth*)
Aviado, D.M. *et al., J. Pharmacol.*, 1983, **14**, 47 (*rev, pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1551
De Simone, C. *et al., Int. J. Immunopharmacol.*, 1991, **13**, 19 (*rev, Inosine pranobex*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 548; 1379
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IDE000

Inosinic acid, 8CI I-39

[131-99-7]
5′-Inosinic acid, 9CI. Inosine 5′-dihydrogen phosphate. Inosine 5′-monophosphate. Inosine 5′-phosphate. Inosine 5′-phosphoric acid. IMP. E630



$C_{10}H_{13}N_4O_8P$ 348.208
Syrup which solidifies to a glass on drying. $[\alpha]_D^{20}$ -18.5 (c, 3.0, Ba salt in 2.5% HCl). pK_{a1} 2.4; pK_{a2} 6.4.

► LD_{50} (rat, orl) 16000 mg/kg. NM7519000

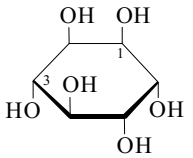
Di-Na salt: [4691-65-0] *Disodium inosinate. E631*
Flavour enhancer. Mp 175° dec. (as monohydrate).

► NM7519500

Levene, P.A. *et al., J. Biol. Chem.*, 1935, **111**, 313
Kalckar, H.M. *et al., J. Biol. Chem.*, 1947, **167**, 429
Korn, E.D. *et al., J. Biol. Chem.*, 1955, **217**, 875 (*synth*)
Takaku, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1844 (*synth*)
Nagashima, N. *et al., Acta Cryst. B*, 1974, **30**, 320 (*cryst struct*)
Evans, F.E. *et al., J.A.C.S.*, 1975, **97**, 3215 (*conformn, pmr*)
Williams, T.J. *et al., Arch. Biochem. Biophys.*, 1976, **172**, 490 (*cmr*)
Brown, E.A. *et al., Acta Cryst. B*, 1980, **36**, 2597 (*cryst struct*)
Watanabe, E. *et al., Anal. Chim. Acta*, 1984, **164**, 139
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1362
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 895
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXE500; IDE200

chiro-Inositol, 9CI, 8CI I-40

(1α,2α,3β,4α,5β,6β)-Cyclohexanehexol. 1,2,4/3,5,6-Inositol. Chiroinositol



D-*form*

$C_6H_{12}O_6$ 180.157

D-*form* [643-12-9]
d-*Inositol. Matezodambose*
Mp 248°. $[\alpha]_D$ +65 (H_2O).

2-O-α-D-Galactopyranoside: [79391-04-1] *2-O-α-D-Galactopyranosyl-D-chiro-inositol.* ***Fagopyritol B$_1$***
$C_{12}H_{22}O_{11}$ 342.299
Isol. from soya beans (*Glycine max*) and jojoba beans (*Simmondsia chinensis*) and also from buckwheat (*Fagopyrum esculentum*). Powder. Mp 165-170° dec. $[\alpha]_D$ +170. $[\alpha]_D^{24}$ +130 (c, 0.5 in H_2O).

2-O-[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranoside]: [116261-02-0] ***Fagopyritol B$_2$***
$C_{18}H_{32}O_{16}$ 504.441
Constit. of sugar beet (*Beta vulgaris*) and buckwheat (*Fagopyrum esculentum*). $[\alpha]_D^{20}$ +177.2.

2-O-[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranosyl-(1→6)-α-D-galactopyranoside]: [208708-11-6] ***Fagopyritol B$_3$***
$C_{24}H_{42}O_{21}$ 666.583
Constit. of buckwheat (*Fagopyrum esculentum*). Proposed struct..

3-Me: [10284-63-6] *3-O-Methyl-D-chiro-inositol.* ***D-Pinitol***. *Matezitol. Sennitol. Cathartomannitol*
$C_7H_{14}O_6$ 194.184
Widely distributed in plants. Mp 185-186°. $[\alpha]_D^{20}$ +67 (c, 2.5 in H_2O).

4-Me, 2-O-α-D-galactopyranoside: [64290-91-1] ***Galactopinitol A***
$C_{13}H_{24}O_{11}$ 356.326
Constit. of soya bean seeds and numerous other plant spp. in the Leguminosae. Viscous syrup. $[\alpha]_D^{25}$ +180 (c, 0.2 in H_2O).

4-Me, 2-O-β-D-galactopyranoside: [88199-72-8] ***Galactopinitol B***
$C_{13}H_{24}O_{11}$ 356.326
Constit. of soya beans.

3-Me, 2-O-α-D-galactopyranoside: [79391-03-0] *2-O-α-D-Galactopyranosyl-3-O-methyl-D-chiro-inositol*
$C_{13}H_{24}O_{11}$ 356.326
Constit. of soya beans. Powder. $[\alpha]_D$ +159.

4-Me, 2-O-[α-D-galactopyranosyl-(1→6)-α-D-galactopyranoside]: [88167-26-4] ***Ciceritol***
$C_{19}H_{34}O_{16}$ 518.468
Constit. of chick pea seeds (*Cicer arietinum*), lentil seeds (*Lens esculenta*) and other plant spp. in the Leguminosae.

4-Me, 2-O-[α-D-galactopyranosyl-(1→6)-α-D-galactopyranosyl-(1→6)-α-D-galactopyranosyl-(1→6)-α-D-galactopyranoside]: [92675-08-6] ***6′′-O-α-D-Galactopyranosylciceritol***
$C_{25}H_{44}O_{21}$ 680.61
Isol. from chickpeas.

3-O-α-D-Galactopyranoside: [209287-65-0] *3-O-α-D-Galactopyranosyl-D-chiro-inositol.* ***Fagopyritol A$_1$***
$C_{12}H_{22}O_{11}$ 342.299
Isol. from buckwheat seeds (*Fagopyrum esculentum*).

3-O-[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranoside]: ***Fagopyritol A$_2$***
$C_{18}H_{32}O_{16}$ 504.441
Constit. of buckwheat (*Fagopyrum esculentum*).

3-O-[α-D-Galactopyranosyl-(1→6)-α-D-galactopyranosyl-(1→6)-α-D-galactopyranoside]: ***Fagopyritol A$_3$***
$C_{24}H_{42}O_{21}$ 666.583
Constit. of *Fagopyrum esculentum* (buckwheat).

L-*form* [551-72-4]
l-*Inositol. Laevoinositol. Levoinositol*
Widely distributed in higher plants predominantly as its monomethyl ether. Mp 246°. $[\alpha]_D$ -65 (H_2O).

2-Me: [642-38-6] *2-O-Methyl-L-chiro-inositol.* ***L-Quebrachitol***
$C_7H_{14}O_6$ 194.184
Widely distributed in plants. Mp 191°. $[\alpha]_D^{20}$ -80.3 (H_2O).

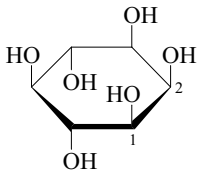
3-Me: [3559-00-0] *3-O-Methyl-L-chiro-inositol.* ***L-Pinitol***
$C_7H_{14}O_6$ 194.184
Present in tarragon (*Artemisia dracunculus*). Mp 186°. $[\alpha]_D$ -65 (c, 2 in H_2O).

Angyal, S.J. *et al., J.C.S.*, 1952, 686-695 (*Pinitol, Quebrachitol, struct*)
Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1956, **243**, 1913-1915 (*L-Pinitol, isol*)
Angyal, S.J. *et al., J.C.S.*, 1962, 2985-2991 (*Quebrachitol*)
Kindl, H. *et al., Prog. Chem. Org. Nat. Prod.*, 1966, **24**, 149-205 (*rev*)
Beverage, R.J. *et al., Aust. J. Chem.*, 1977, **30**, 1583-1590 (*Galactosylpinitol*)
Garegg, P.J. *et al., Carbohydr. Res.*, 1981, **90**, 61-69 (*Galactosylpinitol*)
Schweizer, T.F. *et al., Carbohydr. Res.*, 1981, **95**, 61-71 (*2-galactoside, 4-Me 5-galactoside*)
Quemener, B. *et al., Phytochemistry*, 1983, **22**, 1745-1751 (*Ciceritol*)
Nicolas, P. *et al., Carbohydr. Res.*, 1984, **131**, 331-334 (*6′′-α-D-Galactosylciceritol*)
Shiomi, N. *et al., Agric. Biol. Chem.*, 1988, **52**, 1587-1588 (*Fagopyritol B_2*)
Ley, S.V. *et al., Tetrahedron*, 1989, **45**, 3463-3476 (*Pinitol, synth*)
Mondal, D.N. *et al., J. Indian Chem. Soc.*, 1993, **70**, 651-652 (*Pinitol, config, pmr*)
Agrawal, P.K. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 803-805 (*Quebrachitol, isol, pmr, cmr*)
Kiddle, J.J. *et al., Chem. Rev.*, 1995, **95**, 2189-2202 (*rev, Quebrachitol*)
Acena, J.L. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 3535-3544 (*D-Pinitol, synth*)
Ogawa, K. *et al., Carbohydr. Res.*, 1997, **302**, 219-221 (*Galactosylpinitol*)
Obendorf, R.L. *et al., Carbohydr. Res.*, 2000, **328**, 623-627 (*Fagopyritol A_1*)
Steadman, K.J. *et al., Carbohydr. Res.*, 2001, **331**, 19-25 (*Fagopyritols A_2, A_3*)

myo-Inositol, 9CI, 8CI I-41

[87-89-8]

[6917-35-7]
(1α,2α,3α,4β,5α,6β)-Cyclohexanehexol. meso-*Inositol. Dambose. Nucitol. 1,2,3,5/4,6-Inositol.* i-*Inositol. Inositol. Mesoinositol. Phaseomannitol. Myoinositol. Isoinositol. Many other names*



$C_6H_{12}O_6$ 180.157

The parent compd. exhibits a plane of symmetry (C(2)/C(5)). Unsymmetrically substituted derivs. on C(1), C(3), C(4), C(6) are chiral and care is necessary. The direction of numbering (1- vs. 3-) specifies the absolute configuration, The numbering shown above is for D-*myo*-inositol acc. to IUPAC convention, but the opposite scheme has been used in the past. Of common occurrence in plants and animals . Obt. comly. from phytic acid in corn steep liquor. Dietary supplement. Mp 225°.

▶ Toxic.

Hexaphosphate: [83-86-3]

[7776-28-5, 14306-25-3, 70981-46-3] myo-*Inositol hexakis(phosphate).* ***Phytic acid***. *Fytic acid, INN. Alkalovert. Phytin. Phyton*
$C_6H_{18}O_{24}P_6$ 660.036
Widely distributed in many higher plants. The Ca salt is used as a sequestrant in food flavouring. Straw-coloured syrup. Other salts also documented.

▶ NM7525000

1-O-β-D-Glucopyranoside: [4539-73-5] *1-O-β-D-Glucopyranosyl*-myo-*inositol.* ***Glucinol***
$C_{12}H_{22}O_{11}$ 342.299
Occurs in vascular tissues of higher plants. Mp 252-260°. $[\alpha]_D^{25}$ -17.5 (H_2O).

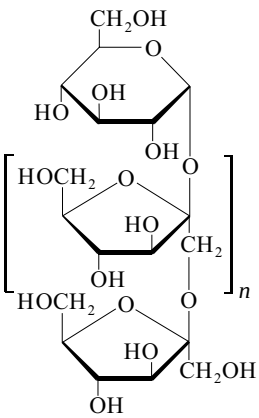
[3615-82-5, 7205-52-9, 17211-15-3, 21667-10-7, 23784-11-4, 39907-99-8, 56083-79-5, 68247-19-8, 105182-27-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 173C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 266A (*nmr*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem.*, 1959, **14**, 135 (*rev*)
Gorin, P.A.J. *et al., Can. J. Chem.*, 1965, **43**, 2259 (*Glucinol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 280 (*bibl*)
Wells, W.W. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **24**, 50 (*rev*)
Isbrandt, L.R. *et al., J.A.C.S.*, 1980, **102**, 3144-3148 (*hexaphosphate, conformn*)
Hopf, H. *et al., CA*, 1981, **94**, 13612n (*occur, Glucinol*)
Angyal, S.J. *et al., Carbohydr. Res.*, 1982, **100**, 43 (*cmr*)
Holub, B.J. *et al., Annu. Rev. Nutr.*, 1986, **6**, 563 (*rev*)

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 540; 588; 8197 (*synonyms*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 695; 1309; 1379
Billington, D.C. *et al., The Inositol Phosphates*, VCH Weinheim, 1993,
Lu, P.J. *et al., Biochemistry*, 1994, **33**, 11586-11597 (*phosphates*)
Barrientos, L.G. *et al., Carbohydr. Res.*, 1996, **296**, 39-54 (*pmr, conformn, phosphates*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 416-417; 1394-1395
Bauman, A.T. *et al., Tet. Lett.*, 1999, **40**, 4489-4492 (*Phytic acid, pmr, conformn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HFG550; PIB250; IDE300

Inulin, 9CI, 8CI, BAN, USAN I-42

[9005-80-5]
Dahlin. Plant starch



n approx. 30, MW approx. 5000. Contains Inulobiose, I-43 as a repeating structural unit with mostly glucose as terminal group. Yields D-Fructose and D-Glucose on acid hydrol.. Present in Jerusalem artichoke (*Helianthus tuberosus*) and in other members of Compositae. $[\alpha]_D^{20}$ -40 (c, 2.0 in H_2O). Log P -7.77 (uncertain value) (calc). For other related storage polysaccharides see Levan, Sinistrin and Phlean, P-323. Other storage polysaccharides which have been isol. from various species and given trivial names include Secalin and Asparagosin from asparagus.

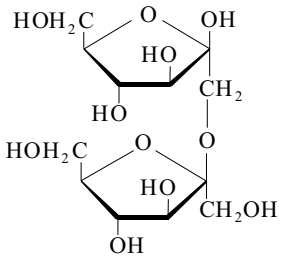
Per-Ac: [59818-02-9]
$[\alpha]_D^{20}$ -34 (c, 1.6 in $CHCl_3$).

Per-Me:
Mp 140°. $[\alpha]_D^{20}$ -55 (c, 1.0 in $CHCl_3$).

Haworth, W.N. *et al., J.C.S.*, 1932, 2384
McDonald, E.J. *et al., Adv. Carbohydr. Chem.*, 1946, **2**, 254 (*isol*)
Bacon, J.S.D. *et al., Biochem. J.*, 1951, **48**, 114
Percival, E.G.V. *et al., Structural Carbohydr. Chem.*, 2nd Ed., 1962, 274 (*struct*)
Aspinall, G.O. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 157 (*synth*)
Ovodov, Yu.S. *et al., Dokl. Akad. Nauk SSSR*, 1968, **178**, 1338; *CA*, **69**, 44141a (*pmr*)
Kennedy, J.F. *et al., Carbohydr. Res.*, 1973, **26**, 401
Hultman, E. *et al., Clin. Biochem. Princ. Methods*, (Eds., Curtius, H. *et al*), Berlin, 1974, **2**, 908; *CA*, **82**, 13173b (*rev*)
Newkome, G.R. *et al., Carbohydr. Res.*, 1976, **48**, 1
Jarrell, H.C. *et al., Carbohydr. Res.*, 1979, **76**, 45-57 (*cmr*)
Marchessault, R.H. *et al., Can. J. Chem.*, 1980, **58**, 2415 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 776
Van Loo, J. *et al., Crit. Rev. Food Sci. Nutr.*, 1995, **35**, 525-552 (*rev*)
Heyer, A.G. *et al., Carbohydr. Res.*, 1998, **313**, 165-174 (*enzymic synth*)

Inulobiose I-43

[470-58-6]
1-O-β-D-Fructofuranosyl-D-fructose. Difructan



$C_{12}H_{22}O_{11}$ 342.299
Constit. of *Artemisia absinthium* (wormwood) leaves and *Artemisia dracunculus* (tarragon) roots. $[\alpha]_D^{20}$ -72.4 (c, 2.7 in H_2O) (-32.5). Sweeter than sucrose.

β-Furanose-*form*

Octa-Ac:
$C_{28}H_{38}O_{19}$ 678.597
$[\alpha]_D^{20}$ -14.2 (c, 1.5 in $CHCl_3$) (-6.5).

Pazur, J.H. *et al., J.A.C.S.*, 1953, **75**, 3458 (*synth, octa-Ac*)
Schlubach, H.H. *et al., Annalen*, 1954, **588**, 192 (*isol*)
Andersen, B. *et al., Acta Chem. Scand.*, 1967, **21**, 828 (*occur*)
Lombard, A. *et al., CA*, 1976, **85**, 74938p (*occur*)
Senda, T. *et al., CA*, 1990, **113**, 170368v (*synth*)
Calub, T.M. *et al., Carbohydr. Res.*, 1990, **207**, 221 (*conformn*)

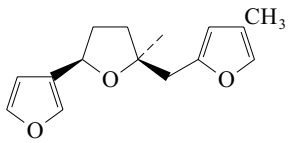
3-Iodopropanoic acid, 9CI I-44

[141-76-4]
3-Iodopropionic acid, 8CI
ICH_2CH_2COOH
$C_3H_5IO_2$ 199.976
Used as a feed additive for ruminants. Glittering leaflets (H_2O). V. sol. EtOH, Et_2O, sol. hot H_2O, v. spar. sol. cold H_2O. pK_a 4.09 (18°).

▶ UF4900000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 510D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 796B (*nmr*)
Hannerz, E. *et al., Ber.*, 1926, **59**, 1367 (*synth*)
Grishchuk, A.P. *et al., Zh. Obshch. Khim.*, 1961, **31**, 2396 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IEY000

Ipomeabisfuran I-45

[92541-62-3]
2,3,4,5-Tetrahydro-5-methyl-5-[(4-methyl-2-furanyl)methyl]-2,3′-bifuran, 9CI



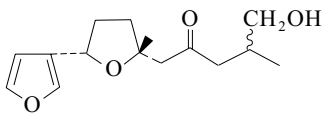
$C_{15}H_{18}O_3$ 246.305
Isol. from *Ipomoea batatas* (sweet potato) infected with *Ceratocystis fimbriata*. Sol. $CHCl_3$, MeOH; poorly sol. H_2O.

[55721-94-3]

Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1155 (*isol*)
Ito, I. *et al., Agric. Biol. Chem.*, 1984, **48**, 159 (*isol*)
Schneider, J.A. *et al., Phytochemistry*, 1984, **23**, 759 (*isol*)

Ipomeamaronol I-46

[26767-96-4]

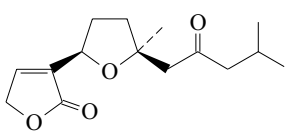


$C_{15}H_{22}O_4$ 266.336
Constit. of sweet potato tubers infected with *Ceratocystis fimbriata*. Viscous oil. Abs. config. not detd., not clear whether it is a hydroxylated deriv. of Ngaione or Ipomeamarone (see Ngaione).

▶ SA9070000
Yang, D.T.C. *et al., Phytochemistry*, 1971, **10**, 1653 (*isol, struct*)
Afzal, M. *et al., Heterocycles*, 1986, **24**, 2943-2961 (*pmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 733

Ipomeamaronolide I-47

[92448-61-8]
2,3,4,5-Tetrahydro-5-methyl-5-(4-methyl-2-oxopentyl)-[2,3′-bifuran]-2′(5′H)-one, 9CI

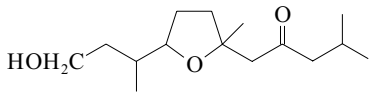


$C_{15}H_{22}O_4$ 266.336
Isol. from *Ipomoea batatas* (sweet potato) infected with *Ceratocystis fimbriata*. $[\alpha]_D$ +31 (CH_2Cl_2).

Schneider, J.A. *et al., Phytochemistry*, 1984, **23**, 759

Ipomeatetrahydrofuran I-48

[92448-62-9]
4-Methyl-1-[tetrahydro-5-(3-hydroxy-1-methylpropyl)-2-methyl-2-furanyl]-2-pentanone, 9CI



$C_{15}H_{28}O_3$ 256.384
Isol. from *Ipomoea batatas* (sweet potato) infected with *Ceratocystis fimbriata*. $[\alpha]_D$ +1 (CH_2Cl_2).

Schneider, J.A. *et al., Phytochemistry*, 1984, **23**, 759

Iprobenfos, BSI I-49

[26087-47-8]
O,O-*Bis(1-methylethyl)* S-*phenylmethyl phosphorothioate, 9CI.* S-*Benzyl* O,O-*diisopropyl phosphorothioate, 8CI. Kitazin P. Kitazin L. IBP*

$PhCH_2SP(O)[OCH(CH_3)_2]_2$

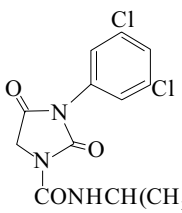
$C_{13}H_{21}O_3PS$ 288.347
Systemic rice fungicide. Yellow oil. $Bp_{0.04}$ 126°. n_D 1.5106.

▶ LD_{50} (rat, orl) 490 mg/kg. TE6550000

Tomizawa, C. *et al., J. Environ. Sci. Health, Part B*, 1976, **11**, 231 (*metab*)
U.S. Pat., 1977, 4 064 200; *CA*, **88**, 89353 (*synth*)
Torii, S. *et al., J.O.C.*, 1979, **44**, 2938 (*synth, ir, pmr*)
Shigetomi, Y. *et al., Anal. Chim. Acta*, 1983, **152**, 301 (*use*)
Pesticide Manual, 11th edn., 1997, No. 427
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BKS750

Iprodione, ANSI, BSI, ISO I-50

[36734-19-7]
3-(3,5-Dichlorophenyl)-N-*(1-methylethyl)-2,4-dioxo-1-imidazolidinecarboxamide, 9CI. Glycophene. Iprodial. Rovral. Verisan*



$C_{13}H_{13}Cl_2N_3O_3$ 330.169
Agricultural and horticultural fungicide. Cryst. Mp 136°.

▶ LD_{50} (rat, orl) 3500 mg/kg. NI8870000

U.K. Pat., 1970, 1 312 536; *CA*, **77**, 19647c
Lacroix, L. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1980, **11**, 247 (*props*)
Belafdal, O. *et al., J.O.C.*, 1989, **54**, 4193 (*pmr*)
Gardyan, C. *et al., Z. Lebensm.-Unters. - Forsch.*, 1991, **192**, 40 (*detn*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A234
Pesticide Manual, 11th edn., 1997, No. 428
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GIA000

Iron I-51

[7439-89-6]
Ferrum (L.)

Fe 55.847

Atomic No. 26. Ground state electron config. $[Ar]3d^64s^2$. Known to ancient civilisations. 10 Isotopes reported of which 4 are stable, the most common being ^{56}Fe (91.6%). 4th most abundant element in earth's crust (62,000 ppm) with traces in sea water. Most important of all metals. Four allotropic forms (α, β,γ, δ) with transition temps. 770°, 928°, 1530°. α-Form (bcc) is magnetic; β-form (also bcc) is not magnetic. The following forms of Fe are used as nutrient supplements: carbonyl iron derived by decompn. of $Fe(CO)_5$; electrolytic iron derived by electrodeposition; reduced iron obtained by a chem. process. Silvery white metal, rel. soft when pure. Traces of impurities have profound effect on physical props. (steels). Rapidly oxidised, esp. in damp air (rust). Attacked by dil. acids (→ H_2). Passivated by HNO_3. Mp 1535°. Bp 3000° (2750°).

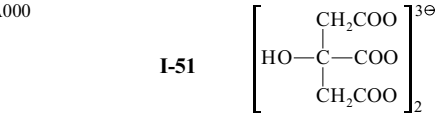
▶ Potentially toxic in all forms and by all routes of exposure, e.g. arc welder's lung. Ultrafine powdered metal is pyrophoric. NO4565500

[12596-02-0, 12596-03-1, 12596-04-2, 12663-83-1, 12663-84-2, 12663-85-3, 12663-86-4, 12663-87-5, 14067-02-8, 14067-08-4, 14067-09-5, 14067-10-8, 14127-53-8, 14127-54-9, 14127-55-0, 15438-31-0, 16603-85-3, 16904-22-6, 16904-25-9, 16941-36-9, 16941-64-3, 16941-65-4, 20074-52-6, 20074-52-6, 37240-35-0, 37366-92-0, 99007-60-0]

Mellor Compr. Treat. Inorg. Theor. Chem., 1932, **12**, 482; 1934, **13**, 1; 1935, **14**, 1 (*rev, bibl*)
Weeks, M.E. *et al., Discovery of the Elements*, J. Chem. Educ., 6th Ed., 1956, 3 (*history*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **3**, 979 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 735; 754 (*rev, bibl*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon Press, Oxford, 1986, 1242 (*rev*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1466
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1409-1411; 1414-1415
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 106; 242
Gmelin Handbook Inorg. Chem., Syst. No. 59, AI/II parts 1-8, (*rev, bibl*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1129 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IGK800

Iron(*III*) ammonium citrate I-52

[1185-57-5]
*Ammonium iron(*III*) 2-hydroxy-1,2,3-propanetricarboxylate, 8CI. Iron ammonium citrate. Ferric ammonium citrate. Soluble ferric citrate. E381*



$C_{12}H_{22}FeN_3O_{14}$ 488.164

Composition variable. Anticaking agent, dietary iron supplement. May be used in infant formulas. Garnet red scales or brown powder; deliquescent; light-sensitive. Sol. H_2O; insol. EtOH.

▶ GE7540000

[87524-94-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1282B (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, 1022 (*rev, bibl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, FAS700
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 975
Food Chemicals Codex, 4th Ed., 1996, **IV**, 147-148 (*anal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1096-1097 (*use, props*)

Iron(*II*) carbonate ($FeCO_3$) I-53

[563-71-3]

[10290-71-8]
Iron carbonate

$FeCO_3$

$CFeO_3$ 115.856
Nutrient supplement. Grey solid. Insol. H_2O; sol. acids to give CO_2; sol. H_2O saturated with CO_2 to give $Fe(HCO_3)_2$ which then oxidises. Dec. yielding CO_2 + FeO at 200°.

Mineral-*form* [14476-16-5]
Siderite. *Chalybite. Spathic iron ore*
Yellow-brown to dark brown, or grey rhombohedral cryst. Dec. on heating.

Hydrate:
Sl. sol. H_2O. Dec. on heating.

Gmelin Handbook Inorg. Chem., Syst. No. 59, 1929, **B2**, 502 (*bibl*)
Goldin, D.M. *et al., J. Therm. Anal.*, 1984, **29**, 139 (*thermal dec*)
Srivastava, K.K.P. *et al., Phys. Rev. B*, 1985, **32**, 3282 (*Mössbauer*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1107-1108
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FBH100

Iron(*III*) chloride I-54

[7705-08-0]

[24290-40-2]
Ferric chloride. Iron trichloride

$FeCl_3$

Cl_3Fe 162.205
Has the BiI_3 struct. in solid state; Fe_2Cl_6 molecules in the gas phase below 700°. Mononuclear above 750°. Nutrient supplement. Hygroscopic dark green or black cryst. Aq. solns. are strongly acidic. Sol. H_2O to give hydrates. Sol. MeOH, Et_2O. Mp 303° dec. Bp 315°.

▶ OES: long-term 1 mg m^{-3} (as Fe); short-term 2 mg m^{-3} (as Fe). Irritant. Locally corrosive in presence of moisture. LD_{50} (rat, orl) 1872 mg/kg. LJ9100000

Hexahydrate: See Tetraaquadichloroiron(*III*)(1+) in *The Combined Chemical Dictionary.*

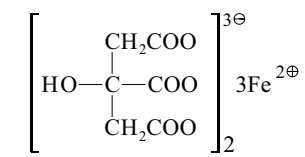
Compd. with graphite: [68896-16-2] *Graphite compd. with iron chloride ($FeCl_3$), 9CI. Iron chloride ($FeCl_3$) compd. with graphite. $FeCl_3$-graphite intercalate*Wide range of composition. Struct. contains layers of C and layers of $FeCl_3$. May contain Fe^{II}.

[10025-77-1, 18497-67-1]

Gmelin Handbook Inorg. Chem., *Syst. No.* 59, 1929, **B1**, 221 (*bibl, rev*)
Inorg. Synth., 1950, **3**, 191; 1957, **5**, 153; 1963, **7**, 163 (*synth*)
Bardawil, A.B. *et al., Inorg. Chem.*, 1964, **3**, 149 (*synth*)
Colton, R. *et al., Halides of the First Row Transition Metals*, Wiley, N.Y., 1969, 273 (*bibl, rev*)
Hosking, C.S. *et al., Aust. Paediatr. J.*, 1970, **6**, 92 (*tox*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **3**, 1641 (*synth*)
Inagaki, M. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1987, **84**, 1439-1442; *CA*, **109**, 15459 (*compd with graphite*)
Ibrahim, A.K. *et al., Phys. Rev. B: Condens. Matter*, 1987, **35**, 1860-1868 (*compd with graphite, magnetism*)
Yazami, R. *et al., Synth. Met.*, 1987, **20**, 383-386 (*compd with graphite, reactions*)
Abou Aly, A.I. *et al., Synth. Met.*, 1989, **34**, 479-484 (*compd with graphite, props*)
Wang, Z.D. *et al., Carbon*, 1991, **29**, 423-427 (*compd with graphite, Mössbauer*)
El-Shazly, O. *et al., J. Phys. Chem. Solids*, 1991, **52**, 643-646 (*compd with graphite, synth, props*)
Stolzenberg, A.M. *et al., Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley*, 1991, **14**, 881
Kalucki, K. *et al., Stud. Surf. Sci. Catal.*, 1991, **63**, 487-496; *CA*, **115**, 190720 (*compd with graphite, use*)
Wang, Z.D. *et al., Synth. Met.*, 1991, **44**, 165-176 (*compd with graphite*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1370
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2875-2883 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1097-1098
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 3835
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 742
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAU000; FAV000

Iron(*II*) citrate I-55

[23383-11-1]
Iron(II) 2-hydroxy-1,2,3-propanetricarboxylate. Iron citrate†. Ferrous citrate. Ferrutope



$C_{12}H_{10}Fe_3O_{14}$ 545.744
Dietary supplement.

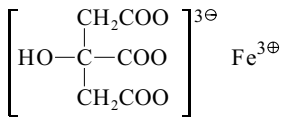
[64521-35-3]

U.K. Pat., 1962, 906 418, (*RP Scherer*); *CA*, **58**, 2187h (*synth*)
Wiltink, W.F. *et al., Clin. Chim. Acta*, 1966, **14**, 320 (*pharmacol*)
Fedorko, M.E. *et al., Exp. Cell Res.*, 1975, **95**, 385 (*pharmacol*)
Anghileri, L.J. *et al., Eur. J. Nucl. Med.*, 1985, **10**, 288
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, FBJ075
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1163
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1108

Iron(*III*) citrate I-56

[3522-50-7]

[28633-45-6]
Iron(III) 2-hydroxy-1,2,3-propanetricarboxylate. Iron citrate†. Ferric citrate, INN, JAN



$C_6H_5FeO_7$ 244.948
Indefinite composition. Nutrient supplement. Light-sensitive red scales or brown powder.
Pentahydrate: [6043-74-9]
Light-sensitive red brown. Insol. EtOH; sol. H_2O. Composition varies.
Triaqua complex: Triaqua[hydrogencitrato(3-)]iron, T-446

[54063-42-2]

Gmelin Handbook Inorg. Chem., *Syst. No.* 59, 1930, 541 (*bibl*)
Takashima, Y. *et al., Bull. Chem. Soc. Jpn.*, 1965, **38**, 1688 (*Mössbauer*)
Schaich, K.M. *et al., Lipids*, 1988, **23**, 570
Stolzenberg, A.M. *et al., Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley*, 1991, **14**, 876
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1098

Iron(*III*) diphosphate ($Fe_4(P_2O_7)_3$) I-57

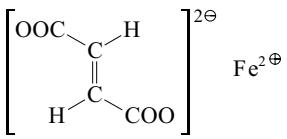
[10058-44-3]
Iron diphosphate. Ferric diphosphate. Ferric pyrophosphate. Iron(III) pyrophosphate
$Fe_4(P_2O_7)_3$
$Fe_4O_{21}P_6$ 745.218
Obt. as hydrate. Nutrient supplement used in bread fortification and infant formulas.
Hydrate:
Yellow-white powder. Insol. H_2O; sol. dil. acid. Freq. confused with the sodium citrate form below.
Sodium citrate complex:Ferric pyrophosphate - sodium citrate
Food additive. Light-sensitive green cryst. Sol. H_2O; insol. EtOH. Formulated as $Fe_4(P_2O_7)_3.nH_2O$ combined with sodium citrate.

[10402-25-2]

Gmelin Handbook Inorg. Chem., *Syst. No.* 59, 1929, 777 (*bibl*)
Takashima, Y. *et al., Bull. Chem. Soc. Jpn.*, 1965, **38**, 1684 (*Mössbauer*)
Rabinowitz, I.N. *et al., J.A.C.S.*, 1966, **88**, 4346 (*Mössbauer*)
Leitsin, V.A. *et al., Zh. Neorg. Khim.*, 1966, **11**, 278 (*soln spp*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1102-1103 (*use, props*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, No. 1339
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAZ525

Iron(*II*) fumarate I-58

[141-01-5]
Iron(II) (E)-1,2-butenedioate. Iron fumarate. Ferrous fumarate, JAN, USAN†. Feostat. Ferrocap. Toleron. Many other names



$C_4H_2FeO_4$ 169.904
Nutrient supplement. Air-stable red-brown solid. Insol. EtOH; sl. sol. H_2O. Mp 280°.
▶ LD_{Lo} (wmn, orl) 400 mg/kg. LD_{50} (rat, orl) 3850 mg/kg. LT1950000

[7705-12-6]

Weaver, *et al., Am. J. Med. Sci.*, 1961, **241**, 296 (*tox*)
Prabhakaran, P. *et al., Indian J. Chem.*, 1969, **7**, 266 (*synth*)
Tenenbein, M. *et al., Hum. Toxicol.*, 1988, **7**, 281 (*tox*)
Stolzenberg, A.M. *et al., Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley*, 1991, **14**, 880
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 976
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1108-1110
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FBJ100; IHB675

Iron(*II*) lactate I-59

[5905-52-2]
Iron(II) 2-hydroxypropanoate. Iron lactate†. Ferrous lactate. Ferro-Drops
$Fe[OOCCH(OH)CH_3]_2$
$C_6H_{10}FeO_6$ 233.988
Generally obt. as trihydrate. Nutrient supplement. May be used in infant formulas.
▶ OD5525000
Trihydrate:
Food supplement. Deliquescent, light-sensitive green cryst. Sol. H_2O; insol. EtOH.

Gmelin Handbook Inorg. Chem., *Syst. No.* 59, 1930, **B3**, 532 (*rev, bibl*)
Takashima, Y. *et al., Bull. Chem. Soc. Jpn.*, 1965, **38**, 1688 (*Mössbauer*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1111-1112 (*props, use*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1340

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LAL000

Iron(*III*) oxide (Fe_2O_3) I-60

[1309-37-1]

Iron oxide†. Diiron trioxide. Ferric oxide. Red ferric oxide. Red iron oxide. C.I. Pigment red 101. C.I. Pigment red 102

Fe_2O_3

Fe_2O_3 159.692

Food colourant esp. for sausage casings and pet food (dogs, cats). Also used as a constit. of paper/board food packaging materials. Dark red powder. Insol. H_2O. Synthetic iron oxide is available in a range of hues including yellows, browns, reds, and blacks under numerous synonyms.

► NO7400000

Monohydrate: [12168-55-7] *Iron oxide yellow*

Resistant to alkali. Precipitated pigment with fine particle size. Intensely yellow in colour.

Dihydrate: [50811-63-7]

$Fe_2H_4O_5$ 195.723

Trihydrate: [58799-87-4]

Hydrate: [12259-21-1]

Red-brown amorphous powder. Sol. acid; insol. H_2O.

α-form [1317-60-8]

[12191-78-5]

Haematite. *Hematite*

Fe(*III*) ions occupy octahedral holes in corundum-type lattice.Red-brown solid; steel grey to black cryst. Insol. H_2O; sol. HCl, H_2SO_4. Mp 1565°. Paramagnetic. Also occurs in a pseudomorphic form as Martite.

β-form

Cubic.Annealing at 500° produces α-form.

γ-form [12134-66-6]

Maghemite

Struct. derived from a spinel with Fe(*III*) ions in both tetrahedral and octahedral holes.Ferromagnetic; easily interconverted with Fe_3O_4 Iron(*II*,*III*) oxide (Fe_3O_4).

Inorg. Synth., 1939, **1**, 185; 1946, **2**, 215 (*synth*)
Nouveau Trait&ee de Chimie Min&eerale, 1967, 615 (*bibl*)
Ben-Dor, L. *et al., Acta Cryst. B*, 1976, **32**, 667 (*struct*)
Wells, A.F. *et al., Structural Inorg. Chem.*, 5th Ed., OUP, Oxford, 1984, 544 (*bibl*)
Sherman, D.M. *et al., Phys. Chem. Miner.*, 1985, **12**, 161; *CA*, **103**, 181095y (*electronic struct*)
Ram, S. *et al., J. Mater. Sci.*, 1991, **26**, 523 (*magnetism, co-cryst with BaO*)
Armelao, L. *et al., J. Mater. Chem.*, 1995, **5**, 79 (*synth*)
Cornell, R.M. *et al., The Iron Oxides*, Wiley-VCH, 1996, (*book*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1099-1101
Gmelin Handbook Inorg. Chem., *Syst. No.* 59, **B1**, 63 (*rev, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IHD000; IHF000

Iron phosphate ($FePO_4$) I-61

[10045-86-0]

[10402-24-1, 31096-47-6, 58782-48-2]

Iron(3+) phosphate (1:1), 9CI, 8CI. Iron phosphate†. Ferric phosphate. Ferric orthophosphate

$FePO_4$

FeO_4P 150.818

Nutrient supplement. Shows transition at 17K between two antiferromagnetic phases.

► LD_{50} (rat, orl) >5000 mg/kg.

[22047-20-7, 51833-68-2, 58694-82-9, 111672-13-0]

Gmelin Handbook Inorg. Chem., *Syst. No.* 59, 1931, **B4**, 773 (*synth, rev bibl*)
Jameson, R.F. *et al., J.C.S.*, 1954, 28 (*synth*)
Remy, *et al., C. R. Hebd. Seances Acad. Sci.*, 1961, **253**, 2699 (*synth*)
Griffith, W.P. *et al., J.C.S.(A)*, 1970, 286 (*Raman*)
Kotlova, A.G. *et al., Zh. Neorg. Khim.*, 1971, **16**, 41; 1972, **17**, 315; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1971, **16**, 21; 1972, **17**, 165 (*synth, props*)
Eshchenko, L.S. *et al., Zh. Neorg. Khim.*, 1973, **18**, 909; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1973, **18**, 478 (*synth, ir*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, FAZ500
Prodan, I.E. *et al., Zh. Neorg. Khim.*, 1989, **34**, 1860; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1989, **34**, 1056 (*synth, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1101-1102

Iron(*III*) sodium diphosphate (1:1:1), 9CI I-62

[10045-87-1]

*Iron(*III*) sodium pyrophosphate, 8CI*

$FeNaO_7P_2$ 252.78

Dietary supplement. Dimorphic.

Gamondes, J.P. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1969, **269**, 1532-1535; 1971, **272**, 49-52 (*synth, cryst struct, dimorphism*)
Lee, K. *et al., J. Food Sci.*, 1980, **45**, 711-715 (*use*)

Iron(*III*) sulfate ($Fe_2(SO_4)_3$) I-63

[10028-22-5]

[10124-49-9, 15244-10-7]

Ferric sulfate. Ferric trisulfate. Iron persulfate. Ferriclear

$Fe_2(SO_4)_3$

$Fe_2O_{12}S_3$ 399.885

Known in monoclinic and rhombohedral modifications. Flavouring agent. Yellow cryst. or grey-white powder. Sl. sol. H_2O; soly. increased if trace $FeSO_4$ present. Thermal dec. to $Fe_2O_3 + SO_3$; forms $[Fe(OH_2)_6]^{3\oplus}$ in soln., stabilised by $H^{\oplus}$ ion.

► NO8505000

Hexahydrate:

$Fe_2H_{12}O_{18}S_3$ 507.976

Purple.

Nonahydrate:Paracoquimbite. Coquimbite

$Fe_2H_{18}O_{21}S_3$ 562.022

Pale violet cryst., dimorphic. Various other (synthetic) hydrates also known including tri-, penta-, hexa- and dodecahydrates.

Hydrosulfate:Rhomboclase

$FeH_9O_{12}S_2$ 321.043

White to pink powder; mineral may be yellow/green cryst. Sol. H_2O. Mp 80° (loses H_2O). Formulated as HFe(*III*)$(SO_4)_2.4H_2O$ or as $Fe_2O_3.4SO_3.9H_2O$.

Double salt with ammonium sulfate: See Ammonium iron(*III*) sulfate ($(NH_4)Fe(SO_4)_2$) in *The Combined Chemical Dictionary.*

Posnjak, E. *et al., J.A.C.S.*, 1922, **44**, 1965 (*formn, phys props*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 59, 1929, 439 (*bibl, rev*)
Vertes, A. *et al., Proc. Symp. Coord. Chem., 3rd*, 1970, **1**, 477 (*hydrol, Mössbauer*)
Kiyama, M. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 1680 (*hydrol, magnetism, props, spectrophotometry*)
Masse, R. *et al., Bull. Soc. Fr. Mineral. Cristallogr.*, 1973, **96**, 346 (*struct*)
Moore, P.B. *et al., Neues Jahrb. Mineral., Abh.*, 1974, **121**, 208; *CA*, **81**, 9697u (*struct*)
Hedley, A. *et al., Water Treat. Exam.*, 1974, **23**, 389 (*use, manuf, rev, bibl*)
Christidis, P.C. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1975, **141**, 233 (*struct*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1997, **4**, 2890-2892 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1104
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FBA000

Iron(*II*) sulfate ($FeSO_4$) I-64

[7720-78-7]

[10124-49-9]

Ferrous sulfate, JAN, USAN. Feosol

$FeSO_4$

FeO_4S 151.911Component of Formalox, Cytoferin and Mediatric. $^{59}FeSO_4$ used as radioactive agent (Ferrous sulfate Fe 59, USAN). Paramagnetic, $\mu_{eff} = 4.9\mu_B$.

► Effects of excessive oral or parenteral iron therapy (which may be delayed) include gastrointestinal, renal, and hepatic toxicities. Average human lethal dose from ingestion *ca.* 200-500 mg Fe/kg. LD_{50} (rat, orl) 319 mg/kg. Exp. reprod. and teratogenic effects. OES: long-term 1 mg m^{-3} (as Fe); short-term 2 mg m^{-3} (as Fe).
NO8500000

Monohydrate: [13463-43-9]

[17375-41-6]

Tetrahydrate:

Hexahydrate: [42120-27-4] *Iron(*II*) sulfate hexahydrate. Ferrous sulfate hexahydrate. Hexaaquairon(2+) sulfate*

$FeH_{12}O_{10}S$ 260.002

Heptahydrate: [7782-63-0]

[15491-23-3] *Iron vitriol. Copperas. Green vitriol. Sal chalybis*

$FeH_{14}O_{11}S$ 278.017

Nutrient supplement. Hygroscopic blue-green cryst. Sol. H_2O to give $[Fe(H_2O)_6]^{2\oplus}$; acidic soln. insol. EtOH. Mp 64°. Loses $7H_2O$ at 300°. μ_{eff} =

5.22μ_B.

► NO8510000

Basic sulfate: See Iron(*III*) hydroxide sulfate ($Fe(OH)(SO_4)$) in *The Combined Chemical Dictionary.*

Double salt with ammonium sulfate: See Ammonium iron(*II*) sulfate ($(NH_4)_2Fe(SO_4)_2$) in *The Combined Chemical Dictionary.*

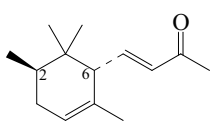
Glycine complex: [17169-60-7] ***Ferroglycine sulfate***. *Plesmet*. *Kelferon*. *Ferronord*. *Ferro sanol*. *Glyferro*. *Pleniron*

[7782-63-0, 20908-72-9]

Fraenckel, F. *et al., Z. Anorg. Allg. Chem.*, 1907, **55**, 223
Gmelin Handbook Inorg. Chem., *Syst. No.* 59, 1929, **B2**, 394 (*bibl*)
U.K. Pat., 1958, 802 565, (*Dr. Schwarz Arzneimittelfabrik*); *CA*, **53**, 9583d (*ferroglycine sulfate*)
Baur, W.H. *et al., Acta Cryst.*, 1964, **17**, 1167 (*cryst struct, heptahydrate*)
Figgis, B.N. *et al., Prog. Inorg. Chem.*, 1964, **6**, 177 (*magnetism*)
Tyagi, R.N. *et al., Indian J. Pure Appl. Phys.*, 1973, **11**, 698 (*Mössbauer*)
Lowenheim, F.A. *et al., Industrial Chemicals*, (Eds.), 4th Ed., Wiley-Interscience, N.Y., 1975, 418 (*synth*)
Zimmermann, R. *et al., Phys. Rev. B*, 1975, **12**, 3902 (*struct*)
Elinder, C.-G. *et al., Handb. Toxicol. Met.*, (Eds. Friberg, L. *et al*), 2nd edn., Elsevier, 1986, **2**, 276 (*tox, rev*)
Pelovski, Y. *et al., J. Therm. Anal.*, 1990, **36**, 1727 (*thermal dec*)
Crichton, R.R. *et al., Inorganic Biochemistry of Iron Metabolism*, Ellis Horwood, 1991, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 976
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2888-2889 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1113
Pesticide Manual, 12th edn., 2000, No. 346
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FBN100; FBO000

α-Irone I-65

[79-69-6]
4-(2,5,6,6-Tetramethyl-2-cyclohexen-1-yl)-3-buten-2-one, 9CI. FEMA 2597



(2*R*,6*R*) - *form*

$C_{14}H_{22}O$ 206.327
Flavouring ingredient.

► EN0335000

(2*R*,6*R*)-*form* [35124-14-2]
(-)-trans-*form*
Oil. $[\alpha]_D^{20}$ -410 ($CHCl_3$).

7,8-Dihydro: [124886-68-6] **trans-*Dihydro-α-irone***
$C_{14}H_{24}O$ 208.343
Oil.

(2*R*,6*S*)-*form* [35124-13-1]
(+)-cis-*form*
Oil. $Bp_{0.3}$ 90-96°. $[\alpha]_D^{20}$ +109 ($CHCl_3$).

(2*S*,6*S*)-*form* [90242-81-2]
(+)-trans-*form*
Oil. $[\alpha]_D$ +420 (CH_2Cl_2).

(2*S*,6*R*)-*form* [89888-03-9]
(-)-cis-*form*
Oil. $[\alpha]_D$ -96.3.

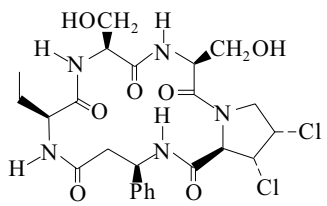
7,8-Dihydro: [132437-13-9] **cis-*Dihydro-α-irone***
$C_{14}H_{24}O$ 208.343
Oil.

7,8-Epoxide: [124886-69-7] ***Epoxy*-cis-*dihydro-α-irone***
$C_{14}H_{22}O_2$ 222.327
Oil.

Barton, D.H.R. *et al., J.C.S.*, 1960, 271-272 (*isol, synth, bibl*)
Rautenstrauch, V. *et al., Helv. Chim. Acta*, 1971, **54**, 1776-1788; 1984, **67**, 325-331 (*isol, struct, bibl*)
Shenvi, V.B. *et al., Some Recent Dev. Chem. Nat. Prod.*, 1972, 1-5 (*rev*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1973, **56**, 1874-1882 (*abs config*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 551 (*rev, tox*)
Torii, S. *et al., J.O.C.*, 1980, **45**, 16-20 (*synth*)
Miyashita, M. *et al., J.C.S. Perkin 1*, 1982, 1303-1309 (*synth*)
Krick, W. *et al., Helv. Chim. Acta*, 1984, **67**, 318-323 (*cd*)
Nussbaumer, C. *et al., J.O.C.*, 1987, **52**, 2096-2098 (*(±)-cis-α-irone, synth*)
Maurer, B. *et al., Helv. Chim. Acta*, 1989, **72**, 1400-1415 (*iris germanica constit, isol, pmr, cmr, bibl*)
Ohtsuka, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2540-2544 (*synth*)
Schulte-Elte, K.H. *et al., Helv. Chim. Acta*, 1992, **75**, 759-765 (*(±)-form, synth*)
Chapuis, C. *et al., Helv. Chim. Acta*, 1993, **76**, 2070-2088 (*bibl, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 374
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1408-1409
Brenna, E. *et al., Helv. Chim. Acta*, 1999, **82**, 2246-2259 (*synth*)
Aleu, J. *et al., Eur. J. Org. Chem.*, 2000, 3031-3038 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IGW500

Islanditoxin I-66

[10089-09-5]
Cyclic(3-phenyl-β-alanyl-α-aminobutyryl-serylseryl-3,4-dichloroprolyl), 9CI

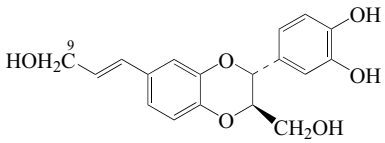


$C_{24}H_{31}Cl_2N_5O_7$ 572.444
Mycotoxin prod. by the common food storage mould *Penicillium islandicum*. Needles (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 250-251° dec. $[\alpha]_D^{21}$ -47.7 (c, 1.99 in AcOH). Similar chemical and biological characteristics to Cyclochlorotine, C-441 λ_{max} 253 ; 259 ; 265 (MeOH) (Berdy). λ_{max} 268 (NH_4OH) (Berdy).

► LD_{50} (mus, scu) 4.7 mg/kg.
Ghosh, A.C. *et al., J. Het. Chem.*, 1980, **17**, 1809 (*rev*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 712

Isoamericanol A I-67

[121620-06-2]
Isoamericanol



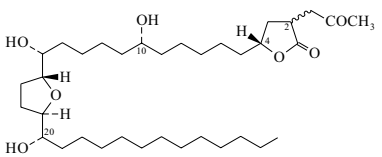
$C_{18}H_{18}O_6$ 330.337
Isol. from the seeds of *Phytolacca americana* (pokeberry). Prims (Me_2CO/EtOAc). Mp 157-159°. Racemic λ_{max} 218 (ε 26800); 224 (ε 24400); 234 (ε 21100); 250 (ε 16700); 290 (ε 14600); 310 (ε 19500); 330 (ε 19500) (EtOH).

9-Aldehyde: [109063-85-6] ***Isoamericanin A***
$C_{18}H_{16}O_6$ 328.321
Isol. from seeds of *Phytolacca americana* (pokeberry). Mp 177-178°.

Hasegawa, T. *et al., Chem. Lett.*, 1987, 329 (*Isoamericanin A*)
Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 252 (*Isoamericanol A*)
She, X. *et al., J. Chem. Res., Synop.*, 1999, 100-101 (*synth*)
She, X. *et al., Synth. Commun.*, 1999, **29**, 2625-2628 (*synth, pmr*)
Gu, W.X. *et al., Chin. Chem. Lett.*, 2001, **12**, 485-486 (*synth*)
Takahashi, H. *et al., Heterocycles*, 2002, **56**, 245-256 (*synth*)
Waibel, R. *et al., Phytochemistry*, 2003, **62**, 805-811 (*isol, pmr, cmr, struct*)

Isoannonacin A I-68

[123266-22-8]
Annonacin-A-one



$C_{35}H_{64}O_7$ 596.886
Constit. of *Annona muricata* (soursop) and *Asimina triloba* (pawpaw). Mp 91-92°. $[\alpha]_D$ +20 (c, 0.2 in $CHCl_3$).

20-Epimer: ***Isoannonacin***
$C_{35}H_{64}O_7$ 596.886
Isol. from *Annona muricata* (soursop) and *Asimina triloba* (pawpaw). Cryst. Sol. MeOH, C_6H_6, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O. Mp 96-98°. $[\alpha]_D^{20}$ +24.8 (c, 0.1 in MeOH). Obt. as a mix. of 2,4-*cis*- and *trans*-isomers.

10-Ketone, 20-epimer: [123266-23-9] ***Isoannonacin-10-one***
$C_{35}H_{62}O_7$ 594.871
Cryst. Sol. MeOH, $CHCl_3$, C_6H_6; fairly

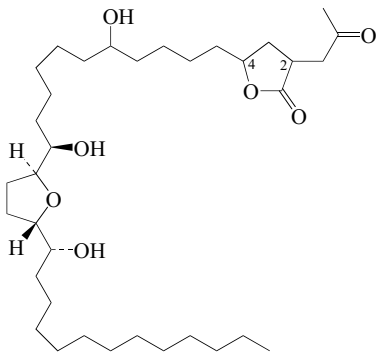
sol. hexane; poorly sol. H_2O. Mp 103.5°. $[\alpha]_D^{20}$ +19.8 (c, 0.05 in MeOH). A mix. of 2,4-*cis*- and *trans*-isomers.

[152784-18-4, 152784-19-5, 152784-21-9, 152784-22-0]

Xu, L.-X. *et al., J.O.C.*, 1989, **54**, 5418 (*isol, pmr, cmr, struct*)
Zhao, G.-X. *et al., Phytochemistry*, 1993, **33**, 1065 (*isol, struct*)
Wu, F.E. *et al., J. Nat. Prod.*, 1995, **58**, 1430 (*isol, pmr, cmr*)

Isoannoreticuin I-69

[142474-61-1]

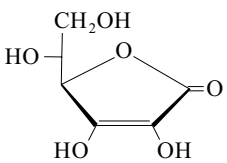


$C_{35}H_{64}O_7$ 596.886
Acetogenin isol. from *Annona reticulata* (custard apple). Amorph. powder. $[\alpha]_D^{24}$ +9.7 (c, 0.33 in $CHCl_3$). Isol. as 2,4-*cis*- and *trans*-isomers λ_{max} 210 (EtOH) (Berdy).

Wu, Y.-C. *et al., Heterocycles*, 1992, **34**, 667-674 (*isol, pmr, cmr*)

Isoascorbic acid I-70

erythro-*Hex-2-enonic acid 1,4-lactone, 9CI, 8CI. Araboascorbic acid. Isovitamin C. Erythorbic acid. Saccharosonic acid. Erycorbin. Glucosaccharonic acid*



D-*form*

$C_6H_8O_6$ 176.126

D-*form* [89-65-6]
E315. FEMA 2410
Prod. from glucose by *Penicillium* spp. Antioxidant for foods and soft drinks. Flavouring ingredient; colouring preservative/antioxidant in fruit and meat products. Mp 168° dec. $[\alpha]_D^{20}$ -22 (H_2O).
▶ KF3015000

Na salt: [6381-77-7] *Sodium erythorbate. E316*
Antioxidant, antimicrobial agent, appearance control agent, curing accelerator for baked goods, meat and cured meat products. Restricted use in Japan. Cryst. powder. $[\alpha]_D^{25}$ +95.5 → +98 (H_2O).

5,6-O-Isopropylidene:5,6-O-Isopropylidene-D-erythro-hex-2-enono-1,4-lactone
$C_9H_{12}O_6$ 216.19
Mp 187-189°. $[\alpha]_D^{25}$ +26.5 (c, 1.0 in H_2O).

5,6-O-Cyclohexylidene:5,6-O-Cyclohexylidene-D-erythro-hex-2-enono-1,4-lactone
$C_{12}H_{16}O_6$ 256.255
Mp 176-178°. $[\alpha]_D^{25}$ -17.8 (c, 1.0 in Me_2CO) (>98% ee).

L-*form* [26094-91-7]
Prisms (Me_2CO/MeOH/petrol). Mp 168° dec. $[\alpha]_D^{20}$ +19 (c, 0.9 in H_2O). $[\alpha]_D^{20}$ +17 (c, 0.6 in MeOH).

Na salt:
Cryst. powder. $[\alpha]_D^{20}$ -94 (c, 0.7 in H_2O).

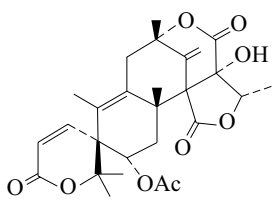
3-Me:3-O-Methyl-L-erythro-hex-2-enono-1,4-lactone
$C_7H_{10}O_6$ 190.152
Needles (MeOH/Et_2O). Mp 120-122°. $[\alpha]_D^{19}$ +42 (c, 0.72 in MeOH).

[7378-23-6, 63524-04-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 707A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1150B (*nmr*)
Maurer, K. *et al., Ber.*, 1934, **67**, 1239-1241 (*D-form, synth*)
Reichstein, T. *et al., Helv. Chim. Acta*, 1934, **17**, 510-520 (*D-form, L-form, L-Me*)
Baird, D.K. *et al., J.C.S.*, 1934, 62-67 (*L-form, synth*)
Esselen, W.B. *et al., Ind. Eng. Chem.*, 1945, **37**, 295-306 (*rev, use*)
Takahashi, T. *et al., Nature (London)*, 1960, **188**, 411-412 (*isol*)
Takahashi, T. *et al., Biochim. Biophys. Acta*, 1961, **51**, 410-412 (*biosynth*)
Azarnia, N. *et al., Acta Cryst. B*, 1972, **28**, 2157-2161 (*D-form, cryst struct*)
Carlsen, P.H.J. *et al., Acta Chem. Scand.*, 1995, **49**, 297-300 (*isopropylidene, cyclohexylidene*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 209
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 931-932; 2554-2555 (*use, props*)

Isoaustin I-71

[85066-64-4]
5-(Acetyloxy)-17-de(acetyloxy)austin, 9CI

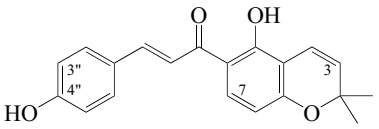


$C_{27}H_{32}O_9$ 500.544
Mycotoxin from of *Penicillium diversum*. Cryst. Mp 290° dec. $[\alpha]_D^{22}$ +172.3 (c, 0.35 in $CHCl_3$). λ_{max} 240 (ε 7400) (MeOH) (Berdy).

Simpson, T.J. *et al., J.C.S. Perkin 1*, 1982, 2687

Isobavachromene I-72

[52801-22-6]
1-(5-Hydroxy-2,2-dimethyl-2H-1-benzopyran-6-yl)-3-(4-hydroxyphenyl)-2-propen-1-one, 9CI. 5-Hydroxy-6-(4-hydroxycinnamoyl)-2,2-dimethylchromene. 4-Hydroxylonchocarpin



$C_{20}H_{18}O_4$ 322.36
Orange-red needles (hexane/EtOAc). Mp 207-208°. λ_{max} 202 (log ε 4.16); 230 (log ε 4.32); 280 (log ε 4.15); 375 (log ε 4.59) (MeOH).

7-Methoxy: [189299-05-6] ***Xanthohumol C**. Dehydrocycloxanthohumol*
$C_{21}H_{20}O_5$ 352.386
Constit. of the female inflorescence of hops (*Humulus lupulus*). Red needles. λ_{max} 285 ; 298 (sh) ; 371 (MeOH).

7-Methoxy, 3ξ-hydroxy, 3,4-dihydro: [189308-10-9] ***Xanthohumol B**. Dehydrocycloxanthohumol hydrate*
$C_{21}H_{22}O_6$ 370.401
Constit. of hops (*Humulus lupulus*). λ_{max} 205 (log ε 4.47); 370 (log ε 4.35) (EtOH).

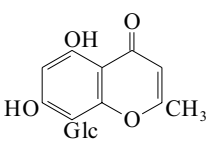
*7-Methoxy, 4ξ-hydroxy, 3,4-dihydro:**Isoxanthohumol B**. Isodehydrocloxanthohumol hydrate*
$C_{21}H_{22}O_6$ 370.401
Constit. of hops (*Humulus lupulus*).

[56083-03-5]

Lupi, A. *et al., Farmaco, Ed. Sci.*, 1975, **30**, 449 (*synth*)
Braz Filho, R. *et al., Phytochemistry*, 1975, **14**, 1454 (*isol*)
Delle Monache, F. *et al., Phytochemistry*, 1978, **17**, 1812 (*isol*)
Tomita, K. *et al., Cryst. Struct. Commun.*, 1982, **11**, 221 (*cryst struct*)
Stevens, J.F. *et al., Phytochemistry*, 1997, **44**, 1575-1585; 2000, **759**, 775 (*Xanthohumols*)
Tabata, N. *et al., Phytochemistry*, 1997, **46**, 683-687 (*Xanthohumol B*)
Ettteldorf, N. *et al., Z. Naturforsch., C*, 1999, **54**, 610-612 (*Isoxanthohumol B*)
Stevens, J.F. *et al., Phytochemistry*, 2000, **53**, 759-775 (*Xanthohumols*)

Isobiflorin I-73

[152041-16-2]
8-β-D-Glucopyranosyl-5,7-dihydroxy-2-methyl-4H-1-benzopyran-4-one. 8-Glucosyl-5,7-dihydroxy-2-methylchromone. 8-C-Glucopyranosylnoreugenin. Clove 3



$C_{16}H_{18}O_9$ 354.313
Constit. of *Syzygium aromaticum* (clove). Needles + ½H_2O (H_2O). Mp 183-184°. $[\alpha]_D$ +22.7 (c, 0.5 in MeOH). λ_{max} 209 (log ε 4.33); 251 (log ε 4.24); 257 (log ε 4.26); 296 (log ε 3.76) (MeOH).

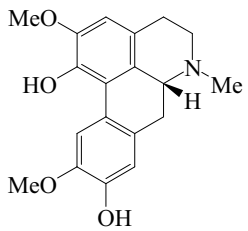
6″-O-(3,4,5-Trihydroxybenzoyl): [152041-17-3]
$C_{23}H_{22}O_{13}$ 506.419

Constit. of *Syzygium aromaticum* (clove). Amorph. powder +½ H_2O. $[\alpha]_D^{28}$ -54.9 (c, 1 in H_2O).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1232 (*isol, pmr, cmr, struct*)
Zhang, Y. *et al., Phytochemistry*, 1997, **45**, 401-403 (*isol, uv, ir, pmr, cmr, ms*)
Okamura, N. *et al., Phytochemistry*, 1998, **49**, 219-223 (*isol, uv, pmr, cmr*)
Toda, M. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 294-298 (*isol*)

Isoboldine I-74

1,9-Dihydroxy-2,10-dimethoxyaporphine. N-Methylaurelliptine



(*R*)-*form*

$C_{19}H_{21}NO_4$ 327.379

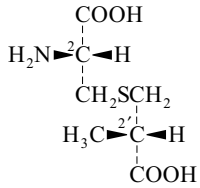
(*S*)-*form* [3019-51-01]
Alkaloid from *Sassafras* and from the leaves of *Peumus boldus* (boldo). Flavouring ingredient. Mp 178-180° dec. $[\alpha]_D^{13}$ +54 (c, 0.20 in EtOH). λ_{max} 219 (ϵ 38020); 280 (ϵ 14454); 304 (ϵ 16220) (MeOH) (Berdy).

N-*De-Me:* [23599-69-1] *1,9-Dihydroxy-2,10-dimethoxynoraporphine.* ***Laurelliptine****. Norisoboldine*
$C_{18}H_{19}NO_4$ 313.352
Alkaloid from *Zizyphus jujuba* (Chinese date). Cryst. (C_6H_6/EtOH). Mp 190-192°. $[\alpha]_D^{21}$ +47.3 (c, 1.0 in EtOH).

Clezy, P.S. *et al., Aust. J. Chem.*, 1966, **19**, 135 (*isol, uv, pmr, Isoboldine, Laurelliptine*)
Johns, S.R. *et al., Aust. J. Chem.*, 1966, **19**, 2331; 1969, **22**, 1277 (*isol, uv, pmr, Isoboldine, Laurelliptine*)
Chan, W.W.C. *et al., J.C.S.(C)*, 1966, 753 (*synth, ir, uv, pmr*)
Jackson, A.H. *et al., J.C.S.(C)*, 1966, 2061 (*synth, uv, pmr*)
Wada, K. *et al., J. Agric. Food Chem.*, 1968, **16**, 471
Brown, G.M. *et al., Acta Cryst. B*, 1977, **33**, 2051 (*cryst struct, abs config*)
Kametani, T. *et al., J.A.C.S.*, 1977, **99**, 3805 (*synth*)
Roques, R. *et al., Acta Cryst. B*, 1978, **34**, 837 (*cryst struct, Laurelliptine*)
Ricca, G.S. *et al., Gazz. Chim. Ital.*, 1979, **109**, 1 (*cmr, pmr*)
Marsaioli, A.J. *et al., Phytochemistry*, 1979, **18**, 165 (*cmr*)

Isobuteine I-75

[4746-40-1]
S-(2-Carboxypropyl)cysteine, 9CI. 3-[(2-Carboxypropyl)thio]alanine. β-Isobuteine



(2*R*,2′*S*)-*form*

$C_7H_{13}NO_4S$ 207.25

(2*R*,2′*S*)-*form* [66512-75-2]
Occurs naturally as a component of the tripeptide *S*-(2-carboxypropyl)glutathione in onion and in garlic. Cryst. (Me_2CO aq.). Mp 196-198° dec. $[\alpha]_D^{25}$ -66.1 (c, 2.5 in H_2O). $[\alpha]_D^{25}$ -44.3 (c, 2.4 in 2.5*M* HCl). Other diastereoisomers also known.

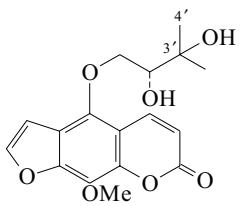
S,S-*Dioxide:* [66403-99-4] *3-[(2-Carboxypropyl)sulfonyl]alanine, 9CI*
$C_7H_{13}NO_6S$ 239.249
Blades (H_2O). Mp 174° dec. (gas evolution). $[\alpha]_D^{25}$ -24 (c, 1.7 in H_2O).

[6852-42-2, 66429-71-8, 66512-76-3]

Virtanen, A.I. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1960, **322**, 8 (*isol*)
Granroth, B. *et al., Acta Chem. Scand.*, 1967, **21**, 1654 (*bisynth*)
Carson, J.F. *et al., J.C.S. Perkin 1*, 1977, 1964 (*synth, pmr*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 433 (*occur*)
Parry, R.J. *et al., J.A.C.S.*, 1985, **107**, 2512 (*synth, abs config*)

Isobyakangelicin I-76

[50791-60-1]



$C_{17}H_{18}O_7$ 334.325

(*R*)-*form*
Cryst. Mp 132.5-133°. $[\alpha]_D^{23}$ +16 (c, 0.1 in Py).

3′-O-β-D-Glucopyranoside:
$C_{23}H_{28}O_{12}$ 496.467
Constit. of *Angelica archangelica* (angelica). Noncryst. $[\alpha]_D^{25}$ +29 (c, 0.09 in MeOH).

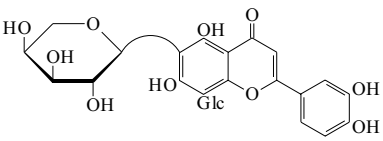
2′-O-Angeloyl:
$C_{22}H_{24}O_8$ 416.427
$[\alpha]_D^{20}$ -1.6 ($CHCl_3$).

3′-Deoxy, 3′,4′-didehydro: [80508-43-6] ***Apaensin***
$C_{17}H_{16}O_6$ 316.31
Cryst. Mp 143-145°. $[\alpha]_D^{20}$ +35 ($CHCl_3$).

Sun, H. *et al., Yunnan Zhiwu Yanjiu*, 1981, **3**, 279; *CA*, **96**, 48961 (*Apaensin*)
Thastrup, O. *et al., Phytochemistry*, 1983, **22**, 2035
Vuorela, H. *et al., Planta Med.*, 1988, **54**, 538 (*deriv*)

Isocarlinoside I-77

[83151-90-0]
6-α-L-Arabinopyranosyl-2-(3,4-dihydroxyphenyl)-8-β-D-glucopyranosyl-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. 6-Arabinopyranosyl-8-glucopyranosyl-3′,4′,5,7-tetrahydroxyflavone. 6-Arabinopyranosyl-8-glucopyranosylluteolin. 6-Arabinosyl-8-glucosylluteolin



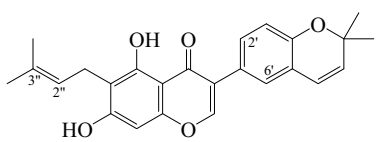
$C_{26}H_{28}O_{15}$ 580.498
Isol. from *Glycine max* (soybean).

3′-Me ether: ***6-Arabinopyranosyl-8-β-D-glucopyranosyl-4′,5,7-trihydroxy-3′-methoxyflavone***
$C_{27}H_{30}O_{15}$ 594.525
Probable struct..

Linard, A. *et al., Phytochemistry*, 1982, **21**, 797 (*isol, spectra*)
Salmenkallio, S.S. *et al., Phytochemistry*, 1982, **21**, 2990 (*deriv*)
Jay, M. *et al., Phytochemistry*, 1984, **23**, 1153 (*isol*)

Isochandalone I-78

[121747-90-8]
3-(2,2-Dimethyl-2H-1-benzopyran-6-yl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI



$C_{25}H_{24}O_5$ 404.462
Amorph. powder.

2′-Hydroxy: ***Kraussianone B***
$C_{25}H_{24}O_6$ 420.461
Cryst. Mp 162-168°.

6′-Hydroxy: [100462-54-2] ***Angustone B***
$C_{25}H_{24}O_6$ 420.461
Cryst. (Et_2O/petrol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 160-161°. λ_{max} 231 (sh) (log ϵ 4.36); 271 (log ϵ 4.51); 310 (sh) (log ϵ 3.98) (MeOH) (Berdy). λ_{max} 272 ; 344 (MeOH-NaOH) (Berdy).

2′,3″-Dihydroxy, 2″,3″-dihydro: ***Kraussianone C***
$C_{25}H_{26}O_7$ 438.476
Orange-yellow cryst. Mp 218-220°. Softens at 156°.

3″,6′,-Dihydroxy, 2″,3″-dihydro: [181476-22-2] ***Kanzonol T***
$C_{25}H_{26}O_7$ 438.476
Constit. of *Glycyrrhiza glabra* (licorice). Granules (C_6H_6/Me_2CO). Mp 205-209°. λ_{max} 214 (log ϵ 4.22); 225 (sh) (log ϵ 4.18); 268 (log ϵ 4.23); 305 (sh) (log ϵ 3.86) (MeOH).

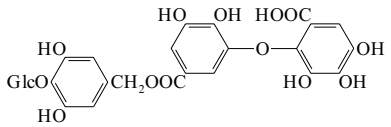
$\Delta^{3''}$-Isomer, 2″-hydroxy: ***Ulexin A***
$C_{25}H_{24}O_6$ 420.461

Cryst. (EtOAc/hexane). Mp 167-169°. $[\alpha]_D$ -9.8 (c, 0.11 in $CHCl_3$). λ_{max} 226 (ε 114320); 238 (ε 110000); 269 (ε 119740); 326 (ε 39900) (MeOH).

Lane, G.A. *et al., Phytochemistry*, 1987, **26**, 295-300 (*Angustone B*)
Tahara, S. *et al., Phytochemistry*, 1989, **28**, 901-911 (*isol, uv, pmr*)
Fukai, T. *et al., Phytochemistry*, 1996, **43**, 531-532 (*Kanzonol T*)
Maximo, P. *et al., Z. Naturforsch., C*, 2000, **55**, 506-510 (*Ulexin A*)
Drewes, S.E. *et al., Phytochemistry*, 2002, **59**, 739-747 (*Kraussianones B,C*)

Isochesnatin I-79

[115356-00-8]

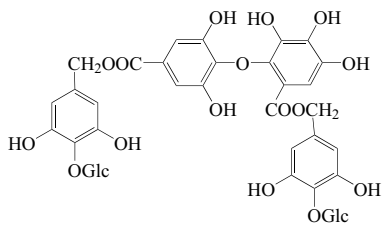


$C_{27}H_{26}O_{18}$ 638.492
Isol. from the leaf of *Castanea mollissima* (Chinese chestnut). Off-white amorph. powder + $1\frac{1}{2}H_2O$. $[\alpha]_D^{20}$ -20.9 (c, 0.65 50% aq. MeOH).

Feng, H. *et al., Phytochemistry*, 1988, **27**, 1185 (*struct, pmr, cmr*)

Isochestanin I-80

[115356-01-9]

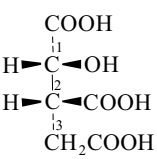


$C_{40}H_{42}O_{26}$ 938.756
Constit. of *Castanea mollissima* (Chinese chestnut). Off-white powder. $[\alpha]_D^{20}$ -84.8 (c, 1 in Me_2CO aq.).

Feng, H. *et al., Phytochemistry*, 1988, **27**, 1185-1189 (*isol, pmr, cmr*)

Isocitric acid I-81

[320-77-4]
1-Hydroxy-1,2,3-propanetricarboxylic acid. 1-Hydroxytricarballylic acid. 3-Carboxy-3,4-dideoxypentaric acid, 9CI



(1*R*,2*R*)-*form*

$C_6H_8O_7$ 192.125
Note differing numbering systems. The one shown here is based on the hydroxypropanetricarboxylic acid name. In the older lit. there appears to be some confusion in the application of the *erythro*/*threo* and D/L-stereodescriptors and these should be avoided.pK_{a1} 3.28; pK_{a2} 4.71; pK_{a3} 6.4 (25°). pK_{a1} 3.02; pK_{a2} 4.28; pK_{a3} 5.75 (25°).

(1*R*,2*R*)-*form* [30810-51-6]
(-)-erythro-*form. (-)-Alloisocitric acid*
Found in lemon juice. $[\alpha]_D$ -34.1 (c, 0.5-1 in H_2O).

1,4-Lactone:Tetrahydro-5-oxo-2,3-furandicarboxylic acid
$C_6H_6O_6$ 174.11
Mp 143°. $[\alpha]_D$ -40.5 (H_2O).

(1*R*,2*S*)-*form* [6061-97-8] *(+)*-threo-*form. (+)-Isocitric acid*
Found in fruit juices. Occurs in blackberry. Mp 105°. $[\alpha]_D$ +30.6 (H_2O).

Di-Me ester:
$C_8H_{12}O_7$ 220.179
Mp 106°. $[\alpha]_D^{20}$ -63.

Tri-Et ester:
$C_{12}H_{20}O_7$ 276.286
Liq. Bp_{10} 180-181°.

Triamide:
$C_6H_{11}N_3O_4$ 189.171
Mp 204° dec.

1,4-Lactone: [43009-34-3]
Mp 154°. $[\alpha]_D$ -61.1 (H_2O).

(1*S*,2*S*)-*form* *(+)*-erythro-*form. (+)-Alloisocitric acid*
$[\alpha]_D$ +34.6.

1,4-Lactone:
Mp 143°. $[\alpha]_D$ +41 (c, 4.8 in H_2O).

1,4-Lactone, di-Me ester:
$C_8H_{10}O_6$ 202.163
Mp 49-50°. $[\alpha]_D^{27}$ +56.2 (c, 0.85 in MeOH).

(1*S*,2*R*)-*form* [55582-48-4] *(-)*-threo-*form. (-)-Isocitric acid*
$[\alpha]_D$ -30 (H_2O).

1,4-Lactone: [27584-86-7]
Cryst. (EtOH/toluene). Mp 156-157°. $[\alpha]_D$ +60.9 (H_2O).

(1*RS*,2*RS*)-*form* [344-79-6] *(±)*-erythro-*form. (±)-Alloisocitric acid*

1,4-Lactone: [3118-83-0]
Mp 153°.

(1*RS*,2*SR*)-*form* [18979-21-0] *(±)*-threo-*form. (±)-Isocitric acid*

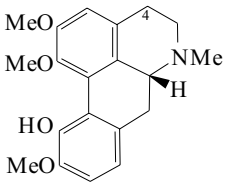
1,4-Lactone: [4702-32-3]
$C_6H_6O_6$ 174.11
Mp 161°.

[1637-73-6]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1145A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 704C (*ir, lactone*)
Kaneko, T. *et al., Chem. Ind. (London)*, 1960, 1187; 1188 (*struct*)
Vickery, H.B. *et al., J. Biol. Chem.*, 1962, **237**, 1739 (*nomencl*)
Patterson, A.L. *et al., J.A.C.S.*, 1962, **84**, 309 (*cryst struct*)
Clark, R.B. *et al., Crop Sci.*, 1969, **9**, 341 (*isol*)
Lehninger, A.L. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1978, **75**, 1690 (*metab*)

Isocorydine I-82

11-Hydroxy-1,2,10-trimethoxyaporphine. Artabotrin. Luteanine†



(*R*)-*form*

$C_{20}H_{23}NO_4$ 341.406

(*R*)-*form* [55056-91-2]
Amorph. powder. Mp 78-80°. $[\alpha]_D^{25}$ -190 (c, 0.02 in $CHCl_3$).

α-N-*Oxide:* [25405-80-5] ***Isocorydine* N-oxide**
$C_{20}H_{23}NO_5$ 357.405
Amorph. solid or gum. Mp 228-229° (as hydrochloride). The *M. velutina* isolate (confusingly called (-)-Isocorydine *N*-oxide by the authors), to which the opt. rotn. refers, is the only isolate with determined stereochem. It appears to have different stereochem from the *B. integerrima* isolate (no opt. rotn. reported) to which the Mp refers. λ_{max} 221 (log ε 4.31); 268 (log ε 3.87); 306 (log ε 3.46) (MeOH).

N-*De-Me:* [194923-28-9]
Alkaloid from *Annona cherimola* (cherimoya). Brown powder. Mp 200-203°. $[\alpha]_D^{24}$ -46 (c, 0.5 in $CHCl_3$). λ_{max} 223 ; 265 ; 309 (no solvent reported).

N-*De-Me,* N-*(methoxycarbonyl):* [344928-15-0] N-*Methoxycarbonylnorisocorydine.* ***Romucosine H***
$C_{21}H_{23}NO_6$ 385.416
Alkaloid from *Annona cherimola* (cherimoya). Amorph. brown powder. Mp 230-233°. $[\alpha]_D^{24}$ -43 (c, 0.01 in $CHCl_3$). λ_{max} 222 (log ε 4.39); 270 (log ε 4.19); 310 (log ε 3.8) (EtOH).

(*S*)-*form* [475-67-2]
Alkaloid from *Peumus boldus* (boldo). Poorly sol. hexane. Mp 185°. $[\alpha]_D^{23}$ +215 (c, 1 in $CHCl_3$). λ_{max} 210 ; 267 ; 302 (MeOH) (Berdy).
▶ LD_{50} (rat, ipr) 10.9 mg/kg. CE1057950

Hydrochloride: [13552-72-2]
Mp 215-218° (dec.). $[\alpha]_D^{20}$ +170 (c, 0.5 in $CHCl_3$).

N-*Me:* [25342-82-9] ***Menisperine.*** N-*Methylisocorydine. Chakranine*
$C_{21}H_{26}NO_4^{\oplus}$ 356.441
Prisms (EtOH)(as chloride). Mp 217-218° dec. (slow heating)(chloride) Mp 235° (rapid heating)(chloride). $[\alpha]_D^{15}$ +146.3 (c, 0.17 in $CHCl_3$).

N-*De-Me:* [475-70-7] ***Norisocorydine.*** *Sanjoinine Ib*
$C_{19}H_{21}NO_4$ 327.379
Alkaloid from *Peumus boldus* (boldo). Mp 203-205° (as hydrobromide). $[\alpha]_D^{20}$ +158.5 (c, 0.1 in EtOH) (hydrobromide). Free base unstable.

4R-*Hydroxy:* [151271-85-1] ***Rhopalotine.*** *Crabbine*
$C_{20}H_{23}NO_5$ 357.405
Cryst. (MeOH). Mp 191°. $[\alpha]_D$ +162 (c,

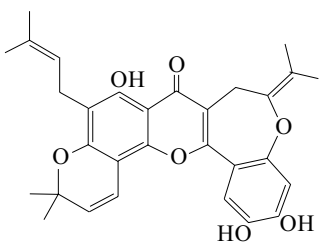
0.2 in MeOH).

(±)-*form* [36284-37-4]
Mp 151-152°.

Gadamer, J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1911, **249**, 641 (*isol*)
Comin, J. *et al., J.O.C.*, 1954, **19**, 1774 (*Isocorydine, Menisperine, isol, uv, struct*)
Ruegger, A. *et al., Helv. Chim. Acta*, 1959, **42**, 754 (*Norisocorydine*)
Katritzky, A.R. *et al., J.C.S.*, 1960, 1950 (*Menisperine, ir, pmr, struct*)
Kuck, A.M. *et al., J.O.C.*, 1961, **26**, 5253 (*synth, uv*)
Albonico, S.M. *et al., J.C.S.(C)*, 1966, 1340 (*ord, derivs*)
Jackson, A.H. *et al., J.C.S.(C)*, 1966, 2181 (*ms*)
Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 1277 (*isol, pmr*)
Groebel, A. *et al., Planta Med.*, 1970, **18**, 66 (*Menisperine, isol, uv, pmr, ms*)
Bhakuni, D.S. *et al., Phytochemistry*, 1972, **11**, 1819 (*Norisocorydine, isol, uv, pmr, ms*)
Karimov, A. *et al., Khim. Prir. Soedin.*, 1978, **14**, 419; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 360 (*Isocorydine N-oxide*)
Marsaioli, A.J. *et al., Phytochemistry*, 1979, **18**, 165 (*cmr, derivs*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80 (*cd*)
Toure, S. *et al., Acta Cryst. C*, 1985, **41**, 1827 (*cryst struct*)
Sariyar, G. *et al., Planta Med.*, 1990, **56**, 232 (*Rhopalotine*)
Ribár, B. *et al., Acta Cryst. C*, 1992, **48**, 945 (*cryst struct*)
Yang, M.H. *et al., Phytochemistry*, 1993, **33**, 943 (*Crabbine*)
You, M. *et al., J. Nat. Prod.*, 1995, **58**, 598 (*isol, (R)-Isocorydine*)
Lee, S.-S. *et al., J. Nat. Prod.*, 1996, **59**, 55 (*cd*)
Chen, C.Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 1997, **44**, 313 (*R-Norisocorydine*)
Rasoanaivo, P. *et al., Planta Med.*, 1998, **64**, 58 (*Norisocorydine, cmr*)
Hasan, C.M. *et al., Nat. Prod. Lett.*, 2000, **14**, 393-397 (*α-N-oxide*)
Chen, C.-Y. *et al., Phytochemistry*, 2001, **56**, 753-757 (*Romucosine H*)

Isocycloheterophyllin I-83

[49794-94-7]



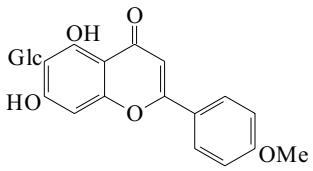
$C_{30}H_{30}O_7$ 502.563
Unusual type of cyclised flavone. Constit. of wood of *Artocarpus heterophyllus* (jackfruit). Yellow needles (C_6H_6). Mp 231°.

Tri-Me ether: [42923-75-1]
Mp 180-182°.

Rao, A.V.R. *et al., Indian J. Chem.*, 1973, **11**, 298 (*isol, nmr, ms*)

Isocytisoside I-84

[4328-19-2]
6-β-D-Glucopyranosyl-5,7-dihydroxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI. 6-Glucopyranosyl-5,7-dihydroxy-4′-methoxyflavone. 4′-O-Methylisovitexin



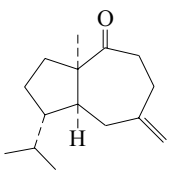
$C_{22}H_{22}O_{10}$ 446.41
Mp 225-227°. $[\alpha]_D$ -22.7 (c, 0.23 in Py).

2″-O-α-L-Rhamnopyranosyl: [64271-11-0]
***Isomargaritene**. Semiaquilinoside*
$C_{28}H_{32}O_{14}$ 592.552
Isol. from *Fortunella margarita* (oval kumquat) and *Fortunella japonica* (round kumquat). Yellow needles. Mp 218-220°.

Chopin, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 1007-1009 (*Isomargaritene*)
Kumamoto, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 2613-2618 (*Isomargaritene*)
Liu, Y. *et al., Zhongcaoyao*, 1999, **30**, 5-7 (*Semiaquilinoside*)

7(14)-Isodaucen-10-one I-85

[73809-82-2]
4(14)-Salvialen-1-one

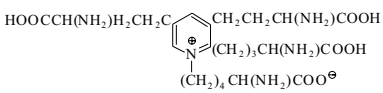


$C_{15}H_{24}O$ 220.354
Constit. of Clary sage oil (*Salvia sclarea*). Cryst. Mp 31-32°. $[\alpha]_D^{20}$ +59.7 (c, 1.6 in $CHCl_3$).

Maurer, B. *et al., Helv. Chim. Acta*, 1983, **66**, 2223

Isodesmosine I-86

[991-01-5]
2-(4-Amino-4-carboxybutyl)-1-(5-amino-5-carboxypentyl)-3,5-bis(3-amino-3-carboxypropyl)pyridinium, 9CI

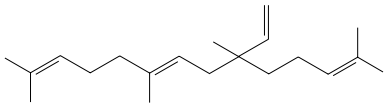


$C_{24}H_{39}N_5O_8$ 525.601
Degradn. prod. of Elastin which, together with Desmosine, D-93, is believed to be responsible for cross-linking the polypeptide chains of Elastin to form insoluble elastic fibres.

Anwar, R.A. *et al., Nature (London)*, 1966, **210**, 1254 (*struct*)
Starcher, B.C. *et al., Prep. Biochem.*, 1975, **5**, 455 (*isol, purifn*)

Isodigeranyl I-87

[5981-30-6]
9-Ethenyl-2,6,9,13-tetramethyl-2,6,12-tetradecatriene, 9CI. 2,6,9,13-Tetramethyl-9-vinyl-2,6,12-tetradecatriene, 8CI

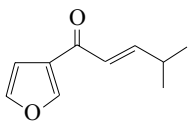


$C_{20}H_{34}$ 274.489
Isol. from bergamot oil. Bp_{10} 185°. n_D^{20} 1.4821.

Souček, M. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 2551 (*isol*)

Isoegomaketone I-88

[34348-59-9]
1-(3-Furanyl)-4-methyl-2-penten-1-one, 9CI



$C_{10}H_{12}O_2$ 164.204
Constit. of the seeds of *Perilla frutescens* (perilla). Oil. Bp_1 77-80°.

▶ SB3921000

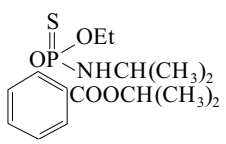
2,4-Dinitrophenylhydrazone:
Red solid (MeOH). Mp 179-180°.

Dihydro: 1-(3-Furanyl)-4-methyl-1-pentanone, F-117

Ito, H. *et al., Yakugaku Zasshi*, 1964, **84**, 1123 (*isol, struct*)
Massy-Westropp, R.A. *et al., Aust. J. Chem.*, 1966, **19**, 891 (*synth*)
Abdulla, R.F. *et al., J.O.C.*, 1978, **43**, 4248 (*synth*)
Pillot, J.-P. *et al., Tet. Lett.*, 1980, 4717 (*synth*)
Watanabe, E. *et al., Bull. Chem. Soc. Jpn.*, 1982, **52**, 3225 (*synth*)

Isofenphos, BSI I-89

[25311-71-1]
1-Methylethyl 2-[[ethoxy[(1-methylethyl)amino]phosphinothioyl]oxy]benzoate, 9CI. O-Ethyl O-2-isopropoxycarbonylphenyl isopropylphosphoramidothioate. Amaze. Oftanol



$C_{15}H_{24}NO_4PS$ 345.399
Agricultural insecticide with contact and stomach action. Oil. V. spar. sol. H_2O. d_4^{20} 1.13. $Bp_{0.01}$ 120°.

▶ LD_{50} (rat, orl) 28 mg/kg; LD_{50} (rat, skn) 188 mg/kg. VO4395500

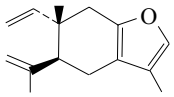
[31120-85-1, 103982-06-5, 103982-07-6, 117176-66-6]

U.K. Pat., 1967, 1 224 323; *CA*, **74**, 125186z (*synth*)
Homeger, B. *et al., Meded. Fac. Landbouwwet., Rijksuniv. Gent*, 1974, **39**, 789 (*activity*)
Agrochemicals Handbook, Royal Society of Chemistry, 1983, A236

Ripley, B.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 1084 (*glc*)
Meji, M. *et al., Nippon Noyaku Gakkaishi*, 1984, **9**, 675; 1986, **11**, 447 (*synth, activity, isomers*)
Gorder, G.W. *et al., J. Agric. Food Chem.*, 1986, **34**, 941 (*activity, isomers*)
Suprock, J.F. *et al., J. Assoc. Off. Anal. Chem.*, 1987, **70**, 1014 (*glc*)
Pesticide Manual, 11th edn., 1997, No. 430
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IMF300

Isogermafurene I-90

[17910-09-7]
Isofuranogermacrene. Curzerene



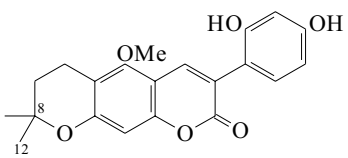
$C_{15}H_{20}O$ 216.322
Isol. from *Curcuma zedoaria* (zedoary), present to some extent in nearly all *Curcuma* spp.. Oil. $[\alpha]_D^{20}$ -0.7 (c, 0.87 in $CHCl_3$). Probably an artifact λ_{max} 210 (log ϵ 3.8) (EtOH).

5-Epimer: [74838-24-7] ***Neocurzene***
$C_{15}H_{20}O$ 216.322

Ishii, H. *et al., Tetrahedron*, 1968, **24**, 625 (*isol*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1970, **18**, 752-755 (*isol, abs config*)
Lu, Y.-C. *et al., CA*, 1981, **94**, 7575r (*Neocurzerene*)
Miyashita, M. *et al., Chem. Lett.*, 1981, 593 (*synth*)

Isoglycycoumarin I-91

[117038-82-1]
*3-(2,4-Dihydroxyphenyl)-7,8-dihydro-5-methoxy-8,8-dimethyl-2*H*,6*H*-benzo[1,2-b:5,4-b′]dipyran-2-one, 9CI*



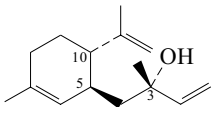
$C_{21}H_{20}O_6$ 368.385
Isol. from *Glycyrrhiza glabra* (licorice) and *Glycyrrhiza uralensis* (Chinese licorice). Mp 235° dec.

7-Hydroxy: [197303-94-9] ***Isolicopyranocoumarin***
$C_{21}H_{20}O_7$ 384.385
Constit. of *Glycyrrhiza* sp.. Pale yellow needles. Mp 251°.

12-Hydroxy: [117038-80-9] ***Licopyranocoumarin***
$C_{21}H_{20}O_7$ 384.385
Isol. from *Glycyrrhiza* sp.. Yellow cryst. Sol. MeOH, $CHCl_3$. Mp 137°. $[\alpha]_D$ +14 (c, 1 in Me_2CO). Log P 2.64 (calc). C-8 config. not determined λ_{max} 211 (ϵ 41686); 352 (ϵ 16220) (MeOH) (Berdy).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2286; 1989, **37**, 3005 (*isol, pmr*)
Zeng, L. *et al., J. Chromatogr.*, 1990, **513**, 247 (*isol*)
Zeng, L. *et al., Zhiwu Xuebao*, 1991, **33**, 124 (*isol*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1485-1492 (*Isolicopyranocoumarin*)

Isohumbertiol I-92

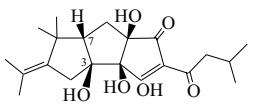


$C_{15}H_{24}O$ 220.354
(3ξ,5ξ,10ξ)-*form*
9,10-Didehydro: ***Isohumbertiol***†
Found as glycosides in *Eriobotrya japonica* (loquat).
9,10-Didehydro, O-*[α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [143376-49-2]
$C_{39}H_{62}O_{18}$ 818.908
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ -40 (c, 1 in MeOH).
9,10-Didehydro, O-*[α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-[(4-hydroxy-3-methoxycinnamoyl(E))-(→4)-α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [143363-61-5]
$C_{49}H_{70}O_{21}$ 995.079
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ -72 (c, 1 in MeOH).

Weyerstahl, P. *et al., Annalen*, 1992, 1325 (*isol, pmr, cmr, synth*)
De Tommasi, N. *et al., J. Nat. Prod.*, 1992, **55**, 1025 (*glycosides*)

Isohumulinone A I-93

[83680-60-8]



Relative configuration

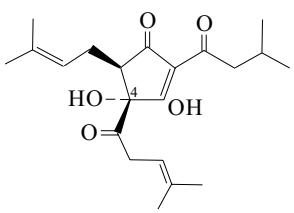
$C_{21}H_{30}O_6$ 378.464
Bitter principle present in beer. Cryst. ($CHCl_3$). Mp 202-204°.

3,7-Diepimer: [83651-39-2] *Isohumulinone B*
$C_{21}H_{30}O_6$ 378.464
Bitter principle present in beer. Cryst. ($CHCl_3$/petrol). Mp 151-153°.

Elvidge, J.A. *et al., J.C.S. Perkin 1*, 1982, 1791

Isohumulone A I-94

[467-72-1]
Isohumulone A_2. Photoisohumulone



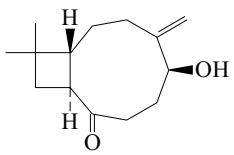
$C_{21}H_{30}O_5$ 362.465
Bitter principle present in beer. Cryst. Mp 62-63°. $[\alpha]_D$ -7.7 (c, 6 in MeOH).

4-Epimer: [1534-03-8] *Isohumulone B. Isohumulone A_1*
Found in beer as isom. prod. of Humulone. Pale yellow oil. $[\alpha]_D$ +46.3 (c, 6 in MeOH).

Laws, D.R.J. *et al., J.C.S.(C)*, 1971, 2412

Isokobusone I-95

[24173-72-6]
6-Hydroxy-15-nor-7(14)-caryophyllen-3-one

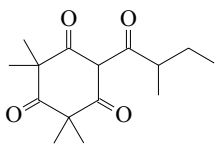


$C_{14}H_{22}O_2$ 222.327
Constit. of *Cyperus rotundus* (nutgrass). Cryst. (Et_2O). Mp 108-109°. $[\alpha]_D$ -40.1 (c, 3.1 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1969, **17**, 1390
Heymann, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 138 (*isol, pmr, cmr*)

Isoleptospermone I-96

[7375-66-8]
2,2,4,4-Tetramethyl-6-(2-methyl-1-oxobutyl)-1,3,5-cyclohexanetrione

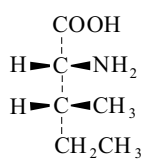


$C_{15}H_{22}O_4$ 266.336
Enolised β-diketone. Constit. of *Leptospermum scoparium* (red tea). Pale yellow oil. λ_{max} 238 (log ϵ 3.83); 279 (log ϵ 4.04) (MeOH).

Ghisalberti, E.L. *et al., Phytochemistry*, 1996, **41**, 7-22 (*occur*)
Van Klink, J.W. *et al., Phytochemistry*, 1999, **62**, 487-489 (*isol, synth, uv, ir, pmr, cmr, ms*)

Isoleucine I-97

[7004-09-3]
2-Amino-3-methylpentanoic acid. Ile. 3-Methylnorvaline



(2*R*,3*R*)-*form*

$C_6H_{13}NO_2$ 131.174
(2*R*,3*R*)-*form* [319-78-8]
D-erythro-*form*. D-*Isoleucine*
Mp 283-284° dec. $[\alpha]_D^{20}$ -12.2 (c, 3.2 in H_2O). $[\alpha]_D$ -41 (c, 1 in 5*M* HCl).
▶NR4700000
(2*R*,3*S*)-*form* [1509-35-9]
D-threo-*form*. D-*Alloisoleucine*

Mp 274-275° dec. $[\alpha]_D^{25}$ -15.6 (c, 2 in H_2O). $[\alpha]_D$ -38.4 (c, 4 in 6*M* HCl). pK_{a1} 2.2; pK_{a2} 9.62 (25°, H_2O).

►BA2930000

(2*S*,3*R*)-*form* [1509-34-8]

L-threo-*form*. *Alloisoleucine*

Mp 278° dec. $[\alpha]_D^{25}$ +15.7 (c, 2 in H_2O). $[\alpha]_D^{25}$ +34.9 (c, 4 in 4*M* HCl). $[\alpha]_D$ +40.5 (c, 1 in 5*M* HCl). pK_{a1} 2.32; pK_{a2} 9.76 (25°).

►BA2933000

(2*S*,3*S*)-*form* [73-32-5]

L-erythro-*form*. *L-Isoleucine*

Dietary supplement, nutrient. Cryst. (EtOH aq.). Mod. sol. H_2O (4.12 g/100 g at 25°). Mp 285-286° dec. $[\alpha]_D$ +16.3 (H_2O). $[\alpha]_D$ +51.8 (5*M* HCl). pK_{a2} 9.68 (NH_2). Isoelectric point 6.02. Bitter taste.

►NR4705000

(2*RS*,3*RS*)-*form* [443-79-8]

(±)-erythro-*form*. (±)-*Isoleucine*. *FEMA 3295*

Flavouring ingredient, dietary supplement, nutrient. Cryst. (EtOH). Sl. sol. H_2O. Mp 275° (sealed tube). pK_{a2} 9.7 (25°, 0.5*M* KCl).

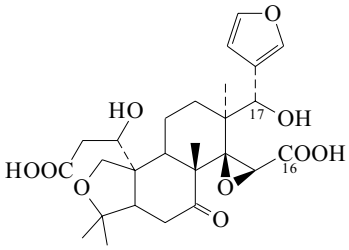
(2*RS*,3*SR*)-*form* [3107-04-8]

(±)-threo-*form*. (±)-*Alloisoleucine*

[4125-98-8, 10466-56-5, 18598-74-8]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 489C (*pmr, Isoleucine*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 575D (*ir, Isoleucine*)
Greenstein, J.P. *et al., Biochem. Prep.*, 1953, **3**, 84
Org. Synth., Coll. Vol., 3, 1955, 495
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2043 (*rev*)
Torii, K. *et al., Acta Cryst. B*, 1971, **27**, 2237 (*cryst struct*)
Armstrong, F.B. *et al., Chem. Comm.*, 1974, 351 (*biosynth*)
Son, T.D. *et al., J.A.C.S.*, 1974, **96**, 1484 (*cmr, Isoleucine*)
Bycroft, B.W. *et al., Chem. Comm.*, 1975, 988 (*synth*)
MacDonald, J.C. *et al., Can. J. Chem.*, 1976, **54**, 1226 (*pmr, Alloisoleucine*)
Rabenstein, D.L. *et al., J. Magn. Reson.*, 1976, **24**, 27 (*cmr*)
Kricheldorf, H.R. *et al., Org. Magn. Reson.*, 1979, **12**, 414 (*N-15 nmr*)
Komatsubara, S. *et al., Prog. Ind. Microbiol.*, 1986, **24**, 233 (*rev*)
Oppolzer, W. *et al., Tet. Lett.*, 1986, **27**, 831 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, IKX000; IKX010
Lauterwein, J. *et al., J. Phys. C: Solid State Phys.*, 1991, **95**, 3804 (*O-17 nmr*)
Groth, U. *et al., Annalen*, 1993, 715 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 593
Lloyd-Williams, P. *et al., J.C.S. Perkin 1*, 1994, 1969 (*synth, Alloisoleucine*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **21**, 403
Görbitz, C.H. *et al., Acta Cryst. C*, 1996, **52**, 1464; 1754 (*cryst struct, L-Isoleucine, L-Leucine*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1472-1474
Portonovo, P. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 1451-1455 (*D-Alloisoleucine, synth, pmr, cmr*)
Belzecki, C. *et al., Synth. Commun.*, 2000, **30**, 2245-2252 (*synth, Alloisoleucine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IKX000; IKX010

Isolimonic acid I-98



$C_{26}H_{34}O_{10}$ 506.549

Normally obt. as the 16,17-lactone, to which the name Isolimonic acid is applied (but the glucoside of the open-chain acid is called Isolimonic acid glucoside). Constit. of *Citrus* spp..

16→17-Lactone: [74729-97-8]
$C_{26}H_{32}O_9$ 488.533
Constit. of *Citrus* spp..

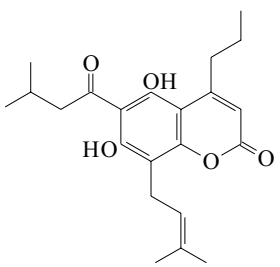
17-O-*β*-D-*Glucopyranoside:*
$C_{32}H_{44}O_{15}$ 668.691
Constit. of *Citrus aurantium*.

Bennett, R.D. *et al., Phytochemistry*, 1980, **19**, 2417; 1991, **30**, 3803

Isomammein I-99

[478-67-1]

*5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-6-isovaleryl-8-(3-methyl-2-butenyl)-4-propylcoumarin, 8CI. Mammea B/AA*



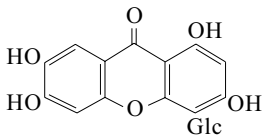
$C_{22}H_{28}O_5$ 372.46
Constit. of *Mammea americana* (mamey) seeds. Yellow cryst. Mp 109° (119-121°).

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248; 1987, 317 (*isol, ir, uv, pmr, ms, synth*)

Isomangiferin I-100

[24699-16-9]

*4-β-D-Glucopyranosyl-1,3,6,7-tetrahydroxy-9*H*-xanthen-9-one, 9CI. 4-Glucosyl-1,3,6,7-tetrahydroxyxanthone*



$C_{19}H_{18}O_{11}$ 422.345
Constit. of *Mangifera indica* (mango). Pale-yellow needles (MeOH). Mp 260° dec. $[\alpha]_D$ +5.5 (Py).

Octa-Ac:
Cryst. ($CHCl_3$/hexane). Mp 203-204°. $[\alpha]_D$ -64.7 ($CHCl_3$).

O-*β*-D-*Glucopyranosyl (1):* [50315-13-4] ***Glucoisomangiferin***. *4*-O-*(Glucosylglucosyl)-1,3,6,7-tetrahydroxyxanthone*
$C_{25}H_{28}O_{16}$ 584.487

O-*β*-D-*Glucopyranosyl (2):Isomangiferin* O-*glucoside*
$C_{25}H_{28}O_{16}$ 584.487A disaccharide of partially detd. struct. having a further Glc residue attached to the glucosyl group. Not clear if this is identical with Glucoisomangiferin.

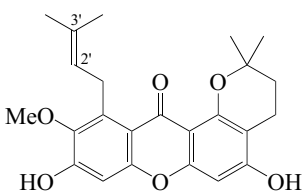
3-Me ether: [83118-66-5] *3*-O-*Methylisomangiferin*. ***Isochinomin***
$C_{20}H_{20}O_{11}$ 436.371
Constit. of *Mangifera indica* (mango). Trivial name is misleading.

7-Me ether: [83159-39-1] ***7*-O-*Methylisomangiferin***
$C_{20}H_{20}O_{11}$ 436.371
Pale-yellow needles (MeOH). Mp 247-248°. $[\alpha]_D^{20}$ +11.4 (c, 1.0 in Py).

Aritami, M. *et al., Tet. Lett.*, 1969, 941 (*isol, struct*)
Prox, A. *et al., Annalen*, 1970, **732**, 199 (*ms*)
Aritami, M. *et al., Annalen*, 1970, **734**, 91 (*ms*)
Smith, D.M. *et al., Phytochemistry*, 1971, **10**, 2117 (*Isomangiferin O-glucoside*)
Glyzin, V.I. *et al., Khim. Prir. Soedin.*, 1973, **9**, 434; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 409 (*Glucoisomangiferin*)
Arisawa, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1609 (*isol*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2342 (*isol*)
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*occur*)
Imperato, F. *et al., Can. J. Bot.*, 1991, **69**, 218 (*Isochinomin*)

1-Isomangostin I-101

[19275-44-6]



$C_{24}H_{26}O_6$ 410.466
Constit. of *Garcinia mangostana* (mangosteen). Mp 245-249°. λ_{max} 244 (ε 38000); 254 (ε 33100); 307 (ε 24550); 345 (ε 10700) (EtOH) (Berdy).

2′,3′-Dihydro, 3′-hydroxy: [26063-95-6] ***1-Isomangostin hydrate***
$C_{24}H_{28}O_7$ 428.481
Constit. of *Garcinia mangostana* (man-

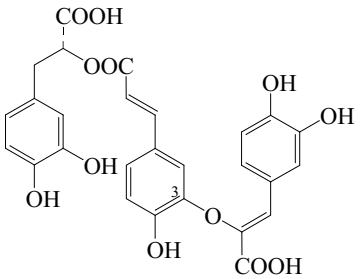
gosteen). Cryst. (CH_2Cl_2). Mp 261-263° (255-257°). Incorrectly named in CA.

[110558-92-4]

Mahabusarakam, W. *et al., J. Nat. Prod.*, 1987, **50**, 474 (*isol, pmr*)

Isomelitric acid A I-102

3′-O-(8″-Z-Caffeoyl)rosmarinic acid. Isoschizotenuin E



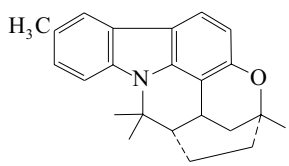
$C_{27}H_{22}O_{12}^{\oplus}$ 538.464

Isomeric with Melitric acid A, S-20. Constit. of the leaves of *Thymus vulgaris* (thyme). $[\alpha]_D^{22}$ +40.3 (c, 1.2 in MeOH). λ_{max} 217 (sh) ; 231 (sh) ; 291 ; 322 (MeOH).

Dapkevicius, A. *et al., J. Nat. Prod.*, 2002, **65**, 892-896 (*isol, pmr, cmr, ms*)

Isomurrayazoline I-103

[85547-20-2]

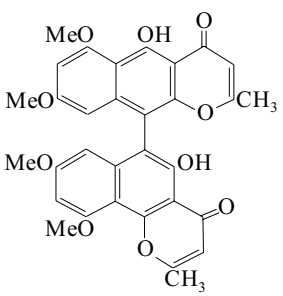


$C_{23}H_{25}NO$ 331.457

Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6/$CHCl_3$). Mp 269-270°. $[\alpha]_D$ -7.33 ($CHCl_3$).

Bhattacharya, L. *et al., Phytochemistry*, 1982, **21**, 2432 (*isol, uv, ir, pmr, ms, struct*)

Isonigerone I-104



$C_{32}H_{26}O_{10}$ 570.551

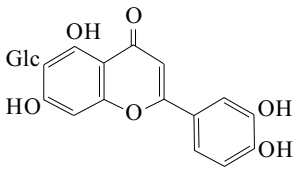
Mycotoxin from *Aspergillus niger* isol. from infected peanuts. Orange solid ($CHCl_3$/MeOH). Mp 330°. $[\alpha]_D^{20}$ -93.1 (c, 0.74 in $CHCl_3$). λ_{max} 228 (ϵ 50100); 248 (ϵ 56200); 279 (ϵ 66100); 390 (ϵ 9550) (MeOH) (Derep).

Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1980, 2474 (*isol, uv, ir, pmr, cmr, struct*)

Isoorientin I-105

[4261-42-1]

*2-(3,4-Dihydroxyphenyl)-6-β-D-glucopyranosyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. 6-*C*-Glucopyranosyl-3′,4′,5,7-tetrahydroxyflavone. 6-*C*-β-D-Glucopyranosylluteolin. Homoorientin. Lespecapitoside. Lutonaretin*



$C_{21}H_{20}O_{11}$ 448.382

Light yellow needles or pale yellow-green powder. Mp 237-239°. $[\alpha]_D^{20}$ +30.8 (c, 1.2 in Py). $[\alpha]_D^{22}$ +30 (c, 0.5 in EtOH).

6″-O-α-L-Rhamnopyranosyl: [108602-35-3] *Isoorientin 6″-rhamnoside. Luteolin 6-*C*-rutinoside*
$C_{27}H_{30}O_{15}$ 594.525
Isol. from wheat leaves (*Triticum* sp.).

2″-O-β-D-Glucopyranosyl: [55196-48-0] *3′,4′,5,7-Tetrahydroxy-6-*C*-sophorosylflavone.* ***Meloside L***
$C_{27}H_{30}O_{16}$ 610.524
Constit. of the leaves of melon (*Cucumis melo*) and rice (*Oryza sativa*). Cryst. (MeOH). Mp 212°.

*2″-O-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl]:* [220948-74-3]
$C_{36}H_{36}O_{18}$ 756.67
Isol. from rice leaves (*Oryza sativa*) exposed to enhanced levels of UV-B.

2″-O-[3,4-Dihydroxycinnamoyl-(→?)-β-D-glucopyranosyl]: [39384-49-1] ***Meloside l***
$C_{36}H_{36}O_{19}$ 772.669
Isol. from melon leaves (*Cucumis melo*).

*2″-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl]:* [220948-75-4]
$C_{37}H_{38}O_{19}$ 786.696
Isol. from rice leaves (*Oryza sativa*) exposed to enhanced levels of UV-B.

7-O-β-D-Glucopyranoside: [35450-86-3] ***Lutonarin***
$C_{27}H_{30}O_{16}$ 610.524
Found in barley seedlings (*Hordeum vulgare*) and other plants in Gramineae, Leguminosae and Lemnaceae. Bright yellow cryst. Mp 239-242° (235°).

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [35450-87-4] ***Wyomin***. *Isoorientin 7-rutinoside*
$C_{33}H_{40}O_{20}$ 756.667
Isol. from wheat leaves (*Triticum aestivum*).

6″-O-[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranosyl]:Isoorientin 6″-diglucoside
$C_{33}H_{40}O_{21}$ 772.666
Isol. from wheat leaves (*Triticum* sp.).

2″-Ac: [131508-00-4] ***2″-O-Acetylisoorientin***
$C_{23}H_{22}O_{12}$ 490.42
Isol. from sorrel leaves (*Rumex acetosa*). Yellow needles (MeOH aq.). Mp 209-210°. $[\alpha]_D^{22}$ +11.4 (c, 0.35 in MeOH).

2″,6″-Di-Ac: [131507-98-7] ***2″,6″-Di-O-acetylisoorientin***
$C_{25}H_{24}O_{13}$ 532.457
Isol. from sorrel leaves (*Rumex acetosa*). Yellow needles (MeCN aq.). Mp 180-182°. $[\alpha]_D^{22}$ +4.8 (c, 0.42 in MeOH).

*6″-O-(3,4-Dihydroxy-*E*-cinnnamoyl):6″-Caffeoylisoorientin*
$C_{30}H_{26}O_{14}$ 610.527
Constit. of *Vitex agnus-castus* (agnus castus). Pale yellow powder. Mp 224-226°. $[\alpha]_D$ -51 (c, 0.5 in MeOH). The *E*-config. was not specifically cited for the *Gentiana arisanensis* isolate, but it appears to be identical with the *E*-form from *Vitex agnus-castus* λ_{max} 210 (ϵ 350); 245 (ϵ 180); 275 (ϵ 166); 300 (ϵ 151); 325 (ϵ 230) (MeOH).

4′-Me ether: [15822-82-9] *6-β-D-Glucopyranosyldiosmetin*
$C_{22}H_{22}O_{11}$ 462.409
Isol. from lemon peel (*Citrus limon*), not found in oranges. Cryst. (MeOH). Mp 243-245°.

*4″-Me ether, 6″-O-(3,4-dihydroxycinnamoyl)(*E*-):*
$C_{31}H_{28}O_{14}$ 624.554
Constit. of *Vitex agnus-castus* (agnus castus). Pale yellow powder (MeOH). Mp 224-226°. $[\alpha]_D$ -44.1 (c, 0.3 in MeOH). λ_{max} 245 ; 272 (sh) ; 295 (sh) ; 336 (MeOH).

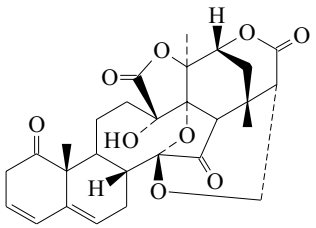
3′,7-Di-Me ether: [74198-15-5] *6-β-D-Glucopyranosyl-4′,5-dihydroxy-3′,7-dimethoxyflavone*
$C_{23}H_{24}O_{11}$ 476.436
Isol. from sugar cane mill syrup (*Saccharum*).

[57788-32-6, 61460-25-1, 62249-40-5, 79078-23-2]

Gentili, B. *et al., J.O.C.*, 1968, **33**, 1571 (*4′-Me ether*)
Julian, E.A. *et al., Phytochemistry*, 1971, **10**, 3185 (*7-rutinoside*)
Monties, B. *et al., CA*, 1972, **78**, 133423x (*Melosides*)
Hostettmann, K. *et al., Helv. Chim. Acta*, 1975, **58**, 130 (*2″-glucosyl*)
Hostettmann, M. *et al., Phytochemistry*, 1978, **17**, 2083 (*rev*)
Mabry, T.J. *et al., J. Nat. Prod.*, 1984, **47**, 127 (*3′,7-di-Me ether*)
Chulia, A.J. *et al., J. Nat. Prod.*, 1985, **48**, 480 (*6″-glucosyl derivs*)
Harborne, J.B. *et al., Plant Syst. Evol.*, 1986, **154**, 251-257 (*6″-diglucoside, 6″-rhamnoside*)
Kato, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2277 (*Acetylisoorientin*)
Krauze-Baranowska, M. *et al., Phytochemistry*, 1995, **39**, 727 (*Lutonarin*)
Kuo, S.-H. *et al., Phytochemistry*, 1996, **41**, 309 (*6″-Caffeoylisoorientin*)
Hirobe, C. *et al., Phytochemistry*, 1997, **46**, 521-524 (*caffeoyl esters*)
Markham, K.R. *et al., Phytochemistry*, 1998, **49**, 1913-1919 (*2″-cinnamoylglucosyl derivs*)

Isophysalin B I-106

[26435-77-8]

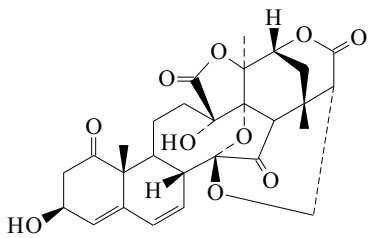


$C_{28}H_{30}O_9$ 510.54
Constit. of *Physalis alkekengi* (winter cherry). Amorph. solid. $[\alpha]_D$ -86 (c, 0.37 in MeOH). λ_{max} 227 (ϵ 6166) (MeOH) (Berdy).

Sunayama, R. *et al., Phytochemistry*, 1993, **34**, 529 (*isol, pmr, cmr*)

Isophysalin G I-107

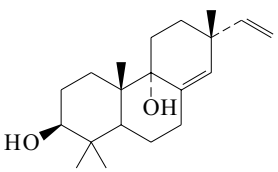
[152221-21-1]



$C_{28}H_{30}O_{10}$ 526.539
Constit. of *Physalis alkekengi* (winter cherry). Amorph. solid. $[\alpha]_D$ -32 (c, 0.19 in $CHCl_3$).

Sunayama, R. *et al., Phytochemistry*, 1993, **34**, 529 (*isol, pmr, cmr*)

8(14),15-Isopimaradiene-3,9-diol I-108



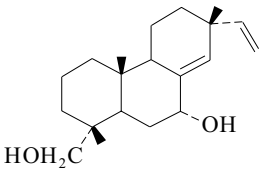
$C_{20}H_{32}O_2$ 304.472

(3β,9α)-*form* [150943-96-7]
Oryzalexin E
Phytoalexin from rice leaves. Needles. Mp 123-124°. $[\alpha]_D^{25}$ -26 (c, 0.1 in MeOH).

Kato, H. *et al., Phytochemistry*, 1993, **33**, 79-81 (*isol, pmr, cmr*)

8(14),15-Isopimaradiene-7,18-diol I-109

[292060-24-3]
8(14),15-Sandaracopimaradiene-7,18-diol



$C_{20}H_{32}O_2$ 304.472
Oil. $[\alpha]_D^{20}$ +63.8 (c, 0.03 in $CHCl_3$). λ_{max} 248 (log ϵ 3.2) (MeOH).

7α-*form* [82190-51-0]
Cryst. (C_6H_6). Mp 86-87°. $[\alpha]_D$ -87.1 (c, 0.05 in MeOH).

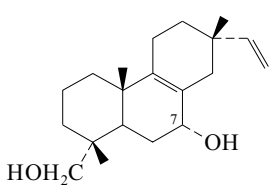
18-Carboxylic acid:7α-Hydroxy-8(14),15-isopimaradien-18-oic acid. ***7α-Hydroxysandaracopimaric acid***
Isol. from *Juniperus communis* (juniper). Oil (as Me ester). $[\alpha]_D$ -41 (c, 0.8 in $CHCl_3$) (Me ester).

18-Carboxylic acid, 7-ketone: ***7-Oxo-8(14),15-isopimaradien-18-oic acid***. *7-Oxosandaracopimaric acid*
$C_{20}H_{28}O_3$ 316.439
Oil. $[\alpha]_D^{20}$ +63.8 (c, 0.3 in $CHCl_3$). λ_{max} 248 (log ϵ 3.2) (MeOH).

18-Carboxylic acid, 7-ketone, Me ester:
$C_{21}H_{30}O_3$ 330.466
Cryst. (EtOAc/petrol). Mp 87-90°. $[\alpha]_D^{20}$ -40 (c, 0.15 in $CHCl_3$).

de Pascual Teresa, J. *et al., Phytochemistry*, 1980, **19**, 1153 (*7-hydroxysandaracopimaric acid*)
de Kimpe, N. *et al., J.O.C.*, 1982, **47**, 3628 (*isol, cryst struct*)
Hakizamungu, E. *et al., Phytother. Res.*, 1982, **2**, 207 (*activity*)
Van Puyvelde, L. *et al., J. Ethnopharmacol.*, 1986, **17**, 269-273 (*activity*)
Esquivel, B. *et al., J. Nat. Prod.*, 1987, **50**, 738 (*7-Oxosandaracopimaric acid*)
Van Puyvelde, L. *et al., Planta Med.*, 1987, **53**, 156-158 (*activity*)
Van Puyvelde, L. *et al., J. Ethnopharmacol.*, 1988, **24**, 233-239 (*activity*)
Van Dunkel, F. *et al., Planta Med.*, 1990, **56**, 645 (*activity*)
Chang, L.C. *et al., J. Nat. Prod.*, 2000, **63**, 1235-1238 (*7-Oxo-8(14),15-isopimaradien-18-oic acid*)

8,15-Isopimaradiene-7,18-diol I-110



$C_{20}H_{32}O_2$ 304.472

7α-*form* [114191-58-1]
Oil. $[\alpha]_D$ +54.5 (c, 2.3 in $CHCl_3$).

7β-*form* [114191-60-5]
Cryst. (Et_2O). Mp 95-97°. $[\alpha]_D$ +29.5 (c, 0.9 in $CHCl_3$).

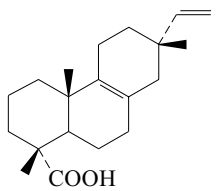
7-Ketone: [110201-62-2] ***18-Hydroxy-8,15-isopimaradien-7-one***
$C_{20}H_{30}O_2$ 302.456
Oil. $[\alpha]_D$ +85.4 (c, 1 in $CHCl_3$).

18-Carboxylic acid, 7-ketone: [114191-62-7] ***7-Oxo-8,15-isopimaradien-18-oic acid***
Isol. from *Juniperus communis* (juniper). Oil (as Me ester). $[\alpha]_D$ +77.6 (c, 0.8 in $CHCl_3$).

de Pascual Teresa, J. *et al., Phytochemistry*, 1980, **19**, 1153-1156; 1987, **26**, 1481
Urones, J.G. *et al., Phytochemistry*, 1988, **27**, 523
Chang, L.C. *et al., J. Nat. Prod.*, 2000, **63**, 1235-1238 (*7-Oxo-8,15-isopimaradien-18-oic acid*)

8,15-Isopimaradien-18-oic acid I-111

[3625-01-2]
Δ⁸-Isopimaric acid



$C_{20}H_{30}O_2$ 302.456
Found in resin of *Pinus* spp. esp. *Pinus edulis* (pinon). Cryst. Mp 105-106°. $[\alpha]_D$ +94 (c, 1.14 in $CHCl_3$). $[\alpha]_D$ +118 (c, 1 in EtOH).

Me ester:
Cryst. (MeOH). Mp 68-70°. $[\alpha]_D$ +118 (c, 1.0 in EtOH).

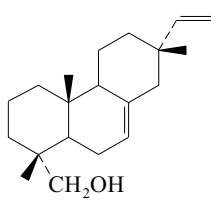
***ent*-form**

18-Alcohol: **ent-*8,15-Isopimaradien-18-ol***
$C_{20}H_{32}O$ 288.472
Oil. $[\alpha]_D^{25}$ +40.5 (c, 2 in $CHCl_3$).

Edwards, O.E. *et al., Can. J. Chem.*, 1959, **37**, 760 (*synth*)
ApSimon, J.W. *et al., Chem. Comm.*, 1966, 361 (*pmr*)
Joye, N.M. *et al., J.O.C.*, 1966, **31**, 320 (*occur, struct*)
Garbarino, J.A. *et al., Phytochemistry*, 1990, **29**, 3037 (*deriv*)

7,15-Isopimaradien-18-ol I-112

[1686-64-2]



$C_{20}H_{32}O$ 288.472
Cryst. (MeOH aq. or by subl.). Mp 85-86°. $[\alpha]_D$ -24.6 (c, 1 in $CHCl_3$).

18-Aldehyde: [1686-63-1] ***7,15-Isopimaradien-18-al***
$C_{20}H_{30}O$ 286.456
Cryst. Mp 35-37°. $[\alpha]_D^{22}$ -15.

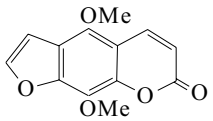
18-Carboxylic acid: [5835-26-7] *7,15-Isopimaradien-18-oic acid.* ***Isopimaric acid***. *Isodextropimaric acid. Micropinic acid*
$C_{20}H_{30}O_2$ 302.456
Isol. from *Pinus palustris* (pitch pine). Cryst.(EtOH). Mp 162-164°. $[\alpha]_D^{24}$ 0.

Antkowiak, W. *et al., Can. J. Chem.*, 1965, **43**, 1257 (*struct*)
Wenkert, E. *et al., J.O.C.*, 1965, **30**, 713 (*pmr*)

Grant, P.K. *et al., Aust. J. Chem.*, 1967, **20**, 969 (*isol, struct*)
Wenkert, E. *et al., J.A.C.S.*, 1972, **94**, 4367 (*cmr*)
Bohlmann, F. *et al., Chem. Ber.*, 1976, **109**, 1446 (*Isopimaric acid*)
Chang, L.C. *et al., J. Nat. Prod.*, 2000, **63**, 1235-1238 (*activity*)

Isopimpinellin I-113

[482-27-9]
*4,9-Dimethoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. 4,9-Dimethoxy-7-oxofuro[3,2-*g*]chromene. 4,9-Dimethoxypsoralen*

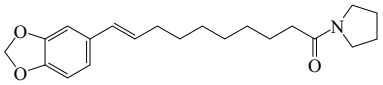


$C_{13}H_{10}O_5$ 246.219
Present in the seeds of *Pastinaca sativa* (parsnip). Golden-yellow needles (MeOH). Mp 147-148° Mp 151°. λ_{max} 222 (ϵ 25120); 240 (ϵ 13490); 248 (ϵ 15850); 268 (ϵ 20900); 311 (ϵ 13800) (EtOH) (Berdy).

Barnes, C.S. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
Sheinker, Y.N. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 1382 (*pmr*)
Ahluwalia, V.K. *et al., Indian J. Chem.*, 1971, **9**, 194 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1378 (*occur*)
Talapatra, S.K. *et al., Phytochemistry*, 1973, **12**, 236; 2312
Austin, D.J. *et al., Phytochemistry*, 1973, **12**, 1657 (*biosynth*)
Kutney, J.P. *et al., Tetrahedron*, 1973, **29**, 2645; 2661; 2673 (*biosynth*)
Voigt, D. *et al., J. Prakt. Chem.*, 1977, **319**, 767 (*ms*)
Elgamal, M.H.A. *et al., Phytochemistry*, 1979, **18**, 139 (*cmr*)
Innocenti, G. *et al., Phytochemistry*, 1983, **22**, 2207-2209 (*biosynth*)

Isopiperolein B I-114

1-[10-(1,3-Benzodioxol-5-yl)-1-oxo-9-decenyl]pyrrolidine. 10-(3,4-Methylenedioxyphenyl)-9-decenoic acid pyrrolidide

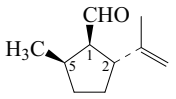


$C_{21}H_{29}NO_3$ 343.465
Alkaloid from the berries of *Piper nigrum* (pepper). Yellow oil. λ_{max} 260 (no solvent reported).

Srinivas, P.V. *et al., Phytochemistry*, 1999, **52**, 957-958

2-Isopropenyl-5-methylcyclopentanecarboxaldehyde I-115

[1753-98-6]
2-Methyl-5-(1-methylethenyl)cyclopentanecarboxaldehyde. Photocitral



(1*RS*,2*RS*,5*RS*)-*form*

$C_{10}H_{16}O$ 152.236

(1*RS*,2*RS*,5*RS*)-*form* [59121-31-2]

[1125-49-1]
Photocitral A
Present, presumably in enantiomeric forms, in photodegraded lemon and orange oils and in other plants. Oil. Bp_8 87°.

2,4-Dinitrophenylhydrazone:
Yellow needles (2-propanol). Mp 115-116°.

(1*RS*,2*RS*,5*SR*)-*form* [55253-28-6] cis,cis-*form. FEMA 3645*
Flavouring ingredient. Liq. with minty camphorous odour. Bp_{13} 102-108°. n_D^{20} 1.4763.

(1*RS*,2*SR*,5*RS*)-*form* [55253-27-5] trans,trans-*form*
Characterised spectroscopically.

(1*RS*,2*SR*,5*SR*)-*form* [1125-48-0] *Epiphotocitral A*
Present in photodegraded lemon and orange oil. Also present in essential oil of *Pelargonium citronellum*.

[43219-98-3]

Cookson, R.C. *et al., Tetrahedron*, 1963, **19**, 1995 (*synth*)
Büchi, G. *et al., J.A.C.S.*, 1965, **87**, 1589-1593 (*Photocitral A, synth, config, pmr*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1976, **59**, 1797-1802; 1984, **67**, 1198-1203 (*synth, isol, pmr, ms*)
Sakai, T. *et al., J.O.C.*, 1981, **46**, 4774 (*synth*)
Demarne, F.E. *et al., J. Essent. Oil Res.*, 1993, **5**, 233-238 (*detn, Photocitral A, Epiphotocitral A*)
Venskutonis, P.R. *et al., Dev. Food Sci.*, 1995, **37**, 833-847 (*detn, glc*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 408 (*cis,cis-form, props, use*)
Yuku, I. *et al., J. Agric. Food Chem.*, 1997, **45**, 463-466 (*formn in lemon oil*)

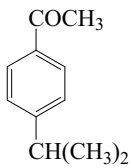
Isopropyl acetate, 8CI I-116

[108-21-4]
1-Methylethyl acetate, 9CI. FEMA 2926
$H_3CCOOCH(CH_3)_2$
$C_5H_{10}O_2$ 102.133
Isol. from ripening melons, apples, bananas, blackcurrants, other fruits and grape oil. Also present in cheddar cheese, soybean, beer, red wine, white wine and plum brandy. Flavouring ingredient. Colourless liq. with sweet apple-like flavour on dilution. Spar. sol. H_2O, misc. EtOH, Et_2O. $Bp_{734.299988}$ 88-91°.
▶ Highly flammable, fl. p. 2/4°, autoignition temp. 460°. Eye and respiratory tract irritant. High vapour conc. narcotic. LD_{50} (rat, orl) 3000 mg/kg, OES: short-term 200 ppm. AI4930000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 899C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 601B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 608A (*ir*)
Caswell, L.R. *et al., J.O.C.*, 1976, **41**, 3312 (*uv*)
Minato, H. *et al., Chem. Lett.*, 1977, 413 (*synth*)
Benoit, F.M. *et al., Org. Mass Spectrom.*, 1977, **12**, 78 (*ms*)
Yabumoto, K. *et al., Food Chem.*, 1978, **3**, 7 (*isol*)
Couperos, P.A. *et al., Org. Magn. Reson.*, 1978, **11**, 590 (*cmr*)
Ergorov, I.A. *et al., Prikl. Biokhim. Mikrobiol.*, 1978, **14**, 135 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, INE100
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 758
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 256 (*tox*)

4′-Isopropylacetophenone I-117

[645-13-6]
1-[4-(1-Methylethyl)phenyl]ethanone, 9CI. p-*Acetylcumene. Methyl* p-*cumyl ketone. Cuminone. FEMA 2927*



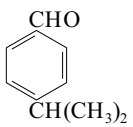
$C_{11}H_{14}O$ 162.231
Flavouring ingredient. Liq. with an odour reminiscent of orris and basil. d^{15} 0.98. Bp 254° $Bp_{0.8}$ 68-72°.

Oxime:
$C_{11}H_{15}NO$ 177.246
Mp 70-71°.

Matlock, J.O. *et al., J. Polym. Sci.*, 1961, **49**, 533 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 410
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1482-1483

4-Isopropylbenzaldehyde I-118

[122-03-2]
4-(1-Methylethyl)benzaldehyde, 9CI. p-*Mentha-1,3,5-trien-1-al.* ***Cuminaldehyde.*** *Cumaldehyde. Cuminal. Cuminic aldehyde. FEMA 2341*



$C_{10}H_{12}O$ 148.204
Found in many essential oils, including eucalyptus, cumin and cassia. Also present in grilled or roast beef and cognac. Flavouring agent. Liq. with pungent cumin-like odour and taste. d_4^{25} 0.98. Bp 235-236° Bp_{10} 103-104°. n_D^{20} 1.5301.
▶ Skin irritant. LD_{50} (rat, orl) 1390 mg/kg. CU7000000

(E)-Oxime: [3717-17-7]
$C_{10}H_{13}NO$ 163.219
Cryst. (EtOH). Mp 52° Mp 61°.

(Z)-Oxime:

$C_{10}H_{13}NO$ 163.219
Prisms. Mp 112°.

Semicarbazone: [950-07-2]
Leaflets. Mp 210-211° Mp 222°.

Phenylhydrazone: [10407-16-6]
Needles (petrol or EtOH). Mp 137-138°.

4-Nitrophenylhydrazone:
Cryst. (EtOH). Mp 190°.

2,4-Dinitrophenylhydrazone: [1906-70-3]
Red needles (C_6H_6). Mp 241°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 939B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 109D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1289B (*ir*)
Penfold, A.R. *et al., J.C.S.*, 1922, **121**, 266
Bert, L. *et al., Bull. Soc. Chim. Fr.*, 1925, **37**, 1397
Bert, L. *et al., C. R. Hebd. Seances Acad. Sci.*, 1942, **215**, 276
Ger. Pat., 1971, 2 062 522; *CA*, **75**, 63417 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 395 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COE500

Isopropylbenzene, 8CI I-119

[98-82-8]
1-Methylethylbenzene, 9CI. Cumene. Cumol. 2-Phenylpropane

$PhCH(CH_3)_2$

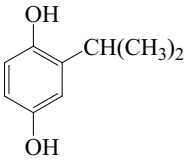
C_9H_{12} 120.194
Trace constit. of ginger oil (*Zingiber officinale*). Liq. d_4^{20} 0.86. Mp -96.9°. Bp 152-153°.

▶ Eye and mucous membrane irritant. Potential narcotic action at high vapour conc. CNS depressant. LD_{50} (rat, orl) 1400 mg/kg; LD_{50}(rat, ihl) 8000 ppm (4 h exposure). GR8575000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 2B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 932A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 850A (*ir*)
Meyer, H. *et al., Monatsh. Chem.*, 1929, **53-4**, 725 (*synth*)
Slanina, S.J. *et al., J.A.C.S.*, 1935, **57**, 1547 (*synth*)
Adv. Chem. Ser., 1955, **15**, 18 (***props***)
Nigam, M.C. *et al., Can. J. Chem.*, 1964, **42**, 2610 (*isol*)
Schaefer, T. *et al., Can. J. Chem.*, 1988, **66**, 1495 (*pmr, conformn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COE750
Lee, E.W. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 96 (*rev, tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 348
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 190

2-Isopropyl-1,4-benzenediol I-120

[2349-71-5]
2-(1-Methylethyl)-1,4-benzenediol, 9CI. Isopropylhydroquinone, 8CI. 1,4-Dihydroxy-2-isopropylbenzene. 2,5-Dihydroxycumene. 2-Isopropylquinol



$C_9H_{12}O_2$ 152.193
Antioxidant for fats and oils. Needles (C_6H_6 or by subl.). Mp 129-131°.

Di-Ac:
$C_{13}H_{16}O_4$ 236.267
Liq. d^{20} 1.1. Bp_3 136-140°.

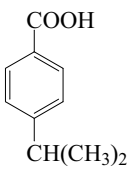
4-Me ether: [13522-86-6] *2-Isopropyl-4-methoxyphenol*
$C_{10}H_{14}O_2$ 166.219
Liq. Bp_1 105°.

Di-Me ether: [4132-71-2] *2-Isopropyl-1,4-dimethoxybenzene*
$C_{11}H_{16}O_2$ 180.246
Liq. Bp_{11} 122-124°.

Zenker, N. *et al., J.O.C.*, 1959, **24**, 1351 (*synth*)
Bogolyubskii, V.A. *et al., Zh. Obshch. Khim.*, 1962, **32**, 869; *CA*, **58**, 2391 (*synth*)

4-Isopropylbenzoic acid I-121

[536-66-3]
4-(1-Methylethyl)benzoic acid, 9CI. Cuminic acid. Cumic acid



$C_{10}H_{12}O_2$ 164.204
Constit. of various plant spp. incl. *Cuminum cyminum* (cumin), *Ferula* spp. and *Perilla frutescens* (perilla). Needles (hexane) or plates (EtOH). d_4 1.16. Mp 117-118°. pK_{a1} 4.36 (25°).

Me ester: [20185-55-1]
$C_{11}H_{14}O_2$ 178.23
Bp_{14} 126°.

Et ester: [19024-50-1]
$C_{12}H_{16}O_2$ 192.257
Bp 263-264° $Bp_{13.5}$ 134-135°.

Chloride: [21900-62-9]
$C_{10}H_{11}ClO$ 182.649
Bp 256-258°.

Amide: [619-76-1]
$C_{10}H_{13}NO$ 163.219
Mp 158-160° (153°).

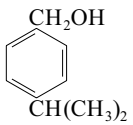
Nitrile: [13816-33-6] *4-(1-Methylethyl)-benzonitrile, 9CI. 1-Cyano-4-isopropylbenzene. 4-Cyanocumene. Cuminyl nitrile*
$C_{10}H_{11}N$ 145.204
Liq. $Bp_{0.7}$ 85°.

▶ Skin irritant. LD_{50} (rat, orl) 3900 mg/kg. DI4650000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1073C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1326B (*ir*)
Bert, L. *et al., Bull. Soc. Chim. Fr.*, 1925, **37**, 1397
Beckwith, A.L.J. *et al., Aust. J. Chem.*, 1965, **18**, 1023 (*synth*)
Ger. Pat., 1973, 2 138 283; *CA*, **78**, 97333
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1983, **21**, 837 (*rev, tox, nitrile*)
Popielarz, R. *et al., J.A.C.S.*, 1990, **112**, 3068 (*nitrile*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IOD050

4-Isopropylbenzyl alcohol I-122

[536-60-7]
4-(1-Methylethyl)benzenemethanol, 9CI. p-*Cymen-7-ol, 8CI.* p-*Mentha-1,3,5-trien-7-ol.* ***Cuminyl alcohol****. Cumic alcohol. FEMA 2933*



$C_{10}H_{14}O$ 150.22
Flavouring ingredient. Isol. from oils of *Cuminum cyminum* (cumin). Liq. with an intense caraway-like odour and an aromatic, burning taste. d^{20} 0.98. Bp 246° Bp_{20} 140°. n_D^{24} 1.5220.

▶ Skin irritant. LD_{50} (rat, orl) 1020 mg/kg. GZ7260000

O-*[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside]:* ***Coleoside***
$C_{22}H_{34}O_{11}$ 474.504
Yellow solid.

Ac: [59230-57-8]
$C_{12}H_{16}O_2$ 192.257
$Bp_{16.5}$ 136°.

▶ DA4977000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1133B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 349A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1057C (*ir*)
Bert, L. *et al., Bull. Soc. Chim. Fr.*, 1925, **37**, 1397; 1577
Palfray, L. *et al., C. R. Hebd. Seances Acad. Sci.*, 1936, **203**, 1523
Seidel, C.F. *et al., Helv. Chim. Acta*, 1944, **27**, 663 (*isol*)
v. Sydow, E. *et al., Acta Chem. Scand.*, 1963, **17**, 2504 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 871 (*rev, tox*)
van Tamelen, E.E. *et al., J.A.C.S.*, 1974, **96**, 5290
Ahmed, B. *et al., Phytochemistry*, 1988, **27**, 3309
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 411
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1486-1487
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQI250

5-Isopropylbicyclo[3.1.0]hexan-2-one, 8CI I-123

[513-20-2]
5-(1-Methylethyl)bicyclo[3.1.0]hexan-2-one, 9CI. Sabina ketone



(−)-*form*

$C_9H_{14}O$ 138.209

Constit. of various plant spp. incl. *Artemisia* sp., *Daucus carota* (carrot).

(-)-*form* [4498-01-5]

Liq. or prisms (H_2O). Characteristic odour. Spar. sol. H_2O, sol. EtOH. Mp 17°. Bp_{17} 97.5°. $[\alpha]_D^{21.6}$ -25.64 (homogeneous).

Semicarbazone:

Amorph. powder or cryst. (MeOH). Mp 135-137°. $[\alpha]_D^{15.6}$ +137.5 (c, 1.0 in MeOH).

2,4-Dinitrophenylhydrazone:

Orange needles (MeOH/$CHCl_3$). Mp 124°. $[\alpha]_D$ +135.2 (c, 1.0 in $CHCl_3$).

(±)-*form* [38981-64-5]

Sol. H_2O, Et_2O. Bp_5 70°.

Semicarbazone:

Cryst. (MeOH aq.). Mp 156-157°.

2,4-Dinitrophenylhydrazone: [28892-22-0]

Orange-red needles ($CHCl_3$/MeOH). Mp 175-176.5°.

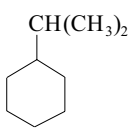
[110716-99-9]

Short, A.G. *et al., J.C.S.*, 1939, 1415 (*synth*)
Daly, J.W. *et al., J.A.C.S.*, 1958, **60**, 6330 (*abs config*)
Wheeler, J.W. *et al., J.O.C.*, 1969, **34**, 545 (*synth, ir, pmr*)
Mori, K. *et al., Tetrahedron*, 1970, **26**, 2821 (*synth, ir, pmr*)
Russell, G.A. *et al., J.A.C.S.*, 1971, **93**, 1452 (*synth, ir, pmr*)
Alexandre, C. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2241 (*synth*)
Gaoni, Y. *et al., Tetrahedron*, 1972, **28**, 5525 (*synth, ms, pmr*)
Hamon, D.P.G. *et al., Aust. J. Chem.*, 1987, **40**, 1321 (*synth*)
Mash, E.A. *et al., Tetrahedron*, 1987, **43**, 679 (*synth*)

Isopropylcyclohexane, 8CI I-124

[696-29-7]

(1-Methylethyl)cyclohexane, 9CI. 2-Cyclohexylpropane



C_9H_{18} 126.241

Found in *Carica papaya* (papaya). Oily liq. d^{20} 0.8. Fp -89.8. Bp 154.7° (150-153°). n_D^{20} 1.4410.

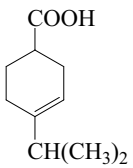
▶ Autoignition temp. 248/283°. GV5030000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 49B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 35D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 51B (*ir*)
Matsubara, K. *et al., J.C.S.*, 1905, 661 (*synth*)
Adv. Chem. Ser., 1955, **15**, 452 (***props***)
Adams, J.Q. *et al., Prepr.- Am. Chem. Soc., Div. Pet. Chem.*, 1972, **17**, C4 (*cmr*)
Green, M.M. *et al., Adv. Mass Spectrom.*, 1978, **7A**, 149 (*ms*)
Miller, L.L. *et al., J.O.C.*, 1978, **43**, 2059 (*synth*)

4-Isopropyl-3-cyclohexene-1-carboxylic acid I-125

[56424-87-4]

4-(1-Methylethyl)-3-cyclohexene-1-carboxylic acid, 9CI. 1,2,5,6-Tetrahydrocuminic acid. p-*Menth-3-ene-7-oic acid. FEMA 3731*



$C_{10}H_{16}O_2$ 168.235

(±)-*form* [71298-42-5]

Cryst. (hexane) with cuminic/sweaty odour. Mp 65-66°.

(ξ)-*form*

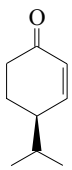
Flavouring ingredient. Present in cumin oil.

Nazarov, I.N. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1959, 1595-1604; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1959, 1536-1544 (*synth*)
Mander, L.N. *et al., Aust. J. Chem.*, 1979, **32**, 823-832 (*synth*)
Eur. Pat., 1984, 110 362; *CA*, **101**, 116599k (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 742 (*use*)

4-Isopropyl-2-cyclohexen-1-one, 8CI I-126

[500-02-7]

4-(1-Methylethyl)-2-cyclohexen-1-one, 9CI. ***Cryptone****. FEMA 3939*



(*R*)-*form*

$C_9H_{14}O$ 138.209

(*R*)-*form* [2158-59-0]

Present in many plants incl. Angelica root, black pepper, lavender and cardamom. Oil with characteristic woody odour. Bp_{10} 98-100°. $[\alpha]_D$ -119.3 (EtOH).

Semicarbazone:

Cryst. (MeOH). Mp 186°. $[\alpha]_D$ -27 (c, 2 in $CHCl_3$).

2,4-Dinitrophenylhydrazone:

Cryst. (MeOH). Mp 135-136° (132°). $[\alpha]_D^{20}$ +4.8 (c, 5 in $CHCl_3$).

(*S*)-*form* [100295-52-1]

$[\alpha]_D$ +64.57 (EtOH).

(±)-*form* [2158-61-4]

Flavouring agent for candies. Liq. with characteristic, woody odour. $Bp_{2.8}$ 78°.

Semicarbazone:

Plates (MeOH). Mp 196-196.5° dec.

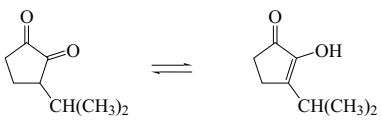
2,4-Dinitrophenylhydrazone:

Orange-red plates (EtOH). Mp 136-136.5°.

Galloway, A.S. *et al., J.C.S.*, 1936, 1595 (*isol*)
Berry, P.A. *et al., J.C.S.*, 1937, 1448 (*isol, S-form*)
Birch, A.J. *et al., Annu. Rep. Prog. Chem., Sect. B*, 1950, **47**, 190 (*abs config*)
Naves, Y.R. *et al., Perfum. Essent. Oil Res.*, 1950, **41**, 441; *CA*, **45**, 4889 (*isol*)
Soffer, M.D. *et al., J.A.C.S.*, 1955, **77**, 1003 (*synth, uv*)
Stadler, P.A. *et al., Helv. Chim. Acta*, 1960, **43**, 1601 (*isol*)
Mukherji, G. *et al., J.C.S.*, 1963, 2402 (*synth, uv*)
Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1969, 588 (*synth*)
Fisher, R.D. *et al., J.A.C.S.*, 1973, **95**, 3646 (*synth, ir, pmr*)
Friedrich, E. *et al., Angew. Chem.*, 1977, **89**, 426 (*synth*)
Mancini, I. *et al., Gazz. Chim. Ital.*, 1988, **118**, 447 (*synth*)
Hawley, R.C. *et al., Synth. Commun.*, 1990, **20**, 1159 (*resoln*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 906 (*use*)

3-Isopropyl-1,2-cyclopentanedione I-127

2-Hydroxy-3-isopropyl-2-cyclopenten-1-one. 2-Hydroxy-3-(1-methylethyl)-2-cyclopenten-1-one, 9CI



$C_8H_{12}O_2$ 140.182

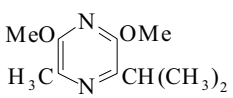
Enol-form predominates. Volatile constit. of roasted Arabica coffee beans. Cryst. (Et_2O/petrol) with sweet, burnt odour. Mp 82-83° (66-68°).

Maignan, C. *et al., Bull. Soc. Chim. Fr.*, 1974, 2035-2039 (*synth, pmr, uv*)
Stetter, H. *et al., Tet. Lett.*, 1980, **21**, 3479-3482 (*synth*)
Arnarp, J. *et al., Acta Chem. Scand., Ser. B*, 1986, 839-854 (*occur, synth, pmr, ms*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*occur, ms, coffee*)

2-Isopropyl-3,5-dimethoxy-6-methylpyrazine I-128

[32021-42-4]

2,6-Dimethoxy-3-methyl-5-(1-methylethyl)pyrazine, 9CI



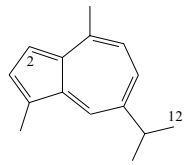
$C_{10}H_{16}N_2O_2$ 196.249

Constit. of Galbanum oil.

Burrell, J.W.K. *et al., Chem. Ind. (London)*, 1970, 1409 (*synth*)
Takken, H.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 638 (*synth*)

7-Isopropyl-1,4-dimethylazulene I-129

[489-84-9]
1,4-Dimethyl-7-(1-methylethyl)azulene, 9CI. 1,3,5,7,9-Guaiapentaene. ***Guaiazulene****.* S-*Guaiazulene. Kessazulene. Azulon. Eucazulene. Azunol*



$C_{15}H_{18}$ 198.307
Obt. from essential oils, e.g. chamomile oil. Blue-violet plates (EtOH) or blue oil. Mp 31.5°. Bp_{12} 167-168°. Log P 5.74 (calc). λ_{max} 286 ; 292 ; 350 ; 377 ; 600 ($CHCl_3$) (Berdy). λ_{max} 556 ; 581 ; 603 ; 632 (Et_2O).

▶ LD_{50} (rat, orl) 1550 mg/kg. CO4790000

1,3,5-Trinitrobenzene complex: [4968-29-0]
Black needles (EtOH). Mp 151-151.5°.

Picrate:
Black needles (EtOH). Mp 122-122.5°.

2-Chloro: [90052-60-1] *2-Chloro-1,3,5,7,9-guaiapentaene. 3-Chloro-7-isopropyl-1,4-dimethylazulene.* ***3-Chloroguaiazulene***
$C_{15}H_{17}Cl$ 232.752
λ_{max} 246 (ϵ); 293 (ϵ); 307 (ϵ); 352 (ϵ); 369 (ϵ); 620 (ϵ) ($CHCl_3$) (Derep).

2-Bromo: [90052-61-2] *2-Bromo-1,3,5,7,9-guaiapentaene. 3-Bromo-7-isopropyl-1,4-dimethylazulene.* ***3-Bromoguaiazulene***
$C_{15}H_{17}Br$ 277.203
Oil.

12-Bromo: [90052-62-3] *12-Bromo-1,3,5,7,9-guaiapentaene. 7-(2-Bromo-1-methylethyl)-1,4-dimethylazulene, 9CI.* ***Ehuazulene***
$C_{15}H_{17}Br$ 277.203
Oil. $[\alpha]_D$ +2 (hexane). λ_{max} 245 (ϵ); 286 (ϵ); 293 (ϵ); 305 (sh) (ϵ); 352 (ϵ); 369 (ϵ); 608 (ϵ) ($CHCl_3$) (Derep).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **2**, 40B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **1**, 955D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 877B (*ir*)
Plattner, P.A. *et al., Helv. Chim. Acta*, 1949, **32**, 2137; 2452 (*synth*)
Šorm, F. *et al., Coll. Czech. Chem. Comm.* , 1951, **16**, 168; 626 (*isol, synth*)
Caujolle, F. *et al., Ann. Pharm. Fr.* , 1952, **10**, 412 (*pharmacol*)
Herz, A. *et al., Arzneim.-Forsch.* , 1953, **3**, 253 (*pharmacol*)
Jacob, T.M. *et al., Tetrahedron*, 1964, **20**, 2821 (*uv, synth*)
Llinas, J.R. *et al., Can. J. Chem.* , 1975, **53**, 2911 (*pmr, cmr*)
Hoffmann, W. *et al., Tet. Lett.* , 1975, 533 (*synth*)
Mukherjee, D. *et al., J.A.C.S.* , 1979, **101**, 251 (*synth*)
Fusetani, N. *et al., Experientia*, 1981, **37**, 680 (*isol*)
Li, M.K.W. *et al., Tet. Lett.* , 1984, **25**, 587 (*derivs*)
Vidal-Ollivier, E. *et al., J. Chromatogr.* , 1989, **463**, 227 (*hplc*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1688
Kourounakis, A.P. *et al., Arch. Pharm. (Weinheim, Ger.)* , 1997, **330**, 7 (*pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DSJ800

2-Isopropyl-2,3-dimethylbutanoic acid I-130

[23119-04-2]
2,3-Dimethyl-2-(1-methylethyl)butanoic acid, 9CI. 2,2-Diisopropylpropanoic acid
$[(H_3C)_2CH]_2C(CH_3)COOH$
$C_9H_{18}O_2$ 158.24
Liq. Mp 49.5-50.5°.

Et ester: [63791-89-9]
$C_{11}H_{22}O_2$ 186.294
Bp_{38} 100-102°.

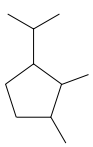
Methylamide: [51115-67-4] N*,2,3-Trimethyl-2-(1-methylethyl)butanamide, 9CI. 2-Isopropyl-*N*,2,3-trimethylbutyramide. FEMA 3804*
$C_{10}H_{21}NO$ 171.282
Physiol. stem cooling agent used in food; its effect is similar to that of menthol but without the strong minty flavour. Flavouring agent for chewing gum and candies. Cryst. solid with cooling menthol-type flavour. Mp 56-64°.

[55519-33-0]

Tsia, L. *et al., J.A.C.S.* , 1957, **79**, 2530-2533 (*synth*)
U.K. Pat. , 1976, 1 421 744; *CA* , **84**, 150224z (*methylamide, synth*)
Watson, H.R. *et al., J. Soc. Cosmet. Chem.* , 1978, **29**, 185-200 (*methylamide, props, synth, SAR*)
Lion, C. *et al., Tetrahedron* , 1979, **35**, 2077-2079 (*synth, Et ester*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 921 (*methylamide*)

1-Isopropyl-2,3-dimethylcyclopentane I-131

[489-20-3]
1,2-Dimethyl-3-(1-methylethyl)cyclopentane, 9CI. Osmane. Nepetane. Iridane



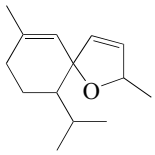
$C_{10}H_{20}$ 140.268
Claimed to have been isol. from flowers of *Osmanthus fragrans* (sweet osmanthus) but this was prob. erroneous.. 2 pure stereoisomers prepd., others obt. as mixts..

[36208-14-7, 36208-15-8, 36208-16-9, 36208-17-0]

Sisido, K. *et al., J.O.C.* , 1966, **31**, 2795 (*synth, bibl*)
Kepner, R.E. *et al., J. Chromatogr.* , 1972, **66**, 229

10-Isopropyl-2,7-dimethyl-1-oxaspiro[4.5]deca-3,6-diene I-132

[89079-92-5]
2,7-Dimethyl-10-(1-methylethyl)-1-oxaspiro[4.5]deca-3,6-diene, 9CI. Neocaspirene



$C_{14}H_{22}O$ 206.327
Fragrance ingredient with a blackcurrant-like aroma.

Eur. Pat. , 1983, 94 722; *CA* , **100**, 120864q (*synth, use*)

2-Isopropylfuran, 8CI I-133

[10599-59-4]
2-(1-Methylethyl)furan, 9CI

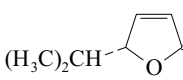


$C_7H_{10}O$ 110.155
Constit. of carob (*Ceratonia siliqua*), coffee and Chinese quince fruit (*Chaenomeles speciosa*) aromas. Bp 107.4-108.4° Bp_{38} 33°.

Heyns, K. *et al., Tetrahedron* , 1966, **22**, 2223 (*ms*)
Gouesnard, J.P. *et al., Bull. Soc. Chim. Fr.* , 1969, 4452 (*synth*)
Ibragimov, I.I. *et al., Khim. Geterotsikl. Soedin.* , 1973, **9**, 1434; *Chem. Heterocycl. Compd. (Engl. Transl.)* , 1973, **9**, 1300 (*synth*)
Menicagli, R. *et al., Chim. Ind. (Milan)* , 1976, **58**, 880 (*synth*)
Vitzthum, O.G. *et al., Z. Lebensm.-Unters. -Forsch.* , 1976, **160**, 277-291 (*isol*)
Gribble, G.W. *et al., Tet. Lett.* , 1988, **29**, 6227 (*synth*)

5-Isopropyl-2(5*H*)-furanone, 8CI I-134

[56767-19-2]
*5-(1-Methylethyl)-2(5*H*)-furanone, 9CI*



(*R*)-*form*

$C_7H_{10}O_2$ 126.155
Lit. unclear over the sign of opt. rotn. of enantiomers.

(R)-form [98878-30-9]
Liq. $Bp_{0.1}$ 78-79°. $[\alpha]_D^{21}$ -121 (c, 2 in dioxan) (98% ee).

(S)-form [98878-24-1]
Liq. $Bp_{0.1}$ 78-79°. $[\alpha]_D^{21}$ +121 (c, 2 in dioxan) (98% ee).

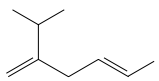
(ξ)-form [100019-33-8]
Component of 'hydrogenation flavour' formed on storage of deodorised hydrogenated soybean oil. Liq.

Yasuda, K. *et al., J. Am. Oil Chem. Soc.* , 1975, **52**, 307 (*isol*)
Franck-Neumann, M. *et al., Angew. Chem., Int. Ed.* , 1985, **97**, 995 (*R-form, S-form, synth*)

Pecunioso, A. *et al., Tetrahedron*, 1990, **46**, 7497 (*synth, pmr, cmr, ir, ms*)
Beckmann, M. *et al., Tetrahedron: Asymmetry*, 1990, **1**, 335 (*S-form, synth*)
Craig, D. *et al., Tet. Lett.*, 1992, **33**, 7445 (*synth*)
Wegener, B. *et al., Tetrahedron: Asymmetry*, 1993, **4**, 345 (*S-form, synth*)
Bonete, P. *et al., J.O.C.*, 1994, **59**, 3202 (*synth, pmr, cmr, ms, ir, tlc*)
Renard, M. *et al., Tetrahedron*, 2001, **57**, 2597-2608 (*R-form, synth*)

2-Isopropyl-1,4-hexadiene, 8CI I-135

6-Methyl-5-methylene-2-heptene, 9CI. Salvene



(E)-form

C_9H_{16} 124.225

Salvene originally descr. as a thujane. Present in oil of sage (*Salvia officinalis*), probably as artifact of decarbonylation of thujanes.

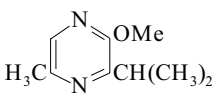
[33746-69-9, 33746-70-2]

Brieskorn, C.H. *et al., Annalen*, 1964, **676**, 171 (*isol*)
Laurence, B.M. *et al., Parfums, Cosmet. Savons Fr.*, 1971, **1**, 256; *CA*, **75**, 80186b (*isol*)
Dillenberger, Z. *et al., Helv. Chim. Acta*, 1978, **61**, 1856 (*synth, pmr*)
Cooke, R.J. *et al., J.A.C.S.*, 1981, **103**, 7317 (*synth, bibl*)

3-Isopropyl-2-methoxy-5-methylpyrazine I-136

[32021-41-3]

2-Methoxy-5-methyl-3-(1-methylethyl)pyrazine, 9CI



$C_9H_{14}N_2O$ 166.222

Constit. of Galbanum oil.

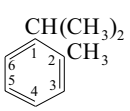
Burrell, J.W.K. *et al., Chem. Ind. (London)*, 1970, 1409 (*synth*)
Takken, H.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 638 (*synth*)

1-Isopropyl-2-methylbenzene I-137

[527-84-4]

[25155-15-1]

1-Methyl-2-(1-methylethyl)benzene, 9CI. o-*Isopropyltoluene.* o-*Cymene.* o-*Mentha-1,3,5-triene*



$C_{10}H_{14}$ 134.221

Isol. from *Citrus aurantium* (Seville orange). Liq. Mp -71.54°. Bp 178.15°.

▶ GZ5949900

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 10A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 856D (*ir*)
Adv. Chem. Ser., 1955, **15**, 32 (***props***)
Allen, R.H. *et al., J.A.C.S.*, 1961, **83**, 2799 (*synth*)
Parham, W.E. *et al., Synthesis*, 1976, 116 (*synth, use*)
Hino, M. *et al., Chem. Lett.*, 1977, 277 (*synth*)

1-Isopropyl-3-methylbenzene I-138

[535-77-3]

[25155-15-1]

1-Methyl-3-(1-methylethyl)benzene, 9CI. m-*Isopropyltoluene.* m-*Cymene.* m-*Cymol.* m-*Mentha-1,3,5-triene*

$C_{10}H_{14}$ 134.221

Present in oil of *Ribes nigrum* (blackcurrant). Liq. d^{20} 0.86. Mp -63.75°. Bp 175.14°. n_D^{20} 1.4922.

▶ GZ5949800

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 13A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 858B (*ir*)
Adv. Chem. Ser., 1955, **15**, 33 (***props***)
Allen, R.H. *et al., J.A.C.S.*, 1961, **83**, 2799 (*synth*)
Andersson, J. *et al., Acta Chem. Scand.*, 1964, **18**, 1105 (*isol*)
Org. Synth., Coll. Vol., 5, 1973, 332 (*synth*)
Olah, G.A. *et al., J.O.C.*, 1974, **39**, 2430 (*synth*)
Hino, M. *et al., Chem. Lett.*, 1977, 277 (*synth*)

1-Isopropyl-4-methylbenzene I-139

[99-87-6]

[25155-15-1]

1-Methyl-4-(1-methylethyl)benzene, 9CI. p-*Mentha-1,3,5-triene.* p-*Cymene.* p-*Isopropyltoluene.* p-*Cymol. Camphogene (obsol.). Camphene (obsol.). FEMA 2356*

$C_{10}H_{14}$ 134.221

V. widely distributed in plant oils e.g. terpentine and citrus oils and many others. Used in flavour industries. Liq. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp -67.94°. Bp 177.1°.

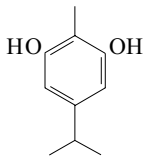
▶ Flammable, fl. p. 47/53°, autoignition temp. 436/445°. Skin and mucous membrane irritant may cause CNS effects by inhalation. LD_{50} (rat, orl) 4750 mg/kg. GZ5950000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 15A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 939D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 859D (*ir*)
Adv. Chem. Ser., 1955, **15**, 34 (***props***)
Allen, R.H. *et al., J.A.C.S.*, 1961, **83**, 2799 (*synth*)
Hall, S.S. *et al., J.O.C.*, 1972, **37**, 760 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 39 (*occur*)
Olah, G.A. *et al., J.O.C.*, 1974, **39**, 2430 (*synth*)
Hino, M. *et al., Chem. Lett.*, 1977, 277 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CQI000
Lee, E.W. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2*, 1990, 105 (*rev, tox*)
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 203

5-Isopropyl-2-methyl-1,3-benzenediol I-140

[4389-62-2]

2-Methyl-5-(1-methylethyl)-1,3-benzenediol, 9CI. p-*Cymene-2,6-diol.* p-*Mentha-1,3,5-triene-2,6-diol.* ***Cymorcin***. *5-Hydroxycarvacrol*



$C_{10}H_{14}O_2$ 166.219

Mp 130-132°. Bp 294°.

Mono-O-β-D-glucopyranoside: [76859-62-6]
$C_{16}H_{24}O_7$ 328.361
Constit. of the seeds of *Carum copticum* (ajowan). Powder. Mp 177-178°.

Di-O-β-D-glucopyranoside:
$C_{22}H_{34}O_{12}$ 490.503
Constit. of fruit of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{23}$ -62 (c, 0.3 in MeOH).

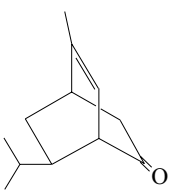
Dibenzoyl:
Mp 80°.

Di-Me ether:
Bp_{20} 142°.

Treibs, W. *et al., Ber.*, 1931, **64**, 2184 (*synth*)
Treibs, W. *et al., J. Prakt. Chem.*, 1933, **138**, 284 (*synth*)
De Fenik, I.J.S. *et al., CA*, 1975, **83**, 103138 (*isol*)
Garg, S.K. *et al., Phytochemistry*, 1980, **19**, 2215 (*isol, glucoside*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*diglucoside*)

7-Isopropyl-5-methylbicyclo[2.2.2]oct-5-en-2-one I-141

[73069-42-8]



$C_{12}H_{18}O$ 178.274

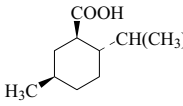
Constit. of *Angelica archangelica* (angelica). Oil. $[\alpha]_D^{20}$ +345 (c, 0.9 in $CHCl_3$).

Escher, S. *et al., Helv. Chim. Acta*, 1979, **62**, 2061

2-Isopropyl-5-methylcyclohexanecarboxylic acid I-142

[39668-86-5]

5-Methyl-2-(1-methylethyl)cyclohexanecarboxylic acid, 9CI



(1*R*,2*S*,5*R*)-*form*

$C_{11}H_{20}O_2$ 184.278

(1*R*,2*S*,5*R*)-*form* [16052-40-7]
Cryst. (MeOH aq.). Mp 62-64°. Subl.10 60. $[\alpha]_D^{20}$ -42.6 (c, 8.16 in EtOH).

Amide:
$C_{11}H_{21}NO$ 183.293
Cryst. (EtOH aq.). Mp 147-148.5°. $[\alpha]_D^{20}$ -50.4 (c, 6.73 in EtOH).

Methylamide:
$C_{12}H_{23}NO$ 197.32
Cryst. (EtOH aq.). Mp 95-97°.

Dimethylamide:
$C_{13}H_{25}NO$ 211.347
Oil. $Bp_{0.01}$ 56-57°.

Ethylamide: [39711-79-0] *Ethyl menthane carboxamide. FEMA 3455*
$C_{13}H_{25}NO$ 211.347
Physiological coolant used in foods, beverages, chewing gum, toiletries, topical pharmaceutical formulations and oral hygiene products. Cryst. (Me_2CO aq.). Mp 91-93° (88°). $[\alpha]_D^{25}$ -46.71 (c, 2.14 in EtOH). Stereochem. not specified by FEMA.

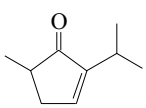
(1*S*,2*R*,5*S*)-*form* [62309-29-9]
$[\alpha]_D^{20}$ +42.3 (c, 8.16 in EtOH).

Anilide: [71376-28-8]
$C_{17}H_{25}NO$ 259.391
Mp 151-152°. $[\alpha]_D^{20}$ +58.7.

Smith, J.G. *et al., J.O.C.*, 1952, **17**, 1116-1121 (*synth*)
Matsumoto, M. *et al., Tet. Lett.*, 1976, 3827-3830 (*anilide*)
Watson, H.R. *et al., J. Soc. Cosmet. Chem.*, 1978, **29**, 185-200 (*ethylamide, synth, props, sar*)
U.S. Pat., 1979, 4 150 052; *CA*, 181430h (*amides, synth, use*)
Pfeiffer, H.P. *et al., Annalen*, 1987, 725-726 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 242 (*ethylamide, props, use*)

2-Isopropyl-5-methyl-2-cyclopenten-1-one, 8CI I-143

[5587-79-1]
5-Methyl-2-(1-methylethyl)-2-cyclopenten-1-one, 9CI. ***Pulegenone***



$C_9H_{14}O$ 138.209
Found in citronella and peppermint oils. Oil. Bp 188.5-189°.

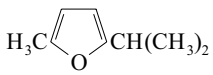
Oxime:
$C_9H_{15}NO$ 153.224
Oil. Bp 237-242°.

Semicarbazone:
Cryst. (MeOH). Mp 183-184°.

Wallach, O. *et al., Annalen*, 1919, **418**, 36 (*synth*)
Vig, O.P. *et al., Indian J. Chem.*, 1963, **1**, 365 (*synth*)
Conia, J.M. *et al., Bull. Soc. Chim. Fr.*, 1970, 2972 (*ir, pmr, uv*)
Saxena, A.K. *et al., Indian Perfum.*, (1-B), 1976, **20**, 1 (*isol*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 867 (*rev tox*)

2-Isopropyl-5-methylfuran I-144

[10504-05-9]
2-Methyl-5-(1-methylethyl)furan



$C_8H_{12}O$ 124.182
Important natural flavour. Oil with strong herbaceous odour. Bp 136° Bp_{60} 58°.

Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)
Eichenberger, H. *et al., Helv. Chim. Acta*, 1976, **59**, 1253 (*cmr*)
Weyerstahl, P. *et al., Annalen*, 1988, 1015 (*synth, pmr, bibl*)

2-Isopropyl-5-methyl-2-hexenal I-145

[35158-25-9]

[69104-96-7, 69104-97-8]
5-Methyl-2-(1-methylethyl)-2-hexenal, 9CI. 2,6-Dimethyl-3-formyl-3-heptene. 2-Isopropyl-3-isobutylacrolein. FEMA 3406. Isodihydrovandulyl aldehyde

$(H_3C)_2CHCH_2CH{=}C(CHO)CH(CH_3)_2$
$C_{10}H_{18}O$ 154.252
Flavouring ingredient. Present in cocoa and preserved *Feijowa sellowiana* fruits. Minor aroma constit. of malted barley. Liq. with sharp cocoa powder-like aroma. d_4^{20} 0.85. Bp 189° $Bp_{2.5}$ 45-50°. n_D^{20} 1.4459. No information on geom. isomerism.

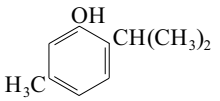
2,4-Dinitrophenylhydrazone:
Mp 138.7°.

Semicarbazone:
Mp 119°.

Tiollais, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1953, **236**, 1798-1799 (*synth*)
Astle, M.J. *et al., J.O.C.*, 1959, **24**, 56-60 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 317 (*use, tox*)
Starodubtseva, V.P. *et al., Subtrop. Kul't.*, 1978, 70-72; *CA*, **90**, 71704b (*occur, feijowa*)
Beal, A.D. *et al., J. Agric. Food Chem.*, 1994, **42**, 2880-2884 (*occur, barley*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 417 (*use*)
Samsudin, M.W. *et al., J. Agric. Food Chem.*, 1996, **44**, 247-250 (*occur*)
Morgan, E.D. *et al., J. Chem. Ecol.*, 1999, **25**, 1395-1409 (*isol, ants*)

2-Isopropyl-5-methylphenol I-146

[89-83-8]
5-Methyl-2-(1-methylethyl)phenol, 9CI. p-*Cymen-3-ol, 8CI. 3-Hydroxy-*p-*cymene. 3-Hydroxy-4-isopropyltoluene. 6-Isopropyl-*m-*cresol.* p-*Mentha-1,3,5-trien-3-ol.* ***Thymol.*** m-*Thymol. Thymianic acid (obsol.). Thymianic camphor (obsol.). FEMA 3066*



$C_{10}H_{14}O$ 150.22
Found in many essential oils. Esp. found in the Labiatae. Rich sources are thyme oil, seed oil of *Ptychotis ajowan* and oils of horsemint (*Monarda punctata*) and *Ocimum* spp. Flavouring ingredient. Plates (EtOAc or AcOH or Me_2CO) with odour of thyme. Sol. MeOH, hexane; poorly sol. H_2O, acids. Mp 51.5°. Bp 233.5° Bp_{10} 115°. pK_{a1} 10.62 (20°). Log P 3.4 (calc).

▶ LD_{50} (rat, orl) 980 mg/kg. XP2275000

Me ether: [1076-56-8] *1-Isopropyl-2-methoxy-4-methylbenzene. 2-Isopropyl-5-methylanisole.* ***Thymol methyl ether***
$C_{11}H_{16}O$ 164.247
Naturally occurring, e.g. in oil of sea fennel (*Crithmum maritimum*) and *Citrus* spp.. Oil with ethereal odour. Bp_{745} 211-212° Bp_{15} 94-96°.

▶ BZ8770000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1087D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 266A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1020D (*ir*)
Fujita, Y. *et al., CA*, 1947, **41**, 3585 (*isol, deriv*)
v. Sydow, E. *et al., Acta Chem. Scand.*, 1963, **17**, 2504 (*ms*)
Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1963, **296**, 353 (*isol, synth, deriv*)
Yamazaki, M. *et al., Chem. Pharm. Bull.*, 1963, **11**, 363 (*biosynth*)
Kraus, M. *et al., Coll. Czech. Chem. Comm.*, 1963, **28**, 1877 (*synth*)
Uldrickies, J. *et al., CA*, 1965, **63**, 11408 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Noall, M.W. *et al., Anal. Biochem.*, 1975, **69**, 10 (*gc*)
Sandell, E.B. *et al., Photometric Determination of Traces of Metals*, General Aspects, Wiley, New York, 1978, 301
Yoshida, T. *et al., Heterocycles*, 1995, **41**, 1923 (*cmr*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1148
Eisenreich, W. *et al., Tetrahedron*, 1997, **38**, 3889-3892 (*biosynth*)
Divakar, K.J. *et al., Org. Prep. Proced. Int.*, 2000, **32**, 92-93 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFX810

5-Isopropyl-2-methylphenol I-147

[499-75-2]
2-Hydroxy-4-isopropyl-1-methylbenzene. p-*Mentha-1,3,5-trien-2-ol. Carvacrol. 2-Hydroxycymene. Cymophenol.* p-*Cymen-2-ol. 5-Isopropyl-*o-*cresol. FEMA 2245*

$C_{10}H_{14}O$ 150.22
Constit. of many essential oils. Esp. found in the Labiatae. Thyme oil (=70%) and Origanum oil (=80%) are rich sources. Flavouring ingredient. Liq. Mp 3.5°. Bp 237-238° Bp_{10} 113°.

▶ Severe skin irritant. LD_{50} (rat, orl) 810 mg/kg. FI1225000

Ac: [6380-28-5]
$C_{12}H_{16}O_2$ 192.257

Found in various essential oils. Bp 245-248°.

3,5-Dinitrobenzoyl:
Cryst. Mp 76-77°.

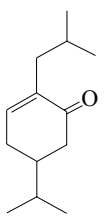
Me ether: [6379-73-3] *4-Isopropyl-2-methoxy-1-methylbenzene. 5-Isopropyl-2-methylanisole*
$C_{11}H_{16}O$ 164.247
Bp 216° Bp_{15} 94°.

Et ether: [4732-13-2] *2-Ethoxy-1-methyl-4-(1-methylethyl)benzene, 9CI. 2-Ethoxy-4-isopropyl-1-methylbenzene. Carvacryl ethyl ether. FEMA 2246*
$C_{12}H_{18}O$ 178.274
Flavouring ingredient. Oil. Bp 235°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 266C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1021B (*ir*)
Guenther, E. *et al., The Essential Oils*, Van Nostrand, N.Y., Vol. 2, 1949, 503 (*rev*)
Ritter, G. *et al., J.A.C.S.*, 1950, **72**, 2381 (*synth*)
Carpenter, E. *et al., J.O.C.*, 1955, **20**, 401 (*isol*)
Enzell, C. *et al., Acta Chem. Scand.*, 1960, **14**, 81; 1961, **15**, 1313 (*isol, deriv*)
Strubell, W. *et al., J. Prakt. Chem.*, 1960, **12**, 27-34 (*Et ether*)
Beckley, H.D. *et al., Org. Mass Spectrom.*, 1968, **1**, 47 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 174 (*occur*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 743 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 106-107 (*Et ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 518-519 (*Et ether*)
Sanabria-Galinda, A. *et al., Rev. Colomb. Quim.*, 1999, **28**, 83-88 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCM000

5-Isopropyl-2-(2-methylpropyl)-2-cyclohexen-1-one I-148

[79862-15-0]
5-(1-Methylethyl)-2-(2-methylpropyl)-2-cyclohexen-1-one, 9CI



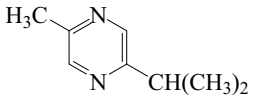
$C_{13}H_{22}O$ 194.316
Constit. of *Anthemis nobilis* (Roman chamomile). Oil.

[79862-34-3]

Thomas, A.F. *et al., Helv. Chim. Acta*, 1981, **64**, 1488

2-Isopropyl-5-methylpyrazine, 8CI I-149

[13925-05-8]
2-Methyl-5-(1-methylethyl)pyrazine, 9CI. FEMA 3554



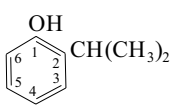
$C_8H_{12}N_2$ 136.196
Present in boiled potato, coffee aroma, cocoa butter, fish sauce and roasted earth-almond (*Cyperus esculentus*). Liq. with peanut-like odour. Bp_{13} 68-70° (as 1:1 mixt. with the 2,6-isomer). n_D^{23} 1.4865.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694-705 (*synth, ms, isol*)
Peer, H.G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 1335-1336 (*synth*)
Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-62; **32(2)**, 64-66; 68-70 (*use*)
Cantalego, M.J. *et al., J. Agric. Food Chem.*, 1997, **45**, 1853-1860 (*glc, detn, earth-almond*)
Ulrich, D. *et al., Am. J. Potato Res.*, 2000, **77**, 111-117 (*glc, detn*)

2-Isopropylphenol I-150

[88-69-7]

[25168-06-3]
2-(1-Methylethyl)phenol, 9CI. o-*Hydroxycumene. FEMA 3461*



$C_9H_{12}O$ 136.193
Flavouring ingredient. d^{20} 1.01. Mp 15-16°. Bp 212-214°. n_D^{20} 1.5315. pK_{a1} 10.31 (25°, 0.1*M* KCl).

▶ SL5900000

Me ether: [2944-47-0] *1-Isopropyl-2-methoxybenzene.* o-*Isopropylanisole*
$C_{10}H_{14}O$ 150.22
d^{16} 0.95. Bp_{751} 198-199°.

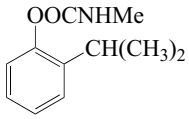
Et ether: [56631-59-5] *1-Ethoxy-2-isopropylbenzene.* o-*Isopropylphenetole*
$C_{11}H_{16}O$ 164.247
d_4^0 0.94. Bp_{762} 208.6-209.6°.

[26967-76-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1070A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 244B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1002A (*ir*)
Yamamoto, O. *et al., Anal. Chem.*, 1972, **44**, 1794 (*nmr*)
Yoneda, N. *et al., Nippon Kagaku Kaishi*, 1977, **6**, 831; *CA*, **87**, 134237n (*synth*)
Iyer, P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 321 (*synth*)
Chang, H.M. *et al., J.O.C.*, 1990, **55**, 3537 (*Me ether, synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 418
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1497
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 757

2-Isopropylphenyl methylcarbamate I-151

[2631-40-5]
2-(1-Methylethyl)phenyl methylcarbamate, 9CI. Isoprocarb, BSI, ISO. O-*Cumenyl methylcarbamate. Etrofolan. Mipcin. MIPC, JMAF*



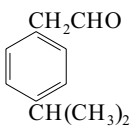
$C_{11}H_{15}NO_2$ 193.245
Agricultural insecticide used on rice, cocoa, sugar cane, vegetables and other crops. Cryst. Insol. H_2O; sol. MeOH, Me_2CO. Mp 88-93°.

▶ LD_{50} (rat, orl) 178 mg/kg. FB7880000

Japan. Pat., 1968, 68 16 973; *CA*, **70**, 57405k
Grou, E. *et al., J. Chromatogr.*, 1983, **260**, 502 (*hplc*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A907
Pesticide Manual, 11th edn., 1997, No. 431
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIA250

4-Isopropylphenylacetaldehyde I-152

[4395-92-0]
4-(1-Methylethyl)benzeneacetaldehyde, 9CI. p-*Cymene-7-carboxaldehyde, 8CI. Cumyl acetaldehyde. Homocuminic aldehyde. Cortexal. FEMA 2954*



$C_{11}H_{14}O$ 162.231
Used in perfumery and food flavouring. Liq. with a wood-sap odour. d_4^{20} 0.97. Bp 243° Bp_{13} 120°. n_D^{20} 1.5109.

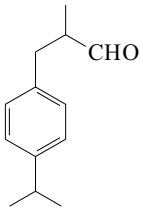
Oxime:
$C_{11}H_{15}NO$ 177.246
Mp 87-88°.

Semicarbazone:
Mp 170°.

Ohloff, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1954, **287**, 258 (*synth, deriv*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 533 (*tox, rev*)

3-(4-Isopropylphenyl)-2-methylpropanal I-153

[103-95-7]
α-Methyl-4-(1-methylethyl)benzenepropanal, 9CI. p-*Isopropyl-α-methylhydrocinnamaldehyde, 8CI. 3-Cumylisobutyraldehyde. Cyclamen aldehyde. FEMA 2743*



$C_{13}H_{18}O$ 190.285

►MW4900000

(±)-*form*

Liq. with odour of cyclamen and lily of the valley. d_4^{20} 0.95. Bp 270° Bp_1 92°.

►Fl. p. 88°.

2,4-Dinitrophenylhydrazone: [14501-58-7] Cryst. Mp 112-112.5°.

Semicarbazone: [7200-97-7] Cryst. Mp 172-172.5°.

(ξ)-*form*

Constit. of blackberries, starfruit and oil of nutmeg; flavouring ingredient.

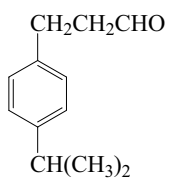
[74648-06-9, 74648-07-0, 80949-77-5]

Naves, Y.R. *et al., Manuf. Chem.*, 1948, **19**, 10 (*rev, synth*)
Beets, M.G.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1951, **70**, 25 (*synth*)
Normant, H. *et al., Bull. Soc. Chim. Fr.*, 1959, 459 (*synth*)
Berends, W. *et al., Perfum. Essent. Oil Res.*, 1967, **58**, 372 (*rev, synth, use*)
Kogami, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 604; 1973, **46**, 3562 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 397 (*rev, use*)
Chalk, A.J. *et al., J.O.C.*, 1976, **41**, 1206 (*synth*)
Garbers, C.F. *et al., S. Afr. J. Chem.*, 1980, **33**, 27 (*synth*)
Yokowo, Y. *et al., Nippon Kagaku Kaishi*, 1981, 1904; *CA*, **96**, 122332 (*synth*)
Virgilio, J.A. *et al., Org. Prep. Proced. Int.*, 1982, **14**, 9 (*synth*)
Nishimura, A. *et al., Nippon Kagaku Kaishi*, 1985, 558; *CA*, **104**, 109137 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 517
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1787-1788

3-(4-Isopropylphenyl)propanal I-154

[7775-00-0]

4-(1-Methylethyl)benzenepropanal, 9CI. FEMA 2957



$C_{12}H_{16}O$ 176.258

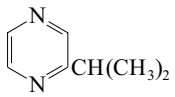
Flavouring ingredient. Liq. with sweet, green, fruity flavour.

Kologrivova, N.E. *et al., CA*, 1972, **78**, 88513p (*props*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 619-620 (*synth*)
Ho, T.-L. *et al., Synth. Commun.*, 1981, **11**, 605-607 (*synth, pmr*)

Isopropylpyrazine I-155

[29460-90-0]

(1-Methylethyl)pyrazine, 9CI. FEMA 3940



$C_7H_{10}N_2$ 122.169

Flavouring ingredient. Oil.

Oerteh, R.P. *et al., Anal. Chem.*, 1972, **44**, 1589 (*Raman*)
Rizzi, G.P. *et al., J.O.C.*, 1974, **39**, 3598 (*pmr, synth*)
Konakahara, T. *et al., Heterocycles*, 1979, **12**, 373

2-[(Isopropylthio)methyl]furan, 8CI I-156

[1883-78-9]

2-[[(1-Methylethyl)thio]methyl]furan, 9CI. Furfuryl isopropyl sulfide. FEMA 3161



$C_8H_{12}OS$ 156.248

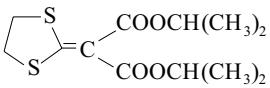
Flavouring ingredient. Liq. with sharp, spicy, mint-like odour. Bp_{12} 79-80°.

Obata, Y. *et al., Agric. Biol. Chem.*, 1965, **29**, 345-350 (*synth, ir, props*)
U.S. Pat., 1965, 3 924 015; *CA*, **84**, 164364g (*synth, use*)

Isoprothiolane, BSI, ISO, JMAF I-157

[50512-35-1]

Bis(1-methylethyl) 1,3-dithiolan-2-ylidenepropanedioate, 9CI. Diisopropyl 1,3-dithiolan-2-ylidenemalonate. Fuji-one. IPT



$C_{12}H_{18}O_4S_2$ 290.404

Agricultural fungicide for rice crops. Cryst. V. spar. sol. H_2O. Mp 50-54.5°.

►LD_{50} (rat, orl) 1190 mg/kg. TY1846000

S-*Oxide, (±)-:* [52303-69-2] *Isoprothiolane sulfoxide*
$C_{12}H_{18}O_5S_2$ 306.403
Needles (hexane/CH_2Cl_2). Mp 85-86°.

S^1,S^3-*Dioxide:* [133188-15-5]
$C_{12}H_{18}O_6S_2$ 322.403
Yellow needles (hexane/CH_2Cl_2). Mp 97-100°.

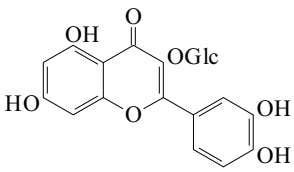
[108114-60-9, 108114-61-0]

Japan. Pat., 1970, 73 33 749; *CA*, **80**, 120903v
Tsumura, T. *et al., Jpn. Pestic. Inf.*, 1976, **27**, 20 (*activity, tox, metab*)
Uchida, M. *et al., Agric. Biol. Chem.*, 1985, **49**, 1127 (*metab*)
Katagiri, N. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3242 (*oxides*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A947
Pesticide Manual, 11th edn., 1997, No. 432

Isoquercitrin I-158

[482-35-9]

2-(3,4-Dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. 3-Glucopyranosyloxy-3′,4′,5,7-tetrahydroxyflavone. Quercetin 3-glucopyranoside. Isoquercetin. Hirsutrin



$C_{21}H_{20}O_{12}$ 464.382

The name Isoquercetin is misleading. Occurs widely in plants. Present in red wine. Yellow needles (MeOH). Mp 238-242°. $[\alpha]_D^{25}$ -19.5 (c, 0.47 in Py). Log P -2.92 (calc).

►DJ2982500

O″-*Sulfate:Quercetin 3-(sulfatoglucoside)*
$C_{21}H_{20}O_{15}S$ 544.446
Isol. from *Phoenix dactylifera* (date).

7-O-D-*Xyloside:* [79592-61-3] *Quercetin-3-glucoside 7-xyloside*
$C_{26}H_{28}O_{16}$ 596.498
Isol. from *Rubus* spp. and *Fragaria* sp..

4′-O-β-D-*Glucopyranoside:* [29125-80-2] *Quercetin 3,4′-diglucoside*
$C_{27}H_{30}O_{17}$ 626.524
Isol. from *Allium cepa* (yellow onion). Yellow needles + $3H_2O$ (MeOH/Me_2CO). Mp 249-251° (223-226°). $[\alpha]_D^{25}$ -54.6 (c, 0.52 in Py).

6″-O-β-D-*Xylopyranosyl:* [142905-18-8]
$C_{26}H_{28}O_{16}$ 596.498
Isol. from *Cistus ladanifer* (labdanum) bee pollen.

4″-O-α-L-*Rhamnopyranosyl:* [123160-33-8]
$C_{27}H_{30}O_{16}$ 610.524
Constit. of *Sambucus racemosa* (red elderberry).

2″-O-*[3,4-Dihydroxycinnamoyl-(→2)-β-D-glucopyranosyl], 7-O-β-D-glucopyranoside:* [151649-67-1] *Quercetin 3-(2-caffeoylsophoroside) 7-glucoside*
$C_{42}H_{46}O_{25}$ 950.81
Present in cabbage.

2″-O-*[4-Hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucopyranosyl], 7-O-β-D-glucopyranoside:* [151649-66-0] *Quercetin 3-(2-feruloylsophoroside) 7-glucoside*
$C_{43}H_{48}O_{25}$ 964.837
Isol. from cabbage.

3″-O-β-D-*Glucopyranosyl:* [171828-58-3] *Quercetin 3-β-laminaribioside*
$C_{27}H_{30}O_{17}$ 626.524
Constit. of *Pteridium aquilinum* (bracken fern). λ_{max} 257 ; 265 (sh) ; 357 (MeOH).

6″-O-*[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranosyl]:* [136449-10-0]
$C_{33}H_{40}O_{21}$ 772.666
Isol. from *Camellia sinensis* (black tea).

2″-O-*[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl]:* [197250-97-8]

$C_{33}H_{40}O_{22}$ 788.666
Constit. of the seeds of *Nigella sativa* (black cumin). Amorph. yellow powder. Sol. H_2O; fairly sol. MeOH; poorly sol. butanol, hexane. λ_{max} 255 ; 265 (sh) ; 355 (MeOH).

▶ LD_{50} (mus, ivn) 62 mg/kg.

2″-O-[4-Hydroxy-3-methoxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl]: [197294-29-4]
$C_{43}H_{48}O_{25}$ 964.837
Constit. of the seeds of *Nigella sativa* (black cumin).

6″-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl]: [61474-16-6] *Quercetin 3-gentiotrioside.* ***Moracetin***
$C_{33}H_{40}O_{22}$ 788.666
Consit. of *Morus alba* (white mulberry). Yellow plates (MeOH/Me_2CO). Mp 211-214° (196-199). $[\alpha]_D^{20}$ -47 (c, 0.25 in DMF).

2″-Ac: [11029-60-0] ***Glyphoside***
$C_{23}H_{22}O_{13}$ 506.419
Isol. from leaves of *Glycyrrhiza glabra* (licorice).

6″-Ac: [54542-51-7]
$C_{23}H_{22}O_{13}$ 506.419
Isol. from *Pinus sylvestris* (Scotch pine).

2″-O-(3,4,5-Trihydroxybenzoyl): [69624-79-9]
$C_{28}H_{24}O_{16}$ 616.488
Isol. from *Polygonum* spp. and *Diospyros kaki* (Japanese persimmon). Yellow needles (MeOH/$CHCl_3$). Mp 208-210°.

3″-O-(4-Hydroxycinnamoyl): [76211-70-6]
$C_{30}H_{26}O_{14}$ 610.527
Isol. from *Pinus sylvestris* (Scotch pine).

*3″,6″-Bis-*O*-(4-hydroxy-*E*-cinnamoyl):* [72691-78-2]
$C_{39}H_{32}O_{16}$ 756.672
Isol. from *Pinus sylvestris* (Scotch pine).

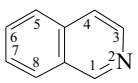
O″-(4-Hydroxy-3-methoxycinnamoyl), 4′-O-β-D-glucopyranoside: [87338-63-4]
$C_{37}H_{38}O_{20}$ 802.695
Isol. from *Crambe tatarica* (tartar bread plant).

[27459-82-1, 53694-45-4, 61405-93-4, 67771-59-9]

Litvinenko, V.I. *et al., CA*, 1966, **66**, 73264 (*Glyphoside*)
Markham, K.R. *et al., Phytochemistry*, 1970, **9**, 2359-2364 (*7-rutinoside, derivs*)
Farkas, L. *et al., Chem. Ber.*, 1974, **107**, 1518-1525 (*synth, diglucosides*)
Wilkins, C.K. *et al., Can. J. Bot.*, 1976, **54**, 2133-2140 (*O″-xylosyl*)
Markham, K.R. *et al., Tetrahedron*, 1978, **34**, 1389-1397 (*cmr*)
Bohm, B.A. *et al., Phytochemistry*, 1979, **18**, 1079-1080 (*O″-xylosyl*)
Ivanova, S.Z. *et al., Khim. Prir. Soedin.*, 1980, **16**, 254; 1984, **20**, 582-589; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 547-553 (*di-4-hydroxycinnamoyl*)
Gehring, E. *et al., Z. Naturforsch., C*, 1980, **35**, 380-383 (*O″-4-hydroxycinnamoyl, 3′,5-di-Me ether*)
Itokawa, H. *et al., Chem. Lett.*, 1982, 49-52 (*ms*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1602-1608 (*2″-gallate*)
Saleh, N.A.M. *et al., Phytochemistry*, 1982, **21**, 1995-2000 (*Quercetin 3-gentiotrioside*)
Aguinagalde, I. *et al., Phytochemistry*, 1982, **21**, 2875-2878 (*derivs*)
Imperato, F. *et al., Chem. Ind. (London)*, 1983, 390-391 (*3-sulfate*)
Reynaud, J. *et al., Pharmazie*, 1985, **40**, 132-133; 1986, **41**, 524-525 (*6″-Ac*)
Saito, N. *et al., Heterocycles*, 1990, **30**, 759-764 (*deriv*)
Webby, R.F. *et al., Phytochemistry*, 1990, **29**, 289-292; 1991, **30**, 2443-2444 (*derivs*)
Nielsen, J.K. *et al., Phytochemistry*, 1994, **34**, 539-544 (*3-acylsophoroside 7-glucosides*)
Imperato, F. *et al., Phytochemistry*, 1995, **40**, 1801-1802 (*Quercetin 3-laminaribioside*)
Merfort, I. *et al., Phytochemistry*, 1997, **46**, 359-363 (*2″-glucosylgalactosyl*)
Fossen, T. *et al., Phytochemistry*, 1998, **47**, 281-285 (*4′-glucoside, 4′,7-diglucoside*)
Afifi, M.-S. *et al., Bull. Fac. Pharm. (Cairo Univ.)*, 1999, **37**, 119-124; *CA*, **132**, 163461j (*isol, activity*)

Isoquinoline, 9CI, 8CI I-159

[119-65-3]
2-Benzazine. Benzopyridine. 2-Aza-naphthalene. FEMA 2978



C_9H_7N 129.161
Flavouring agent. Hygroscopic cryst. or oil. Sol. EtOH, Et_2O, Me_2CO, C_6H_6. d_4^{20} 1.1. Mp 25.5-26°. Bp 242° Bp_{40} 142°. pK_a 5.4 (25°).

▶ Fl. p. >107°. Severe eye and skin irritant. LD_{50} (rat, orl) 360 mg/kg. LD_{50} (rbt, skn) 590 mg/kg. NW6825000

Hydrochloride: [21364-46-5]
Needles (2-propanol/MeOH). Mp 187-189°.

Picrate: [1567-46-0]
Mp 226°.

N-*Oxide:* [1532-72-5]
C_9H_7NO 145.16
Oil, cryst. on cooling (+ $2H_2O$). Sol. H_2O, EtOH. Mp 98° (dihydrate).

N-*Oxide; hydrochloride:*
Needles (EtOH). Mp 180-181°.

N-*Me:1-Methylisoquinolinium(1+)*
$C_{10}H_{10}N^{\oplus}$ 144.196
Cryst. + $1H_2O$ (H_2O) (as iodide). Mp 159° (iodide).

N-*Et:*N-*Ethylisoquinolinium(1+)*
$C_{11}H_{12}N^{\oplus}$ 158.223
Yellow leaflets (EtOH) (as iodide). Mp 148° (iodide).

N-*Propyl:* [86377-01-7] N-*Propylisoquinolinium(1+)*
$C_{12}H_{14}N^{\oplus}$ 172.249
Cryst. (EtOH) (as bromide). Mp 146-148° (bromide). CAS no. refers to bromide.

N-*Dodecyl:* [93-23-2] ***Laurylisoquinolinium(1+), INN.*** *Isothan Q5*
$C_{21}H_{32}N^{\oplus}$ 298.491CAS no. refers to bromide.

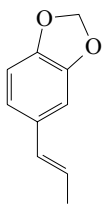
▶ Eye irritant. LD_{50} (rat, orl) 230 mg/kg. NX5250000

N-*Benzyl:*N-*Benzylisoquinolinium(1+)*
$C_{16}H_{14}N^{\oplus}$ 220.293
Mp 175-176° (as iodide).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 877D; 918B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 456B; 484C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1572B (*ir*)
Meisenheimer, J. *et al., Ber.*, 1926, **59**, 1848 (*oxide*)
Manske, R.H.F. *et al., Chem. Rev.*, 1942, **30**, 145 (*rev*)
Black, P.J. *et al., Aust. J. Chem.*, 1966, **19**, 1287 (*pmr*)
Narasimhan, N.S. *et al., Chem. Ind. (London)*, 1967, 120 (*synth*)
Shashidhar, M.A. *et al., Indian J. Pure Appl. Phys.*, 1973, **11**, 73 (*uv*)
Johns, S.A. *et al., Aust. J. Chem.*, 1976, **29**, 1617 (*cmr*)
Raju, A.M. *et al., Indian J. Chem., Sect. A*, 1977, **15**, 1005 (*use*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 532 (*rev*)
Dyke, S.F. *et al., Chem. Heterocycl. Compd.*, 1981, **38**, 1 (*rev*)
Kametani, T. *et al., Chem. Heterocycl. Compd.*, 1981, **38**, 139 (*rev*)
Ferles, M. *et al., Coll. Czech. Chem. Comm.*, 1983, **48**, 1068 (*N-propyl*)
Wagner, H. *et al., Planta Med.*, 1986, 378 (*isol, uv, pmr, ms*)
Daly, J.J. *et al., Acta Cryst. C*, 1987, **43**, 1818 (*hydrochloride, cryst struct*)
Janssen, R.H.A.M. *et al., Phytochemistry*, 1989, **28**, 2833 (*cmr*)
Goto, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1612 (*cryst struct*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 423
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1504-1505
Hensen, K. *et al., Acta Cryst. C*, 1999, **55**, 1565-1567 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IRX000; LBW000

Isosafrole I-160

[120-58-1]
5-(1-Propenyl)-1,3-benzodioxole, 9CI. 1,2-(Methylenedioxy)-4-(1-propenyl)benzene, 8CI



(*E*)-*form*

$C_{10}H_{10}O_2$ 162.188
Isol. from leaves of the curryleaf (*Murraya koenigii*) and from star anise oil (*Illicium religiosum*). Use as a food additive prohibited.

▶ DA5950000

(*E*)-*form* [4043-71-4]
β-Isosafrole
Fp 6.7-6.8. Bp_{768} 252.4-252.7° $Bp_{11.5}$ 123°.

▶ DA5951000

(*Z*)-*form* [17627-76-8]
α-Isosafrole
Liq.

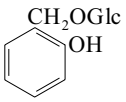
▶ DA5952000

Aldrich Library of ^{13}C and ^{1}H FT NMR

Spectra , 1992, **2**, 232A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 986D (*ir*)
Crymble, C.R. *et al., J.C.S.* , 1911, 451 (*uv*)
Robinson, R. *et al., J.C.S.* , 1927, 2489 (*synth*)
Dutt, S. *et al., CA* , 1958, **52**, 20904 (*isol*)
Willhalm, B. *et al., Tetrahedron*, 1964, **20**, 1185 (*ms*)
Shulgin, A.T. *et al., J. Chromatogr.* , 1967, **30**, 54 (*glc*)
Torii, S. *et al., J.O.C.* , 1984, **49**, 1830 (*synth*)
Sy, L.K. *et al., Phytochemistry*, 1997, **44**, 1099 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IRZ000

Isosalicin I-161

[7724-09-6]

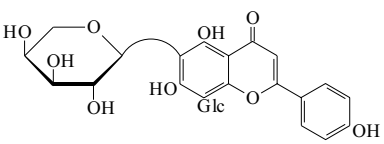


$C_{13}H_{18}O_7$ 286.281
Isol. from flowers of *Filipendula ulmaria* (meadowsweet). Needles + $3H_2O$ (Me_2CO/petrol). Mp 66-68°. $[\alpha]_D^{20}$ -45.2 (anhyd.).

Bourquelot, E. *et al., C. R. Hebd. Seances Acad. Sci.* , 1913, **156**, 1790 (*synth*)
Thieme, H. *et al., Pharmazie*, 1966, **21**, 123 (*isol*)

Isoschaftoside I-162

[52012-29-0]
*6-α-L-Arabinopyranosyl-8-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 6-Arabinopyranosyl-8-glucopyranosyl-4′,5,7-trihydroxyflavone. 6-Arabinosylvitexin*



$C_{26}H_{28}O_{14}$ 564.499
Yellow cryst. (MeOH). Dec. ca. 220°.

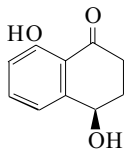
4′-O-*β-D-Glucopyranoside:* [151922-19-9]
Isoschaftoside 4′-glucoside
$C_{32}H_{38}O_{19}$ 726.641
Constit. of *Ceratonia siliqua* (carob).

2‴-O-*(4-Hydroxy-3-methoxycinnamoyl):* [80754-94-5] ***2‴-O-Ferulylisoschaftoside***
$C_{36}H_{36}O_{17}$ 740.67

Biol, M.C. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1974, **279**, 409 (*synth*)
Gaffield, W. *et al., Tetrahedron*, 1978, **34**, 3089 (*cd*)
Theodor, R. *et al., Phytochemistry*, 1981, **20**, 1851-1852 (*2-Ferulylisoschaftoside*)
Linard, A. *et al., Phytochemistry*, 1982, **21**, 797
Batista, M.T. *et al., Phytochemistry*, 1993, **34**, 1191 (*4′-glucoside*)
Wada, S. *et al., Biosci., Biotechnol., Biochem.* , 2000, **64**, 2262-2265 (*isol,pmr,cmr*)

Isosclerone I-163

[62332-73-4]
*3,4-Dihydro-4,8-dihydroxy-1(2*H*)-naphthalenone, 9CI. 4,8-Dihydroxy-1-tetralone. Regiolone. Antibiotic PD6. PD6*



(*R*)-*form*

$C_{10}H_{10}O_3$ 178.187

(R)-form
Sol. C_6H_6, $CHCl_3$; poorly sol. hexane. $[\alpha]_D$ -68 (c, 0.05 in MeOH). λ_{max} 215 (ϵ 17800); 260 (ϵ 10000); 293 (ϵ 5200) (MeOH) (Berdy).

(S)-form [54712-38-8]
Constit. of *Juglans regia* (walnut). Cryst. (petrol). Sol. C_6H_6, $CHCl_3$; fairly sol. EtOAc, EtOH; poorly sol. hexane, H_2O. Mp 74-76° (72°). $[\alpha]_D^{15}$ +19 (c, 0.34 in $CHCl_3$). λ_{max} 215 (ϵ 18200); 260 (ϵ 10000); 343 (ϵ 4265) (MeOH) (Berdy).

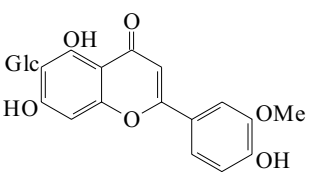
Dibenzoyl:
Mp 125-127°.

(±)-*form* [51114-98-8]
Cryst. (hexane). Mp 70-72°.

Findlay, J.A. *et al., Can. J. Chem.* , 1973, **51**, 3299 (*ir, uv, nmr*)
Morita, T. *et al., Agric. Biol. Chem.* , 1974, **38**, 1501 (*uv, pmr, ms, ord*)
Stipanovic, R.D. *et al., Mycologia*, 1977, **69**, 164
Fujimoto, Y. *et al., Chem. Pharm. Bull.* , 1986, **34**, 1497; 4540 (*isol, synth*)
Talapatra, S.K. *et al., Phytochemistry*, 1988, **27**, 3929 (*isol*)
Venkatasubbaiah, P. *et al., J. Nat. Prod.* , 1991, **54**, 1293 (*isol*)
Fujimoto, H. *et al., Chem. Pharm. Bull.* , 1998, **46**, 423-429 (*isol, pmr, cmr*)
Laurent, D. *et al., Tetrahedron*, 2002, **58**, 9163-9167 (*isol, pmr, cmr*)

Isoscoparin I-164

[20013-23-4]
*6-β-D-Glucopyranosyl-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 6-β-D-Glucopyranosyl-4′,5,7-trihydroxy-3′-methoxyflavone. 6-Glucosyl-4′,5,7-trihydroxy-3′-methoxyflavone*



$C_{22}H_{22}O_{11}$ 462.409
Yellow cryst. Mp 215-217° (207-209° dec.).

7-O-*β-D-Glucopyranoside:* [50307-26-1]
$C_{28}H_{32}O_{16}$ 624.551
Cryst. (MeOH). Mp 210-212°.

2″-O-*β-D-Glucopyranosyl:* [97605-25-9]
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Oryza sativa* (rice).

2″-O-*[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl]:* [99445-33-7]
$C_{37}H_{38}O_{18}$ 770.696
Isol. from rice.

2″-O-*[4-Hydroxy-3-methoxycinnamoyl-(→6)-β-D-glucopyranosyl]:* [97605-26-0]
$C_{38}H_{40}O_{19}$ 800.723
Isol. from rice.

2″-O-*[4-Hydroxy-3-methoxy*-E-*cinnamoyl-(→6)-β-D-glucopyranosyl], 4′*-O-*β-D-glucopyranoside:*
$C_{44}H_{50}O_{24}$ 962.865
Constit. of *Cucumis sativus* (cucumber).

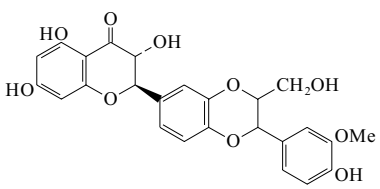
2″-O-*α-L-Rhamnopyranosyl:* [78570-70-4]
$C_{28}H_{32}O_{15}$ 608.552

1″-Epimer: [89759-25-1] *6-α-D-Glucopyranosyl-4′,5,7-trihydroxy-3′-methoxyflavone.* ***(-)-Isoscoparin***
$C_{22}H_{22}O_{11}$ 462.409
Yellow needles (MeOH). Mp 202-204°. $[\alpha]_D^{21}$ -24.8 (c, 0.5 in MeOH). The name (-)-Isoscoparin is a misnomer.

Chopin, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1967, **265**, 1334 (*isol, synth, struct*)
Marston, A. *et al., Helv. Chim. Acta*, 1976, **59**, 2596 (*7-glucoside*)
Gaffield, W. *et al., Tetrahedron*, 1978, **34**, 3089 (*cd*)
Raynaud, J. *et al., Pharmazie*, 1980, **35**, 712 (*isol*)
van Brederode, J. *et al., Z. Naturforsch., C*, 1981, **36**, 486 (*2″-rhamnosyl*)
Boguslavskaya, L.I. *et al., Khim. Prir. Soedin.* , 1983, **19**, 783; *Chem. Nat. Compd. (Engl. Transl.)* , 1983, **19**, 746 (*(-)-Scoparin*)
Besson, E. *et al., Phytochemistry*, 1985, **24**, 1061 (*2″-glucosyl*)
Wu, F. *et al., Chem. Pharm. Bull.* , 1990, **38**, 2281 (*(-)-Scoparin*)
Rahman, K. *et al., Phytochemistry*, 1997, **45**, 1093 (*2″-glucosyl, uv, pmr, ms*)
Abou-Zaid, M.M. *et al., Phytochemistry*, 2001, **58**, 167-172 (*Cucumis sativus glucoside*)

Isosilybin I-165

[72581-71-6]

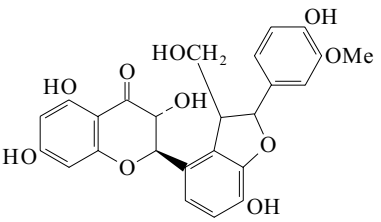


$C_{25}H_{22}O_{10}$ 482.443
Constit. of *Silybum marianum* (milk thistle). Cryst. Mp 239-241°. $[\alpha]_D$ +16.9 (Me_2CO). Component of Silymarin, crude milk thistle extract. λ_{max} 288 ; 322 (MeOH).

Arnone, A. *et al., Chem. Comm.* , 1979, 696 (*isol, struct*)
Merlini, L. *et al., J.C.S. Perkin 1* , 1980, 775 (*synth*)
Meriçli, A.H. *et al., Planta Med.* , 1988, **54**, 44 (*isol*)

Isosilychristin I-166

[77182-66-2]

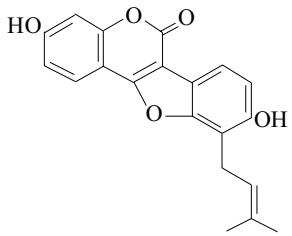


$C_{25}H_{22}O_{10}$ 482.443
Constit. of *Silybum marianum* (milk thistle). Cryst. Mp 155-157°. $[\alpha]_D$ +245 (Py).

Kalonga, M. *et al., Z. Naturforsch., B*, 1981, **36**, 262

Isosojagol I-167

[94390-15-5]
*3,9-Dihydroxy-10-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 9CI. 3,9-Dihydroxy-10-prenylcoumestan*

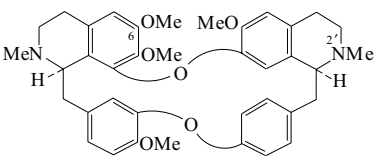


$C_{20}H_{16}O_5$ 336.343
Constit. of *Phaseolus coccineus* (canary grass).

O'Neill, M.J. *et al., Phytochemistry*, 1984, **23**, 2704

Isotetrandrine I-168

[477-57-6]
O-*Methylberbamine*



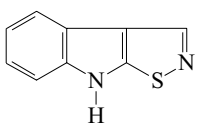
$C_{38}H_{42}N_2O_6$ 622.76
Alkaloids covered by this entry (1*R*,1′*S*-series) are enantiomeric with those included under Peinamine. Alkaloid from *Laurelia sempervirens* (Peruvian nutmeg),. Prisms (MeOH). Mp 182-183°. $[\alpha]_D^{20}$ +150.7 (c, 0.85 in $CHCl_3$). Log P 8.3 (uncertain value) (calc). λ_{max} 218 (ϵ 31600); 240 (sh) (ϵ 15800); 282 (ϵ 12600) (MeOH) (Derep).

▶ LD_{50} (mus, orl) 6400 mg/kg. LD_{50} (mus, ipr) 160 mg/kg. NX7285000

Bick, I.R.C. *et al., Aust. J. Chem.*, 1956, **9**, 111-119; 1980, **33**, 225-228 (*isol*)
Yang, T.-H. *et al., Yakugaku Zasshi*, 1960, **80**, 847-849; *CA*, **54**, 23187i (*isol*)
Battersby, A.R. *et al., J.C.S.*, 1965, 2239-2247 (*uv, ord*)
Falco, M.R. *et al., Tet. Lett.*, 1968, 1953-1959 (*pmr*)
Mitscher, L.A. *et al., Dtsch. Apoth. -Ztg.*, 1971, **111**, 1704 (*activity*)
Baldas, J. *et al., J.C.S. Perkin 1*, 1972, 592-596 (*ms*)
Tackie, A.N. *et al., J. Nat. Prod.*, 1974, **37**, 1-5 (*isol, uv, pmr, ms*)
Kuroda, H. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2413-2420 (*activity*)
Moiseeva, G.P. *et al., Khim. Prir. Soedin.*, 1979, **15**, 818-823; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 723-727 (*cd, abs config*)
Koike, L. *et al., Tet. Lett.*, 1979, 3765-3768 (*cmr*)
Bhakuni, D.S. *et al., Tetrahedron*, 1980, **36**, 2149-2151 (*biosynth*)
Moulis, C. *et al., J. Nat. Prod.*, 1981, **44**, 101-103 (*isol, uv, ir, pmr, ms*)
Nakova, E. *et al., Khim. Prir. Soedin.*, 1985, **21**, 86-91; 91-95; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 83-87; 88-91 (*synth*)
Buck, K.T. *et al., Alkaloids (N.Y.)*, 1987, **30**, 147 (*pharmacol*)

8*H*-Isothiazolo[5,4-*b*]indole, 9CI I-169

[119752-76-0]
Brassilexin



$C_9H_6N_2S$ 174.226
Isol. from leaves of brown mustard (*Brassica juncea*) (Cruciferae). Microcryst. Mp 164-167°. λ_{max} 218 (ϵ 50000); 245 (ϵ 14000); 264 (ϵ 12000) (MeOH) (Derep).

N-*Ac:*
$C_{11}H_8N_2OS$ 216.263
Mp 172-178°.

N-*Methoxy:8-Methoxy-8*H*-isothiazolo[5,4-*b*]indole.* ***Sinalexin***
$C_{10}H_8N_2OS$ 204.252
Isol. from leaves of white mustard (*Sinapis alba*) (Cruciferae) under biotic or abiotic elicitation.

Devys, M. *et al., Tet. Lett.*, 1988, **29**, 6447 (*isol, uv, ir, pmr, cmr, ms, struct*)
Devys, M. *et al., Synthesis*, 1990, 214 (*synth, ir, uv, pmr, ms*)
Pedras, M.S.C. *et al., Phytochemistry*, 1997, **46**, 833-837 (*Sinalexin*)
Pedras, M.S.C. *et al., Phytochemistry*, 2000, **53**, 161-176 (*rev*)
Pedras, M.S.C. *et al., Org. Lett.*, 2001, **3**, 1213-1216 (*synth*)

1-Isothiocyanatobutane, 9CI I-170

[592-82-5]
Butyl isothiocyanate, 8CI. Butyl mustard oil

$H_3C(CH_2)_3NCS$

C_5H_9NS 115.199
Volatile constituent of cabbage and other crucifers arising from enzymic hydrolysis of Butyl glucosinolate, B-234. Liq. Bp 167° Bp_9 58-59°. n_D^{20} 1.4980.

▶ Irritant. NX8420500

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1411A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 874C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 827B (*ir*)
Schmidt, E. *et al., Annalen*, 1954, **585**, 230 (*synth*)
Jensen, K.A. *et al., Acta Chem. Scand.*, 1966, **20**, 2107 (*ms*)
Kessler, H. *et al., Chem. Ber.*, 1978, **111**, 2947 (*cmr*)
Gifford, M. *et al., J.C.S. Perkin 2*, 1985, 157 (*pmr, cmr, N-15 nmr*)
Olejniczak, B. *et al., Synthesis*, 1989, 300 (*synth*)
Yamamoto, T. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 555 (*synth, pmr*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 448

4-Isothiocyanato-1-butene I-171

[3386-97-8]

[34424-44-7]
1-Butene-4-isothiocyanate. 3-Butenyl isothiocyanate. Crotonyl mustard oil. Crotyl mustard oil

$H_2C{=}CHCH_2CH_2NCS$

C_5H_7NS 113.183
Chief volatile isothiocyanate of enzymically treated seeds of *Brassica napus* (rape) and other crucifers. Formed from 3-Butenyl glycosinolate, B-227. Liq. Bp_{26} 78.5° $Bp_{11.5}$ 57.5-58.5°.

Conti, J. *et al., Acta Chem. Scand.*, 1953, **7**, 1271 (*isol*)
Ettlinger, M.G. *et al., J.A.C.S.*, 1955, **77**, 1831 (*isol, synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)
Spurlock, L.A. *et al., J.O.C.*, 1972, **37**, 1162 (*synth*)

7-Isothiocyanato-1-heptene, 9CI I-172

[49776-82-1]
6-Heptenyl isothiocyanate

$H_2C{=}CH(CH_2)_5NCS$

$C_8H_{13}NS$ 155.263
Isol. from a hydrolysate of *Wasabia japonica* (Japanese horseradish).

Kojima, M. *et al., Yakugaku Zasshi*, 1973, **93**, 453; *CA*, **79**, 63527d (*isol, ms*)

1-Isothiocyanatohexane, 9CI I-173

[4404-45-9]
Hexyl isothiocyanate

$H_3C(CH_2)_5NCS$

$C_7H_{13}NS$ 143.252
Isol. from radish (*Raphanus sativus*) and other crucifers. Liq. Bp 210° Bp_{27} 98° Bp_{15} 100°.

Dyson, G.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 421 (*synth*)
Svatek, E. *et al., Acta Chem. Scand.*, 1959, **13**, 442 (*ir, uv*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Jensen, K.A. *et al., Acta Chem. Scand.*, 1966, **20**, 2107 (*ms*)
Kjaer, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1715 (*isol*)
Blotny, G. *et al., Annalen*, 1982, 1927 (*synth*)

Yamamoto, T. *et al., Org. Prep. Proced. Int.*, 1992, **24**, 346; 1994, **26**, 555 (*synth, ir, pmr*)

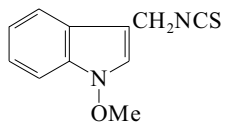
6-Isothiocyanato-1-hexene, 9CI I-174

[49776-81-0]
5-Hexenyl isothiocyanate
$H_2C{=}CH(CH_2)_4NCS$
$C_7H_{11}NS$ 141.237
Isol. from a hydrolysate of Japanese horseradish (*Wasabia japonica*) and from radish (*Raphanus sativus*).

Kojima, M. *et al., Yakugaku Zasshi*, 1973, **93**, 453; *CA*, **79**, 63527d (*isol, ms*)
Kjaer, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1715 (*isol*)

3-(Isothiocyanatomethyl)-1-methoxy-1*H*-indole, 9CI I-175

[126769-93-5]
(1-Methoxyindol-3-yl)methyl isothiocyanate



$C_{11}H_{10}N_2OS$ 218.279
Intermediate in the enzymic hydrolysis of 3-Indolylmethyl glucosinolate, I-35 from rape *Brassica napus*. Unstable. Identified by tlc-ms.

Hanley, A.B. *et al., J.C.S. Perkin 1*, 1990, 2273

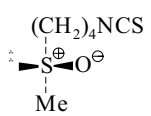
1-Isothiocyanato-4-methylpentane, 9CI I-176

[17608-07-0]
4-Methylpentyl isothiocyanate. Isohexyl isothiocyanate
$(H_3C)_2CH(CH_2)_3NCS$
$C_7H_{13}NS$ 143.252
Isol. from radish (*Raphanus sativus*).

Kaluza, L. *et al., Monatsh. Chem.*, 1909, **30**, 701 (*synth*)
Kjaer, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1715 (*isol, ms*)

1-Isothiocyanato-4-(methylsulfinyl)butane, 9CI I-177

[4478-93-7]
4-(Methylsulfinyl)butyl isothiocyanate. ***Sulforaphane***



(R)-form

$C_6H_{11}NOS_2$ 177.291

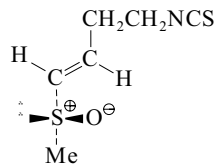
(R)-form
Present in brassicas. Potential nutriceutical. Sol. MeOH, hexane; poorly sol. H_2O. $Bp_{0.03}$ 130-135°. $[\alpha]_D$ -79.3 (c, 1.2 in $CHCl_3$).

(±)-form
Phenylthiourea deriv.:
Mp 126-127°.

Schmid, H. *et al., Helv. Chim. Acta*, 1948, **31**, 1497 (*synth, resoln*)
Procháza, Z. *et al., Coll. Czech. Chem. Comm.*, 1959, **24**, 2429 (*synth*)
Balenovic, K. *et al., Tetrahedron*, 1966, **22**, 2139 (*synth*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359 (*ms*)
Talalay, P. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 2399 (*pharmacol*)
Whitesell, J.K. *et al., J.O.C.*, 1994, **59**, 597 (*synth*)
Chiang, W.C.K. *et al., J. Agric. Food Chem.*, 1998, **46**, 1018-1021 (*anal, glc, ms*)
Jeffery, E.H. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press,, 2001, 169-191

4-Isothiocyanato-1-(methylsulfinyl)-1-butene, 9CI I-178

[592-95-0]
Sulforaphene*. Raphanin. Sulphoraphene*

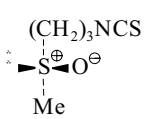


$C_6H_9NOS_2$ 175.275Log P 0.32 (uncertain value) (calc).
► NX8944000

(R)-(E)-form [2404-46-8]
Mustard oil from Glucoraphenin (see 4-(Methylthio)-3-butenyl glucosinolate, M-667) in radish seeds (*Raphanus sativus* var. *alba*). Sol. MeOH, $CHCl_3$, H_2O; fairly sol. Et_2O; poorly sol. hexane. $Bp_{0.015}$ 125-130°. $[\alpha]_D$ -108 (c, 1.427 in $CHCl_3$). λ_{max} 226 (ϵ 2951) (H_2O) (Berdy).
► LD_{50} (mus, ivn) 10 mg/kg.
Schmid, H. *et al., Helv. Chim. Acta*, 1948, **31**, 1017 (*synth*)
Cheung, K.K. *et al., Chem. Comm.*, 1965, 100 (*synth*)
Balenovic, K. *et al., Tetrahedron*, 1966, **22**, 2139 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 418 (*isol*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359 (*ms*)

1-Isothiocyanato-3-(methylsulfinyl)propane, 9CI I-179

[505-44-2]
3-(Methylsulfinyl)propyl isothiocyanate. ***Iberin***



$C_5H_9NOS_2$ 163.264
► LD_{50} (rat, scu) 90 mg/kg. NX8950000

(R)-form [37791-20-1]
Occurs in crucifer seeds. $[\alpha]_D^{18}$ -73.6 (EtOH).
Phenylthiourea deriv.:
Mp 133-134°. $[\alpha]_D^{22.5}$ -45.4 (c, 1.76 in EtOH).

(±)-form
$Bp_{0.05}$ 129-133°.

[84104-27-8]

Karrer, P. *et al., Helv. Chim. Acta*, 1950, **33**, 1237 (*synth*)
Schultz, O.-E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1954, **287**, 404 (*synth*)
Procházka, Z. *et al., Coll. Czech. Chem. Comm.*, 1960, **25**, 1100 (*synth*)
Kjaer, A. *et al., Chem. Comm.*, 1965, 100 (*abs config*)
Kjaer, A. *et al., Phytochemistry*, 1972, **11**, 1502 (*isol*)
Kjaer, A. *et al., Chem. Scr.*, 1982, **20**, 42 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPN100

1-Isothiocyanato-4-(methylthio)butane, 9CI I-180

[4430-36-8]
4-(Methylthio)butyl isothiocyanate. 4-(Methylthio)butyl mustard oil. ***Erucin***†
$MeS(CH_2)_4NCS$
$C_6H_{11}NS_2$ 161.292
Occurs in seeds of salad rocket. Liq. Bp_{12} 136°.

S-*Oxide:* 1-Isothiocyanato-4-(methylsulfinyl)butane, I-177

S-*Dioxide:* [504-84-7] *1-Isothiocyanato-4-(methylsulfonyl)butane. 4-(Methylsulfonyl)butyl isothiocyanate.* ***Erysolin***
$C_6H_{11}NO_2S_2$ 193.29
Needles (Et_2O). Mp 60-60.5°.

Schneider, W. *et al., Annalen*, 1912, **392**, 1 (*isol, deriv*)
Schmid, H. *et al., Helv. Chim. Acta*, 1948, **31**, 1497 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1954, **8**, 295; 1955, **9**, 542; 1963, **17**, 2143 (*isol, synth, ms*)
Benn, M.H. *et al., Can. J. Chem.*, 1986, **64**, 940 (*synth, pmr*)

4-Isothiocyanato-1-(methylthio)-1-butene, 9CI I-181

[51598-96-0]
4-(Methylthio)-3-butenyl isothiocyanate
$MeSCH{=}CHCH_2CH_2NCS$
$C_6H_9NS_2$ 159.276

(E)-form [13028-50-7]
Major component of the pungent principle of radish roots (*Raphanus sativus*). Formed by hydrolysis of 4-(Methylthio)-3-butenyl glucosinolate, M-667. Oil. Poorly sol. hexane. n_D^{25} 1.5815.

S-*Oxide:* 4-Isothiocyanato-1-(methylsulfinyl)-1-butene, I-178

(Z)-form [123954-93-8]
Minor component of radish isol. by glc.

Früs, P. *et al., Acta Chem. Scand.*, 1966, **20**, 698 (*isol*)
Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1972, **91**, 729 (*synth*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359 (*ms*)
Kosemura, S. *et al., Tet. Lett.*, 1993, **34**, 481 (*isol*)

1-Isothiocyanato-10-(methylthio)decane I-182

10-(Methylthio)decyl isothiocyanate
$MeS(CH_2)_{10}NCS$

$C_{12}H_{23}NS_2$ 245.452

S-*Oxide:* [75272-83-2] *1-Isothiocyanato-10-(methylsulfinyl)decane, 9CI. 10-(Methylsulfinyl)decyl isothiocyanate.* ***Camelinin***
$C_{12}H_{23}NOS_2$ 261.452
Isol. from seeds of *Camelina sativa* (false flax).

[39036-84-5]

Kjaer, A. *et al., Acta Chem. Scand.*, 1956, **10**, 1614 (*isol*)
Kjaer, A. *et al., Phytochemistry*, 1972, **11**, 3045 (*isol*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359 (*ms*)

1-Isothiocyanato-2-(methylthio)ethane I-183

[4430-37-9]
2-(Methylthio)ethyl isothiocyanate
$MeSCH_2CH_2NCS$
$C_4H_7NS_2$ 133.238
Present as the glucosinolate in horseradish (*Armoracia lapathifolia*). Liq. Bp_2 85°. n_D^{25} 1.5767.

Kjaer, A. *et al., Acta Chem. Scand.*, 1957, **11**, 1298; 1963, **17**, 2143 (*synth, ms*)
Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)

1-Isothiocyanato-7-(methylthio)heptane, 9CI I-184

[4430-38-0]
7-(Methylthio)heptyl isothiocyanate
$MeS(CH_2)_7NCS$
$C_9H_{17}NS_2$ 203.372
Flavour compound of Japanese horseradish (*Wasabia japonica*). Oil. $Bp_{0.3}$ 117°. n_D^{25} 1.5274.

S-*Oxide:* [129244-98-0] *1-Isothiocyanato-7-(methylsulfinyl)heptane*
$C_9H_{17}NOS_2$ 219.371
Flavour component of Japanese horseradish (*Wasabia japonica*). Oil.

[31456-69-6]

Kjaer, A. *et al., Acta Chem. Scand.*, 1957, **11**, 1298; 1963, **17**, 2143 (*synth, ms*)
Gmelin, R. *et al., Acta Chem. Scand.*, 1970, **24**, 3031 (*deriv*)
Ina, K. *et al., Agric. Biol. Chem.*, 1989, **53**, 537 (*isol, pmr, cmr*)
Etoh, H. *et al., Agric. Biol. Chem.*, 1990, **54**, 1587 (*deriv*)

1-Isothiocyanato-6-(methylthio)hexane, 9CI I-185

[4430-39-1]
6-(Methylthio)hexyl isothiocyanate
$MeS(CH_2)_6NCS$
$C_8H_{15}NS_2$ 189.345
Flavour compd. of Japanese horseradish (*Wasabia japonica*). Liq. $Bp_{0.5}$ 119°. n_D^{25} 1.5336.

S-*Oxide:* [4430-35-7] *1-Isothiocyanato-6-(methylsulfinyl)hexane, 9CI. 6-(Methylsulfinyl)hexyl isothiocyanate*
$C_8H_{15}NOS_2$ 205.345
Mustard oil from dame's violet (*Hesperis matronalis*). Flavour component of Japanese horseradish (*Wasabia japonica*). Oil. $[\alpha]_D^{20}$ -71 (c, 0.84 in $CHCl_3$).

Kjaer, A. *et al., Acta Chem. Scand.*, 1957, **11**, 1298; 1963, **17**, 846; 2143 (*isol, synth, ms*)
Daxenbichler, M.E. *et al., J.O.C.*, 1961, **26**, 4168 (*isol*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359 (*ms*)
Ina, K. *et al., Agric. Biol. Chem.*, 1989, **53**, 535 (*isol, pmr, cmr*)
Etoh, H. *et al., Agric. Biol. Chem.*, 1990, **54**, 1587 (*isol, pmr*)
Pedras, M.S.C. *et al., Phytochemistry*, 1998, **49**, 1959-1965 (*isol, pmr, cmr, ms*)

1-Isothiocyanato-8-(methylthio)octane I-186

[4430-41-5]
8-(Methylthio)octyl isothiocyanate
$MeS(CH_2)_8NCS$
$C_{10}H_{19}NS_2$ 217.399
Flavour component of Japanese horseradish (*Wasabia japonica*). Oil. $Bp_{0.3}$ 122°. n_D^{25} 1.5242.

S-*Oxide(*R-*):* [31456-68-5]

[75272-81-0] *1-Isothiocyanato-8-(methylsulfinyl)octane. 8-(Methylsulfinyl)octyl isothiocyanate.* ***Hirsutin***†
$C_{10}H_{19}NOS_2$ 233.398
Inhibits germination of lettuce seeds and affects the growth of the roots of lettuce seedlings. Yellowish oil. $Bp_{0.3}$ 122°. $[\alpha]_D^{23}$ -47 (c, 0.073 in MeOH). n_D^{25} 1.5242.

Kjaer, A. *et al., Acta Chem. Scand.*, 1957, **11**, 1298; 1958, **12**, 833; 1963, **17**, 2143; 1970, **24**, 3031 (*synth, ms*)
Ina, K. *et al., Agric. Biol. Chem.*, 1989, **53**, 537 (*isol, pmr*)
Kawabata, J. *et al., Agric. Biol. Chem.*, 1989, **53**, 3361 (*S-oxide, isol, synth, ms, uv, ir, pmr*)

1-Isothiocyanato-5-(methylthio)pentane, 9CI I-187

[4430-42-6]
5-(Methylthio)pentyl isothiocyanate. ***Berteroin***
$MeS(CH_2)_5NCS$
$C_7H_{13}NS_2$ 175.318
Prod. by *Wasabia japonica* (Japanese horseradish). Oil. Bp_{10} 155°.

S-*Oxide:* [646-23-1] *1-Isothiocyanato-5-(methylsulfinyl)pentene, 9CI.* ***Alyssin***
$C_7H_{13}NOS_2$ 191.318
Oil. $Bp_{0.02}$ 130°. $[\alpha]_D$ -9 (EtOH). $[\alpha]_D$ -69 ($CHCl_3$).

Kjaer, A. *et al., Acta Chem. Scand.*, 1955, **9**, 1311-1316; 1956, **10**, 1100-1110 (*isol, synth*)
Kjaer, A. *et al., Phytochemistry*, 1973, **12**, 929-933 (*isol*)
Cole, R.A. *et al., Phytochemistry*, 1976, **15**, 759-762 (*isol*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359-367 (*ms*)
Pedras, M.S.C. *et al., Phytochemistry*, 1998, **49**, 1959-1965 (*isol, pmr, cmr, ms*)

1-Isothiocyanato-3-(methylthio)propane, 9CI I-188

[505-79-3]
3-Methylthiopropyl isothiocyanate. ***Ibervirin.*** *FEMA 3312*
$MeSCH_2CH_2CH_2NCS$
$C_5H_9NS_2$ 147.265
Found in hydrolysates of crucifer seeds. Also found in cabbage, cauliflower, kohlrabi, horse radish (*Armoracia lapathifolia*), Japanese horseradish (*Wasabi japonica*) and radish (*Rapharius sativus*). Flavouring ingredient. Liq. with odour of radish. Bp_{12} 120.5-122°.

S-*Oxide:* 1-Isothiocyanato-3-(methylsulfinyl)propane, I-179

S,S-*Dioxide:* [505-34-0] *1-Isothiocyanato-3-(methylsulfonyl)propane, 9CI. Isothiocyanopropyl methyl sulfone. 3-(Methylsulfonyl)propyl isothiocyanate.* ***Cheiroline***
$C_5H_9NO_2S_2$ 179.264
Rhombic prisms. Sol. MeOH, $CHCl_3$; fairly sol. H_2O; poorly sol. hexane. Log P -0.22 (calc).
▶ LD_{50} (mus, ivn) 3 - 7 mg/kg. NX8960000

Kjaer, A. *et al., Acta Chem. Scand.*, 1955, **9**, 1143; 1963, **17**, 2143 (*isol, struct, ms*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)
Kjaer, A. *et al., Phytochemistry*, 1972, **11**, 1502; 3045 (*isol, synth, deriv*)
Kjaer, A. *et al., Chem. Scr.*, 1982, **20**, 42 (*synth*)

1-Isothiocyanatopentane, 9CI I-189

[629-12-9]
Pentyl isothiocyanate. n-*Amyl isothiocyanate*
$H_3C(CH_2)_4NCS$
$C_6H_{11}NS$ 129.226
Isol. from Japanese radish (*Raphanus sativus* var. *niger*) roots. Liq. Bp 191°.

Dyson, G.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1926, **45**, 421 (*synth*)
Svatek, E. *et al., Acta Chem. Scand.*, 1959, **13**, 442 (*ir, uv*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Kjaer, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1715 (*isol*)
Ryu, E.K. *et al., Synth. Commun.*, 1994, **24**, 1101 (*synth, pmr, ms*)

5-Isothiocyanato-1-pentene, 9CI I-190

[18060-79-2]
4-Pentenyl isothiocyanate
$H_2C{=}CHCH_2CH_2CH_2NCS$
C_6H_9NS 127.21
Mustard oil from rape (*Brassica napus*), brown mustard (*Brassica juncea*) and other crucifers. Formed from 4-Pentenyl glucosinolate, P-209. Bp_{12} 75°. n_D^{25} 1.5118.

Kjaer, A. *et al., Acta Chem. Scand.*, 1956, **10**, 1365; 1963, **17**, 2143 (*isol, synth, ms*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)

1-Isothiocyanato-4-phenylbutane I-191

[61499-10-3]
(4-Isothiocyanatobutyl)benzene, 9CI. 4-Phenylbutyl isothiocyanate
$Ph(CH_2)_4NCS$
$C_{11}H_{13}NS$ 191.296
Present as the glucosinolate in *Armoracia lapathifolia* (horseradish). Liq.

v. Braun, J. *et al., Ber.*, 1912, **45**, 2188 (*synth*)

Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)

1-Isothiocyanato-2-phenylethane I-192

[2257-09-2]
(2-Isothiocyanatoethyl)benzene, 9CI. 2-Phenylethyl isothiocyanate. Phenethyl isothiocyanate

$PhCH_2CH_2NCS$

C_9H_9NS 163.243

Hydrolysis product formed by action of myrosinase on 2-Phenylethyl glucosinolate, P-276. Present in mustard oil and extensively distributed in Cruciferae esp. in *Brassica* spp. Nutriceutical. Liq. Bp_{12} 143-145° $Bp_{2.5}$ 106°. Log P 3.31 (calc).

▶ NX9115000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 466A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1423A (*ir*)
v. Braun, J. *et al., Ber.*, 1912, **45**, 2188 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1953, **7**, 1276 (*isol*)
Lichtenstein, E.P. *et al., J. Agric. Food Chem.*, 1964, **12**, 158 (*isol*)
Dieter, M. *et al., Chem. Ber.*, 1965, **98**, 2425 (*synth*)
Antos, K. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 3339 (*synth*)
Bose, A.K. *et al., J. Het. Chem.*, 1979, **16**, 1313-1316 (*synth*)
Suzuki, O. *et al., Biomed. Mass Spectrom.*, 1983, **10**, 430 (*ms*)
Chung, F.-L. *et al., Cancer Res.*, Suppl., 1992, **52**, 2719s-2722s (*pharmacol*)
Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, D.), Sheffield Academic Press, 1998, 29-53 (*rev*)
Olivier, C. *et al., J. Chem. Ecol.*, 1999, **25**, 2687-2701 (*activity, occur*)
Jeffery, E.H. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 169-191
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ISP000

1-Isothiocyanato-3-phenylpropane I-193

[2627-27-2]
(3-Isothiocyanatopropyl)benzene, 9CI. 3-Phenylpropyl isothiocyanate

$PhCH_2CH_2CH_2NCS$

$C_{10}H_{11}NS$ 177.27

Isol. from horseradish. Liq. with weak odour. Bp_{15} 163-166°.

v. Braun, J. *et al., Ber.*, 1912, **45**, 2188 (*synth*)
Heiduschka, A. *et al., J. Prakt. Chem.*, 1931, **132**, 201 (*isol*)

3-Isothiocyanato-1-propene, 9CI I-194

[57-06-7]
Allyl isothiocyanate, USAN. Allyl mustard oil. Carbospol. Mustard oil. Allyspol 75EC. FEMA 2034

$H_2C{=}CHCH_2NCS$

C_4H_5NS 99.156

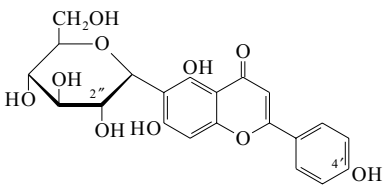
Chief constit. of natural mustard oil. Also found in cooked cabbage, horseradish, etc. Flavouring ingredient. Potential nutriceutical. Oil with very pungent, irritating odour. Sol. EtOH, Et_2O, C_6H_6, sl. sol. H_2O. d_4^{15} 1.02. Fp -80. Bp 151° Bp_{12} 44°.

▶ Flammable, fl. p. 46/297°. Irritant and skin allergen. LD_{50} (rat, orl) 112 mg/kg. LD_{50} (rbt, skn) 88 mg/kg. Exp. reprod. and teratogenic effects. Goitrogenic (antithyroid) activity. Autoclave reacns. between NaSCN and $H_2C{=}CHCH_2Cl$ may explode. NX8225000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 875A (*ir*)
Tollens, B. *et al., Annalen*, 1870, **156**, 134 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)
Langer, P. *et al., Endocrinology (Baltimore)*, 1965, **76**, 151 (*pharmacol*)
Mathias, A. *et al., Tetrahedron*, 1965, **21**, 1073 (*pmr*)
Food Chemicals Codex, 2nd Ed., 1972, 31 (*anal*)
Yanemoto, T. *et al., J. Magn. Reson.*, 1974, **13**, 153 (*synth*)
Mahuja, M. *et al., Indian J. Chem.*, 1976, **11**, 15 (*synth*)
Fenwick, G.R. *et al., CRC Crit. Rev. Food Sci. Nutri.*, 1983, **18**, 123 (*glucosinolates, rev*)
IARC Monog., 1985, **36**, 55; *Suppl*. 7, 56 (*rev, tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1391
Yamamoto, T. *et al., Org. Prep. Proced. Int.*, 1994, **26**, 555 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGJ250
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1378
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 31

Isovitexin I-195

[38953-85-4]
*6-β-D-Glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 6-C-Glucopyranosylapigenin. 6-Glucosylapigenin. Saponaretin. Homovitexin. Avroside*



$C_{21}H_{20}O_{10}$ 432.383

Yellow cryst. (MeOH/EtOAc). Mp 239° (223-224°). $[\alpha]_D$ +16.2 (EtOH). Acid → Vitexin. Isoavroside was assigned the struct. of a geom. isomer of avroside but it is not clear what was meant by this. λ_{max} 271 ; 336 (MeOH).

*7-O-[4-Hydroxy-3,5-dimethoxy-*E*-cinnamoyl-(→6)-β-D-glucopyranoside]:* ***6‴-O-Sinapoylsaponarin***
$C_{38}H_{40}O_{19}$ 800.723
Constit. of young green barley leaves (*Hordeum vulgare* var. *nudum*). Amorph. powder. $[\alpha]_D^{25}$ -144 (c, 0.5 in MeOH aq.). λ_{max} 333 (log ϵ 4.38) (MeOH).

4′,7-Di-O-β-D-glucopyranoside: ***Isovitexin 4′,7-diglucoside***
$C_{33}H_{40}O_{20}$ 756.667
Constit. of young green barley leaves (*Hordeum vulgare* var. *nudum*). Amorph. solid. $[\alpha]_D^{25}$ -51 (c, 0.5 in MeOH).

*7-O-[4-Hydroxy-3,5-dimethoxy-*E*-cinnamoyl-(→6)-glucopyranoside], 4′-O-β-D-glucopyranoside:* [212271-13-1]
$C_{44}H_{50}O_{24}$ 962.865
Constit. of young green barley leaves (*Hordeum vulgare* var. *nudum*). Amorph. powder. $[\alpha]_D^{25}$ -84 (c, 0.5 in MeOH aq.). λ_{max} 329 (log ϵ 4.39) (MeOH).

2″-O-α-L-Arabinopyranosyl: [53382-71-1]
$C_{26}H_{28}O_{14}$ 564.499
Isol. from *Avena sativa* (oats). The pyranose-form has not been confirmed for all isolations.

2″-O-β-D-Glucopyranosyl: [60767-80-8] ***Meloside A***†
$C_{27}H_{30}O_{15}$ 594.525
Constit. of *Oxalis acetosella* (wood sorrel) and many other plants. Amorph. powder. $[\alpha]_D^{20}$ -21 (c, 0.1 in MeOH). Softens at 210°. Meloside A is given the 2″-*O*-D-glucoside struct..

2″-O-β-D-Galactopyranosyl: [101977-24-6]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Secale cereale* (rye).

2″-O-β-D-Glucopyranosyl, O-*(3,4-dihydroxycinnamoyl):* [39384-48-0] ***Meloside a***†
$C_{36}H_{36}O_{18}$ 756.67
Isol. from *Cucumis melo* (melon). Caffeoyl ester of Meloside A.

*2″-O-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl]:*
$C_{36}H_{36}O_{17}$ 740.67
Constit. of *Cucumis sativus* (cucumber). Yellow solid. λ_{max} 273 ; 294 (sh) ; 321 (MeOH).

*2″-O-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl], 4′-O-β-D-glucopyranoside:*
$C_{42}H_{46}O_{22}$ 902.812
Constit. of *Cucumis sativus* (cucumber). Yellow solid. λ_{max} 278 ; 316 (MeOH).

*2″-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl]:* [220948-77-6]
$C_{37}H_{38}O_{18}$ 770.696
Constit. of *Cucumis sativa* (cucumber).

*2″-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl], 4′-O-β-D-glucopyranoside:*
$C_{43}H_{48}O_{23}$ 932.838
Constit. of *Cucumis sativus* (cucumber).

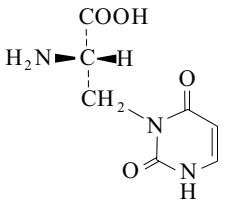
[11018-95-4, 28570-90-3, 29702-25-8, 36025-68-0, 53609-37-3, 61460-24-0, 64813-37-2, 72021-35-3, 77193-99-8, 84842-17-1, 84842-18-2, 87551-96-0, 89961-45-5, 133196-84-6]

Monties, B. *et al., Phytochemistry*, 1976, **15**, 1053 (*Meloside*)
Chopin, J. *et al., Phytochemistry*, 1977, **16**, 2041 (*2″-arabinosyl*)
Dellamonica, G. *et al., Phytochemistry*, 1983, **22**, 2627 (*2″-galactosyl*)
Lin, C.N. *et al., J. Nat. Prod.*, 1997, **60**, 851 (*6″-glucosyl*)

Ohkawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1887-1890 (*Hordeum vulgare saponins*)
Haribal, M. *et al., Phytochemistry*, 1998, **47**, 1237-1240 (*6″-glucosyl*)
Abou-Zaid, M.M. *et al., Phytochemistry*, 2001, **58**, 167-172 (*Cucumis sativus cinnamoylglucosides*)

Isowillardiine I-196

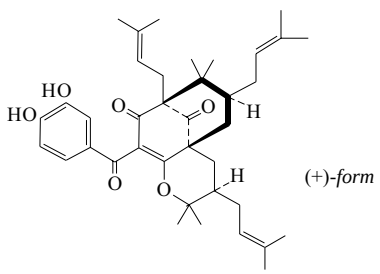
α-Amino-3,6-dihydro-2,6-dioxo-1(2H)-pyrimidinepropanoic acid. β-(2,4-Dihydroxy-3-pyrimidinyl)alanine



$C_7H_9N_3O_4$ 199.166

(*S*)-*form* [21381-33-9]
From seeds of *Pisum sativum* (peas).
Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1968, **32**, 474 (*isol, uv, struct*)
Ashworth, T.S. *et al., Biochem. J.*, 1972, **129**, 897 (*biosynth*)
Janzen, D.H. *et al., Phytochemistry*, 1977, **16**, 223 (*biosynth, tox*)
Al-Baldaw, N.F. *et al., CA*, 1980, **93**, 180253m (*metab*)
Tsuchida, K. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2748 (*synth*)
De Bruyn, A. *et al., Org. Magn. Reson.*, 1991, **29**, 641 (*pmr, cmr*)

Isoxanthochymol I-197



(+)-*form*

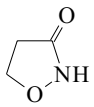
$C_{38}H_{50}O_6$ 602.809
λ_{max} 233 (ϵ 21200); 277 (ϵ 24000); 310 (ϵ 12000) (MeOH) (Derep).

(+)-*form* [52617-33-1]
Constit. of fruit of *Garcinia xanthochymus* (false mangosteen). Yellow needles. Poorly sol. H_2O. Mp 242-244°. $[\alpha]_D^{25}$ +213 (MeOH). $[\alpha]_D^{25}$ +208 (MeOH). λ_{max} 233 (ϵ 22387); 278 (ϵ 26300) (MeOH) (Berdy).

(-)-*form* [71117-97-0]
Isogarcinol. *Cambogin*
Found in the latex of *Garcinia indica* (kokam) and *Garcinia cambogia*. Mp 242-243°. $[\alpha]_D^{25}$ -224 (MeOH) (-209.9). λ_{max} 233 (ϵ 23442); 277 (ϵ 25700); 311 (MeOH) (Berdy).
Karanjgoaker, C.G. *et al., Tet. Lett.*, 1973, 4977 (*isol*)
Venkatswamy, G. *et al., Indian J. Chem.*, 1975, **13**, 1355 (*abs config, uv*)
Rao, A.V.R. *et al., Chem. Ind. (London)*, 1979, 92 (*struct, bibl*)
Baslas, R.K. *et al., Curr. Sci.*, 1979, **48**, 814 (*struct, bibl*)
Krishnamurthy, N. *et al., Tet. Lett.*, 1982, **23**, 2233-2236 (*Isogarcinol, Cambogin*)
Gustafson, K.R. *et al., Tetrahedron*, 1992, **48**, 10093 (*isol, pmr, cmr*)
Iinuma, M. *et al., Biol. Pharm. Bull.*, 1996, **19**, 311-314 (*Isogarcinol*)
Roux, D. *et al., J. Nat. Prod.*, 2000, **63**, 1070-1076 (*isol*)

3-Isoxazolidinone, 9CI I-198

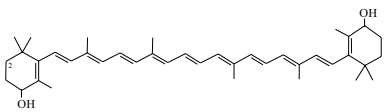
[1192-07-0]
3-Isoxazolidone



$C_3H_5NO_2$ 87.078
Isol. from seedlings of *Canavalia ensiformis* (jack bean). Cryst. Mp 70°.
Shunk, C.H. *et al., J.O.C.*, 1957, **22**, 76 (*synth*)
Olive, J.L. *et al., Bull. Soc. Chim. Fr.*, 1976, 1589 (*synth, pmr*)
Sugii, M. *et al., Phytochemistry*, 1981, **20**, 451 (*isol*)

Isozeaxanthin I-199

[29065-03-0]
β,β-Carotene-4,4′-diol. Aphanicol



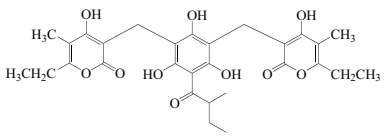
$C_{40}H_{56}O_2$ 568.881
Widespread in marine animals. Additive for salmon feed. Fine red needles (AcOH/petrol). Mp 149-151°.

Diketone: [514-78-3] ***Canthaxanthin***. *β,β-Carotene-4,4′-dione. Chlorellaxanthin. Aphanicin. Euglenanone. Carophyll red. E161g*
$C_{40}H_{52}O_2$ 564.85
Food colouring. Constit. of the edible mushroom (*Cantharellus cinnabarinus*), sea trout, salmon and brine shrimp. Used in broiler chicken feed to enhance the yellow colour of chicken skin. Purple cryst. (C_6H_6/MeOH). Sol. $CHCl_3$, hexane; poorly sol. H_2O. Mp 218°. Identity with Euglenanone is not certain. λ_{max} 470 (E1%/1cm 2250) (cyclohexane) (Berdy).
► FI0330000

Diketone, 2-hydroxy: [100485-10-7] ***2-Hydroxycanthaxanthin***. *2-Hydroxy-β,β-carotene-4,4′-dione*
$C_{40}H_{52}O_3$ 580.849
λ_{max} 470 (Me_2CO).
Isler, O. *et al., Helv. Chim. Acta*, 1956, **39**, 449 (*synth, ir*)
Warren, C.K. *et al., J.C.S.*, 1958, 3986 (*synth*)
Krinsky, N.I. *et al., Arch. Biochem. Biophys.*, 1960, **91**, 271 (*Euglenanone*)
Bodea, C. *et al., Annalen*, 1963, **666**, 189 (*ir*)
Di Accadia, F.D. *et al., Biochem. J.*, 1966, **101**, 735 (*Euglenanone*)
Hertzberg, S. *et al., Phytochemistry*, 1966, **5**, 565
Surmatis, J.D. *et al., Helv. Chim. Acta*, 1970, **53**, 974 (*synth*)
Kjoesen, H. *et al., Acta Chem. Scand.*, 1972, **26**, 2185 (*pmr*)
Gilchrist, B.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1976, **54**, 343 (*biosynth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Rosenberger, M. *et al., J.O.C.*, 1982, **47**, 2130 (*synth*)
Partali, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **82**, 767 (*2-Hydroxycanthaxanthin*)
Foss, P. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 157 (*2-Hydroxycanthaxanthin*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 129; 380 (*bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CBE800

Italidipyrone I-200

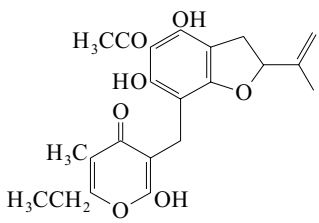
[75680-22-7]



$C_{28}H_{32}O_{10}$ 528.555
Constit. of *Helichrysum italicum* (curry plant). Cryst. ($CHCl_3$/Et_2O). Mp 178-182°. Isol. as a mixt. with its homologue to which the data refers λ_{max} 295 (log ϵ 4.42) ($CHCl_3$).
Haensel, R. *et al., Phytochemistry*, 1980, **19**, 639-644 (*isol, uv, ir, pmr, ms, struct*)
Hirschmann, G.S. *et al., Rev. Latinoam. Quim.*, 1984, **15**, 134-135 (*isol*)

Italipyrone I-201

[75680-21-6]



$C_{22}H_{24}O_7$ 400.427
Constit. of *Helichrysum italicum* (curry plant). Needles ($CHCl_3$/Et_2O). Mp 165°. λ_{max} 293 (log ϵ 4.31) (MeOH). λ_{max} 293 (ϵ 20500) ($CHCl_3$) (Berdy).
Haensel, R. *et al., Phytochemistry*, 1980, **19**, 639 (*isol, uv, ir, pmr, ms*)
Zdero, C. *et al., Phytochemistry*, 1987, **26**, 187 (*struct*)

Ivonine I-202

$C_{29}H_{34}N_7O_9S$ 656.695
Struct. unknown. Alkaloid from the mushroom *Phallus impudicus* (common stinkhorn). Mp 262°.
Stefănescu, P. *et al., Med. Promst. SSSR*, 1960, **14**, 15; *CA*, **55**, 11763i

IWF I-203

Isol. from sugarbeet leaves.

IWF 1 [181380-09-6] Basic monomeric protein containing 99 amino acid residues including 8 cysteines.

IWF 2 [181380-10-9] Protein containing 91 amino acid residues of which 89 are identical with IWF-1.

IWF 4 Peptide containing 30 amino acid residues incl. 6 cysteines and 7 glycines.

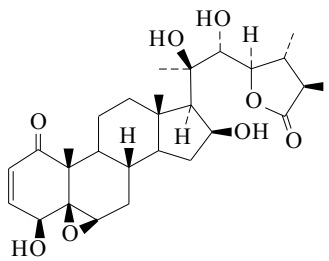
Nielsen, K.K. *et al., Plant Mol. Biol.*, 1996, **31**, 539-552 (*IWF-1, IWF-2, isol, struct*)

Nielsen, K.K. *et al., Plant Physiol.*, 1997, **113**, 83-91 (*IWF-4, isol, struct*)

Ixocarpalactone A I-204

[71801-45-1]

5,6-Epoxy-4,16,20,22-tetrahydroxy-1-oxoergost-2-eno-26,23-lactone. 5,6-Epoxy-4,16,20,22,23-pentahydroxy-1-oxoergost-2-en-26-oic acid, γ-lactone



$C_{28}H_{40}O_8$ 504.619

Constit. of *Physalis ixocarpa* (tomatillo). Cryst. Mp 294-295°. $[\alpha]_D$ +84.

Kirson, I. *et al., J. Chem. Res., Synop.*, 1979, 103

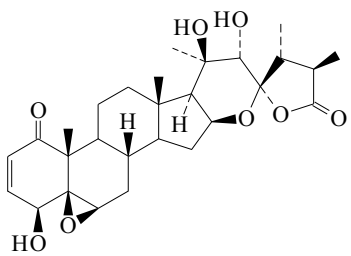
Abdullaev, N.D. *et al., Khim. Prir. Soedin.*, 1986, **22**, 326; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 300 (*pmr, cmr*)

Su, B.-N. *et al., Tetrahedron*, 2002, **58**, 3453-3466 (*cryst struct*)

Ixocarpalactone B I-205

[71801-44-0]

*5,6β;16β,23*S*-Diepoxy-4β,20*R*,22*S*-trihydroxy-1-oxo-5β-ergost-2-eno-26,23*S*-lactone*



$C_{28}H_{38}O_8$ 502.603

Constit. of *Physalis philadelphica (ixocarpa)* (tomatillo). Amorph. powder. Mp 145-148°. $[\alpha]_D^{20}$ -19.6 (c, 0.25 in $CHCl_3$). λ_{max} 215 (log ϵ 3.9); 326 (log ϵ 2021) (MeOH).

4-Ac:

Mp 170-172°. $[\alpha]_D$ +47.2.

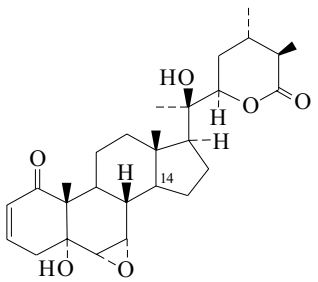
Kirson, I. *et al., J. Chem. Res., Synop.*, 1979, 103

Su, B.-N. *et al., Tetrahedron*, 2002, **58**, 3453-3466 (*isol, pmr, cmr*)

Ixocarpanolide I-206

[108157-59-1]

6,7-Epoxy-5,20,22-trihydroxy-1-oxoergost-2-en-26-oic acid δ-lactone, 9CI. 6,7-Epoxy-5,20-dihydroxy-1-oxowith-2-enolide



$C_{28}H_{40}O_6$ 472.62

Constit. of *Physalis ixocarpa* (tomatillo). Cryst. (MeOH). Mp 252-253°. $[\alpha]_D$ +27 (c, 0.83 in $CHCl_3$).

Stereoisomer: ***Withasomniferol B***

$C_{28}H_{40}O_6$ 472.62

Needles ($CHCl_3$/MeOH). Mp 281-283°. $[\alpha]_D$ -124 (c, 0.5 in $CHCl_3$). λ_{max} 228 (log ϵ 4.18) (EtOH).

14α-Hydroxy: [107221-65-8] *6,7-Epoxy-5,14,20-trihydroxy-1-oxowith-2-enolide.*

14α-Hydroxyixocarpanolide

$C_{28}H_{40}O_7$ 488.62

From the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH). Mp 245-250°. $[\alpha]_D^{20}$ +29 (c, 1.18 in $CHCl_3$).

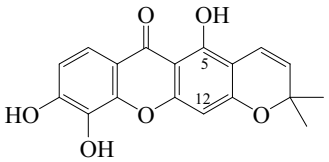
Abdullaev, N.D. *et al., Khim. Prir. Soedin.*, 1986, **22**, 326; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 300 (*isol*)

Vasina, O.E. *et al., Khim. Prir. Soedin.*, 1986, **22**, 596; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 560 (*deriv*)

Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 424-433 (*Withasomniferol B*)

Jacareubin J-1

[3811-29-8]
*5,9,10-Trihydroxy-2,2-dimethyl-2*H,*6*H-*pyrano[3,2-*b*]xanthen-6-one, 9CI*



$C_{18}H_{14}O_6$ 326.305

Systematic numbering shown. These compds. are often numbered as cyclised prenylxanthones with the numbering going round the xanthone nucleus only.Bright yellow prisms (MeOH). Mp 212-214° Mp 256-257° dec. λ_{max} 240 (ϵ 12200); 279 (ϵ 40800); 334 (ϵ 18200) (MeOH) (Berdy). λ_{max} 241 (ϵ 18200); 283 (ϵ 41700); 332 (ϵ 19050) (EtOH) (Berdy).

5-Me ether: [189065-54-1] ***Caloxanthone K***. *1-*O*-Methyljacareubin*
$C_{19}H_{16}O_6$ 340.332
Amorph. yellow powder. λ_{max} 257 (sh) ; 268 ; 300 (sh) ; 350 (sh) (No solvent reported).

Tri-Me ether:
Needles (MeOH). Mp 182-183°.

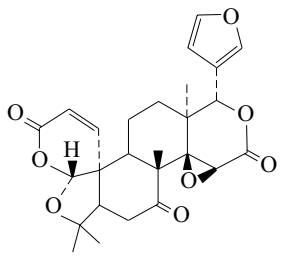
9-Deoxy: [16265-56-8] ***6-Deoxyjacareubin***
$C_{18}H_{14}O_5$ 310.306
Yellow prisms (EtOAc). Mp 212-214°.

12-Methoxy, tri-Me ether: ***Dulxanthone E***
$C_{22}H_{22}O_7$ 398.412
Constit. of *Garcinia dulcis* (mundu). Yelow cubes (EtOAc). Mp 191-192°. λ_{max} 272 (ϵ 4.2); 320 (ϵ 3.75) (MeOH).

King, F.E. *et al., J.C.S.*, 1953, 3932 (*isol, struct*)
Bhak, H.B. *et al., Tetrahedron*, 1963, **19**, 77 (*synth*)
Jefferson, A. *et al., J.C.S.(C)*, 1966, 175 (*synth*)
Locksley, H.D. *et al., J.C.S.(C)*, 1969, 486; 1567; 1971, 3804 (*isol, struct, synth*)
Bandaranayake, W.M. *et al., J.C.S.(C)*, 1971, 811 (*synth*)
Anand, S.M. *et al., Tetrahedron*, 1972, **28**, 987 (*synth*)
Helboe, P. *et al., Acta Chem. Scand.*, 1973, **27**, 2237 (*pmr*)
Iinuma, M. *et al., Heterocycles*, 1997, **45**, 299 (*Caloxanthone K*)
Peres, V. *et al., Phytochemistry*, 1997, **44**, 191 (*rev, occur, 6-Deoxyjacareubin*)
Kosela, S. *et al., Phytochemistry*, 1999, **52**, 1375-1377 (*Dulxanthone E*)
Hou, A.-J. *et al., J. Nat. Prod.*, 2001, **64**, 65-70 (*6-Deoxyjacareubin, activity*)

Jangomolide J-2

[93767-25-0]
Acidissimin†



$C_{26}H_{28}O_8$ 468.502
Constit. of *Flacourtia jangomas* (paniala) and *Limonia acidissima* (wood apple). Cryst. ($CHCl_3$/Et_2O). Mp 282-288°. $[\alpha]_D$ +22 (c, 0.5 in Me_2CO).

Ahmad, J. *et al., Phytochemistry*, 1984, **23**, 1269 (*isol, struct*)
MacLeod, J.K. *et al., J. Nat. Prod.*, 1989, **52**, 882 (*isol, pmr, cmr*)

Janthitrem A J-3

[73561-89-4]

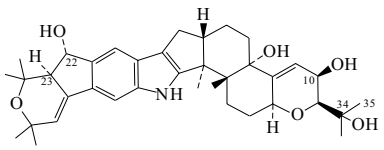
$C_{37}H_{47}NO_6$ 601.781

Struct. unknown. Prod. by *Penicillium janthinellum*. Tremorgenic mycotoxin. Fluorescent.

Gallagher, R.T. *et al., Appl. Environ. Microbiol.*, 1980, **39**, 272 (*isol*)
Lauren, D.R. *et al., J. Chromatogr.*, 1982, **248**, 150
Penn, J. *et al., Phytochemistry*, 1993, **32**, 1431-1434 (*isol, ms*)

Janthitrem E J-4

[90986-50-8]



$C_{37}H_{49}NO_6$ 603.797

Rel. stereochem. at C-22 and C-23 depicted. Prod. by *Penicillium janthinellum*. Tremorgenic mycotoxin. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 228 (ϵ 17700); 265 (ϵ 30000); 330 (ϵ 17000) (MeOH) (Berdy).

10-Ac: [90986-52-0] ***Janthitrem F***
$C_{39}H_{51}NO_7$ 645.834
Prod. by *Penicillium janthinellum*. Tremorgenic mycotoxin. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 228 (ϵ 24200); 265 (ϵ 22400); 330 (ϵ 12200) (MeOH) (Berdy).

22-Deoxy, 10-Ac: [90986-51-9] ***Janthitrem G***
$C_{39}H_{51}NO_6$ 629.835
Prod. by *Penicillium janthinellum*. Tremorgenic mycotoxin. Amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 228 (ϵ 23000); 263 (ϵ 15700); 331 (ϵ 10800) (MeOH) (Berdy).

22-Deoxy, 10-ketone: ***Shearinine B***
$C_{37}H_{47}NO_5$ 585.782
Mp 165-170° dec. $[\alpha]_D$ -76 (c, 0.20 in $CHCl_3$). C-23 config. not defined.

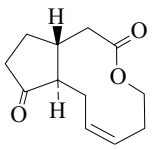
34-Deoxy, 34,35-didehydro: [73561-90-7] ***Janthitrem B***
$C_{37}H_{47}NO_5$ 585.782
Prod. by *Penicillium janthinellum*. Tremorgenic mycotoxin.

22,34-Dideoxy, 34,35-didehydro: [73561-91-8] ***Janthitrem C***
$C_{37}H_{47}NO_4$ 569.783
Prod. by *Penicillium janthinellum*. Tremorgenic mycotoxin. Amorph. solid.

De Jesus, A.E. *et al., J.C.S. Perkin 1*, 1984, 697 (*isol, uv, ir, pmr, cmr, struct*)
Wilkins, A.L. *et al., J. Agric. Food Chem.*, 1992, **40**, 1307 (*struct, config*)
Penn, J. *et al., Phytochemistry*, 1993, **32**, 1431 (*struct*)
Belofsky, G.N. *et al., Tetrahedron*, 1995, **51**, 3959 (*Shearinine B*)

Jasmine ketolactone J-5

[70981-24-7]
*1,4,5,8,8*a,*10,11,11*a-*Octahydrocyclopent[-*d*]oxecin-2,9-dione, 9CI. Jasmine oil ketolactone*

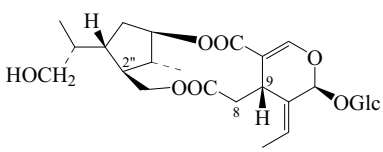


$C_{12}H_{16}O_3$ 208.257
Constit. of Italian jasmine oil (*Jasminum grandiflorum*). Small needles (petrol). Mp 104°. $[\alpha]_D^{20}$ -260 (c, 3.05 in MeOH).

Demole, E. *et al., Helv. Chim. Acta*, 1964, **47**, 1152 (*isol, ir, pmr, ms, struct*)
Kitahara, T. *et al., Agric. Biol. Chem.*, 1984, **48**, 1731 (*synth*)
Shimizu, I. *et al., Tet. Lett.*, 1992, **33**, 4957 (*synth*)
Furstner, A. *et al., Synlett*, 1997, 1010-1012 (*synth*)
Inoue, M. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1122-1124 (*synth*)

Jasminin J-6

[30164-93-3]
Jasmine lactone†



$C_{26}H_{38}O_{12}$ 542.579
Cryst. Mp 159-161°. $[\alpha]_D^{26}$ -245 (c, 1 in EtOH).

O-*β*-*D*-*Glucopyranoside:Jasminin 10″*-O-*β*-*D*-*glucoside*
$C_{32}H_{48}O_{17}$ 704.721
Needles. Mp 153-154°. $[\alpha]_D^{21}$ -236.7 (c, 0.49 in Py).

8,9-Didehydro: [85562-86-3] ***Sambacin***
$C_{26}H_{36}O_{12}$ 540.563
Isol. from *Jasminum sambac* (Arabian jasmine). Cryst. Mp 150-153°.

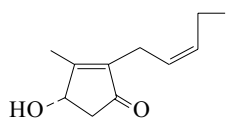
*2″α-Hydroxy:**2″-Hydroxyjasminin***
$C_{26}H_{38}O_{13}$ 558.578
Powder. $[\alpha]_D^{16}$ -160.8 (c, 0.77 in MeOH).

2″α-Hydroxy, carboxylic acid: [123967-69-1] ***Jasmisnyiroside***
$C_{26}H_{36}O_{14}$ 572.562
Cryst. Mp 230-232°. $[\alpha]_D$ -228.2 (MeOH).

Tamikawa, T. *et al., Tetrahedron*, 1970, **26**, 4561 (*struct*)
Inouye, H. *et al., Chem. Pharm. Bull.*, 1974, **22**, 676 (*biosynth*)
Asaka, Y. *et al., Tetrahedron*, 1974, **30**, 3257 (*synth*)
Ross, S. *et al., Fitoterapia*, 1982, **53**, 91 (*Sambacin*)
Utaka, M. *et al., Chem. Lett.*, 1983, 911 (*synth*)
He, Z. *et al., CA*, 1989, **111**, 228945h (*Jasmisnyiroside*)
Tanahashi, T. *et al., Phytochemistry*, 1989, **28**, 1413 (*deriv*)
Takahashi, K. *et al., Acta Cryst. C*, 1991, **47**, 777 (*cryst struct*)
Inouye, K. *et al., Phytochemistry*, 1991, **30**, 1191 (*deriv*)

Jasmolone J-7

[54383-66-3]
4-Hydroxy-3-methyl-2-(2-pentenyl)-2-cyclopenten-1-one, 9CI. Jasmololone



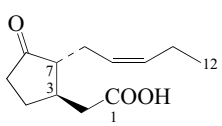
$C_{11}H_{16}O_2$ 180.246
Constit. of oil of *Jasminum grandiflorum* (royal jasmine). Oil.

O-*β-D-Glucopyranoside:*
$C_{17}H_{26}O_7$ 342.388
Constit. of *Mentha spicata* var. *crispa* (spearmint). $[\alpha]_D^{21}$ -25 (c, 0.2 in MeOH).

Pattenden, G. *et al., J.C.S. Perkin 1*, 1974, 1603 (*synth*)
Ficini, P. *et al., Bull. Soc. Chim. Fr.*, 1975, 1811 (*synth*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1975, 1500 (*cmr*)
Sato, T. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 505 (*synth*)
Takahashi, T. *et al., Chem. Lett.*, 1981, 1189 (*synth*)
Yamamura, S. *et al., Phytochemistry*, 1998, **48**, 131-136 (*isol, glucoside*)

Jasmonic acid J-8

[6894-38-8]
3-Oxo-2-(2-pentenyl)cyclopentaneacetic acid, 9CI, 8CI



Absolute Configuration

$C_{12}H_{18}O_3$ 210.272
Esters are present in *Jasminum grandiflorum* (royal jasmine) and are responsible for its odour. Viscous oil. $Bp_{0.001}$ 125°. $[\alpha]_D$ -83.5 (c, 0.97 in $CHCl_3$). n_D^{19} 1.4885.

Me ester: [1211-29-6]
[20073-13-6] *Methyl jasmonate. FEMA 3410*
$C_{13}H_{20}O_3$ 224.299
Flavouring ingredient. From *Jasminum grandiflorum* (royal jasmine). Oil with characteristic odour of jasmine. Prac. insol. H_2O; sol. EtOH. $d^{22.6}$ 1.02. $Bp_{0.001}$ 81-84°. $[\alpha]_D$ -76.5 (c, 3.4 in MeOH). n_D^{22} 1.4730.

11-β-D-Glucopyranosyloxy:β-D-Glucopyranosyl-11-hydroxyjasmonic acid
$C_{18}H_{28}O_9$ 388.414
Constit. of *Solanum tuberosum* (potato). C-11 stereochem. not determined.

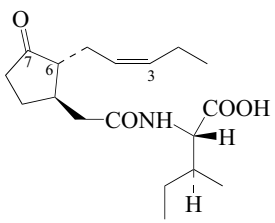
3-Epimer, 4,5-didehydro, Me ester: [59366-47-1]
$C_{13}H_{18}O_3$ 222.283
Constit. of *Jasminum* sp.. $[\alpha]_D^{20}$ +43.8 (c, 0.6 in $CHCl_3$).

[76968-33-7, 77026-92-7, 135911-63-6]

Kaiser, R. *et al., Tet. Lett.*, 1974, 3413-3416 (*4,5-didehydro Me ester*)
Miersch, O. *et al., Phytochemistry*, 1986, **26**, 1037; 1989, **28**, 339-340; 1303-1305; 1992, **31**, 3835 (*isol, derivs*)
Montforts, F.-P. *et al., Helv. Chim. Acta*, 1989, **72**, 1852 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 85S (*rev, tox*)
Sembdner, G. *et al., Annu. Rev. Plant Physiol.*, 1993, **44**, 569 (*rev*)
Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1253 (*derivs*)
Husain, A. *et al., J. Nat. Prod.*, 1993, **56**, 2008 (*isol, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 519 (*Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1789-1790 (*Me ester*)
Kiyota, H. *et al., Phytochemistry*, 1997, **46**, 983-986 (*deriv, synth*)
Jong Sun, U. *et al., Synth. Commun.*, 1997, **27**, 2931-2941 (*synth, stereoisomers*)
Wasternack, C. *et al., Fett/Lipid*, 1998, **100**, 139-146 (*rev*)
Matsuura, H. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 378-382 (*11-Glucosyloxyjasmonic acid*)

N-Jasmonoylisoleucine J-9

[28838-58-6]
N-*[[3-Oxo-2-(2-pentenyl)cyclopentyl]acetyl]isoleucine, 9CI*



$C_{18}H_{29}NO_4$ 323.431
Isol. from *Pinus mugo* (dwarf mountain pine) and *Vicia faba*.

7α-Alcohol: [162854-97-9] N-*[[3-Hydroxy-2-(2-pentenyl)cyclopentyl]acetyl]isoleucine.* N-*(7-Isocucurbinoyl)isoleucine*
$C_{18}H_{31}NO_4$ 325.447
Constit. of the pollen of *Pinus mugo* (dwarf mountain pine).

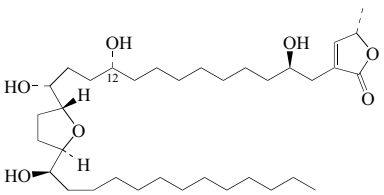
3,4-Dihydro: [28838-59-7] **N-*Dihydrojasmonoylisoleucine***
$C_{18}H_{31}NO_4$ 325.447
Needles (Me_2CO/petrol). Mp 140-141.5°.

*6-Epimer, 3,4-dihydro:***N-*Dihydro-6-isojasmonoylisoleucine***
$C_{18}H_{31}NO_4$ 325.447

Cross, B.E. *et al., J.C.S.(C)*, 1970, 1839 (*struct*)
Knoefel, H.-D. *et al., Phytochemistry*, 1995, **38**, 569 (*isol*)
Miersch, O. *et al., Phytochemistry*, 1999, **50**, 517-523 (*isol*)

Javoricin J-10

[172588-18-0]



$C_{35}H_{64}O_7$ 596.886
Constit. of *Annona muricata* (soursop). Amorph. powder. Mp 70°. $[\alpha]_D^{25}$ +13.6 (c, 0.1 in $CHCl_3$). λ_{max} 217 (ϵ 11800) (MeOH).

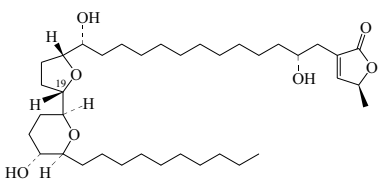
12-Epimer: [172430-57-8] ***Arianacin***
$C_{35}H_{64}O_7$ 596.886
Constit. of *Annona muricata* (soursop). Amorph. powder. Mp 64°. $[\alpha]_D^{25}$ +12.5 (c, 0.1 in $CHCl_3$). λ_{max} 215 (ϵ 12500) (MeOH).

*15-Epimer:**Asitrocin***
$C_{35}H_{64}O_7$ 596.886
Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. Mp 66.5-67.2°. $[\alpha]_D^{22}$ +5.2 (c, 0.01 in CH_2Cl_2). λ_{max} 215 (log ϵ 3.4) (MeOH).

Rieser, M.J. *et al., J. Nat. Prod.*, 1996, **59**, 100 (*isol, uv, ir, pmr, cmr, ms*)
Kim, E.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1503-1506 (*Asitrocin*)

Jimenezin J-11

[204185-17-1]



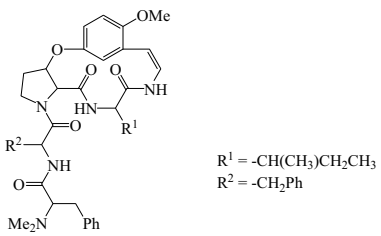
Absolute Configuration

$C_{37}H_{66}O_7$ 622.924
Constit. of the seeds of *Rollinia mucosa* (biriba). Yellow oil. $[\alpha]_D^{20}$ +8.3 (c, 1.2 in MeOH). Stereochem. of C-19 revised in 1999 λ_{max} 210 (log ϵ 3.97) (MeOH).

Chavez, D. *et al., J. Nat. Prod.*, 1998, **61**, 419-421 (*isol, uv, ir, cd, pmr, cmr, ms*)
Takahashi, S. *et al., Org. Lett.*, 1999, **1**, 2025-2028 (*synth*)

Jubanine A J-12

[60375-07-7]



$C_{40}H_{49}N_5O_6$ 695.857
Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Amorph. $[\alpha]_D^{20}$ -326 (c, 0.12 in MeOH). Stereochemistry unspecified.

Dihydro:
Mp 247-249°. $[\alpha]_D^{20}$ -148 (c, 0.06 in MeOH).

N-*De-Me:* [64309-23-5] ***Nummularine H***. N-*Demethyljubanine A*
$C_{39}H_{47}N_5O_6$ 681.83
Needles (MeOH). Mp 194-196°. $[\alpha]_D^{20}$ -343 (c, 0.27 in MeOH).

N-*De-Me,* N-*Ac:*
Cryst. ($CHCl_3$/petrol). Mp 135°. $[\alpha]_D^{20}$ -205 (c, 0.1 in MeOH).

Tschesche, R. *et al., Phytochemistry*, 1976, **15**, 541 (*isol, uv, ir, pmr, ms, struct*)
Tschesche, R. *et al., Chem. Ber.*, 1977, **110**, 2649 (*isol, uv, ir, pmr, ms, struct, Nummularine H*)

Jubanine B J-13

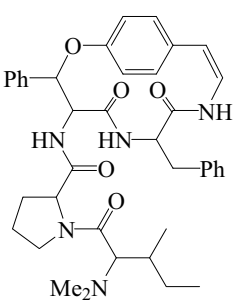
[60375-08-8]
As Jubanine A, J-12 with
$R^1 = R^2 = CH_2Ph$
$C_{43}H_{47}N_5O_6$ 729.874
Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Amorph. $[\alpha]_D^{20}$ -218 (c, 0.28 in MeOH). Stereochemistry unspecified.

N-*De-Me:* **N-*Desmethyljubanine B***
$C_{42}H_{45}N_5O_6$ 715.847

Tschesche, R. *et al., Phytochemistry*, 1976, **15**, 541 (*isol, uv, ir, ms, struct*)
Miana, G.A. *et al., Fitoterapia*, 1985, **56**, 363; *CA*, **105**, 75886p (*deriv*)

Jubanine C J-14

[159226-00-3]



$C_{39}H_{47}N_5O_5$ 665.831
Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Cryst. (MeOH). Mp 233-235° dec. λ_{max} 214 (MeOH).

Tripathi, M. *et al., Fitoterapia*, 2001, **72**, 507-510

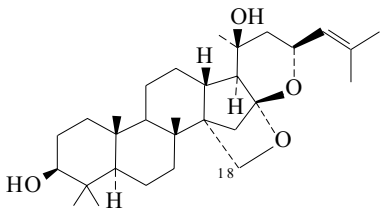
Juglanin J-15

$C_{27}H_{22}O_{18}$ 634.46
Ester of glucose, 2 × gallic acid and hexahydroxydiphenic acid, isomeric with Corilagin. Struct. not fully known. Isol. from walnuts (*Juglans regia*). Powder. Mp 235-237° dec. $[\alpha]_D^{20}$ +52 (H_2O).

Jurd, L. *et al., J.A.C.S.*, 1958, **80**, 2249

Jujubogenin J-16

[54815-36-0]
16,18:16,23-Diepoxydammar-24-ene-3,20-diol



$C_{30}H_{48}O_4$ 472.707
Cryst. (MeOH). Mp 250-252°. $[\alpha]_D^{25}$ -36 (c, 0.069 in EtOH).

3-O-α-L-Arabinopyranoside: [68170-83-2] ***Zizyotin***
$C_{35}H_{56}O_8$ 604.823
Cryst. (MeOH aq.). Mp 255-257° dec.

3,20-Di-O-α-L-arabinopyranoside: [178064-11-4] ***Bacopasaponin A***
$C_{40}H_{64}O_{12}$ 736.938
Needles (EtOAc/MeOH). Mp 256°. $[\alpha]_D$ -90 (c, 1.3 in MeOH).

3-O-β-D-Glucopyranoside, 20-O-α-L-rhamnopyranoside: [79190-13-9] ***Saponin G***
$C_{42}H_{68}O_{13}$ 780.991
Constit. of *Hovenia dulcis* (raisin tree). Needles. Mp 257-259°. $[\alpha]_D$ -33.1 (c, 0.35 in MeOH).

3-O-[α-L-Arabinofuranosyl-(1→3)-α-L-arabinopyranoside]: [58798-94-0] ***Bacoside A1***
$C_{40}H_{64}O_{12}$ 736.938
Needles (MeOH). Mp 240°.

3-O-[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranoside], 20-O-(2,3-di-O-acetyl-α-L-rhamnopyranoside): [73667-51-3] ***Ziziphin***. *Zizyphin*
$C_{51}H_{80}O_{18}$ 981.182
Constit. of leaves of *Zizyphus jujuba* (Chinese date). Cryst. Mp 213-215°. $[\alpha]_D$ -42.3 (c,3.6 in MeOH). Struct. revised in 1991.

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 20-O-α-L-rhamnopyranoside: [79190-14-0] ***Saponin D***
$C_{48}H_{78}O_{17}$ 927.134
Constit. of *Hovenia dulcis* (raisin tree). Needles. Mp 270-272°. $[\alpha]_D$ -48.6 (c, 0.28 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-α-L-arabinopyranoside]: [155545-03-2] ***Rugoside A***
$C_{41}H_{66}O_{13}$ 766.965
Cryst. (MeOH). Mp 224-227° dec.

3-O-[α-L-Arabinofuranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]: [94443-88-6]
$C_{46}H_{74}O_{17}$ 899.08
Cryst. $[\alpha]_D^{25}$ -43 (c, 1 in MeOH).

3-O-[α-L-Arabinofuranosyl-(1→2)-[(4-hydroxy-E-cinnamoyl)-(→2)-β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]: [230285-57-1]
$C_{55}H_{80}O_{19}$ 1045.226

3-O-[α-L-Arabinofuranosyl-(1→2)-[4-hydroxy-Z-cinnamoyl-(→2)-β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]: [230285-55-9]
$C_{55}H_{80}O_{19}$ 1045.226

3-O-[5-O-(Carboxyacetyl)-α-L-arabinofuranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]: [230285-56-0]
$C_{49}H_{76}O_{20}$ 985.127
Amorph. powder. $[\alpha]_D^{25}$ -24 (c, 0.48 in MeOH).

3-O-[α-L-Arabinopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-6-deoxy-α-L-talopyranoside]: [88100-00-9] ***Zizynummin***
$C_{47}H_{76}O_{17}$ 913.107
Cryst. (MeOH). Mp 255-260°. $[\alpha]_D^{20}$ -44.85 (c, 1.00 in MeOH).

3-O-[β-D-Xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]: [68665-70-3] ***Hovenoside I***
$C_{46}H_{74}O_{17}$ 899.08
Constit. of leaves of *Hovenia dulcis* (raisin tree). Cryst. (MeOH). Mp 272-274°. $[\alpha]_D$ -24.2 (c, 0.5 in MeOH).

3-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-2-O-acetyl-α-L-arabinopyranoside]: [87834-09-1] ***Colubrin***
$C_{48}H_{76}O_{18}$ 941.118
Amorph. solid.

3-O-[β-D-Xylopyranosyl-(1→2)-3-O-acetyl-β-D-glucopyranosyl-(1→3)-2-O-acetyl-α-L-arabinopyranoside]: [310871-97-7] ***3′′-Acetylcolubrin***
$C_{50}H_{78}O_{19}$ 983.155
Amorph. powder. $[\alpha]_D^{24}$ -7.4 (c, 0.6 in MeOH).

3-O-[2-O-Acetyl-β-D-xylopyranosyl-(1→2)-3-O-acetyl-β-D-glucopyranosyl-(1→3)-2-O-acetyl-α-L-arabinopyranoside]: [310871-98-8] ***2′′′,3′′-Diacetylcolubrin***
$C_{52}H_{80}O_{20}$ 1025.192
Amorph. powder. $[\alpha]_D^{24}$ -12.5 (c, 0.16 in MeOH).

3-O-[β-D-Xylopyranosyl-(1→2)-3-O-acetyl-6-O-(2E-butenoyl)-β-D-glucopyranosyl-(1→3)-2-O-acetyl-α-L-arabinopyranoside]: [310871-99-9] ***3′′-Acetyl-6′′-crotonylcolubrin***
$C_{54}H_{82}O_{20}$ 1051.23
Amorph. powder. $[\alpha]_D^{24}$ +2 (c, 0.5 in MeOH). λ_{max} 206 (log ε 4.64) (H_2O).

3-O-[α-L-Fucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]: [156985-57-8] ***Christinin A***
$C_{47}H_{76}O_{17}$ 913.107

3-O-[α-D-Fucopyranosyl-(1→2)-[4-sulfo-β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]: [177855-94-6] ***Christinin***

B
$C_{47}H_{76}O_{20}S$ 993.171

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-xylopyranosyl-(1→2)-β-D-xylopyranoside]:* [163974-29-6]
$C_{46}H_{74}O_{16}$ 883.081
Amorph. solid. Mp 188-200°.

3-O-*[2*-O-*Acetyl-α-L-rhamnopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]:* [156408-68-3] ***Zizyphoiside D***
$C_{49}H_{78}O_{18}$ 955.144

3-O-*[3*-O-*Acetyl-α-L-rhamnopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]:* [156408-67-2] ***Zizyphoiside C***
$C_{49}H_{78}O_{18}$ 955.144

3-O-*[4*-O-*Acetyl-α-L-rhamnopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]:* [156436-85-0] ***Zizyphoiside E***
$C_{49}H_{78}O_{18}$ 955.144

3-O-*[β-D-Glucopyranosyl-(1→3)-[α-L-arabinofuranosyl-(1→2)]-α-L-arabinopyranoside], 20*-O-*α-L-arabinopyranoside:* [267895-16-9] ***Bacopasaponin E***
$C_{51}H_{82}O_{21}$ 1031.196
Amorph. powder (MeOH/Et_2O). Mp 266-270° dec. $[\alpha]_D$ -27.7 (c, 0.44 in MeOH).

3-O-*[4-Hydroxy*-E-*cinnamoyl-(→3)-β-D-glucopyranosyl-(1→3)-[α-L-arabinopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [245419-22-1]
$C_{55}H_{80}O_{19}$ 1045.226
Powder. Mp 212°. $[\alpha]_D^{25}$ -79.7 (c, 0.025 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→3)-[α-L-arabinofuranosyl-(1→2)]-β-D-glucopyranoside]:* [157408-08-7] ***Bacoside A3***
$C_{47}H_{76}O_{18}$ 929.107
Amorph. solid.

3-O-*[β-D-Glucopyranosyl-(1→3)-[α-L-arabinopyranosyl-(1→2)]-β-D-glucopyranoside], 20*-O-*α-L-arabinopyranoside:* [267895-17-0] ***Bacopasaponin F***
$C_{52}H_{84}O_{22}$ 1061.222
Amorph. powder (MeOH/Et_2O). Mp 260-264° dec. $[\alpha]_D$ -37.7 (c, 0.44 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→3)-[6-deoxy-β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [146503-30-2] ***Hoduloside III***
$C_{47}H_{76}O_{17}$ 913.107
Constit. of leaves of *Hovenia dulcis* (raisin tree). Needles (MeOH). Mp 297-299°. $[\alpha]_D^{22}$ -36.9 (c, 1 in Py).

3-O-*[β-D-Glucopyranosyl-(1→3)-[6-deoxy-α-L-talopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [77943-56-7] ***Zizyphussaponin I***
$C_{47}H_{76}O_{17}$ 913.107
Cryst. Mp 269-272°. $[\alpha]_D^{18}$ -48.5 (c, 1 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→3)]-α-L-arabinopyranoside]:* [178033-50-6] ***Christinin C***
$C_{47}H_{76}O_{17}$ 913.107

3-O-*[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [77943-83-0] ***Zizyphussaponin II***. *Saponin* C_2
$C_{47}H_{76}O_{17}$ 913.107
Constit. of leaves of *Hovenia dulcis* (raisin tree). Needles (MeOH). Mp 288-290°. $[\alpha]_D^{22}$ 0 (c, 5.8 in Py).

3-O-*[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranoside]:* [146445-92-3] ***Hoduloside V***
$C_{48}H_{78}O_{18}$ 943.133
Constit. of leaves of *Hovenia dulcis* (raisin tree). Needles (MeOH). Mp 215-217°. $[\alpha]_D^{22}$ -31.4 (c, 4.3 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [146445-91-2] ***Hoduloside IV***
$C_{47}H_{76}O_{18}$ 929.107
Constit. of leaves of *Hovenia dulcis* (raisin tree). Needles (MeOH). Mp 246-248°. $[\alpha]_D^{22}$ -12.9 (c, 3.5 in MeOH).

3-O-*[β-D-Arabinopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-[α-L-fucopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [177855-95-7] ***Christinin D***
$C_{52}H_{84}O_{21}$ 1045.223

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [55466-01-8] ***Hovenoside G***
$C_{51}H_{82}O_{21}$ 1031.196
Constit. of leaves of *Hovenia dulcis* (raisin tree). Cryst. $[\alpha]_D$ -26.4 (c, 1 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-[6-deoxy-α-L-talopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [77943-54-5] ***Zizyphussaponin III***
$C_{52}H_{84}O_{21}$ 1045.223
Cryst. Mp 229-233°. $[\alpha]_D^{28}$ -46.5 (c, 0.98 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [55466-05-2] ***Jujuboside B***
$C_{52}H_{84}O_{21}$ 1045.223
Isol. from seeds of *Zizyphus jujuba* (Chinese date). Cryst. Mp 222-225°. $[\alpha]_D^{24}$ -42 (c, 0.5 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→2)-[6*-O-*acetyl-β-D-glucopyranosyl-(1→3)]-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [194737-13-8] ***Acetylzizyphoside B***
$C_{54}H_{86}O_{22}$ 1087.26
Constit. of *Zizyphus jujuba* var. *spinosa*. Cryst. (MeOH aq.). Mp 207-210°. $[\alpha]_D^{28}$ -42.8 (c, 0.3 in MeOH).

3-O-*[6-Deoxy-β-D-galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]:* [68144-21-8] ***Jujuboside B1***
$C_{52}H_{84}O_{21}$ 1045.223
Isol. from seeds of *Zizyphus jujuba* (Chinese date). Mp 223-226°. $[\alpha]_D$ -50.6.

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]:* [184955-70-2] ***Hovacerboside A1***
$C_{53}H_{86}O_{22}$ 1075.249
Cryst. ($CHCl_3$/MeOH). Mp 257-260° dec.

3-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [189136-85-4] ***Jujuboside C***†
$C_{53}H_{86}O_{22}$ 1075.249
Amorph. powder. $[\alpha]_D^{20}$ -48 (c, 0.66 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside]:* [55466-04-1] ***Jujuboside A***
$C_{58}H_{94}O_{26}$ 1207.365
Isol. from seeds of *Zizyphus jujuba* (Chinese date). Cryst. Mp 211-216°. $[\alpha]_D^{24}$ -50.1 (c, 0.43 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [68144-22-9] ***Hovenoside D***
$C_{57}H_{92}O_{26}$ 1193.338
Constit. of leaves of *Hovenia dulcis* (raisin tree). Powder (butanol). Mp 205-210°. $[\alpha]_D$ -29.6 (c, 0.5 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→3)-[α-D-fucopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [194851-84-8] ***Jujuboside A1***
$C_{58}H_{94}O_{26}$ 1207.365
Constit. of *Zizyphus jujuba* var. *spinosa*. Cryst. (MeOH aq.). Mp 223-225°. $[\alpha]_D^{29}$ -47.6 (c, 0.3 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside]:* [194852-14-7] ***Jujuboside C***†
$C_{59}H_{96}O_{27}$ 1237.391
Constit. *Zizyphus jujuba* var. *spinosa*. Cryst. (MeOH aq.). Mp 229-231°. $[\alpha]_D^{29}$ -32.8 (c, 0.3 in MeOH).

Kawai, K.-I. *et al., Acta Cryst. B*, 1974, **30**, 2886-2888 (*cryst struct*)

Inoue, O. *et al., J. Chem. Res., Synop.*, 1978, 144-145 (*cmr, Jujuboside B1*)

Inoue, O. *et al., J.C.S. Perkin 1*, 1978, 1289-1293 (*Hovenosides*)

Kawai, K.-I. *et al., Phytochemistry*, 1978, **17**, 287-289 (*synth*)

Otsuka, H. *et al., Phytochemistry*, 1978, **17**, 1349-1352 (*Jujubosides*)

Okamura, N. *et al., Chem. Pharm. Bull.*, 1981, **29**, 676-683 (*Zizyphussaponins*)

Kimura, Y. *et al., J.C.S. Perkin 1*, 1981, 1923-1927 (*Hoveniasaponins*)

Sharma, S.C. *et al., Phytochemistry*, 1983, **22**, 1469-1471 (*Zizynummin*)

Yoshikawa, K. *et al., Tet. Lett.*, 1991, **32**, 7059-7062 (*Ziziphin, Jujubasaponin I, II, III*)

Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2287-2291 (*Hodulosides*)

Pandey, V.B. *et al., Fitoterapia*, 1993, **64**, 341-343 (*Rugoside A*)

Jain, P. *et al., Phytochemistry*, 1993, **33**, 449-451 (*Bacoside A1*)

Li, D. *et al., J. Nat. Prod.*, 1994, **57**, 218-224 (*Zizyphoisides*)

Rastogi, S. *et al., Phytochemistry*, 1994, **36**, 133-137 (*Bacoside A3*)

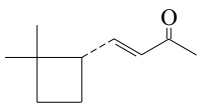
Maurya, S.K. *et al., Pharmazie*, 1995, **50**, 372 (*Zizyotin*)

Simão, S.M. *et al., Quim. Nova*, 1995, **18**, 34-39; *CA*, **123**, 29597u (*Centrosema bracteosum saponin*)

Garai, S. *et al., Phytochemistry*, 1996, **42**, 815-820 (*Bacopasaponin A*)
Mahran, G.E.-D.H. *et al., Planta Med.*, 1996, **62**, 163-165 (*Christinins*)
Liang, Q. *et al., Zhongguo Yaoke Daxue Xuebao*, 1996, **27**, 401-404; *CA*, **126**, 44938m (*Hovacerboside A_1*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1186-1192 (*Jujubosides*)
Renault, J.-H. *et al., Phytochemistry*, 1997, **44**, 1321-1327 (*Jujubosides A and C*)
Li, X.-C. *et al., J. Nat. Prod.*, 1999, **62**, 674-677 (*Colubrina retusa saponins, isol, activity*)
Elsohly, H.N. *et al., J. Nat. Prod.*, 1999, **62**, 1341-1342 (*Colubrina retusa saponin*)
Lee, S.-S. *et al., J. Nat. Prod.*, 2000, **63**, 1580-1583 (*Colubrin derivs*)
Mahato, S.B. *et al., Phytochemistry*, 2000, **53**, 711-714 (*Bacopasaponins*)

Junionone J-17

[51847-79-1]
4-(2,2-Dimethylcyclobutyl)-3-buten-2-one

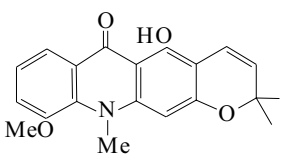


$C_{10}H_{16}O$ 152.236
Constit. of the fruit oil of *Juniperus communis* (juniper).

Thomas, A.F. *et al., Chem. Comm.*, 1973, 746
Gaoni, Y. *et al., Tet. Lett.*, 1982, **23**, 5219 (*synth*)
Gaoni, Y. *et al., J.O.C.*, 1985, **50**, 2948 (*synth*)
Ghosh, A. *et al., Tetrahedron*, 1990, **46**, 3077 (*synth*)

Junosidine J-18

[110883-39-1]
*2,11-Dihydro-5-hydroxy-10-methoxy-2,2,11-trimethyl-6*H*-pyrano[3,2-*b*]acridin-6-one, 9CI*



$C_{20}H_{19}NO_4$ 337.374
Alkaloid from the root bark of *Citrus junos* (yuzu). Orange needles. Mp 188-189°.

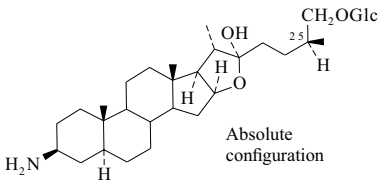
O-*De-Me:* [145940-32-5] ***Yukocitrine***
$C_{19}H_{17}NO_4$ 323.348
Yellow oil.

9-Hydroxy: [100595-86-6] ***Honyumine***
$C_{20}H_{19}NO_5$ 353.374
Alkaloid from the root bark of *Citrus grandis* (pummelo). Yellow granules (Me_2CO). Mp 175-176°.

Wu, T.S. *et al., Heterocycles*, 1986, **24**, 41 (*Honyumine*)
Ju-ichi, M. *et al., Heterocycles*, 1987, **26**, 2077 (*Junosidine*)
Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2123 (*Yukocitrine*)

Jurubine J-19

[14256-61-2]



$C_{33}H_{57}NO_8$ 595.815
Alkaloid from *Solanum torvum* (pea eggplant). Mp 212-214°. $[\alpha]_D^{18}$ -30.9 (c, 1.04 in Py). Paniculine from *Solanum paniculatum* is a mixt. of Jurubine and its C-25 epimer.

N-*Salicylidene:*
Mp 176-177°. $[\alpha]_D$ -34.9 (Py).

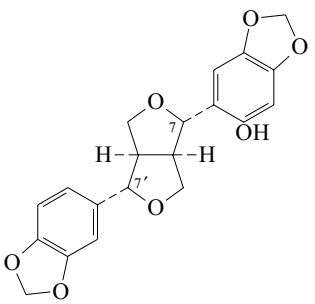
Penta-Ac:
Mp 165-168°. $[\alpha]_D$ -41.1 (Py).

Aglycone: See Spirostan-3-amine in *The Combined Chemical Dictionary.*

Ripperger, H. *et al., Chem. Ber.*, 1967, **100**, 1725 (*isol, ir, ms, pmr, struct*)
Schreiber, K. *et al., CA*, 1968, **69**, 27721 (*isol*)

Justisolin J-20

[74061-79-3]
2-(2-Hydroxy-3,4-methylenedioxyphenyl)-6-(3,4-methylenedioxyphenyl)-3,7-dioxabicyclo[3.3.0]octane. 2-Hydroxy-3′,4′:4,5-bis(methylenedioxy)-7,9′:7′,9-diepoxylignan. Sesaminol



$C_{20}H_{18}O_7$ 370.358
Lignan numbering shown. Found in sesame seed and oxidised sesame oil. Mp 146-148°. $[\alpha]_D^{28}$ +42.7 (c, 0.21 in $CHCl_3$).

O-*β-D-Glucopyranoside:* [153512-13-1]
$C_{26}H_{28}O_{12}$ 532.5
Constit. of sesame seed. $[\alpha]_D^{25}$ -6.24 (c, 1.3 in MeOH).

O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [157469-82-4]
$C_{32}H_{38}O_{17}$ 694.642
Constit. of sesame seed. $[\alpha]_D^{25}$ -25.3 (c, 0.2 in MeOH).

O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]:* [157469-83-5]
$C_{38}H_{48}O_{22}$ 856.784
Constit. of sesame seed. $[\alpha]_D^{25}$ -9.75 (c, 0.3 in H_2O).

7-Epimer: [104319-96-2]
Yellow prisms ($CHCl_3$/MeOH) (as 3,5-dinitrobenzoyl). Mp 169-170° (3,5-dinitrobenzoyl). $[\alpha]_D$ +101.5 (c, 1 in $CHCl_3$) (dinitrobenzoyl).

7-Epimer, O-*[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Cuscutoside B***
$C_{31}H_{36}O_{16}$ 664.616
Pale yellow powder. $[\alpha]_D^{28}$ -7.2 (c, 0.36 in MeOH).

7-Epimer, O-*[β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Cuscutoside A***
$C_{31}H_{36}O_{16}$ 664.616
Pale yellow powder. $[\alpha]_D^{28}$ -25.1 (c, 0.48 in MeOH aq.).

7-Epimer, O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Neocuscutoside C***
$C_{32}H_{38}O_{17}$ 694.642
Powder. $[\alpha]_D^{20}$ -12.5 (c, 0.4 in Py).

7-Epimer, O-*[β-arabinopyranosyl-(1→6)-[β-D-apiofuranosyl-(1→2)]-β-D-glucopyranoside]:* ***Neocuscutoside B***
$C_{36}H_{44}O_{20}$ 796.732
Powder. $[\alpha]_D^{20}$ -20 (c, 0.5 in Py).

7-Epimer, O-*[β-D-glucopyranosyl-(1→4)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Neocuscutoside A***
$C_{37}H_{46}O_{21}$ 826.758
Powder. $[\alpha]_D^{20}$ -19.8 (c, 0.1 in Py).

7′-Epimer:
Mp 160°. $[\alpha]_D$ +138.2 (c, 1 in $CHCl_3$).

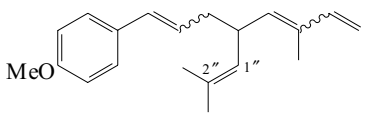
7,7′-Diepimer:Diasesaminol
Mp 194-196°. $[\alpha]_D$ +325.9 (c, 0.1 in $CHCl_3$).

[105616-55-5, 112531-05-2]

Ghosal, S. *et al., Phytochemistry*, 1980, **19**, 332 (*isol, struct*)
Fukuda, Y. *et al., Heterocycles*, 1986, **24**, 923 (*synth*)
Nagata, M. *et al., Agric. Biol. Chem.*, 1987, **51**, 1285 (*synth, cryst struct*)
Katsuzaki, H. *et al., Phytochemistry*, 1994, **35**, 773 (*glycosides*)
Yahara, S. *et al., Phytochemistry*, 1994, **37**, 1755 (*Cuscutosides*)
Xiang, S.-X. *et al., Chin. J. Chem.*, 2001, **19**, 282-285 (*Neocuscutosides*)

Juvocimene 1 J-21

[75539-64-9]
1-Methoxy-4-[6-methyl-4-(2-methyl-1-propenyl)-1,5,7-octatrienyl]benzene, 9CI



$C_{20}H_{26}O$ 282.425
Constit. of the oil of *Ocimum basilicum* (sweet basil).

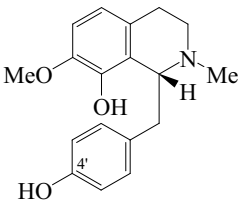
1″,2″-Epoxide: [75539-63-8] ***Juvocimene 2***
$C_{20}H_{26}O_2$ 298.424
Constit. of the oil of *Ocimum basilicum* (sweet basil).

[94668-94-7, 94668-95-8, 94668-96-9]

Nishida, R. *et al., J. Chem. Ecol.*, 1984, **10**, 1435 (*isol, synth*)

Juziphine J-22

Yuziphine. Yuzifine



(*R*)-*form*

$C_{18}H_{21}NO_3$ 299.369

(*R*)-*form* [64091-05-0]
Alkaloid from the leaves of *Zizyphus jujuba* (Chinese date).

N-*Oxide:* [65954-43-0] ***Juziphine* N-*oxide***
$C_{18}H_{21}NO_4$ 315.368
Cryst. (MeOH). Mp 197-198°. $[\alpha]_D$ -29 (MeOH).

N-*De-Me:* [74119-87-2] ***Norjuziphine***
$C_{17}H_{19}NO_3$ 285.342
Plates (MeOH). Mp 199-201°. $[\alpha]_D^{21}$ +17.3 (MeOH).

N-*Me:* [152230-57-4]

[152230-59-6] *1,2,3,4-Tetrahydro-8-hydroxy-1-[(4-hydroxyphenyl)methyl]-7-methoxy-2,2-dimethylisoquinolinium*. ***Oblongine*†**
$C_{19}H_{24}NO_3^{\oplus}$ 314.403
Quaternary alkaloid from stems of *Litsea cubeba* (mountain pepper). Amorph. solid (as perchlorate). Mp 109.5° (perchlorate). $[\alpha]_D^{24}$ -11 (c, 1.0 in MeOH).

(*S*)-*form*

N-*Me:* [60008-01-7]

[60134-32-9]
Mp 160° (as iodide). $[\alpha]_D$ -9.

(±)-*form*

N-*Me:* [97185-37-0]
Cryst. (Me_2CO/petrol) (as iodide). Mp 161° (153-155°) (iodide).

[152321-76-1]

Karimov, A. *et al., Khim. Prir. Soedin.*, 1976, **12**, 117-118 (*Oblongine, isol*)
Ziyaev, R. *et al., Khim. Prir. Soedin.*, 1977, **13**, 239; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 204
Israilov, I.A. *et al., Khim. Prir. Soedin.*, 1977, **13**, 834; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 702
Alimova, M. *et al., Khim. Prir. Soedin.*, 1979, **15**, 874; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 783 (*Norjuziphine*)
Dwuma-Badu, D. *et al., J. Nat. Prod.*, 1983, **46**, 342 (*Oblongine, isol, uv, ir, pmr, ms, struct, synth*)
Hong, H. *et al., Planta Med.*, 1986, 193 (*Norjuziphine*)
Lee, S.S. *et al., J. Nat. Prod.*, 1993, **56**, 1971 (*Oblongine*)
Chen, J.-J. *et al., Planta Med.*, 2001, **67**, 423-427 (*Norjuziphine, isol, pmr, cmr*)

Kallikrein, 9CI K-1

[9001-01-8]

Kallidinogenase, BAN, INN, JAN. *Callicrein. Circuletin. Depot-Glumorin. Diminal†. Glumorin. Onokrein P. Padreatin. Padutin. Prokrein. Sialogastrone. Kininogenin. Kalleone*

► NZ2017050

Nustad, K. *et al., Gen. Pharmacol.*, 1978, **9**, 1 (*rev*)

Obika, L.F.O. *et al., Life Sci.*, 1978, **23**, 765 (*rev*)

Schachter, M. *et al., Pharmacol. Rev.*, 1979, **31**, (*rev*)

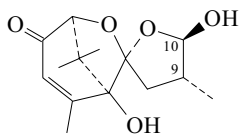
Fritz, H. *et al., Adv. Exp. Med. Biol.*, 1983, **156A**, 1; 13; 29 (*revs*)

Haberlund, G.L. *et al., Kininogenases: Physiological Properties and Pharmacol. Rationale - Exp. Studies*, (Eds.), Schattauer, Stuttgart, 1986, (*book*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1310

Kamahine C K-2

[144841-11-2]



$C_{14}H_{20}O_5$ 268.309

Found in honey from Kamali (*Weinmannia racemosa*). Cryst. (as Ac). Mp 152-154° (Ac).

9-Epimer: [160709-06-8] ***Kamahine A***
$C_{14}H_{20}O_5$ 268.309
Constit. of honey from *Weinmannia racemosa*.

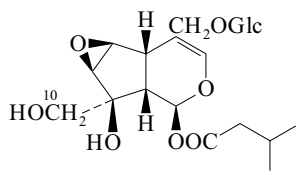
10-Epimer: [160709-07-9] ***Kamahine B***
$C_{14}H_{20}O_5$ 268.309
Constit. of honey from *Weinmannia racemosa*.

Broom, S.J. *et al., Tet. Lett.*, 1992, **33**, 6201 (*isol, pmr, cmr, cryst struct*)

Broom, S.J. *et al., J.O.C.*, 1994, **59**, 6425 (*isol, pmr, cmr*)

Kanokoside A K-3

[64703-85-1]



$C_{21}H_{32}O_{12}$ 476.477

Constit. of *Valeriana officinalis* (valerian) root. Amorph. Mp 58-62° (as penta-Ac). $[\alpha]_D$ -87.5 (MeOH) (penta-Ac).

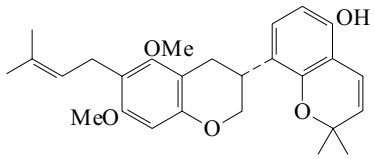
10-O-β-D-Glucopyranoside: [64703-87-3] ***Kanokoside C***
$C_{27}H_{42}O_{17}$ 638.619
From *Valeriana officinalis* (valerian) root. Amorph. Mp 102-105° (as penta-Ac). $[\alpha]_D$ -51.5 (MeOH) (penta-Ac).

Endo, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2140

Nishiya, K. *et al., Phytochemistry*, 1992, **31**, 3511 (*isol, pmr, cmr*)

Kanzonol I K-4

[152546-94-6]



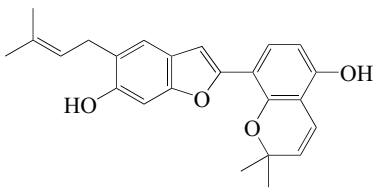
$C_{27}H_{32}O_5$ 436.547

Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Prisms (C_6H_6). Mp 180-185°.

Fukai, T. *et al., Heterocycles*, 1993, **36**, 2565 (*isol, pmr, cmr*)

Kanzonol V K-5

[184584-65-4]



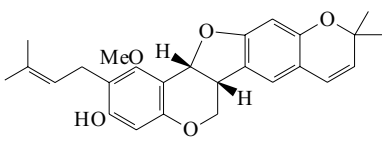
$C_{24}H_{24}O_4$ 376.451

Constit. of *Glycyrrhiza glabra* (licorice). Amorph. powder. λ_{max} 203 (log ϵ 4.38); 230 (sh) (log ϵ 4.1); 272 (sh) (log ϵ 4.06); 282 (log ϵ 4.1); 292 (log ϵ 4.07); 324 (log ϵ 4.14); 340 (sh) (log ϵ 3.97) (MeOH).

Fukai, T. *et al., Phytochemistry*, 1996, **43**, 1119-1124 (*isol, uv, pmr, cmr, ms*)

Kanzonol F K-6

[152511-44-9]



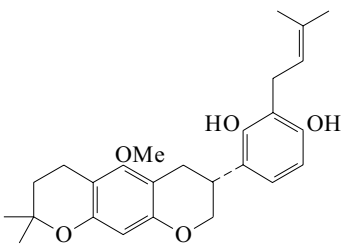
$C_{26}H_{28}O_5$ 420.504

Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. powder. $[\alpha]_D$ -119 (c, 0.035 in MeOH).

Fukai, T. *et al., Heterocycles*, 1993, **36**, 2565 (*isol, pmr, cmr*)

Kanzonol H K-7

[152511-46-1]



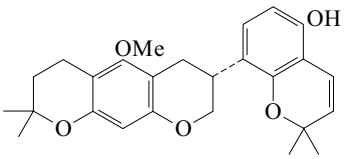
$C_{26}H_{32}O_5$ 424.536

Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Fine prisms (C_6H_6). Mp 198-199°. $[\alpha]_D$ +5 (c, 0.11 in MeOH).

Fukai, T. *et al., Heterocycles*, 1993, **36**, 2565 (*isol, pmr, cmr*)

Kanzonol J K-8

[152511-47-2]



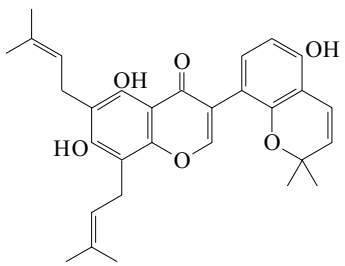
$C_{26}H_{30}O_5$ 422.52

Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow oil. $[\alpha]_D$ +30 (c, 0.06 in MeOH).

Fukai, T. *et al., Heterocycles*, 1993, **36**, 2565 (*isol, pmr, cmr*)

Kanzonol L K-9

[156281-31-1]



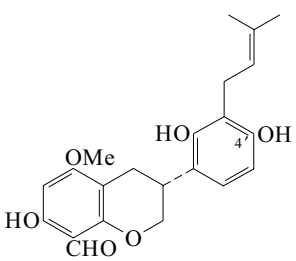
$C_{30}H_{32}O_6$ 488.579

Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow oil. λ_{max} 220 (ϵ 22390); 269 (ϵ 15850); 310 (sh) (ϵ 6170); 340 (sh) (ϵ 2690) (MeOH).

Fukai, T. *et al., Phytochemistry*, 1994, **36**, 225 (*isol, uv, pmr, ms*)

Kanzonol N K-10

[156250-71-4]



$C_{22}H_{24}O_6$ 384.428

Constit. of the roots of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. powder. $[\alpha]_D$ -9 (c, 0.01 in MeOH). λ_{max} 216 ; 291 ; 350 (sh) (EtOH).

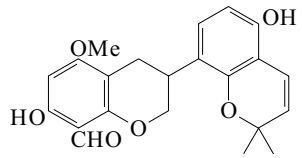
4′-Me ether: [156250-70-3] ***Kanzonol M***
$C_{23}H_{26}O_6$ 398.455
Constit. of the roots of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow

prisms (C_6H_6/Me_2CO). Mp 109-116°. Racemic λ_{max} 296 ; 345 (sh) (EtOH).

Fukai, T. *et al., Heterocycles*, 1994, **38**, 1089 (*isol, uv, pmr, cmr, ms*)

Kanzonol O K-11

[156250-69-0]



$C_{22}H_{22}O_6$ 382.412

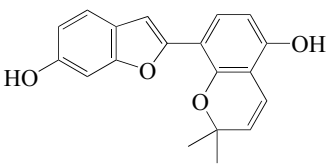
Constit. of the roots of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. powder. $[\alpha]_D$ -10 (c, 0.01 in MeOH). λ_{max} 225 (ϵ 93325); 292 (ϵ 56234); 342 (sh) (ϵ 8320) (MeOH).

Fukai, T. *et al., Heterocycles*, 1994, **38**, 1089 (*isol, uv, ms, cd, pmr, cmr*)

Kanzonol U K-12

[178330-48-8]

*8-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, 9CI. Glabrocoumarone A*



$C_{19}H_{16}O_4$ 308.333

Constit. of *Glycyrrhiza glabra* (licorice). Amorph. powder or needles (MeOH aq.). Mp 192-194°. λ_{max} 205 (log ϵ 4.44); 230 (sh) (log ϵ 4.16); 248 (log ϵ 4.1); 270 (log ϵ 4.32); 281 (log ϵ 4.38); 292 (log ϵ 4.35); 317 (log ϵ 4.45); 350 (sh) (log ϵ 4.02) (MeOH).

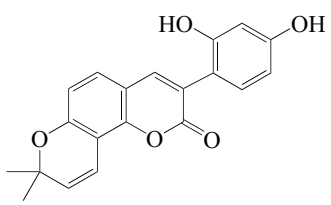
Kinoshita, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1218 (*isol, uv, ir, pmr, cmr*)

Fukai, T. *et al., Phytochemistry*, 1996, **43**, 1119-1124 (*isol, uv, pmr, cmr, ms*)

Kanzonol W K-13

[184584-82-5]

*3-(2,4-Dihydroxyphenyl)-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b′*]dipyran-2-one, 9CI*



$C_{20}H_{16}O_5$ 336.343

Constit. of *Glycyrrhiza glabra* (licorice) roots. Pale yellow needles (C_6H_6) or amorph. powder. Mp 110-112° dec. λ_{max} 220 (log ϵ 4.13); 258 (sh) (log ϵ 3.87); 285 (log ϵ 3.82); 351 (log ϵ 3.91) (MeOH).

*4′-Me ether:3-(2-Hydroxy-4-methoxyphenyl)-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b′*]dipyran-2-one, 9CI.* ***4′-O-Methylkanzonol W***

$C_{21}H_{18}O_5$ 350.37

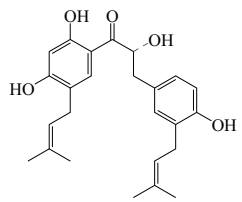
Constit. of *Glycyrrhiza glabra* (licorice). Pale yellow needles (C_6H_6/hexane). Mp 199-200°. λ_{max} 239 (log ϵ 4.38); 256 (sh) (log ϵ 4.15); 290 (log ϵ 4.08); 349 (log ϵ 4.27) (MeOH).

Fukai, T. *et al., Phytochemistry*, 1996, **43**, 1119-1124 (*isol, uv, pmr, cmr, ms*)

Kinoshita, T. *et al., Nat. Prod. Lett.*, 1997, **9**, 289-296 (*4′-O-Methylkanzonol W*)

Kanzonol Y K-14

2-Hydroxy-1-[2,4-dihydroxy-5-(3-methyl-2-butenyl)phenyl]-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-1-propanone. α,2′,4,4′-Tetrahydroxy-3,5′-diprenyldihydrochalcone



Absolute Configuration

$C_{25}H_{30}O_5$ 410.509

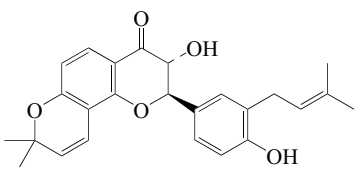
λ_{max} 216 (log ϵ 4.34); 283 (log ϵ 4.12); 329 (log ϵ 3.83) (MeOH).

(R)-form [184584-87-0]

Constit. of *Glycyrrhiza glabra* (licorice). Amorph. powder.

Fukai, T. *et al., Phytochemistry*, 1996, **43**, 1119-1124; 1998, **49**, 2005-2013 (*isol, uv, cd, pmr, cmr, ms, abs config*)

Kanzonol Z K-15



Absolute Configuration

$C_{25}H_{26}O_5$ 406.477

Constit. of *Glycyrrhiza glabra* (licorice). Mp 141-145.5°. $[\alpha]_D^{24}$ -17 (c, 0.06 in MeOH). λ_{max} 206 (log ϵ 4.29); 233 (log ϵ 4.11); 251 (log ϵ 4.1); 268 (log ϵ 4.13); 310 (sh) (log ϵ 3.6) (MeOH).

Fukai, T. *et al., Phytochemistry*, 1998, **49**, 2005-2013 (*isol, uv, cd, pmr, cmr, ms*)

Kapporphin K-16

[112771-37-6]

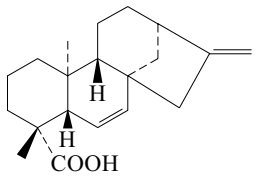
H-Tyr-Ser-Phe-Gly-Gly-OH

$C_{25}H_{31}N_5O_8$ 529.549

Derived from the kappa-chain of immunoglobulin.

Kharchenko, E.P. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1987, **297**, 740 (*isol, struct*)

6,16-Kauradien-19-oic acid K-17



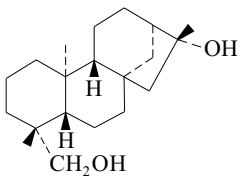
$C_{20}H_{28}O_2$ 300.44

ent-form [77280-78-5]

Prod. by seed extracts of *Cucurbita maxima*.

Hedden, P. *et al., Phytochemistry*, 1981, **20**, 1011

16,19-Kauranediol K-18



$C_{20}H_{34}O_2$ 306.487

(ent-16βOH)-form [70901-55-2]

Plates (C_6H_6). Mp 200-201°. $[\alpha]_D^{22}$ -40.5 (c, 0.4 in EtOH).

19-O-β-D-Glucopyranoside:

$C_{26}H_{44}O_7$ 468.629

Needles. Mp 237-238°. $[\alpha]_D^{22}$ -64 (c, 0.35 in Py).

19-Ac: [30320-70-8]

$C_{22}H_{36}O_3$ 348.525

Isol. from sunflowers.

Di-Ac: [250368-26-4]

$C_{24}H_{38}O_4$ 390.562

Powder. Mp 112-114°. $[\alpha]_D$ -52.5 (c, 0.55 in $CHCl_3$).

19-Aldehyde: [22376-05-2] **ent-*16β-Hydroxy-19-kauranal***

$C_{20}H_{32}O_2$ 304.472

Cryst. (EtOAc/hexane). Mp 169-173°. $[\alpha]_D^{22}$ -68 (c, 0.6 in Me_2CO).

19-Carboxylic acid: [22376-06-3] **ent-*16β-Hydroxy-19-kauranoic acid***

$C_{20}H_{32}O_3$ 320.471

Cryst. Mp 276-278°. $[\alpha]_D$ -117 (c, 0.5 in Py).

19-Carboxylic acid, 16-Me ether: [38308-35-9] **ent-*16β-Methoxy-19-kauranoic acid***

$C_{21}H_{34}O_3$ 334.498

Constit. of *Annona glabra* (pond apple). Powder. Mp 216-219°. $[\alpha]_D^{25}$ -115.1 (c, 0.16 in $CHCl_3$).

Henrick, C.A. *et al., Aust. J. Chem.*, 1964, **17**, 915

Serebryakov, E.P. *et al., Chem. Ind. (London)*, 1968, 1770 (*acid*)

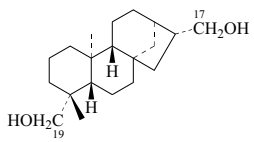
Ekong, D.E.U. *et al., Phytochemistry*, 1969, **8**, 1053 (*isol*)

Pakrashi, S.C. *et al., Indian J. Chem.*, 1970, **8**, 569 (*acid*)

Kalinovskii, A.I. *et al., Org. Mass Spectrom.*, 1970, **3**, 1393 (*ms*)

Serebryakov, E.P. *et al., Tetrahedron*, 1970, **26**, 5215 (*aldehyde*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 2317 (*acetate*)
Satake, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3865
Correa, M.S. *et al., Fitoterapia*, 1998, **69**, 275-276 (*cmr*)
Arriaga-Giner, F.J. *et al., Z. Naturforsch., C*, 1999, **54**, 602-604 (*di-Ac*)
Chen, C.-Y. *et al., J. Nat. Prod.*, 2000, **63**, 1000-1003 (*16-Methoxy-19-kauranoic acid*)

17,19-Kauranediol K-19



(*ent*-16β)-*form*

$C_{20}H_{34}O_2$ 306.487

(*ent*-16β)-*form* [74365-75-6]
Needles (C_6H_6). Mp 180-181°. $[\alpha]_D$ -66 (c, 1.8 in EtOAc).

19-Aldehyde: [41756-43-8] **ent-*17-Hydroxy-16β-kauran-19-al***
$C_{20}H_{32}O_2$ 304.472
Isol. from *Annona squamosa* (sugar apple). Cryst. (Et_2O/petrol). Mp 148°. $[\alpha]_D^{24}$ -45.4 (c, 2.2 in $CHCl_3$).

19-Aldehyde, 17-Ac: [41756-46-1]
$C_{22}H_{34}O_3$ 346.509
Isol. from *Annona squamosa* (sugar apple). Oil.

(*ent*-16α)-*form*

17-Carboxylic acid: [106454-60-8] ent-*19-Hydroxy-16α-kauran-17-oic acid.* ***Annoglabasin E***
$C_{20}H_{32}O_3$ 320.471
Constit. of *Annona glabra* (pond apple). Powder. Mp 206-207°. $[\alpha]_D^{25}$ -53.6 (c, 0.05 in $CHCl_3$/MeOH).

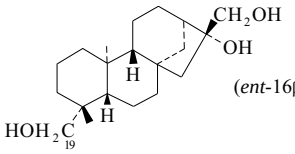
17-Carboxylic acid, 19-Ac: [205312-86-3] ent-*19-Acetoxy-16α-kauran-17-carboxylic acid.* ***Annoglabasin B***
$C_{22}H_{34}O_4$ 362.508
Constit. of *Annona glabra* (pond apple). Needles (MeOH). Mp 106-108°. $[\alpha]_D^{24}$ -41.3 (c, 0.6 in $CHCl_3$).

Dicarboxylic acid, di-Me ester: ***Dimethyl* ent-*16α-kaurane-17,19-dioate***
$C_{22}H_{34}O_4$ 362.508
Constit. of *Annona glabra* (pond apple). Powder. Mp 165-166°. $[\alpha]_D^{25}$ -208.2 (c, 0.15 in $CHCl_3$).

[60761-79-7, 65760-38-5]

Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 841 (*19-aldehyde*)
Kim, Y.-H. *et al., Phytochemistry*, 1995, **39**, 449 (*carboxylic acid esters*)
Chang, F.-R. *et al., J.O.C.*, 1998, **61**, 437-439 (*Annoglabasin B*)
Chen, C.-Y. *et al., J. Nat. Prod.*, 2000, **63**, 1000-1003 (*Annona glabra constit*)

16,17,19-Kauranetriol K-20



(*ent*-16β*OH*)-*form*

$C_{20}H_{34}O_3$ 322.487

(*ent*-16β*OH*)-*form* [58648-76-3]
Cryst. (EtOAc). Mp 224-226°. $[\alpha]_D$ -38 (c, 3 in EtOH).

17-Carboxylic acid, 19-aldehyde, 16-Ac, Me ester: [288627-10-1] ***Annoglabasin D***
$C_{23}H_{34}O_5$ 390.519
Constit. of *Annona glabra* (pond apple). Powder. Mp 138-140°. $[\alpha]_D^{25}$ -68.3 (c, 0.09 in $CHCl_3$).

17,19-Dicarboxylic acid, 16-Ac, 17-Me ester: [288627-09-8] ***Annoglabasin C***
$C_{23}H_{34}O_6$ 406.518
Constit. of *Annona glabra* (pond apple). Powder. Mp 215-217°. $[\alpha]_D^{25}$ -141 (c, 0.18 in $CHCl_3$).

(*ent*-16α*OH*)-*form*

17,19-Di-Ac: [218281-62-0] ***Annocherin A***
$C_{24}H_{38}O_5$ 406.561
Constit. of *Annona cherimola* (cherimoya). Oil. $[\alpha]_D^{24}$ -34 (c, 0.1 in $CHCl_3$). λ_{max} 211 (log ϵ 4.01) (MeOH).

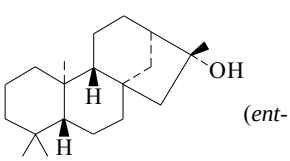
19-Aldehyde, 17-Ac: [177742-55-1] ***Annosquamosin A***
$C_{22}H_{34}O_4$ 362.508
Constit. of *Annona squamosa* (sugar apple). Needles (MeOH). Mp 162-164°. $[\alpha]_D^{24}$ -64 (c, 0.2 in $CHCl_3$).

17-Carboxylic acid, 19-aldehyde, 16-Ac, Me ester: [205312-85-2] *Methyl* ent-*16α-acetoxy-19-oxo-17-kauranoate.* ***Annoglabasin A***
$C_{23}H_{34}O_5$ 390.519
Constit. of *Annona glabra* (pond apple). Amorph. powder. Mp 138-140°. $[\alpha]_D^{24}$ -74.8 (c, 0.22 in $CHCl_3$).

[20547-77-7]

Wu, Y.-C. *et al., J. Nat. Prod.*, 1996, **59**, 635-637 (*Annosquamosin A, cmr*)
Chen, C.-Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 1998, **45**, 629-634 (*Annocherin A*)
Chang, F.-R. *et al., J. Nat. Prod.*, 1998, **61**, 437-439 (*Annoglabasin A*)
Chen, C.-Y. *et al., J. Nat. Prod.*, 2000, **63**, 1000-1003 (*Annoglabasins*)

16-Kauranol K-21



(*ent*-16β)-*form*

$C_{20}H_{34}O$ 290.488

(*ent*-16β)-*form* [5524-17-4]
Kauranol. *α-Kaurene. γ-Podocarprene. Ceruchinol. β-Cryptomerene. Ceruchdiol*
Cryst. (hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 214-215°. $[\alpha]_D$ -45 (c, 0.9 in $CHCl_3$).

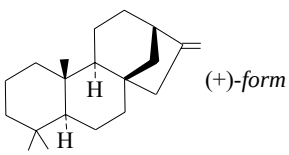
(*ent*-5β,16β)-*form* [63902-40-9] No details. Unprecedented 5-config. May be a drawing error.

(*ent*-16α)-*form* [5354-44-9]
Isol. from sunflowers. Mp 210-211°.

Uchida, S. *et al., J.A.C.S.*, 1916, **38**, 687 (*isol*)
Briggs, L.H. *et al., J.C.S.*, 1950, 955; 1963, 1345 (*isol*)
Huneck, S. *et al., Z. Naturforsch., B*, 1965, **20**, 611; 1966, **21**, 713; 1970, **25**, 227 (*isol*)
Kalinovskii, A.I. *et al., Org. Mass Spectrom.*, 1970, **3**, 1393 (*ms*)
Nilsson, E. *et al., Acta Chem. Scand.*, 1971, **25**, 1486 (*isol*)
Huneck, S. *et al., Phytochemistry*, 1972, **11**, 2429 (*biochem*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 487 (*ent-5β,16β-form*)
Le Quesne, P.W. *et al., Phytochemistry*, 1985, **24**, 1785 (*isol*)
Fraga, B.M. *et al., Phytochemistry*, 1987, **26**, 775 (*cmr*)

16-Kaurene K-22

Kaurene. *Podocarprene*



(+)-*form*

$C_{20}H_{32}$ 272.473

(+)-*form* [10178-84-4]
Cryst. (MeOH). Mp 49°. $[\alpha]_D$ +74 (c, 2.8 in $CHCl_3$).

(-)-*form* [562-28-7]
ent-*form.* α-*Podocarprene.* α-*Podocarpene*
Constit. of *Hordeum vulgare* (barley) and others. Mp 50°. $[\alpha]_D$ -80 (c, 1.0 in $CHCl_3$).

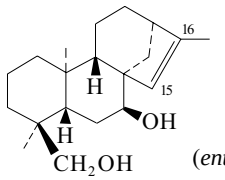
16,17-Epoxide: See 16,17-Epoxykaurane in *The Combined Chemical Dictionary.*

(±)-*form*
Mp 44-47°. $Bp_{0.02}$ 120°.

[469-86-3, 13850-19-6, 34424-57-2, 87759-99-7]

Briggs, L.H. *et al., J.C.S.*, 1963, 1345 (*isol, struct*)
Cross, B.E. *et al., J.C.S.*, 1963, 2937 (*isol, struct*)
Bell, R.A. *et al., J.O.C.*, 1966, **31**, 2530 (*synth*)
Gonzalez, R.B. *et al., An. Quim.*, 1971, **67**, 59 (*ms*)
Tahara, A. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2329 (*synth*)
Hanson, J.R. *et al., J.C.S. Perkin 1*, 1976, 114 (*cmr*)
Overton, K.H. *et al., Prog. Chem. Org. Nat. Prod.*, 1977, **34**, 249 (*biosynth, rev*)
Coates, R.M. *et al., J.A.C.S.*, 1980, **102**, 6358 (*biosynth*)
Hogg, R.W. *et al., Aust. J. Chem.*, 1987, **40**, 469 (*synth*)

15-Kaurene-7,18-diol K-23



(*ent*-7α)-*form*

$C_{20}H_{32}O_2$ 304.472

(*ent*-7α)-*form* [19891-25-9]
Sideridiol
Constit. of *Sideritis* spp.. Cryst. (MeOH aq.). Mp 196-197°. $[\alpha]_D^{20}$ +19 (c, 0.87 in EtOH).

7-Ac: [19885-22-4] ***Siderol***
$C_{22}H_{34}O_3$ 346.509
Constit. of *Sideritis* spp.. Cryst. (petrol). Mp 152-153°. $[\alpha]_D^{20}$ +43 (c, 1.96 in EtOH).

18-Ac: [68349-18-8] ***Sideripol***
$C_{22}H_{34}O_3$ 346.509
Cryst. (petrol). Mp 121-122°.

Di-Ac:
Cryst. (EtOH aq.). Mp 128-129°. $[\alpha]_D^{20}$ +25 (c, 0.66 in $CHCl_3$).

15α,16α-Epoxide: [22338-60-9] ent-*15β,16β-Epoxy-7α,18-kauranediol.*
Sideroxol
$C_{20}H_{32}O_3$ 320.471
Cryst. Mp 245-246°.

15α,16α-Epoxide, 7-Ac: [22338-62-1]
Epoxysiderol
$C_{22}H_{34}O_4$ 362.508
Isol. from *Sideritis* spp..

7-Ketone: [89686-82-8] ent-*18-Hydroxy-15-kauren-7-one.* ***Siderone***
$C_{20}H_{30}O_2$ 302.456
Isol. from *Sideritis syriaca* (Greek mountain tea). Needles (EtOAc). Mp 134-135°.

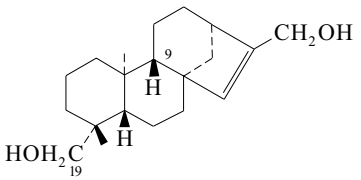
(*ent*-7β)-*form*

15α,16α-Epoxide: [87376-64-5] ent-*15β,16β-Epoxy-7β,18-kauranediol.*
Ucriol
$C_{20}H_{32}O_3$ 320.471
Isol. from *Sideritis syriaca* (Greek mountain tea). Cryst. (EtOAc). Mp 185-186°.

[22338-62-1]

Piozzi, F. *et al., Ric. Sci.*, 1968, **38**, 462 (*Sideroxol*)
Piozzi, F. *et al., Tetrahedron*, 1968, **24**, 4073 (*Sideridiol, Siderol*)
Piozzi, F. *et al., J.C.S. Perkin 1*, 1973, 1164 (*synth*)
Venturella, P. *et al., Fitoterapia*, 1977, **48**, 3 (*Epoxysiderol*)
Venturella, P. *et al., Phytochemistry*, 1978, **17**, 811 (*Sideripol*)
Venturella, P. *et al., Phytochemistry*, 1983, **22**, 600; 2537 (*Ucriol, Siderone*)

15-Kaurene-17,19-diol K-24



$C_{20}H_{32}O_2$ 304.472

***ent*-form** [41473-26-1]
Cryst. Mp 193-195°. $[\alpha]_D$ -37 (EtOH).

19-[3-(4-Hydroxyphenyl)propanoyl]:
[80368-60-1]
$C_{29}H_{40}O_4$ 452.633
Gum. Mp 55° (as diacetate). $[\alpha]_D^{24}$ -13 (c, 0.84 in $CHCl_3$) (diacetate).

19-Carboxylic acid: [35030-38-7] **ent-*17-Hydroxy-15-kauren-19-oic acid***
$C_{20}H_{30}O_3$ 318.455
Isol. from *Aralia cordata* (udo). Cryst. Mp 193-194°. $[\alpha]_D$ -60 (c, 0.3 in MeOH).

19-Carboxylic acid, 15α,16α-epoxide: [93888-88-1]

[88664-27-1] **ent-*15β,16β-Epoxy-17-hydroxy-19-kauranoic acid***
$C_{20}H_{30}O_4$ 334.455
Cryst. (EtOAc/hexane) (as Me ester). Mp 177-179° (Me ester).

19-Carboxylic acid, 17-aldehyde: [77887-58-2] **ent-*17-Oxo-15-kauren-19-oic acid***
$C_{20}H_{28}O_3$ 316.439
Constit. of *Helianthus* spp.. Pale yellow gum. $[\alpha]_D$ -21.9 (c, 1.2 in $CHCl_3$).

17,19-Dicarboxylic acid: [88664-29-3] **ent-*15-Kaurene-17,19-dioic acid***
$C_{20}H_{28}O_4$ 332.439
Isol. from *Helianthus* spp.. Gum (as Me ester).

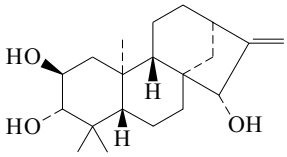
(*ent*-9β)-*form*

19-Carboxylic acid: [74311-12-9] **ent-*17-Hydroxyisokaur-15-en-19-oic acid***
$C_{20}H_{30}O_3$ 318.455
Oil (as Me ester). $[\alpha]_D^{24}$ -40.6 (Me ester). The name isokaurenoic is used to denote the unusual 9-config..

[77887-57-1]

Lloyd, H.A. *et al., Tet. Lett.*, 1967, 4891
Ali, E. *et al., Indian J. Chem.*, 1971, **9**, 1166 (*isol, acid*)
Yahara, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1629 (*isol, acid*)
Misra, R. *et al., Tetrahedron*, 1979, **35**, 985; 2301 (*abs config, isol*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 267; 2399; 1981, **20**, 1907 (*isol*)
Herz, W. *et al., Phytochemistry*, 1983, **22**, 2021 (*epoxide, diacid*)
Harrigan, G.G. *et al., Phytochemistry*, 1994, **36**, 109 (*isol, pmr, cmr*)
Piacenta, S. *et al., Phytochemistry*, 1994, **36**, 991 (*cmr*)
Correa, M.S. *et al., Fitoterapia*, 1998, **69**, 275-276 (*cmr*)

16-Kaurene-2,3,15-triol K-25

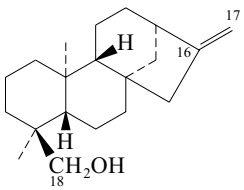


$C_{20}H_{32}O_3$ 320.471

(*ent*-2α,3β,15β)-*form* [140636-09-5]
Isol. from leaves of a blight-resistant rice cultivar. Powder. Mp 191-192°. $[\alpha]_D^{22}$ -19 (c, 0.18 in MeOH).

Watanabe, M. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 113 (*isol, pmr, cmr*)

16-Kauren-18-ol K-26



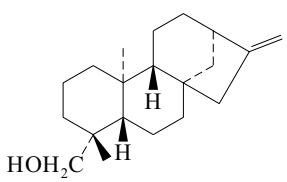
$C_{20}H_{32}O$ 288.472

***ent*-form** [17360-30-4]
Candol B
Constit. of barley. Cryst. Mp 107-108°. $[\alpha]_D$ -75 (c, 1 in $CHCl_3$).

[2300-11-0, 24739-14-8, 33426-17-4]

González, A.G. *et al., Phytochemistry*, 1973, **12**, 2721; 1981, **20**, 846 (*isol, cmr*)
Castro, V. *et al., Phytochemistry*, 1985, **24**, 2450 (*isol*)

16-Kauren-19-ol K-27



$C_{20}H_{32}O$ 288.472

***ent*-form** [2300-11-0]
Constit. of root of *Annona squamosa* (sugar apple). Cryst. (MeOH aq.). Mp 141-142°. $[\alpha]_D$ -75 (c, 2.76 in $CHCl_3$).

Ac: [41756-45-0]
$C_{22}H_{34}O_2$ 330.509
Constit. of *Annona squamosa* (sugar apple). Cryst. (MeOH) or gum. Mp 117-118°. $[\alpha]_D$ -74 (c, 2.3 in $CHCl_3$).

19-Aldehyde: [14046-84-5] **ent-*16-Kauren-19-al***
$C_{20}H_{30}O$ 286.456
Constit. of the root of *Annona squamosa* (sugar apple). Cryst. (petrol). Mp 113-116°. $[\alpha]_D^{24}$ -84.2 (c, 1.05 in $CHCl_3$).

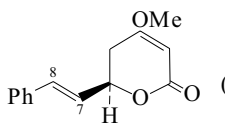
19-Carboxylic acid, Me ester: [41473-15-8]
$C_{21}H_{32}O_2$ 316.483
Isol. from *Helianthus annuus* (sunflower). Cryst. (MeOH). Mp 88-89°. $[\alpha]_D$ -107 (c, 3.2 in $CHCl_3$).

[5095-09-0, 10438-44-5]

Henrick, C.A. *et al., Aust. J. Chem.*, 1964, **17**, 915-933 (*synth*)
Mori, K. *et al., Tetrahedron*, 1968, **24**, 3095-3111 (*synth*)
Kalinowskii, A.I. *et al., Khim. Prir. Soedin.*, 1971, **7**, 281-286; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 269-273 (*acid, ms*)
Piozzi, F. *et al., Phytochemistry*, 1971, **10**, 1164-1166 (*aldehyde, isol*)
Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 841-844 (*isol*)
Yamasaki, K. *et al., Tet. Lett.*, 1976, 1005-1008 (*cmr*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 107-110; 267-271; 2399-2403; 1981, **20**, 1899-1902; 1907-1913; 1982, **21**, 399-403 (*epoxide 19-angeloyl, O-3-(4-hydroxyphenyl)propanoyl, epoxide, aldehyde epoxide, acid epoxide, acid 2-hydroxyethyl ester*)
Brassy, C. *et al., Acta Cryst. C*, 1988, **44**, 528-531 (*acid, cryst struct*)
Mukhopadhyay, G. *et al., Fitoterapia*, 1993, **64**, 7-10 (*acid, pmr, cmr, cryst struct*)
Lu, T. *et al., Phytochemistry*, 1995, **38**, 451-456 (*acid, cmr*)
Wu, Y.-C. *et al., J. Nat. Prod.*, 1996, **59**, 635-637 (*cmr*)
Da Costa, F.B. *et al., Fitoterapia*, 1998, **69**, 86-87 (*activity*)
Gutierrez, S.R. *et al., Rev. Latinoam. Quim.*, 1998, **26**, 71-74 (*isol, activity*)
Batista, R. *et al., Planta Med.*, 1999, **65**, 783-784 (*isol, activity*)
Toyota, M. *et al., J.O.C.*, 2000, **65**, 4565-4570 (*synth*)

Kawain K-28

*5,6-Dihydro-4-methoxy-6-(2-phenylethenyl)-2*H*-pyran-2-one, 9CI. Kavain*



(*R*)-*form*

$C_{14}H_{14}O_3$ 230.263Log P 1.85 (calc).

(*R*)-*form* [500-64-1]
Found in the roots of kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Prisms (Et_2O/MeOH). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. Mp 106° (110°). $Bp_{0.1}$ 195-197°. $[\alpha]_D^{20}$ +105 (EtOH). λ_{max} 245 (ϵ 25500) (EtOH) (Berdy).
► LD_{50} (mus, orl) 1130 mg/kg. UQ0518000

7,8-Dihydro: [587-63-3] ***Marindinin***. *Dihydrokawain*
$C_{14}H_{16}O_3$ 232.279
Found in the roots of kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Prisms (Et_2O/petrol). Mp 56-60°. $[\alpha]_D^{19}$ +30 (EtOH). Log P 2.15 (calc). Has (*S*)-config. (change of Cahn-Ingold-Prelog priorities).
► LD_{50} (mus, orl) 920 mg/kg. UQ0517700

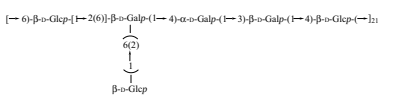
(±)-*form* [3155-48-4]
Cryst. (EtOAc/petrol, THF or Et_2O/MeOH). Mp 146-147°.

7,8-Dihydro: [3384-26-7]
Needles (CCl_4). Mp 73-74°.

[19451-52-6, 19902-90-0, 24576-85-0, 73536-68-2]

Borsche, W. *et al., Ber.*, 1930, **63**, 2414 (*isol*)
van Veen, A.G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1939, **58**, 521 (*Marindinin*)
Haensel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1968, **301**, 369 (*isol, synth, deriv*)
Snatzke, G. *et al., Tet. Lett.*, 1968, 1797 (*abs config*)
Dutta, C.P. *et al., Phytochemistry*, 1972, **11**, 2891 (*isol, ms, pmr*)
Yoshino, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1972, **136**, 66 (*cryst struct*)
Engel, P. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1972, **136**, 453 (*cryst struct, deriv*)
Franca, N.C. *et al., Phytochemistry*, 1973, **12**, 1182-1184 (*isol, deriv*)
Kimura, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 875 (*ir, pmr*)
Achenbach, H. *et al., Chem. Ber.*, 1974, **107**, 735 (*abs config*)
Izawa, T. *et al., Chem. Lett.*, 1975, 161 (*synth*)
Achenbach, H. *et al., Org. Mass Spectrom.*, 1975, **10**, 850 (*ms*)
Reffstrup, T. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 613 (*pmr*)
Israili, Z.H. *et al., J.O.C.*, 1976, **41**, 4070 (*synth*)
Moeller, J. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 671 (*ms*)
Castellino, S. *et al., Tet. Lett.*, 1984, **25**, 4059 (*synth*)
Spino, C. *et al., Tet. Lett.*, 1996, **37**, 6503 (*synth, deriv*)
Ranjith, H. *et al., Phytochemistry*, 2002, **59**, 429-433 (*isol, pmr, cmr, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DLR000; GJI250

Kefiran K-29



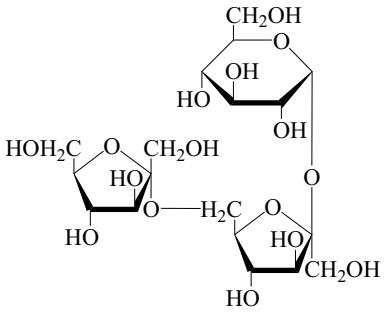
Conts. an equal proportion of galactose and glucose residues. Mol. wt. of 20600 (average of 1127 hexose units). Isol. from Kefir grains, the inoculating material used for conversion of milk into the Russian beverage Kefir. Kefir grains consist of yeast and bacteria, predominantly *Saccharomyces delbruckii* and *Lactobacillus brevis*. About 25% of the dry material consists of the capsular polysaccharide of *Lactobacillus brevis*. Sol. H_2O. $[\alpha]_D$ +68 (c, 1.0 in H_2O).

*Poly(*O*-Me):*
Syrup. $[\alpha]_D$ +18 ($CHCl_3$).

Kooiman, P. *et al., Carbohydr. Res.*, 1968, **7**, 200

Kelose K-30

[138809-76-4]
O-α-D-*Fructofuranosyl-(2→6)-β-D-fructofuranosyl-α-D-glucopyranoside, 9CI*

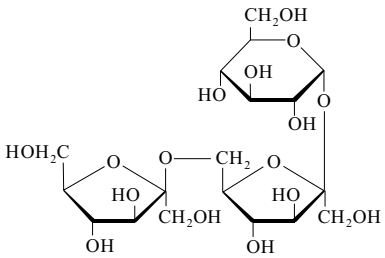


$C_{18}H_{32}O_{16}$ 504.441
Constit. of commercial beet syrup, *Beta vulgaris*.

Swallow, K.W. *et al., J. Agric. Food Chem.*, 1993, **41**, 1587-1592 (*isol, cmr, struct*)

6-Kestose K-31

[562-68-5]
O-β-D-*Fructofuranosyl-(2→6)-β-D-fructofuranosyl α-D-glucopyranoside, 9CI, 8CI. Kestose. 6-Kestotriose*



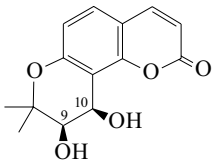
$C_{18}H_{32}O_{16}$ 504.441
A fructan. See Fructans. Widely distributed in cereals and other grasses. Also isol. from onion (*Allium cepa*). Component of Neosugar which is a mixt. with Nystose, N-159 and its 1-fructosyl deriv. used as a dietary constit. for improvement of intestinal flora. Mp 145°. $[\alpha]_D^{20}$ +27.3 (c, 2.19 in H_2O).

Undeca-Me:
$[\alpha]_D^{18}$ +25.8 (c, 4.2 in H_2O).

Albon, N. *et al., J.C.S.*, 1953, 24 (*synth, isol*)
Gross, D. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 360 (*enzymic synth*)
Hammer, H. *et al., Acta Chem. Scand.*, 1968, **22**, 197 (*occur*)
Jeffrey, G.A. *et al., Acta Cryst. B*, 1972, **28**, 257 (*cryst struct*)
Ferretti, V. *et al., Acta Cryst. C*, 1984, **40**, 531 (*cryst struct*)
Liu, J. *et al., Carbohydr. Res.*, 1991, **217**, 43 (*pmr, cmr*)
Buddington, R.K. *et al., Am. J. Clin. Nutr.*, 1996, **63**, 709-719 (*pharmacol, neosugar*)

Khellactone K-32

[518-76-3]
*9,10-Dihydro-9,10-dihydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-b:3,4-b′]dipyran-2-one, 9CI. 3′,4′-Dihydroxy-3′,4′-dihydroseselin*



(9*R*,10*R*)-*form*

$C_{14}H_{14}O_5$ 262.262

Abs. configs. given here are based on the reviews by Murray.

(9*R*,10*S*)-*form* [23458-04-0]

(-)-trans-*form*

Cryst. (Me_2CO/petrol). Mp 185-186°. $[\alpha]_D^{23}$ -6.4 (c, 0.838 in EtOH). $[\alpha]_D^{21}$ -18 (c, 0.901 in $CHCl_3$).

9-O-*(3-Methylbutanoyl):* ***Junosmarin***

$C_{19}H_{22}O_6$ 346.379

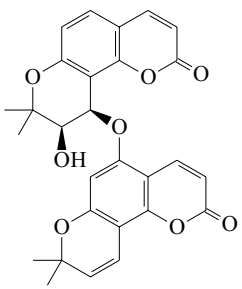
Constit. of *Citrus junos* (yuzu). Oil. $[\alpha]_D$ -16.4 ($CHCl_3$). Registered in CA as identical with Campesterol, which appears to be incorrect.

[6005-18-1, 10182-81-7, 15575-57-2, 76250-53-8]

Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, 1978, **35**, 200; 1991, **58**, 83 (*rev, bibl*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, 400 (*occur, rev*)
Ju-ichi, M. *et al., Heterocycles*, 1986, **24**, 2777 (*Junosmarin*)

Khelmarin D K-33

[175923-64-5]



Relative configuration

$C_{28}H_{24}O_8$ 488.493

Constit. of a cross hybrid of *Citrus paradisi* and *Citrus tangerina* (Rutaceae). Light yellow oil. $[\alpha]_D$ +32.7 (c, 0.2 in $CHCl_3$). λ_{max} 207 ; 220 (sh) ; 285 (sh) ; 294 ; 324 (MeOH).

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1996, **44**, 804-809 (*isol, uv, ir, pmr*)

KHR toxin K-34

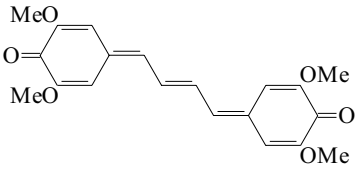
Protein; MW 20kDa. Isol. from yeast *Saccharomyces cerevisiae*.

Goto, K. *et al., Agric. Biol. Chem.*, 1990, **54**, 505 (*isol*)

Kinobeon A K-35

[155239-87-5]

4,4′-(2-Butene-1,4-diylidene)bis(2,6-dimethoxy-2,5-cyclohexadien-1-one), 9CI. 1,4-Bis(3,5-dimethoxy-4-oxo-2,5-cyclohexadienylidene)-2-butene



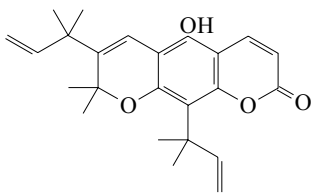
$C_{20}H_{20}O_6$ 356.374

Pigment prod. by cultures of *Carthamus tinctorius* (safflower). Red cryst. Mp 224-226°.

Wakayama, S. *et al., Z. Naturforsch., C*, 1994, **49**, 1 (*isol, uv*)

Kinocoumarin K-36

[119139-65-0]



$C_{24}H_{28}O_4$ 380.483

Constit. of *Citrus medica* (citron). Oil.

Ito, C. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3805

Kitagine K-37

$C_7H_7NO_3$ 153.137

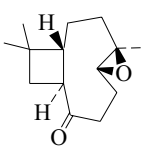
Struct. unknown. Constit. of *Canavalia ensiformis* (jack bean) seeds. Mp 240-242°. Opt. inactive.

Ackermann, D. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1939, **262**, 103 (*isol*)

Kobusone K-38

[24173-71-5]

6,7-Epoxy-15-nor-3-caryophyllanone. Caryophyllene keto epoxide



$C_{14}H_{22}O_2$ 222.327

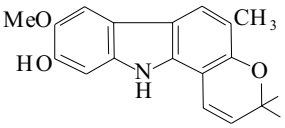
Constit. of *Cyperus rotundus* (nutgrass). Also in lavender oil. Cryst. (petrol). Mp 60-61°. $[\alpha]_D$ -142.2 (c, 3.6 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1957, 2988 (*synth*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1969, **17**, 1390 (*isol, struct*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1983, **66**, 1843 (*isol*)
Heymann, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 138 (*isol, pmr, cmr*)

Koenigine K-39

[28513-33-9]

*3,11-Dihydro-8-methoxy-3,3,5-trimethylpyrano[3,2-*a*]carbazol-9-ol, 9CI. Kenigine*



$C_{19}H_{19}NO_3$ 309.364

Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Cryst. (EtOH), needles (hexane/EtOH). Mp 183-185°.

Me ether: [24123-92-0] ***Koenigicine****. 3,11-Dihydro-8,9-dimethoxy-3,3,5-trimethylpyrano[3,2-*a*]carbazole, 9CI. Koenidine. Koenimbidine. Kenigicine. Kenidine. Kenimbidine*

$C_{20}H_{21}NO_3$ 323.391

Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Cryst. (EtOH). Mp 224-225°. Subl. at 210°/0.5 mm.

O,N-*Di-Me:*

Cryst. (EtOH). Mp 190-191°.

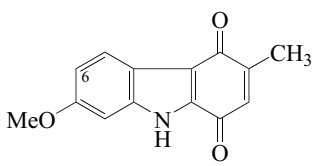
Me ether, dihydro:

Cryst. (hexane). Mp 237°.

Joshi, B.S. *et al., Tetrahedron*, 1970, **26**, 1475 (*isol, struct, uv, ir, pmr, ms*)
Narasimhan, N.S. *et al., Indian J. Chem.*, 1975, **13**, 993 (*isol, uv, ir, pmr, ms, struct, synth*)
Sharma, R.B. *et al., Experientia*, 1980, **36**, 815 (*synth, Koenigicine*)
Bowen, I.H. *et al., Phytochemistry*, 1982, **21**, 433 (*isol, ms*)

Koeniginequinone A K-40

*7-Methoxy-3-methyl-1*H*-carbazole-1,4(9*H*)-dione. 7-Methoxy-3-methyl-1,4-carbazolequinone*



$C_{14}H_{11}NO_3$ 241.246

Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Red needles (C_6H_6/petrol). Mp 240° (dec.). λ_{max} 227 (log ϵ 4.65); 260 (log ϵ 4.51); 286 (sh) (log ϵ 3.8); 387 (log ϵ 3.72) (MeOH).

*6-Methoxy:6,7-Dimethoxy-3-methyl-1*H*-carbazole-1,4(9*H*)-dione.* ***Koeniginequinone B***

$C_{15}H_{13}NO_4$ 271.272

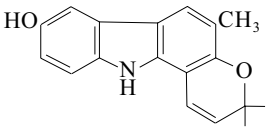
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Reddish-brown needles (C_6H_6/petrol). Mp 256° (dec.). λ_{max} 225 (log ϵ 4.61); 263 (log ϵ 4.39); 293 (sh) (log ϵ 3.21); 464 (log ϵ 3.09) (MeOH).

Saha, C. *et al., Phytochemistry*, 1998, **48**, 363-366 (*isol, synth, uv, ir, pmr*)

Koenine K-41

[28200-63-7]

*3,11-Dihydro-3,3,5-trimethylpyrano[3,2-*a*]carbazol-8-ol, 9CI. Kenine*



$C_{18}H_{17}NO_2$ 279.338
Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6). Mp 250-252°.

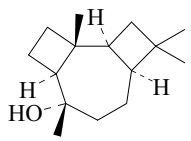
N-*Me:*
Mp 148°.

Me ether: [21087-98-9] ***Koenimbine****. 3,11-Dihydro-8-methoxy-3,3,5-trimethylpyrano[3,2-a]carbazole, 9CI. Kenimbine*
$C_{19}H_{19}NO_2$ 293.365
Alkaloid from leaves and fruits of *Murraya koenigii* (curryleaf tree). Cryst. (hexane or $CHCl_3$/hexane). Mp 194-195°.

Narasimhan, N.S. *et al., Tet. Lett.*, 1968, 5501 (*isol, uv, pmr, ms, struct*)
Kureel, S.P. *et al., Chem. Ind. (London)*, 1970, 1262 (*synth*)
Joshi, B.S. *et al., Tetrahedron*, 1970, **26**, 1475 (*isol, uv, ir, struct*)
Narasimhan, N.S. *et al., Indian J. Chem.*, 1975, **13**, 993 (*isol, uv, ir, pmr, ms, struct, synth*)
Roy, S. *et al., J. Indian Chem. Soc.*, 1981, **58**, 1212 (*isol*)

Koraiol K-42

[72188-51-3]
2,6,10,10-Tetramethyltricyclo[7.2.0.0^{2,5}]undecan-6-ol, 9CI. Korayol

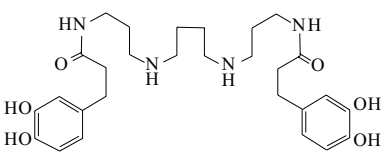


$C_{15}H_{26}O$ 222.37
Constit. of *Pinus koraiensis* (Korean pine). Cryst. (pentane/Et_2O). Mp 92.5-93°. $[\alpha]_D^{20}$ +31.7 (c, 11 in $CHCl_3$).

Khan, V.A. *et al., Khim. Prir. Soedin.*, 1979, 652-658

Kukoamine A K-43

[75288-96-9]
1,14-Bis(dihydrocaffeoyl)spermine



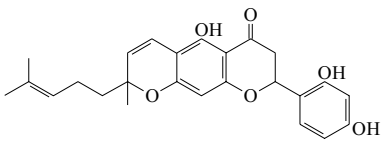
$C_{28}H_{42}N_4O_6$ 530.663
Alkaloid from the root bark of *Lycium chinense* (Chinese boxthorn). Noncryst. λ_{max} 284 (ε) (possibly MeOH, not reported) (Derep).

N^1*-De(dihydrocaffeoyl),* N^5*-dihydrocaffeoyl:* [164991-67-7] ***Kukoamine B***
$C_{28}H_{42}N_4O_6$ 530.663
Pale yellow powder.

Funayama, S. *et al., Tet. Lett.*, 1980, **21**, 1355 (*isol, uv, pmr, cmr, struct*)
Chantrapromma, K. *et al., Tet. Lett.*, 1981, **22**, 23 (*synth*)
Funayama, S. *et al., Phytochemistry*, 1995, **38**, 1529 (*Kukoamine B*)
Karigiannis, G. *et al., Tet. Lett.*, 1998, **39**, 5117-5120 (*synth*)

Kuwanol C K-44

[123702-94-3]

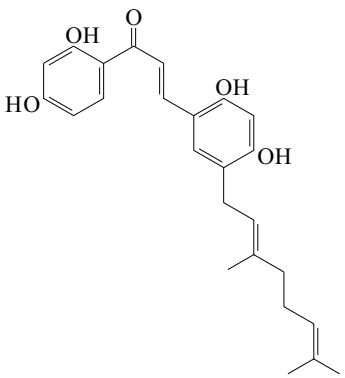


$C_{25}H_{26}O_6$ 422.477
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{22}$ -10 (c, 0.31 in EtOH).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 807

Kuwanol D K-45

[123702-93-2]
5-Geranyl-2,2′,4,4′-tetrahydroxychalcone

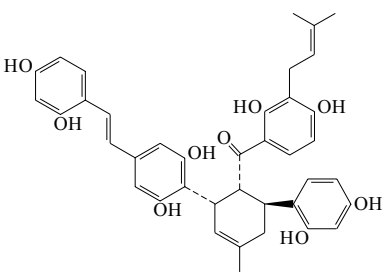


$C_{25}H_{28}O_5$ 408.493
Constit. of *Morus alba* (white mulberry). Yellow amorph. powder.

Hano, Y. *et al., Heterocycles*, 1989, **29**, 807

Kuwanol E K-46

[125850-38-6]

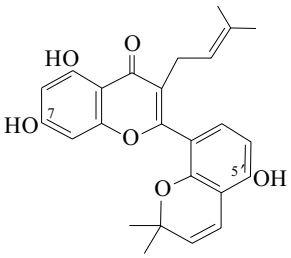


$C_{39}H_{38}O_9$ 650.724
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{20}$ +171 (c, 0.018 in EtOH).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 2035 (*isol, pmr, cmr*)

Kuwanon A K-47

[62949-77-3]
5,7-Dihydroxy-2-(5-hydroxy-2,2-dimethyl-2H-1-benzopyran-8-yl)-3-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI



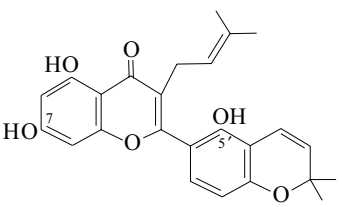
$C_{25}H_{24}O_6$ 420.461
Constit. of the root bark of *Morus alba* (white mulberry). Amorph. powder.

5′,7-Di-Ac:
Mp 167-169°.

Nomura, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 529; 1978, **26**, 1453 (*isol, ms, uv*)

Kuwanon B K-48

[62949-78-4]
5,7-Dihydroxy-2-(5-hydroxy-2,2-dimethyl-2H-1-benzopyran-6-yl)-3-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI



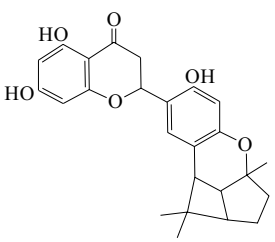
$C_{25}H_{24}O_6$ 420.461
Constit. of the root bark of *Morus alba* (white mulberry). Mp 250-254°.

5,7-Di-Ac:
Mp 125-127°.

Nomura, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 529; 1978, **26**, 1453 (*isol, uv, pmr, ir*)

Kuwanon D K-49

[67172-84-3]



Probable structure

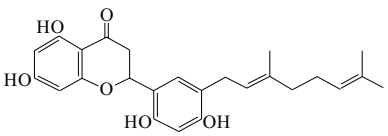
$C_{25}H_{26}O_6$ 422.477
Constit. of the root of *Morus alba* (white mulberry). Prisms (Et_2O/MeOH). Mp 230-232°. $[\alpha]_D$ 0.

Nomura, T. *et al., Heterocycles*, 1978, **9**, 745 (*isol, uv, ir, ms, pmr, cmr*)

Kuwanon E K-50

[68401-05-8]

2-[5-(3,7-Dimethyl-2,6-octadienyl)-2,4-dihydroxyphenyl]-2,3-dihydro-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. 2′,4′,5,7-Tetrahydroxy-5′-geranylflavanone



$C_{25}H_{28}O_6$ 424.493

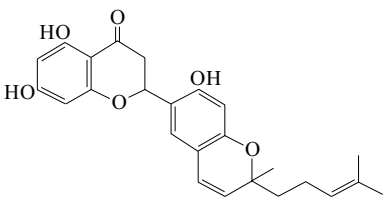
Constit. of *Morus alba* (white mulberry). Prisms (Et_2O/hexane). Mp 132-136°. $[\alpha]_D$ 0.

Nomura, T. *et al., Heterocycles*, 1978, **9**, 1295 (*isol, ms, ir, uv, pmr, cmr*)

Kuwanon F K-51

[71344-07-5]

5,7,7′-Trihydroxy-2′-methyl-2′-(4-methyl-3-pentenyl)-(2,6′-bi-2H-1-benzopyran)-4(3H)-one, 9CI



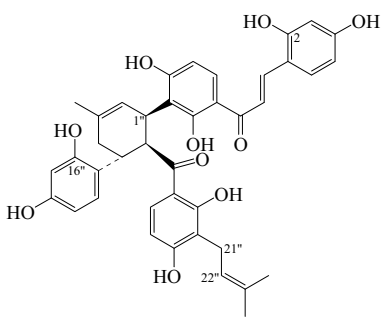
$C_{25}H_{26}O_6$ 422.477

Constit. of *Morus alba* (white mulberry). Powder. $[\alpha]_D^{20}$ +0.5 (c, 1.1 in MeOH).

Nomura, T. *et al., Heterocycles*, 1979, **12**, 943 (*uv, ms, pmr, isol*)

Kuwanon J K-52

[83709-26-6]



$C_{40}H_{38}O_{10}$ 678.734

These kuwanons are Diels-Alder products derived from natural chalcones. Metab. of tissue cultures of *Morus alba* (white mulberry). Yellow amorph. powder. Sol. MeOH, EtOAc; poorly sol. hexane, H_2O. $[\alpha]_D^{17}$ +85 (c, 0.04 in MeOH). λ_{max} 298 (ϵ 20000); 390 (ϵ 29500) (EtOH) (Berdy).

2-Deoxy: [89803-85-0] ***Kuwanon R***
$C_{40}H_{38}O_9$ 662.735
Pigment from culture cells of *Morus alba* (white mulberry). Yellow amorph. powder. $[\alpha]_D^{17}$ +56 (c, 0.165 in Me_2CO).

2-Deoxy, $\Delta^{21'',22''}$-Isomer: ***Artonin X***
$C_{40}H_{38}O_9$ 662.735
Constit. of the bark of *Artocarpus heterophyllus* (jackfruit). Yellow powder. $[\alpha]_D^{22}$ +12 (c, 0.08 in MeOH).

16″-Deoxy: [89803-86-1] ***Kuwanon Q***
$C_{40}H_{38}O_9$ 662.735
Pigment from culture cells of *Morus alba* (white mulberry). Yellow amorph. powder. $[\alpha]_D^{16}$ +160 (c, 0.081 in Me_2CO).

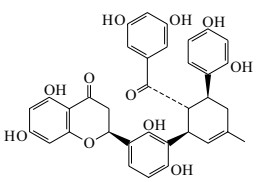
2,16″-Dideoxy: [89803-84-9] ***Kuwanon V***
$C_{40}H_{38}O_8$ 646.735
Pigment from culture cells of *Morus alba* (white mulberry). Yellow amorph. powder. $[\alpha]_D^{23}$ +145 (c, 0.11 in Me_2CO).

1″-Epimer: [81381-68-2] ***Kuwanon I***
$C_{40}H_{38}O_{10}$ 678.734
Constit. of *Morus alba* (white mulberry). Yellow powder. Sol. MeOH, DMF, EtOH; fairly sol. Me_2CO, Et_2O, EtOAc; poorly sol. H_2O, hexane, $CHCl_3$, CH_2Cl_2. $[\alpha]_D^{14}$ -454 (c, 0.035 in MeOH). λ_{max} 266 (sh) (log ϵ 4.16); 290 (log ϵ 4.33); 320 (sh) (log ϵ 4.28); 390 (log ϵ 4.47) (EtOH). λ_{max} 290 ; 390 (MeOH) (Berdy).

Ueda, S. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3042 (*isol*)
Nomura, T. *et al., Planta Med.*, 1982, **46**, 167-174 (*Kuwanon I*)
Ikuta, J. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2471 (*isol, derivs*)
Shinomiya, K. *et al., Phytochemistry*, 1995, **40**, 1317 (*Artonin X*)

Kuwanon L K-53

[88524-65-6]



Absolute configuration

$C_{35}H_{30}O_{11}$ 626.615

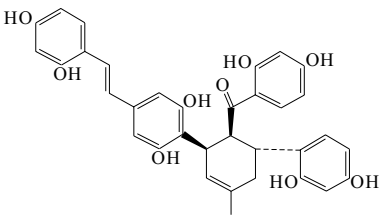
Constit. of *Morus alba* (white mulberry). Amorph. Sol. MeOH, EtOAc, Et_2O; poorly sol. H_2O, hexane. $[\alpha]_D^{22}$ -227 (c, 0.04 in MeOH). λ_{max} 286 (ϵ 23600) (MeOH) (Berdy).

2,3-Didehydro, 3-(3-methyl-2-butenyl):
[88524-66-7] ***Kuwanon K***
$C_{40}H_{36}O_{11}$ 692.718
From *Morus alba* (white mulberry). Amorph. $[\alpha]_D$ -218 (c, 0.016 in MeOH).

Nomura, T. *et al., Planta Med.*, 1983, **47**, 151 (*isol*)
Hano, Y. *et al., Heterocycles*, 1988, **27**, 75 (*abs config*)

Kuwanon Y K-54

[105016-28-2]



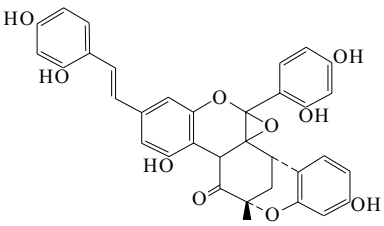
$C_{34}H_{30}O_9$ 582.606

Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{22}$ +172 (c, 0.129 in EtOH).

Hano, Y. *et al., Heterocycles*, 1986, **24**, 2603

Kuwanon Z K-55

[104931-21-7]

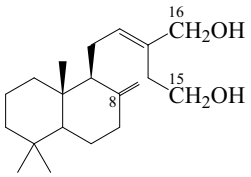


$C_{34}H_{26}O_{10}$ 594.573

Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{22}$ +40.5 (c, 0.0543 in EtOH).

Hano, Y. *et al., Heterocycles*, 1986, **24**, 2603

8(17),12-Labdadiene-15,16-diol L-1



12*E*-form

$C_{20}H_{34}O_2$ 306.487

(12*E*)-*form*

16-Aldehyde: ***15-Hydroxy-8(17),12*E*-labdadien-16-al***
$C_{20}H_{32}O_2$ 304.472
Oil. $[\alpha]_D^{20}$ +20 (c, 0.1 in $CHCl_3$).

15,16-Dialdehyde: [104263-85-6] ***8(17),12-Labdadiene-15,16-dial***
$C_{20}H_{30}O_2$ 302.456
Constit. of *Alpinia galanga* (greater galangal). Oil. $[\alpha]_D^{20}$ +16 (c, 0.23 in MeOH).

15,16-Dialdehyde, 8β,17-epoxide: [71641-23-1] *8β,17-Epoxy-12*E*-labdene-15,16-dial*. ***Aframodial***. *Miogadial*. *ZT*
$C_{20}H_{30}O_3$ 318.455
Constit. of *Zingiber officinale* (ginger). Cryst. (C_6H_6/petrol). Mp 90-92°. $[\alpha]_D$ +28.1 (c, 1.41 in $CHCl_3$).

15,16-Dialdehyde, 15-dimethyl acetal:
[284022-04-4] *15,15-Dimethoxy-8(17),12-labdadien-16-al*. ***Calcaratarin A***
$C_{22}H_{36}O_3$ 348.525
Oil. $[\alpha]_D^{21}$ +12.4 (c, 0.08 in $CHCl_3$). λ_{max} 235 (log ϵ 4.01) (MeCN).

15-Carboxylic acid, 16-aldehyde: [176050-48-9] *16-Oxo-8(17),12-labdadien-15-oic acid*. ***Zerumin A***
$C_{20}H_{30}O_3$ 318.455
Yellow oil or gum. $[\alpha]_D$ +15 (c, 0.06 in EtOH) (10.8). λ_{max} 237 (log ϵ 4.13) (MeOH).

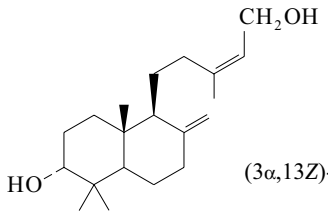
(*ent*-12*E*)-*form*

15,16-Dialdehyde: [77346-42-0]
Oil. $[\alpha]_D^{25}$ -15 (c, 0.04 in EtOH).

[84413-88-7]

Kimbu, S.F. *et al., J.C.S. Perkin 1*, 1979, 1303 (*epoxide*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3452-3454 (*Alpinia speciosa constit*)
Kim, T.H. *et al., Chem. Comm.*, 1983, 730 (*synth*)
Itokawa, H. *et al., Phytochemistry*, 1988, **27**, 435-438 (*Alpinia formosana constit*)
Firman, K. *et al., Phytochemistry*, 1988, **27**, 3887-3891 (*Curcuma heyneana constit*)
Morita, H. *et al., Planta Med.*, 1988, **54**, 117-120 (*Alpinia galanga constit, activity*)
Hokawa, H. *et al., Planta Med.*, 1988, **54**, 311-315 (*Hedychium coronaruim constit, activity*)
Singh, M. *et al., Planta Med.*, 1988, **65**, 2-8 (*review*)
Xu, H. *et al., Phytochemistry*, 1996, **42**, 149 (*Zerumin A*)
Sy, L.-K. *et al., J. Nat. Prod.*, 1997, **60**, 904-908 (*dialdehyde, pmr, cmr*)
Zhou, B.N. *et al., J. Nat. Prod.*, 1997, **60**, 1287-1293 (*16-Oxolabdadienoic acid*)
Jung, M. *et al., Tet. Lett.*, 1997, **38**, 2871 (*synth*)
Ngo, K.S. *et al., Phytochemistry*, 1998, **47**, 1117-1123 (*8,17-Epoxy-12-labdene-15,16-dial, pmr, cmr*)
Singh, M. *et al., Planta Med.*, 1999, **65**, 2-8 (*rev*)
Kong, L.-Y. *et al., J. Nat. Prod.*, 2000, **63**, 939-942 (*Calcaratarin A*)
Nyasse, B. *et al., Pharmazie*, 2000, **55**, 703-704 (*Aframodial, cmr*)
Abe, M. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 2698-2700 (*Miogadial*)

8(17),13-Labdadiene-3,15-diol L-2



(3α,13*Z*)-form

$C_{20}H_{34}O_2$ 306.487

(3α,13*Z*)-*form*

Cryst. (C_6H_6). Mp 65°.

15-Ac:
$C_{22}H_{36}O_3$ 348.525
Cryst. (C_6H_6). Mp 86°.

(3β,13*E*)-*form*

Di-O-*β*-D-*glucopyranoside:* ***Gomojoside J***
$C_{32}H_{54}O_{12}$ 630.771
Amorph. powder. $[\alpha]_D$ -56.3 (c, 0.24 in MeOH). λ_{max} 212 (ϵ 1290) (MeOH) (Berdy).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{32}H_{54}O_{11}$ 614.772
Needles (MeOH aq.). Mp 128-132°. $[\alpha]_D$ -32.1 (c, 0.15 in MeOH).

15-Carboxylic acid: [63399-38-2] *3β-Hydroxy-8(17),13*E*-labdadien-15-oic acid*. ***Alepterolic acid***
$C_{20}H_{32}O_3$ 320.471
Cryst. (Et_2O). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 157.5-158.5°. $[\alpha]_D^{20}$ +40.7 (c, 0.2 in $CHCl_3$).

15-Carboxylic acid, 3-Ac: [63399-37-1] ***3β-Acetoxy-8(17),13*E*-labdadien-15-oic acid***
$C_{22}H_{34}O_4$ 362.508
Cryst. (Et_2O/petrol). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 161-162°.

(*ent*-3β,13*E*)-*form*

Cryst. ($CHCl_3$). Mp 161-163°. $[\alpha]_D^{18}$ -29 (c, 0.56 in $CHCl_3$).

3,15-Di-O-*β*-D-*glucopyranoside:* ***Goshonoside F7***
$C_{32}H_{54}O_{12}$ 630.771
Constit. of *Rubus foliolosus* (Ceylon raspberry). Powder. $[\alpha]_D^{18}$ -47.7 (c, 0.55 in MeOH).

15-Carboxylic acid: **ent-*3β-Hydroxy-8(17),13-labdadien-15-oic acid***
$C_{20}H_{32}O_3$ 320.471

3-Ketone: **ent-*15-Hydroxy-8(17),13-labdadien-3-one***
$C_{20}H_{32}O_2$ 304.472
Needles (MeOH). Mp 110-112°. $[\alpha]_D^{19}$ -20.1 (c, 1.6 in $CHCl_3$).

(*ent*-3β,13*Z*)-*form*

15-Carboxylic acid: [74559-97-0] ent-*3β-Hydroxy-8(17),13Z-labdadien-15-oic acid*
$C_{20}H_{32}O_3$ 320.471
Oil (as Me ester). $[\alpha]_D^{24}$ -2.8 (c, 0.5 in $CHCl_3$) (Me ester).

15-Carboxylic acid, 3-ketone, 8α,17-epoxide: [74513-98-7] **ent-*8β,17-Epoxy-3-oxo-13Z-labden-15-oic acid***
$C_{20}H_{30}O_4$ 334.455
Oil (as Me ether). $[\alpha]_D$ 0 (Me ether).

(*ent*-3α,13*E*)-*form*

Cryst. Mp 162-163°. $[\alpha]_D^{25}$ -24.6 (c, 0.5 in $CHCl_3$).

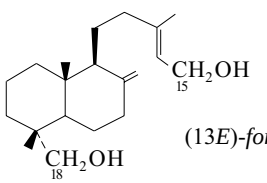
Cyclic malonyl ester: See 7,13-Corymbidienolide in *The Combined Chemical Dictionary.*

Dimeric malonyl ester: See Corymbivillosol in *The Combined Chemical Dictionary.*

[84711-18-2]

Braun, S. *et al., Tetrahedron*, 1977, **33**, 145
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1997
Wollenweber, E. *et al., Z. Naturforsch., C*, 1982, **37**, 1283 (*Alepterolic acid*)
Armstrong, R.J. *et al., Can. J. Chem.*, 1986, **64**, 584 (*synth, bibl*)
Pandita, K. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 453 (*isol*)
Dhar, K.L. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 911 (*isol, pmr, cmr*)
Ohtani, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2443 (*isol, pmr, cmr*)
Iwagawa, T. *et al., Phytochemistry*, 1992, **31**, 1311 (*Gomojoside J*)
Mizuno, R. *et al., Chem. Pharm. Bull.*, 1995, **43**, 5 (*rhamnosylglucoside, isol, pmr, cmr*)
Konishi, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 229 (*3-ketone*)
Anjaneyulu, A.S.R. *et al., Phytochemistry*, 2000, **55**, 891-901 (*pmr, cmr*)

8(17),13-Labdadiene-15,18-diol L-3



(13*E*)-form

$C_{20}H_{34}O_2$ 306.487

(13*E*)-*form* [26296-35-5]

[28644-65-7]
Kayadiol. *4-Epiagathadiol*. *4*-epi-*Agathadiol*. *Copaiferadiol*
Cryst. (Me_2CO/hexane). Mp 114.5-115.5°. $[\alpha]_D$ +45.8 (c, 1.4 in $CHCl_3$).

15,18-Dicarboxylic acid: [33123-07-8] *8(17),13-Labdadiene-15,18-dioic acid*. ***Dehydropinifolic acid***
$C_{20}H_{30}O_4$ 334.455
Constit. of *Pinus sylvestris* (Scotch pine). Cryst. (Me_2CO/diisopropyl ether). Mp 190-192°. $[\alpha]_D$ +39 (c, 1.6 in EtOH).

(*ent*-13*E*)-*form*

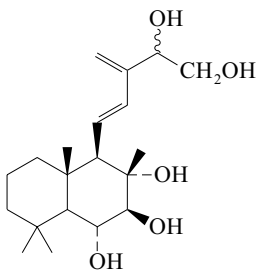
15,18-Di-O-*β*-D-*glucopyranoside:* [90851-27-7] ***Goshonoside F4***
$C_{32}H_{54}O_{12}$ 630.771
Constit. of *Rubus foliolosus* (Ceylon raspberry). Powder. $[\alpha]_D^{18}$ -45.2 (c, 1.85

in MeOH).

18-Carboxylic acid, 15,18-di-O-β-D-glucopyranoside: [90851-26-6] ***Goshonoside F3***
$C_{32}H_{52}O_{13}$ 644.755
Constit. of *Rubus foliolosus* (Ceylon raspberry). Powder. $[\alpha]_D^{18}$ -36.5 (c, 0.75 in MeOH).

Norin, T. *et al., Acta Chem. Scand.*, 1971, **25**, 607 (*Dehydropinifolic acid*)
Tanaka, T. *et al., Phytochemistry*, 1984, **23**, 615 (*Goshonosides*)

11,13(16)-Labdadiene-6,7,8,14,15-pentol L-4



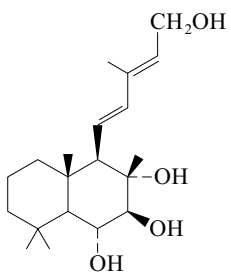
$C_{20}H_{34}O_5$ 354.486

(6α,7β,8α,11*E*,14ξ)(1)-*form* [114437-32-0] ***Sterebin G***
Constit. of *Stevia rebaudiana* (stevia). Powder. $[\alpha]_D$ -5.9 (c, 0.5 in MeOH).

(6α,7β,8α,11*E*,14ξ)(2)-*form* [114927-19-4] ***Sterebin H***
From *Stevia rebaudiana* (stevia). Powder. $[\alpha]_D$ -6.7 (c, 0.5 in MeOH). 14-Epimer of Sterebin G.

Oshima, Y. *et al., Phytochemistry*, 1988, **27**, 624

11,13-Labdadiene-6,7,8,15-tetrol L-5



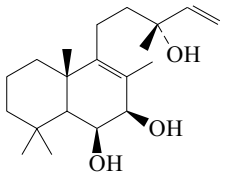
$C_{20}H_{34}O_4$ 338.486

(6α,7β,8α,11*E*,13*E*)-*form* [114343-74-7] ***Sterebin E***
Constit. of *Stevia rebaudiana* (stevia). Powder. $[\alpha]_D$ +29.9 (c, 0.17 in MeOH).

(6α,7β,8α,11*E*,13*Z*)-*form* [114489-87-1] ***Sterebin F***
Constit. of *Stevia rebaudiana* (stevia). Powder. $[\alpha]_D$ +40.3 (c, 0.16 in MeOH).

Oshima, Y. *et al., Phytochemistry*, 1988, **27**, 624

8,14-Labdadiene-6,7,13-triol L-6



$C_{20}H_{34}O_3$ 322.487

(6β,7β,13*R*)-*form*

6-Ac:
$C_{22}H_{36}O_4$ 364.524
$[\alpha]_D^{24}$ +30 (c, 4.4 in $CHCl_3$).

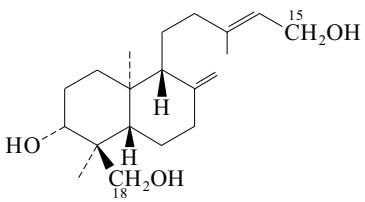
6,7-Di-Ac: [260792-29-8]
$C_{24}H_{38}O_5$ 406.561
Constit. of *Vitex agnus-castus* (agnus castus). $[\alpha]_D^{20}$ +1.1 (c, 1 in $CDCl_3$). λ_{max} 205 (log ϵ 1) (MeOH).

7-Ketone:6,13-Dihydroxy-8,14-labdadien-7-one

7-Ketone, 6-Ac:
$C_{22}H_{34}O_4$ 362.508

Zdero, C. *et al., Phytochemistry*, 1991, **30**, 3683 (*isol, pmr, cmr*)
Hoberg, E. *et al., Phytochemistry*, 1999, **52**, 1555-1558 (*di-Ac*)

8(17),13-Labdadiene-3,15,18-triol L-7



$C_{20}H_{34}O_3$ 322.487

(ent*-3β,13*E*)-*form
Cryst. ($CHCl_3$). Mp 141-143°. $[\alpha]_D^{18}$ -29 (c, 0.98 in $CHCl_3$).

15-O-β-D-Glucopyranoside: [90851-24-4] ***Goshonoside F1***
$C_{26}H_{44}O_8$ 484.629
Constit. of *Rubus foliolosus* (Ceylon raspberry). Cryst. (MeCN aq.). Mp 95-98°. $[\alpha]_D^{18}$ -55.6 (c, 1.91 in MeOH).

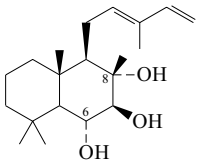
18-O-β-D-Glucopyranoside: [90851-25-5] ***Goshonoside F2***
$C_{26}H_{44}O_8$ 484.629
Constit. of *Rubus foliolosus* (Ceylon raspberry). Powder. $[\alpha]_D^{18}$ -30.4 (c, 0.96 in MeOH).

15,18-Di-O-β-D-glucopyranoside: [90851-28-8] ***Goshonoside F5***
$C_{32}H_{54}O_{13}$ 646.771
Constit. of *Rubus foliolosus* (Ceylon raspberry). Powder. $[\alpha]_D^{18}$ -45.2 (c, 1.85 in MeOH).

15-O-[α-L-Arabinofuranosyl(1→6)-β-D-glucopyranoside]: [138614-60-5] ***Goshonoside F6***
$C_{31}H_{52}O_{12}$ 616.745
Constit. of *Rubus foliolosus* (Ceylon raspberry). Powder. $[\alpha]_D^{18}$ -28.4 (c, 0.56 in MeOH).

Tanaka, T. *et al., Phytochemistry*, 1984, **23**, 615 (*isol, pmr, cmr*)
Ohtani, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2443 (*isol, pmr, cmr*)

12,14-Labdadiene-6,7,8-triol L-8



(6α,7β,8α,12*E*)-*form*

$C_{20}H_{34}O_3$ 322.487

(6α,7β,8α,12*E*)-*form* [70387-38-1] ***6α-Hydroxynidorellol***
Oil.

*6-Angeloyl:**6α-Angeloyloxynidorellol***
$C_{25}H_{40}O_4$ 404.589
Cryst. Mp 114-115°. $[\alpha]_D$ -34.8 ($CHCl_3$).

(6α,7β,8β,12*Z*)-*form* [62868-75-1] ***Austroinulin***
Isol. from *Stevia rebaudiana* (stevia). Needles (MeOH). Mp 74-77°. $[\alpha]_D^{25}$ +33.6 (c, 0.48 in $CHCl_3$). $[\alpha]_D^{14}$ +24 (c, 0.50 in $CHCl_3$).

6-Ac: [75207-46-4] *6α-Acetoxy-12,14-labdadiene-7β,8β-diol*
$C_{22}H_{36}O_4$ 364.524
Isol. from *Stevia rebaudiana* (stevia). Cryst. (EtOAc). Mp 173-174°. $[\alpha]_D^{25}$ +36.8 (c, 0.46 in $CHCl_3$).

7-Ac:7β-Acetoxy-12,14-labdadiene-6α,8β-diol
$C_{22}H_{36}O_4$ 364.524
From *Stevia rebaudiana* (stevia). Needles (hexane). Mp 148-149°. $[\alpha]_D^{16}$ +14.9 (c, 0.67 in $CHCl_3$).

(6β,7β,8α,12*E*)-*form* [92694-04-7] ***Crotomachlin***. *6β,7β-Dihydroxy-12*E*-abienol*
Oil. $[\alpha]_D^{24}$ +10 (c, 0.25 in $CHCl_3$). λ_{max} 232 (ϵ 18000) (EtOH) (Derep).

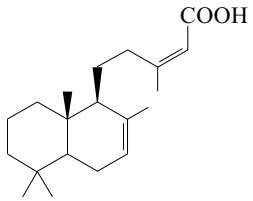
7-Ac:7β-Acetoxy-12,14-labdadiene-6β,8α-diol
$C_{22}H_{36}O_4$ 364.524
Oil.

(ent*-6α,7β,8ξ,12*Z*)-*form

6-Ac: [73947-04-3] ***Stevinsol***
$C_{22}H_{36}O_4$ 364.524

Bohlmann, F. *et al., Chem. Ber.*, 1977, **110**, 1034 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1769; 1984, **23**, 1190 (*isol*)
Sholichin, M. *et al., Phytochemistry*, 1980, **19**, 326 (*isol*)
Ortega, A. *et al., Rev. Latinoam. Quim.*, 1980, **11**, 45 (*Stevinsol*)
Quijano, L. *et al., Phytochemistry*, 1982, **21**, 1369 (*isol*)
Darise, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 133 (*isol, struct, abs config*)
Herlem, D. *et al., Tet. Lett.*, 1993, **34**, 5587 (*synth*)

7,13-Labdadien-15-oic acid L-9



(13*Z*)-*form*

$C_{20}H_{32}O_2$ 304.472

(13*Z*)-*form*

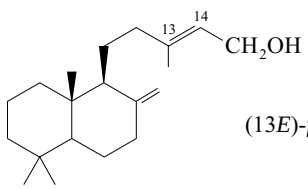
(*ent*-13*E*)-*form* [14022-43-6]
7,13-Eperudien-15-oic acid
Constit. of *Hymenaea courbaril* (copinol).

Me ester:
Oil. $[\alpha]_D^{22}$ -26.4 (c, 1.2 in $CHCl_3$).

p-*Phenylphenacyl ester:*
Cryst. Mp 109-111°. $[\alpha]_D$ -29.8 (c, 0.155 in $CHCl_3$).

Bevan, C.W.L. *et al., J.C.S.(C)*, 1968, 1067 (*isol*)
Imamura, P.M. *et al., Phytochemistry*, 1977, **16**, 1842 (*cmr*)
Tsichirtzis, F. *et al., Phytochemistry*, 1991, **30**, 211 (*isol, pmr, cmr*)

8(17),13-Labdadien-15-ol L-10



(13*E*)-*form*

$C_{20}H_{34}O$ 290.488

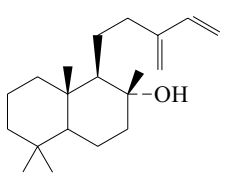
(*ent*-13*E*)-*form* [21738-29-4]
Oil. $[\alpha]_D$ -15.5 (c, 0.46 in $CHCl_3$).

15-Carboxylic acid: [20257-75-4] ent-*8(17),13*E-*Labdadien-15-oic acid*. ***Copalic acid***
$C_{20}H_{32}O_2$ 304.472
Constit. of *Hymenaea courbaril* (copinol). Oil. $Bp_{0.005}$ 160°. $[\alpha]_D$ -6.9 (c, 1.15 in $CHCl_3$).

[14022-42-5]

Nakano, T. *et al., J.O.C.*, 1961, **26**, 167 (*Copalic acid*)

13(16),14-Labdadien-8-ol L-11



8α-*form*

$C_{20}H_{34}O$ 290.488

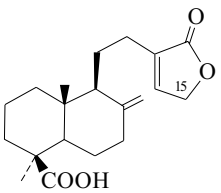
8α-*form* [10207-79-1]
Isoabienol
Constit. of the needles of *Pinus sylvestris* (Scotch pine). Cryst. Mp 68-68.5°. $[\alpha]_D^{20}$ -6.4 ($CHCl_3$).

(*ent*-8α)-*form*
Cryst. Mp 50-51°. $[\alpha]_D^{20}$ -0.49 (c, 1 in $CHCl_3$).

Ekman, R. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 921 (*Isoabienol*)
Cabrera, E. *et al., Phytochemistry*, 1983, **22**, 2779 (*isol*)
Toyota, M. *et al., Phytochemistry*, 1989, **28**, 3415 (*isol, pmr, cmr*)

8(17),13-Labdadien-16,15-olid-19-oic acid L-12

[40433-82-7]
Demethylpinusolide. Pinusolidic acid. Pinosolide acid. Pinusolic acid



$C_{20}H_{28}O_4$ 332.439
Gum.

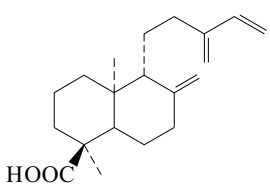
Me ester: [31685-80-0]

[443965-67-1] ***Pinusolide***
$C_{21}H_{30}O_4$ 346.466
Constit. of the oleorosin of *Pinus koraiensis* (Korean pine). Fine needles (petrol). Mp 83-84°. $[\alpha]_D^{23}$ +24 (MeOH). Confusion in ref. and CA about *Thuja orientalis* consitit..

15ξ-Hydroxy:15-Hydroxy-8(17),13-labdadien-16,15-olid-19-oic acid. ***15-Hydroxypinusolidic acid***
$C_{20}H_{28}O_5$ 348.438
Cryst. Mp 74-75°. $[\alpha]_D^{23}$ +30.5 (c, 1 in $CHCl_3$).

Raldugin, V.A. *et al., Khim. Prir. Soedin.*, 1970, **6**, 541; *Chem. Nat. Compd. (Engl. Transl.)*, 559 (*isol, struct, synth*)
Calderón, J.S. *et al., Phytochemistry*, 1987, **26**, 2639 (*isol*)
Kuo, Y.-H. *et al., Heterocycles*, 1990, **31**, 1705 (*15-Hydroxypinusolidic acid*)
Mehta, B.K. *et al., Indian J. Chem., Sect. B*, 2002, **41**, 1088-1092 (*Thuja orientalis ester*)

8(17),13(16),14-Labdatrien-18-oic acid L-13



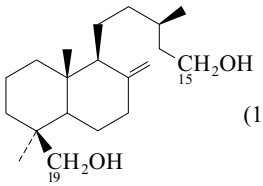
$C_{20}H_{30}O_2$ 302.456

ent*-*form
Isol. from seed pods of *Hymenaea courbaril* (copinol).

Me ester:
$[\alpha]_D^{25}$ -17.5 (c, 0.4 in $CHCl_3$).

Khoo, S.F. *et al., Tetrahedron*, 1973, **29**, 3379
Martins, D. *et al., Phytochemistry*, 1999, **51**, 813-817 (*pmr, cmr*)

8(17)-Labdene-15,19-diol L-14



(13*R*)-*form*

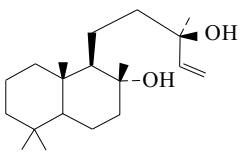
$C_{20}H_{36}O_2$ 308.503

(13*S*)-*form*
Cryst. Mp 99-100°. $[\alpha]_D^{25}$ +32.6 (c, 0.9 in $CHCl_3$).

Dialdehyde: [70901-87-0] *8(17)-Labdene-15,19-dial*. ***Junicedral***
$C_{20}H_{32}O_2$ 304.472
Isol. from *Juniperus communis* (juniper). Oil. $[\alpha]_D$ +16.1 (c, 0.99 in $CHCl_3$).

De Pascual Teresa, J. *et al., An. Quim.*, 1974, **70**, 1015; 1977, **73**, 568 (*Junicedral*)

14-Labdene-8,13-diol L-15



(8α,13*R*)-*form*

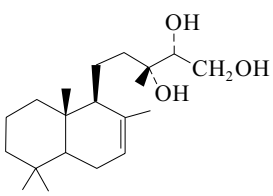
$C_{20}H_{36}O_2$ 308.503

(8α,13*S*)-*form* [515-03-7]
Sclareol
Constit. of *Salvia sclarea* (clary sage). Cryst. (petrol). Mp 105.5-106°. $[\alpha]_D^{18}$ -6.25 (EtOH).
▶ QK0301900

Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 971 (*Sclareol, pmr, cmr*)
Topçu, G. *et al., Phytochemistry*, 1999, **50**, 1195-1199 (*Sclareol, activity*)
Singh, M. *et al., Planta Med.*, 1999, **65**, 2-8 (*review*)
Demetzos, C. *et al., Planta Med.*, 1999, **65**, 77-78 (*Sclareol, activity*)

7-Labdene-13,14,15-triol L-16

13,14,15-Trihydroxy-7-labdene



$C_{20}H_{36}O_3$ 324.503

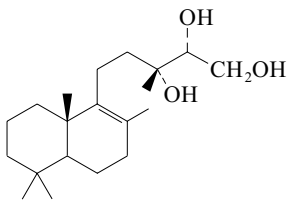
(13*R*,14*R*)-*form*
Constit. of *Madia sativa* (Chile tarweed). Gum. $[\alpha]_D^{24}$ +4.1 (c, 1.0 in $CHCl_3$).

(*ent*-13*R*,14*S*)-*form*
Cryst. (EtOAc/hexane). Mp 89-90°. $[\alpha]_D$ +3 (c, 5.0 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1103
Maldonado, E. *et al., Phytochemistry*, 1994, **35**, 721 (*isol, pmr, cmr, cryst struct*)

8-Labdene-13,14,15-triol L-17

13,14,15-Trihydroxy-8-labdene



$C_{20}H_{36}O_3$ 324.503

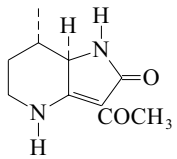
(13*R*,14*R*)-*form*

Constit. of *Madia sativa* (Chile tarweed). Gum.

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1103

Laccarin L-18

[175669-28-0]



Relative configuration

$C_{10}H_{14}N_2O_2$ 194.233

Alkaloid from fruit bodies of the mushroom *Laccaria vinaceoavellanea*. Powder. $[\alpha]_D^{31}$ +188 (c, 0.47 in $CHCl_3$). λ_{max} 235 (ϵ 11220); 293 (ϵ 11750) (MeOH) (Berdy).

Matsuda, M. *et al., Heterocycles*, 1996, **43**, 685 (*isol, uv, ir, pmr, cmr, struct*)

Lacidin A L-19

[158191-48-1]

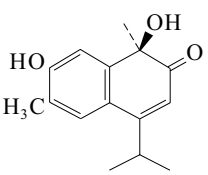
Prod. by *Lactobacillus acidophilus* OSU133. Bacteriocin.

Liao, C.C. *et al., J. Food Saf.*, 1994, **14**, 87-101 (*isol*)

Lacinilene C L-20

[41653-72-9]

1,7-Dihydroxy-1,6-dimethyl-4-(1-methylethyl)-2(1H)-naphthalenone, 9CI. 1,7-Dihydroxy-4-isopropyl-1,6-dimethyl-2(1H)-naphthalenone



(*R*)-*form*

$C_{15}H_{18}O_3$ 246.305

Isol. from *Gossypium hirsutum* (cotton) bracts. Mp 62-63°. The abs. config. has been detd.; the (*R*)-enantiomer is dextrorotatory but there is no indication in the literature as to which enantiomer occurs naturally λ_{max} 250 (ϵ 11600); 339 (ϵ 5710) (H_2O) (Derep). λ_{max} 249 (ϵ 11700); 341 (ϵ 6380) (MeOH) (Derep).

Me ether: [72843-51-7]
$C_{16}H_{20}O_3$ 260.332

From *Gossypium hirsutum* (cotton). Cryst. (CCl_4), also descr. as yellow oil. Mp 100-102°. One natural sample is definitely racemic. Posn. of methylation not indicated.

Jeffs, P.W. *et al., J.O.C.*, 1975, **40**, 2958
Stipanovic, R.D. *et al., Phytochemistry*, 1975, **14**, 1041 (*ms, ir, uv, struct*)
McCormick, J.P. *et al., J.O.C.*, 1984, **49**, 34 (*synth*)
Stipanovic, R.D. *et al., J.O.C.*, 1986, **51**, 2500 (*abs config*)
Krohn, K. *et al., J.O.C.*, 1998, **63**, 4140-4142 (*synth*)
Abraham, K.J. *et al., Phytochemistry*, 1999, **52**, 829 (*activity*)

Lactacins L-21

Peptide bacteriocins. Prod. by *Lactobacillus acidophilus*.

Lactacin B [86836-29-5]
λ_{max} 211 (H_2O) (Berdy).

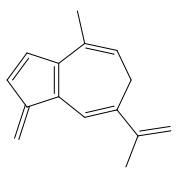
Lactacin F [107950-55-0]

Barefoot, S.F. *et al., Appl. Environ. Microbiol.*, 1983, **45**, 1808-1815 (*Lactacin B*)
Barefoot, S.F. *et al., Antimicrob. Agents Chemother.*, 1984, **26**, 328-334 (*Lactacin B*)
Muriana, P.M. *et al., Appl. Environ. Microbiol.*, 1991, **57**, 114-121 (*Lactacin F*)

Lactarofulvene L-22

[18454-60-9]

1,6-Dihydro-7-isopropenyl-4-methyl-1-methyleneazulene, 8CI. 1,6-Dihydro-4-methyl-1-methylene-7-(1-methylethenyl)azulene



$C_{15}H_{16}$ 196.291

Constit. of *Lactarius deliciosus*. Unstable orange liq.

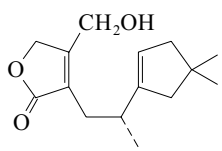
Betelli, D.J. *et al., Tetrahedron*, 1968, **24**, 2079

Lactaronecatorin A L-23

[62824-38-8]

[58757-91-8]

8-Hydroxy-8,9-seco-2(9),6-lactaradien-5,14-olide. Blennin C



$C_{15}H_{22}O_3$ 250.337

Identity of Lactaronecatorin A with Blennin C not confirmed. Constit. of *Lactarius blennius* (slimy milk cap). Pale-yellow oil. $[\alpha]_D^{20}$ -73 ($CHCl_3$). λ_{max} 316 (MeOH) (Berdy).

Aldehyde: [108888-55-7] *8-Oxo-8,9-seco-2(9),6-lactaradien-5,14-olide*
$C_{15}H_{20}O_3$ 248.321

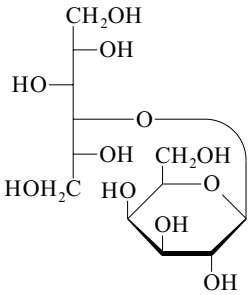
Daniewski, W.M. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1975, **23**, 639 (*isol*)
Vidari, G. *et al., Phytochemistry*, 1976, **15**, 1953 (*isol, struct*)
De Bernardi, M. *et al., Tetrahedron*, 1986, **42**, 4277 (*abs config*)
Pang, Z. *et al., Tet. Lett.*, 1992, **33**, 6863 (*aldehyde*)

Lactitol, BAN, INN L-24

[585-86-4]

[81025-04-9]

4-O-β-D-Galactopyranosyl-D-glucitol, 9CI. Emportal. Floralac. Importal. Oponaf. Portolac. E966



$C_{12}H_{24}O_{11}$ 344.315

Artificial sweetener used in foods. Sweetness 0.4 x sucrose. Cryst. + 1, 2 or $3H_2O$. Mp 95-98° (monohydrate). Log P -6.86 (calc). A food additive petition for GRAS status has been filed with the FDA.

▶ LD_{50} (rat, orl) 27500 mg/kg. LZ4392000

[81025-03-8]

Hoagland, P.D. *et al., Carbohydr. Res.*, 1979, **74**, 135 (*cmr*)
Van Velthuijsen, J.A. *et al., J. Agric. Food Chem.*, 1979, **27**, 680 (*rev, synth, props, use*)
Kanters, J.A. *et al., Acta Cryst. C*, 1990, **46**, 2408 (*cryst struct*)
Van Velthuijsen, J.A. *et al., Food Sci. Technol.*, 1991, **48**, 283 (*rev*)
Kivikoski, J. *et al., Carbohydr. Res.*, 1992, **223**, 45; 53; 189 (*cryst struct*)
Sinkledam, E.J. *et al., J. Am. Coll. Toxicol.*, 1992, **11**, 165; 189; 209; 219; 233; 249 (*tox*)
Christiansen-Brams, I. *et al., J. Carbohydr. Chem.*, 1992, **11**, 813 (*synth, pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1043
Peruche, B. *et al., Pharm. Ztg.*, 1993, **138**, 40 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1533-1534 (*props*)

Lactobin A L-25

Peptide containing 50 unmodified amino acid residues. Prod. by *Lactobacillus amylovorus* isol. from corn steep liquor. Bacteriocin.

Contreras, B.G.L. *et al., Appl. Environ. Microbiol.*, 1997, **63**, 13-20 (*isol*)

Lactocins L-26

[80619-55-2]

Polypeptides. Prod. by *Lactobacillus* sp.. Bacteriocins with potential food uses.

Lactocin A1 [81209-57-6]
Prod. by *Lactobacillus acidophilus*.

Lactocin D [147230-10-2]

Prod. by *Lactobacillus lactis*.

Lactocin S [125387-34-0]
Prod. by *Lactobacillus sake* L45.

Lactocin 27 [51109-86-5]
Prod. by *Lactobacillus helveticus* LP27.

Lactocin 705 [162163-97-5]
Prod. by *Lactobacillus casei* CRL705. Consists of 2 peptide chains, α and β, of 33 residues each.

Lactocin P 109
Prod. by *Lactobacillus plantarum*. Bacteriocin.

Lactocin C183

Upreti, G.C. *et al., Antimicrob. Agents Chemother.*, 1973, **4**, 487-494 (*Lactocin 27, isol*)
Filippov, V.A. *et al., Antibiotiki (Moscow)*, 1980, **25**, 837-840; 1981, **26**, 843-847 (*Lactocin C183, Lactocin P109, Lactocin A1*)
Moertvedt, C.I. *et al., Appl. Environ. Microbiol.*, 1991, **57**, 1829-1834 (*Lactocin S, isol*)
Parente, E. *et al., J. Appl. Bacteriol.*, 1992, **73**, 290-298 (*Lactocin D, isol*)
Vignolo, G.M. *et al., J. Appl. Bacteriol.*, 1995, **78**, 5-10 (*Lactocin 705, isol*)
Wozzo, S.A. *et al., FEMS Microbiol. Lett.*, 2000, **185**, 157-161 (*Lactocin 705, struct*)

Lactococcin L-27

[138636-34-7]

Peptide bacteriocins. Prod. by *Lactococcus lactis*. Bacteriocins with potential food uses.

Lactococcin A [138860-83-0]
Prod. by *Lactobacillus lactis* ssp. *cremoris* LMG 2130. Appears to be identical to Diplococcin.

Lactococcin B [145421-17-6]
Prod. by *Lactobacillus lactis* ssp. *cremoris* 9B4.

Lactococcin D53 [162430-02-6]
Prod. by *Lactobacillus lactis* D53.

Lactococcin G [144246-40-2]
Prod. by *Lactobacillus lactis* ssp. *lactis* LMG 2081. Bacteriocin activity depends on the complementary action of two peptides, α (39 aminoacids) and β (35 aminoacids).

Lactococcin K3113 [201057-95-6]
Prod. by *Lactobacillus lactis* LAB3113 isol. from kimchi.

Lactococcin M
Prod. by *Lactobacillus lactis* ssp. *cremoris* 9B4.

Lactococcin R [211431-23-1]
Prod. by *Lactobacillus lactis* ssp. *cremoris* R, isol. from radishes.

Lactococcin 140 [157243-29-3]
Prod. by *Lactobacillus lactis* 140NWC.

Lactococcin 972 [182892-95-1]
Prod. by *Lactobacillus lactis* ssp. *lactis* IPLA 972.

Holo, H. *et al., J. Bacteriol.*, 1991, **173**, 3879-3887 (*Lactococcin A*)
Van Belkum, M.J. *et al., Appl. Environ. Microbiol.*, 1992, **58**, 572-577 (*Lactococcin B*)
Nissen-Meyer, J. *et al., J. Bacteriol.*, 1992, **174**, 5686-5692 (*Lactococcin G*)
Parente, E. *et al., Appl. Microbiol. Biotechnol.*, 1994, **41**, 388-394 (*Lactococcin 140*)
McDougall, L.A. *et al., Int. J. Food Microbiol.*, 1994, **24**, 295-308 (*Lactococcin D53*)
Venema, K. *et al., Int. Dairy J.*, 1995, **5**, 815-832 (*rev*)
Shin, J.Y. *et al., J. Food Sci. Nutr.*, 1997, **2**, 101-108 (*Lactococcin K3113*)
Yildirim, Z. *et al., Lett. Appl. Microbiol.*, 1998, **26**, 297-304 (*Lactococcin R*)
Martinez, B. *et al., Microbiology (Reading, U.K.)*, 2000, **146**, 949-955 (*Lactococcin 972*)

β-Lactoglobulin L-28

[52503-66-9]

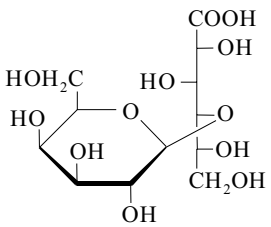
[9045-23-2, 9066-45-9, 50863-91-7, 50863-92-8, 176521-75-8, 176521-76-9, 176521-77-0]

Protein containing 162 amino acid residues of which four are Cys. The monomeric form has Mw 18000, but a dimeric form is also known. At least five genetic variants have been identified in cows, of which the A and B variants are the most important. These differ at positions 64 and 118, where Asp and Val respectively in variant A are substituted by Gly and Ala in variant B. Both variants have two disulfide bridges and one free cysteine. Numerous species variants are also known. The major whey protein in the milk of cows and many other mammals, comprising about 50% of the total protein. A major component of whey concentrates (obtained by ultrafiltration) and whey solids (obtained by spray drying), used to improve the functional and nutritional properties of many foodstuffs. Undergoes ready thermal denaturation and crosslinking with casein and other proteins in whey to form a coagulate known as lactalbumin (not to be confused with α-lactabumin) which is also used for protein fortification of foods.

McKenzie, H.A. *et al., Biochemistry*, 1972, **11**, 4539-4547 (*struct*)
Braunitzer, G. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1972, **353**, 832-834; 1973, **354**, 867-878 (*struct*)
Monaco, H.L. *et al., J. Mol. Biol.*, 1987, **197**, 695-706 (*cryst struct*)
Encyclopedia of Food Science, Food Technology and Nutrition, (eds. Macrae, R. *et al*), Academic Press, 1993, 3075-3079; 4889-4894 (*rev*)
Heddleson, R.A. *et al., J. Agric. Food Chem.*, 1997, **45**, 2369-2373 (*isol*)
Brownlow, S. *et al., Structure (London)*, 1997, **5**, 481-494 (*cryst struct*)
Belloque, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 1805-1813 (*conformn, pmr*)

Lactonic acid L-29

4-O-β-Galactopyranosylgluconic acid, 9CI. Lactobionic acid, 8CI



$C_{12}H_{22}O_{12}$ 358.299

D-*form* [96-82-2]

Ca salt: [5001-51-4] *Calcium lactobionate*
Firming agent used in dry pudding mixtures. Pentahydrate. $[\alpha]_D^{20}$ +23.7 (c, 6.28 in H_2O).

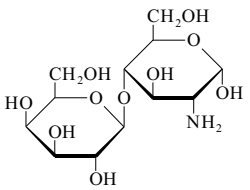
1,5-Lactone:Lactono-1,5-lactone
$C_{12}H_{20}O_{11}$ 340.283
Mp 195-196° dec. $[\alpha]_D^{20}$ +54 → +22 (c, 5.0 in H_2O).

*Octa-Me, Me ester:Methyl octa-*O*-methyl-D-lactonate*
$C_{21}H_{40}O_{12}$ 484.54
$Bp_{0.05}$ 157-164°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 460B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 525D (*ir*)
Haworth, W.N. *et al., J.C.S.*, 1927, 544 (*Me octa-Me*)
Isbell, H.S. *et al., Bur. Standards J. Research*, 1933, **11**, 713 (*Ca salt, lactone, synth*)
Nishizuka, Y. *et al., J. Biol. Chem.*, 1960, **235**, PC13 (*enzymic synth*)
Cook, W.J. *et al., Acta Cryst. B*, 1973, **29**, 215 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 395-396

Lactosamine L-30

[13000-25-4]
*2-Amino-2-deoxy-4-*O*-(β-D-galactopyranosyl)-D-glucose, 9CI. β-D-Galactopyranosyl-(1→4)-2-amino-2-deoxy-D-glucose. 4-*O*-β-D-Galactosyl-D-glucosamine*



α-Pyranose-*form*

$C_{12}H_{23}NO_{10}$ 341.314
Isol. from human milk. Growth factor for *Lactobacillus bifidus*. $[\alpha]_D^{21.5}$ +78.2 (3 min) → +63.1 (3h) (c, 1.25 in H_2O).

N-*Ac:* [32181-59-2]

[77304-67-7] N-*Acetyllactosamine*
$C_{14}H_{25}NO_{11}$ 383.352
Structural unit in higher oligosaccharides present in human milk. Cryst. (2-propanol/MeOH). Mp 170-171° (168-170°). $[\alpha]_D^{20}$ +50 → +28.5 (c, 0.6 in 90% MeOH aq.). $[\alpha]_D^{19}$ +48.3 (3 min) → +27.4 (equilib.) (c, 0.5 in H_2O).

α-Pyranose-*form*

Octa-Ac: [36954-63-9]
$C_{28}H_{39}NO_{18}$ 677.612
Mp 224-225°. $[\alpha]_D$ +61.5 (+57.7) ($CHCl_3$).

[4307-58-8, 36954-63-9]

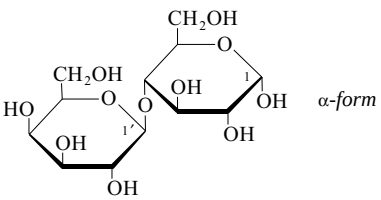
Kuhn, R. *et al., Chem. Ber.*, 1954, **87**, 1547; 1961, **94**, 842; 1259 (*synth*)
Zilliken, F. *et al., J. Biol. Chem.*, 1954, **208**, 299; 1955, **217**, 79 (*synth*)
Zilliken, F. *et al., Arch. Biochem. Biophys.*, 1955, **54**, 398 (*isol*)
Okuyama, T. *et al., CA*, 1961, **55**, 18817; 1962, **57**, 8880 (*synth*)
Cote, R.H. *et al., Nature (London)*, 1961, **178**, 1171 (*isol*)
Spiro, R.G. *et al., J. Biol. Chem.*, 1962, **237**, 646
Dmitriev, B.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1973, 2365-2366; *Bull. Acad. Sci.*

USSR, Div. Chem. Sci. (Engl. Transl.), 1973, 2310-2311 (*synth*)
Johnson, G. *et al., Carbohydr. Res.*, 1975, **39**, 271-281 (*N-Ac, synth*)
Jacquinet, J.C. *et al., Carbohydr. Res.*, 1976, **46**, 138 (*synth, hepta-Ac*)
Takamura, T. *et al., Chem. Pharm. Bull.*, 1979, **27**, 721-725 (*N-Ac, synth*)
Longchambon, F. *et al., Acta Cryst. B*, 1981, **37**, 601-607 (*N-Ac, cryst struct*)
Alais, J. *et al., Carbohydr. Res.*, 1981, **93**, 164 (*N-Ac*)
Wong, C.-H. *et al., J.O.C.*, 1982, **41**, 5416-5418 (*N-Ac, synth*)
Ajisaka, K. *et al., Carbohydr. Res.*, 1988, **180**, 35 (*synth*)
Goux, W.J. *et al., Carbohydr. Res.*, 1988, **184**, 47 (*cmr*)
Orlando, R. *et al., Anal. Chem.*, 1990, **62**, 2388 (*ms*)
Lattová, E. *et al., Carbohydr. Res.*, 1992, **235**, 289 (*synth, N-Ac*)
Herrmann, G.F. *et al., Angew. Chem., Int. Ed.*, 1993, **32**, 1342 (*synth*)
Wiemann, T. *et al., Carbohydr. Res.*, 1994, **257**, C1 (*synth, N-Ac*)
Wrodnigg, T.M. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 827-828 (*synth*)
Endo, J. *et al., Carbohydr. Res.*, 1999, **316**, 179-183 (*N-Ac, biomanuf, pmr*)
Yoon, J.H. *et al., Carbohydr. Res.*, 2000, **327**, 377-383 (*N-Ac, enzymic synth*)
Hara, Y. *et al., Carbohydr. Res.*, 2001, **330**, 65-71 (*biosynth*)

Lactose L-31

[63-42-3]

[64044-51-5]
4-O-β-D-Galactopyranosyl-D-glucose, 9CI, 8CI. Milk sugar. Lactobiose. Tablettose. Lactin



α-*form*

$C_{12}H_{22}O_{11}$ 342.299
Occurs in mammalian milk (human 6-7%, cow 4-5%), fruits of sapodilla *Achras sapota*, and a few other plants. Nutrient. Obt. industrially from whey. Sweetness 0.68 × sucrose.

► Exp. teratogen. Gastrointestinal effects if intestinal lactase activity is diminished. Mixtures with strong oxidants are explosive. May cause allergy in sensitive patients. OD9625000

[10039-26-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 194D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 307A (*nmr*)
Venkataraman, R. *et al., Arch. Biochem. Biophys.*, 1958, **75**, 443 (*isol*)
Clamp, J.R. *et al., Adv. Carbohydr. Chem.*, 1961, **16**, 159 (*rev*)
Chumbalov, T.K. *et al., Khim. Prir. Soedin.*, 1966, **2**, 284; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 230 (*isol*)
Pazur, J.H. *et al., The Carbohydrates*, Academic Press, 1970, **2A**, 69
Roberts, J.D. *et al., J.A.C.S.*, 1971, **93**, 4463 (*cmr*)
Vazquez, I.M. *et al., Carbohydr. Res.*, 1973, **26**, 351
Hough, L. *et al., Pure Appl. Chem.*, 1977, **49**, 1069 (*rev*)
Bradbury, J.H. *et al., Carbohydr. Res.*, 1979, **71**, 15 (*pmr*)
Pfeffer, P.E. *et al., J.A.C.S.*, 1979, **101**, 1265 (*cmr*)
Thelwall, L.A.W. *et al., Dev. Food Carbohydr.*, Applied Science Publ., 1980, **2**, 275 (*rev*)
Takeo, K. *et al., Carbohydr. Res.*, 1983, **121**, 163 (*synth*)
Brittain, H.G. *et al., Anal. Profiles Drug Subst.*, 1991, **20**, 369 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 252-261
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1370
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LAR000

Lactostrepcin L-32

[86595-91-7]
Prod. by non-nisin producing strains of *Streptococcus lactis*. Bacteriocin.

Kosak, W. *et al., J. Dairy Res.*, 1978, **45**, 247-257 (*isol*)
Dobrzanski, W.T. *et al., Microbiology (Washington, D.C.)*, 1982, 225-229 (*isol*)

Lactostrepcin 5 L-33

[96697-31-3]
Prod. by *Streptococcus cremoris* 202. Bacteriocin.

Zajdel, J.K. *et al., Appl. Environ. Microbiol.*, 1985, **49**, 969-974 (*isol*)

Lactoyllactic acid L-34

[517-52-2]

[923-17-1, 1115-79-3]
1-Carboxyethyl 2-hydroxypropanoate, 9CI. 2-Lactylic acid

$HOCH(CH_3)COOCH(CH_3)COOH$
$C_6H_{10}O_5$ 162.142
Preparations are doubtless mixts. of diastereomers.Viscous liq.

Me ester: [36395-19-4]
$C_7H_{12}O_5$ 176.169
Oil. Bp_{10} 111°.

Et ester: [65002-62-2]
$C_8H_{14}O_5$ 190.196
Viscous liq. Bp_{10} 116°.

O-*Octadecanoyl, Na salt:* [25383-99-7]

[14440-80-3] *Sodium stearoyl 2-lactylate*
$C_{24}H_{43}NaO_6$ 450.59
Used in foods as a dough strengthener, emulsifier, stabiliser, surface active agent, formulation aid, processing aid and texturiser.

O-*Octadecanoyl, Ca salt:* [5793-94-2]

[14440-80-3] *Calcium stearoyl 2-lactylate*
$C_{48}H_{86}CaO_{12}$ 895.278
Used in foods as an emulsifier, texturiser, surface-tension control agent and dough conditioner.

U.S. Pat., 1945, 2 371 281; *CA*, **39**, 4089 (*esters*)
Rehberg, C.E. *et al., J.A.C.S.*, 1952, **74**, 1609 (*esters*)
Thompson, J.B. *et al., Cereal Chem.*, 1954, **31**, 296-302; 1955, **32**, 493-498 (*salts, manuf, use*)
U.S. Pat., 1956, 2 733 252; *CA*, **50**, 6818g (*sodium stearoyl*)
Fed. Regist., 1965, **30**, 12070; 1966, **31**, 13793 (*use*)
Elliger, C.A. *et al., J. Agric. Food Chem.*, 1979, **27**, 527-528 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 426-427; 2609-2610 (*salts*)

Lactyltrimethylammonium betaine L-35

[68688-60-8]
(2-Carboxy-2-hydroxyethyl)trimethylarsonium hydroxide inner salt, 9CI. β-Trimethylarsonium lactate

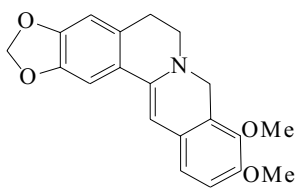
$Me_3As^{\oplus}CH_2CH(OH)COO^{\ominus}$
$C_6H_{13}AsO_3$ 208.088
Occurs free in the lobster *Homarus americanus*. Plates (EtOH/Et_2O). Mp 199-201°.

Cooney, R.V. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1978, **75**, 4262
Cooney, R.V. *et al., Chemosphere*, 1980, **9**, 335 (*biosynth*)
Summons, R.E. *et al., Phosphorus Sulfur Relat. Elem.*, 1982, **13**, 133 (*synth, ms, ir*)

Lambertine L-36

[120834-89-1]

[119420-08-5]
Dihydroberberine



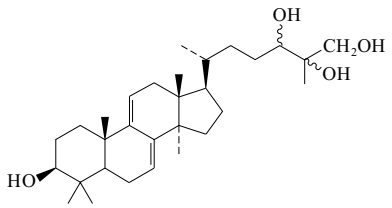
$C_{20}H_{19}NO_4$ 337.374
Alkaloid from *Berberis vulgaris* (barberry). Yellow needles (MeOH or Me_2CO). Mp 163-164°. λ_{max} 280 (log ϵ 4.21); 368 (log ϵ 4.3) (no solvent reported).

N-*Me:* [47474-50-0]

[26668-90-6] **N-*Methyllambertine***. N-*Methyldihydroberberine. 7,8-Dihydro*-N-*methylberberine*
$C_{21}H_{22}NO_4^{\oplus}$ 352.409
Cryst. (as chloride). Mp 210-212° (chloride).

Chatterjee, R. *et al., J. Indian Chem. Soc.*, 1955, **32**, 609 (*isol, uv, struct, synth*)
Onda, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2365-2371 (*deriv, synth*)
Dobhal, M.P. *et al., Pharmazie*, 1988, **43**, 659-660 (*isol, pmr, cmr*)
Yusupov, M.M. *et al., Khim. Prir. Soedin.*, 1990, **26**, 128-129; *Chem. Nat. Compd. (Engl. Transl.)*, **105**, 106 (*isol*)
Yusupov, M.M. *et al., Khim. Prir. Soedin.*, 1993, **29**, 53-59; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 43-48 (*Didhydromethylberberine, isol, deriv*)

Lanosta-7,9(11)-diene-3,24,25,26-tetrol L-37



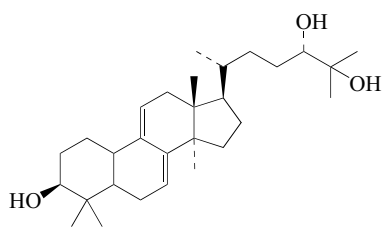
$C_{30}H_{50}O_4$ 474.723

3β-*form*
Ganoderiol A
Constit. of *Ganoderma lucidum* (reishi). Needles ($CHCl_3$). Mp 232-234°. $[\alpha]_D^{23}$ +20 (c, 0.1 in EtOH).

3-Ketone: [106518-63-2] *24,25,26-Trihydroxylanosta-7,9(11)-dien-3-one.* ***Ganodermanontriol***
$C_{30}H_{48}O_4$ 472.707
Constit. of *Ganoderma lucidum* (reishi). Cryst. Mp 168-170°. $[\alpha]_D^{24}$ +41 (c, 0.2 in MeOH).

Sato, H. *et al., Agric. Biol. Chem.*, 1986, **50**, 2887 (*isol*)
Fujita, A. *et al., J. Nat. Prod.*, 1986, **49**, 1122 (*isol*)

Lanosta-7,9(11)-diene-3,24,25-triol L-38



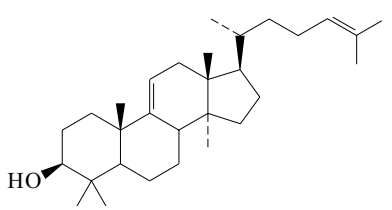
$C_{30}H_{50}O_3$ 458.723

(3β,24*S*)-*form* [107900-79-8]
Lucidumol B
Constit. of *Ganoderma lucidum* (reishi). Plates ($CHCl_3$). Mp 209-211°. $[\alpha]_D$ +53 (c, 0.04 in MeOH).

3-Ketone:24,25-Dihydroxylanost-7,9(11)-dien-3-one. ***Ganodermanondiol***
$C_{30}H_{48}O_3$ 456.707
Constit. of *Ganoderma lucidum* (reishi). Needles (MeOH). Mp 182-183°. $[\alpha]_D^{23}$ +45.8 (c, 0.5 in $CHCl_3$).

Fujita, A. *et al., J. Nat. Prod.*, 1986, **49**, 1122 (*Ganodermanondiol*)
Min, B.S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1607-1612 (*Lucidumol B*)

Lanosta-9(11),24-dien-3-ol L-39

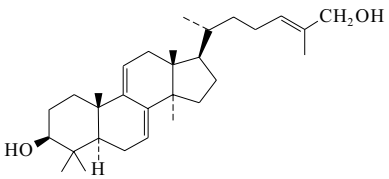


$C_{30}H_{50}O$ 426.724

3β-*form* [514-45-4]
Parkeol
Constit. of *Butyrospermum parkii* (shea). Cryst. (Et_2O/MeOH). Mp 162-165°. $[\alpha]_D$ +76.8 (c, 1 in $CHCl_3$).

Schreiber, K. *et al., Tetrahedron*, 1964, **20**, 1803 (*struct*)
v. Tamelen, E.E. *et al., J.A.C.S.*, 1972, **94**, 8225 (*synth*)
Itoh, T. *et al., Steroids*, 1976, **27**, 275 (*pmr*)

Lanosta-7,9(11),24-triene-3,26-diol L-40



$C_{30}H_{48}O_2$ 440.708

See note under 3,22-Dihydroxylanosta-7,9(11),24-trien-26-oic acid, D-525.

(3β,24*E*)-*form* [104700-96-1]
Ganoderol B. *Ganodermadiol*
Constit. of fungus *Ganoderma lucidum* (reishi). Needles (MeOH). Mp 171-173°. $[\alpha]_D^{25}$ +61 (c, 0.18 in $CHCl_3$).

3-Ketone: [104700-97-2] *26-Hydroxylanosta-7,9(11),24*E*-trien-3-one.* ***Ganoderol A***. *Ganodermenonol*
$C_{30}H_{46}O_2$ 438.692
Constit. of *Ganoderma lucidum* (reishi). Leaflets (MeOH). Mp 109-111° (99-101°). $[\alpha]_D^{23}$ +38.96 (c, 1 in $CHCl_3$).

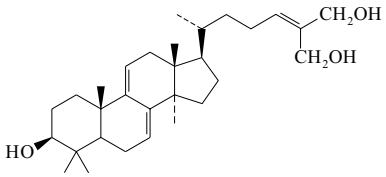
3-Ketone, 26-aldehyde: [104700-98-3] *3-Oxolanosta-7,9(11),24*E*-trien-26-al.* ***Ganoderal A***
$C_{30}H_{44}O_2$ 436.676
Constit. of *Ganoderma lucidum* (reishi). Leaflets (MeOH). Mp 127-128°. $[\alpha]_D^{25}$ +27 (c, 0.21 in $CHCl_3$).

3-Ketone, 26-carboxylic acid: [104759-35-5] *3-Oxolanosta-7,9(11),24*E*-trien-26-oic acid.* ***Tyromycic acid***. *Ganoderic acid S*†
$C_{30}H_{44}O_3$ 452.676
Constit. of *Ganoderma lucidum* (reishi). Rods (MeOH). Mp 173-175° (168-169°). $[\alpha]_D$ +45 ($CHCl_3$). Ganoderic acid S appears to be identical with the prev. known Tyromycic acid λ_{max} 226 (ε 13800); 233 (ε 1549); 243 (ε 17780); 252 (ε 9550) (MeOH) (Berdy).

[16929-95-6]

Gaudamer, A. *et al., Bull. Soc. Chim. Fr.*, 1967, 1844 (*Tyromycic acid*)
Morigiwa, A. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3025 (*isol*)
Arisawa, M. *et al., J. Nat. Prod.*, 1986, **49**, 621; 1988, **51**, 54 (*isol, pmr, cmr*)

Lanosta-7,9(11),24-triene-3,26,27-triol L-41



$C_{30}H_{48}O_3$ 456.707

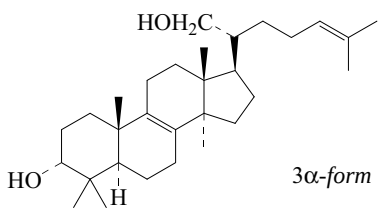
3β-*form* [105300-28-5]
Ganodermatriol
Constit. of *Ganoderma lucidum* (reishi). Plates. Mp 180-190°. $[\alpha]_D^{20}$ +9 (c, 0.04 in EtOH).

Tri-Ac:
Cryst. (MeOH). Mp 98-100°.

3-Ketone: [114567-47-4] *26,27-Dihydroxylanosta-7,9(11),24-trien-3-one.* ***Ganoderiol F***
$C_{30}H_{46}O_3$ 454.692
Metab. of *Ganoderma lucidum* (reishi). Pale yellow plates ($CHCl_3$/MeOH). Mp 116-120°. $[\alpha]_D^{21}$ +42 (c, 0.1 in MeOH).

Sato, H. *et al., Agric. Biol. Chem.*, 1986, **50**, 2887 (*isol*)
Arisawa, M. *et al., J. Nat. Prod.*, 1986, **49**, 621; 1988, **51**, 54 (*isol, pmr, cmr*)
Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 367 (*Ganoderiol F*)

Lanost-8,24-diene-3,21-diol L-42



$C_{30}H_{50}O_2$ 442.724

3α-*form* [267649-99-0]
Needles ($CHCl_3$). Mp 71-72°. $[\alpha]_D^{27}$ -12.7 (c, 0.3 in $CHCl_3$).

*3-Ac, 21-*O*-β-D-xylopyranoside:* [267649-97-8] ***Tsugarioside B***
$C_{37}H_{60}O_7$ 616.877
Constit. of *Ganoderma tsugae* (red reishi). Needles ($CHCl_3$). Mp 135-137°. $[\alpha]_D^{27}$ +7.6 (c, 0.1 in $CHCl_3$).

21-Carboxylic acid: ***3-Hydroxylanost-8,24-dien-21-oic acid***
$C_{30}H_{48}O_3$ 456.707
Powder. Mp 149-153°. $[\alpha]_D^{21}$ +29 (c, 1 in $CHCl_3$).

21-Carboxylic acid, Ac: [174391-64-1]
$C_{32}H_{50}O_4$ 498.745
Powder. Mp 192-194°. $[\alpha]_D^{21}$ +14 (c, 1 in $CHCl_3$).

21-Carboxylic acid, Ac, Me ester:
Needles (Me_2CO aq.). Mp 135-137°. $[\alpha]_D$ +7 ($CHCl_3$).

*21-Carboxylic acid, 3-*O*-(3-hydroxy-4-methoxycarbonyl-3-methylbutanoyl):* [174324-47-1] ***Fomitopsic acid***
$C_{37}H_{58}O_7$ 614.861

Powder. Mp 147°. $[\alpha]_D^{21}$ +5 (c, 1 in $CHCl_3$).

3β-*form*

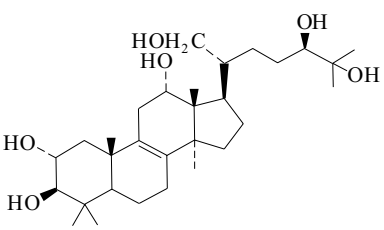
21-Carboxylic acid: [24160-36-9] ***Trametenolic acid***. *Trametenolic acid B*
$C_{30}H_{48}O_3$ 456.707
Metab. of *Ganoderma tsugae* (red reishi). Cryst. Mp 258-261°. $[\alpha]_D$ +40.2.

21-Carboxylic acid, Ac: ***Tsugaric acid A***
$C_{32}H_{50}O_4$ 498.745
Isol. from *Ganoderma tsugae* (red reishi). Needles (MeOH/$CHCl_3$). Mp 181-182°. $[\alpha]_D^{27}$ +6 (c, 0.1 in $CHCl_3$).

*21-Carboxylic acid, 3-Ac, 21-*O*-β-D-glucopyranosyl ester:* [205119-13-7]
$C_{38}H_{60}O_9$ 660.887
Constit. of *Ganoderma tsugae* (red reishi). Needles. Mp 188-190°. $[\alpha]_D^{25}$ +21 (c, 0.1 in MeOH).

Beereboom, J.J. *et al., J.C.S.*, 1957, 3437-3441 (*3α-acid*)
Halsall, T.G. *et al., J.C.S.*, 1959, 2036-2040 (*Trametenolic acid*)
Kempska, K. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1962, **36**, 1453-1457 (*Trametenolic acid*)
Batta, A.K. *et al., J.C.S. Perkin 1*, 1975, 451-455 (*Trametenolic acid*)
Keller, A.C. *et al., Phytochemistry*, 1996, **41**, 1041-1046 (*Fomitopsis isolates*)
Lin, C.-N. *et al., Phytochemistry*, 1997, **46**, 1143-1146 (*Tsugaric acid A*)
Tanaka, N. *et al., J. Nat. Prod.*, 1998, **61**, 193-197 (*Trametenolic acid, pmr, cmr*)
Gan, K.-H. *et al., J. Nat. Prod.*, 1998, **61**, 485-487 (*Tsugaric acid A glucosyl ester*)
Su, H.-J. *et al., J. Nat. Prod.*, 2000, **63**, 514-516 (*Tsugarioside B, isol, activity*)

Lanost-8-ene-2,3,12,21,24,25-hexol L-43



$C_{30}H_{52}O_6$ 508.737

(2α,3β,12α,24*R*)-*form* [65694-19-1]
Fasciculol C
Constit. of mushrooms *Naematoloma fasciculare* and *Naematoloma sublateritum*. Cryst. (MeCN). Mp 242-244° (185-187°). $[\alpha]_D^{20}$ +73.48 (MeOH). λ_{max} 207 (ε 6000) (EtOH) (Berdy).

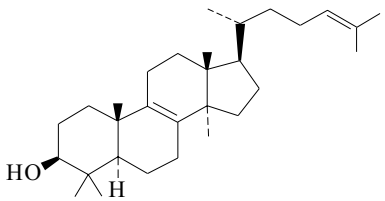
*2-*O*-(3-Hydroxy-3-methylglutaroyl) (*S*-):* [261638-76-0] ***Fasciculic acid F***
$C_{36}H_{60}O_{10}$ 652.864

2-Ketone: [348611-64-3] *3,12,21,24,25-Pentahydroxylanost-8-en-2-one.* ***Sublateriol B***
$C_{30}H_{50}O_6$ 506.721
Amorph. powder. $[\alpha]_D^{32}$ +89.7 (c, 0.2 in MeOH).

Ikeda, M. *et al., Agric. Biol. Chem.*, 1977, **41**, 1803 (*isol*)
De Bernardini, M. *et al., J. Nat. Prod.*, 1981, **44**, 351 (*isol*)
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2176 (*isol*)
Kubo, I. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3821-3825 (*isol*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2001, **49**, 589-594 (*Sublateriol B*)

Lanosterol L-44

[79-63-0]
Lanosta-8,24-dien-3-ol. 4,4,14-Trimethylcholesta-8,24-dien-3-ol. Isocholesterol. Kryptosterol. Cryptosterol



$C_{30}H_{50}O$ 426.724
Constit. of wool fat used e.g. as chewing-gum softener. Also from yeast. Cryst. (MeOH/Me_2CO). Mp 140-141°. $[\alpha]_D^{17}$ +58 ($CHCl_3$).

▶ OE3360000

*3-*O*-Sulfate:*
$C_{30}H_{50}O_4S$ 506.789
Mp 199-200° (as K salt).

Ac:
$C_{32}H_{52}O_2$ 468.762
Mp 131-133°. $[\alpha]_D^{20}$ +62.5 (c, 1.12 in $CHCl_3$).

Sobel, A.E. *et al., J.A.C.S.*, 1941, **63**, 1259 (*sulfate*)
Voser, W. *et al., Helv. Chim. Acta*, 1952, **35**, 66; 2414 (*struct*)
Hemmert, F. *et al., Bull. Soc. Chim. Fr.*, 1966, 976 (*pmr*)
Legrand, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1966, **262**, 1290 (*cd*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1969, **332**, (*synth*)
Shishibori, T. *et al., Chem. Lett.*, 1973, 1289 (*biosynth*)
Boar, R.B. *et al., J.C.S. Perkin 1*, 1973, 1583 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1995, **117**, 11819 (*biosynth*)
Joubert, B.M. *et al., Org. Lett.*, 2000, **2**, 339-341 (*biosynth*)
Hess Jr., B.A. *et al., Org. Lett.*, 2003, **5**, 165-167 (*biosynth*)

Lansamide I L-45

N-*Methyl-3-phenyl-*N-*(2-phenylethenyl)-2-propenamide, 9CI.* N-*Methyl-*N-*styryl-cinnamamide*
PhCH=CHNMeCOCH=CHPh
$C_{18}H_{17}NO$ 263.338

(*E*,*E*)-*form* [77527-97-0]
Alkaloid from the leaves and seeds of *Clausena lansium* (wampee). Mp 124-125° (119-120°).

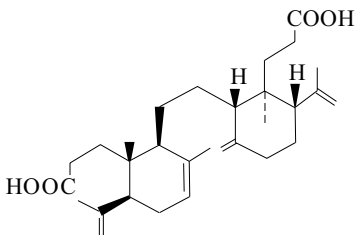
(*Z*,*E*)-*form* [121817-37-6]
Lansiumamide B. N-*Methyl-*N-cis-*styrylcinnamamide*
Isol. from seeds of *Clausena lansium* (wampee). Yellowish plates (Et_2O). Mp 72-73°.

N-*De-Me:* [121817-36-5] ***Lansiumamide A***. N-cis-*Styrylcinnamamide*
$C_{17}H_{15}NO$ 249.312
Isol. from seeds of *Clausena lansium* (wampee). Pale yellow needles (cyclohexane/Et_2O). Mp 121-123°.

Prakash, D. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 1075 (*isol, uv, ir, pmr, ms, struct, synth*)
Lin, J.-H. *et al., Phytochemistry*, 1989, **28**, 621 (*Lansiumamides*)
Stefanuti, I. *et al., Tet. Lett.*, 2000, **41**, 3735-3738 (*synth*)

Lansic acid L-46

[19954-99-5]
3,4;21,22-Bisseco-4(23),7,14(27),22(29)-onoceratetraene-3,21-dioic acid

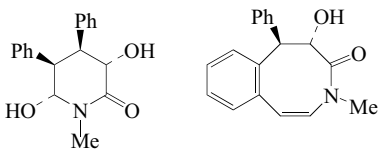


$C_{30}H_{46}O_4$ 470.691
Constit. of *Lansium domesticum* (langsat). Cryst. Mp 182-184°. $[\alpha]_D$ -7 ($CHCl_3$).

Kiang, A.K. *et al., Tet. Lett.*, 1967, 3571 (*isol*)
Habaguchi, K. *et al., Tet. Lett.*, 1968, 3731 (*struct*)
Nishizawa, M. *et al., Tet. Lett.*, 1984, **25**, 5071 (*synth*)

Lansimide 2 L-47

[119574-06-0]



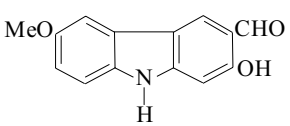
Relative Configurations

$C_{18}H_{36}N_2O_5$ 360.493
A 1:1 complex of cyclic amides. Constit. of *Clausena lansium* (wampee). Cryst. (MeOH/C_6H_6). Racemic.

Lakshmi, V. *et al., Indian Drugs*, 1988, **26**, 105-106 (*isol*)
Ji, X. *et al., Acta Cryst. C*, 1992, **48**, 1082-1085 (*conformn, cryst struct*)

Lansine L-48

[74606-99-8]
*2-Hydroxy-6-methoxy-9*H*-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-2-hydroxy-6-methoxycarbazole*



$C_{14}H_{11}NO_3$ 241.246
Alkaloid from the leaves of *Clausena lansium* (wampee). Mp 225-226°.

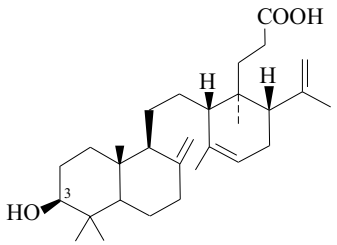
Me ether: [51971-09-6] *2,6-Dimethoxy-9*H*-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-2,6-dimethoxycarbazole.* ***Glycozolidal***
$C_{15}H_{13}NO_3$ 255.273
Mp 185°.

8-Methoxy: [182261-81-0] *2-Hydroxy-6,8-dimethoxy-9*H*-carbazole-3-carboxaldehyde. 3-Formyl-2-hydroxy-6,8-dimethoxycarbazole.* ***Clausine B***
$C_{15}H_{13}NO_4$ 271.272
Yellow needles (Me_2CO). Mp 228-229°. λ_{max} 210 (log ϵ 4.28); 235 (log ϵ 4.3); 269 (sh) (log ϵ 4.24); 278 (log ϵ 4.32); 304 (log ϵ 4.36); 357 (log ϵ 3.83) (MeOH).

Sharma, R.B. *et al., Chem. Ind. (London)*, 1980, 158 (*synth*)
Prakash, D. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 1075 (*isol, uv, ir, pmr, ms, struct*)
Bhattacharyya, P. *et al., J. Nat. Prod.*, 1985, **48**, 465 (*Me ether*)
Wu, T.-S. *et al., Phytochemistry*, 1996, **43**, 133 (*Clausine B*)

Lansiolic acid L-49

[87453-43-8]
3-Hydroxy-21,22-seco-8(26),14,22(29)-onoceratrien-21-oic acid



$C_{30}H_{48}O_3$ 456.707

Me ester:
Syrup. $[\alpha]_D^{19}$ +34.9 (c, 1.36 in $CHCl_3$).

*3-(*N*-Acetyl-β-D-glucosaminide):* [82537-86-8] ***Lansioside A***
$C_{38}H_{61}NO_8$ 659.902
Constit. of *Lansium domesticum* (langsat). Cryst. (EtOH). Mp 174-175°. $[\alpha]_D^{15}$ +26.5 (c, 1.06 in EtOH).

3-O-*β-D-Glucopyranoside:* [87453-34-7] ***Lansioside B***
$C_{36}H_{58}O_8$ 618.849
From *Lansium domesticum* (langsat). Amorph. solid. $[\alpha]_D^{23}$ +12.5 (c, 1.5 in EtOH).

3-O-*β-D-Xylopyranoside:* [87453-35-8] ***Lansioside C***
$C_{35}H_{56}O_7$ 588.823
From *Lansium domesticum* (langsat). Cryst. ($CHCl_3$/hexane). Mp 124.5-126°. $[\alpha]_D^{24}$ +12.4 (c, 0.76 in EtOH).

Nishizawa, M. *et al., J.O.C.*, 1983, **48**, 4462

Ficus Latex peptide 1 L-50

[124903-89-5]
FLP 1

H-Ala-Val-Asn-Pro-Ile-Arg-OH

$C_{29}H_{52}N_{10}O_8$ 668.792
Isol. from the latex of *Ficus carica* (fig). $[\alpha]_D^{25}$ -118 (c, 0.3 in H_2O).

Maruyama, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 2763 (*isol, struct, props*)

Ficus Latex peptide 2 L-51

[124925-14-0]
FLP 2

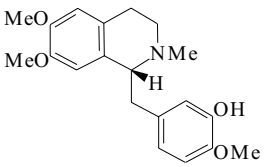
H-Leu-Tyr-Pro-Val-Lys-OH

$C_{31}H_{50}N_6O_7$ 618.772
Isol. from the latex of *Ficus carica* (fig). $[\alpha]_D^{25}$ -77 (c, 0.8 in H_2O).

Maruyama, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 2763 (*isol, struct, props*)

Laudanidine L-52

Tritopine. Laudanine



(*R*)-*form*

$C_{20}H_{25}NO_4$ 343.422
The name Laudanine was originally applied to the racemate.

(R)-form [301-21-3]
Alkaloid from *Papaver somniferum* (opium poppy). Mp 184-185°. $[\alpha]_D^{28}$ -101 (EtOH).

Picrate:
Mp 174-175°.

Ac:
Mp 98°.

(S)-form [3122-95-0]
Mp 181-182°. $[\alpha]_D^{28}$ +134 (c, 0.51 in MeOH). $[\alpha]_D$ +87 (c, 0.56 in $CHCl_3$).

N-*Me:* **N-*Methyllaudanidinium***
$C_{21}H_{28}NO_4^{\oplus}$ 358.456
Amorph. solid (as iodide). $[\alpha]_D^{23}$ +72 (c, 0.04 in MeOH).

Me ether: Laudanosine, L-53

(±)-*form* [85-64-3] ***Laudanine***
Alkaloid from *Papaver somniferum* (opium poppy). Mp 166-167°. Log P 2.91 (calc).

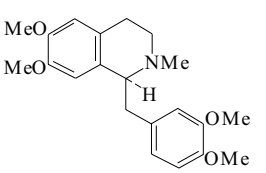
Picrate:
Mp 176-177°.

Benzoyl:
Mp 156-157°.

Späth, E. *et al., Monatsh. Chem.*, 1926, **47**, 733-740 (*synth*)
Wu, J. *et al., J. Nat. Prod.*, 1977, **40**, 593-601 (*isol, uv, pmr*)
Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 2299-2309 (*N-Methyllaudanidinium*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 1073

Laudanosine L-53

N-*Methyltetrahydropapaverine. Laudanine methyl ether*



(*S*)-*form*

$C_{21}H_{27}NO_4$ 357.449

(R)-form [85-63-2]
Mp 83-85°. $[\alpha]_D^{20}$ -85 (c, 0.45 in EtOH).

(S)-form [2688-77-9]
Alkaloid from *Papaver somniferum* (opium poppy). Mp 89°. $[\alpha]_D^{25}$ +103 (EtOH). $[\alpha]_D$ +52 ($CHCl_3$).

Methiodide:
Mp 225-227° (218-221°). $[\alpha]_D$ +120.

(±)-*form* [1699-51-0]
Mp 114-115° (67-70°).

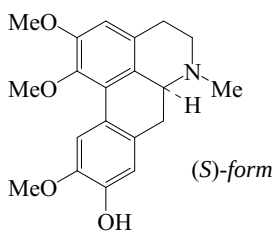
► NX5070000

Hydrochloride:
Mp 123°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1318A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 667C (*nmr*)
Cymerman-Craig, J. *et al., Tetrahedron*, 1966, **22**, 1335-1339 (*uv, ord, config*)
Elliott, I.W. *et al., J. Het. Chem.*, 1970, **7**, 1229-1230 (*synth*)
Preininger, V. *et al., Alkaloids (N.Y.)*, 1975, **15**, 207 (*pharmacol*)
Konda, M. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1025-1031; 1977, **25**, 69-74 (*synth, ir, pmr, ms*)
Singh, S.P. *et al., J. Het. Chem.*, 1978, **15**, 541-544 (*cmr*)
Takano, S. *et al., Chem. Comm.*, 1982, 769-770 (*synth*)
Czarnocki, Z. *et al., Can. J. Chem.*, 1986, **64**, 2205-2210 (*synth*)
Gawley, R.E. *et al., Tet. Lett.*, 1988, **29**, 301-302 (*synth*)
Gottlieb, L. *et al., J.O.C.*, 1990, **55**, 5659-5662 (*synth*)
Coppola, G.M. *et al., J. Het. Chem.*, 1991, **28**, 1769-1772 (*synth*)
Comins, D.L. *et al., Tet. Lett.*, 1991, **32**, 2995-2996 (*synth*)
Takano, S. *et al., Heterocycles*, 1993, **35**, 47-52 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1200
Kitamura, M. *et al., J.O.C.*, 1994, **59**, 297-310 (*synth*)
Comins, D.L. *et al., Tetrahedron*, 1997, **48**, 16327-16340 (*synth*)

Lauroscholtzine L-54

*5,6,6*a*,7-Tetrahydro-1,2,10-trimethoxy-6-methyl-4*H*-dibenzo[*d,e*]quinolin-9-ol, 9CI. 9-Hydroxy-1,2,10-trimethoxyaporphine.* N-*Methyllaurotetanine. Rogersine*



(*S*)-*form*

$C_{20}H_{23}NO_4$ 341.406

(S)-form [2169-44-0]
Mp 100-105°. $[\alpha]_D$ +111 (c, 0.86 in MeOH).

► CE1057900

β-N-*Oxide:* [100010-00-2] **N-*Methyllaurotetanine β*-N-*oxide***
$C_{20}H_{23}NO_5$ 357.405
Amorph. $[\alpha]_D^{25}$ +49 (c, 0.15 in MeOH).

N-*De-Me:* [128-76-7] *9-Hydroxy-1,2,10-*

trimethoxynoraporphine. ***Laurotetanine.*** *Litsoene*
$C_{19}H_{21}NO_4$ 327.379
Alkaloid from the leaves of *Peumus boldus* (boldo). Mp 125°. $[\alpha]_D$ +95 (c, 0.50 in EtOH). λ_{max} 219 ; 282 ; 304 (MeOH) (Berdy).
► RB6025000

N-*De-Me, hydrochloride:*
Mp 245°.

N-*Me:* [6872-88-4] ***Xanthoplanine***
$C_{21}H_{26}NO_4^{\oplus}$ 356.441
Quaternary alkaloid from *Litsea cubeba* (mountain pepper). Mp 207-209° (as iodide). $[\alpha]_D^{21}$ +62 (c, 0.83 in EtOH).

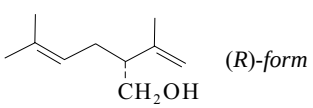
(±)-*form* [38849-65-9]
Mp 199-202° dec. (143-144°).

N-*De-Me:* [65877-55-6]
$C_{19}H_{21}NO_4$ 327.379

Ruegger, A. *et al., Helv. Chim. Acta*, 1959, **42**, 754 (*isol, uv, Laurotetanine*)
Ishii, H. *et al., Yakugaku Zasshi*, 1961, **81**, 238 (*Xanthoplanine*)
Pachler, K.G.R. *et al., Tetrahedron*, 1965, **21**, 2159 (*struct, pmr, Laurotetanine*)
Albonico, S.M. *et al., J.C.S.(C)*, 1966, 1340 (*uv, ord, Xanthoplanine*)
Kametani, T. *et al., J.C.S. Perkin 1*, 1972, 1435 (*synth, specra, derivs*)
Govindachari, T.R. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 873 (*synth, Laurotetanine*)
Marsaioli, A.J. *et al., Phytochemistry*, 1979, **18**, 165 (*cmr, Xanthoplanine*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80 (*cd, Laurotetanine, N-Methyllaurotetanine*)
Montgomery, C.T. *et al., J. Nat. Prod.*, 1985, **48**, 833 (*N-Methyllaurotetanine β-N-oxide*)
Hara, H. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1946 (*synth*)
Lee, S.S. *et al., J. Nat. Prod.*, 1993, **56**, 1971 (*isol, uv, ir, pmr, Xanthoplanine*)
Lee, S.-S. *et al., J. Nat. Prod.*, 1996, **59**, 55 (*cd*)
Chen, J.-J. *et al., Planta Med.*, 2000, **66**, 251-256 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LBO200; TKX700

Lavandulol L-55

5-Methyl-2-(1-methylethenyl)-4-hexen-1-ol, 9CI. 2-Isopropenyl-5-methyl-4-hexen-1-ol



(*R*)-*form*

$C_{10}H_{18}O$ 154.252

(*R*)-*form* [498-16-8]
Constit. of French lavender oil. Bp_{13} 94-95°. $[\alpha]_D^{20}$ -10.7 (c, 1.01 in MeOH) (opt. pure).
► MP8623000

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Kenposide B***
$C_{21}H_{36}O_{10}$ 448.509
Constit. of *Hovenia dulcis* (raisin tree). Oil. $[\alpha]_D$ -41.6 (c, 4.5 in MeOH).

(*S*)-*form* [50373-53-0]
$[\alpha]_D^{20}$ +10.11 (neat) (opt. pure). Inactive as a pheromone.

O-*(3-Methyl-2-butenoyl):* [337465-11-9] ***Lavandulyl senecioate***
$C_{15}H_{24}O_2$ 236.353

(±)-*form* [1845-51-8]
d_4^{17} 0.88. Bp_6 100-101°. n_D^{17} 1.4710.

Ac: [25905-14-0]
$C_{12}H_{20}O_2$ 196.289
d_4^{20} 0.98. Bp_{12} 143-144°. n_D^{20} 1.4560.
► Skin irritant.

[20777-39-3]

Schinz, H. *et al., Helv. Chim. Acta*, 1947, **30**, 1483 (*synth*)
Soucek, M. *et al., Coll. Czech. Chem. Comm.*, 1959, **24**, 3802 (*abs config*)
Baba, S.N. *et al., Tetrahedron*, 1966, **22**, 903 (*synth, rev*)
Banthorpe, D.V. *et al., Phytochemistry*, 1977, **16**, 85 (*biosynth*)
Bertrand, M. *et al., Tet. Lett.*, 1977, 1785 (*synth*)
Kramer, A. *et al., Helv. Chim. Acta*, 1982, **65**, 293 (*synth, ir, pmr, bibl*)
Takano, S. *et al., J.O.C.*, 1985, **50**, 931 (*synth*)
Celebuski, J. *et al., Tetrahedron*, 1985, **41**, 5741 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 55S (*rev, tox*)
Yoshikawa, K. *et al., Phytochemistry*, 1993, **34**, 1431 (*Kenposide B*)
Imai, T. *et al., Chem. Comm.*, 1994, 277 (*synth*)
Piva, O. *et al., J.O.C.*, 1995, **60**, 7879 (*synth*)
Fleming, I. *et al., Tet. Lett.*, 1996, **37**, 6929 (*synth*)
Mino, T. *et al., J.O.C.*, 1997, **62**, 734 (*synth*)
Hinkens, D.M. *et al., Tet. Lett.*, 2001, **42**, 1619-1621 (*Lavandulyl senecioate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LCA100

Grifola frandosa Lectin L-56

GFL
Monomeric glycoprotein, MW 33 kDa. Isol. from fruiting bodies of *Grifola frondosa* (maitake). *N*-Acetylgalactosamine-specific lectin.

Kawagishi, H. *et al., Biochim. Biophys. Acta*, 1990, **1034**, 247-252 (*isol*)

Legnodulic acid L-57

Struct. unknown. Constit. of the root nodules of *Vicia faba*. Hexagonal plates. Mp 250° dec.

Ishida, Y. *et al., Yakugaku Zasshi*, 1959, **79**, 790; *CA*, **53**, 19049h (*isol*)

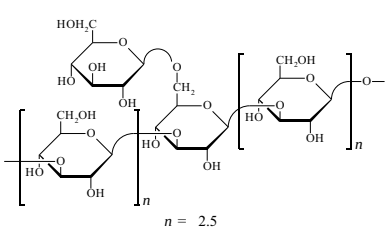
LEM JLS 18 L-58

The water-sol. lignin-rich fraction of LEM, the extract of the solid culture medium of *Lentinus edodes* mycelia. Isol. from *Lentinus edodes* (shiitake).

Yamamoto, Y. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1909-1912 (*isol*)

Lentinan L-59

[37339-90-5]



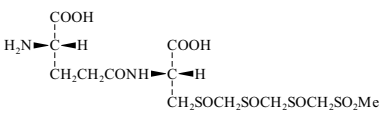
A highly (1→6) branched (1→3)β-D-glucan. Elaborated by the fungus *Lentinus edodes* (shiitake). Launched 1986. Powder. Sol. H_2O, DMSO; fairly sol. H_2O; poorly sol. EtOH, hexane. Forms nonelastic gel in aq. suspensions.

[114285-68-6]

Chihara, G. *et al., Nature (London)*, 1969, **222**, 687; 1971, **229**, 634 (*isol, pharmacol*)
Sasaki, T. *et al., Carbohydr. Res.*, 1976, **47**, 99 (*pharmacol*)
Bluhm, T.L. *et al., ACS Symp. Ser.*, 1977, **48**, 105 (*cryst struct*)
Saito, H. *et al., Carbohydr. Res.*, 1979, **74**, 227-240 (*cmr, struct*)
Saito, H. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2093 (*conform, cmr*)
Tsukagoshi, S. *et al., Drugs of Today (Barcelona)*, 1988, **24**, 91 (*rev*)
Suzuki, M. *et al., Int. J. Immunopharmacol.*, 1994, **16**, 463 (*rev*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1721
Gordon, M. *et al., J. Med. (Westbury, N.Y.)*, 1998, **29**, 305-330 (*pharmacol*)

Lentinic acid L-60

[12705-98-5]



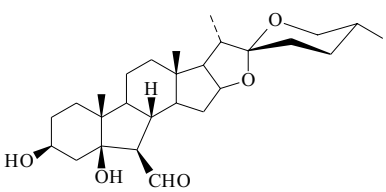
$C_{12}H_{22}N_2O_{10}S_4$ 482.577
Isol. from the mushroom *Lentinus edodes*.

Diastereoisomer: [74958-22-8] ***Epilentinic acid***
$C_{12}H_{22}N_2O_{10}S_4$ 482.577
Like Lentinic acid, conts. 2 L-amino acid residues, therefore is epimeric with Lentinic acid at one or more sulfoxide functions.

Yasumoto, K. *et al., Agric. Biol. Chem.*, 1971, **35**, 2059
Gmelin, R. *et al., Phytochemistry*, 1980, **19**, 553

Leontogenin L-61

6β-Formyl-B-nor-5β,25R-spirostane-3β,25-diol

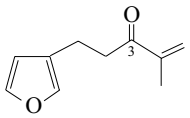


$C_{27}H_{42}O_5$ 446.626
Constit. of *Tacca leontopetaloides* (Polynesian arrowroot). Gum.

Abdel-Aziz, A. *et al., Phytochemistry*, 1990, **29**, 2623 (*isol, pmr, ir, cmr, ms*)

Lepalone L-62

[80445-58-5]
5-(3-Furyl)-2-methyl-1-penten-3-one



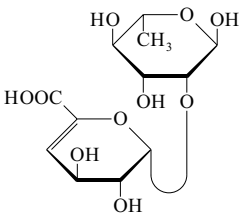
$C_{10}H_{12}O_2$ 164.204
Constit. of Roman camomile oil (*Anthemis nobilis*). Oil.

3-Alcohol: [72075-28-6] *α-(1-Methylethenyl)-3-furanpropanol, 9CI. 5-(3-Furyl)-2-methyl-1-penten-3-ol.* ***Lepalol***
$C_{10}H_{14}O_2$ 166.219
Oil with pleasant odour. Bp_4 108-111°. n_D^{20} 1.4925. Opt. inactive.

Mikhailova, N.S. *et al., Khim. Prir. Soedin.*, 1979, 322; *Chem. Nat. Compd. (Engl. Transl.)*, 278 (*Lepalol*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1981, **64**, 2393 (*Lepalone*)

Lepidimoic acid L-63

[157676-09-0]
*6-Deoxy-2-O-(4-deoxy-β-L-*threo*-hex-4-enopyranuronosyl)-L-mannose, 9CI. Lepidimoide*



α-Pyranose-*form*

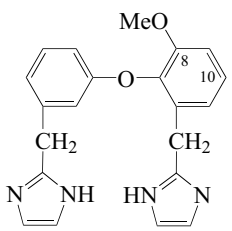
$C_{12}H_{18}O_{10}$ 322.268
Isol. from seeds of *Lepidium sativum* (garden cress). Oil, amorph. powder (as Na salt). $[\alpha]_D^{19}$ +87.8 (c, 0.03 in D_2O). Strictly the Na salt is named Lipodimoide.

[145039-76-5]

Hasegawa, K. *et al., Plant Physiol.*, 1992, **100**, 1059-1061 (*isol*)
Kosemura, S. *et al., Tet. Lett.*, 1993, **34**, 2653-2656 (*abs config, synth*)
Yamada, K. *et al., Phytochemistry*, 1995, **39**, 1031-1032; 1996, **41**, 671 (*occur, activity*)
Yokotani-Tomita, K. *et al., Phytochemistry*, 1998, **47**, 1-2 (*isol, pmr*)
Hirose, K. *et al., Tet. Lett.*, 2003, **44**, 2171-2173 (*synth*)

Lepidine L-64

[100108-65-4]



$C_{21}H_{20}N_4O_2$ 360.415
Alkaloid from the seeds of *Lepidium sativum* (garden cress). Cryst. (CH_2Cl_2/MeOH).

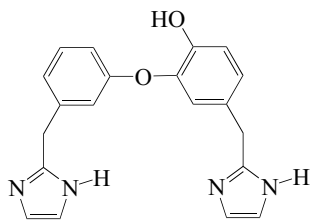
O-*De-Me:* ***Lepidine B***
$C_{20}H_{18}N_4O_2$ 346.388
Alkaloid from *Lepidium sativum* (garden cress). Yellow cryst. (CH_2Cl_2/MeOH). Mp 212-214°.

8-Demethoxy, 10-hydroxy: ***Lepidine D***
$C_{20}H_{18}N_4O_2$ 346.388
Alkaloid from *Lepidium sativum* (garden cress). Yellow cryst. (CH_2Cl_2/MeOH). Mp 202-204°.

8-Demethoxy, 10-methoxy: ***Lepidine C***
$C_{21}H_{20}N_4O_2$ 360.415
Alkaloid from *Lepidium sativum* (garden cress). Yellow cryst. (CH_2Cl_2/MeOH). Mp 194-195°.

Bahroun, A. *et al., J. Soc. Chim. Tunis.*, 1985, **2**, 15; *CA*, **104**, 65910g
Maier, U.H. *et al., Phytochemistry*, 1998, **49**, 1791-1795 (*isol, pmr, cmr, ms*)

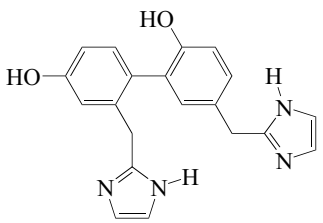
Lepidine E L-65



$C_{20}H_{18}N_4O_2$ 346.388
Alkaloid from the seeds of *Lepidium sativum* (garden cress). Yellow cryst. (CH_2Cl_2/MeOH). Mp 196-198°.

Maier, U.H. *et al., Phytochemistry*, 1998, **49**, 1791-1795 (*isol, pmr, cmr, ms*)

Lepidine F L-66

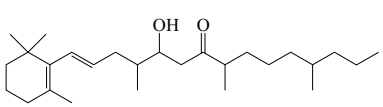


$C_{20}H_{18}N_4O_2$ 346.388
Alkaloid from the seeds of *Lepidium sativum* (garden cress). Pale yellow cryst. (CH_2Cl_2/MeOH). Mp 245-247°.

Maier, U.H. *et al., Phytochemistry*, 1998, **49**, 1791-1795 (*isol, pmr, cmr, ms*)

Lepidiumterpenoid L-67

[255833-56-8]



$C_{27}H_{48}O_2$ 404.675
Unusual irregular terpenoid. Constit. of *Lepidium sativum* (garden cress). Cryst. ($CHCl_3$). Mp 120-121°. λ_{max} 204 (log ε 2.8); 263 (log ε 0.9) (MeOH).

Pande, S.D. *et al., Pharmazie*, 1999, **54**, 851-853 (*isol, pmr, cmr*)

Leptin L-68

[169494-85-3]

[177404-21-6]
Ob gene product

A 16-kDa peptide hormone with 167 amino acid residues. Implicated in the regulation of food intake, energy expenditure and whole-body energy balance.

Human-*form* [177404-21-6]

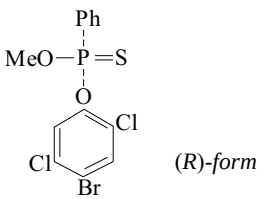
N-*Methionyl:* [186018-45-1]

[177404-22-7] ***Metreleptin, INN, USAN.*** N-*Methionylleptin (human)*

Zhang, X.-Y. *et al., Nature (London)*, 1994, **372**, 425-432; 1995, **377**, 530-532; 1996, **382**, 589 (*cloning, activity*)
Caro, J.F. *et al., Diabetes*, 1996, **45**, 1455-1462 (*activity*)
Bray, G.A. *et al., Lancet*, 1996, **348**, 140-141 (*activity*)
Meinders, A.E. *et al., Neth. J. Med.*, 1996, **49**, 247-252 (*rev*)
U.K. Pat., (Rockefeller Univ.), 1996, 2 292 382; *CA*, **125**, 26940f (*metreleptin*)
Frohbeck, G. *et al., Clin. Physiol.*, 1998, **18**, 399-419 (*rev*)
Prolo, P. *et al., Int. J. Biochem. Cell Biol.*, 1998, **30**, 1285-1290 (*rev*)
Houseknecht, K. *et al., J. Anim. Sci.*, 1998, **76**, 1405-1420 (*rev*)
Marti, A. *et al., J. Physiol. Biochem.*, 1999, **55**, 43-49 (*rev*)
Schwartz, M.W. *et al., Nature (London)*, 2000, **404**, 661-671 (*rev*)

Leptophos, BSI L-69

[21609-90-5]
O-*4-Bromo-2,5-dichlorophenyl* O-*methyl phenylphosphonothioate, 9CI. Phosvel. Abar*



(*R*)-*form*

$C_{13}H_{10}BrCl_2O_2PS$ 412.07
▶ V. toxic if swallowed and in contact with skin. LD_{50} (rat, orl) 19 mg/kg. LD_{50} (rat, skn) 44 mg/kg. Exp. teratogen. Exp. neurotoxic effects. TB1720000

(R)-form
Mp 88-90°. $[\alpha]_D^{24}$ +46.13 (c, 10.6 in C_6H_6).
▶ More toxic (housefly, mouse) than (*S*)-form.

(S)-form
Mp 88-90°. $[\alpha]_D^{24}$ -46.26 (c, 10 in C_6H_6) (98% op).
▶ Shows more delayed neurotoxic effect (hen) than (*R*)-form.

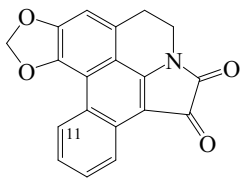
(±)-form
Agricultural insecticide, now superseded. Cryst. (EtOH). V. sol. hexane, Me_2CO, v. spar. sol. H_2O. Mp 71-72°. Stable at pH 1-7, dec. at pH >7. Degraded by uv.
▶ Exhibits delayed neurotoxicity; causes

irreversible ataxia.

U.K. Pat., 1965, 1 197 111; *CA*, **71**, 81519s
Holmstead, R.L. *et al., Arch. Environ. Contam. Toxicol.*, 1973, **1**, 133 (*metab, tlc, ms*)
Steurbaut, W. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 791 (*synth, ir, pmr*)
Lee, R.W. *et al., Arch. Environ. Contam. Toxicol.*, 1976, **4**, 443 (*metab*)
Busch, K.L. *et al., Appl. Spectrosc.*, 1978, **32**, 388 (*ms*)
Hollingshaus, J.G. *et al., J. Agric. Food Chem.*, 1979, **27**, 1197 (*tox*)
Pesticide Manual, 6th edn., 1979, 318
Lapp, R.L. *et al., Cryst. Struct. Commun.*, 1980, **9**, 65 (*cryst struct*)
Allahyari, R. *et al., J. Agric. Food Chem.*, 1980, **28**, 594 (*enantiomers, synth, tox*)
Francis, B.M. *et al., J. Environ. Sci. Health, Part B*, 1982, **17**, 611 (*tox*)
Purnanand, R.K.D. *et al., Synthesis*, 1983, 731 (*synth, ir, pmr*)
Baker, S.M. *et al., J. Agric. Food Chem.*, 1995, **43**, 503-506 (*cryst struct*)
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1086
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LEN000

Lettowianthine L-70

Annobraine



$C_{19}H_{11}NO_4$ 317.3

Alkaloid from *Annona glabra* (pond apple). Dark red solid ($CHCl_3$); red needles ($CHCl_3$). Mp 314-317° dec. (265-267°). λ_{max} 254 (log ϵ 4.02); 293 (log ϵ 3.42); 323 (sh) (log ϵ 3.5); 333 (log ϵ 3.55); 365 (log ϵ 3.23); 509 (log ϵ 3.07) (MeOH) (Lettowianthine). λ_{max} 232 (sh) (log ϵ 3.97); 253 (log ϵ 4.37); 280 (log ϵ 3.8); 291 (log ϵ 3.84); 333 (log ϵ 3.64); 355 (sh) (log ϵ 3.43); 373 (log ϵ 3.2) (EtOH) (Annobraine).

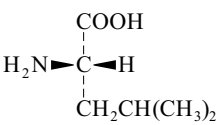
*11-Hydroxy:**11-Hydroxylettowianthine***
$C_{19}H_{11}NO_5$ 333.3
Dark red amorph. solid. λ_{max} 260 (log ϵ 4.09); 292 (log ϵ 3.48); 311 (sh) (log ϵ 3.28); 355 (log ϵ 3.25); 505 (log ϵ 3.02) (MeOH).

Chang, F.R. *et al., J. Chin. Chem. Soc. (Taipei)*, 2000, **47**, 913-920 (*Annobraine*)
Nkunya, M.H.H. *et al., Phytochemistry*, 2000, **53**, 1067-1073 (*Lettowianthine, 11-Hydroxylettowianthine*)

Leucine, 9CI, USAN L-71

[7005-03-0]

2-Amino-4-methylpentanoic acid. 2-Aminoisocaproic acid. 4-Methylnorvaline. Leu. Chenopodine



(*S*)-*form*

$C_6H_{13}NO_2$ 131.174
$[\alpha]_D^{16}$ +14 (c,1.3 in H_2O). Log P -1.67 (calc). Derivs. useful in peptide synth. are listed elsewhere.

(*S*)-*form* [61-90-5]
L-form. FEMA 3297
Flavouring ingredient; dietary supplement, nutrient. Plates (EtOH aq.). Spar. sol. H_2O (2.3 g/100 cm^3 at 25°). Mp 337° (293-295°) dec. $[\alpha]_D^{20}$ -10.42 (H_2O). $[\alpha]_D^{15}$ +17.3 (20% HCl). pK_{a1} 2.33; pK_{a2} 9.74 (25°). Log P -1.67 (calc). Isoelectric point 5.98. Bitter taste.
► Exp. reprod. and teratogenic effects (v. large doses). OH2850000

(±)-*form* [328-39-2]
Dietary supplement, nutrient. Plates (H_2O). V. spar. sol. EtOH. Mp 293-295° (sealed tube). pK_{a1} 2.33; pK_{a2} 9.74 (25°).

[5845-53-4, 10466-61-2, 13366-40-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 575A; 575B; 575C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 875B (*nmr*)
Fischer, E. *et al., Ber.*, 1900, **33**, 2370; 2377; 1901, **34**, 445; 1905, **38**, 615; 3997; 4002
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 31), Wiley, N.Y., 1961, 2075; 2750; 2758 (*rev*)
Heyns, K. *et al., Annalen*, 1963, **667**, 194 (*ms*)
Di Blasio, B. *et al., Acta Cryst. B*, 1975, **31**, 601; 2941 (*cryst struct*)
Oguri, T. *et al., Chem. Pharm. Bull.*, 1975, **23**, 167 (*synth*)
Harding, M.M. *et al., Acta Cryst. B*, 1976, **32**, 633 (*cryst struct*)
Kovalev, V.N. *et al., Khim. Prir. Soedin.*, 1985, **21**, 724; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 687 (*isol*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, LER000; LES000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 597
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 429
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1567-1569
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LER000; LES000

Leucocidin R1 L-72

[171172-66-0]

Struct. unknown. Prod. by *Leuconostoc paramesenteroides* NM-14 isol. from an aged cream sample. Bacteriocin.

Malik, R.K. *et al., Microbiol., Aliments, Nutr.*, 1994, **12**, 443-448 (*isol*)

Leucocins L-73

Polypeptide bacteriocins.

Leucocin A [139069-78-6]
KYYGNGVHCTKSGCSVNWGEAFSAGVHRLANGGNGFW
Linear polypeptide with 37 AA's. See ref. for struct.. Bacteriocin prod. by *Leuconostoc gelidum* VAL187. Isol. from vacuum-packaged meat.

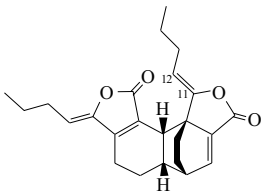
Leucocin D La54a
Prod. by *Leuconostoc carnosum* La54a isol. from meat.

Leucocin F10 [184973-27-1]
Prod. by *Leuconostoc carnosum* isol. from fermented meat.

[145170-91-8, 145170-92-9]

Hastings, J.W. *et al., J. Appl. Bacteriol.*, 1991, **70**, 127 (*Leucocin A, isol*)
Henkel, T. *et al., J.A.C.S.*, 1992, **114**, 1898 (*Leucocin A, pmr, struct*)
Hastings, J.W. *et al., Int. J. Food Microbiol.*, 1994, **24**, 75-81 (*Leucocin D La54A*)
Parente, E. *et al., Int. J. Food Microbiol.*, 1996, **33**, 231-243 (*Leucocin F10*)

Levistolide L-74



(11*Z*)-*form*

$C_{24}H_{28}O_4$ 380.483

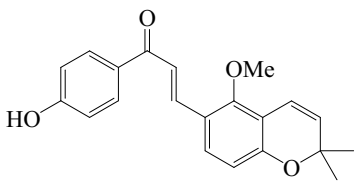
(11*E*)-*form* [89708-24-7]
Levistolide B
Constit. of *Levisticum officinale* (lovage).

(11*Z*)-*form* [89708-23-6]
Levistolide A
Constit. of *Levisticum officinale* (lovage). Cryst. (Et_2O/hexane). Mp 112-113°.

(11*Z*)-(±)-*form* [88182-33-6]
Diligustilide
Cryst. Mp 123°.

Kaouadji, M. *et al., Tet. Lett.*, 1983, **24**, 4677 (*Diligustilide*)
Cichy, M. *et al., Annalen*, 1984, 397
Delgado, G. *et al., Heterocycles*, 1988, **27**, 1305 (*Diligustilide*)
Ogawa, Y. *et al., Heterocycles*, 1997, **45**, 1869-1872 (*synth, pmr*)
Rios, M.Y. *et al., Tetrahedron*, 1998, **54**, 3355-3366 (*Diligustilide, synth*)

Licoagrochalcone B L-75

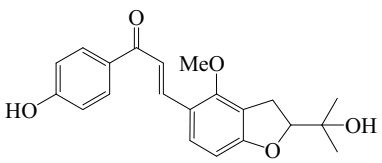


$C_{21}H_{20}O_4$ 336.387

Isol. from hairy root cultures of *Glycyrrhiza glabra* (licorice). Yellow powder. λ_{max} 290 (log ϵ 3.7); 350 (log ϵ 3.73) (MeOH).

Li, W. *et al., Phytochemistry*, 2000, **55**, 447-456

Licoagrochalcone D L-76

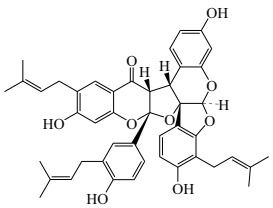


$C_{21}H_{22}O_5$ 354.402

Isol. from hairy root cultures of *Glycyrrhiza glabra*. Yellow powder. $[\alpha]_D^{24}$ -8.7 (c, 0.23 in $CHCl_3$). λ_{max} 260 (log ε 3.83); 300 (sh) (log ε 3.87); 356 (log ε 4.16) (MeOH).

Li, W. *et al., Phytochemistry*, 2000, **55**, 447-456

Licoagrodin L-77



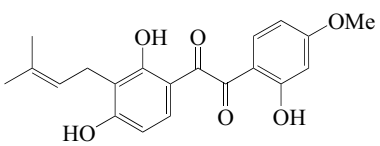
Relative Configuration

$C_{45}H_{44}O_9$ 728.837
Isol. from hairy root cultures of *Glycyrrhiza glabra* (licorice). Yellow powder. Racemic λ_{max} 230 (sh) (log ε 4.49); 280 (log ε 4.23); 326 (log ε 3.93) (MeOH).

Li, W. *et al., Phytochemistry*, 2000, **55**, 447-456

Licoagrodione L-78

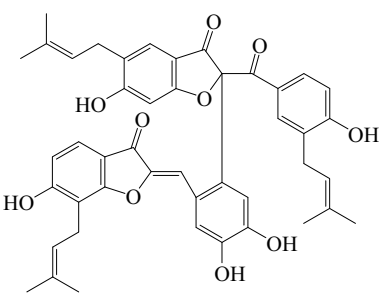
1-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)-phenyl]-2-(2-hydroxy-4-methoxyphenyl)ethanedione



$C_{20}H_{20}O_6$ 356.374
Constit. of hairy root cultures of *Glycyrrhiza glabra* (licorice). Yellow powder. λ_{max} 234 (sh) (log ε 4.26); 290 (log ε 4.3); 326 (log ε 4.3) (MeOH).

Li, W. *et al., Planta Med.*, 1998, **64**, 746-747 (*isol, uv, pmr, cmr*)

Licoagrone L-79

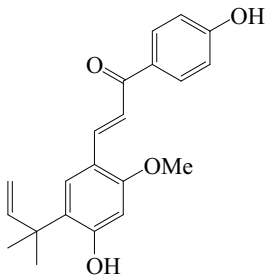


$C_{45}H_{42}O_{10}$ 742.821
Isol. from hairy root cultures of *Glycyrrhiza glabra*. Orange powder. Racemate λ_{max} 230 (sh) (log ε 4.55); 278 (log ε 4.46); 324 (log ε 4.41); 396 (log ε 4.25) (MeOH).

Asada, Y. *et al., Phytochemistry*, 1999, **50**, 1015-1019 (*isol, uv, ir, pmr, cmr, ms*)

Licochalcone A L-80

[58749-22-7]
3-[5-(1,1-Dimethyl-2-propenyl)-4-hydroxy-2-methoxyphenyl]-1-(4-hydroxyphenyl)-2-propen-1-one, 9CI. 5-(1,1-Dimethylallyl)-4,4′-dihydroxy-2-methoxychalcone

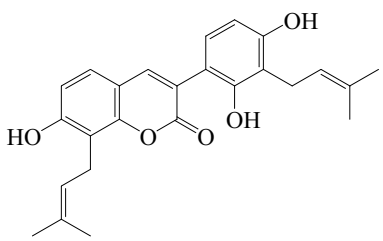


$C_{21}H_{22}O_4$ 338.402
Constit. of the roots of *Glycyrrhiza glabra* (licorice). Yellow needles. Mp 101-102°. Log P 4.26 (calc). Unusual 'retroflavonoid' hydroxylation pattern.

Saitoh, T. *et al., Tet. Lett.*, 1975, 4461; 4463 (*isol, struct, biosynth*)
Khan, S.A. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 276 (*synth*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2286 (*activity*)
Shibata, S. *et al., Planta Med.*, 1991, **57**, 221 (*pharmacol*)
Islam, A. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 713 (*synth*)
Chen, M. *et al., Antimicrob. Agents Chemother.*, 1994, **38**, 1339; 1470 (*activity*)
Feldbaek, N. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 449 (*synth*)

Licocoumarin A L-81

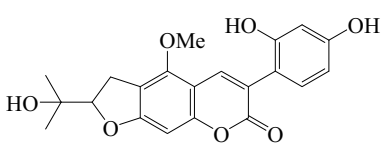
3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)-phenyl]-7-hydroxy-8-(3-methyl-2-butenyl)-2H-1-benzopyran-2-one



$C_{25}H_{26}O_5$ 406.477
Constit. of *Glycyrrhiza glabra* (licorice). Amorph. yellow solid. λ_{max} 252 (log ε 3.81); 352 (log ε 4.24) (MeOH).

Baba, M. *et al., Heterocycles*, 1999, **51**, 387-391 (*isol, uv, pmr, cmr, ms*)

Licofuranocoumarin L-82

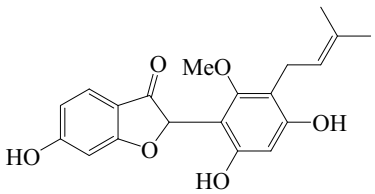


$C_{21}H_{20}O_7$ 384.385
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow needles. Mp 242°. $[\alpha]_D$ -4.2 (c, 1 in EtOH). λ_{max} 212 (log ε 4.61); 254 (log ε 3.95); 354 (log ε 4.24) (MeOH).

Hatano, T. *et al., Phytochemistry*, 2000, **55**, 959-963

Licofuranone L-83

[161099-38-3]
2-[4,6-Dihydroxy-2-methoxy-3-(3-methyl-2-butenyl)phenyl]-6-hydroxy-3(2H)-benzofuranone, 9CI

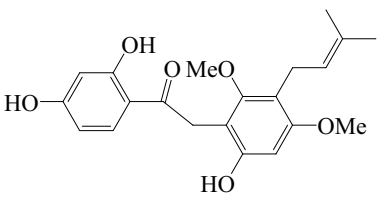


$C_{20}H_{20}O_6$ 356.374
Constit. of licorice (*Glycyrrhiza* sp.). Needles + $^1/_2H_2O$. Mp 162°. Racemic λ_{max} 212 (log ε 4.69); 232 (sh) (log ε 4.32); 272 (log ε 4.12); 317 (log ε 3.92); 331 (sh) (log ε 3.84) (MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1238-1243

Licoriphenone L-84

[129280-36-0]



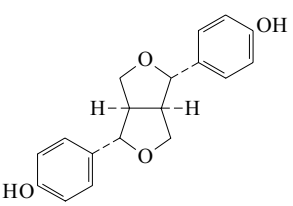
$C_{21}H_{24}O_6$ 372.417
Constit. of licorice (*Glycyrrhiza* sp.). Needles (Et_2O/hexane). Mp 136-138°.

*4-O-De-Me:**Glicophenone***
$C_{20}H_{22}O_6$ 358.39
Constit. of Chinese licorice, *Glycyrrhiza uralensis*. Needles. Mp 145°. λ_{max} 209 (log ε 4.64); 230 (sh) (log ε 4.21); 276 (log ε 4.13); 313 (log ε 3.63) (MeOH).

Kiuchi, F. *et al., Heterocycles*, 1990, **31**, 629-636 (*Licoriphenone*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1286-1292 (*Glicophenone*)

Ligballinol L-85

4,4′-(Tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl)bisphenol, 9CI. 2,6-Bis-(4-hydroxyphenyl)-3,7-dioxabicyclo[3.3.0]octane. 4,4′-Dihydroxy-7,9′:7′,9-diepoxylignan



(+)-*form*

$C_{18}H_{18}O_4$ 298.338

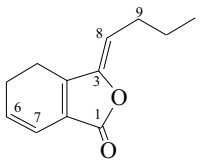
(+)-*form*
Stress metabolite of cell cultures of *Vigna angularis* (azuki bean). Needles. $[\alpha]_D$ +25.3.

(-)-*form* [55332-75-7]
Needles ($CHCl_3$). Mp 264-266°. $[\alpha]_D$ -7.1 (c, 1.61 in MeOH). Abs. config. and struct. doubtful.

Rao, M.M. *et al., Tetrahedron*, 1974, **30**, 3309 (*isol*)
Kobayashi, M. *et al., Phytochemistry*, 1983, **22**, 1257 (*isol*)

Ligustilide L-86

[4431-01-0]
*3-Butylidene-4,5-dihydro-1(3*H*)-isobenzofuranone, 9CI. 3-Butylidene-4,5-dihydrophthalide, 8CI*



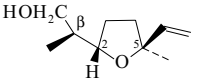
$C_{12}H_{14}O_2$ 190.241
Constit. of *Angelica* spp. Oil. Bp_6 168-169°. λ_{max} 320 (ε 2400) (MeOH) (Berdy).

9-Angeloyloxy: [112899-64-6] ***Angeloylsenkyunolide F***
$C_{17}H_{20}O_4$ 288.343
Constit. of *Angelica acutiloba* (Dong Dang Gui). Oil. $[\alpha]_D$ +26 (c, 0.7 in $CHCl_3$).

Stahl, E. *et al., Naturwissenschaften*, 1967, **54**, 118 (*isol*)
Mitsuhashi, H. *et al., CA*, 1969, **71**, 88456 (*isol*)
Nikonov, G.K. *et al., Khim. Prir. Soedin.*, 1971, **7**, 387; *Chem. Nat. Compd. (Engl. Transl.)*, 373 (*isol*)
Yamagishi, T. *et al., CA*, 1975, **83**, 84751; 1976, **84**, 132662 (*isol*)
Yamagishi, T. *et al., Yakugaku Zasshi*, 1977, **97**, 237 (*isol*)
Tsuchida, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4460 (*Angeloylsenkyunolide F*)
Naito, T. *et al., Phytochemistry*, 1992, **31**, 639 (*isol, abs config*)
Li, S. *et al., Synth. Commun.*, 1993, **23**, 2061; 2909 (*synth, deriv*)
Beck, J.J. *et al., J. Nat. Prod.*, 1995, **58**, 1047 (*synth, pmr*)
Ogawa, Y. *et al., Synlett*, 1995, 871 (*synth*)

Lilac alcohol L-87

5-Ethenyltetrahydro-β,5-dimethyl-2-furanethanol, 9CI



(β*S*,2*S*,5*S*)-*form*

$C_{10}H_{18}O_2$ 170.251
Incorrectly named as 5-Ethenyltetrahydro-α,5-dimethyl-2-furanethanol in 8CI.
Constit. of dried woodruff and coriander oil aroma. May also be present in honeys from certain flowers. Opt. rotns. are those measured for natl. lilac alcohols, which were obt. only in small amts. Somewhat different values were obt. for synthetic material of both enantiomeric series synth. from (+)- and (-)-linalool.

(β*S*,2*S*,5*S*)-*form* [33081-34-4]
Lilac alcohol a
$[\alpha]_D^{23}$ +12.2 (c, 4.1 in $CHCl_3$).

(β*R*,2*S*,5*S*)-*form* [33081-35-5]
Lilac alcohol b
$[\alpha]_D^{23}$ -6.6 (c, 3.6 in $CHCl_3$).

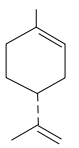
(β*R*,2*R*,5*S*)-*form* [33081-36-6]
Lilac alcohol c
$[\alpha]_D^{23}$ -1.4 (c, 1.8 in $CHCl_3$).

(β*S*,2*R*,5*S*)-*form* [33081-37-7]
Lilac alcohol d
$[\alpha]_D^{23}$ +4.3 (c, 1.7 in $CHCl_3$).

Wakayama, S. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3183 (*isol, synth*)
Lamparsky, D. *et al., Perfum. Flavor.*, 1988, **13**, 17-18 (*detn, coriander*)
Woerner, M. *et al., Z. Lebensm.-Unters. - Forsch.*, 1991, **193**, 317-320 (*detn, chromatog*)
Wilkins, A.L. *et al., J. Agric. Food Chem.*, 1993, **41**, 873-878 (*occur, honey*)

Limonene L-88

[138-86-3]
1-Methyl-4-(1-methylethenyl)cyclohexene, 9CI. 4-Isopropenyl-1-methylcyclohexene. p-*Mentha-1,8-diene. Citrene. Hesperidene. Diisoprene. Terpilene. Kautschine. Cinene. Cynene. Cajeputene. Isoterebentine. Carvene. FEMA 2633*



(*R*)-*form*

$C_{10}H_{16}$ 136.236
Found in over 300 essential oils, the (*R*)-form is the most widespread, followed by the racemate and then the (*S*)-form. Extensively used in the flavour industry.
► OS8100000

(*R*)-*form* [5989-27-5]
Major constit. of oil of orange rind, dill oil, oil of cumin, bergamot, caraway, lemon balm and lemon. Obt. comly. from orange oil on a large scale (ca. 50000 T/a). Flavouring agent. Nutriceutical with anticancer props.. Oil, with lemon-like odour. Bp_{20} 71°. $[\alpha]_D^{20}$ +126.8.
► LD_{50} (rat, orl) 4400 mg/kg. Exp. reprod. and teratogenic effects (large doses). GW6360000

(*S*)-*form* [5989-54-8]
Constit. of pine needle oil. Also present in ginger, nutmeg, pepper, mace, coriander and other herbs and spices. Oil. Sol. MeOH, hexane; poorly sol. H_2O. Bp 177.6-177.8°. $[\alpha]_D$ -122.6.
► Skin irritant. OS8350000

(±)-*form* [7705-14-8]
Dipentene
Constit. of many essential oils. Oil. Bp 178°.
► Flammable, fl. p. 45/53°, autoignition temp. 237°. Skin irritant.

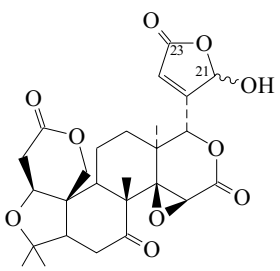
Diepoxide: [96-08-2] *1-Methyl-4-(2-methyloxiranyl)-7-oxabicyclo[4.1.0]heptane, 9CI. 1,2:8,9-Diepoxymethane. Dipentene diepoxide*
$C_{10}H_{16}O_2$ 168.235
Bp 242°. Coml. product undoubtedly a mixt. of diastereoisomers. Opt. active preparations, not fully characterised stereochemically, have also been reported.

[6876-12-6, 9003-73-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 43B; 43C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 70C; 71A; 71B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 63D; 64A (*ir*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Pawson, B.A. *et al., Chem. Comm.*, 1968, 1057 (*abs config*)
Verghese, J. *et al., Perfum. Essent. Oil Res.*, 1968, **59**, 439 (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 53; 54 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Nijaura, N. *et al., Chem. Lett.*, 1974, 1411 (*synth*)
Mukhamedovoa, L.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1974, **23**, 404-406; 1977, **26**, 2066-2070; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1974, **23**, 370-373; 1977, **26**, 1911-1915 (*diepoxides*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 825; 1978, **16**, 809 (*rev, tox*)
Org. Synth., 1977, **56**, 101 (*synth*)
Thomas, A.F. *et al., Nat. Prod. Rep.*, 1989, **6**, 291 (*rev*)
IARC Monog., 1993, **56**, 135 (*rev, tox*)
Pyun, H.-J. *et al., J.O.C.*, 1993, **58**, 3998 (*biosynth*)
Coates, R.M. *et al., Chem. Comm.*, 1997, 2079-2080 (*biosynth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1581-1584 (*occur, use*)
Rani, K. *et al., Fitoterapia*, 1998, **69**, 337-348 (*biosynth*)
Nakamura, H. *et al., J.O.C.*, 2002, **67**, 5124-5137 (*synth*)
Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 313
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 376
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LFU000; MCC250; MCC500

Limonexic acid L-89

[99026-99-0]
Limonexin. Shihulimonin A



$C_{26}H_{30}O_{10}$ 502.517
Constit. of *Citrus* spp.. Mp 285-286° dec. $[\alpha]_D^{25}$ -127. Photooxidn. prod. of Limonin, L-90, therefore prob. artifact.

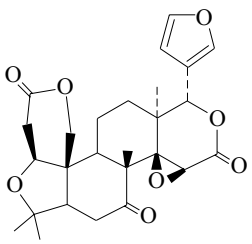
21-Me ether: [364615-53-2] *21*-O-*Methyllimonexic acid*
$C_{27}H_{32}O_{10}$ 516.544
Needles. Mp 296-298°. $[\alpha]_D$ -54 (c, 0.025 in CH_2Cl_2).

21-Oxo, 23ξ-alcohol: [113164-90-2] ***Isolimonexic acid***
$C_{26}H_{30}O_{10}$ 502.517
Needles (EtOAc). Mp 295°. $[\alpha]_D$ -65 (c, 0.13 in MeOH). Error in struct. diag. of ref..

Dreyer, D.L. *et al., Tetrahedron*, 1965, **21**, 75-87 (*Limonexic acid, pmr, bibl*)
Kondo, Y. *et al., Yakugaku Zasshi*, 1985, **105**, 742-746 (*Limonexic acid*)
Ng, K.M. *et al., J. Nat. Prod.*, 1987, **50**, 1160-1163 (*Isolimonexic acid*)
Lee, S.-Y. *et al., Nat. Med. (Tokyo)*, 1999, **53**, 255-258 (*cryst struct*)
Gai, L. *et al., Yaoxue Xuebao*, 2001, **36**, 743-745 (*Shihulimonin A*)
Biavatti, M.W. *et al., Z. Naturforsch., C*, 2001, **56**, 570-574 (*21-O-Methyllimonexic acid*)

Limonin L-90

[1180-71-8]
Limone†. *Citrolimonin. Evodine*†. *Dictamnolactone. Obaculactone*



$C_{26}H_{30}O_8$ 470.518
Isol. from oranges and other citrus fruits (*Citrus* spp.).. Cryst. (CH_2Cl_2/2-propanol). Mp 298°. $[\alpha]_D$ -125 (Me_2CO). λ_{max} 207 (ϵ 7000); 285 (ϵ 38) (EtOH) (Berdy).

Deepoxy: ***Desoxylimonin***
$C_{26}H_{30}O_7$ 454.519
Isol. from grapefruit seeds. Cryst. (Me_2CO/EtOH). Mp 323-325°. $[\alpha]_D$ -39 (c, 1.08 in $CHCl_3$). Conts. a double bond in place of the epoxide function.

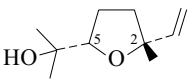
12α-Hydroxy: [120693-65-4] ***12α-Hydroxylimonin***
$C_{26}H_{30}O_9$ 486.518
Powder. $[\alpha]_D^{20}$ -134 (c, 1 in $CHCl_3$). λ_{max} 205 (log ϵ 3.76) (MeOH).

Schechter, M. *et al., J.A.C.S.*, 1940, **62**, 1307
Barton, D.H.R. *et al., J.C.S.*, 1961, 255 (*struct*)
Arnott, S. *et al., J.C.S.*, 1961, 4183 (*cryst struct*)
Dreyer, D.L. *et al., J.O.C.*, 1965, **30**, 749; 1966, **31**, 2279 (*Desoxylimonin, pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 3903 (*bibl, occur*)
Maier, V.P. *et al., Citrus Sci. Technol.*, 1977, **1**, 355 (*rev*)
Herman, Z. *et al., Phytochemistry*, 1985, **24**, 2911 (*biosynth*)
Sugimoto, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4453-4461 (*12α-Hydroxylimonin*)
Patra, A. *et al., J. Indian Chem. Soc.*, 1988, **65**, 205 (*pmr, cmr*)
Takahashi, K. *et al., Acta Cryst. C*, 1990, **46**, 425 (*cryst struct*)
Guthrie, N. *et al., ACS Symp. Ser.*, 2000, **758**, 164-174 (*activity*)

Linalyl oxide L-91

[60047-17-8]

[1365-19-1]
5-Ethenyltetrahydro-α,α,5-trimethyl-2-furanmethanol, 9CI. Tetrahydro-2-methyl-5-(1-hydroxy-1-methylethyl)-2-vinylfuran. Epoxydihydrolinalool. Epoxylinalool. Linalool epoxide. Linalool monoxide. Linalool 3,6-oxide. FEMA 3746



(2*R*,5*S*)-*form*

$C_{10}H_{18}O_2$ 170.251
Isol. from *Citrus paradisi* (grapefruit), *Thea sinensis* (tea) and many other sources. Flavouring ingredient. Normally occurs with Tetrahydro-3-hydroxy-2,2,6-trimethyl-6-vinylpyran, T-92 to which it is closely related and to which the older synonyms also refer.
► LD_{50} (rat, orl) 1150 mg/kg. LD_{50} (rbt, skn) 2500 mg/kg, Exp. severe skin irritant. OI7782000

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:*

[158699-10-6, 158799-49-6] *Linalool 3,6-oxide primeveroside*
$C_{21}H_{36}O_{11}$ 464.509
Constit. of *Camellia sinensis* var. *sinensis* (tea). Obt. as a mixt. of *cis*- and *trans*-isomers.

(2*R*,5*S*)-*form* [4031-48-5]
(-)-cis-*form*
Oil. $[\alpha]_D$ -12.1.
(2*S*,5*S*)-*form* [41720-60-9]
(+)-trans-*form*
Oil. $[\alpha]_D^{20}$ +3.4.
(2*RS*,5*RS*)-*form* [128441-10-1]

[34995-77-2]
(±)-trans-*form. Linalool oxide A*
Oil.

(2*RS*,3*SR*)-*form* [128441-08-7]

[5989-33-3]
(±)-cis-*form. Linalool oxide B*
Oil.

[11063-77-7, 11063-78-8, 23007-29-6, 41720-55-2]

Felix, D. *et al., Helv. Chim. Acta*, 1963, **46**, 1513-1536 (*synth*)
Attaway, J.A. *et al., Phytochemistry*, 1966, **5**, 1273-1279 (*occur*)
Rychnovsky, S.D. *et al., J.A.C.S.*, 1981, **103**, 3963-3964 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1983, **21**, 863-864 (*rev, tox*)
Utaka, M. *et al., Tet. Lett.*, 1983, **24**, 2567-2570 (*synth*)
Howell, A.R. *et al., J.C.S. Perkin 1*, 1990, 2715-2720 (*synth*)
Meou, A. *et al., Synthesis*, 1990, 752-753 (*2R,5S-form, 2S,5S-form, synth, ir, pmr, cmr*)
Moon, J.H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1742-1744 (*primeverosides*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 452
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1587-1588
Fournier-Nguefack, C. *et al., Tetrahedron*, 1997, **53**, 4353-4362 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LFY500

Linecin L-92

[90015-48-8]

[132823-03-1]
Linecin A

Polypeptide. Bacteriocin prod. by *Breviabacterium linens*.

Kato, F. *et al., Agric. Biol. Chem.*, 1984, **48**, 193-200; 1991, **55**, 161-166 (*isol*)

Linocin M 18 L-93

[158854-12-7]

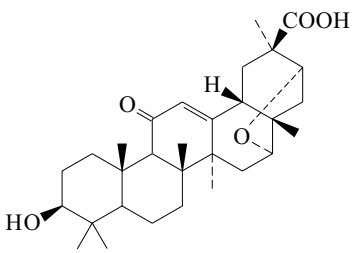
H-Met-Asn-Asn-Leu-Tyr-Arg-Glu-Leu-Ala-Pro-Ile-Pro-Gly-Pro-Ala-Ala-Ala-Glu-Ile-OH

$C_{91}H_{146}N_{24}O_{43}S$ 2296.355
Bacteriocin prod. by *Brevibacterium linens* M 18.

Valdes-Stauber, N. *et al., Appl. Environ. Microbiol.*, 1994, **60**, 3809 (*isol, struct, props*)

Liquoric acid L-94

16,21-Epoxy-3-hydroxy-11-oxo-12-oleanen-30-oic acid. Licoric acid

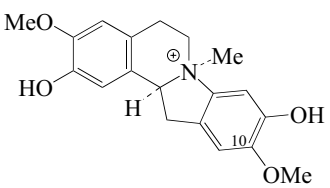


$C_{30}H_{44}O_5$ 484.675
Minor constit. of liquorice root (*Glycyrrhiza glabra*). Cryst. ($CHCl_3$/MeOH) (as Me ester). Mp 260-263° (Me ester). $[\alpha]_D$ +155.2 ($CHCl_3$) (Me ester).

Elgamal, M.H.A. *et al., Tetrahedron*, 1965, **21**, 2109

Litcubine L-95

[172924-22-0]



$C_{19}H_{22}NO_4^{\oplus}$ 328.387
Alkaloid from the roots of *Litsea cubeba* (mountain pepper). Amorph. solid (as perchlorate). $[\alpha]_D^{25.5}$ -111 (c, 1.0 in MeOH). λ_{max} 233 (sh) (log ϵ 4.06); 287 (log ϵ 3.96)

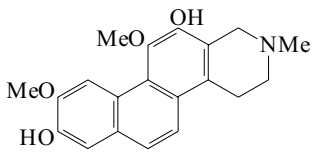
(MeOH). λ_{max} 249 (log ϵ 4.14); 304 (log ϵ 3.99) (MeOH + NaOH).

10-O-De-Me: [172924-24-2] ***Litcubinine***
$C_{18}H_{20}NO_4^{\oplus}$ 314.36
Alkaloid from the roots of *Litsea cubeba* (mountain pepper). Amorph. solid (as perchlorate). $[\alpha]_D^{25.5}$ -144 (c, 0.5 in MeOH). λ_{max} 234 (sh) (log ϵ 4.03); 290 (log ϵ 3.99) (MeOH). λ_{max} 248 (log ϵ 4.1); 305 (log ϵ 4.08) (MeOH/NaOH).

Lee, S.S. *et al., J. Nat. Prod.*, 1996, **59**, 80-82

Litebamine L-96

[137031-56-2]
1,2,3,4-Tetrahydro-9,11-dimethoxy-2-methylnaphth[2,1-f]isoquinoline-8,12-diol, 9CI

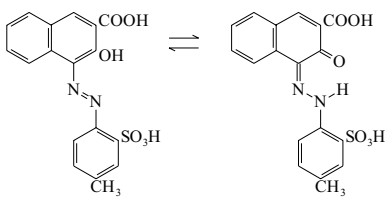


$C_{20}H_{21}NO_4$ 339.39
Alkaloid from *Litsea cubeba* (mountain pepper). Cryst. (MeOH). Mp 218-220°.

Wu, Y.-C. *et al., Tet. Lett.*, 1991, **32**, 4169 (*isol, pmr, cmr, ir, uv, struct*)
Lee, S.-S. *et al., Tet. Lett.*, 1992, **33**, 6309 (*synth*)
Hara, H. *et al., Tetrahedron*, 1995, **51**, 10189 (*synth*)

Lithol Rubine L-97

[16014-23-6]
3-Hydroxy-4-[(4-methyl-2-sulfophenyl)azo]-2-naphthalenecarboxylic acid, 9CI. Litholrubine BK. C.I. 15850. C.I. Pigment red 57. E180



$C_{18}H_{14}N_2O_6$ 354.318
Hydrazone tautomer predominates in solid state for Ca salt. Food dye.

Di-Na salt: [5858-81-1]
Red powder with yellow tint.

Ca salt: [5281-04-9] *C.I. Pigment red 57:1*
Bluish-red powder.

Colour Index, 3rd Edn., 1971, **4**, 4085 (*rev*)
Ger. Pat., 1980, 2 845 073; *CA*, **93**, 73767k (*Na salt*)
Ger. Pat., 1984, 3 336 247; *CA*, **101**, 112421y (*Ca salt*)
Eur. Pat., 1986, 202 906; *CA*, **106**, 215574h (*Ca salt*)
Harris, R.K. *et al., J.C.S. Perkin 2*, 1987, 1383 (*Ca salt, cmr, N-15 nmr*)
East Ger. Pat., 1992, 298 256; *CA*, **116**, 237367b (*Ca salt*)

Locust bean gum L-98

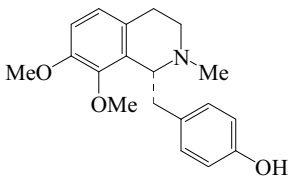
[9000-40-2]
Gum locust bean. Carob bean gum. Carob gum

Consists of a high-MW polysaccharide with a main chain of 1,4-linked D-mannose units and side chains of D-galactose. Stabiliser, thickener.

Merck Index, 12th edn., 1996, 5584
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 494-497

Longifolidine L-99

1,2,3,4-Tetrahydro-1-(4-hydroxybenzyl)-7,8-dimethoxy-1-methylisoquinoline



(*R*)-*form*

$C_{19}H_{23}NO_3$ 313.396

(R)-form [77480-17-2]
Pale yellow amorph. solid. $[\alpha]_D^{20}$ -72 (c, 0.2 in EtOH).

N-*Me:* [152230-58-5] ***8-O-Methyloblongine***
$C_{20}H_{26}NO_3^{\oplus}$ 328.43
Alkaloid from stems of *Litsea cubeba* (mountain pepper). Amorph. solid (as perchlorate). Mp 102° (perchlorate). $[\alpha]_D^{24}$ -12 (c, 1.0 in MeOH).

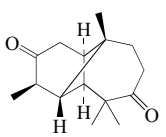
(±)-form
Cryst. (Et_2O). Mp 166-168°.

Grethe, G. *et al., Helv. Chim. Acta*, 1970, **53**, 874 (*synth, uv, ir, pmr, ms*)
Bick, I.R.C. *et al., Aust. J. Chem.*, 1981, **34**, 195 (*isol, uv, ir, pmr, ms, struct*)
Lee, S.S. *et al., J. Nat. Prod.*, 1993, **56**, 1971 (*8-O-Methyloblongine*)

4,10-Longipinanedione L-100

[88198-34-9]

[81915-98-2]
2,4-Longipinanedione



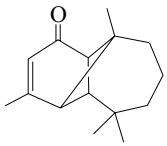
Absolute Configuration

$C_{15}H_{22}O_2$ 234.338
Constit. of the flowers of *Tanacetum vulgare* (tansy). Cryst. (Et_2O/petrol). Mp 113.5-114.5°. λ_{max} 212 ; 290 (no solvent reported).

Todorova, I.O.M. *et al., Phytochemistry*, 1983, **22**, 1775-1777 (*isol, uv, ir, pmr, cmr, cd, cryst struct*)

3-Longipinen-5-one L-101

[64180-68-3]
1-Oxo-α-longipinene. ***Vulgarone B***



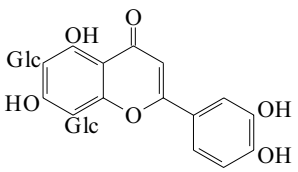
$C_{15}H_{22}O$ 218.338
Constit. of essential oil of *Chrysanthemum vulgare* (tansy). Oil or cryst. Mp 35.5-36°. $[\alpha]_D$ +63.4 (c, 1.1 in $CHCl_3$). $[\alpha]_D^{24}$ +81.3 (c, 3.1 in $CHCl_3$).

[65556-52-7]

Bohlmann, F. *et al., Chem. Ber.*, 1977, **110**, 3572
Uchio, Y. *et al., Tetrahedron*, 1978, **34**, 2893
Baig, M.A. *et al., Fitoterapia*, 1989, **60**, 373-375 (*isol, pmr, cmr*)
Yokochi, A.F.T. *et al., Acta Cryst. E*, 2001, **57**, o99-o101 (*cryst struct*)

Lucenin 2 L-102

[29428-58-8]
2-(3,4-Dihydroxyphenyl)-6,8-di-β-D-glucopyranosyl-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. 6,8-Diglucopyranosyl-3′,4′,5,7-tetrahydroxyflavone. 6,8-Diglucopyranosyl-luteolin. 6,8-Diglucosylluteolin



$C_{27}H_{30}O_{16}$ 610.524
Mp 265-267° dec. (240° dec.). $[\alpha]_D^{20}$ +16 (c, 0.062 in Py). $[\alpha]_D$ +67 (c, 6 in Py).

7-O-α-L-Rhamnopyranoside: [29432-27-7]
$C_{33}H_{40}O_{20}$ 756.667
Isol. from *Linum usitatissimum* (flax).

3′-O-β-D-Glucopyranoside:
$C_{33}H_{40}O_{21}$ 772.666

4′-Me ether: [98813-28-6] ***6,8-Diglucopyranosyl-3′,5,7-trihydroxy-4′-methoxyflavone.*** *6,8-Diglucopyranosyldiosmetin. 6,8-Diglucosyldiosmetin*
$C_{28}H_{32}O_{16}$ 624.551
Isol. from peelings of *Citrus limon* (lemon). Gelatinous ppt.

3′-Me ether: [63975-58-6] *6,8-Diglucopyranosyl-4′,5,7-trihydroxy-3′-methoxyflavone.* ***Stellarin 2***
$C_{28}H_{32}O_{16}$ 624.551

Seikel, M.K. *et al., Phytochemistry*, 1966, **5**, 439 (*isol*)
Gentili, B. *et al., J.O.C.*, 1968, **33**, 1571 (*deriv*)
Ibrahim, R.K. *et al., Phytochemistry*, 1970, **9**, 1855 (*7-Rhamnoside*)
Zoll, A. *et al., Plant. Med. Phytother.*, 1974, **8**, 134 (*Stellarin 2*)
Osterdahl, B.G. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 93 (*isol, struct*)
Gaffield, W. *et al., Tetrahedron*, 1978, **34**, 3089 (*cd*)
Bouillant, M.L. *et al., Phytochemistry*, 1979, **18**, 1043 (*Stellarin 2*)
Kumamoto, H. *et al., CA*, 1985, **103**, 183426 (*deriv*)
Basile, A. *et al., Phytochemistry*, 1999, **52**, 1479 (*isol, activity*)

Lucernic acid L-103

[56283-67-1]

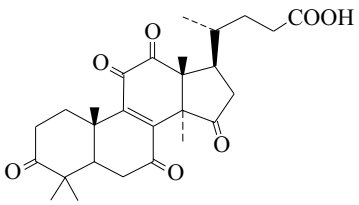
Triterpene sapogenin of unknown struct.. Constit. of *Medicago sativa* (alfalfa).

Berrang, B. *et al., Phytochemistry*, 1974, **13**, 2253 (*isol*)

Lucidenic acid D_1 L-104

[97653-95-7]

4,4,14-Trimethyl-3,7,11,12,15-pentaoxo-5α-chol-8-en-24-oic acid, 9CI. 3,7,11,12,15-Pentaoxo-25,26,27-trisnorlanost-8-en-24-oic acid



$C_{27}H_{34}O_7$ 470.561

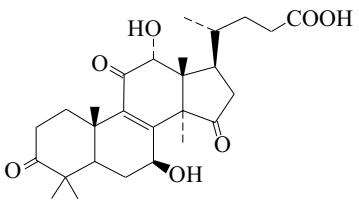
Constit. of *Ganoderma lucidum* (reishi). Cryst. Mp 229-231°. $[\alpha]_D^{22}$ +84 (c, 0.1 in EtOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 1547

Lucidenic acid E_1 L-105

[97673-89-7]

7β,12α-Dihydroxy-4,4,14-trimethyl-3,11,15-trioxochol-8-en-24-oic acid, 9CI. 7β,12α-Dihydroxy-3,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid



$C_{27}H_{38}O_7$ 474.593

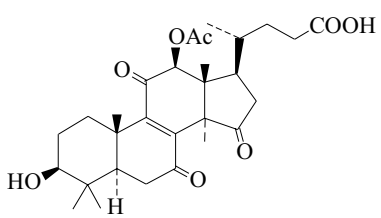
Constit. of *Ganoderma lucidum* (reishi). Cryst. (EtOAc). Mp 216-219°. $[\alpha]_D^{20}$ +229 (c, 0.2 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 1547

Lucidenic acid E_2 L-106

[98665-17-9]

12β-Acetoxy-3β-hydroxy-4,4,14-trimethyl-7,11,15-trioxochol-8-en-24-oic acid, 9CI. 12β-Acetoxy-3β-hydroxy-7,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid. Lucidenic acid E



$C_{29}H_{40}O_8$ 516.63

Constit. of *Ganoderma lucidum* (reishi).

Me ester:

Yellow needles. Mp 140-144°. $[\alpha]_D$ +86 ($CHCl_3$).

3-Ketone: [98665-16-8] *12β-Acetoxy-4,4,14-trimethyl-3,7,11,15-tetraoxochol-8-en-24-oic acid, 9CI. 12β-Acetoxy-3,7,11,15-tetraoxo-25,26,27-trisnorlanost-8-en-24-oic acid.* ***Lucidenic acid D2****. Lucidenic acid D*

$C_{29}H_{38}O_8$ 514.614

Constit. of *Ganoderma lucidum* (reishi). Pale yellow amorph. powder. $[\alpha]_D^{22}$ +70.2 (c, 0.62 in $CHCl_3$). λ_{max} 253 (ε 9120) (EtOH) (Derep).

3-Ketone, Me ester:

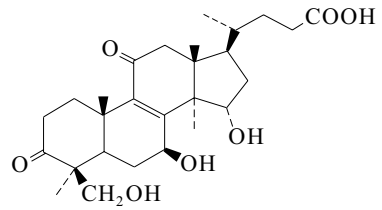
Amorph. $[\alpha]_D$ +136 ($CHCl_3$).

Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2624 (*Lucidenic acid E2*)

Komodo, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4829-4835 (*Lucidenic acid D2*)

Lucidenic acid G L-107

7β,15α,29-Trihydroxy-3,11-dioxo-25,26,27-trinorlanost-8-en-24-oic acid



$C_{27}H_{40}O_7$ 476.609

Metab. of *Ganoderma lucidum* (reishi).

Me ester:

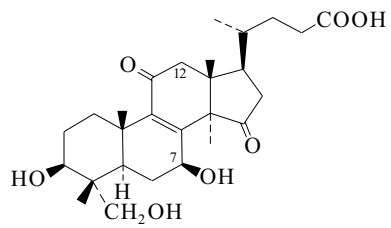
Syrup. $[\alpha]_D^{21}$ +127 (c, 0.2 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 509

Lucidenic acid H L-108

[110241-25-3]

3β,7β-Dihydroxy-4α-hydroxymethyl-4β,14α-dimethyl-11,15-dioxo-5α-chol-8-en-24-oic acid, 9CI. 3β,7β,28-Trihydroxy-11,15-dioxo-25,26,27-trisnorlanost-8-en-24-oic acid



$C_{27}H_{40}O_7$ 476.609

Constit. of *Ganoderma lucidum* (reishi). Cryst. (EtOAc/hexane) (as Me ester). Mp 190-192° (Me ester). $[\alpha]_D^{23}$ +136 (c, 0.2 in MeOH) (Me ester).

7-Ketone: [110241-27-5] *3β-Hydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, 9CI. 3β,28-Dihydroxy-7,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid.* ***Lucidenic acid I***

$C_{27}H_{38}O_7$ 474.593

Constit. of *Ganoderma lucidum* (reishi). Pale yellow syrup (as Me ester). $[\alpha]_D^{23}$ +118 (c, 0.1 in MeOH) (Me ester).

7-Ketone, 12β-hydroxy:3β,12β-Dihydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, 9CI. 3β,12β,28-Trihydroxy-7,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid. ***Lucidenic acid J***

$C_{27}H_{38}O_8$ 490.592

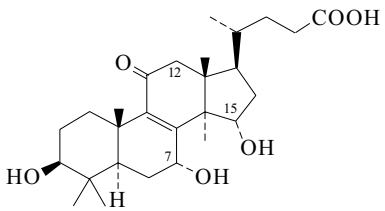
Constit. of *Ganoderma lucidum* (reishi). Pale yellow syrup (as Me ester). $[\alpha]_D^{25}$ +78 (c, 0.1 in MeOH) (Me ester).

Nishitoba, T. *et al., Phytochemistry*, 1987, **26**, 1777

Lucidenic acid M L-109

[110241-33-3]

3β,7α,15α-Trihydroxy-4,4,14α-trimethyl-11-oxo-5α-chol-8-en-24-oic acid, 9CI. 3β,7α,15α-Trihydroxy-11-oxo-25,26,27-trisnorlanost-8-en-24-oic acid



$C_{27}H_{42}O_6$ 462.625

Constit. of *Ganoderma lucidum* (reishi).

7,15-Diketone, 12β-hydroxy: [110267-45-3] *3β,12β-Dihydroxy-4,4,14α-trimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, 9CI. 3β,12β-Dihydroxy-7,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid.* ***Lucidenic acid L***

$C_{27}H_{38}O_7$ 474.593

Constit. of *Ganoderma lucidum* (reishi).

3,7,15-Triketone, 12α-hydroxy:12α-Hydroxy-4,4,14α-trimethyl-3,7,11,15-tetraoxo-5α-chol-8-en-24-oic acid, 9CI. 12α-Hydroxy-3,7,11,15-tetraoxo-25,26,27-trisnorlanost-8-en-24-oic acid. ***Lucidenic acid K***

$C_{27}H_{36}O_7$ 472.577

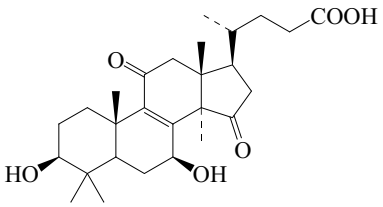
Constit. of *Ganoderma lucidum* (reishi).

Nishitoba, T. *et al., Phytochemistry*, 1987, **26**, 1777

Lucidenic acid N L-110

[364622-33-3]

3,7-Dihydroxy-4,4,14-trimethyl-11,15-dioxochol-8-en-24-oic acid. 3,7-Dihydroxy-25,26,27-trinor-11,15-dioxolanost-8-en-24-oic acid. Lucidenic acid LM1



$C_{27}H_{40}O_6$ 460.609

Same struct. assigned to Lucidenic acids N and LM1 although props. are not in good agreement. Constit. of *Ganoderma lucidum* (reishi). Powder (CH_2Cl_2). Mp 202-204° (130-131°). $[\alpha]_D$ +119.5 (c, 0.23 in $CHCl_3$). $[\alpha]_D^{25}$ +140 (c, 0.014 in Me_2CO). λ_{max} 251 (log ϵ 3.9) (MeOH).

3,7-Diketone: [98665-18-0] *4,4,14-Trimethyl-3,7,11,15-tetraoxochol-8-en-24-oic acid. 25,26,27-Trinor-3,7,11,15-tetraoxolanost-8-en-24-oic acid.* ***Lucidenic acid F***

$C_{27}H_{36}O_6$ 456.578

Constit. of *Ganoderma lucidum* (reishi).

3,7-Diketone, Me ester: [98665-10-2] ***Methyl lucidenate F***

$C_{28}H_{38}O_6$ 470.605

Constit. of *Ganoderma lucidum* (reishi). Yellow needles (MeOH). Mp 208-211° (205-207°). $[\alpha]_D$ +195 ($CHCl_3$) (+120). λ_{max} 224 ; 251 (MeOH).

Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2624 (*Lucidenic acid F*)

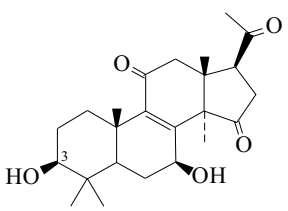
Wu, T.S. *et al., J. Nat. Prod.*, 2001, **64**, 1121-1122 (*Lucidenic acid N, Methyl lucidenate F*)

Luo, J. *et al., Yaoxue Xuebao*, 2001, **36**, 595-598 (*Lucidenic acid LM1*)

Lucidone A L-111

[97653-92-4]

3β,7β-Dihydroxy-4,4,14-trimethyl-5α-pregn-8-ene-11,15,20-trione, 9CI. 3β,7β-Dihydroxy-22,23,24,25,26,27-hexanorlanost-8-ene-11,15,20-trione



$C_{24}H_{34}O_5$ 402.53

Constit. of *Ganoderma lucidum* (reishi). Amorph. powder. Mp 280-283°. $[\alpha]_D^{24}$ +210 (c, 0.2 in $CHCl_3$).

3-Ketone: [97653-93-5] *7β-Hydroxy-4,4,14-trimethyl-5α-pregn-8-ene-3,11,15,20-tetrone.* ***Lucidone B***

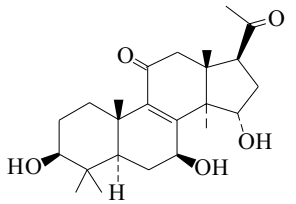
$C_{24}H_{32}O_5$ 400.514

From *Ganoderma lucidum* (reishi). Cryst. (EtOAc). Mp 270-271°. $[\alpha]_D^{22}$ +278 (c, 0.2 in $CHCl_3$).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 1547

Lin, C.-N. *et al., Phytochemistry*, 1993, **32**, 1549-1551 (*cmr*)

Lucidone C L-112



$C_{24}H_{36}O_5$ 404.545

Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{24}$ +145 (c, 0.2 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 809

Luffin L-113

Proteins. Isol. from the seeds of *Luffa cylindrica* (smooth luffa). Sol. H_2O.

Luffin a [160674-53-3] Approx. 250 amino acid residues.

Luffin b [160674-54-4] Approx. 250 amino acid residues.

Kamenosono, M. *et al., Agric. Biol. Chem.*, 1988, **52**, 1223-1227 (*isol*)

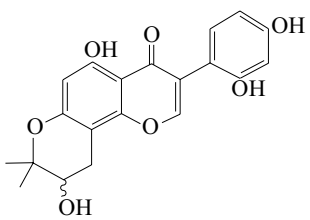
Islam, M.R. *et al., Agric. Biol. Chem.*, 1990, **54**, 1343-1345; 2967-2978; 1991, **55**, 229-238 (*struct*)

Yeung, H.W. *et al., Int. J. Pept. Protein Res.*, 1991, **38**, 15-19 (*isol*)

Lunatone L-114

[104363-13-5]

*3-(2,4-Dihydroxyphenyl)-9,10-dihydro-5,9-dihydroxy-8,8-dimethyl-4*H,*8*H-*benzo[1,2-b:3,4-b′]dipyran-4-one, 9CI*

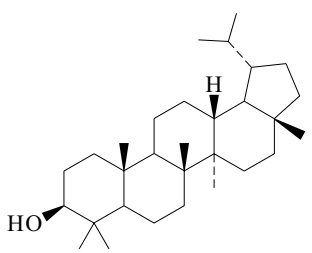


$C_{20}H_{18}O_7$ 370.358

Constit. of *Phaseolus lunatus* (butter bean).

O'Neill, M.J. *et al., Phytochemistry*, 1986, **25**, 1315

3-Lupanol L-115



$C_{30}H_{52}O$ 428.74

3β-*form* [3186-86-5]

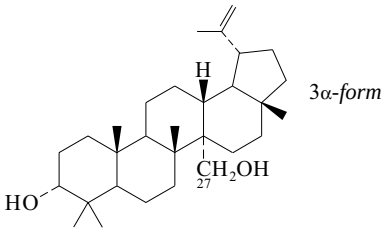
Constit. of *Sorghum bicolor* (sorghum). Cryst. (Py). Mp 201-202°. $[\alpha]_D^{22}$ -17.3.

Palmer, M.A. *et al., Phytochemistry*, 1977, **16**, 459 (*isol*)

Ayer, W.A. *et al., Tetrahedron*, 1984, **40**, 2069 (*pmr, cmr*)

Chaturvedi, S.K. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 562 (*isol, ms*)

20(29)-Lupene-3,27-diol L-116



3α-*form*

$C_{30}H_{50}O_2$ 442.724

3α-*form*

Needles ($C_6H_6/CHCl_3$). Mp 260-262°.

27-Carboxylic acid: [198014-94-7] *3α-Hydroxy-20(29)-lupen-27-oic acid.* ***Bacosine***

$C_{30}H_{48}O_3$ 456.707

3β-*form* [58940-21-9]

Constit. of *Sapium sebiferum* (Chinese tallowtree). Cryst. (MeOH). Mp 214-215°. $[\alpha]_D$ +67 (c, 0.5 in MeOH).

27-Carboxylic acid: [2566-80-5] ***3β-Hydroxy-20(29)-lupen-27-oic acid***

$C_{30}H_{48}O_3$ 456.707

Cryst. (MeOH). Mp 307-308°. $[\alpha]_D^{25}$ +31 (Py).

Hui, W.-H. *et al., J.C.S. Perkin 1*, 1976, 23

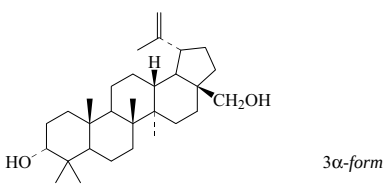
Misra, T.N. *et al., Phytochemistry*, 1983, **22**, 2557

Del Castillo, J.B. *et al., Fitoterapia*, 1986, **57**, 61

Jain, N. *et al., Phytochemistry*, 1994, **35**, 1070 (*isol, pmr, cmr*)

Ahmed, B. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 620-625 (*Bacosine*)

20(29)-Lupene-3,28-diol L-117



3α-*form*

$C_{30}H_{50}O_2$ 442.724Log P 8.53 (uncertain value) (calc).

3β-*form* [473-98-3]

Betulin. *Betulinol (obsol.). Trochol*

Constit. of *Corylus avellana* (filbert) and *Vicia faba*. Cryst. Mp 251-252°. $[\alpha]_D^{15}$ +20 (Py). Pharmacol. active isomer.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 567C (*nmr*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1493G (*ir*)

Ruzicka, L. *et al., Helv. Chim. Acta*, 1939, **22**, 1523; 1941, **24**, 529

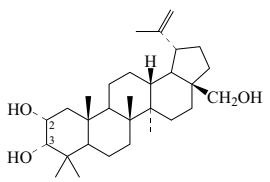
Davy, G.S. *et al., J.C.S.*, 1951, 2696 (*struct*)

Lehn, J.M. *et al., Bull. Soc. Chim. Fr.*, 1962, 1137 (*pmr*)

Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688 (*ms*)

Aplin, R.T. *et al., J.C.S.*, 1963, 3269 (*isol*)
Das, S.C. *et al., Chem. Ind. (London)*, 1971, 1331 (*epimer*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2024 (*occur*)
Bandopadhyay, M. *et al., Phytochemistry*, 1972, **11**, 1511 (*isol*)
Herz, W. *et al., Phytochemistry*, 1972, **11**, 3061 (*epimer*)
Bhaltacharyya, J. *et al., Phytochemistry*, 1976, **15**, 432 (*isol*)
Sholichin, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1006 (*cmr*)
Hayek, E.W.H. *et al., Phytochemistry*, 1989, **28**, 2229-2242 (*rev*)
Tietze, L.F. *et al., Annalen*, 1991, 1245-1249 (*synth*)
Tinto, W.F. *et al., J. Nat. Prod.*, 1992, **55**, 963-966 (*cmr*)

20(29)-Lupene-2,3,28-triol L-118



(2α,3α)-*form*

$C_{30}H_{50}O_3$ 458.723

(2α,3α)-*form*

28-Carboxylic acid: [97762-86-2] *2,3-Dihydroxy-20(29)-lupen-28-oic acid.* ***3-Epialphitolic acid***
$C_{30}H_{48}O_4$ 472.707
Cryst. ($CHCl_3$/MeOH). Mp 298-300°.

(2α,3β)-*form* [169134-54-7]
Constit. of *Rheum rhabarbarum* (rhubarb). Needles (MeOH). Mp 258-260°. $[\alpha]_D$ +11 (c, 0.6 in $CHCl_3$/MeOH). λ_{max} 261 (log ϵ 3.87); 296 (log ϵ 3.65) (MeOH).

3,28-Dihexadecanoyl: [169134-55-8]
$C_{62}H_{110}O_5$ 935.548
Constit. of *Rheum rhabarbarum* (rhubarb). Wax. $[\alpha]_D$ +5 (c, 0.75 in $CHCl_3$/MeOH).

28-Carboxylic acid: [19533-92-7] ***Alphitolic acid***
$C_{30}H_{48}O_4$ 472.707
Cryst. (C_6H_6) (as Me ester). Mp 233-235° (Me ester). $[\alpha]_D$ -11 (Me ester). $[\alpha]_D^{25}$ -4 (c, 1.0 in py) (free acid).

28-Carboxylic acid, 2-(3,4-dihydroxybenzoyl): [182682-95-7] *2-O-Protocatechuoylalphitolic acid*
$C_{37}H_{52}O_7$ 608.814
Constit. of *Zizyphus jujuba* (Chinese date). Cryst. $[\alpha]_D^{23}$ -9 (c, 0.43 in MeOH). Mp >300° λ_{max} 261 (log ϵ 3.87); 296 (log ϵ 3.65) (MeOH).

*28-Carboxylic acid, 3-(4-hydroxy-*E*-cinnamoyl):* [67911-62-0] ***3-O-p-trans-Coumaroylalphitolic acid***
$C_{39}H_{54}O_6$ 618.852
Constit. of the fruit of *Ziziphus jujuba* (Chinese date). Needles ($CHCl_3$/MeOH). Mp 279-282°. $[\alpha]_D^{28}$ -33 (c, 3.75 in Py).

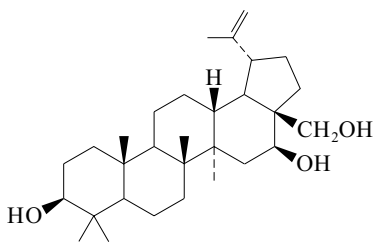
*28-Carboxylic acid, 3-(4-hydroxy-*Z*-cinnamoyl):* [67911-64-2] ***3-O-p-cis-Coumaroylalphitolic acid***
$C_{39}H_{54}O_6$ 618.852
Constit. of the fruit of *Ziziphus jujuba* (Chinese date). Needles ($CHCl_3$/MeOH). Mp 208-210°. $[\alpha]_D^{24}$ +40 (c, 0.8 in Py).

28-Carboxylic acid, 3-(3,4-dihydroxycinnamoyl): [182682-96-8] *2α-Hydroxypyracrenic acid*
$C_{39}H_{54}O_7$ 634.851
Constit. of *Zizyphus jujuba* (Chinese date). Cryst. (MeOH) (as tri-Ac). Mp 225° (tri-Ac). $[\alpha]_D^{23}$ -13 (c, 1.35 in $CHCl_3$).

*28-Carboxylic acid, 3-(4-hydroxy-3-methoxy-*E*-cinnamoyl):* ***Eucalyptic acid***
$C_{40}H_{56}O_7$ 648.878
Needles ($CHCl_3$/MeOH). Mp 280-281°. $[\alpha]_D^{27}$ +39 (c, 0.1 in MeOH).

Cheung, H.T. *et al., J.C.S.(C)*, 1968, 1047
Yagi, A. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1798-1802 (*3-p-Coumaroylalphitolic acids*)
Kumar, N.S. *et al., Phytochemistry*, 1985, **24**, 1337 (*isol*)
Kuang, H.X. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2232 (*isol, pmr, cmr*)
Schmidt, J. *et al., Phytochemistry*, 1995, **40**, 527 (*isol, pmr, cmr*)
Lee, S.-S. *et al., Phytochemistry*, 1996, **43**, 847 (*esters*)
Siddiqui, B.S. *et al., Planta Med.*, 1997, **63**, 47 (*Eucalyptic acid*)
Kashiwada, Y. *et al., J. Nat. Prod.*, 1998, **61**, 1090-1095 (*Alphitolic acid, activity*)
Schühly, W. *et al., Planta Med.*, 1999, **65**, 740; 1959 (*Alphitolic acid, activity*)
Braca, A. *et al., Planta Med.*, 2000, **66**, 768-769 (*Alphitolic acid, activity*)

20(29)-Lupene-3,16,28-triol L-119



$C_{30}H_{50}O_3$ 458.723

(3β,16β)-*form* [61229-18-3]
Heliantriol B2
Constit. of *Calendula officinalis* (pot marigold), *Helianthus annuus* (sunflower) and *Stenocereus thurberi* (organ pipe cactus). Cryst. (MeOH). Mp 300-301°. $[\alpha]_D$ +8 (c, 0.4 in $CHCl_3$).

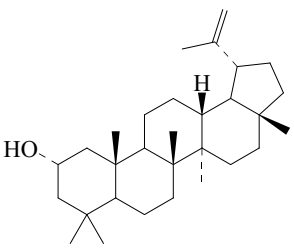
3-Tetradecanoyl: [357419-32-0] *Heliantriol B_2 myristate*
$C_{44}H_{76}O_4$ 669.082
Amorph. solid.

3-Hexadecanoyl: [147000-40-6] *Heliantriol B_2 palmitate*
$C_{46}H_{80}O_4$ 697.136
Amorph. Mp 120-121°. $[\alpha]_D^{20}$ +8.45.

28-Carboxylic acid: [205439-97-0] *3,16-Dihydroxy-20(29)-lupen-28-oic acid.* ***16β-Hydroxybetulinic acid***
$C_{30}H_{48}O_4$ 472.707
Amorph. powder. Mp 271-274°. $[\alpha]_D$ -14.3 (c, 0.34 in MeOH).

Errington, S.G. *et al., Aust. J. Chem.*, 1976, **29**, 1809 (*isol, pmr*)
Wenkert, E. *et al., Org. Magn. Reson.*, 1978, **11**, 337 (*cmr*)
St Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 2465 (*isol*)
Kircher, H.W. *et al., Phytochemistry*, 1980, **19**, 2707 (*isol*)
Diaz, J.G. *et al., Phytochemistry*, 1992, **31**, 3471 (*hexadecanoyl*)
Hu, L. *et al., Zhiwu Xuebao*, 1997, **39**, 85-90; *CA*, **127**, 231901b (*hexadecanoyl*)
Ye, Y. *et al., J. Nat. Prod.*, 1998, **61**, 456-460 (*16-Hydroxybetulinic acid*)
Ukiya, M. *et al., J. Agric. Food Chem.*, 2001, **49**, 3187-3197 (*tetradecanoyl*)

20(29)-Lupen-2-ol L-120

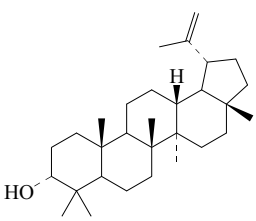


$C_{30}H_{50}O$ 426.724

2α-*form* [254892-57-4]
Palestinol
Constit. of the leaves of *Salvia triloba* (Greek sage).

Firdous, S. *et al., Fitoterapia*, 1999, **70**, 326-327 (*isol, pmr, cmr*)

20(29)-Lupen-3-ol L-121



3α-*form*

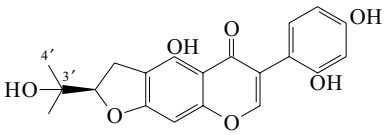
$C_{30}H_{50}O$ 426.724

3β-*form* [545-47-1]
Lupeol. *Monogynol B. Fagarasterol. β-Viscol. Cautchicol. Xanthosterin. Clerodol*
Cryst. (Me_2CO/MeOH aq.). Mp 215-216°. $[\alpha]_D$ +26.4 ($CHCl_3$). Log P 10.51 (uncertain value) (calc).

3-O-[β-D-Xylopyranosyl-(1→4)-β-D-glucopyranoside]: [111216-33-2] ***Lupeoside***
$C_{41}H_{68}O_{10}$ 720.982
Constit. of the seeds of jack bean (*Canavalia ensiformis*).

Mukharya, D. *et al., Acta Cienc. Indica, Chem.*, 1985, **11**, 24 (*Lupeoside*)

Lupinisoflavone B L-122



$C_{20}H_{18}O_7$ 370.358

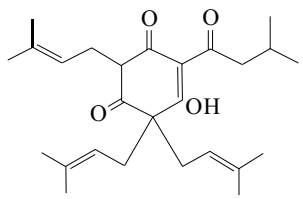
(R)-form [91681-64-0]
Pale-yellow prisms. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 245-247°. $[\alpha]_D^{23}$ 0 (c, 0.101 in MeOH). λ_{max} 215 (ϵ 35500); 263 (ϵ 27600) (MeOH) (Berdy). λ_{max} 280 (MeOH-NaOH) (Berdy).

3″-Deoxy, 3″,4″-didehydro: [93373-45-6] ***Lupinisoflavone A***
$C_{20}H_{16}O_6$ 352.343
Isol. from *Cajanus cajan* (pigeon pea). Pale yellow needles. Mp 189-191°. $[\alpha]_D^{23}$ +74 (c, 0.108 in MeOH). Abs. config. not certain, given here by analogy with Lupinisoflavone B.

Dahiya, J.S. *et al., Phytochemistry*, 1984, **23**, 871
Tahara, S. *et al., Phytochemistry*, 1984, **23**, 1889

Lupulone L-123

[468-28-0]
β-Lupulinic acid. β-Bitter acid. β-Lupulic acid



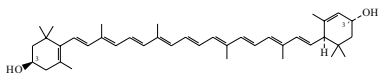
$C_{26}H_{38}O_4$ 414.584
Constit. of hops. Cryst. (MeOH). Sol. MeOH, hexane; fairly sol. H_2O. Mp 93°. λ_{max} 229 (E1%/1cm 350); 275 ; 340 (MeOH) (Berdy). λ_{max} 221 (E1%/1cm 550); 355 (E1%/1cm 450) (MeOH-NaOH) (Berdy).

► LD_{50} (mus, scu) 600 mg/kg , LD_{50} (mus, orl) 1800 mg/kg. OK5950000

Levaditi, C. *et al., C. R. Hebd. Seances Soc. Biol. Ses Fil.*, 1949, **143**, 1474 (*props*)
Balwé, T. *et al., Chem. Ber.*, 1966, **99**, 3277 (*struct*)
Teuber, M. *et al., Arch. Mikrobiol.*, 1973, **94**, 159 (*props*)
Drawert, F. *et al., Phytochemistry*, 1974, **13**, 2749 (*biosynth*)
Molyneux, R.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 1201 (*pmr*)
Drawert, F. *et al., Phytochemistry*, 1976, **15**, 1689; 1695 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LIU000

Lutein L-124

[127-40-2]
Xanthophyll. β,ϵ-Carotene-3,3′-diol. Lutein A



$C_{40}H_{56}O_2$ 568.881
Pigment from egg yolk and leaves. Found in all higher plants. Nutriceutical with anticancer and antioxidation props. Potentially useful for the treatment of age-related macular degeneration (AMD) of the eye. Coppery cryst. (MeOH). Mp 196°. $[\alpha]_{643.9}^{18}$ +160 ($CHCl_3$). Other stereoisomers have been distinguished λ_{max} 420 ; 444 ; 472 (MeOH) (Berdy).

Dihexadecanoyl: [547-17-1] ***Xantofyl palmitate, INN***. *Helenien, JAN. Adaptinol. Aptinol. Heligal. Xantophyll dipalmitate. E161b*
$C_{72}H_{116}O_4$ 1045.706
Food colourant for butter and bakery products. Red cryst. (EtOH). Mp 92°.

Di-Me ether: [53779-13-8] *3,3′-Dimethoxy-β,ϵ-carotene. Lutein dimethyl ether. Xanthophyll dimethyl ether*
$C_{42}H_{60}O_2$ 596.935
Cryst. (MeOH/Et_2O). Mp 162-163° (155°). λ_{max} 267 ; 428 ; 433 ; 480 (dioxan).

3′-Ketone: [97134-08-2] *3-Hydroxy-β,ϵ-caroten-3′-one.* ***Philosamixanthin***. *3′-O-Didehydrolutein*
$C_{40}H_{54}O_2$ 566.865
Isol. from marine fish eggs. Red needles (petrol). Mp 168-170°. λ_{max} 449 ; 477 (Me_2CO).

5,6-Epoxide: See Lutein epoxide in *The Combined Chemical Dictionary.*

7′,8′-Dihydro: [169275-78-9] ***7′,8′-Dihydrolutein***
$C_{40}H_{58}O_2$ 570.897

3′-Epimer: [52842-48-5] ***3′-Epilutein***. *Calthaxanthin*
$C_{40}H_{56}O_2$ 568.881
Isol. from plants and animals (e.g. *Potamon dehaari*, Yellowtail Fish). Mp 162-163°. $[\alpha]_D^{20}$ +88 (EtOH). λ_{max} 420 ; 444 ; 472 (no solvent reported).

6′-Epimer: [97169-07-8]
$C_{40}H_{56}O_2$ 568.881
λ_{max} 420 ; 444 ; 472 (petrol).

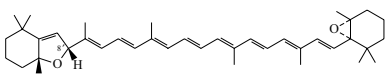
3′,6′-Diepimer: [89673-72-3]
$C_{40}H_{56}O_2$ 568.881
λ_{max} 420 ; 444 ; 472 (petrol).

[15904-92-4, 105452-20-8]

Kuhn, R. *et al., Naturwissenschaften*, 1930, **18**, 754 (*isol*)
Ohta, T. *et al., Chem. Pharm. Bull.*, 1959, **7**, 254-255 (*isol*)
Jensen, S.L. *et al., Acta Chem. Scand.*, 1966, **20**, 1703-1709 (*di-Me ether*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1844; 1845 (*occur*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1974, **57**, 631-656; 1979, **62**, 2817-2824 (*abs config, synth, di-Me ether, synth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97-102 (*cmr*)
Weedon, B.C.L. *et al., Pure Appl. Chem.*, 1976, **47**, 161-171 (*synth*)
Davies, B.H. *et al., Int. Rev. Biochem.*, 1977, **14**, 51 (*rev*)
Mayer, H. *et al., Helv. Chim. Acta*, 1980, **63**, 1451-1455 (*synth*)
Baranyai, M. *et al., Tetrahedron*, 1981, **37**, 203-207 (*cmr*)
Vecchi, M. *et al., Helv. Chim. Acta*, 1982, **65**, 1050-1058 (*Calthaxanthin, hplc, pmr*)
Milborrow, B.V. *et al., Phytochemistry*, 1982, **21**, 2853-2857 (*synth, Philosamixanthin*)
Miki, W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 195-201 (*Calthaxanthin, occur, biosynth*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779-789 (*stereoisomers, Philosamixanthin*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 133; 136; 232; 302 (*bibl*)
Chopra, M. *et al., Ann. N.Y. Acad. Sci.*, 1993, **691**, 246-249 (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1428
Bui, M.H. *et al., J. Chromatogr., B: Biomed. Appl.*, 1994, **654**, 129 (*hplc*)
Egeland, E.S. *et al., Phytochemistry*, 1995, **40**, 515 (*7′,8′-Dihydrolutein*)
Sliwka, H.-R. *et al., Acta Chem. Scand.*, 1996, **50**, 637 (*synth*)
Okai, Y. *et al., Cancer Lett. (Shannon, Irel.)*, 1996, **100**, 235-240; *CA*, **128**, 223350u (*activity*)
Largo, G. *et al., Philipp. J. Sci.*, 1997, **126**, 107-115; *CA*, **128**, 306237w (*activity*)
Ragasa, C.Y. *et al., Philipp. J. Sci.*, 1997, **126**, 199-206; *CA*, **129**, 313379 (*activity*)
Deli, J. *et al., Helv. Chim. Acta*, 1998, **81**, 1815-1819 (*Lutein, pmr, cmr*)

Luteochrome L-125

[6821-08-5]
5,6:5′,8′-Diepoxy-5,5′,6,8′-tetrahydro-β,β-carotene



(5R,5′R,6S,8′R)-form

$C_{40}H_{56}O_2$ 568.881

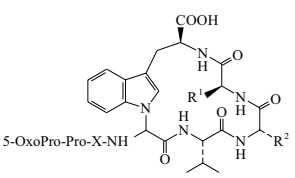
(5R,5′R,6S,8′R)-form
Constit. of *Ipomoea batatas* (sweet potato). Orange cryst. (Et_2O/MeOH). Mp 170-171°.

(5R,5′R,6S,8′S)-form
From *Ipomoea batatas* (sweet potato). Orange cryst. (Et_2O/MeOH). Mp 161-163°.

[96290-86-7, 96290-88-9, 124150-18-1]

Acemoglu, M. *et al., Helv. Chim. Acta*, 1984, **67**, 2226 (*synth*)
Bicudo de Almeida, L. *et al., Helv. Chim. Acta*, 1986, **69**, 1554 (*isol*)

Lyciumin L-126



Lyciumin A X = Tyr R^1 = CH_2OH, R^2 = H
B X = Trp R^1 = CH_2OH, R^2 = H
C X = Tyr R^1 = CH_2OH, R^2 = CH_2Ph
D X = Tyr R^1 = $CH(CH_3)CH_2CH_3$, R^2 = H

Lyciumin A [125708-06-7]

$C_{42}H_{51}N_9O_{12}$ 873.918
Isol. from root bark of *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D$ +10.1. λ_{max} 273 (ϵ); 281 (ϵ); 291 (ϵ) (solvent not reported) (Derep).

Lyciumin B [125756-66-3]
$C_{44}H_{52}N_{10}O_{11}$ 896.955
Isol. from *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D$ +3.5. λ_{max} 281 (ϵ); 291 (ϵ) (solvent not reported) (Derep).

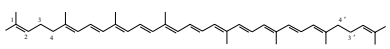
Lyciumin C [150394-23-3]
$C_{49}H_{57}N_9O_{12}$ 964.042
Isol. from *Lycium chinense* (Chinese boxthorn). Powder. Sol. MeOH, $CHCl_3$; poorly sol. hexane, H_2O. $[\alpha]_D^{24}$ -11.9 (c, 0.97 in DMSO). λ_{max} 230 ; 235 ; 292 ; 418 ; 438 (MeOH) (Berdy).

Lyciumin D [150415-40-0]
$C_{45}H_{57}N_9O_{11}$ 899.999
Isol. from *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D^{25}$ -8.4 (c, 0.45 in DMSO).

Yahara, S. *et al., Tet. Lett.*, 1989, **30**, 6041 (*isol*)
Schmidt, U. *et al., Chem. Comm.*, 1992, 1353 (*synth*)
Yahara, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 703 (*isol, pmr, cmr, struct*)
Morita, H. *et al., Tetrahedron*, 1996, **52**, 2795 (*pmr, conformn, config*)

Lycopene L-127

2,6,10,14,19,23,27,31-Octamethyl-2,6,8,10,12,14,16,18,20,22,24,26,30-dotriacontatridecaene. ψ,ψ-Carotene, 9CI. Solanorubin. Dicarotene. Lycopine. E160



$C_{40}H_{56}$ 536.882
Used as food colouring.

(*all-E*)-*form* [502-65-8]
Constit. of tomatoes and many other fruits. Nutriceutical with antioxidant props.. Long red needles or prisms (petrol). Mp 175°.

*1,2*S*-Epoxide:* [51599-09-8] ***1,2-Epoxy-1,2-dihydrolycopene***. *1,2-Epoxy-1,2-dihydro-ψ,ψ-carotene*
$C_{40}H_{56}O$ 552.882
Isol. from tomatoes.

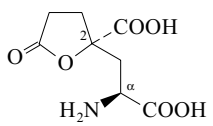
5,6-Epoxide: [51599-10-1] ***5,6-Epoxy-5,6-dihydrolycopene***. *5,6-Epoxy-5,6-dihydro-ψ,ψ-carotene*
$C_{40}H_{56}O$ 552.882
Constit. of tomatoes.

(7*Z*,7′*Z*,9*Z*,9′*Z*)-*form* [2361-24-2]
Prolycopene
Constit. of tomatoes (*Lycopersicon esculentum*). Also in other fruits. Red prisms (C_6H_6/MeOH); red-orange flaky cryst. (hexane/EtOH). Mp 111°. λ_{max} 232 ; 255 ; 295 ; 437 (hexane).

Karrer, P. *et al., Helv. Chim. Acta*, 1950, **33**, 1349 (*synth*)
Isler, O. *et al., Helv. Chim. Acta*, 1956, **39**, 463 (*synth*)
Enzell, C.R. *et al., Acta Chem. Scand.*, 1969, **23**, 727 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1818; 1820 (*occur*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759 (*isol*)
Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*Prolycopene*)
Pfander, H. *et al., Helv. Chim. Acta*, 1984, **67**, 964; 968 (*epoxide, isol, synth*)
Ritacco, R.P. *et al., J. Agric. Food Chem.*, 1984, **32**, 296
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 31 (*bibl*)
Pattenden, G. *et al., Tet. Lett.*, 1987, **28**, 5751 (*synth*)
Hengartner, U. *et al., Helv. Chim. Acta*, 1992, **75**, 1848 (*synth*)
Stahl, W. *et al., Arch. Biochem. Biophys.*, 1996, **336**, 1-9 (*rev*)
Bramley, P. M. *et al., Phytochemistry*, 2000, **54**, 233-236 (*rev*)

Lycoperdic acid L-128

[69086-72-2]
α-Amino-2-carboxytetrahydro-5-oxo-2-furanpropanoic acid, 9CI



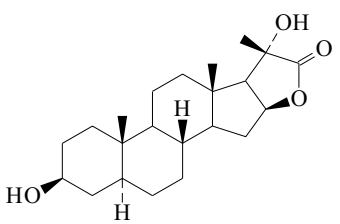
Absolute configuration

$C_8H_{11}NO_6$ 217.178
Isol. from the mushroom *Lycoperdon perlatum* (common puffball). Needles (H_2O). Mp 200-201°. $[\alpha]_D^{20}$ +14.9 (c, 0.47 in H_2O). $[\alpha]_D$ +36.5 (c, 1.37 in 1*M* HCl).

Lamotte, J. *et al., Acta Cryst. B*, 1978, **34**, 3635 (*cryst struct*)
Rhugenda-Banga, N. *et al., Phytochemistry*, 1979, **18**, 482 (*isol, synth*)
Yoshifuji, S. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1617 (*synth, pmr, cmr, cd*)
Masaki, H. *et al., Tet. Lett.*, 2000, **41**, 4801-4804 (*synth*)
Makino, K. *et al., Tetrahedron*, 2002, **58**, 9737-9740 (*synth, pmr, cmr*)

Lycopersiconolide L-129

[110612-29-8]
*3β,16β,20*S*-Trihydroxy-5α-pregnane-20-carboxylic acid 22,16-lactone. 3β,20*S*-Dihydroxy-5α-pregnane-20,16β-carbolactone*

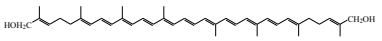


$C_{22}H_{34}O_4$ 362.508
Constit. of tomato roots. Needles ($CHCl_3$/MeOH). Mp 295-297°. $[\alpha]_D^{20}$ -48 (c, 0.088 in MeOH).

Nagaoka, T. *et al., Phytochemistry*, 1987, **26**, 2113

Lycophyll L-130

[19891-75-9]
ψ,ψ-Carotene-16,16′-diol. 16,16′-Dihydroxylycopene



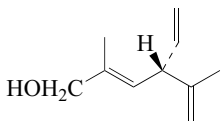
$C_{40}H_{56}O_2$ 568.881
Constit. of *Lycopersicon esculentum* (tomato). Violet-red cryst. (C_6H_6/MeOH). Mp 191°.

Deoxy: [19891-74-8] ***Lycoxanthin***. *ψ,ψ-Caroten-16-ol. 16-Hydroxylycopene. Lycopen-16-ol*
$C_{40}H_{56}O$ 552.882
Red-brown cryst. (Et_2O/petrol). Mp 170°.

Kelly, M. *et al., Acta Chem. Scand.*, 1971, **25**, 1607 (*stereochem*)
Kjosen, H. *et al., Acta Chem. Scand.*, 1972, **26**, 4121 (*isol, synth*)

Lyratol L-131

4-Ethenyl-2,5-dimethyl-2,5-hexadien-1-ol. 2,5-Dimethyl-4-vinyl-2,5-hexadien-1-ol



(*S,E*)-*form*

$C_{10}H_{16}O$ 152.236

(*S,E*)-*form* [19889-92-0]
Oil. Bp_2 105°. $[\alpha]_D$ +62.3 (c, 4.6 in $CHCl_3$).

Ac: [79549-21-6]
$C_{12}H_{18}O_2$ 194.273
Constit. of *Artemisia vulgaris* (mugwort).

Propanoyl: [79507-85-0]

[20384-05-8]
$C_{13}H_{20}O_2$ 208.3
Constit. of *Artemisia vulgaris* (mugwort).

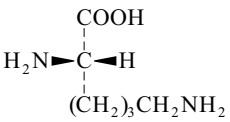
1-Carboxylic acid: [17152-12-4] *4-Ethenyl-2,5-dimethyl-2,5-hexadienoic acid, 9CI. 2,5-Dimethyl-4-vinyl-2,5-hexadienoic acid*. ***Lyratic acid***. *Lyratoic acid*
$C_{10}H_{14}O_2$ 166.219
Bp_4 110°. The *S*-config. does not appear to have been explicitly detd. but is assumed here. No opt. rotn. reported.

(*S,Z*)-*form*
Ac: [79549-24-9]
Constit. of *Artemisia vulgaris* (mugwort).

Devgan, O.N. *et al., Curr. Sci.*, 1967, **36**, 205 (*isol*)
Devgan, O.N. *et al., Tetrahedron*, 1969, **25**, 3217 (*struct*)
Sucrow, W. *et al., Tet. Lett.*, 1970, 4725 (*synth*)
Bamboria, B.K. *et al., Indian J. Chem.*, 1971, **9**, 186 (*isol*)
Näf-Müller, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1424 (*esters*)

Lysine, 9CI, INN, USAN L-132

[6899-06-5]
2,6-Diaminohexanoic acid. Lys



(*S*)-*form*

$C_6H_{14}N_2O_2$ 146.189Log P -3.42 (calc).

(S)-form [56-87-1]

[39665-12-8]

L-form. L-Lysine. FEMA 3847

Dietary supplement, nutrient. Found widely in protein hydrolysates, e.g. casein, egg albumen, fibrin, gelatin, beet molasses. Flavouring agent for a variety of foods. Needles (EtOH aq.). V. sol. H_2O; spar. sol. EtOH. Mp 224-225° dec. (darkens at 210°). $[\alpha]_D$ +19.7 (H_2O). $[\alpha]_D$ +37.9 (5*M* HCl). pK_{a3} 10.54 (25°, 0.1*M* $NaClO_4$). Isoelectric point pH 10.56 at 0°, 9.74 at 25°. Flat taste. Undergoes thermal condensation polym. to give poly(L-lysine).

► Exp. reprod. and teratogenic effects (v. large doses). OL5540000

Hydrochloride: [10098-89-2]

[657-27-2] ***Lysine hydrochloride, USAN***

Dietary supplement, nutrient. Mp 235-236°.

► LD_{50} (rat, orl) 10000 mg/kg. OL5650000

N^2*-Galacturonopyranoside:* [220718-56-9]

$C_{12}H_{22}N_2O_8$ 322.314

Possible constit. of plant cell walls incl. tomato and spinach.

N^6*-D-Galacturonopyranoside:* [220718-57-0]

$C_{12}H_{22}N_2O_8$ 322.314

Possible constit. of plant cell walls incl. tomato and spinach.

N^6*-Ac:* [692-04-6]

$C_8H_{16}N_2O_3$ 188.226

Isol. from sugarbeet (*Beta vulgaris*). $[\alpha]_D^{20}$ +4 (c, 5 in H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 587C; 587D; 588B; 783A; 783C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 890C; 1279A (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 74; 76; 374 (*synth*)
Galat, A. *et al., J.A.C.S.*, 1947, **69**, 86 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 32), Wiley, N.Y., 1961, 2097 (*rev*)
Bugayong, R.R. *et al., Acta Cryst. B*, 1972, **28**, 3214 (*cryst struct*)
Fowden, L. *et al., Phytochemistry*, 1972, **11**, 2271 (N^6*-Ac*)
Sifniades, S. *et al., J.A.C.S.*, 1976, **98**, 3738 (*synth*)
Sodek, L. *et al., Phytochemistry*, 1976, **15**, 1903 (*biosynth*)
Amino, Y. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 613 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1044
Perrone, P. *et al., Phytochemistry*, 1998, **49**, 1879-1890 (*galacturonosides*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LJM700; LJN000; LJO000

Lysinoalanine L-133

[18810-04-3]

N^6*-(2-Amino-2-carboxyethyl)lysine, 9CI*

$HOOCCH(NH_2)CH_2NH(CH_2)_4CH(NH_2)COOH$

$C_9H_{19}N_3O_4$ 233.267

Nephrotoxic food contaminant. Has the L-lysine config. but most samples appear to be diastereoisomeric mixts..

► Nephrotoxic.

Hydrochloride (1:2):

Cryst. (EtOH aq.). Mp 176-178°. $[\alpha]_D^{25}$ +15 (c, 2 in 2*M* HCl).

N^ϵ*-2,4-Dinitrophenyl:*

Cryst. (EtOH aq.). Mp 180-182°. $[\alpha]_D^{25}$ +10.4 (c, 2.5 in 2*M* HCl).

[4418-81-9, 23250-50-2, 63116-88-1, 63121-95-9, 63121-98-2]

Okuda, T. *et al., Chem. Ber.*, 1965, **98**, 1164 (*synth*)
Tas, A.C. *et al., Lebensm.-Wiss. Technol.*, 1976, **9**, 360-362; *CA*, **87**, 23703s (*synth*)
Gross, E. *et al., Adv. Chem. Ser.*, (*Food Proteins, Symp.*), 1977, **160**, 37 (*rev*)
Woodard, J.C. *et al., Food Cosmet. Toxicol.*, 1977, **15**, 109; *CA*, **87**, 68619k (*synth*)
Finley, J.W. *et al., J. Agric. Food Chem.*, 1977, **25**, 1421 (*synth*)
Maga, J.A. *et al., J. Agric. Food Chem.*, 1984, **32**, 955-964 (*rev*)
Jonker, D. *et al., Food Chem. Toxicol.*, 1993, **31**, 125-136 (*tox*)
Friedman, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 1295-1319 (*rev, food chem*)

Lysopine L-134

[34522-31-1]

N^2*-(1-Carboxyethyl)lysine*

$H_2N(CH_2)_4CH(COOH)NHCH(CH_3)COOH$

$C_9H_{18}N_2O_4$ 218.252

L-form

Isol. from crown gall tumours of various plants incl. tomato, jerusalem artichoke and salsify. Needles + $2H_2O$ (EtOH aq.). Mp 157-160° Mp 240° dec. (double Mp). $[\alpha]_D$ +18 (c, 1.40 in H_2O). Both nat. and synthetic material consisted of mixts. of diastereoisomers.

Lioret, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1957, **244**, 2171 (*isol*)
Biemann, K. *et al., Biochim. Biophys. Acta*, 1960, **40**, 369 (*struct, ms, synth*)
Kemp, J.D. *et al., Plant Physiol.*, 1978, **62**, 26 (*synth, biosynth*)

Lysozyme L-135

[9001-63-2]

[12671-19-1]

N-*Acetylmuramylhydrolase. Peptidoglycan* N-*acetylmuramoylhydrolase. Muramidase. E.C. 3.2.1.17. E1105*

A protein consisting of a single linear chain of 129 amino acid residues cross-linked by four cystine disulfide bridges. For full structure see Jollés, J. *et al*. Preservative. Prevents late blowing in semi-hard cheeses due to *Clostridium tyrobutyricum*.

► OL5987000

Hydrochloride: [9066-59-5] *Acdeam. Antalzyme. Immunozima. Lanzyme. Leftose. Murazyme. Neutase*

[52219-07-5]

Jollés, P. *et al., Proc. R. Soc. London*, 1967, **167**, 650 (*primary struct*)
Philips, D.C. *et al., Proc. R. Soc. London, B*, 1967, **167**, 378 (*cryst struct*)
Hamaguchi, K. *et al., Proteins: Struct. Funct.*, 1972, **1**, 85 (*rev*)
Campbell, I.D. *et al., Proc. R. Soc. London, A*, 1975, **345**, 23 (*pmr*)
Moult, J. *et al., Methods Mol. Biol.*, 1976, **100**, 179 (*tertiary struct*)
Fernadez-Souse, J.H. *et al., Biochim. Biophys. Acta*, 1978, **523**, 430 (*isol*)
Ataka, M. *et al., Biopolymers*, 1979, **18**, 507 (*ir*)
Ikehara, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2202 (*gene synth*)
Redfield, C. *et al., Biochemistry*, 1988, **27**, 122; 1990, **29**, 7201 (*nmr, conformn*)
McKenzie, H.A. *et al., Adv. Protein Chem.*, 1991, **41**, 173 (*rev*)
Kachalova, G. *et al., FEBS Lett.*, 1991, **284**, 91 (*cryst struct*)

LZ 8 L-136

Ling Zhi-8

Protein containing 110 amino acid residues including an acetylated *N*-terminal serine. Isol. from a mycelial extract of the Oriental medical fungus Ling Zhi (*Ganoderma lucidum*). Sol. EtOAc, MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 290 (E1%/1cm 25) (MeOH) (Berdy).

Kino, K. *et al., J. Biol. Chem.*, 1989, **264**, 472-478 (*isol*)
Tanaka, S. *et al., J. Biol. Chem.*, 1989, **264**, 16372-16377 (*struct*)

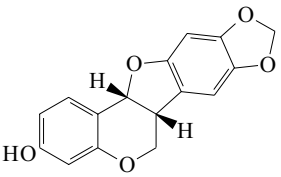
M1 M-1

Basic protein, MW 5677 Da. A gamma-thionin showing antifungal activity isol. from seeds of yellow mustard, *Sinapis alba*.

Neumann, G.M. *et al., Int. J. Pept. Protein Res.*, 1996, **47**, 437-446 (*isol, struct*)

Maackiain M-2

6a,12a-Dihydro-6H-[1,3]dioxolo[5,6]benzofuro[3,2-c][1]benzopyran-3-ol, 9CI. 3-Hydroxy-8,9-methylenedioxypterocarpan. 7-Hydroxy-4′,5′-methylenedioxypterocarpan (obsol.). Demethylpterocarpin. Inermin



(−)-*form*

$C_{16}H_{12}O_5$ 284.268
λ_{max} 282 (ϵ 3800); 287 (ϵ 4460) (MeOH) (Berdy).

(-)-*form* [2035-15-6]
Widespread in the Leguminosae subfamily. Constit. of *Trifolium pratense* (red clover). Leaflets (MeOH aq.). Sol. MeOH, dioxan, C_6H_6, bases; poorly sol. H_2O. Mp 179-181°. $[\alpha]_D^{22}$ -260 (c, 1.0 in Me_2CO). λ_{max} 280 (ϵ 4420); 286 (ϵ 5120); 310 (ϵ 8500) (EtOH) (Berdy).

O-*β-D-Glucopyranoside:* [6807-83-6] ***Trifolirhizin***
$C_{22}H_{22}O_{10}$ 446.41
Isol. from *Trifolium pratense* (red clover). Rods + 1MeOH (MeOH). Sol. MeOH, Me_2CO; fairly sol. H_2O. Mp 142-144° dec. $[\alpha]_D^{20}$ -183 (c, 1.5 in EtOH). λ_{max} 280 (ϵ 7330); 285 (ϵ 4560); 310 (ϵ 7310) (MeOH) (Berdy). λ_{max} 280 (ϵ 3900); 285 (ϵ 4700); 310 (ϵ 8000) (EtOH) (Berdy).

O-*(6′-O-Malonyl-β-D-glucopyranoside):* [135574-57-1] *6′-Malonyltrifolirhizin*
$C_{25}H_{24}O_{13}$ 532.457
Constit. of *Cicer arietinum* (chickpea).

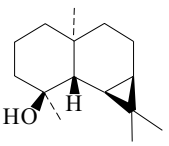
O-*β-D-Galactopyranoside:* [114761-94-3]
$C_{22}H_{22}O_{10}$ 446.41
Isol. from *Trifolium pratense* (red clover).

[22091-18-5, 22973-29-1]

Bredenberg, J.B. *et al., Acta Chem. Scand.*, 1961, **15**, 696; 936 (*Trifolirhizin*)
Suginome, H. *et al., Experientia*, 1962, **18**, 161 (*isol, ir, uv, pmr*)
Shibata, S. *et al., Chem. Pharm. Bull.*, 1963, **11**, 167 (*isol, uv, ir*)
Ito, S. *et al., Chem. Comm.*, 1965, 595 (*abs config*)
Pachler, K.G.R. *et al., Tetrahedron*, 1967, **23**, 1817 (*nmr*)
Kukui, K. *et al., Experientia*, 1968, **24**, 536 (*synth, ir, uv*)
Harper, S.H. *et al., J.C.S.(C)*, 1969, 1109 (*isol*)
Dewick, P.M. *et al., Phytochemistry*, 1975, **14**, 979; 1977, **16**, 93; 1978, **17**, 1751 (*isol, biosynth*)
Horino, H. *et al., Chem. Comm.*, 1976, 500 (*synth*)
Pelter, A. *et al., J.C.S. Perkin 1*, 1976, 2475 (*cmr*)
Dewick, P.M. *et al., Phytochemistry*, 1977, **16**, 93 (*biosynth*)
Komatsu, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1274 (*isol*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*occur*)
Al-Ani, H.A.M. *et al., J.C.S. Perkin 1*, 1984, 2831 (*biosynth*)
Jain, A.K. *et al., J. Indian Chem. Soc.*, 1988, **65**, 69 (*galactoside*)
Ozaki, Y. *et al., J.C.S. Perkin 1*, 1989, 1219 (*synth*)
Nabei-Bidhendi, G. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 366 (*synth*)
Yamamoto, H. *et al., Phytochemistry*, 1991, **30**, 1732; 4213 (*6′-Malonyltrifolirhizin*)
Bedir, E. *et al., Phytochemistry*, 1999, **51**, 1017-1020 (*isol, pmr, cmr*)

Maaliol M-3

[527-90-2]
Maalialcohol



$C_{15}H_{26}O$ 222.37
Constit. of *Valeriana officinalis* (valerian). Cryst. (EtOH). Mp 103.5-105°. $[\alpha]_D$ +18.4 (c, 1.1 in EtOH).

4-Epimer: [489-27-0] ***4-Epimaaliol***
$C_{15}H_{26}O$ 222.37
$[\alpha]_D^{20}$ +2 (c, 0.5 in $CHCl_3$).

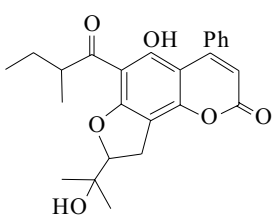
ent-form [77171-53-0] ent-*Maaliol*
Mp 98-99°. $[\alpha]_D$ -37.8 (c, 4 in $CHCl_3$).

Büchi, G. *et al., J.A.C.S.*, 1959, **81**, 1968 (*struct*)
Bates, R.B. *et al., J.A.C.S.*, 1960, **82**, 2327 (*synth*)
Büchi, G. *et al., Tet. Lett.*, 1962, 827 (*abs config*)
Asakawa, Y. *et al., Phytochemistry*, 1980, **19**, 2141 (*ent-Maaliol*)
Barnekow, D.E. *et al., J.A.C.S.*, 1989, **111**, 3511 (*synth, pmr, cmr*)
Nishiya, K. *et al., Phytochemistry*, 1992, **31**, 3511 (*isol, pmr, cmr*)
Gijsen, H.J.M. *et al., Tetrahedron*, 1994, **50**, 4733 (*synth*)
Weyerstahl, P. *et al., Annalen*, 1995, 1039 (*4-Epimaaliol*)

MAB 3 M-4

[30390-13-7]

[38703-28-5]
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2H-furo[2,3-h]-1-benzopyran-2-one, 9CI. Mammea A/AB cyclo F

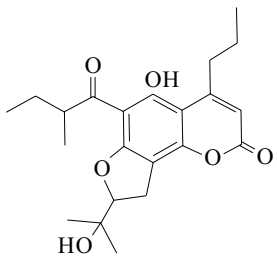


$C_{25}H_{26}O_6$ 422.477
Constit. of *Mammea americana* (mamey). Yellow cryst. Mp 134° dec., 115-117°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248-2254 (*isol, ir, uv, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317-331 (*synth*)
Guilet, D. *et al., J. Nat. Prod.*, 2001, **64**, 563-568 (*isol, cmr*)

MAB 4 M-5

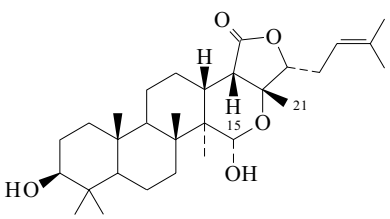
[30390-15-9]
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxobutyl)-4-propyl-2H-furo[2,3-h]-1-benzopyran-2-one, 9CI. Mammea B/AB cyclo F



$C_{22}H_{28}O_6$ 388.46
Isol. from seeds of *Mammea americana* (mamey). Cryst. (Et_2O/hexane). Mp 92-94° (83-84°).

Carpenter, I. *et al., J.C.S.(C)*, 1971, 3783 (*isol, uv, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248; 1987, 317 (*isol, ir, pmr, ms, synth*)

Mabiogenin M-6



$C_{30}H_{48}O_5$ 488.706

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: ***Mabioside C***
$C_{42}H_{68}O_{14}$ 796.991
Constit. of *Colubrina elliptica* (mabi). $[\alpha]_D$ -4 (c, 0.04 in MeOH).

15-Ketone, 21-hydroxy, 3-O-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: ***Mabioside B***†
$C_{42}H_{66}O_{15}$ 810.974
Constit. of *Colubrina elliptica* (mabi). Amorph. $[\alpha]_D$ -7.5 (c, 0.26 in MeOH). Mabioside B assigned by two different groups.

3-O-[α-L-Rhamnopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]: ***Mabioside B***†
$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Colubrina elliptica* (mabi). $[\alpha]_D$ -6 (c, 0.05 in MeOH).

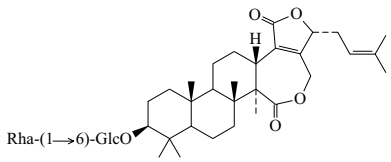
3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 15-O-β-D-glucopyranoside: [143672-61-1] ***Mabioside A***

$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Colubrina elliptica* (mabi). Needles (Me_2CO/MeOH). Mp 230-234°. $[\alpha]_D$ -23.7 (c, 0.12 in MeOH).

Seaforth, C.E. *et al., Tet. Lett.*, 1992, **33**, 4111 (*isol, pmr, cmr*)
Tinto, W.F. *et al., Magn. Reson. Chem.*, 1993, **31**, 859 (*isol, pmr, cmr*)
Oulad-Ali, A. *et al., Nat. Prod. Lett.*, 1993, **2**, 203 (*Mabioside B*)

Mabioside C M-7

[156980-54-0]

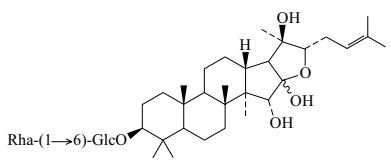


$C_{42}H_{64}O_{14}$ 792.959
Constit. of *Colubrina elliptica* (mabi). Amorph. powder. $[\alpha]_D$ -15.6 (c, 0.25 in MeOH).

Oulad-Ali, A. *et al., Phytochemistry*, 1994, **36**, 445 (*isol, pmr, cmr*)

Mabioside D M-8

[156980-55-1]

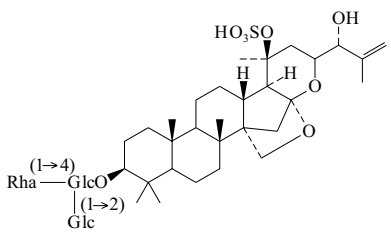


$C_{42}H_{70}O_{14}$ 799.007
Constit. of *Colubrina elliptica* (mabi). Amorph. powder. $[\alpha]_D$ -17 (c, 0.22 in MeOH).

Oulad-Ali, A. *et al., Phytochemistry*, 1994, **36**, 445 (*isol, pmr, cmr*)

Mabioside E M-9

[156980-56-2]

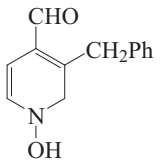


$C_{48}H_{78}O_{22}S$ 1039.197
Constit. of *Colubrina elliptica* (mabi). Amorph. powder. $[\alpha]_D$ -19.8 (c, 0.1 in MeOH).

Oulad-Ali, A. *et al., Phytochemistry*, 1994, **36**, 445 (*isol, pmr, cmr*)

Macaridine M-10

3-Benzyl-1,2-dihydro-1-hydroxy-4-pyridinecarboxaldehyde. 3-Benzyl-4-formyl-1,2-dihydro-1-hydroxypyridine

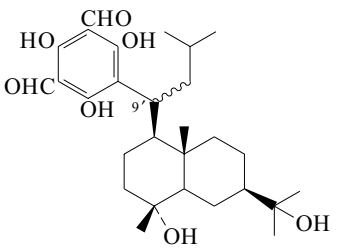


$C_{13}H_{13}NO_2$ 215.251
Alkaloid from the tubers of *Lepidium meyenii* (maca). Amorph. solid. λ_{max} 208 (log ϵ 4.07); 255 (sh) (log ϵ 3.76); 294 (log ϵ 4.14) (MeOH).

Muhammad, I. *et al., Phytochemistry*, 2002, **59**, 105-110 (*isol*)

Macrocarpal I M-11

[179388-54-6]



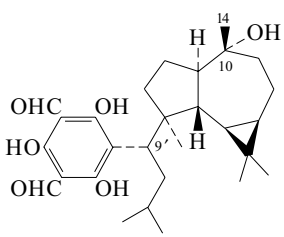
$C_{28}H_{42}O_7$ 490.636
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Pale yellow powder. $[\alpha]_D$ -49.1 (c, 0.028 in EtOH).

9′-Epimer: [179603-47-5] ***Macrocarpal J***
$C_{28}H_{42}O_7$ 490.636
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Pale yellow powder. $[\alpha]_D$ -62.5 (c, 0.048 in EtOH).

Osawa, K. *et al., J. Nat. Prod.*, 1996, **59**, 823-827 (*isol, pmr, cmr*)
Osawa, K. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1216-1217 (*abs config*)

Macrocarpal B M-12

[142698-60-0]



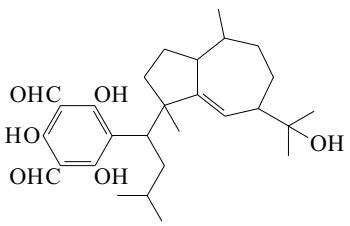
$C_{28}H_{40}O_6$ 472.62
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. Mp 198-200°. $[\alpha]_D^{24}$ -17.5 (c, 1.2 in EtOH).

10-Deoxy, 10,14-didehydro: [142628-53-3] ***Macrocarpal C***
$C_{28}H_{38}O_5$ 454.605
Isol. from *Eucalyptus globulus* (Tasmanian blue gum). Amorph. solid. $[\alpha]_D^{24}$ -3 (c, 0.92 in EtOH).

9′-Epimer: [132951-90-7] ***Macrocarpal A***
$C_{28}H_{40}O_6$ 472.62
Plates. Mp 198-200°. $[\alpha]_D^{20}$ -94.7 (c, 0.275 in EtOH). λ_{max} 288 (ϵ 10000) (EtOH/HCl) (Derep). λ_{max} 302 (ϵ 16000); 369 (ϵ 2500) (EtOH/NaOH) (Derep). λ_{max} 275 (ϵ 13000); 393 (ϵ 5600) (EtOH) (Derep).

Murata, M. *et al., Agric. Biol. Chem.*, 1990, **54**, 3221 (*isol, pmr, cmr, cryst struct*)
Yamakoshi, Y. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1570 (*isol, pmr, cmr*)
Nishizawa, M. *et al., Tet. Lett.*, 1992, **33**, 2983 (*isol, pmr, cmr, cryst struct*)
Tanaka, T. *et al., Chem. Comm.*, 1997, 2401-2402 (*synth*)
Tanaka, T. *et al., J.O.C.*, 1998, **63**, 9782-9793 (*synth*)

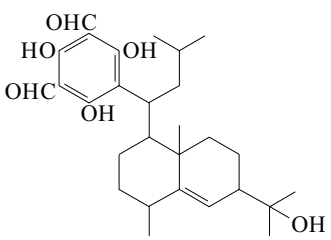
Macrocarpal D M-13



$C_{28}H_{40}O_6$ 472.62
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Amorph. solid. $[\alpha]_D^{21}$ -13.2 (c, 1 in EtOH).

Nishizawa, M. *et al., Tet. Lett.*, 1992, **33**, 2983 (*isol, pmr, cmr*)

Macrocarpal E M-14

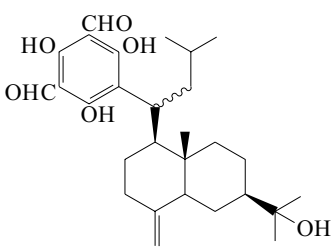


$C_{28}H_{40}O_6$ 472.62
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Amorph. solid. $[\alpha]_D^{21}$ -7.2 (c, 1.7 in EtOH).

Nishizawa, M. *et al., Tet. Lett.*, 1992, **33**, 2983 (*isol, pmr, cmr*)

Macrocarpal H M-15

[179388-53-5]



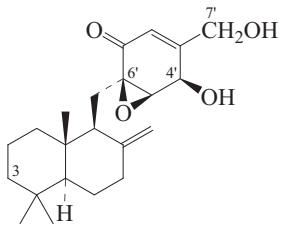
$C_{28}H_{40}O_6$ 472.62

Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Pale yellow powder. $[\alpha]_D$ -39.2 (c, 0.02 in EtOH).

Osawa, K. *et al., J. Nat. Prod.*, 1996, **59**, 823-827 (*isol, pmr, cmr*)
Osawa, K. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1216-1217 (*abs config*)

Macrophorin A M-16

[85754-70-7]



$C_{22}H_{32}O_4$ 360.492
Prod. by *Macrophoma* fruit rot of apple. Cryst. (Me_2CO/C_6H_6). Mp 127-128°. $[\alpha]_D^{20}$ +29 (MeOH). λ_{max} 237 (MeOH).

4′-O-Malonyl: [220229-94-7] ***Macrophorin G***
$C_{25}H_{34}O_7$ 446.539
Amorph. solid.

7′-O-Malonyl: [220229-90-3] ***Macrophorin E***
$C_{25}H_{34}O_7$ 446.539
Amorph. solid. $[\alpha]_D$ +24 (c, 0.5 in MeOH).

7′-O-(3-Hydroxy-3-methylglutaroyl)(S-): [92279-92-0] ***Macrophorin D***
$C_{28}H_{40}O_8$ 504.619
From *Macrophoma* fruit rot. Gum. Sol. MeOH, EtOAc, bases; poorly sol. H_2O, hexane. $[\alpha]_D^{21}$ +31 (c, 1.7 in MeOH). λ_{max} 231 (MeOH) (Berdy). λ_{max} 235 (MeOH/NaOH) (Berdy).

4′-Ketone: [349147-29-1] ***4′-Oxomacrophorin A***. *EC-B*
$C_{22}H_{30}O_4$ 358.477
Yellow oil. $[\alpha]_D$ +10.2 (c, 0.3 in MeOH). λ_{max} 219 (log ϵ 3.87); 268 (sh) (log ϵ 3.33) (MeOH).

4′-Ketone, 7′-O-(3-hydroxy-3-methylglutaroyl)(S-): [349147-28-0] ***4′-Oxomacrophorin D***. *EC-A*
$C_{28}H_{38}O_8$ 502.603
Yellow oil. $[\alpha]_D^{25}$ +35.5 (c, 0.3 in MeOH). λ_{max} 221 (log ϵ 3.97); 260 (sh) (log ϵ 3.47) (MeOH).

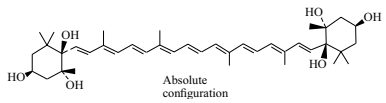
3-Oxo: [85764-12-1] ***Macrophorin B***
$C_{22}H_{30}O_5$ 374.476
From *Macrophoma* fruit rot. Cryst. Mp 107-110°. $[\alpha]_D$ +11.5 (MeOH).

3β-Hydroxy: [85764-11-0] ***Macrophorin C***
$C_{22}H_{32}O_5$ 376.492
From *Macrophoma* fruit rot. Cryst. Mp 113-116°. $[\alpha]_D$ +23 (MeOH).

Sassa, T. *et al., Agric. Biol. Chem.*, 1983, **47**, 187-189; 1984, **48**, 1923-1925 (*isol, struct*)
Sassa, T. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2260-2262 (*Macrophorins E,G*)
Fujimoto, H. *et al., J. Nat. Prod.*, 2001, **64**, 1234-1237 (*4′-Oxomacrophorin A, 4′-Oxomacrophorin D, abs config*)

Mactraxanthin M-17

[86105-69-3]
5,5′,6,6′-Tetrahydro-β,β-carotene-3,3′,5,5′,6,6′-hexol



$C_{40}H_{60}O_6$ 636.91
Constit. of Japanese edible surf clam (*Mactra chinensis*). Deep orange needles. Mp 232-233°.

Matsuno, T. *et al., Tet. Lett.*, 1983, **24**, 911
Buchecker, R. *et al., Helv. Chim. Acta*, 1984, **67**, 2043 (*synth, struct*)

Magnesium carbonate, BAN, JAN, USAN M-18

[546-93-0]

[2090-64-4]
Carbonic acid magnesium salt, 8CI. E504
$MgCO_3$
$CMgO_3$ 84.314
Isotypic with $CaCO_3$ (calcite). pH-control agent; drying agent; buffer and anticaking agent. White powder; dec. on heating with CO_2 loss. Readily dissolves in aq. acids forming the corresp. salts. Prac. insol. H_2O (0.011 g per 100 cm^3); insol. Me_2CO, NH_3(l). Mp 350° dec. ΔH_f° -1112 kJ mol^{-1}; ΔG_f° -1028 kJ mol^{-1}; S° 65.9 J K^{-1} mol^{-1}.
▶ ACGIH TLV-TWA 10 mg/m^3. OM2470000

Dihydrate: [5145-48-2] *Barringtonite*
CH_4MgO_5 120.345
Triclinic cryst.

Trihydrate: [14457-83-1]

[5145-46-0, 23389-33-5] *Nesquehonite*
CH_6MgO_6 138.36
Monoclinic cryst. Spar. sol. H_2O (0.18 g per 100 cm^3 at 16°). Mp 165°.

Pentahydrate:

[5145-47-1, 61042-72-6] *Lansfordite*
Monoclinic cryst. Spar. sol. H_2O (0.38 g per 100 cm^3 at 20°). ΔH_f° -2584 kJ mol^{-1}.

Mineral-*form* [13717-00-5] ***Magnesite***
Member of calcite group of minerals.Colourless to yellow to brown cryst.

[39409-82-0]

Fenoglio, M. *et al., Atti Accad. Naz. Lincei, Cl. Sci. Fis., Mat. Nat., Rend.*, 1936, **24**, 219 (*cryst struct, pentahydrate*)
Cohen, A. *et al., Helv. Chim. Acta*, 1939, **22**, 449 (*synth*)
Duval, R. *et al., Bull. Soc. Chim. Fr.*, 1943, 517 (*ir*)
Kinsolving, *et al., Am. Mineral.*, 1950, **35**, 127 (*cryst struct, trihydrate*)
Graf, D.L. *et al., Am. Mineral.*, 1961, **46**, 1283 (*cryst struct*)
Vinogradova, L.M. *et al., Prib. Tekh. Eksp.*, 1971, 191; *CA*, **75**, 119239 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **14**, 618 (*rev*)
Belyaev, E.K. *et al., Zh. Fiz. Khim.*, 1978, **52**, 2709 (*ir, thermochem*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 612 (*thermochem data*)
Washington, N. *et al., Antacids and Anti-Reflux Agents*, CRC Press, Boca Raton, 1991, (*book*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 274-277
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1225
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1616-1620
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAC650

Magnesium chlorate(*V*) ($Mg(ClO_3)_2$) M-19

[10326-21-3]
Chloric acid, magnesium salt, 8CI
$Mg(ClO_3)_2$
Cl_2MgO_6 191.207
Powerful desiccant and defoliant (esp. for cotton, soft fruit, potato, rice and wheat). Extremely hygroscopic colourless cryst. V. sol. H_2O.
▶ FO0175000

Hexahydrate: [7791-19-7]
$Cl_2H_{12}MgO_{12}$ 299.298
Colourless cubic cryst. V. sol H_2O (129 g per 100 cm^3 at 18°); sol. EtOH. Mp 40°.
▶ FO0200000

Rocchiccioli, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1956, **242**, 2922 (*ir*)
U.S.S.R. Pat., 1957, 107541; *CA*, 1958, **52**, 4122e (*synth*)
Martynov, Yu.M. *et al., Khim. Promst. (Moscow)*, 1958, 420; *CA*, 1960, **54**, 11363b (*manuf*)
Monev, G. *et al., Khim. Ind. (Sofia)*, 1959, **31**, 66; *CA*, **53**, 20671f (*manuf*)
Weigel, D. *et al., Bull. Soc. Chim. Fr.*, 1963, 2087 (*cryst struct, hexahydrate*)
Moshier, R.W. *et al., Inorg. Chem.*, 1964, **3**, 199 (*Cl-35 nqr*)
Gardiner, D.J. *et al., J. Phys. Chem.*, 1973, **77**, 640 (*Raman, anhydr, hexahydrate*)
Ovcharov, P.K. *et al., Agrokhimiya*, 1982, 110; *CA*, **96**, 137887 (*use, defoliant*)
U.S. Pat., 1986, 4 600 451; *CA*, **105**, 175403 (*use, explosives*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAE000

Magnesium chloride ($MgCl_2$), 8CI, USAN M-20

[7786-30-3]
Magnesium chloride. E511
$MgCl_2$
Cl_2Mg 95.21
$CdCl_2$ struct.. Flavouring agent and nutrient supplement. Hygroscopic white rhombohedral cryst. V. sol. H_2O (54.3 g per 100 cm^3 at 20°; 72.7 g per 100 cm^3 at 100°), sol. EtOH (7.4 g per 100cm^3 at 30°). Mp 714°. Bp 1412°. ΔH_f°-641.6 kJ mol^{-1}; ΔG_f°-592.1 kJ mol^{-1}; S° 89.6 J K^{-1} mol^{-1}.
▶ Irritant. OM2800000

Hexahydrate: [7791-18-6]

[13778-96-6] *Hexaaquamagnesium(2+) dichloride.* ***Bischofite***
$Cl_2H_{12}MgO_6$ 203.302

Colourless monoclinic cryst. Dec. on heating → lower hydrates and accompanying hydrol. V. sol. H_2O (167 g per 100 cm^3 at 25°, 367 g per 100 cm^3); sol. EtOH. ΔH_f° -2499 kJ mol^{-1}; ΔG_f° -2115 kJ mol^{-1}, S° 366 J K^{-1} mol^{-1}.

►OM2975000

Hexahydrate, molecular composite with β-cyclodextrin:

Mineral-*form* [15230-53-2]

Chloromagnesite

Koczkás, J.V. *et al., Z. Phys.*, 1929, **59**, 274 (*uv*)
Büchler, A. *et al., J. Chem. Phys.*, 1958, **29**, 121 (*ir*)
Ferrari, A. *et al., Acta Cryst.*, 1963, **16**, 846 (*cryst struct*)
Takahashi, A. *et al., J. Phys. Soc. Jpn.*, 1973, **35**, 1346 (*pmr, hexahydrate*)
Sorrell, C.A. *et al., J. Chem. Eng. Data*, 1974, **19**, 31 (*cryst struct, hexahydrate*)
Ergin, Yu.V. *et al., Zh. Strukt. Khim.*, 1974, **15**, 391 (*magnetism*)
Hadenfeldt, C. *et al., Z. Naturforsch., B*, 1975, **30**, 165 (*synth*)
Gurevich, L.M. *et al., Zh. Strukt. Khim.*, 1977, **18**, 858 (*ir, hexahydrate*)
Pribylov, K.P. *et al., Zh. Neorg. Khim.*, 1978, **23**, 1764 (*thermal dec, hexahydrate*)
Lai, Y. *et al., Synthesis*, 1981, 585 (*uses*)
Dubessy, J. *et al., Chem. Geol.*, 1982, **37**, 137; *CA*, 1983, **98**, 26988 (*Raman, hexahydrate*)
Kimura, H. *et al., Enerugi, Shigen*, 1985, **6**, 528; *CA*, 1986, **106**, 92081 (*heat storage*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 810 (*thermochem data*)
Naumann, R. *et al., Thermochim. Acta*, 1985, **92**, 673 (*thermal dec, hexahydrate*)
CA, 1986, **104**, 92081 (*thermal, dec, hexahydrate*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2178D
Nicolis, I. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 2381 (*cyclodextrin composite, cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1620-1621
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAE250; MAE500

Magnesium hydroxide, 8CI, USAN M-21

[1309-42-8]

Milk of magnesia. E528

$Mg(OH)_2$

H_2MgO_2 58.32

Has CdI_2 struct.. Used in foods as a dietary supplement, pH control agent and processing aid. Amorph. powder or colourless hexagonal cryst. Readily dissolves in aq. acids forming corresp. salts. Dec. on heating at 350° → MgO + H_2O. Prac. insol. H_2O (9×10^{-4} g per 100 cm^3 at 18°; 4×10^{-3} g per 100 cm^3 at 100°). Component of Ascriptin, Camalox, Fermalox, Gelusil, Maalox Plus, Mylanta and Oxaine M. ΔH_f° -925 kJ mol^{-1}; ΔG_f° -834 kJ mol^{-1}; S° 63.2 J K^{-1} mol^{-1}.

►LD_{50} (rat, orl) 8500 mg/kg. OM3570000

Mineral-*form* [1317-43-7]

Brucite

►QO4930000

[37317-08-1]

Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, No. 539, 1956, **6**, 30 (*cryst struct*)
Krishnamurti, D. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1959, **50**, 223 (*ir, Raman*)
Lippincott, E.R. *et al., J. Chem. Phys.*, 1964, **41**, 3006 (*pmr*)
U.S. Pat., 1964, 3 127 241, (*Dow*); *CA*, **60**, 14155h
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 908 (*synth*)
Brindley, G.W. *et al., Phys. Chem. Miner.*, 1984, **10**, 187 (*ir*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1267 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2179C (*haz*)
Washington, N. *et al., Antacids and Anti-Reflux Agents*, CRC Press, Boca Raton, 1991, (*book*)
Mofenson, H.C. *et al., J. Toxicol. Clin. Toxicol.*, 1991, **29**, 215 (*tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 889
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1624-1625
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAG750; NBT000

Magnesium lactate M-22

[18917-93-6]

[151566-85-7, 179308-96-4]

[Bis(2-hydroxy-O)propanoato-O]magnesium. Lactic acid magnesium salt. Magnesium 2-hydroxypropanoate

$Mg[OOCCH(OH)CH_3]_2$

$C_6H_{10}MgO_6$ 202.446

No modern reports on synth., struct. or props. Degree of hydration uncertain. Buffering agent; dough conditioner; dietary supplement. White solid + $2H_2O$ or $6H_2O$. Sol. H_2O; sl. sol. EtOH.

Merck Index, 12th edn., 1996, No. 5708
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1157

Magnesium oxide (MgO) M-23

[1309-48-4]

Magnesium oxide. Calcined brucite. Magnesia. E530

MgO

MgO 40.304

NaCl struct.. Added to food as a nutrient supplement, anticaking agent, firming agent, or lubricant and release agent. Moisture-sensitive colourless cubic cryst. Pract. insol. H_2O (8.6×10^{-3} g per 100 cm^3 at 30°); insol. EtOH; sol. acids. Mp 2832°. Bp 3600°. ΔH_f° -601.2 kJ mol^{-1}; ΔG_f° -568.9 kJ mol^{-1}; S° 26.92 J K^{-1} mol^{-1}.

►OM3850000

Mineral-*form* [1317-74-4]

Periclase

Usually colourless to grey-yellow cubic cryst.

[12274-68-9]

Skinner, *et al., Am. Mineral.*, 1957, **42**, 39 (*cryst struct*)
Kammori, O. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1967, **16**, 1050; *CA*, 1968, **69**, 6597 (*ir*)
Hanso, W.F. *et al., J. Appl. Phys.*, 1972, **43**, 1661 (*uv*)
Schramm, S. *et al., J.A.C.S.*, 1983, **105**, 2483 (*O-17 nmr*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1469 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2180C
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 278-279
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **5**, 3205-3206 (*use*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1226
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1627-1628
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAH500

Magnesium perchlorate M-24

[10034-81-8]

[64010-42-0]

Magnesium chlorate(VII). Perchloric acid, magnesium salt, 8CI. Chloric(VII) acid magnesium salt

$Mg(ClO_4)_2$

Cl_2MgO_8 223.206

Feeding stock additive. Colourless deliquescent solid. Dec. on heating with formation of MgO. V. sol. H_2O (99.3 g per 100 cm^3 at 25°), EtOH (24.0 g per 100cm^3 at 25°). ΔH_f° -569 kJ mol^{-1}; ΔG_f° -432 kJ mol^{-1}; S° 213 J K^{-1} mol^{-1}.

►Oxidiser, irritant. Potentially explosive when mixed with org. or organomet. compds.. SC8925000

Hexahydrate: [13446-19-0] *Hexaaquamagnesium(2+) perchlorate*

$Cl_2H_{12}MgO_{14}$ 331.297

Colourless orthorhombic cryst. Dec. on heating with H_2O loss. (Pseudo-hexagonal) struct. ΔH_f° -2446 kJ mol^{-1}; ΔG_f° -1863 kJ mol^{-1}; S° 521 J K^{-1} mol^{-1}.

►Oxidiser, irritant.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1254A (*ir*)
West, C. *et al., Z. Kristallogr.*, 1935, **91**, 480 (*cryst struct, hexahydrate*)
Miller, F.A. *et al., Anal. Chem.*, 1952, **24**, 1253 (*ir*)
Weil, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 2510 (*Raman*)
Balicheva, T.G. *et al., Zh. Strukt. Khim.*, 1964, **5**, 29 (*ir, hexahydrate*)
Gazarov, R.A. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1975, **222**, 859 (*hydrate, pmr*)
Heubel, P. *et al., J. Solution Chem.*, 1979, **8**, 283 (*Mg-25 nmr*)
Patel, M.B. *et al., J. Raman Spectrosc.*, 1983, **14**, 406 (*hydrate, Raman*)
Ishitani, O. *et al., J.C.S. Perkin 1*, 1985, 1527 (*uses*)
Agarwal, A. *et al., J. Raman Spectrosc.*, 1985, **16**, 303 (*hydrate, polymorphs, Raman*)
White, M.A. *et al., J. Chem. Phys.*, 1986, **84**, 3484 (*hydrate, polymorphs, ir*)
Devlin, D.J. *et al., Thermochim. Acta*, 1986, **104**, 159 (*anhyd, hydrate, thermal dec*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2180D (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PCE000

Magnesium phosphate ($Mg(HPO_4)$) M-25

[7757-86-0]

[10043-83-1]

Magnesium phosphate (1:1), 9CI, 8CI. Magnesium hydrogenphosphate. Phosphoric acid, magnesium salt (1:1), 8CI

$Mg(HPO_4)$

$HMgO_4P$ 120.284

Anhydrous salt not obt. pure by thermal dehydration of hydrates because of simultaneous structural dehydration to give condensed salts. Used in foods as a nutritional source of Mg and P, pH control agent, dietary supplement, flow aid and leavening agent. Dec. on heating to 650° with evolution of H_2O and formation of $Mg_2P_2O_7$. In addition to the tri- and hepta-hydrates, a monohydrate and a hexahydrate have been reported.

Trihydrate: [7782-75-4]
Diamond-shaped rhombs. Sol. acids; spar. sol. H_2O. Loses $3H_2O$ at 130-300°, and 0.5 H_2O at 300-580° depending on heating rate, with formation of $Mg_2P_2O_7$ before much water driven off. Can lose 2.4 H_2O during vacuum drying. Orthorhombic. At pH 7.9 → Magnesium phosphate ($Mg_3(PO_4)_2$), M-26. Cryst. struct. possesses markedly distorted $PO_4^{3\ominus}$ tetrahedra, layers of which alternate with octahedrally coordinated Mg ions. Loses H_2O on grinding.

Heptahydrate: [13446-22-5]
Long, colourless prisms. Sol. acids; spar. sol. H_2O; insol. EtOH. Easily loses $4H_2O$.

Mineral-*form* [14654-11-6]
Newberyite
Essentially the trihydrate.Short colourless, transparent prismatic or tubular cryst. with vitreous lustre. Closely related is Hannayite.

Mineral-*form* [14654-10-5]
Phosphorrosslerite. Phosphoroesslerite
Essentially the heptahydrate.Normally pale yellowish, monoclinic prismatic cryst. with vitreous lustre (when fresh). Readily loses $4H_2O$.

[19154-49-5, 38894-14-3]

Hägele, G. *et al., Zentralbl. Mineral., Geol. Palentol.*, 1939, **A2**, 97 (*cryst struct, heptahydrate*)
Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1951, 709; 713 (*minerals*)
Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Sutor, D.J. *et al., Acta Cryst.*, 1967, **23**, 418 (*cryst struct, trihydrate*)
Brekhunets, A.G. *et al., Dokl. Akad. Nauk BSSR*, 1969, **13**, 1005; *CA*, 1970, **72**, 237517 (*pmr, trihydrate*)
Il'yasova, A.K. *et al., CA*, 1971, **75**, 12753 (*ir, trihydrate*)
Duff, E.J. *et al., J.C.S.(A)*, 1971, 2736 (*synth*)
Pirogov, Yu.A. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1972, **8**, 878; *Inorg. Mater. (Engl. Transl.)*, 1972, **8**, 763 (*props*)
Shchegrov, L.N. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1973, **9**, 1783; *Inorg. Mater. (Engl. Transl.)*, 1973, **9**, 1587 (*synth, props*)
Havel, J. *et al., Chem. Scr.*, 1974, **5**, 164 (*synth*)
Krylov, O.S. *et al., Zh. Prikl. Khim. (Leningrad)*, 1975, **48**, 422 (*thermal dec, trihydrate*)
Kotlova, A.G. *et al., Term. Anal. Miner. 1978*, 1978, 128 (*synth, hydrates*)
Abbona, F. *et al., Acta Cryst. B*, 1979, **35**, 2514 (*cryst struct*)
Pechkovskii, V.V. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1979, **15**, 957; *Inorg. Mater. (Engl. Transl.)*, 1979, **15**, 750 (*ir, Raman*)
Boistelle, R. *et al., J. Cryst. Growth*, 1981, **54**, 275 (*synth, struct, morphology*)
Komornicki, S. *et al., Bull. Pol. Acad. Sci., Chem.*, 1985, **33**, 127; *CA*, **103**, 115081 (*thermal stability*)
Abbona, F. *et al., J. Cryst. Growth*, 1986, **74**, 581 (*synth, trihydrate*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr, F-19 nmr, trihydrate*)
Andraptseva, N.M. *et al., Zh. Neorg. Khim.*, 1988, **33**, 2506; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1988, **33**, 1435 (*synth, ir, cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1629-1630
Afanas'eva, V.A. *et al., Zh. Neorg. Khim.*, 1998, **43**, 392-396; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1998, **43**, 330-334 (*ir*)
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1157
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAH775

Magnesium phosphate ($Mg_3(PO_4)_2$) M-26

[7757-87-1]

[10043-83-1]

Magnesium phosphate (3:2), 9CI, 8CI, USAN. Magnesium orthophosphate. Phosphoric acid, magnesium salt (2:3), 8CI. Magnesium phosphate tribasic

$Mg_3(PO_4)_2$

$Mg_3O_8P_2$ 262.858

Additional hydrates thought to be formed as intermediates in dehydration sequences, with $x H_2O$, x = 1, 3, 5, 11. Used in foods as a nutrient supplement and pH control agent. Iridescent, orthorhombic cryst. Sol. acids; insol. H_2O. Mp 1348°. ΔH_f° -3775 kJ mol^{-1}; ΔG_f° -3503 kJ mol^{-1}; S° 188 J K^{-1} mol^{-1}.

Tetrahydrate: [13465-22-0]
Prac. insol. H_2O. ΔH_f° -4023 kJ mol^{-1}.

Pentahydrate: [10233-87-1] Loses $3H_2O$ at 220°.

Heptahydrate: [26062-72-6] Loses 5 H_2O at 190°, and remainder of H_2O of cryst. at → 420°, ending at 440-530°.

Octahydrate: [13446-23-6]
The most stable hydrate. Possesses nuclear coord. H_2O. Prac. insol. (H_2O). Two kinds of cryst. lattice known, both monoclinic. H_2O molecules coord. by cation are non-equiv. Dehydrates in three stages at 110°, 280° and 370°.

Decahydrate: [10102-35-9]
Possesses nuclear coord. H_2O as well as H_2O of cryst. Said to occur in aq. solns..

Docosahydrate: [53408-95-0]
Colourless plates. Possesses nuclear coord. H_2O as well as H_2O of cryst. Triclinic unit cell. P–O 153.9-154.9 pm, OPO 108.6-110.5°. Mg–O 205-210.6 pm. Stable in air, unstable in aq. → octahydrate. Vacuum drying removes $18H_2O$. Otherwise, $20H_2O$ are lost at 150° and $1H_2O$ at 280°. Completely dehydrates at 320-600°.

Mineral-*form* [16225-79-9]
Bobierite
Essentially the octahydrate. Monoclinic, and closely related to the vivianite group. Octahedral edge-sharing dimers $Mg_2O_6(H_2O)_4$ and independent $MgO_2(H_2O)_4$ octahedra (Mg–O 203.0-213.9 pm) are linked by PO_4 tetrahedra (PbO 153.5-155.9 pm, OPO 107.2-112.0°). Complex sheets differ in one direction only from those of synthetic compound.Minute acicular or fibrous, transparent colourless cryst.

[10233-87-1, 53408-95-0]

Dana's System of Mineralogy, 7th Ed., Wiley, N.Y., 1951, 753
Taylor, A.W. *et al., Trans. Faraday Soc.*, 1963, **59**, 1585 (*synth, props*)
Nord, A.G. *et al., Acta Chem. Scand.*, 1968, **22**, 1466 (*cryst struct*)
Eanes, E.D. *et al., Calcif. Tissue Res.*, 1968, **2**, 38 (*synth*)
Termine, J.D. *et al., Calcif. Tissue Res.*, 1974, **15**, 55 (*ir Raman*)
Vol'khin, V.V. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1976, **12**, 1634; *Inorg. Mater. (Engl. Transl.)*, 1976, **12**, 1340 (*props*)
Schroeder, L.W. *et al., J. Phys. Chem.*, 1978, **82**, 2335 (*synth, cryst struct*)
Kanazawa, T. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 3713 (*synth, cryst struct*)
Bar-On, P. *et al., J. Agric. Food Chem.*, 1979, **27**, 152 (*manuf*)
Pechkovskii, V.V. *et al., Zh. Neorg. Khim.*, 1979, **24**, 651; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 363 (*cryst struct*)
Mazghouri, M. *et al., Thermochim. Acta*, 1981, **47**, 125 (*props*)
Catti, M. *et al., Z. Kristallogr.*, 1981, **155**, 53 (*synth, cryst struct*)
Takagi, S. *et al., Am. Mineral.*, 1986, **71**, 1229 (*cryst struct*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Théorodoret, *et al., Rev. Chim. Miner.*, 1987, **24**, 478 (*synth, struct*)
Lopatin, S.I. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1989, **25**, 645; *Inorg. Mater. (Engl. Transl.)*, 1989, **25**, 556 (*ms*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 857
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1631

Magnesium silicate (Mg_2SiO_4) M-27

[10034-94-3]

Magnesium orthosilicate. E553a

Mg_2SiO_4

Mg_2O_4Si 140.693

Normally has the olivine struct. (α-phase). High-pressure modified spinel (β-phase) and spinel (γ-phase) structs. exist. Anticaking and coating agent. Cryst. Insol. H_2O. Mp 1910°.

Mineral-*form* [15118-03-3]
Forsterite
Green, lemon yellow, white orthorhombic cryst.

[1343-88-0]

Deer, W.A. *et al., Rock Forming Minerals*, Longman, 1962, **1A**, 1 (*mineral*)
Horiuchi, H. *et al., Am. Mineral.*, 1981, **66**, 568 (*cryst struct*)
Lager, G.A. *et al., J. Appl. Crystallogr.*, 1981, **14**, 137 (*cryst struct, olivine-form*)
Sasaki, S. *et al., J. Geophys. Res., B*, 1982, **87**, 7829 (*cryst struct, spinel-form*)
Handke, M. *et al., J. Mol. Struct.*, 1982, **79**, 353 (*ir, Raman*)
Piriou, B. *et al., Am. Mineral.*, 1983, **68**, 426 (*Raman, olivine-form*)
Schramm, S. *et al., J.A.C.S.*, 1984, **106**, 2502 (*O-17 nmr*)
Weiden, N. *et al., Z. Naturforsch., A*, 1985, **40**, 126 (*Si-29 nmr*)
McMillan, P. *et al., Am. Mineral.*, 1987, **72**, 361 (*Raman, spinel-form*)
Petricevic, V. *et al., Appl. Phys. Lett.*, 1988, **52**, 1040 (*use*)
Burlitch, J.M. *et al., Chem. Mater.*, 1991, **3**, 692 (*synth, use*)
Park, D.G. *et al., Chem. Mater.*, 1993, **5**, 518 (*synth, uv-vis, powder struct, epr, sem*)
Yeager, K.E. *et al., Chem. Mater.*, 1993, **5**, 525 (*synth, Si-29 nmr, Raman*)

Magnesium sulfate heptahydrate M-28

[10034-99-8]
Sulfuric acid, magnesium salt, heptahydrate, 8CI. Bitter salts. Magnesium sulfate, JAN, USAN

$MgSO_4.7H_2O$

$H_{14}MgO_{11}S$ 246.475

Used in foods as a flavour enhancer, nutrient supplement and processing aid. Colourless orthorhombic cryst. Dec. on heating → monohydrate and then anhyd. $MgSO_4$. V. sol. H_2O (71 g per 100 cm^3 at 20°); spar. sol. EtOH. Piezoelectric. ΔH_f° -3389 kJ mol^{-1}; ΔG_f° -2872 kJ mol^{-1}; S° 372 J K^{-1} mol^{-1}.

►OM4508000

Mineral-*form* [14457-55-7]
Epsomite. *Epsom salts*
Named after deposit in Epsom, England.Colourless transparent cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1264C (*ir*)
Baur, W.H. *et al., Acta Cryst.*, 1964, **17**, 1361 (*cryst struct*)
Heide, K. *et al., Naturwissenschaften*, 1965, **52**, 183 (*thermal dec*)
Diem, P. *et al., Phys. Kondens. Mater.*, 1968, **7**, 76 (*ir*)
Hillaire, P. *et al., C. R. Hebd. Seances Acad. Sci. Ser. B*, 1971, **273**, 255 (*Raman*)
Ferraris, G. *et al., J.C.S. Dalton*, 1973, 816 (*cryst struct, nd*)
Lallemant, M. *et al., Rev. Chim. Miner.*, 1974, **11**, 113 (*dissn press*)
Skokanova, Z. *et al., Czech. J. Phys., Sect. B (Engl. Transl.)*, 1978, **28**, 220 (*magnetism*)
Yaroslavtsev, A.B. *et al., Koord. Khim.*, 1981, **7**, 697 (*pmr, thermal dec*)
Phadnis, A.B. *et al., Thermochim. Acta*, 1981, **43**, 249 (*thermal dec*)
Calleri, M. *et al., Acta Cryst. B*, 1984, **40**, 218 (*abs config, cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 857
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1635-1636

Magnesium trisilicate, USAN M-29

[39365-87-2]

[14987-04-3]
Trimax. Sellagen. Magnosil. E553a

$Mg_2Si_3O_8$

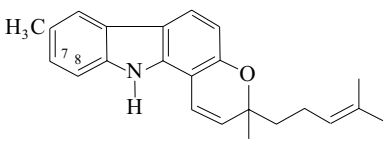
$Mg_2O_8Si_3$ 260.862

Anticaking and coating agent. White powder. Component of Azolid A, Gaviscon, Malcotabs, Tricreamalate and Trisogel.

Glass, N. *et al., Q. J. Pharm. Pharmacol.*, 1936, **9**, 445
U.S. Pat., 1966, 3 272 594
Washington, N. *et al., Antacids and Anti-Reflux Agents*, CRC Press, 1991, (*book*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 283-284
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1226
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1632-1633
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 7th edn., Van Nostrand Reinhold*, 1989, 2154

Mahanimbicine M-30

3,11-Dihydro-3,8-dimethyl-3-(4-methyl-3-pentenyl)pyrano[3,2-a]carbazole, 9CI. Isomahanimbine



$C_{23}H_{25}NO$ 331.457

(+)-*form* [28305-77-3]
Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Mp 142°. $[\alpha]_D^{30}$ +18.6 (c, 0.86 in $CHCl_3$).

7-Hydroxy: [138876-26-3] ***Pyrafoline D***. *Isomahanine*
$C_{23}H_{25}NO_2$ 347.456
Alkaloid from seeds of *Murraya koenigii* (curryleaf tree). Pale brown powder, cryst. (CH_2Cl_2/petrol). Mp 184°. $[\alpha]_D$ 0 (MeOH). Pyrafoline D descr. as brown powder, Isomahanine as cryst. with indicated Mp. Opt. rotn. refers to Pyrafoline D. The samples have not been compared.

(±)-*form* [28305-78-4]
Mp 140°. Racemate.

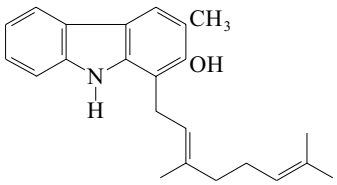
8-Methoxy: [134779-19-4] ***Murrayamine C***†
$C_{24}H_{27}NO_2$ 361.483
Syrup.

[26871-46-5]

Kureel, S.P. *et al., Chem. Ind. (London)*, 1970, 958 (*uv, ir, pmr, struct, synth*)
Joshi, B.S. *et al., Tetrahedron*, 1970, **26**, 1475 (*isol, uv, ir, pmr, struct*)
Narasimhan, N.S. *et al., Indian J. Chem.*, 1975, **13**, 993 (*isol, uv, ir, pmr, ms, struct*)
Narasimhan, N.S. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 329 (*synth*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1668 (*Pyrafoline D*)
Wu, T.-S. *et al., Phytochemistry*, 1991, **30**, 1048 (*Murrayamine C*)
Reisch, J. *et al., Phytochemistry*, 1992, **31**, 2877 (*Isomahanine*)
Itoigawa, M. *et al., J. Nat. Prod.*, 2000, **63**, 893-897 (*activity*)

Mahanimbilol M-31

[77156-13-9]
Mahanimbinol



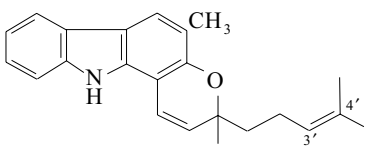
$C_{23}H_{27}NO$ 333.472

The struct. was first assigned to Mahanimbinol but Reisch *et al* assigned it to Mahanimbilol with different spectroscopic props. The struct. of Mahanimbinol is therefore currently unresolved. Alkaloid from *Murraya koenigii* (curryleaf tree). Pale yellow oil.

Rao, A.V.R. *et al., Chem. Ind. (London)*, 1980, 697 (*Mahanimbinol*)
Reisch, J. *et al., Phytochemistry*, 1994, **36**, 1073 (*Mahanimbilol*)
Meragelman, K.M. *et al., J. Nat. Prod.*, 2000, **63**, 427 (*activity*)

Mahanimbine M-32

3,11-Dihydro-3,5-dimethyl-3-(4-methyl-3-pentenyl)pyrano[3,2-a]carbazole, 9CI



$C_{23}H_{25}NO$ 331.457

(+)-*form* [21104-28-9]
Alkaloid from the fruits and leaves of *Murraya koenigii* (curryleaf tree). Cryst. (hexane). Mp 94-95°. $[\alpha]_D$ +40.6 (c, 2.1 in $CHCl_3$). $[\alpha]_D$ +52 ($CHCl_3$).

N-*Me:*
Needles (EtOH). Mp 120°.

N-*Et:*
Cryst. (EtOH). Mp 96°.

3′,4′-Dihydro, 4′-hydroxy: [30048-24-9] ***Mahanimbinine***
$C_{23}H_{27}NO_2$ 349.472
Alkaloid from leaves of *Murraya koenigii* (curryleaf tree). Mp 179°.

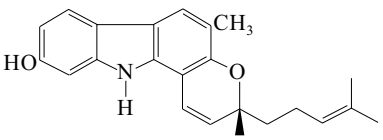
$\Delta^{4'}$-Isomer, 3′-hydroxy: [73385-58-7] ***Murrayamine C***
$C_{23}H_{25}NO_2$ 347.456
Pale yellow oil. This struct. was formerly assigned erroneously to Mahanimboline. The pmr data of the compd. isol. by Roy *et al* (1979) are different from those reported for Murrayamine C (see Mahanimbicine, M-30), which has now been assigned this struct..

(±)-*form* [24948-14-9]
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (hexane). Mp 72-73° Mp 75-76° Mp 94-95°.

Narasimhan, N.S. *et al., Tet. Lett.*, 1968, 5501 (*uv, pmr, ms, struct*)
Kureel, S.P. *et al., Experientia*, 1970, **26**, 1055 (*Mahanimbinine*)
Joshi, B.S. *et al., Tetrahedron*, 1970, **26**, 1475 (*isol, uv, ir, pmr, struct*)
Bandaranyake, W.M. *et al., J.C.S. Perkin 1*, 1974, 998 (*synth*)
Roy, S. *et al., Phytochemistry*, 1974, **13**, 2893 (*isol, uv, ir, pmr*)
Narasimhan, N.S. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 329; 430 (*isol, uv, ir, pmr, ms, struct, synth*)
Bhattacharyya, P. *et al., J. Indian Chem. Soc.*, 1978, **55**, 308 (*isol, uv, ir*)
Roy, S. *et al., Chem. Ind. (London)*, 1979, 669 (*Mahanimboline*)
Ito, C. *et al., Phytochemistry*, 1992, **31**, 1083 (*Murrayamine C*)
Meragelman, K.M. *et al., J. Nat. Prod.*, 2000, **63**, 427-428 (*isol, cmr*)
Itoigawa, M. *et al., J. Nat. Prod.*, 2000, **63**, 893-897 (*activity*)

Mahanine M-33

3,11-Dihydro-3,5-dimethyl-3-(4-methyl-3-pentenyl)pyrano[3,2-a]carbazol-9-ol, 9CI



(*R*)-*form*

$C_{23}H_{25}NO_2$ 347.456

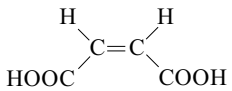
(*R*)-*form* [28360-49-8]
Alkaloid from the leaves of *Murraya koenigii* (curry leaf tree). Fluffy cryst. (petrol). Mp 98-100°. $[\alpha]_D$ -24.4.

(*S*)-*form* [134876-75-8]
Needles (Me_2CO). Mp 95-96°. $[\alpha]_D$ +34 (c, 2 in $CHCl_3$). λ_{max} 221 (ϵ 73300); 240 (ϵ 81200); 294 (ϵ 64600); 325 (ϵ 4500); 342 (ϵ 4800); 357 (ϵ 3450) (MeOH) (Berdy).

Narasimhan, N.S. *et al., Indian J. Chem.*, 1975, **13**, 993 (*isol, uv, ir, pms, ms, struct*)
Atta-ur-Rahman, *et al., Fitoterapia*, 1988, **59**, 494 (*pmr, cmr*)
Wu, T.-S. *et al., Phytochemistry*, 1991, **30**, 1048 (*isol, pmr*)
Itoigawa, M. *et al., J. Nat. Prod.*, 2000, **63**, 893-897 (*activity*)

Maleic acid, 8CI M-34

[110-16-7]
(Z)-2-Butenedioic acid, 9CI. cis-*Ethylene-1,2-dicarboxylic acid*



$C_4H_4O_4$ 116.073

For (*E*)-form see Fumaric acid, F-86.Prisms (H_2O) with repulsive astringent taste. Sol. H_2O, EtOH, Et_2O, Me_2CO. Mp 138-139°. pK_{a1} 1.65; pK_{a2} 5.61 (25°,H_2O). On heating above the Mp is converted partly to Fumaric acid, F-86 and partly to the anhydride.

► Skin, mucous membrane, and severe eye irritant. LD_{50} (rat, orl) 708 mg/kg. LD_{50} (rbt, skn) 1560 mg/kg. OM9625000

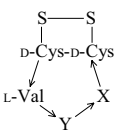
Homopolymer: [26099-09-2]
Limescale prevention additive for boiler water. Permitted additive in foods.

[142-44-9, 371-47-1, 1330-76-3, 6915-18-0, 18016-19-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 503A; 644B; 644C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 787A; 992A; 992B; 992C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 689A; 689B; 689D (*ir*)
Bhattacharyya, A. *et al., J. Appl. Chem.*, 1958, **8**, 728 (*manuf*)
Rodd's Chem. Carbon Compd. (2nd edn.), 1965, **1D**, 340 (*rev, synth, props*)
Gillo-Tos, M. *et al., Kunststoffe*, 1966, **56**, 409-412 (*gc*)
Chiusoli, G.P. *et al., Chem. Ind. (London)*, 1968, 977 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
James, M.N.G. *et al., Acta Cryst. B*, 1974, **30**, 1249 (*cryst struct*)
Compton, D.A.C. *et al., J.C.S. Perkin 2*, 1975, 400 (*Raman*)
Vogeli, U. *et al., Org. Magn. Reson.*, 1975, **7**, 617 (*nmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **15**, 893 (*rev*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4969
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DED600; DJO200; DSL800; MAK900

Malformin M-35

[53571-13-4]



malformin						
	A_1	X =	L-Ile ,	Y =	D-Leu
	A_2	X =	L-Val ,	Y =	D-Leu
	A_4	X =	L-Val ,	Y =	D-Ile
	B_{1a}	X =	L-*allo*-Ile ,	Y =	D-Leu
	B_{1b}	X =	L-Leu ,	Y =	D-Leu
	B_2	X =	L-Leu ,	Y =	D-Val
	B_3	X =	L-Leu ,	Y =	D-Ile
	B_4	X =	L-Ile ,	Y =	D-Ile
	B_5	X =	L-Ile ,	Y =	D-Val
	C	X =	L-Leu ,	Y =	D-Leu

Cyclic peptide antibiotic complex. Prod. by *Aspergillus niger*. Isol. from mould damaged rice. Mp 0°. $[\alpha]_D^{24}$ +58.6 (c, 0.5 in DMF). Dec. >300°.

Malformin A, 9CI [3022-92-2]
Malformin A_1. Cyclic (D-cysteinyl-D-cysteinyl-L-valyl-D-leucyl-L-isoleucyl)-cyclic(1→2)-disulfide, 9CI

$C_{23}H_{39}N_5O_5S_2$ 529.724
Sol. MeOH, butanol; fairly sol. Me_2CO, EtOAc; poorly sol. $CHCl_3$, H_2O, hexane. Mp 300° dec. $[\alpha]_D^{24}$ +58.6 (c, 0.5 in DMF). $[\alpha]_D^{25}$ -39 (2-methoxyethanol). Major component of Malformin complex. Contains 12% Malformin A_2 which is biol. inactive λ_{max} 252 (ϵ 475) (EtOH) (Derep). λ_{max} 220 (ϵ 4100) (MeOH) (Berdy).

► LD_{50} (mus, ipr) 3.1 mg/kg. ON7050000

Malformin A_2 [83680-20-0]
$C_{22}H_{37}N_5O_5S_2$ 515.697
$[\alpha]_D$ -49.5 (c, 0.73 in 2-methoxyethanol).

Malformin A_4
$C_{22}H_{37}N_5O_5S_2$ 515.697

Malformin B_1 [138875-32-8]
$C_{23}H_{39}N_5O_5S_2$ 529.724
$[\alpha]_D^{25}$ -40.3 (c, 0.72 in 2-methoxyethanol). Minor component. Has been separated into 2 components B_{1a} and B_{1b}.

Malformin B_2 [138797-31-6]
$C_{22}H_{37}N_5O_5S_2$ 515.697
Amorph. Sol. EtOH, MeOH, EtOAc; poorly sol. H_2O, hexane. λ_{max} 220 (MeOH) (Berdy).

Malformin B_3
$C_{23}H_{39}N_5O_5S_2$ 529.724

Malformin B_4
$C_{23}H_{39}N_5O_5S_2$ 529.724

Malformin B_5
$C_{23}H_{37}N_5O_5S_2$ 527.708

Malformin C [59926-78-2]
Malformin A_3
$C_{23}H_{39}N_5O_5S_2$ 529.724
Amorph. Mp 300° dec. $[\alpha]_D^{25}$ -37.4 (c, 1.01 in DMSO). Poss. identical with B_{1b}.

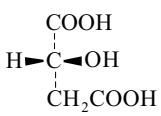
► LD_{50} (mus, ipr) 0.9 mg/kg. ON7060000

[11004-48-1, 130392-01-7, 130392-02-8]

Curtis, R.W. *et al., Science (Washington, D.C.)*, 1958, **128**, 661
Tekeuchi, S. *et al., Phytochemistry*, 1967, **6**, 287 (*isol*)
Bodanszky, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1974, **71**, 2791 (*struct, synth*)
Stahl, G.L. *et al., Diss. Abstr. Int., B*, 1975, **36**, 2817 (*synth, struct*)
Bodanszky, M. *et al., J. Antibiot.*, 1976, **29**, 549 (*ms*)
Anderegg, R.J. *et al., J.A.C.S.*, 1976, **98**, 3365 (*isol, spectra, struct*)
Bodanszky, M. *et al., Int. J. Pept. Protein Res.*, 1982, **20**, 16 (*struct, bibl, conformn*)
Hall, D. *et al., J. Comput. Chem.*, 1982, **3**, 89 (*conformn*)
Chandrasekaran, R. *et al., Conform. Biol.*, (Srinivasan, R., Ed.,), Adenine Press, New York, 1983, (*conformn, rev*)
Sugawara, F. *et al., Tet. Lett.*, 1990, **31**, 4337 (*pmr, struct*)
Kim, K.W. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 240; 787 (*isol, pmr, struct*)
Varoglu, M. *et al., J. Nat. Prod.*, 2000, **63**, 41-43 (*Malformin C, isol, pmr, cmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 671; 673; 675; 678

Malic acid, 8CI M-36

[6915-15-7]
Hydroxybutanedioic acid, 9CI. Hydroxysuccinic acid. E296



(*R*)-*form*

$C_4H_6O_5$ 134.088
Mainly used as an acidifier in a wide range of food, such as fruit drinks, jams, sweet and sour sauces, boiled sweets, chewing gum. Occasionally used as a metal ion chelator in wine or in hard water. Flavour

enhancer.

►Skin and severe eye irritant. ON7175000

(R)-form [636-61-3]

D-form

This enantiomer of rare occurrence; reported from fruits and leaves of *Hibiscus sabdariffa* (roselle) although there are many more isolations of malic acid with no opt. rotn. given and some may be of the *R*-form. Cryst. (Et_2O). Sol. H_2O, EtOH, Me_2CO. Mp 101° (97-99°). $[\alpha]_D$ +2.92 (MeOH). $[\alpha]_D^{20}$ +28.4 (c, 5.5 in Py) (>99.8% ee). pK_{a1} 5.26 (25°, H_2O).

►ON7260000

Di-Na salt: [138-09-0]

$[\alpha]_D$ +8.29 (H_2O).

►ON7350000

(S)-form [97-67-6]

L-form. FEMA 2655

Occurs naturally in apples and various other fruits. Flavour enhancer, pH control agent. Cryst. (Me_2CO). V. sol. EtOH, spar. sol. Et_2O. Mp 104-105° (100°). $[\alpha]_D^{21}$ -2.3 (c, 8.5 in H_2O). $[\alpha]_D^{20}$ -28.7 (c, 5.5 in Py) (>99.8% ee). pK_{a1} 3.46; pK_{a2} 5.1. Dec. at *ca*. 140°. Specific rotn. concn. dependent. See (±)-form for food use.

Di-Et ester: [691-84-9] *FEMA 2374*

Flavouring agent. Present in guava fruit, papaya, kiwifruit, raspberry, chicory and various wines and spirits. Oil. Bp_{10} 120°. $[\alpha]_D$ -10.2 (neat). $[\alpha]_D$ +6 (c, 2.3 in $CHCl_3$).

Dibutyl ester: [2385-79-7] *Dibutyl malate*

$C_{12}H_{22}O_5$ 246.303

Isol. from tamarind fruits (*Tamarindus indica*). Oil. $[\alpha]_D$ -9.8 (c, 1 in Me_2CO).

O-*Benzoyl:* [22138-51-8] *Benzoylmalic acid*

$C_{11}H_{10}O_6$ 238.196

Constit. of alfalfa (*Medicago sativa*). Cryst. Mp 142° (136-138°).

O-*(3,4-Dihydroxycinnamoyl):* [53755-04-7] ***(S)-Phaselic acid***. *Caffeoylmalic acid*

$C_{13}H_{12}O_8$ 296.233

Isol. from leaves of French bean (*Phaseolus vulgaris*) and from *Trifolium pratense* (red clover). Yellowish hygroscopic glass. $[\alpha]_D^{20}$ +31.5 (c, 1.36 in H_2O). $[\alpha]_D^{25}$ +28.3 (H_2O).

(±)-form [617-48-1]

Acidulant, antioxidant, flavouring agent, flavour enhancer. Not for use in baby foods (GRAS). Cryst. Sol. MeOH, Me_2CO, H_2O. Mp 131-133°. pK_{a1} 3.4; pK_{a2} 5.81 (25°, H_2O).

[149-61-1, 676-46-0, 3105-51-9, 4387-09-1, 22138-22-3, 39015-77-5, 68303-40-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 522A; 522B; 522C (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 811B; 1041B (*nmr*)

Aldrich Library of NMR Spectra, **2**, 172B (*pmr*)

Sadtler Standard C-13 NMR Spectra, 4652 (*cmr*)

Pratt, D.S. *et al., Philipp. J. Sci.*, 1912, **7**, 201; *Chem. Zentralbl.*, 1913, 645 (*isol, R-form*)

McKenzie, A. *et al., J.C.S.*, 1923, **123**, 2875 (*synth, resoln*)

Scarpati, M.L. *et al., Gazz. Chim. Ital.*, 1960, **90**, 212 (*Phaselic acid*)

Kryger, L. *et al., Acta Chem. Scand.*, 1972, **26**, 2349 (*cryst struct, abs config*)

Rodd's Chem. Carbon Compd. (2nd edn.), 1976, **1E**, 224 (*rev*)

Yoshihara, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 2427 (*Benzoylmalic acid*)

Shiba, T. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 899 (*resoln*)

Wynberg, H. *et al., J.A.C.S.*, 1982, **104**, 166 (*synth*)

Braud, C. *et al., Polym. Prepr. (Am. Chem. Soc., Div. Polym. Chem.)*, 1983, **24**, 71 (*rev, polymer*)

van der Sluis, P. *et al., Acta Cryst. C*, 1985, **41**, 956; 1989, **45**, 1406 (*cryst struct*)

Larchevêque, M. *et al., Synth. Commun.*, 1986, **16**, 183 (*synth, derivs*)

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MAN000

Santaniello, E. *et al., J.C.S. Perkin 1*, 1991, 601 (*esters*)

Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **13**, 1063 (*rev*)

Ushio, K. *et al., Biotechnol. Lett.*, 1992, **14**, 795 (*synth*)

Hahn, R. *et al., Planta Med.*, 1993, **59**, 71; 189 (*Phaselic acid*)

Koert, U. *et al., Chem. Ber.*, 1994, **127**, 1447 (*di-Et ester*)

Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 285-286

Eck, R. *et al., Tetrahedron*, 1994, **50**, 13641-13654 (*synth, R-form, S-form*)

Kobayashi, A, *et al., Z. Naturforsch., C*, 1996, **51**, 233 (*isol, dibutyl ester*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 817; 1637-1639 (*use, occur, props, di-Et ester*)

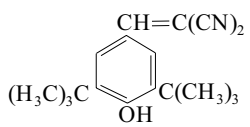
Kuo, Y.-H. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1211-1214 (*isol, di-Et ester*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAN000

Malonoben, ANSI, BSI, ISO M-37

[10537-47-0]

*[[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]propanedinitrile, 9CI. 2,6-Di-*tert*-butyl-4-(2,2-dicyanovinyl)phenol. 2-(3,5-Di-*tert*-butyl-4-hydroxybenzylidene)malononitrile. SF 6847*



$C_{18}H_{22}N_2O$ 282.385

Agricultural acaricide, now superseded. Cryst. (petrol). Mp 141-143° (131-132°). pK_a 6.84.

►LD_{50} (rat, orl) 87 mg/kg; LD_{50} (rbt, skn) 226 mg/kg. OO3737000

Mueller, E. *et al., Annalen*, 1961, **645**, 53 (*synth*)

U.K. Pat., 1966, 1 185 509; *CA*, **70**, 67175z

Itoh, M. *et al., J. Chem. Phys.*, 1978, **69**, 816 (*cryst struct*)

Walton, B.T. *et al., Pestic. Biochem. Physiol.*, 1979, **12**, 23 (*synth, activity*)

Katsumi, I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 1619 (*synth*)

Miyoshi, H. *et al., Biochim. Biophys. Acta*, 1987, **891**, 293; 1988, **935**, 312 (*activity*)

Gazit, A. *et al., J. Med. Chem.*, 1989, **32**, 2344 (*synth, pharmacol*)

Pesticide Manual, 9th edn., 1991, No. 7740

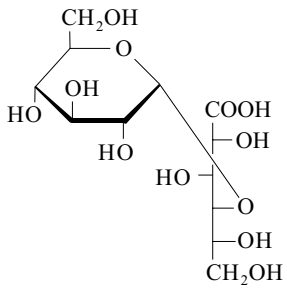
Miyoshi, H. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 269 (*conformn, bibl*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DED000

Maltobionic acid M-38

[534-42-9]

4-O-α-D-Glucopyranosyl-D-gluconic acid, 9CI, 8CI. Maltonic acid



$C_{12}H_{22}O_{12}$ 358.299

Used as an additive in instant food preparations. $[\alpha]_D^{20}$ +98.3 (H_2O).

Ca salt:

$[\alpha]_D^{20}$ +97.5 (H_2O).

*Octa-Me, Me ester:Methyl octa-*O*-methylmaltobionate*

$C_{21}H_{40}O_{12}$ 484.54

$Bp_{0.05}$ 170-173°. $[\alpha]_D$ +120.8 ($CHCl_3$).

Glattfeld, J.K.E. *et al., J.A.C.S.*, 1918, **40**, 973 (*synth*)

Haworth, W.N. *et al., J.C.S.*, 1926, 3094 (*Me ester octa-Me*)

Carlsson, B. *et al., Anal. Chim. Acta*, 1968, **43**, 47 (*chromatog*)

Japan. Pat., 1973, 20 314, (*Hayashibara*); *CA*, **80**, 26091g (*synth, use*)

Maltodextrin, 9CI M-39

[9050-36-6]

[52769-80-9, 54077-26-8]

Polysccharide consisting of D-glucose units linked primarily by α-1,4-bonds and having a reducing sugar content (dextrose equivalent) of less than 20%. Nonsweet nutritive food additive used as a reduced calorie fat replacement. Also used as a stabiliser, thickener and encapsulating agent in food products. Powder, granules or conc. soln. Mp 240° dec.

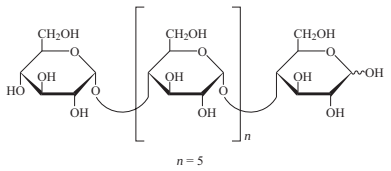
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **9**, 599; **23**, 289-601; 559; 569 (*use*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1643-1644 (*props, use*)

Maltoheptaose M-40

[34620-78-5]

O-α-D-Glucopyranosyl-(1→4)-[O-α-D-glucopyranosyl-(1→4)]$_5$-D-glucose. Amyloheptaose



$n = 5$

$C_{42}H_{72}O_{36}$ 1153.009
Maltooligosaccharide mixtures are important food additives (sweeteners, gelling agents and viscosity modifiers). V. sol. H_2O; insol. EtOH. $[\alpha]_D$ +175.5 (c, 2 in H_2O).

Tricosa-Ac: [114715-54-7]

[84814-32-4]
$C_{88}H_{118}O_{59}$ 2119.865
Powder.

β-Pyranose-*form*

2-Chloro-4-nitrophenyl glycoside: [90826-64-5]
$C_{48}H_{74}ClNO_{38}$ 1308.549

Friebolin, H. *et al., Makromol. Chem.*, 1976, **177**, 845-858 (*cmr*)
Henkel, E. *et al., Fresenius' Z. Anal. Chem.*, 1984, **317**, 753-754 (*chloronitrophenyl glycoside, use*)
Oguma, T. *et al., Agric. Biol. Chem.*, 1991, **55**, 1661-1662
Hitchkiss, A.T. *et al., Carbohydr. Res.*, 1993, **242**, 1-9 (*synth*)
Sakairi, N. *et al., J.C.S. Perkin 1*, 1995, 437-443 (*tricosa-Ac*)
Sugiyama, H. *et al., Carbohydr. Res.*, 2000, **325**, 177-182 (*pmr, conformn*)

Maltohexaose, 8CI M-41

[34620-77-4]
O-α-D-*Glucopyranosyl-(1→4)-[*O-α-D-*glucopyranosyl-(1→4)]$_4$-*D-*glucose, 9CI. Amylohexaose*
As Maltoheptaose, M-40 with
$n = 4$
$C_{36}H_{62}O_{31}$ 990.867
Constit. of corn starch. Amylolysis prod. from starch. Maltooligosaccharide mixtures are important food additives (sweeteners, gelling agents and viscosity modifiers). $[\alpha]_D^{25}$ +182 (c, 1 in H_2O).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 311B (*nmr*)
Whistler, R.L. *et al., J.A.C.S.*, 1955, **77**, 5761-5762 (*isol*)
French, D. *et al., J. Chem. Res.*, 1966, **24**, 68-75 (*isol*)
Beadle, J.B. *et al., J. Agric. Food Chem.*, 1969, **17**, 904-906 (*glc*)
Friebolin, H. *et al., Makromol. Chem.*, 1976, **177**, 845-858 (*cmr*)
Eur. Pat., 1995, 670 368; *CA*, **123**, 221799 (*synth*)
Sugiyama, H. *et al., Carbohydr. Res.*, 2000, **325**, 177-182 (*pmr, conformn*)

Maltopentaose, 8CI M-42

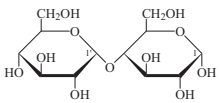
[34620-76-3]
O-α-D-*Glucopyranosyl-(1→4)-[*O-α-D-*glucopyranosyl-(1→4)]$_3$-*D-*glucose, 9CI. Amylopentaose*
As Maltoheptaose, M-40 with
$n = 3$
$C_{30}H_{52}O_{26}$ 828.725
Constit. of corn syrup. Amylolysis prod. from starch. Maltooligosaccharide mixtures are important food additives (sweeteners, gelling agents and viscosity modifiers). Cryst. + H_2O. Sol. H_2O; fairly sol. EtOH, Me_2CO; poorly sol. EtOAc, hexane. Mp 78° (hydrate). $[\alpha]_D^{25}$ +176.4 (c, 1.0 in H_2O).

[1668-09-3]

Whistler, R.L. *et al., J.A.C.S.*, 1955, **77**, 1017 (*isol*)
Beadle, J.B. *et al., J. Agric. Food Chem.*, 1969, **17**, 904 (*glc*)
Robyt, J.F. *et al., J. Biol. Chem.*, 1970, **245**, 3917
Friebolin, H. *et al., Makromol. Chem.*, 1976, **177**, 845 (*cmr*)
Moates, G.K. *et al., Carbohydr. Res.*, 1997, **299**, 91-94 (*struct, props*)
Sugiyama, H. *et al., Carbohydr. Res.*, 2000, **325**, 177-182 (*pmr, conformn*)

Maltose, 9CI, 8CI M-43

[69-79-4]
4-O-α-D-Glucopyranosyl-D-glucose, 9CI. Finetose. Maltobiose. Malt sugar



α-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
Sweetening agent, dietary supplement. Occurs in some plants as hydrolytic dec. prod. of starch. Prod. in high yield (80%) by the action of diastase (α- and β-amylase) on starch, a process used in brewing. Cryst. + $1H_2O$ (β-form). Mp 102-103°. $[\alpha]_D$ +112 → +130 (H_2O).
► LD_{50} (rat, orl) 35000 mg/kg. OO5250000

[6363-53-7, 74135-02-7]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 910C (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 195A (*ir*)
Fischer, E. *et al., Ber.*, 1901, **34**, 2885; 1902, **35**, 840
Bates, F.J. *et al., Polarimetry, Saccharimetry and the Sugars*, U.S. Dept. of Commerce, Natl. Bur. Stand., 1942, 742
Conchie, J. *et al., Adv. Carbohydr. Chem.*, 1957, **12**, 180 (*rev*)
Wolfrom, M.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 334 (*purifn*)
Pazur, J.H. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 335 (*enzymic synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 647 (*occur*)
Usui, T. *et al., J.C.S. Perkin 1*, 1973, 2425 (*conformn, cmr, Me gly*)
St.-Jacques, M. *et al., J.A.C.S.*, 1976, **98**, 4386 (*pmr*)
Tarelli, E. *et al., Dev. Food Carbohydr.*, Applied Science Publ., 1980, 187
Khan, R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1981, **39**, 214 (***rev***)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1044
Tang, J. *et al., Spectrosc. Lett.*, 1995, **28**, 261 (*cmr, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1646-1647
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAO500

Maltotetraose, 8CI M-44

[34612-38-9]
O-α-D-*Glucopyranosyl-(1→4)-[*O-α-D-*glucopyranosyl-(1→4)-]$_2$-*D-*glucose, 9CI. Amylotetraose*
As Maltoheptaose, M-40 with
$n = 2$
$C_{24}H_{42}O_{21}$ 666.583
Constit. of corn syrup. Product of action of α-amylase on starch. Maltooligosaccharide mixtures are important food additives (sweeteners, gelling agents and viscosity modifiers). Amorph. Sol. H_2O, MeOH; fairly sol. EtOH, 2-propanol, butanol; poorly sol. Me_2CO, hexane. Mp 169.5-173° dec. $[\alpha]_D$ +165.5 (c, 5.0 in H_2O). $[\alpha]_D$ +177 (H_2O).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 311A (*nmr*)
Whistler, R.L. *et al., J.A.C.S.*, 1954, **76**, 1671 (*isol*)
Whyte, J.N.C. *et al., Anal. Biochem.*, 1971, **42**, 476 (*pmr*)
Kondo, H. *et al., J. Antibiot.*, 1975, **28**, 157 (*isol*)
Tanaka, M. *et al., J. Antibiot.*, 1975, **28**, 920 (*biosynth*)
Friebolin, H. *et al., Makromol. Chem.*, 1976, **177**, 845 (*cmr*)
Sugiyama, H. *et al., Carbohydr. Res.*, 2000, **325**, 177-182 (*pmr, conformn*)

Maltotriose, 8CI M-45

[1109-28-0]
α-D-Glucopyranosyl-(1→4)-α-D-glucopyranosyl-(1→4)-D-glucose, 9CI. Amylotriose
As Maltoheptaose, M-40 with
$n = 1$
$C_{18}H_{32}O_{16}$ 504.441
Constit. of corn syrup. Amylolysis prod. from starch. Maltooligosaccharide mixtures are important food additives (sweeteners, gelling agents and viscosity modifiers). $[\alpha]_D^{23}$ +160 (in H_2O).

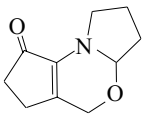
β-Undeca-Ac: [35396-13-5]
Cryst. (EtOH). Mp 134-136°. $[\alpha]_D^{25}$ +86 (c, 1.6 in $CHCl_3$).

Thompson, A. *et al., J.A.C.S.*, 1952, **74**, 3612 (*struct*)
Pazur, J.H. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 337 (*enzymic synth*)
Kamerling, J.P. *et al., Tetrahedron*, 1972, **28**, 3037 (*pmr*)
Colson, P. *et al., J.A.C.S.*, 1974, **96**, 8081 (*conformn, cmr*)
Sugiyama, H. *et al., Carbohydr. Res.*, 2000, **325**, 177-182 (*pmr, conformn*)
Damager, I. *et al., Synthesis*, 2002, 418-426 (*β-undeca-Ac*)

Maltoxazine M-46

[80933-73-9]

[111261-77-9]
*1,2,3,3*a*,6,7-Hexahydrocyclopenta[*d*]pyrrolo[2,1-*b*][1,3]oxazin-8(5*H*)-one, 9CI. 8-Oxo-1,2,3,3*a*,5,6,7,8-octahydrocyclopenta[*d*]pyrrolo[2,1-*b*][1,3]oxazine. Daechualkaloid A*

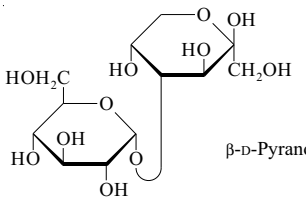


$C_{10}H_{13}NO_2$ 179.218
Aroma substance isol. from malt. Alkaloid from fruit of Chinese jujube *Zizyphus jujuba* var. *inermis* (Rhamnaceae). Amorph. Mp 52°. $[\alpha]_D^{22}$ +0.3 (c, 0.82 in $CHCl_3$). Rapidly becomes resinous in soln. The small opt. rotn. and the Mp. were reported for Daechalkaloid A.

Tressl, R. *et al., Helv. Chim. Acta*, 1982, **65**, 483 (*Maltoxazine*)
Han, B.H. *et al., Tet. Lett.*, 1987, **28**, 3957 (*Daechualkaloid A*)

Maltulose M-47

[17606-72-3]
4-O-α-D-Glucopyranosyl-D-fructose, 9CI



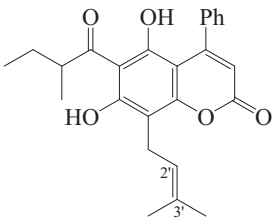
β-D-Pyranose-*form*

$C_{12}H_{22}O_{11}$ 342.299
An aq. soln. at 25° contains 64% β-pyr, 12% α-fur, 22.5% β-fur and 1.5% ketone. Isol. from honey, beer and from the products formed by the action of an α-amylase on liver glycogen. Originates partly by epimerisation of maltose and partly by transglucosylation during the hydrolysis of sucrose by D-glucosidases present in yeast and honey. Cryst. + $1H_2O$ (dioxan/MeOH). Mp 113-115° dec Mp 200-202°. $[\alpha]_D^{20}$ +58 → +64 (c, 1.6 in H_2O). $[\alpha]_D^{20}$ +51.9 (c, 1.5 in H_2O).

Peat, S. *et al., Biochem. J.*, 1952, **51**, xvii (*isol*)
Hough, L. *et al., J.C.S.*, 1953, 2005 (*synth*)
MacWilliam, I.C. *et al., Chem. Ind. (London)*, 1959, 364 (*occur*)
Täufel, A. *et al., Carbohydr. Res.*, 1967, **5**, 223 (*enzymic synth*)
Pfeffer, P.E. *et al., Carbohydr. Res.*, 1982, **102**, 11 (*cmr*)
Hicks, K.B. *et al., Carbohydr. Res.*, 1983, **112**, 37 (***synth, hplc***)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)
Lichtenthaler, F.W. *et al., J.C.S. Perkin 2*, 1990, 1489 (*equilib*)

Mammea A/AB M-48

[7058-70-0]
*5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methylbutyryl)-4-phenylcoumarin, 8CI. MAB 1*



$C_{25}H_{26}O_5$ 406.477
Constit. of *Mammea americana* (mamey) seeds. Yellow needles (hexane). Mp 107-108°.

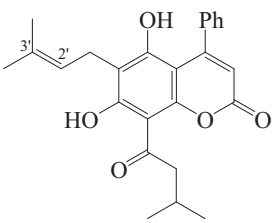
2′,3′-Dihydroxy, 2′,3′-dihydro: ***Dispardiol B***
$C_{25}H_{28}O_7$ 440.492
Amorph. solid. Racemate λ_{max} 234 (log ε 4.22); 284 (log ε 4.43); 355 (log ε 3.93); 426 (log ε 3.59) (EtOH).

Δ$^{3'}$-Isomer, 2′-hydroxy: [221379-36-8] ***Disparinol B***
$C_{25}H_{26}O_6$ 422.477
Yellow oil. Racemate.

Crombie, L. *et al., J.C.S.(C)*, 1967, 2553 (*isol, uv, ir, pmr, ms*)
Carpenter, I. *et al., J.C.S.(C)*, 1971, 3783 (*isol, uv, ir, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317 (*synth*)
Guilet, D. *et al., Phytochemistry*, 2001, **58**, 571-575 (*Dispardiol B*)

Mammea A/BA M-49

[5224-54-4]
*5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-8-isovaleryl-6-(3-methyl-2-butenyl)-4-phenylcoumarin, 8CI*



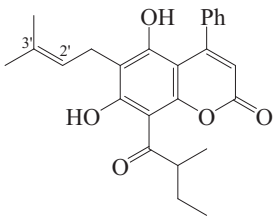
$C_{25}H_{26}O_5$ 406.477
Constit. of *Mammea americana* (mamey) seeds. Needles (hexane). Mp 125-126°.

Δ$^{3'}$-Isomer, 2′-hydroxy: [221379-39-1] ***Isodisparinol A***
$C_{25}H_{26}O_6$ 422.477
Yellow oil. Racemate.

Crombie, L. *et al., J.C.S.(C)*, 1967, 2553 (*isol, uv, ir, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317 (*synth*)
Guilet, D. *et al., Heterocycles*, 1999, **51**, 67-76 (*Isodisparinol A*)

Mammea A/BB M-50

[6916-62-7]
*5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methylbutyryl)-4-phenylcoumarin, 8CI*



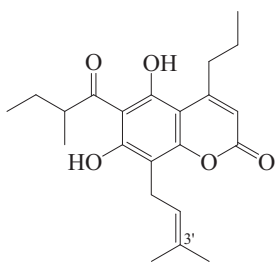
$C_{25}H_{26}O_5$ 406.477
Constit. of *Mammea americana* (mamey) seeds. Needles (hexane). Mp 124-125°.

Δ$^{3'}$-Isomer, 2′-hydroxy: [221379-41-5] ***Isodisparinol B***
$C_{25}H_{26}O_6$ 422.477
Yellow oil. Racemate.

Crombie, L. *et al., J.C.S.(C)*, 1967, 2553 (*isol, uv, ir, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317 (*synth*)
Guilet, D. *et al., Heterocycles*, 1999, **51**, 67-76 (*Isodisparinol B*)

Mammea B/AB M-51

[30390-12-6]
*5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-8-(3-methylbutryl)-6-(2-methylbutryl)-4-propylcoumarin, 8CI. MAB 2*



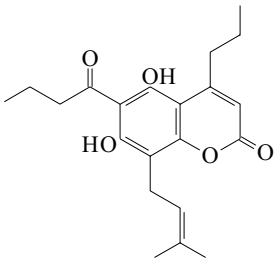
$C_{22}H_{28}O_5$ 372.46
Constit. of *Mammea americana* (mamey) seeds. Yellow cryst. Mp 115-116°.

Δ$^{3'}$-Isomer, 2′-hydroxy: ***Disparpropylinol B***
$C_{22}H_{28}O_6$ 388.46
Yellow cryst. (hexane/EtOAc). Mp 111-112°. Racemate λ_{max} 236 (log ε 3.96); 286 (log ε 4.2); 329 (log ε 3.85) (EtOH).

Carpenter, I. *et al., J.C.S.(C)*, 1971, 3783 (*isol, uv, ir, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248; 1987, 317 (*isol, uv, ir, pmr, ms, synth*)
Guilet, D. *et al., Phytochemistry*, 2001, **58**, 571-575 (*Disparpropylinol B*)

Mammea B/AC M-52

[38537-84-7]
*5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 9CI. 6-Butyryl-5,7-dihydroxy-8-isopentenyl-4-propylcoumarin*

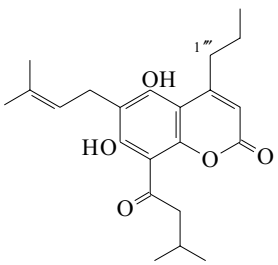


$C_{21}H_{26}O_5$ 358.433
Constit. of *Mammea americana* (mamey) seeds. Yellow cryst. Mp 127-128.5°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1972, 2248; 1987, 317 (*isol, uv, ir, pmr, ms, synth*)

Mammea B/BA M-53

[521-38-0]
*5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-8-isovaleryl-6-(3-methyl-2-butenyl)-4-propylcoumarin, 8CI. Ferruol B*



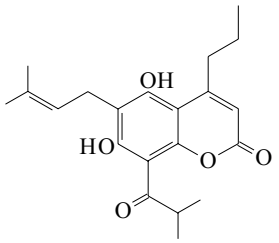
$C_{22}H_{28}O_5$ 372.46
Constit. of *Mammea americana* (mamey) seeds. Needles (hexane). Sol. hexane; poorly sol. H_2O. Mp 127°. Mammein has been shown to consist of a mixt. of Mammeas B/BA and B/BC λ_{max} 244 ; 249 ; 255 ; 261 ; 334 (MeOH) (Berdy).

1‴-Acetoxy: [111321-13-2] ***Mammea El BA***
$C_{24}H_{30}O_7$ 430.497
Isol. from seeds of *Mammea americana* (mamey). Sol. hexane; fairly sol. CCl_4; poorly sol. H_2O. Mp 50-53°. $[\alpha]_D^{24}$ -28.5 (EtOH). λ_{max} 222 (ϵ 63000); 294 (ϵ 24500); 320 (ϵ 15500) (HCl) (Berdy). λ_{max} 225 (ϵ 17800); 258 (ϵ 11500); 332 (ϵ 37150) (NaOH) (Berdy).

Crombie, L. *et al., J.C.S.(C)*, 1967, 2545 (*isol, ir, uv, ms, pmr*)
Crombie, L. *et al., J.C.S. Perkin 2*, 1972, 2255 (*Mammea E/BA*)
Chrichton, E.G. *et al., Phytochemistry*, 1978, **17**, 1783 (*isol, uv, ir, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317; 345 (*synth*)

Mammea B/BD M-54

[98216-05-8]
*5,7-Dihydroxy-7-(3-methyl-2-butenyl)-8-(2-methyl-2-oxopropyl)-3-propyl-2*H*-1-benzopyran-2-one. 5,7-Dihydroxy-8-(2-methyl-1-oxopropyl)-7-prenyl-3-propylcoumarin*

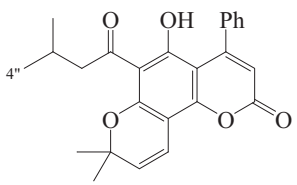


$C_{21}H_{26}O_5$ 358.433
Isol. from *Mammea americana* (mamey). Related to the Mammeins.

Games, D.E. *et al., Tet. Lett.*, 1972, 3187
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317 (*synth*)

Mammeigin M-55

[2289-11-4]
*5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b′*]dipyran-2-one, 9CI. 5-Hydroxy-6-isovaleryl-8,8-dimethyl-4-phenyl-2*H*,8*H*-benzo[1,2-*b*,3,4-*b′*]dipyran-2-one, 8CI. Mammea A/A cyclo D*



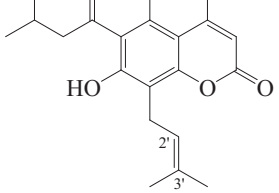
$C_{25}H_{24}O_5$ 404.462
Constit. of *Mammea americana* (mamey). Yellow needles (hexane). Mp 144-145°.

*4″-Hydroxy:**4″-Hydroxymammeigin***
$C_{25}H_{24}O_6$ 420.461
Yellow needles (hexane/$CHCl_3$). Mp 174-176°. λ_{max} 232 (log ϵ 4.53); 284 (log ϵ 4.6); 335 (log ϵ 3.94) (MeOH).

Crombie, L. *et al., J.C.S.(C)*, 1967, 2553 (*isol, ir, uv, pmr, ms*)
Games, D.E. *et al., Tet. Lett.*, 1972, 3187-3190 (*isol*)
Bala, K.R. *et al., Phytochemistry*, 1975, **14**, 265 (*isol, synth, uv*)
Gramacho, R. da S. *et al., Phytochemistry*, 1999, **51**, 579-581 (*4″-Hydroxymammeigin*)
Cruz, F.G. *et al., J. Braz. Chem. Soc.*, 2001, **12**, 117-122 (*isol*)

Mammeisin M-56

[18483-64-2]
*5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-8-isopentenyl-6-isovaleroyl-4-phenylcoumarin. Mammea A/AA*



$C_{25}H_{26}O_5$ 406.477
Constit. of *Mammea americana* (mamey). Solvated yellow cryst. Mp 98-109°. λ_{max} 236 (ϵ 13490); 285 (ϵ 19050); 332 (ϵ 2040) (MeOH) (Berdy). λ_{max} 240 ; 303 ; 394 ; 428 (MeOH-NAOH) (Berdy).

Di-Ac:
Mp 122-124°.

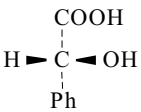
Di-Me ether:
Mp 86-89°.

Δ³′-Isomer, 2′-hydroxy: [221379-33-5] ***Disparinol A***
$C_{25}H_{26}O_6$ 422.477
Yellow needles (hexane/EtOAc). Mp 115-116°. Racemate.

Djerassi, C. *et al., J.O.C.*, 1961, **26**, 1180 (*isol, struct*)
Crombie, L. *et al., J.C.S.(C)*, 1967, 2553 (*pmr, ms*)
Bala, K.R. *et al., Phytochemistry*, 1971, **10**, 1131 (*synth*)
Bhattacharya, G.C. *et al., Indian J. Phys.*, 1975, **49**, 65 (*cryst struct*)
Crichton, E.G. *et al., Phytochemistry*, 1978, **17**, 1783 (*cmr*)
Bordoloi, M. *et al., Phytochemistry*, 1997, **44**, 939 (*isol*)
Guilet, D. *et al., Heterocycles*, 1999, **51**, 67-76 (*Disparinol A*)

Mandelic acid M-57

[90-64-2]
α-Hydroxybenzeneacetic acid, 9CI. 2-Hydroxy-2-phenylacetic acid. α-Hydroxyphenylacetic acid. Phenylglycollic acid. Amygdalic acid



(R)-form

$C_8H_8O_3$ 152.149
Prior to 1923 confusion existed between the (*R*)- and (*S*)-forms.
▶ OO6300000
(R)-form [611-71-2]
D-form (obsol.)
Plates. Mp 133°. $[\alpha]_D^{20}$ -159.73 (EtOH). $[\alpha]_D$ -187.44 (AcOH). pK_a 3.37. Slowly racemises at 160°.

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [190323-48-9] ***Lucuminic acid***
$C_{19}H_{26}O_{12}$ 446.407
Constit. of *Calocarpum sapota* (marmalade plum). Powder.

(S)-form [17199-29-0]
L-form (obsol.)
Plates. Mp 133.8°. $[\alpha]_D^{20}$ +156.57 (H_2O).

O-*β-D-Glucopyranoside:*
Constit. of *Sambucus nigra* (elderberry). Oil. $[\alpha]_D$ +6. λ_{max} 279 (EtOH).

[1701-77-5, 14007-02-4, 66996-75-6, 79416-45-8, 123403-21-4]

Takeda, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 697-699 (*Lucuminic acid*)
D'Abrosca, B. *et al., Phytochemistry*, 2001, **58**, 1073-1081 (*S-form glucoside, isol*)

Manganese(*II*) chloride ($MnCl_2$) M-58

[7773-01-5]

Manganese chloride†. *Manganese dichloride*

$MnCl_2$

Cl_2Mn 125.843

Hexagonal $CdCl_2$ type struct.. Nutrient supplement. Pink cryst. V. sol. H_2O. Mp 654°. Bp 1225°. Obeys Curie-Weiss law above 15°, $\mu_{eff} = 5.73\mu_B$. Forms large number of adducts with O and N donor ligands.

▶ LD_{50}(rat, orl) 770 mg/kg. Exp. reprod. and teratogenic effects. OO9625000

[11132-78-8]

Starr, C. *et al., Phys. Rev.*, 1940, **58**, 977
Osthoff, R.C. *et al., J.A.C.S.*, 1954, **76**, 4732 (*synth*)
Schafer, H. *et al., Z. Anorg. Allg. Chem.*, 1959, **300**, 278 (*bp*)
Chisholm, R.C. *et al., J. Chem. Phys.*, 1962, **36**, 972 (*synth*)
Ferrari, A. *et al., Acta Cryst.*, 1963, **16**, 846 (*struct*)
Corbett, J.D. *et al., J. Inorg. Nucl. Chem.*, 1963, **25**, 1287 (*mp*)
Gutmann, V. *et al., Monatsh. Chem.*, 1967, **98**, 276 (*synth*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 56, 1978, **C5**, 4; 1983, **C10**, 29 (*rev, bibl, uv-vis*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **5**, 3227-3229 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1652-1653
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, MAR000

Manganese hypophosphite M-59

[10043-84-2]

*Manganese(*II*) hydrogen phosphite. Manganese phosphinate*

$Mn(H_2PO_2)_2$

$H_4MnO_4P_2$ 184.915

Dietary supplement. Inhibitor of *Clostridium botulinum* in smoked meat prods.. Pale pink granules or powder.

Monohydrate: [7783-16-6]
$H_6MnO_5P_2$ 202.93
Pink cryst. Stable to 250°.

Ger. Pat., 1974, 1 669 509; *CA*, **82**, 99903z (*stabilizer, use*)
Golub, A.M. *et al., Ukr. Khim. Zh. (Russ. edn.)*, 1977, **43**, 1019-1021; *CA*, **87**, 210380w (*synth*)
Weakley, T.J.R. *et al., Acta Cryst. B*, 1979, **35**, 42-45 (*cryst struct*)
U.S. Pat., 1981, 4 282 260; *CA*, **95**, 131194a (*preservative, use*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MAS815
Marcos, M.D. *et al., J. Alloys Compd.*, 1992, **188**, 133-137 (*cryst struct*)

Manganese oxide (MnO), 11CI M-60

[1344-43-0]

Manganese oxide†. *Cassel green. Manganese green. C.I. 77726*

MnO

MnO 70.937

Basic oxide. Exists in the Mn–O system in the range $MnO_{1.00}$ to *ca.* $MnO_{1.15}$. Cubic NaCl type struct. with Mn–O 222.3 pm. Dietary supplement. Bright green powder. Insol. H_2O. Mp 1850°. Takes up oxygen if left to stand in air, becoming brown. Relatively easily reduced to Mn by metals but not by H_2 or CO. Paramagnetic at r.t., becomes antiferromagnetic at *ca.* 120°. Below Néel temp. lattice becomes rhombohedral. Tetragonal high pressure modification also known.

▶ OP0900000

Mineral-*form* [1313-12-8]
Manganosite

Belongs to periclase group of minerals.Emerald green cryst., becoming black on exp.

Moore, T.E. *et al., J.A.C.S.*, 1950, **72**, 856 (*synth, magnetism, cryst struct*)
Glasser, F.P. *et al., Am. J. Sci.*, 1958, **256**, 398 (*mp*)
Howe, A.T. *et al., Q. Rev., Chem. Soc.*, 1967, **21**, 507 (*magnetism*)
Hush, N.S. *et al., Prog. Inorg. Chem.*, 1968, **10**, 259 (*uv-vis*)
Finsley, D.M. *et al., J. Therm. Anal.*, 1971, **3**, 43 (*synth*)
Goodenough, J.B. *et al., Prog. Solid State Chem.*, 1971, **5**, 145 (*magnetism*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 56, 1973, **C1**, 14 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **14**, 844 (*uses, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, MAT250

Manganese(*II*) sulfate ($MnSO_4$), 11CI M-61

[7785-87-7]

[10124-55-7, 15244-36-7]
Manganese sulfate, USAN

$MnSO_4$

MnO_4S 151.002

Contains tetragonally distorted MnO_6 octahedra; four Mn–O 225, two Mn–O 211 pm. Nutrient supplement. Pale pink cryst. thermally v. stable. Dec. above 700° to form SO_2, SO_3 and Mn oxides. Sol. H_2O; sl. sol. MeOH, EtOH. Mp 710° (at 4850 atm.). Other phases exist at high temps. and press. $\mu_{eff} = 5.7\mu_B$ (77-600K).

▶ OP1050000

Dihydrate: [13465-25-3]
Pink cryst. Not v. stable.

Tetrahydrate: [10101-68-5]
Pink cryst. Monoclinic struct. similar to $MgSO_4.4H_2O$.

▶ OP1200000

Pentahydrate: [13465-27-5]
Pink triclinic cryst. $\mu_{eff} = 5.9\mu_B$.

Mineral-*form* [52717-37-0]
Szmikite

Monoclinic struct. Kieserite group of minerals.Greyish white, brownish white, rose red.

Monohydrate: [10034-96-5] $\mu_{eff} = 5.74\mu_B$.

▶ OP0893500

Mineral-*form* [73347-41-8]
Mallardite

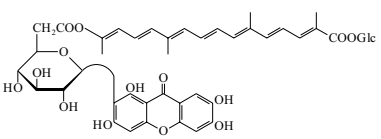
Monoclinic struct. Melanterite group of minerals.Pale rose. Vitreous. Dehydrates rapidly becoming opaque and mealy. Sol. H_2O.

Heptahydrate: [13492-24-5]
Pink cryst. Monoclinic struct. Metastable orthorhombic form can be obtained if cryst. soln. seeded with $MgSO_4.7H_2O$.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1262D (*ir*)
Baur, W.H. *et al., Acta Cryst.*, 1962, **15**, 815 (*cryst struct*)
Will, G. *et al., Acta Cryst.*, 1965, **19**, 854 (*synth, cryst struct*)
Hezel, A. *et al., Spectrochim. Acta*, 1966, **22**, 1949 (*ir*)
Ben-Dar, L. *et al., Inorg. Chim. Acta*, 1967, **1**, 49 (*dta*)
Allain, Y. *et al., J. Appl. Phys.*, 1968, **39**, 1124 (*magnetism*)
Lohr, L.L. *et al., J. Chem. Phys.*, 1968, **49**, 3516 (*uv*)
Brégeault, J.-M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1969, **268**, 2165 (*struct*)
Kirfel, A. *et al., High Temp. High Pressures*, 1974, **6**, 525 (*cryst struct*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 56, 1976, **C6**, 81 (*rev, bibl*)
Will, G. *et al., Fortschr. Mineral.*, 1981, **59**, 31 (*cryst struct*)
Roberts, W.M. *et al., Encyclopaedia of Minerals*, 2nd Ed.; Van Nostrand, 1990, 519; 841 (*rev, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1657-1658
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAU250; MAU750

Mangicrocin M-62

[122575-51-3]



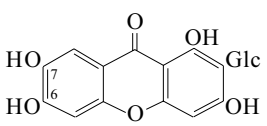
$C_{45}H_{50}O_{19}$ 894.879
Constit. of saffron. $[\alpha]_D^{28}$ +17.5 (c, 0.53 in MeOH).

Ghosal, S. *et al., J. Chem. Res., Synop.*, 1989, 70

Mangiferin M-63

[4773-96-0]

*2-β-D-Glucopyranosyl-1,3,6,7-tetrahydroxy-9*H*-xanthen-9-one, 9CI. Euxanthogen. Chinomine. Alpizarin. Hedysaride. Mannipherin. Chedisaride*



$C_{19}H_{18}O_{11}$ 422.345

Mannipherin is a CA misprint and Chedisaride appears to be an alternative transliteration of Hedysaride from the Russian. Constit. of *Mangifera indica* (mango). Pale yellow needles (EtOH aq.). Mp 278-280° (270-272° dec.). $[\alpha]_D^{32}$ +32 (EtOH aq.). λ_{max} 240 ; 241 (ϵ

18200); 257 (ϵ 19500); 315 (ϵ 9600); 316 ; 364 ; 365 (ϵ 8500) (MeOH) (Berdy). λ_{max} 247 ; 270 ; 271 ; 389 ; 390 (MeOH-NAOH) (Berdy).

► OP1927800

6′-O-(3,4,5-Trihydroxybenzoyl): [92631-82-8] ***Mangiferin 6′-gallate***
$C_{26}H_{22}O_{15}$ 574.451
Isol. from leaves of *Mangifera indica* (mango). Yellow granular solid + ½H_2O (H_2O). $[\alpha]_D^{30}$ -35.2 (c, 0.2 in MeOH).

3-Me ether: [21794-66-1] ***Homomangiferin***. *3-O-Methylmangiferin*
$C_{20}H_{20}O_{11}$ 436.371
Constit. of *Mangifera indica* (mango). Mp 255-257°.

[74484-89-2]

Haynes, L.J. *et al., J.C.S.(C)*, 1966, 1685 (*pmr, struct*)
Nott, P.E. *et al., Phytochemistry*, 1967, **6**, 741; 1597 (*struct, uv, ir, synth*)
Bhatia, V.K. *et al., Tetrahedron*, 1967, **23**, 1363 (*isol, uv, ir*)
Glyzina, G.S. *et al., Khim. Prir. Soedin.*, 1969, **5**, 322; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 272 (*isol*)
Prox, A. *et al., Annalen*, 1970, **732**, 199 (*ms*)
Fujita, M. *et al., Tet. Lett.*, 1977, 4503 (*biosynth*)
Ghosal, S. *et al., Phytochemistry*, 1978, **17**, 2119 (*Homomangiferin*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2676 (*Mangiferin 6-gallate*)
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*occur*)
Wada, H. *et al., Chem. Pharm. Bull.*, 1995, **43**, 461 (*isol, pmr*)

Mannan, 9CI, 8CI M-64

[9036-88-8]

$C_6H_{10}O_5$ 162.142

A polysaccharide containing 95% or more mannose units which are (1→4) linked in the β-pyranosyl form with some α-D-galactopyranosyl units (1→6) linked along the main chain. The type of mannan depends on the ratio D-mannose: D-galactose; Galactomannan 1.04-5.26: 1; Mannan A 50:1; Mannan B 90:1. Polymeric. Minimum formula given. Found in custard apples. Widely used in food industry, e.g. in the preparation of rice substitutes and in jellies. Thickening agent. $[\alpha]_D^{18}$ -44.58 (c, 0.83 in 1*N* NaOH).

► LD_{50} (mus, ivn) 2000 mg/kg. OP1949500

Per-Ac:
Powder. Mp 128-145°. $[\alpha]_D$ -3 ($CHCl_3$).

Patterson, J. *et al., J.C.S.*, 1923, **123**, 1147
Hess, K. *et al., Annalen*, 1928, **466**, 18
Gorin, P.A.J. *et al., Can. J. Chem.*, 1973, **51**, 2375 (*cmr*)
Marchessault, R.M. *et al., Adv. Carbohydr. Chem. Biochem.*, 1976, **33**, 398 (*cryst struct*)
Dey, P.M. *et al., Adv. Carbohydr. Chem. Biochem.*, 1978, **35**, 341
Fox, J.E. *et al., Thickening and Gelling Agents for Food*, (ed. Imeson, A.), 2nd edn., Blackie, 1997, 262-283 (*rev*)

Mannan *endo*-1,4-β-mannosidase, 9CI M-65

[37288-54-3]

1,4-β-D-Mannan mannanohydrolase. endo-*1,4-β-Mannonase. E.C. 3.2.1.78*

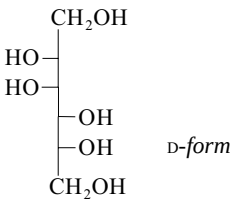
Enzyme. Used to reduce the viscosity of coffee extract in the manuf. of instant coffee.

Reese, E.T. *et al., Can. J. Microbiol.*, 1965, **11**, 167-183 (*isol*)
Eriksson, A.F.C. *et al., Acta Chem. Scand.*, 1968, **22**, 1924-1934 (*isol*)

D-Mannitol M-66

[87-78-5]

Mannite. manno-*Hexitol. Kurrine (obsol.)*



D-*form*

$C_6H_{14}O_6$ 182.173

► OP2050000

D-***form*** [69-65-8]

Cordycepic acid. Manita. Osmitrol. Resectisol. E421

Permitted bulk sweetener for foods. Sweetening agent. Food additive, used as anticaking agent, lubricant, for stabiliser and thickener, and for other uses in food processing. Needles. Sol. H_2O, Py; sl. sol. EtOH; insol. Et_2O. Mp 166°. $Bp_{3.5}$ 295°. $[\alpha]_D^{25}$ -0.21 (c, 17.6 in H_2O). $[\alpha]_D^{25}$ +28.61 (c, 10 in 12.8% borax aq.). pK_{a1} 13.29 (25°). Log P -4.67 (calc). Cordycepic acid was originally given the struct. of a stereoisomer of quinic acid.

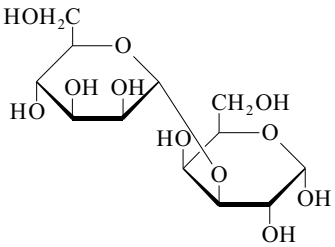
► Human systemic effects when used therapeutically, LD_{50} (rat, orl) 13500 mg/kg. OP2060000

[45007-61-2, 61453-77-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 186C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 289C; 401A; 401B; 404A (*nmr*)
Lohmar, R. *et al., Carbohydr. Res.*, 1949, **4**, 211 (*rev*)
Kolthoff, I.M. *et al., Volumetric Analysis*, Interscience, NY, 1954, **2**, (*use*)
Wright, L. *et al., J.O.C.*, 1961, **26**, 1588 (*synth*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 148 (*occur*)
Brimacombe, J.S. *et al., The Carbohydrates*, Academic Press, 1972, **1A**, 479
Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, (*use*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **1**, 754 (*rev*)
Makkee, M. *et al., Starch/Staerke*, 1985, **37**, 136 (*rev, synth*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 901; 902
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1658 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HER000; MAW250; MAW800

3-*O*-α-D-Mannopyranosyl-D-galactose, 9CI M-67

[71869-57-3]

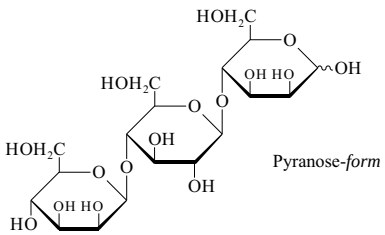


$C_{12}H_{22}O_{11}$ 342.299
Isolated from enzymic hydrolysate of peach gum. $[\alpha]_D^{20}$ +135.9 (c, 1.0 in H_2O) (+42.1).

Kardosova, A. *et al., Coll. Czech. Chem. Comm.*, 1979, **44**, 2250
Torgov, V.I. *et al., Bioorg. Khim.*, 1985, **11**, 83; *Sov. J. Bioorg. Chem. (Engl. Transl.)*, 1985, **11**, 47 (*synth, deriv*)

β-D-Mannopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-D-mannose, 8CI M-68

[28152-46-7]



Pyranose-*form*

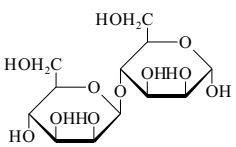
$C_{18}H_{32}O_{16}$ 504.441
Isol. from enzymic reaction on *Amorphophallus konjac* glucomannan (devil's tongue). $[\alpha]_D^{23}$ -5.8 (c, 2.2 in H_2O). $[\alpha]_D^{25}$ -8 (c, 0.4 in H_2O).

Aspinall, G.O. *et al., J.C.S.*, 1962, 214
Kato, K. *et al., Carbohydr. Res.*, 1973, **29**, 469
Tomoda, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1807 (*isol*)
Usui, T. *et al., Agric. Biol. Chem.*, 1979, **43**, 863 (*cmr*)
Koleva, M. *et al., CA*, 1981, **95**, 165582r (*isol*)
Shimizu, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 949 (*isol*)
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1988, **52**, 519 (*synth*)

4-*O*-β-D-Mannopyranosyl-D-mannose, 9CI, 8CI M-69

[14417-51-7]

Mannobiose



α-Pyranose-*form*

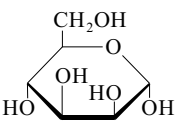
$C_{12}H_{22}O_{11}$ 342.299
The major repeating unit in the mannose chains of plant mannans, galacto and

glucomannans. Isol. from partial acid hydrolysates of ivory nut (*Phytelephas macrocarpa*) mannan, guaran (*Cyamopsis* sp.), palmyra palm nut mannan (*Borassus flabellifer*), fenugreek (*Trigonella foenumgraecum*), lucerne (*Medicago sativa*) galactomannans, western hemlock wood cellulose (*Tsuga heterophylla*), white spruce (*Picea glauca*), *Larix decidua, Pinus strobus* and red maple (Acer rubrum) glucomannans and *Pinus taeda* hemicellulose. Also from the mucilage in the bulbs of *Narcissus tazetta*, the exocellular yeast mannan of *Rhodotorula glutinis* and from *Sesbania aegyptiaca* seeds. Cryst. (MeOH). Mp 203-204° (198-199°). $[\alpha]_D^{30}$ -8 (c, 1.6 in H_2O) (-2.3, -4). Some sources report a hydrate, Mp 122-124°.

Courtois, J.E. *et al., Bull. Soc. Chim. Biol.*, 1958, **40**, 2031 (*isol*)
Mukherjee, A.K. *et al., Can. J. Chem.*, 1961, **39**, 1408 (*isol*)
Kato, K. *et al., Agric. Biol. Chem.*, 1969, **33**, 1446 (*isol, struct*)
Kamerling, J.P. *et al., Tetrahedron*, 1971, **27**, 4275; 1972, **28**, 3037 (*ms, pmr*)
Gorin, P.A.J. *et al., Carbohydr. Res.*, 1975, **39**, 3 (*isol, cmr*)
Usui, T. *et al., Agric. Biol. Chem.*, 1979, **43**, 863 (*cmr*)
Bhattarcharyya, S.B. *et al., Phytochemistry*, 1983, **22**, 161 (*isol*)
Sheldrick, B. *et al., Carbohydr. Res.*, 1984, **132**, 1 (*cryst struct*)

Mannose, 9CI, 8CI M-70

[31103-86-3]
Seminose. Carubinose



α-D-Pyranose-*form*

$C_6H_{12}O_6$ 180.157

A 4*M* aq. soln. at 36° contains 63.7% α-pyr, 35.5% β-pyr, 0.6% α-fur, and 0.2% β-fur.

D-*form* [3458-28-4]
Occurs in trace amounts in apples and peaches. Obt. from the hydrolysates of D-mannans of the corms of *Amorphophallus konjac* (devil's tongue). pK_{a1} 12.08 (25°).

α-D-Pyranose-*form* [7296-15-3]

[27710-20-9]
Mp 133°. $[\alpha]_D^{25}$ +29.3 → +14.5 (c, 1 in H_2O).

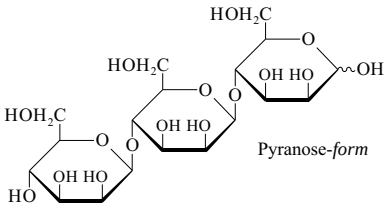
β-D-Pyranose-*form* [7322-31-8]
Mp 132° dec. $[\alpha]_D^{20}$ -17 → +14.6 (c, 4 in H_2O).

[12773-34-1, 36972-23-3, 37738-80-0, 41767-04-8, 41847-42-1, 41847-43-2, 41847-45-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 188B; 191B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 299A; 299B; 1058A (*nmr*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 298; 324 (*rev, derivs*)
Isbell, H.S. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 145 (*α-D-form, isol*)
Levine, S. *et al., Carbohydr. Res.*, 1968, **6**, 382; 1969, **10**, 468 (*β-D-pyr, synth, β-D-pyr-penta-Ac*)
Schaffer, R. *et al., The Carbohydrates*, 1972, **1A**, 69 (*occur*)
Wilbur, D.J. *et al., J.A.C.S.*, 1977, **99**, 5450 (*equilib*)
Bock, K. *et al., Annu. Rep. NMR Spectrosc.*, (Webb, G.A. ed.), Acad. Press, London and New York, 1982, **13**, 37; 41 (*pmr, cmr*)
Horton, D. *et al., Carbohydr. Res.*, 1982, **105**, 145 (*cmr*)

Mannotriose M-71

[28173-52-6]
β-D-Mannopyranosyl-(1→4)-β-D-mannopyranosyl-(1→4)-D-mannose, 9CI, 8CI



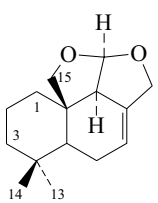
$C_{18}H_{32}O_{16}$ 504.441
Constit. of Palmyra palm (*Borassus flabellifer*) and from commercial soybean syrup. Cryst. (EtOH). Mp 167° Mp 211-213° (219°). $[\alpha]_D^{25}$ -21 (c, 3.0 in H_2O).

Trihydrate:
Mp 137-137.5°.

Aspinall, G.O. *et al., J.C.S.*, 1958, 215; 1962, 214 (*isol*)
Tyminski, A. *et al., J.A.C.S.*, 1960, **82**, 2823
Perila, O. *et al., Can. J. Chem.*, 1961, **39**, 815
Mukherjee, A.K. *et al., Can. J. Chem.*, 1961, **39**, 1408
Kato, K. *et al., Carbohydr. Res.*, 1973, **29**, 469
Tomoda, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1807 (*isol*)
Usui, T. *et al., Agric. Biol. Chem.*, 1979, **43**, 863 (*cmr*)
Tanaka, R. *et al., CA*, 1982, **97**, 24116w (*occur*)
Shimizu, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 949 (*isol*)
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1983, **47**, 2391 (*isol, props*)
Bhattacharyya, S.B. *et al., Phytochemistry*, 1983, **22**, 161 (*isol*)
Mackie, W. *et al., Int. J. Biol. Macromol.*, 1986, **8**, 43 (*cryst struct*)
Park, G.G. *et al., CA*, 1989, **110**, 171717h (*occur*)
Takano, Y. *et al., CA*, 1991, **115**, 278391c (*occur, cmr, hplc*)

Marasmene M-72

[124869-12-1]



$C_{15}H_{22}O_2$ 234.338
Metab. of *Marasmius oreades* (fairy ring mushroom). Needles. Mp 70-74°. $[\alpha]_D^{24}$ +57 (c, 0.07 in MeOH).

3-Oxo: [124894-87-7] ***Marasmen-3-one***
$C_{15}H_{20}O_3$ 248.321
Metab. of *Marasmius oreades* (fairy ring mushroom). Cryst. (CH_2Cl_2/hexane). Mp 135-138°. $[\alpha]_D^{24}$ -1.6 (c, 1 in MeOH).

15-Oxo: Marasmone, M-73

3β-Hydroxy: [124869-08-5] ***3β-Hydroxymarasmene***
$C_{15}H_{22}O_3$ 250.337
Metab. of *Marasmius oreades* (fairy ring mushroom). Microcryst. solid. Mp 129-133°. $[\alpha]_D^{24}$ +34 (c, 1.05 in MeOH).

13-Hydroxy: [124869-09-6] ***13-Hydroxymarasmene***
$C_{15}H_{22}O_3$ 250.337
Metab. of *Marasmius oreades* (fairy ring mushroom). Microcryst. Mp 147-150°. $[\alpha]_D^{24}$ +3.7 (C, 0.2 in MeOH).

14-Hydroxy: [124987-02-6] ***14-Hydroxymarasmene***
$C_{15}H_{22}O_3$ 250.337
Metab. of *Marasmius oreades* (fairy ring mushroom). Prisms (CH_2Cl_2/hexane). Mp 162.5-163°. $[\alpha]_D^{24}$ +23.8 (c, 0.32 in MeOH).

15-Hydroxy, 3-oxo: [124894-86-6] ***15-Hydroxymarasmen-3-one***
$C_{15}H_{20}O_4$ 264.321
Metab. of *Marasmius oreades* (fairy ring mushroom). Oil.

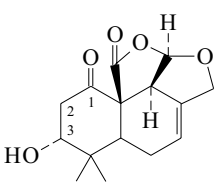
1α,15-Dihydroxy: [124869-04-1] ***1α,15-Dihydroxymarasmene***
$C_{15}H_{22}O_4$ 266.336
Metab. of *Marasmius oreades* (fairy ring mushroom). Cryst. (EtOAc/hexane). Mp 152-155°.

3α,15-Dihydroxy: [124869-03-0] ***3α,15-Dihydroxymarasmene***
$C_{15}H_{22}O_4$ 266.336
Metab. of *Marasmius oreades* (fairy ring mushroom). Cryst. (EtOAc/hexane). Mp 146-147°.

Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371 (*isol, pmr, cmr*)
Kuschel, A. *et al., J. Antibiot.*, 1994, **47**, 733; 1017 (*1α,15-Dihydroxymarasmene*)

Marasmone M-73

[122458-04-2]



$C_{15}H_{18}O_5$ 278.304
Constit. of *Marasmius oreades* (fairy ring mushroom). Foam. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{24}$ +74.6 (c, 1.44 in MeOH).

3-Deoxy, 2,3-didehydro: [122458-06-4] ***Anhydromarasmone***
$C_{15}H_{16}O_4$ 260.289
Constit. of *Marasmius oreades* (fairy ring mushroom). Cryst. (CH_2Cl_2/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 194-196°. $[\alpha]_D^{24}$ -59.8 (c, 0.4 in MeOH). λ_{max} 215 ; 245 ; 331 (ε 1000)

(MeOH) (Berdy).

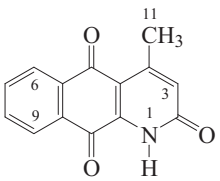
1α-Alcohol: [122458-07-5] ***Dihydromarasmone***
$C_{15}H_{20}O_5$ 280.32
Constit. of *Marasmius oreades* (fairy ring mushroom). Prisms (EtOAc/CH_2Cl_2/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 164-165°. $[\alpha]_D^{24}$ +28 (c, 0.5 in MeOH).

1α-Alcohol, 3-ketone: [122458-05-3] ***Isomarasmone***
$C_{15}H_{18}O_5$ 278.304
Constit. of *Marasmius oreades* (fairy ring mushroom). Prisms ($CHCl_3$). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 247-250°.

Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 773 (*isol, pmr, cmr, cryst struct*)

Marcanine A M-74

[157463-84-8]
4-Methylbenzo[g]quinoline-2,5,10(1H)-trione, 9CI. 4-Methyl-1H-1-aza-2,9,10-anthracenetrione. Griffiazanone B



$C_{14}H_9NO_3$ 239.23
Alkaloid from *Annona glabra* (pond apple). Yellow needles. Mp 240-242° Mp 249-251°. Mp >300°.

3-Methoxy: [104696-15-3] *3-Methoxy-4-methylbenzo[g]quinoline-2,5,10(1H)-trione, 9CI.* ***Dielsiquinone***
$C_{15}H_{11}NO_4$ 269.256
Yellow-green amorph. powder. Mp 250-252°.

3-Methoxy, N-*Me:* ***Marcanine B***
$C_{16}H_{13}NO_4$ 283.283
Orange powder. λ_{max} 272 (log ϵ 4.36); 299 (sh) (log ϵ 4.08); 320 (sh) (log ϵ 3.86); 419 (log ϵ 3.3) (MeOH).

6-Hydroxy, 3-methoxy: ***Marcanine D***
$C_{15}H_{11}NO_5$ 285.256
Yellow powder. λ_{max} 275 (log ϵ 4.2); 295 (log ϵ 4.05) (MeOH).

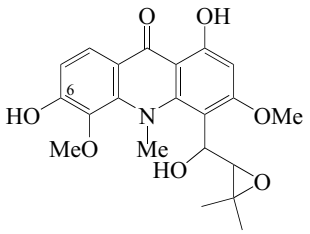
9-Hydroxy, 3-methoxy, N-*Me:* ***Marcanine E***
$C_{16}H_{13}NO_5$ 299.282
Orange powder. λ_{max} 274 (log ϵ 4.13); 300 (log ϵ 3.95) (MeOH).

11-Hydroxy, 3-methoxy, N-*Me:* ***Marcanine C***
$C_{16}H_{13}NO_5$ 299.282
Orange powder. λ_{max} 272 (log ϵ 4.23); 306 (sh) (log ϵ 3.97); 323 (sh) (log ϵ 3.82); 419 (log ϵ 3.19) (MeOH).

Goulart, M.O.F. *et al., Phytochemistry*, 1986, **25**, 1691-1695 (*Dielsiquinone*)
Marcos, A. *et al., Tetrahedron*, 1994, **50**, 12941-12952 (*synth*)
Zhang, Y.J. *et al., Chin. Chem. Lett.*, 1998, **9**, 1029-1032 (*Griffiazanone B*)
Soonthornchareonnon, N. *et al., J. Nat. Prod.*, 1999, **62**, 1390-1394 (*isol*)
Chang, F.-R. *et al., J. Chin. Chem. Soc. (Taipei)*, 2000, **47**, 913-920 (*isol, pmr, cmr*)

Margrapine A M-75

[185417-68-9]



$C_{21}H_{23}NO_7$ 401.415
Alkaloid from roots of Marsh grapefruit (*Citrus paradisi*). Yellow oil. $[\alpha]_D$ -16.7 (c, 0.036 in $CHCl_3$). λ_{max} 225 (sh) ; 264 ; 295 (sh) ; 331 ; 381 (EtOH).

6-Me ether: [185417-69-0] ***Margrapine B***
$C_{22}H_{25}NO_7$ 415.442
From roots of Marsh grapefruit (*Citrus paradisi*). Yellow oil. $[\alpha]_D$ -37.5 (c, 0.008 in $CHCl_3$). λ_{max} 226 (sh) ; 264 ; 331 ; 375 (EtOH).

Takemura, Y. *et al., Heterocycles*, 1996, **43**, 2483 (*isol, uv, ir, pmr, cmr, ms, struct*)

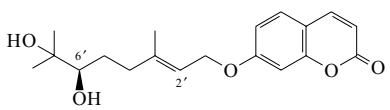
Maricin M-76

[90015-49-9]
Bacteriocin prod. by *Brevibacterium maris*.

Kato, F. *et al., Agric. Biol. Chem.*, 1984, **48**, 193-200

Marmin M-77

7-[(6,7-Dihydroxy-3,7-dimethyl-2-octenyl)oxy]-2H-1-benzopyran-2-one, 9CI



(*R*)-*form*

$C_{19}H_{24}O_5$ 332.396
(*R*)-*form* [14957-38-1]
Constit. of grapefruit peel and bael fruit (*Aegle marmelos*). Cryst. (EtOAc). Mp 123-124°. $[\alpha]_D$ +25 (EtOH).

6′-O-β-D-Glucopyranoside: [55062-36-7] ***Diversoside***
$C_{25}H_{34}O_{10}$ 494.538
Cryst. Mp 154-155°. $[\alpha]_D^{20}$ +10 (EtOH).

6′-O-Formyl: [144398-51-6] ***6′-O-Formylmarmin***
$C_{20}H_{24}O_6$ 360.406
Constit. of *Citrus hassaku*. Viscous oil. $[\alpha]_D^{14}$ +8.9 (c, 1 in EtOH).

6′-O-Angeloyl: [71899-66-6]
$C_{24}H_{30}O_6$ 414.497
Oil. $[\alpha]_D^{20}$ +19 ($CHCl_3$).

6′-O-(4-Geranyloxy-2-hydroxycinnamoyl): [142628-36-2]
$C_{38}H_{46}O_8$ 630.777
Constit. of *Citrus hassaku* juice oil. Viscous oil. $[\alpha]_D^{26}$ +72 (c, 1.0 in EtOH).

7′-Me ether: [144424-82-8] ***7′-O-Methylmarmin***
$C_{20}H_{26}O_5$ 346.422
Constit. of *Citrus hassaku* and *Aegle marmelos* (bael fruit). Needles (hexane). Mp 65°. $[\alpha]_D^{14}$ +23 (c, 1 in EtOH).

6′-Ketone: [36413-96-4] ***Dehydromarmin***
$C_{19}H_{22}O_5$ 330.38
Cryst. Mp 76.5-78°.

2′,3′-Dihydro, 5′-oxo: [115806-87-6] *7-[(6,7-Dihydroxy-3,7-dimethyl-5-oxooctyl)oxy]-2H-1-benzopyran-2-one*
$C_{19}H_{24}O_6$ 348.395
Oil. $[\alpha]_D$ -28.6 (c, 0.21 in $CHCl_3$). Abs. config. not detd..

(*S*)-*form* [61347-54-4]
Cryst(MeOH/Et_2O). Mp 117-118°. $[\alpha]_D^{25}$ -14 (c, 0.32 in EtOH).

7′-O-β-D-Glucopyranoside: [169790-23-2] ***Pituranthoside***
$C_{25}H_{34}O_{10}$ 494.538
Prisms (MeOH aq.). Mp 185-186°. $[\alpha]_D^{26}$ +12 (c, 0.5 in MeOH).

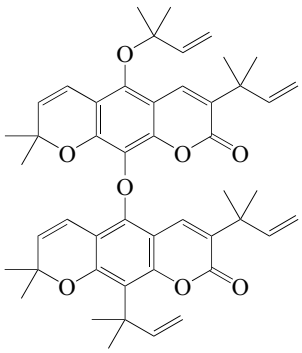
7′-Deoxy, 7′-chloro: [169869-82-3] ***Chloromarmin***
$C_{19}H_{23}ClO_4$ 350.841
Constit. of *Aegle marmelos* (bael fruit). Oil. $[\alpha]_D^{24}$ +27.3 (c, 0.8 in EtOH).

4′α-Hydroxy, 6′-O-β-D-glucopyranoside: [169626-23-7] ***Aeglin***
$C_{25}H_{34}O_{11}$ 510.537
Constit. of *Aegle marmelos* (bael fruit). Cryst. ($CHCl_3$/MeOH aq.). Mp 218-219°. $[\alpha]_D^{24}$ +25.9 (c, 0.6 in EtOH). Possesses (4′*R*,5′*R*)-config..

Chatterjea, A. *et al., J.C.S.*, 1959, 1922 (*isol, uv*)
Chatterjea, A. *et al., Tet. Lett.*, 1967, 471 (*struct, uv, ir, pmr, ms*)
Coates, R.M. *et al., Tetrahedron*, 1970, **26**, 5699 (*synth, pmr*)
Dreyer, D.L. *et al., Phytochemistry*, 1972, **11**, 763-767 (*Dehydromarmin*)
Kamilov, K.M. *et al., Khim. Prir. Soedin.*, 1974, **10**, 781; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 800 (*isol*)
Yamada, S.N. *et al., Tet. Lett.*, 1976, 2557 (*synth*)
Banerji, J. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 496 (*synth*)
Yamada, Y. *et al., Agric. Biol. Chem.*, 1987, **51**, 1105-1110 (*activity*)
Bevalot, F. *et al., Phytochemistry*, 1988, **27**, 1547 (*2′,3′-dihydro*)
Aziz, M. *et al., Tetrahedron*, 1988, **44**, 101 (*synth*)
Masuda, T. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1257 (*O-Methylmarmin*)
Ohashi, K. *et al., Chem. Lett.*, 1995, 881 (*Aeglin, Chloromarmin*)
Halim, A.F. *et al., Phytochemistry*, 1995, **40**, 927 (*Pituranthoside*)
Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, 2002, **83**, 1 (*rev*)

Marshdimerin M-78

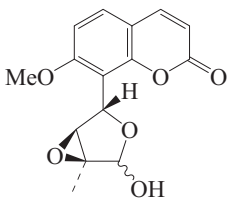
[192189-93-8]



$C_{48}H_{54}O_8$ 758.95
Constit. of the roots of *Citrus paradisi* (grapefruit). Oil. λ_{max} 230 ; 269 (sh) ; 276 ; 328 ; 348 (sh) (MeOH).

Takemura, Y. *et al., Heterocycles*, 1997, **45**, 1169-1172 (*isol, uv, ir, pmr, cmr*)

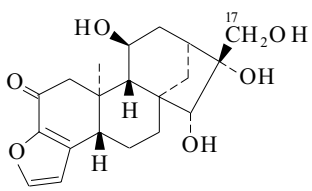
Marshrin M-79



$C_{15}H_{14}O_6$ 290.272
Constit. of the roots of Marsh grapefruit (*Citrus paradisi*). Cubes. Mp 200-203°. $[\alpha]_D^{24}$ +2.6 (c, 0.31 in Py). λ_{max} 218 (sh) ; 251 ; 257 ; 322 (EtOH).

Takemura, Y. *et al., Heterocycles*, 1999, **51**, 851-855 (*isol, uv, ir, pmr, cmr, ms*)

Mascarol M-80



$C_{20}H_{26}O_6$ 362.422

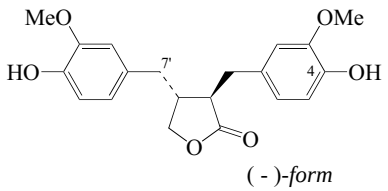
17-O-*β*-D-*Glucopyranoside:* [55465-97-9] ***Mascaroside***
$C_{26}H_{36}O_{11}$ 524.564
Bitter principle from green beans of Malagasy coffee (*Coffea vianneyi*). Cryst. Mp 277-278°. $[\alpha]_D$ -187 (H_2O).

15-Deoxy, 11-O-*β*-D-*glucopyranoside:* [70717-95-2] ***Mozambioside***
$C_{26}H_{36}O_{10}$ 508.564
Isol. from beans of arabica coffee (*Coffea arabica*) and wild coffee sp. (*Coffea pseudozanguebariae*). Cryst. (H_2O). Mp 179.4-180.3°.

Ducruix, A. *et al., Chem. Comm.*, 1975, 396 (*Mascaroside*)
Richter, H. *et al., Chem. Ber.*, 1979, **112**, 1088 (*Mozambioside*)
Prewo, R. *et al., Phytochemistry*, 1990, **29**, 990 (*cryst struct, Mozambioside*)

Matairesinol M-81

*Dihydro-3,4-bis[(4-hydroxy-3-methoxyphenyl)methyl]-2(3*H*)-furanone, 9CI. Dihydro-3,4-divanillyl-2(3*H*)-furanone, 8CI. 4,4′-Dihydroxy-3,3′-dimethoxylignan-9,9′-olide*



(-)-*form*

$C_{20}H_{22}O_6$ 358.39

(-)-*form* [580-72-3]
Needles (EtOH or AcOH). Sol. EtOH, $CHCl_3$; fairly sol. C_6H_6, Et_2O, toluene; poorly sol. hexane, H_2O. Mp 119° (anhyd.). $[\alpha]_D$ -40 (c, 0.1 in EtOH). λ_{max} 230 ; 280 (EtOH) (Berdy).

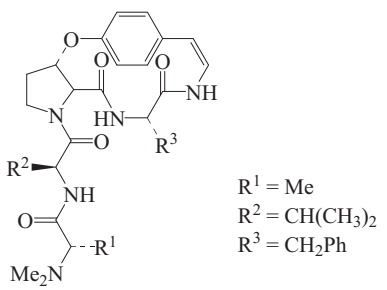
4′-O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [211115-82-1]
$C_{31}H_{40}O_{15}$ 652.648
Constit. of safflower oil cake *Carthamus tinctorius*. Mp 115-116.5°. $[\alpha]_D^{18}$ -86.3 (c, 0.5 in MeOH). λ_{max} 229 (ϵ 6900); 280 (ϵ 2500) (MeOH).

[29764-17-8, 41948-08-7]

Nagatsu, A. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1044-1047 (*4′-apiosylglucoside*)

Mauritine A M-82

[38478-72-7]



R^1 = Me
R^2 = $CH(CH_3)_2$
R^3 = CH_2Ph

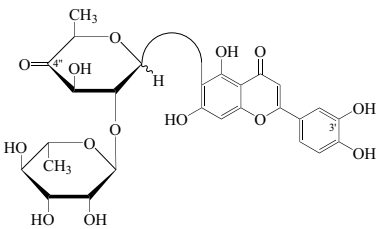
$C_{32}H_{41}N_5O_5$ 575.706
Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Rhombs (CH_2Cl_2/petrol). Mp 104°. $[\alpha]_D^{20}$ -315 (c, 0.33 in MeOH).

N-*De-Me:* [55609-23-9] ***Mauritine F***
$C_{31}H_{39}N_5O_5$ 561.68
Needles ($CHCl_3$/petrol). Mp 222-225°. $[\alpha]_D^{20}$ -285 (c, 0.15 in MeOH).

Tschesche, R. *et al., Tet. Lett.*, 1972, 2609 (*isol, ms, struct*)
Tschesche, R. *et al., Annalen*, 1974, 1694 (*Mauritine F*)
Tschesche, R. *et al., Phytochemistry*, 1974, **13**, 1633; 1976, **15**, 541 (*isol*)
Tschesche, R. *et al., Tetrahedron*, 1975, **31**, 2944 (*isol, Mauritine F*)
Kirfel, A. *et al., Z. Naturforsch., B*, 1976, **31**, 279 (*cryst struct*)
Laib, T. *et al., Tet. Lett.*, 2000, **41**, 7645-7649 (*synth*)

Maysin M-83

[70255-49-1]
*2,6-Anhydro-1-deoxy-5-*O*-(6-deoxy-α-L-mannopyranosyl)-6-*C*-[2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-6-yl]-*xylo*-3-hexulose, 9CI. 3′,4′,5,7-Tetrahydroxy-6-[α-L-rhamnopyranosyl(1→2)-2,6-anhydro-1-deoxy-*xylo*-3-hexulopyranosyl]flavone*



$C_{27}H_{28}O_{14}$ 576.51
Isol. from corn silk (*Zea mays*). Cryst. (MeOH/Me_2CO). Sol. H_2O, MeOH; poorly sol. Me_2CO, hexane. Mp *ca.*° 225 dec. λ_{max} 258 (ϵ 19000); 272 (ϵ 14800); 352 (ϵ 14450) (MeOH) (Berdy).

3′-Me ether: [74158-05-7] ***Maysin 3′-methyl ether***. *3′-Methoxymaysin(incorr.)*
$C_{28}H_{30}O_{14}$ 590.537
Isol. from corn silk (*Zea mays*).

3′-Deoxy: [74158-04-6] *3′-Deoxymaysin*. ***Apimaysin***
$C_{27}H_{28}O_{13}$ 560.51
Isol. from corn silk (*Zea mays*).

4″α-Alcohol: [170079-82-0] **eq-*4″-Hydroxymaysin***
$C_{27}H_{30}O_{14}$ 578.526
Isol. from corn silk (*Zea mays*). Mp 212°.

4″β-Alcohol: [170079-83-1] **ax-*4″-Hydroxymaysin***
$C_{27}H_{30}O_{14}$ 578.526
Isol. from corn silk (*Zea mays*). Dark yellow powder.

4″β-Alcohol, 3′-Me ether: [169132-06-3] **ax-*4″-Hydroxy-3′-methoxymaysin***
$C_{28}H_{32}O_{14}$ 592.552
Isol. from corn silk (*Zea mays*). Mp 192°.

Waiss, A.C. *et al., J. Econ. Entomol.*, 1979, **72**, 256 (*isol, props*)
Elliger, C.A. *et al., Phytochemistry*, 1980, **19**, 293 (*isol*)
Snook, M.E. *et al., J. Agric. Food Chem.*, 1995, **43**, 2740 (*isol, cmr*)

MBP 1 M-84

[143179-53-7]
Basic peptide with 33 amino acid residues. Isol. from maize kernels (*Zea mays*).

Duvick, J.P. *et al., J. Biol. Chem.*, 1992, **267**, 18814-18820 (*isol, struct*)

Mecarbam, BSI M-85

[2595-54-2]
Ethyl 6-ethoxy-2-methyl-3-oxo-7-oxa-5-

thia-2-aza-9-phosphanonanoate 6-sulfide, 9CI. S-*(*N-*Ethoxycarbonyl*-N-*methylcarbamoylmethyl)* O,O-*diethyl phosphorodithioate. Ethyl [[(diethoxyphosphinothioyl)thio]acetyl]-methylcarbamate. Murfotox. Pestan*

$(EtO)_2P(S)SCH_2CONMeCOOEt$

$C_{10}H_{20}NO_5PS_2$ 329.377

Agricultural insecticide and acaricide with sl. systemic props.. Pale yellow oil. Spar. sol. H_2O. d_{20}^{20} 1.22. $Bp_{0.02}$ 144°. n_D^{20} 1.5138.

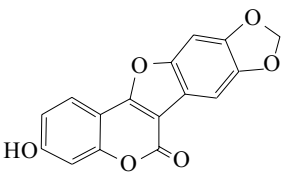
▶ LD_{50} (rat, orl) 36 mg/kg. LD_{50} (rat, skn) 380 mg/kg. FB3850000

U.K. Pat., 1957, 867 780; *CA*, **55**, 25756h (*synth, use*)
Krijgsman, W. *et al., J. Chromatogr.*, 1976, **117**, 201 (*glc*)
Lynch, V.P. *et al., Pestic. Sci.*, 1981, **12**, 65 (*synth, props*)
Charalambous, J. *et al., Phosphorus Sulfur Relat. Elem.*, 1984, **19**, 267 (*ms*)
Pesticide Manual, 11th edn., 1997, No. 458
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1160
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DJI000

Medicagol M-86

[1983-72-8]

*3-Hydroxy-6*H-*[1,3]dioxolo[5,6]benzofuro[3,2-*c*][1]-benzopyran-6-one, 9CI. 7-Hydroxy-11,12-methylenedioxycoumestan. 7-Hydroxy-5′,6′-methylenedioxybenzofurano[3′,2′:3,4]coumarin. 3-Hydroxy-8,9-methylenedioxycoumestan*



$C_{16}H_8O_6$ 296.236

Found in alfalfa (*Medicago sativa*) having viral leaf spot infections. Also from *Cicer arietinum* (chick pea) and *Trifolium pratense* (red clover). Cryst. by subl.; needles (MeOH). Mp 324-325° (337°).

Ac:
Needles. Mp 262-263°.

Me ether: [3862-34-8] *3-Methoxy-8,9-methylenedioxycoumestan.* ***Flemichapparin C***
$C_{17}H_{10}O_6$ 310.262
Needles (EtOH). Mp 272°. λ_{max} 314 (ϵ 10000); 384 (ϵ 18400) (EtOH) (Berdy).

Livingston, A.L. *et al., J.O.C.*, 1965, **30**, 2353 (*isol, synth, uv, pmr*)
Takai, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2488 (*isol, uv, ir, pmr*)
Adityachaudhury, N. *et al., Phytochemistry*, 1973, **12**, 425 (*deriv*)
Farkas, L. *et al., Acta Chim. Acad. Sci. Hung.*, 1974, **82**, 225 (*synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Tang, Y.-P. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 1-5 (*isol, uv, pmr, cmr*)

Mediolacin M-87

[90015-50-2]

Bacteriocin prod. by *Corynebacterium mediolanum*.

Kato, F. *et al., Agric. Biol. Chem.*, 1984, **48**, 193-200

Megacins M-88

[9010-73-5]

Proteins. Prod. by *Bacillus megatherium*. Bacteriocins with potential food uses.

Megacin A19213 [87806-18-6]
Prod. by *Bacillus megatherium* ATCC 19213. Comprises 2 polypeptide subunits.

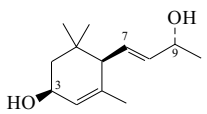
Megacin Cx [39340-85-7]
Prod. by *Bacillus megatherium* 337. Monomeric protein, MW 210KDa.

Megacin FW337 [57285-15-1]
Prod. by *Bacillus megatherium* 337.

[12710-15-5]

Holland, I.B. *et al., Biochem. J.*, 1961, **78**, 641-648 (*isol*)
Walker, F.J. *et al., Spores*, 1975, **6**, 586-591 (*Megacin FW337*)
Brusilow, N.S. *et al., J. Biol. Chem.*, 1981, **256**, 159-164 (*Megacin Cx*)
Von Tersch, M.A. *et al., J. Bacteriol.*, 1983, **155**, 866-871 (*Megacin A19213*)

4,7-Megastigmadiene-3,9-diol M-89



(3*S*,7*E*,9*R*)-*form*

$C_{13}H_{22}O_2$ 210.316

(3*S*,7*E*,9*R*)-*form* [68072-60-6]
Oil. $[\alpha]_D$ +272 (c, 0.29 in $CHCl_3$).

9-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:
$C_{24}H_{40}O_{11}$ 504.573
Constit. of *Cydonia vulgaris* (quince).

3-Ketone, 9-O-β-D-glucopyranoside:
$C_{19}H_{30}O_7$ 370.442
Isol. from raspberry (*Rubus idaeus*) and the leaves of Dalmatian sage (*Salvia officinalis*). Oil. $[\alpha]_D^{20}$ +58.6 (c, 1.5 in MeOH).

3-Ketone, 9-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [143363-62-6]
$C_{24}H_{38}O_{11}$ 502.558
Constit. of *Eriobotrya japonica* (loquat).

3-Ketone, 9-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [290308-51-9] ***Eriojaposide A***
$C_{24}H_{38}O_{11}$ 502.558
Constit. of *Eriobotrya japonica* (loquat). Amorph. powder. $[\alpha]_D$ +26.7 (c, 1 in MeOH). λ_{max} 238 (log ϵ 4.08) (MeOH).

3-Ketone, 9-O-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [351412-97-0] ***Eriojaposide B***
$C_{25}H_{40}O_{11}$ 516.584
Constit. of *Eriobotrya japonica* (loquat). Amorph. powder. $[\alpha]_D^{23}$ +33.5 (c, 1 in MeOH). λ_{max} 234 (log ϵ 4.01) (MeOH).

(3*S*,7*E*,9*S*)-*form* [66890-49-1]
Oil.

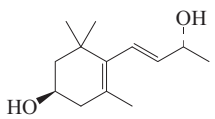
3-Ketone, 9-O-β-D-glucopyranoside:
Constit. of raspberry (*Rubus idaeus*) and leaves of sage (*Salvia officinalis*). Amorph. powder.

3-Ketone, 9-O-[β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]: ***Salvionoside B***
$C_{24}H_{38}O_{11}$ 502.558
Amorph. powder. $[\alpha]_D^{24}$ +49.2 (c, 0.49 in MeOH). λ_{max} 237 (ϵ 11470) (MeOH).

Aasen, A.J. *et al., Acta Chem. Scand.*, 1973, **27**, 2107
Aasen, A.J. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 285
Behr, D. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 391
Murakami, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 866-868 (*3-ketone 9-glucoside*)
Takuzawa, O. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1907 (*synth*)
De Tommasi, N. *et al., J. Nat. Prod.*, 1992, **55**, 1025 (*glycosides*)
Pabst, A. *et al., Phytochemistry*, 1992, **31**, 1649-1652 (*Rubus idaeus glucosides*)
Neugebauer, W. *et al., Nat. Prod. Lett.*, 1995, **6**, 177 (*glucoside*)
De Tommasi, N. *et al., J. Agric. Food Chem.*, 1996, **44**, 1676 (*isol, pmr, cmr*)
Wang, M. *et al., J. Agric. Food Chem.*, 1998, **46**, 2509-2511 (*3-ketone glucoside, isol, nmr*)
Ito, H. *et al., J. Nat. Prod.*, 2001, **64**, 737-740 (*Eriojaposides*)

5,7-Megastigmadiene-3,9-diol M-90

3-Hydroxy-β-ionol



(3*R*,7*E*,9*R*)-*form*

$C_{13}H_{22}O_2$ 210.316

(3*R*,7*E*,9*R*)-*form*

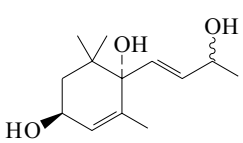
3,9-Di-O-β-D-glucopyranoside: [232601-22-8] ***Platanionoside***
$C_{25}H_{42}O_{12}$ 534.6
Amorph. powder. $[\alpha]_D^{25}$ -42.9 (c, 0.56 in MeOH). λ_{max} 231 (log ϵ 3.71) (MeOH).

(3ξ,7*E*,9ξ)-*form*

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [137606-56-5]
$C_{25}H_{42}O_{12}$ 534.6
Constit. of *Cydonia oblonga* (quince).

Winterhalter, P. *et al., Phytochemistry*, 1991, **30**, 3021-3025 (*isol, pmr, cmr*)
Tamaki, A. *et al., J. Nat. Prod.*, 1999, **62**, 1074-1076 (*Platanionoside B*)

4,7-Megastigmadiene-3,6,9-triol M-91



$C_{13}H_{22}O_3$ 226.315

(3β,6α,7*E*,9ξ)-*form*
3β,6α-Dihydroxy-α-ionol

9-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [177261-72-2]
$C_{24}H_{40}O_{12}$ 520.573
Constit. of *Cydonia vulgaris* (quince).

7,8-Dihydro, 9-O-β-D-glucopyranoside: [177261-75-5]
$C_{19}H_{34}O_8$ 390.473
Constit. of *Cydonia vulgaris* (quince).

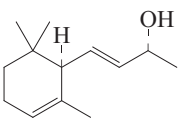
7,8-Dihydro, 9-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [177261-73-3]
$C_{24}H_{42}O_{12}$ 522.589
Constit. of *Cydonia vulgaris* (quince).

De Tommasi, N. *et al., J. Agric. Food Chem.*, 1996, **44**, 1676-1681 (*isol, pmr, cmr*)

4,7-Megastigmadien-9-ol M-92

[25312-34-9]

[472-78-6]
4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-ol, 9CI



$C_{13}H_{22}O$ 194.316

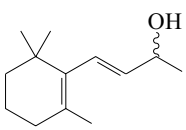
(6*R*,7*E*,9*R*)-*form*
α-Ionol. *FEMA 3624*
Present in grape and raspberry. Flavouring ingredient. Oil.
►EM9630050

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{24}H_{40}O_{10}$ 488.574
Constit. of *Rubus idaeus* (raspberry) fruit.

Ac: [52210-18-1]
$C_{15}H_{24}O_2$ 236.353
d 0.86. Bp_{15} 134°. n_D^{21} 1.4713. The coml. prod. may be a mixt. of stereoisomers.

Aasen, A.J. *et al., Acta Chem. Scand.*, 1973, **27**, 2107 (*Ac*)
Pabst, A. *et al., Phytochemistry*, 1992, **31**, 2043 (*isol, pmr, cmr, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 372
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1401

5,7-Megastigmadien-9-ol M-93



$C_{13}H_{22}O$ 194.316

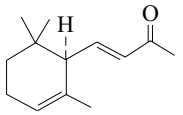
(7*E*,9ξ)-*form*

O-*β-D-Glucopyranoside:* [146610-77-7]
$C_{19}H_{32}O_6$ 356.458
Constit. of *Passiflora edulis* (passion fruit).

Herderich, M. *et al., Nat. Prod. Lett.*, 1993, **2**, 227 (*isol, pmr, cmr, synth*)

4,7-Megastigmadien-9-one M-94

[127-41-3]
4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, 9CI. ***α-Ionone***. *Parmone. FEMA 2594*



(R)-(E)-form

$C_{13}H_{20}O$ 192.3
►Fl. p. 113°.

(*R*)-(*E*)-*form* [24190-29-2]
Constit. of many essential oils. Flavouring agent with woody-violet fragrance. Oil with woody-violet fragrance. Bp_{28} 146.5-147.5°. $[\alpha]_D^{23}$ +347. n_D^{25} 1.5000. Coml. Ionone contains β-Ionone and other substances.

Oxime:
Cryst. Mp 89-90°.

7,8-Dihydro: [39721-65-8]

[31499-72-6] *4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-butanone, 9CI, 8CI. 4-Megastigmen-9-one. Dihydro-α-ionone. FEMA 3628*
$C_{13}H_{22}O$ 194.316
Flavouring ingredient for artificial fruit flavours. Present in peaches, raspberry, *Rubus* hybrid fruits, Chinese scented green tea and alfalfa extract. Bp_3 98-99°. $[\alpha]_D^{22}$ +138.4 (c, 0.615 in EtOH). n_D^{22} 1.4763. *R*-Config. confirmed only for the violet oil isolate.

(*R*)-(*Z*)-*form*
Bp_1 72-72.5°. n_D^{25} 1.4890.

(±)-(*E*)-*form*
Bp_{28} 146.5-147.5°. n_D^{20} 1.5041.

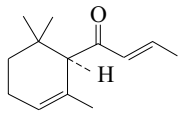
7,8-Dihydro: [49749-39-5]
Oil. d_4^{20} 0.92. Bp 234°. n_D^{20} 1.4778.

[8013-90-9]

Naves, Y.R. *et al., Perfum. Essent. Oil Res.*, 1964, **55**, 658,667 (*occur*)
Fordham, W.D. *et al., Rep. Prog. Appl. Chem.*, 1968, **53**, 264 (*rev*)
Food Chemicals Codex, 2nd Ed., 1972, **2**, 391 (*anal*)
Uhde, G. *et al., Helv. Chim. Acta*, 1972, **55**, 2621-2625 (*dihydro, occur*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1973, **56**, 1874 (*abs config*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 549 (*rev, tox*)
Takeda, R. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 1125-1132 (*dihydro, synth, pmr*)
Yamanishi, T. *et al., Dev. Food Sci.*, 1988, **17**, 181-190 (*dihydro, occur, glc*)
Mori, K. *et al., Annalen*, 1991, 1053-1056 (*dihydro, R-form, synth, pmr, cmr*)
Qing, N. *et al., Magn. Reson. Chem.*, 1991, **29**, 459 (*pmr, cmr*)
Fehr, C. *et al., Helv. Chim. Acta*, 1992, **34**, 1023 (*synth*)
Sumitani, H. *et al., J. Agric. Food Chem.*, 1994, **42**, 785-790 (*dihydro, occur, glc*)
Pfander, H. *et al., Aust. J. Chem.*, 1995, **48**, 145 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 165; 373 (*rev*)
Brenna, E. *et al., J.C.S. Perkin 1*, 1998, 4129-4134 (*synth*)
Alea, J. *et al., J.C.S. Perkin 1*, 1999, 271-278 (*synth*)

4,8-Megastigmadien-7-one M-95

1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one, 9CI. 6-(2-Butenoyl)-1,5,5-trimethylcyclohexene



(R,E)-form

$C_{13}H_{20}O$ 192.3

(*R,E***)-*form*** [28102-28-5]
Cryst. (pentane). Mp 27.5-28°. $[\alpha]_D^{20}$ +487 ($CHCl_3$).

(*S,E***)-*form*** [116497-11-1]
α-Damascone
Detected as minor constit. of black tea leaves (nearly racemic mixt.). Cryst. (pentane) with fruity apple-plum-rose odour (threshold 1ppb). Mp 22-23°. $Bp_{0.001}$ 77-80°. $[\alpha]_D^{24}$ -510 (c, 1.92 in $CHCl_3$).

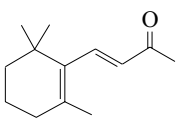
[72748-70-0]

Demole, E. *et al., Helv. Chim. Acta*, 1970, **53**, 541-551 (*synth*)
Schulte-Elte, K.H. *et al., Helv. Chim. Acta*, 1973, **56**, 310-320 (*synth*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1973, **56**, 1503-1513 (*synth*)
Mandai, T. *et al., J.O.C.*, 1984, **49**, 3403-3406 (*synth*)
Fehr, C. *et al., J.A.C.S.*, 1988, **110**, 6909-6911 (*synth, enantiomers*)
König, W.A. *et al., Tetrahedron*, 1989, **45**, 7003-7006 (*isol, abs config*)
Azzari, E. *et al., J.O.C.*, 1990, **55**, 1106-1108 (*synth*)
Werkhoff, P. *et al., Lebensm. Unters. Forsch.*, 1991, **192**, 111-115 (*gc, enantiomers, organoleptic props*)
Mori, K. *et al., Tetrahedron*, 1993, **49**, 1871-1878 (*synth, S-form*)

5,7-Megastigmadien-9-one M-96

[79-77-6]

[14901-07-6]
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one, 9CI. ***β-Ionone***. *Boronione. FEMA 2595*



$C_{13}H_{20}O$ 192.3
Found in many essential oils including oil of *Boronia megastigma* (brown boronia) and coml. ionone. Flavouring agent. Oil. Bp_{24} 150-151°.
►Fl. p. 112°. LD_{50} (rat, orl) 4590 mg/kg.
EN0350000

Semicarbazone:
Cryst. Mp 149°.

Thiosemicarbazone: [2302-90-1]
$C_{14}H_{23}N_3S$ 265.422
Cryst. Sol. common org. solvs.; spar. sol. H_2O. Mp 167-169°.

9-Alcohol: [22029-76-1]

[53078-25-4, 81801-17-4] *β-Ionol*
$C_{13}H_{22}O$ 194.316

Flavouring ingredient. Bp_2 105°. The *S*-enantiomer has been synthesised.

► EM9630000

9-Alcohol, 9-Ac: [22030-19-9] *β-Ionyl acetate. FEMA 3844*
$C_{15}H_{24}O_2$ 236.353
Flavouring agent. Liq. with raspberry-like odour. d_4^{19} 0.94. $Bp_{14.5}$ 136.5° Bp_2 120°. n_D^{19} 1.4765.

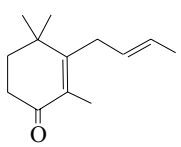
7,8-Dihydro: [17283-81-7] *4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone, 9CI. 5-Megastigmen-9-one. Dihydro-β-ionone*
$C_{13}H_{22}O$ 194.316
Component of peach aroma. Oil. $Bp_{0.01}$ 47-49°.

7,8-Dihydro, semicarbazone:
Mp 161-163°.

[8013-90-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 444D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 686B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 531B (*ir*)
Naves, Y.R. *et al., Perfum. Essent. Oil Res.*, 1964, **55**, 658,667 (*occur*)
Thomas, A.F. *et al., Tet. Lett.*, 1967, 5129 (*ms*)
Shervi, V.B. *et al., Some Recent Dev. Chem. Nat. Prod.*, (Rangoswami, S. etal, Ed.), Prentice-Hall, India, 1972, 1 (*rev*)
Guzman, M. *et al., Inf. Quim. Anal.*, 1973, **23**, 209; *CA*, **80**, 103445e (*synth, ir, use*)
Ishihara, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 439 (*synth*)
Schmidt, C. *et al., Can. J. Chem.*, 1974, **52**, 1732 (*β-Ionol*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367 (*cmr*)
Noyori, R. *et al., J.A.C.S.*, 1984, **106**, 6717-6725 (*S-β-Ionol, synth*)
Khai, B.T. *et al., Chem. Ber.*, 1993, **126**, 2265-2268 (*synth, ir, pmr, ms, dihydro*)
Herlem, D. *et al., Tetrahedron*, 1993, **49**, 607-618 (*synth, ir, pmr, dihydro*)
Bury, P. *et al., Tetrahedron*, 1994, **50**, 8793-8808 (*synth, ir, pmr, cmr, dihydro*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 837-841 (*use*)
Vani, P.V.S.N. *et al., Synth. Commun.*, 2001, **31**, 219-224 (*synth, pmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IFX000

5,8-Megastigmadien-4-one M-97



$C_{13}H_{20}O$ 192.3

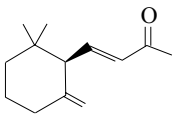
(*E*)-*form* [67401-26-7]
Constit. of *Nicotiana tabacum* and *Passiflora edulis* (passion fruit). Oil.

(*Z*)-*form* [67401-25-6]
Constit. of *Passiflora edulis* (passion fruit). Oil.

Demole, E. *et al., Helv. Chim. Acta*, 1979, **62**, 67
Boulin, B. *et al., Tetrahedron*, 2000, **56**, 3927-3932 (*synth*)

5(13),7-Megastigmadien-9-one M-98

[79-76-5]
*4-(2,2-Dimethyl-6-methylenecyclohexyl)-3-buten-2-one, 9CI. **γ-Ionone**. FEMA 3175*



(*R*)-*form*

$C_{13}H_{20}O$ 192.3
Flavouring agent.

(*R*)-*form* [24190-32-7]
Oil. $[\alpha]_D^{20}$ -15.6 (EtOH).

(*S*)-*form* [64129-96-0]
Constit. of *Tamarindus indica* (tamarind). Oil. $[\alpha]_D^{20}$ +19.5 (EtOH).

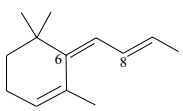
Semicarbazone:
Cryst. Mp 144-144.5°.

[8013-90-9, 84847-77-8]

Buchecker, R. *et al., Helv. Chim. Acta*, 1973, **56**, 2548 (*abs config*)
Mukaiyama, T. *et al., Chem. Lett.*, 1976, 1033 (*synth*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 1271 (*synth, abs config*)
Leyendecker, F. *et al., Tetrahedron*, 1987, **43**, 85 (*synth*)
Audran, G. *et al., Tet. Lett.*, 1993, **34**, 3417 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 374
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1405
Fuganti, C. *et al., Helv. Chim. Acta*, 2000, **83**, 2761-2768 (*synth*)

4,6,8-Megastigmatriene M-99

6-(2-Butenylidene)-1,5,5-trimethyl-1-cyclohexene



(6*E*,8*E*)-*form*

$C_{13}H_{20}$ 176.301

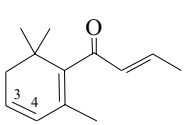
(6*E*,8*E*)-*form* [51468-86-1]
Constit. of *Passiflora edulis* (passion fruit). Oil.

(6*Z*,8*E*)-*form* [51468-85-0]
Constit. of *Passiflora edulis* (passion-fruit). Oil.

Barjot, J. *et al., Bull. Soc. Chim. Fr.*, 1973, 3187 (*synth*)
Whitfield, F.B. *et al., Aust. J. Chem.*, 1979, **32**, 891 (*isol*)

3,5,8-Megastigmatrien-7-one M-100

[23726-93-4]
*1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one. **Damascenone**. β-Damascenone*



$C_{13}H_{18}O$ 190.285
From *Rosa damascena* and many other sources. Oil. Bp_{13} 116-118°.

3,4-Dihydro: [23726-91-2]

[35044-68-9] *5,8-Megastigmatrien-7-one. **β-Damascone***
$C_{13}H_{20}O$ 192.3
Constit. of tea and rose oils. $Bp_{0.001}$ 52°.

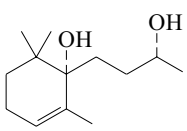
► EN0340000

*3,4-Dihydro, 3-hydroxy:3-Hydroxy-5,8-megastigmadien-7-one. **3-Hydroxy-β-damascone***
$C_{13}H_{20}O_2$ 208.3
Liq. Racemic.

*3,4-Dihydro, 4-hydroxy:4-Hydroxy-5,8-megastigmadien-7-one. **4-Hydroxy-β-damascone***
$C_{13}H_{20}O_2$ 208.3
Oil.

Hollenstein, B. *et al., Helv. Chim. Acta*, 1972, **55**, 2030 (*cmr*)
Mori, K. *et al., Agric. Biol. Chem.*, 1973, **37**, 2907 (*4-Hydroxy-β-damascone*)
Schulte-Elte, K.H. *et al., Helv. Chim. Acta*, 1973, **56**, 310 (*synth*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1973, **56**, 1503 (*synth*)
Ayyar, K.S. *et al., J.C.S. Perkin 1*, 1975, 1727 (*synth*)
Kitahara, T. *et al., Agric. Biol. Chem.*, 1979, **43**, 2351 (*synth*)
Torii, S. *et al., J.O.C.*, 1979, **44**, 3412 (*synth*)
Pellicciari, R. *et al., J.C.S. Perkin 1*, 1981, 2566 (*synth*)
Bolt, A.J.N. *et al., Phytochemistry*, 1983, **22**, 613 (*Hydroxydamascone*)
Fehr, Ch. *et al., Helv. Chim. Acta*, 1986, **69**, 228 (*synth*)
Azzari, E. *et al., J.O.C.*, 1990, **55**, 1106 (*synth*)
Kutney, J.P. *et al., Can. J. Chem.*, 1992, **70**, 2094 (*synth*)
Sarandeses, L.A. *et al., J.O.C.*, 1992, **57**, 2757 (*synth, β-Damascone*)
Unnikrishnan, P.A. *et al., Org. Prep. Proced. Int.*, 1993, **25**, 687 (*synth, β-Damascone*)
Puglisi, C.J. *et al., Tet. Lett.*, 2001, **42**, 6937-6939 (*synth*)

4-Megastigmene-6,9-diol M-101



$C_{13}H_{24}O_2$ 212.331

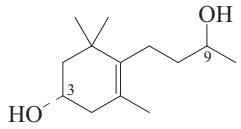
(6α,9*R*)-*form*
7,8-Dihydro-6α-hydroxy-α-ionol

9-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [177261-74-4]
$C_{24}H_{42}O_{11}$ 506.589
Constit. of *Cydonia vulgaris* (quince).

De Tommasi, N. *et al., J. Agric. Food Chem.*, 1996, **44**, 1676-1681 (*isol, pmr, cmr*)

5-Megastigmene-3,9-diol M-102

3-Hydroxy-7,8-dihydro-β-ionol



3α-*form*

$C_{13}H_{24}O_2$ 212.331
Gum. $[\alpha]_D^{23}$ -84.4 (c, 0.48 in MeOH).

(3β,9*R*)-*form*

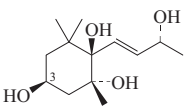
9-O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [347852-04-4]
$C_{24}H_{42}O_{11}$ 506.589
Constit. of leaves of *Camellia sinensis* var. *sinensis* (China tea). $[\alpha]_D^{27}$ -7.2 (c, 1 in MeOH).

(3ξ,9ξ)-*form* [221547-14-4]
Tsangane L
Oil. $[\alpha]_D^{25}$ -33.8 (c, 0.5 in $CHCl_3$).

3-O-*β-D-Glucopyranoside:* [143775-68-2]
Isol. from sloe tree leaves (*Prunus spinosa*). Potential aroma compd.. $[\alpha]_D^{20}$ -83.6 (c, 0.5 in MeOH).

Bilia, A.R. *et al., J. Nat. Prod.*, 1993, **56**, 2142 (*isol, pmr, cmr*)
Ma, S.-J. *et al., Phytochemistry*, 2001, **56**, 819-825 (*apiosylglucoside*)

7-Megastigmene-3,5,6,9-tetrol M-103



(3*S*,5*R*,6*R*,7*E*,9*R*)-*form*

$C_{13}H_{24}O_4$ 244.33

(3*S*,5*R*,6*R*,7*E*,9*R*)-*form*

3-O-*β-D-Glucopyranoside:* [141897-12-3]
Kiwiionoside*. Stratioside II*
$C_{19}H_{34}O_9$ 406.472
Constit. of *Actinidia chinensis* (kiwifruit). $[\alpha]_D$ +24.7 (c, 0.1 in MeOH).

(3*S*,5*R*,6*R*,7*E*,9*S*)-*form* [276870-26-9]
Amorph. powder. $[\alpha]_D^{26}$ -25.7 (c, 1.52 in MeOH).

(3*S*,5*R*,6*R*,7*E*,9ξ)-*form*
Aripuanin
$[\alpha]_D$ -30.4 (c, 0.53 in MeOH).

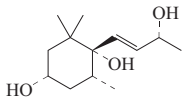
3-O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [178273-38-6] ***Alangionoside O***
$C_{24}H_{42}O_{13}$ 538.588
Amorph. powder. $[\alpha]_D^{22}$ -50.6 (c, 1 in MeOH).

(3*S*,5*S*,6*S*,7*E*,9ξ)-*form* [180322-35-4]
Amorph. powder.

Murai, F. *et al., Planta Med.*, 1992, **58**, 112 (*isol, pmr, cmr, cryst struct*)
Pérez, C. *et al., Nat. Prod. Lett.*, 1996, **8**, 1-6 (*isol, pmr, cmr*)
Della Greca, M. *et al., Nat. Prod. Lett.*, 1996, **8**, 83 (*Stratioside II*)
Kijima, H. *et al., Phytochemistry*, 1996, **42**, 723 (*Alangionoside O*)
Nascimento, M. *et al., Fitoterapia*, 1999, **70**, 628-629 (*Aripuanin, pmr, cmr*)
Takeda, Y. *et al., Chem. Pharm. Bull.*, 2000, **48**, 752-754 (*Euscaphis japonica constit*)

7-Megastigmene-3,6,9-triol M-104

3,6-Dihydroxy-5,6-dihydro-β-ionol



(3*S*,5*R*,6*R*,7*E*,9*R*)-*form*

$C_{13}H_{24}O_3$ 228.331

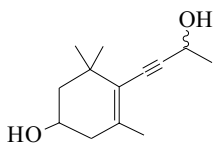
(3*S*,5*R*,6*S*,7*E*,9ξ)-*form*
Syrup. $[\alpha]_D$ -10.1 (c, 1 in $CHCl_3$).

9-O-*β-D-Glucopyranoside:*
$C_{19}H_{34}O_8$ 390.473
Constit. of *Averrhoa carambola* (carambola). May be identical with Alangionoside A above.

Lutz, A. *et al., Nat. Prod. Lett.*, 1993, **3**, 95 (*9-glucoside*)

5-Megastigmen-7-yne-3,9-diol M-105

[58023-72-6]
3-Hydroxy-7,8-didehydro-β-ionol



$C_{13}H_{20}O_2$ 208.3
$[\alpha]_D^{17}$ -82.6 (c, 0.27 in EtOH).

3-O-*β-D-Glucopyranoside:* [62512-27-0]
$C_{19}H_{30}O_7$ 370.442
Constit. of Riesling wine.

9-O-*β-D-Glucopyranoside:* [62512-26-9]
$C_{19}H_{30}O_7$ 370.442
Constit. of Riesling wine and Rose petals. $[\alpha]_D$ -32.6 (c, 0.19 in MeOH) (as penta-Ac). λ_{max} 226 (MeOH) (as penta-Ac).

Fujimori, T. *et al., Phytochemistry*, 1975, **14**, 2095
Straubinger, M. *et al., J. Agric. Food Chem.*, 1997, **45**, 4053-4056 (*9-glycoside*)
Baderschneider, B. *et al., Nat. Prod. Lett.*, 1997, **10**, 111-114 (*glycosides*)

Melaninocin M-106

[76930-38-6]

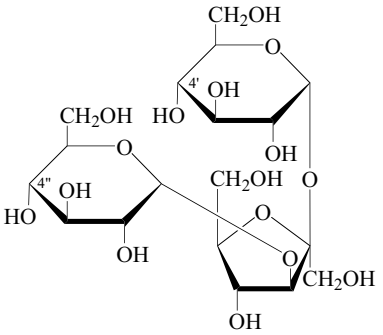
Struct. unknown. Bacteriocin prod. by *Bacteroides melaninogenicus*.

Nakamura, T. *et al., Infect. Immun.*, 1981, **31**, 28-32 (*isol*)

Melezitose, 8CI M-107

[597-12-6]

[10030-67-8]
O-*α-D-Glucopyranosyl-(1→3)-β-D-fructofuranosyl α-D-glucopyranoside, 9CI. Melizitose*



$C_{18}H_{32}O_{16}$ 504.441
Constit. of honey. Dihydrate. Mp 153-154°. $[\alpha]_D^{20}$ +88.2 (H_2O). Dimorphic.

Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Mp 117°. $[\alpha]_D$ +104 (c, 1.0 in $CHCl_3$).

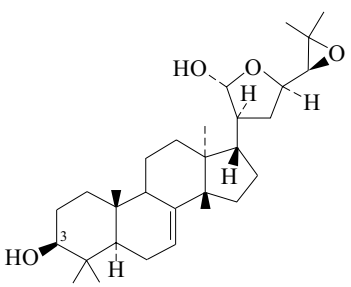
Undeca-Me:
$C_{29}H_{54}O_{16}$ 658.736
$Bp_{0.01}$ 236°. $[\alpha]_D$ +114 (MeOH).

4′,4″-Di-O-*β-D-glucopyranosyl:* ***Diglucomelezitose***
$C_{30}H_{52}O_{26}$ 828.725

Leitch, G.C. *et al., J.C.S.*, 1927, 588
Hudson, C.S. *et al., Adv. Carbohydr. Chem.*, 1946, **2**, 2 (*rev*)
Richtmyer, N.K. *et al., J.O.C.*, 1946, **11**, 610 (*struct*)
Hehre, E.J. *et al., Arch. Biochem. Biophys.*, 1952, **36**, 158 (*occur*)
Moor, J. *et al., Org. Mass Spectrom.*, 1974, **9**, 903 (*ms*)
Anteunis, M. *et al., Carbohydr. Res.*, 1975, **44**, 101 (*pmr*)
Avenel, D. *et al., Acta Cryst. B*, 1976, **32**, 2598 (*cryst struct*)
Bequart, J. *et al., Carbohydr. Res.*, 1982, **111**, 9 (*cryst struct*)
Wei, Y.A. *et al., J. Agric. Food Chem.*, 1997, **45**, 3481-3486 (*Diglucomelezitose*)

Melianol M-108

[16838-01-0]
*21*R,*23*R:*24S,25-Diepoxytirucall-7-ene-3β,21*R-*diol*



$C_{30}H_{48}O_4$ 472.707
Cryst. (Me_2CO/pentane). Mp 194-195°. $[\alpha]_D$ -38 (c, 1 in $CHCl_3$).

3-Ac: [5532-42-3] ***Turraeanthin***
$C_{32}H_{50}O_5$ 514.744
Cryst. (MeOH/$CHCl_3$). Mp 218-220°. $[\alpha]_D$ +3 (c, 1 in $CHCl_3$).

3-O-*Alkanoyl:* ***Lipomelianol***
Cryst. ($CHCl_3$/MeOH). Mp 54-55°. $[\alpha]_D^{20}$ -3 (c, 0.18 in $CHCl_3$). Alkanoyl residues consist of stearoyl, palmitoyl,

myristoyl and lauroyl. Behaves as a single compound.

3-Ketone: [6553-27-1] ***Melianone***. *24,25-Epoxyflindissone. Cneorin NP_{37}*
$C_{30}H_{46}O_4$ 470.691
Cryst. ($CHCl_3$/pentane). Mp 232-233°. $[\alpha]_D$ -62 (c, 1 in $CHCl_3$).

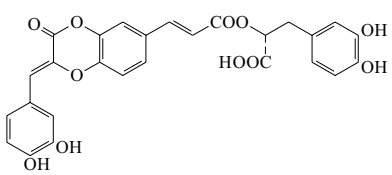
1,2-Didehydro: ***Murrayenol***
$C_{30}H_{46}O_4$ 470.691
Isol. from roots of *Murraya koenigii* (curry leaf tree). Mp 234-236°.

[81177-21-1]

Bevan, C.W.L. *et al., J.C.S.(C)*, 1967, 820 (*isol*)
Lavie, D. *et al., J.C.S.(C)*, 1967, 1347 (*isol*)
Lyons, C.W. *et al., Chem. Comm.*, 1975, 517 (*struct*)
Polonsky, J. *et al., Isr. J. Chem.*, 1977, **16**, 16 (*cmr*)
Mondon, A. *et al., Tet. Lett.*, 1981, 4467 (*Cneorin NP_{37}*)
Nakanishi, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 100 (*isol*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1053 (*Melianone, cmr*)
Srivastava, J.K. *et al., J. Indian Chem. Soc.*, 1993, **70**, 655 (*Murrayenol*)

Melitric acid B M-109

[153765-46-9]

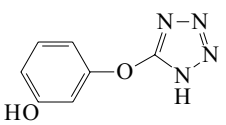


$C_{27}H_{20}O_{11}$ 520.448
Constit. of *Melissa officinalis* (lemon balm). Light brown powder + $1^1/_2H_2O$. Mp 133-135°. $[\alpha]_D^{24}$ +119.7 (c, 0.33 in MeOH).

Agata, I. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1608 (*isol, pmr, cmr*)

Melizame, INN, USAN M-110

[26921-72-2]
3-(1H-Tetrazol-5-yloxy)phenol, 9CI. 5-(3-Hydroxyphenoxy)-1H-tetrazole. Lilly 56063



$C_7H_6N_4O_2$ 178.15
Sweetener. Never marketedCryst. (H_2O). Mp 141-143°. Log P 1.15 (calc).

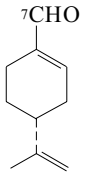
Na salt:
Mp 130-135° (as dihydrate).

U.S. Pat., 1970, 3 515 727, (*Eli Lilly*); *CA*, **72**, 120260t (*synth, use*)
Ger. Pat., 1973, 2 250 960, (*Procter and Gamble*); *CA*, **79**, 9775 (*use*)

p-Mentha-1,8-dien-7-al M-111

[2111-75-3]
4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde, 9CI. 4-Isopropenyl-1-cyclohexene-1-carboxaldehyde. ***Perillaldehyde.***

Perillaaldehyde



(*R*)-*form*

$C_{10}H_{14}O$ 150.22
▶ Skin irritant. LD_{50} (mus, orl) 1720 mg/kg. GW2967000

(R)-form [5503-12-8]
Flavouring agent. Isol. from tangerine (*Citrus reticulata*) and other plants. Oil. Bp_9 99-104°. $[\alpha]_D$ +137.

Oxime:
$C_{10}H_{15}NO$ 165.235
Cryst. Mp 102°.

7-Carboxylic acid: [7694-45-3] p-*Mentha-1,8-dien-7-oic acid.* ***Perillic acid***
$C_{10}H_{14}O_2$ 166.219
Cryst. (EtOH). Mp 132-133°. Bp_{10} 164-165°. $[\alpha]_D^{20}$ -146.

7-Carboxylic acid, Me ester: [54298-90-7]
$Bp_{0.5}$ 81-83°.

7-Carboxylic acid, β-D-glucopyranosyl ester: ***Perilloside B***
$C_{16}H_{24}O_7$ 328.361
Constit. of perilla (*Perilla frutescens*). Needles ($CHCl_3$/Et_2O). Mp 154-155°. $[\alpha]_D^{22}$ -57.1 (c, 0.645 in MeOH). λ_{max} 220 (ϵ 10500) (MeOH) (Berdy).

(S)-form [18031-40-8]
Constit. of *Perilla nankinensis* and gingergrass oils. Oil. Bp_{10} 104-105°. $[\alpha]_D^{20}$ -145.8.
▶ GW2967200

(E)-Oxime: [30950-27-7] *Perilla sugar. Perillartine*
$C_{10}H_{15}NO$ 165.235
Sweetening agent. V. sweet cryst. Mp 102°. Bp_{12} 147-148°.
▶ LD_{50} (rat, orl) 2500 mg/kg. GW2975000

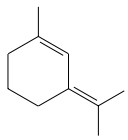
(Z)-Oxime:
$C_{10}H_{15}NO$ 165.235
Cryst. Mp 129°.

[6611-91-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 477A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 745C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 568A (*ir*)
Ritter, J.J. *et al., J.A.C.S.*, 1950, **72**, 2381 (*synth, Perillic acid*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1968, **45**, 615 (*synth*)
Acton, E.M. *et al., Experientia*, 1970, **26**, 473 (*struct*)
Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 545 (*stereochem*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Tori, K. *et al., Tet. Lett.*, 1975, 2199 (*pmr*)
Regan, J.W. *et al., J. Agric. Food Chem.*, 1976, **24**, 377 (*Perillic acid*)
Tius, M.A. *et al., Synth. Commun.*, 1988, **18**, 1905 (*synth*)
Fujita, T. *et al., Phytochemistry*, 1993, **34**, 1545 (*Perilloside B*)
McGeady, P. *et al., J. Nat. Prod.*, 2002, **65**, 953-955 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DKX100; PCJ000

m-Mentha-1,3(8)-diene M-112

[17092-80-7]
1-Methyl-3-(1-methylethylidene)cyclohexene, 9CI. ***Sylveterpinolene***

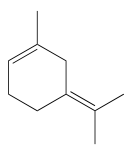


$C_{10}H_{16}$ 136.236
Isol. from *Pinus sylvestris* (Scotch pine). Bp 88°. n_D^{20} 1.5132.

Cocker, W. *et al., J.C.S.(C)*, 1968, 489 (*synth*)
Muraleedharan, N.V. *et al., J. Indian Chem. Soc.*, 1972, **49**, 289 (*synth*)
Bardyshev, I.I. *et al., Khim. Prir. Soedin.*, 1974, **10**, 318; *Chem. Nat. Compd. (Engl. Transl.)*, 325 (*isol*)

m-Mentha-1(6),3(8)-diene M-113

[25946-29-6]
1-Methyl-5-(1-methylethylidene)cyclohexene. ***5-Isosylveterpinolene***



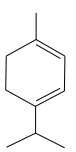
$C_{10}H_{16}$ 136.236
Constit. of black pepper oil (*Piper nigrum*). Oil.

Nussbaumer, C. *et al., Helv. Chim. Acta*, 1999, **82**, 53-58 (*isol, pmr, cmr, synth*)

p-Mentha-1,3-diene M-114

[99-86-5]

[1329-99-3]
1-Methyl-4-(1-methylethyl)-1,3-cyclohexadiene. 1-Isopropyl-4-methyl-1,3-cyclohexadiene. ***α-Terpinene****. FEMA 3558*



$C_{10}H_{16}$ 136.236
Constit. of many essential oils e.g. *Citrus, Eucalyptus* and *Juniperus* spp. Oil of *Litsea ceylanica* is a major source (20%). Flavouring agent. Oil with lemon odour. Bp_{755} 173.5-174.8°. n_D^{20} 1.4780.
▶ LD_{50} (rat, orl) 1680 mg/kg. OS8060000

[8013-00-1]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 64A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 47B (*ir*)

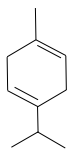
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 69C (*ir*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Bardyshev, I.I. *et al., Khim. Prir. Soedin.*, 1969, **5**, 123; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 106 (*occur, ir, uv*)
Degny, E. *et al., Bull. Soc. Chim. Fr.*, 1972, 4770 (*synth*)
Verghese, J. *et al., Flavour Ind.*, 1972, **3**, 252 (*rev*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 873 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MLA250

p-Mentha-1,4-diene M-115

[99-85-4]

[1329-99-3]

1-Methyl-4-(1-methylethyl)-1,4-cyclohexadiene, 9CI. 1-Isopropyl-4-methyl-1,4-cyclohexadiene. ***γ-Terpinene****. Crithmene. Moslene. FEMA 3559*



$C_{10}H_{16}$ 136.236
Constit. of many essential oils e.g. *Citrus*, *Eucalyptus*, *Mentha*, *Pinus* spp. Ajowan seed oil (*Carum copticum*) is a major source. Oil with characteristic lemon odour. Bp 183°.
► Skin irritant. LD_{50} (rat, orl) 3650 mg/kg. OS8070000

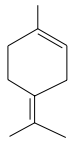
[8013-00-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 47C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 64B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 69D (*ir*)
Briggs, L.H. *et al., J.O.C.*, 1948, **6**, 1 (*isol*)
Ryhage, R. *et al., Acta Chem. Scand.*, 1963, **17**, 2025 (*ms*)
Wrolstad, R.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 507 (*ir*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 47 (*occur*)
Verghese, J. *et al., Indian Perfum.*, 1974, **18**, 53 (*rev*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 875 (*rev, tox*)
Bond, A.D. *et al., Acta Cryst. E*, 2001, **57**, o1032-o1033 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCB750

p-Mentha-1,4(8)-diene M-116

[586-62-9]

1-Methyl-4-(1-methylethylidene)cyclohexene, 9CI. 4-Isopropylidene-1-methylcyclohexene. ***Terpinolene****. FEMA 3046*



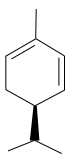
$C_{10}H_{16}$ 136.236
Constit. of many essential oils e.g. *Citrus, Mentha, Juniperus, Myristica* spp. Parsnip oil (*Pastinaca sativa*) is a major source (40-70%). Flavouring ingredient. Oil with sweet pine/citrus odour. d_{20}^{20} 0.86. Bp 186°. n_D^{20} 1.4900.
► Flammable, fl. p. 38°, LD_{50} (rat, orl) 4390 mg/kg. WZ6870000

Thomas, A.F. *et al., Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Wrolstad, R.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 507 (*isol, ir*)
Verghese, J. *et al., Perfum. Essent. Oil Res.*, 1967, **58**, 638 (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 51 (*occur*)
Krapcho, A.P. *et al., J.O.C.*, 1974, **39**, 1322 (*synth*)
Mathew, C.P. *et al., J. Indian Chem. Soc.*, 1975, **52**, 997 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 877 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBE000

p-Mentha-1,5-diene M-117

[99-83-2]

2-Methyl-5-(1-methylethyl)-1,3-cyclohexadiene. 5-Isopropyl-2-methyl-1,3-cyclohexadiene. ***α-Phellandrene****. FEMA 2856*



(*R*)-*form*

$C_{10}H_{16}$ 136.236
► Flammable, fl. p. 49°. Severe human skin irritant. LD_{50} (rat, orl) 5700 mg/kg. OS8080000

(R)-form [4221-98-1]
Constit. of oils of pimento, bay, *Citrus*, *Juniperus*, *Mentha*, and other essential oils. Oil of *Zanthoxylum alatum* is a major source (50%). Flavouring agent. Oil. Bp 174°. $[\alpha]_D^{20}$ -217.

(S)-form [2243-33-6]
Flavouring agent. Constit. of many essential oils including bitter fennel, elemi and ginger-grass oils. Oil of *Ridolfia segetum* is a major source (85%). Oil. Bp 175-176°. $[\alpha]_D$ +49.1.

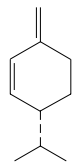
[13811-01-3]

Ryhage, R. *et al., Acta Chem. Scand.*, 1963, **17**, 2025 (*ms*)
Snatzke, G. *et al., Tet. Lett.*, 1966, 4551 (*abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 48 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 843 (*rev, tox*)
Singaram, B. *et al., Perfum. Flavor.*, 1978, **2**, 33 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 644 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCC000

p-Mentha-1(7),2-diene M-118

[555-10-2]

3-Methylene-6-(1-methylethyl)cyclohexene. 3-Isopropyl-6-methylenecyclohexene. ***β-Phellandrene***



(*R*)-*form*

$C_{10}H_{16}$ 136.236
Widely distributed in essential oils (*Angelica*, *Eucalyptus*, *Lavandula*, *Mentha*, *Pinus* spp.). Flavour ingredient.
► Flammable, fl. p. 49°.

(R)-form [6153-17-9]
Oil. Bp 172-174°. $[\alpha]_D$ -74.4. n_D^{20} 1.4826.

(S)-form [6153-16-8]
Oil. Bp 171-172°. $[\alpha]_D$ +75.

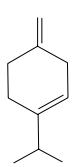
[51941-36-7]

Acheson, G.G. *et al., J.C.S.*, 1949, 812 (*struct*)
Mitzner, B.M. *et al., J.O.C.*, 1962, **27**, 3359 (*synth*)
Ryhage, R. *et al., Acta Chem. Scand.*, 1963, **17**, 2025 (*ms*)
Deorha, D.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **82**, 137 (*synth*)
Bardyshev, I.I. *et al., Khim. Prir. Soedin.*, 1967, **3**, 282; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 237 (*ir, uv*)
Verghese, J. *et al., Perfum. Essent. Oil Res.*, 1967, **58**, 868 (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 49 (*occur*)
Miller, D.R. *et al., J. Chem. Ecol.*, 1990, **16**, 2519
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 791

p-Mentha-1(7),3-diene M-119

[99-84-3]

4-Methylene-1-(1-methylethyl)cyclohexene. 1-Isopropyl-4-methylenecyclohexene. ***β-Terpinene***



$C_{10}H_{16}$ 136.236
Constit. of Juniper and *Myrica gale* (bog myrtle) oils. Oil. Bp 173-174°. $[\alpha]_D^{20}$ +3.

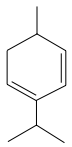
[8013-00-1]

Wallach, O. *et al., Annalen*, 1908, **362**, 288
Corbett, R.E. *et al., J. Sci. Food Agric.*, 1959, **10**, 198 (*isol*)

Mitzner, B.M. *et al., J.O.C.*, 1962, **27**, 3359 (*synth*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Verghese, J. *et al., Indian Perfum.*, 1974, **18**, 39 (*rev*)

p-Mentha-2,4-diene M-120

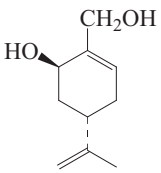
[586-68-5]
5-Methyl-2-(1-methylethyl)-1,3-cyclohexadiene. 2-Isopropyl-5-methyl-1,3-cyclohexadiene



$C_{10}H_{16}$ 136.236
Constit. of Valencia orange oil. Oil. Bp_{25} 56°.

Hunter, G.L.K. *et al., J.O.C.*, 1964, **29**, 498

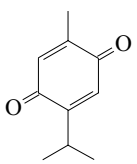
p-Mentha-1,8-diene-6,7-diol M-121



$C_{10}H_{16}O_2$ 168.235
(4*S*,6*R*)-*form* [402593-56-0]
Amorph. powder. $[\alpha]_D^{22}$ +36 (c, 0.2 in MeOH).
7-O-β-D-Glucopyranoside: [402593-54-8]
$C_{16}H_{26}O_7$ 330.377
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{24}$ +12 (c, 0.4 in MeOH).
Matsumura, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 66-72 (*isol, pmr, cmr*)

p-Mentha-3,6-diene-2,5-dione, 8CI M-122

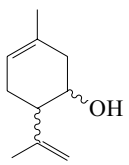
[490-91-5]
2-Methyl-5-(1-methylethyl)-2,5-cyclohexadiene-1,4-dione, 9CI. 2-Isopropyl-5-methyl-1,4-benzoquinone. p-*Cymene-2,5-dione.* ***Thymoquinone****. Thymoil*



$C_{10}H_{12}O_2$ 164.204
Major constit. of seed oil of black cumin, *Nigella sativa* (24%). Bright yellow cryst. (pentane) with penetrating odour. Sol. MeOH, Et_2O; fairly sol. $CHCl_3$; poorly sol. H_2O. Mp 44-45°. Steam-volatile λ_{max} 276 (ε 2610); 282 (ε 2450) (EtOH) (Berdy).
► LD_{50} (rat, ipr) 10 mg/kg. GU5330000
Dioxime:
$C_{10}H_{14}N_2O_2$ 194.233
Cryst. (EtOH). Mp 235°.
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 714A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 543B (*ir*)
Henderson, G.G. *et al., J.C.S.*, 1910, 1659 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 498; 511 (*synth*)
Flaig, W. *et al., Z. Naturforsch., B*, 1955, **10**, 668 (*uv*)
Flaig, W. *et al., Annalen*, 1959, **626**, 215 (*ir*)
El-Dakhakhny, M. *et al., Planta Med.*, 1963, **11**, 465 (*isol*)
Norris, R.K. *et al., Aust. J. Chem.*, 1966, **19**, 617 (*pmr*)
Jacobsen, N. *et al., J.C.S. Perkin 2*, 1979, 569 (*synth, pmr, ms*)
Liebeskind, L.S. *et al., J.O.C.*, 1992, **57**, 4345 (*synth, pmr, ir*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IQF000

p-Mentha-1(6),8-dien-3-ol M-123

[20019-62-9]
3-Methyl-6-(1-methylethenyl)-3-cyclohexen-1-ol, 9CI. p-*Mentha-1,8-dien-5-ol*



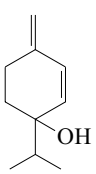
$C_{10}H_{16}O$ 152.236
Isol. from lemongrass oil. $Bp_{2.5}$ 64-65°. Obt. as a mixt. of *cis* and *trans*-forms. No props. of individual stereoisomers reported.

[55820-19-4, 58461-28-2]

Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1961, 1881 (*isol*)
Cant, P.A.E. *et al., Aust. J. Chem.*, 1975, **28**, 621 (*synth, pmr*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)

p-Mentha-1(7),2-dien-4-ol M-124

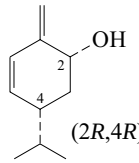
4-Methylene-1-(1-methylethyl)-2-cyclohexen-1-ol, 9CI. 1-Isopropyl-4-methylene-2-cyclohexen-1-ol



$C_{10}H_{16}O$ 152.236
(ξ)-*form*
Isol. from black pepper oil.
Debrauwere, J. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 167 (*isol, ms, pmr*)

p-Mentha-1(7),5-dien-2-ol M-125

[30681-15-3]
2-Methylene-5-(1-methylethyl)-3-cyclohexen-1-ol, 9CI. ***Yabunikkeol***

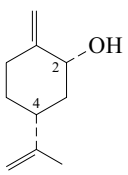


(2*R*,4*R*)-*form*

$C_{10}H_{16}O$ 152.236
(2*R*,4*R*)-*form* [29332-99-8]
(+)-cis-*form*
Cryst. Mp 41-42° (34°). Bp 228°. $[\alpha]_D^{20}$ +56 (c, 1.0 in $CHCl_3$). $[\alpha]_D^{20}$ +35 (c, 0.30 in EtOH).
(2*S*,4*R*)-*form* [29332-98-7]
(-)(EtOH)-trans-*form*
Constit. of *Piper nigrum* (pepper). Oil. Bp 226°. $[\alpha]_D^{20}$ -28 (c, 0.52 in EtOH). $[\alpha]_D^{20}$ +5 (c, 0.81 in $CHCl_3$).
Ac:
$C_{12}H_{18}O_2$ 194.273
Constit. of *Angelica archangelica* (angelica). Oil. $[\alpha]_D^{20}$ -55 (c, 0.8 in $CHCl_3$).
Fujita, Y. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 1599 (*isol*)
Debrauwere, J. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 167 (*isol, pmr*)
Escher, S. *et al., Helv. Chim. Acta*, 1979, **62**, 2061 (*isol, synth, uv, ir, pmr*)
Montiel, V. *et al., Synth. Commun.*, 1987, **17**, 993 (*synth*)

p-Mentha-1(7),8-dien-2-ol M-126

[35907-10-9]
2-Methylene-5-(1-methylethenyl)cyclohexanol, 9CI. 5-Isopropenyl-2-methylenecyclohexanol



(2*R*,4*R*)-*form*

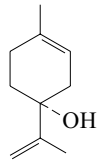
$C_{10}H_{16}O$ 152.236
Ac: Menthadienyl acetate. FEMA 3848
$C_{12}H_{18}O_2$ 194.273
Flavouring agent for candies. Mixt. of *cis*- and *trans*-isomers.
(2*R*,4*R*)-*form* [10374-04-6]
(2*S*,4*R*)-*form* [2102-62-7]
Isol. from *Zanthoxylum piperitum* (Japanese pepper tree).

[21391-84-4, 22626-43-3]

Ohloff, G. *et al., Angew. Chem.*, 1961, **73**, 578 (*synth*)
Sakai, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1945 (*isol*)

p-Mentha-1,8-dien-4-ol M-127

[3419-02-1]
4-Methyl-1-(1-methylethenyl)-3-cyclohexen-1-ol, 9CI



(*R*)-*form*

$C_{10}H_{16}O$ 152.236
Isol. from Japanese pepper tree (*Zanthoxylum piperitum*), yuzu (*Citrus junos*), and spearmint (*Mentha spicata*) oils.

(*R*)-*form* [38630-70-5]
$[\alpha]_D^{20}$ +10 (c, 1 in EtOH).

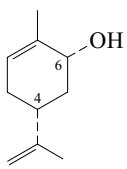
(±)-*form* [28342-82-7]
Bp_5 81-82°.

[73069-45-1]

Sakai, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1945 (*isol*)
Birch, A.J. *et al., Aust. J. Chem.*, 1969, **22**, 2037 (*synth*)
Jensen, H.P. *et al., J.O.C.*, 1975, **40**, 264 (*synth*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Naya, Y. *et al., Heterocycles*, 1978, **10**, 29 (*isol*)
Delay, F. *et al., Helv. Chim. Acta*, 1979, **62**, 2168 (*synth, pmr*)

p-Mentha-1,8-dien-6-ol M-128

[99-48-9]
2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-ol. 5-Isopropenyl-2-methyl-2-cyclohexen-1-ol. ***Carveol****. FEMA 2247*



(4*R*,6*R*)-*form*

$C_{10}H_{16}O$ 152.236
Present in oil of grapefruit (*Citrus paradisi*), mandarin (*Citrus reticulata*), blackcurrant berries, celery, black tea, dill, caraway seeds and lamb's lettuce. Flavouring agent.

► LD_{50} (rat, orl) 3000 mg/kg. OS8400000

Ac: [97-42-7] *Carvyl acetate. FEMA 2250*
$C_{12}H_{18}O_2$ 194.273
Flavouring ingredient.

Propanoyl: [97-45-0] *Carvyl propionate. FEMA 2251*
$C_{13}H_{20}O_2$ 208.3
Flavouring ingredient with a sweet, fruity, minty taste. Oil with sweet fruity-minty taste.

(4*R*,6*R*)-*form* [2102-59-2]
(-)-cis-*form*
Constit. of Valencia orange oil (*Citrus sinensis*). Flavouring agent. Cryst. (hexane). Mp 24-25°. $[\alpha]_D$ -30 (c, 2.1 in MeOH).

O-*β*-D-*Glucopyranoside:* [74284-29-0]
$C_{16}H_{26}O_6$ 314.378

(4*R*,6*S*)-*form* [2102-58-1]
(-)-trans-*form*
Constit. of Valencia orange essence oil. Flavouring ingredient. Oil. Bp_{10} 102.2-102.4°. $[\alpha]_D$ -213.

O-*β*-D-*Glucopyranoside:* [113349-30-7]
$C_{16}H_{26}O_6$ 314.378
Constit. of *Citrus* spp. and ginger mint *Mentha gentilis cardiaca*.

(4*S*,6*R*)-*form* [18383-51-2]
(+)-trans-*form*
Oil. Bp_4 80-80.5°. $[\alpha]_D^{20}$ +217.1.

O-*β*-D-*Glucopyranoside:* [114673-98-2]
$C_{16}H_{26}O_6$ 314.378
Constit. of *Citrus* spp..

(4*S*,6*S*)-*form* [7632-16-8]
(+)-cis-*form*
Constit. of dill seed oil (*Anethum graveolens*). Oil. $Bp_{5.5}$ 87-88°. $[\alpha]_D$ +30.4 (c, 2 in MeOH).

(4*RS*,6*RS*)-*form*
(±)-cis-*form*
Bp_{16} 108°. n_D^{19} 1.4779.

4-Nitrobenzoyl:
Mp 94°.

(4*SR*,6*SR*)-*form* [5157-78-8] *(±)*-trans-*form*
Bp_{16} 108°. n_D^{19} 1.4956.

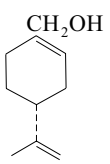
4-Nitrobenzoyl:
Mp 101°.

[1197-06-4, 1197-07-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 165C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 261A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 241C (*ir*)
Naves, Y.R. *et al., Helv. Chim. Acta*, 1964, **47**, 1617 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1055 (*rev, tox*)
Grandi, R. *et al., Tetrahedron*, 1974, **30**, 4037 (*synth*)
Voisin, D. *et al., Bull. Soc. Chim. Fr.*, 1975, 375 (*synth*)
Ackermann, I.E. *et al., Annalen*, 1989, 79 (*synth, glucosides*)
Shimizu, S. *et al., J. Essent. Oil Res.*, 1990, **2**, 81 (*glucoside*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 107; 109-110
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 520-521; 525-526
Bouwmeester, H.J. *et al., Phytochemistry*, 1999, **50**, 243-248 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKY250

p-Mentha-1,8-dien-7-ol M-129

[536-59-4]
4-(1-Methylethenyl)-1-cyclohexene-1-methanol, 9CI. 1-Hydroxymethyl-4-isopropenylcyclohexene. ***Perilla alcohol****. Perillyl alcohol. Dihydrocuminyl alcohol. Perillic alcohol. Perillol. NSC 641066*



(*R*)-*form*

$C_{10}H_{16}O$ 152.236

► Severe skin irritant. LD_{50} (rat, orl) 2100 mg/kg. OS8395000

Ac: [15111-96-3] *Perillyl acetate. FEMA 3561*
$C_{12}H_{18}O_2$ 194.273
Flavouring ingredient.

(*R*)-*form* [57717-97-2]
Isol. from caraway seed oil. $[\alpha]_D$ +85.6.

(*S*)-*form* [18457-55-1]
Occurs in a variety of essential oils, e.g. lavender. Oil. Bp 244.5° Bp_{11} 118-121°. $[\alpha]_D$ -97.5.

α-Naphthylurethane:
Cryst. Mp 146-147°.

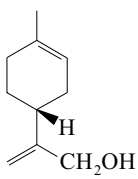
O-*β*-D-*Glucopyranoside:* ***Perilloside A***
$C_{16}H_{26}O_6$ 314.378
Constit. of *Perilla frutescens* (perilla). Needles. Mp 114.5-115°. $[\alpha]_D^{22}$ -92.7 (c, 0.77 in MeOH).

[66141-69-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 153D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 260C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 226A (*ir*)
Kergomard, A. *et al., Bull. Soc. Chim. Fr.*, 1958, 393 (*synth*)
Naves, Y.-R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1959, **249**, 306 (*isol*)
Büchi, G. *et al., J.A.C.S.*, 1969, **91**, 6473 (*abs config*)
v. Sydow, E. *et al., Arch. Mass Spectral Data*, 1970, **1**, 436 (*ms*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Fujita, T. *et al., Phytochemistry*, 1992, **31**, 3265 (*Perilloside A*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2137-2138 (*Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PCI550

p-Mentha-1,8-dien-10-ol M-130

4-Methyl-α-methylene-3-cyclohexeneethanol. p-*Mentha-1,8(10)-dien-9-ol. Limonen-10-ol*



(*R*)-*form*

$C_{10}H_{16}O$ 152.236

(*R*)-*form* [38142-45-9]
$Bp_{8.5}$ 101-103°. $[\alpha]_D^{20}$ +112 (neat). $[\alpha]_D^{20}$ +107 (c, 0.15 in MeOH).

3,5-Dinitrobenzoyl:
Mp 71-72°.

Aldehyde: **p-*Mentha-1,8-dien-10-al***
$C_{10}H_{14}O$ 150.22
$[\alpha]_D^{20}$ +70 (c, 0.88 in MeOH). n_D^{20} 1.4998.

Aldehyde, 2,4-dinitrophenylhydrazone:
Mp 178-179°.

Aldehyde, semicarbazone:
Mp 117-118°.

(*S*)-*form*
$[\alpha]_D^{25}$ -65.5 (c, 0.74 in EtOH). $n_D^{25.5}$ 1.4993.

Ac: [15593-88-1]
$C_{12}H_{18}O_2$ 194.273
Isol. from grapefruit, lemon and mandarin oils. $Bp_{1.5}$ 102-104°. $[\alpha]_D$ -46.8 (c,

0.72 in EtOH).

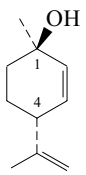
(±)-*form* [3269-90-7]
$Bp_{2.5}$ 112° (lit. gives a pressure range). $[\alpha]_D^{12}$ +15.16 (c, 5.13 in EtOH). n_D^{26} 1.4830.

Ac: [15111-97-4]
Isol. from *Citrus natsudaidai* oil.

Ogata, Y. *et al., Kogyo Kagaku Zasshi*, 1953, **56**, 861 (*synth*)
Ruegg, R. *et al., Recherches*, 1966, **15**, 3 (*synth, pmr*)
Vig, O.P. *et al., Indian J. Chem.*, 1967, **5**, 475 (*synth*)
Mitzner, B.M. *et al., Appl. Spectrosc.*, 1968, **22**, 34 (*ir*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1970, **53**, 770 (*synth*)
Moshonas, M.G. *et al., J. Agric. Food Chem.*, 1971, **19**, 769 (*isol, Ac*)
Dubovenko, Zh.V. *et al., Khim. Prir. Soedin.*, 1973, **9**, 120; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 118 (*isol, alcohol, aldehyde*)
Nomura, M. *et al., Nippon Kagaku Kaishi*, 1979, 305 (*synth*)

p-Mentha-2,8-dien-1-ol M-131

1-Methyl-4-(1-methylethenyl)-2-cyclohexen-1-ol, 9CI. 4-Isopropenyl-1-methyl-2-cyclohexen-1-ol



(1*R*,4*R*)-*form*

$C_{10}H_{16}O$ 152.236

(1*R*,4*R*)-*form* [52154-82-2]
Isol. from gingergrass oil (*Cymbopogon martini*) and various *Citrus* oils. Metabolic and oxidn. prod. of Limonene, L-88. $Bp_{6.5}$ 86.5°. n_D^{20} 1.4881. This is the *cis*-form acc. to most authors but the *trans*-form in CA.

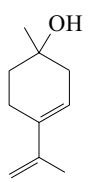
(1*S*,4*R*)-*form* [22972-51-6]
Isol. from gingergrass (*Cymbopogon*) and *Citrus* oils. Mp 18°. Bp_{12} 90°. $[\alpha]_D^{20}$ +67.3. n_D^{20} 1.4900.

[3886-78-0, 7212-40-0, 22771-44-4]

Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1960, 37 (*isol*)
Schenk, G.O. *et al., Annalen*, 1964, **674**, 93 (*synth*)
Wang, W. *et al., J. Chem. Res., Synop.*, 1998, 42-43 (*synth, pmr, cmr*)

p-Mentha-3,8-dien-1-ol M-132

[55708-38-8]
1-Methyl-4-(1-methylethenyl)-3-cyclohexen-1-ol, 9CI



$C_{10}H_{16}O$ 152.236

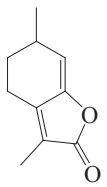
(ξ)-*form*
Isol. from black pepper oil.

Sakuda, Y. *et al., Nippon Kagaku Zasshi*, 1960, **81**, 1891; 1961, **82**, 117 (*synth*)
Debrauwer, J. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 167 (*isol, ms, pmr*)

p-Mentha-2,4(8)-dien-9,3-olide M-133

[80417-97-6]

[75640-26-5]
5,6-Dihydro-3,6-dimethyl-2(4H)-benzofuranone, 9CI. Dehydromenthofurolactone. FEMA 3755



$C_{10}H_{12}O_2$ 164.204

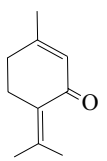
(±)-*form*
Liq. with hay and coumarin-like odour/flavour. Mp 30-32°. Bp_{24} 166-167°.

(ξ)-*form*
Flavouring ingredient.

Woodward, R.B. *et al., J.A.C.S.*, 1950, **72**, 399-403 (*synth*)
Yamamoto, M. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 2366-2370 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 153 (*use*)
Naf, R. *et al., Flavour Fragrance J.*, 1998, **13**, 203-208 (*isol*)
Adams, T.B. *et al., Food Chem. Toxicol.*, 1998, **36**, 249-278 (*tox*)

p-Mentha-1,4(8)-dien-3-one M-134

[491-09-8]
*3-Methyl-6-(1-methylethylidene)-2-cyclohexen-1-one, 9CI. 6-Isopropylidene-3-methyl-2-cyclohexenone. **Piperitenone**. Pulespenone. 3-Terpinolenone. FEMA 3560*



$C_{10}H_{14}O$ 150.22
Flavouring agent. Present in grapefruit juice lemon juice, orange juice, spearmint oil and peppermint oil. Oil. Bp 233° Bp_{14} 120-122°.

1,2-Epoxide: 1,2-Epoxy-*p*-menth-4(8)-en-3-one, E-170

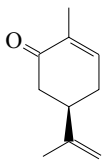
3-Alcohol: [6753-08-8] p-*Mentha-1,4(8)-dien-3-ol*. ***3-Terpinolenol***
$C_{10}H_{16}O$ 152.236

3-Alcohol, 4,8-epoxide: [263844-44-6] ***4,8-Epoxy*-p-*menth-1-en-3-ol***
$C_{10}H_{16}O_2$ 168.235
Oil. $[\alpha]_D^{20}$ -0.5 (c, 1.5 in $CHCl_3$).

Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1963, 681 (*isol*)
Nigam, M.C. *et al., Can. J. Chem.*, 1965, **43**, 521 (*isol*)
Beereboom, J.J. *et al., J.O.C.*, 1966, **31**, 2026 (*synth*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Naves, Y.R. *et al., Riv. Ital. Essenze, Profumi, Piante Off., Aromi, Saponi, Cosmet., Aerosol*, 1976, **58**, 136 (*rev*)
Tanowitz, B.D. *et al., J. Nat. Prod.*, 1984, **47**, 739 (*isol, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 442
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2229
Becker, H. *et al., Z. Naturforsch., C*, 1999, **54**, 997-1004 (*3-alcohol epoxide*)

p-Mentha-1,8-dien-6-one M-135

[99-49-0]
*2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one, 9CI. 5-Isopropenyl-2-methyl-2-cyclohexen-1-one. **Carvone, BSI**. Carvol (obsol.). Talent. FEMA 2249*



(*R*)-*form*

$C_{10}H_{14}O$ 150.22
Flavouring ingredient. Log P 2.01 (calc).
▶ LD_{50} (rat, orl) 1640 mg/kg. OS8575000

(*R*)-*form* [6485-40-1]
Constit. of spearmint (*Mentha crispa*) costmary, kuromoji and other oils. Flavouring ingredient. Oil. Bp 230-231°. $[\alpha]_D$ -62.46.
▶ LD_{50} (rat, orl) 1640 mg/kg. OS8650000

Oxime:
$C_{10}H_{15}NO$ 165.235
Cryst. (MeOH). Mp 72°. $[\alpha]_D^{18}$ -39.3 (EtOH).

(*S*)-*form* [2244-16-8]
Constit. of dill (*Anethum graveolens*) and caraway (*Carum carvi*) oils. Flavouring ingredient. Oil. Bp 230°. $[\alpha]_D^{20}$ +61.2.
▶ Skin irritant. OS8670000

Oxime:
Cryst. (MeOH). Mp 72°. $[\alpha]_D^{17}$ +39.5 (EtOH).

(±)-*form* [22327-39-5]
Flavouring ingredient. Constit. of gingergrass oil. Oil. Bp 231°.

Oxime:
Cryst. (MeOH). Mp 93-94°.

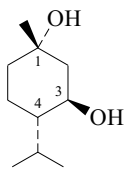
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 449C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 694A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 539C (*ir*)
Ronayne, J. *et al., J.A.C.S.*, 1966, **88**, 5288 (*pmr*)
Honwad, V.K. *et al., Indian J. Chem.*, 1967, **5**, 234 (*synth*)
Schevitz, R.W. *et al., Chem. Comm.*, 1969, 711 (*abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 557 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1057; 1978, **16**, 673 (*rev, tox*)

Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Oonk, H.A.J. *et al., Acta Cryst. B*, 1976, **32**, 500 (*cryst struct*)
Paris, M. *et al., Riv. Ital. Essenze, Profumi, Piante Off., Aromi, Saponi, Cosmet., Aerosol*, 1976, **58**, 473-476; *CA*, 1977, **86**, 21707b (*R-form, occur*)
Singaram, B. *et al., Perfum. Flavor.*, 1977, **2**, 47-51 (*synth, rev*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 673 (*rev, tox, S-form*)
Akhita, A. *et al., Phytochemistry*, 1980, **19**, 1433 (*biosynth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MCD379; MCD500
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1350; 1361; 1416
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 109 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 522 (*rev*)
Rani, K. *et al., Fitoterapia*, 1998, **69**, 337-348 (*biosynth*)
Bouwmeester, H.J. *et al., Phytochemistry*, 1999, **50**, 243-248 (*biosynth*)
Pesticide Manual, 12th edn., 2000, No. 122
McGeady, P. *et al., J. Nat. Prod.*, 2002, **65**, 953-955 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCM100; CCM120; MCD250

p-Menthane-1,3-diol M-136

[1612-98-2]

[10219-67-7, 17948-62-8, 42963-13-3, 42963-14-4, 42963-15-5, 107133-86-8]
1-Methyl-4-(1-methylethyl)-1,3-cyclohexanediol, 9CI. 4-Isopropyl-1-methyl-1,3-cyclohexanediol



(1*S*,3*R*,4*R*)-*form*

$C_{10}H_{20}O_2$ 172.267

(1*S*,3*R*,4*R*)-*form* [58342-65-7]
Isol. from peppermint oil. Mp 165°. $Bp_{1.5}$ 83-86°. $[\alpha]_D^{25}$ -34 (c, 0.9 in $CHCl_3$).

(1*S*,3*S*,4*R*)-*form* [58342-64-6]
$[\alpha]_D^{20}$ +18.8 (c, 0.48 in $CHCl_3$). n_D^{20} 1.4667.

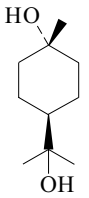
(1*S*,3*S*,4*S*)-*form* [107133-85-7]
Cryst. Mp 75°. $[\alpha]_D$ +31.3 (c, 0.46 in MeOH).

[10219-67-7, 17948-62-8, 42963-13-3, 42963-14-4, 42963-15-5]

Katsuhara, J. *et al., Kogyo Kagaku Zasshi*, 1966, **69**, 1170-1171; *CA*, **65**, 17006h (*isol, abs config*)
Paris, C. *et al., J. Chromatogr. Sci.*, 1972, **10**, 402-411 (*glc*)
Nagasawa, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 2083-2084 (*ir, pmr, ms*)
Sorochinskaya, E.I. *et al., Zh. Obshch. Khim.*, 1975, **45**, 2537-2546 (*synth*)
Gacs-Baitz, E. *et al., J. Chem. Res., Synop.*, 1985, 350 (*cmr*)

p-Menthane-1,8-diol, 8CI M-137

[80-53-5]
*4-Hydroxy-α,α,4-trimethylcyclohexanemethanol, 9CI. 4-(1-Hydroxy-1-methylethyl)-1-methylcyclohexanol. Dipenteneglycol. **Terpin, BAN**. Terpinol†*



(1*RS*,4*RS*)-*form*

$C_{10}H_{20}O_2$ 172.267Log P 1.03 (calc).
▶Flammable, fl. p. 43°.

(1*RS*,4*RS*)-*form* [565-48-0]
cis-*form*
Isol. from fruits of California peppertree (*Schinus molle*). Prisms or plates (EtOAc). Spar. sol. H_2O. Mp 104-105°. Bp 263-265°. Originally assigned the *trans*-config..

Monohydrate: [2451-01-6]

[16485-15-7]
Rhombic pyramids (H_2O). Mp 116-117°.

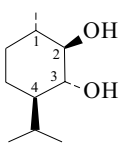
(1*RS*,4*SR*)-*form* [565-50-4] trans-*form*
Found in Chinese anise and sweet fennel oil. Mp 158-159°. Bp 258°. Hygroscopic, forms hydrate, Mp 123° (sealed tube), which loses H_2O at 70-80°. Originally assigned the *cis*-config..

Di-Ac:
Bp_{14} 145°.

Barnes, C.S. *et al., Aust. J. Chem.*, 1958, **11**, 134-146 (*config, bibl*)
Peyron, L. *et al., Bull. Soc. Chim. Fr.*, 1969, 339 (*isol*)
Pertoldi, M. *et al., CA*, 1970, **73**, 91168 (*isol*)
Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 914-917 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 2029
Hassan, M.M.A. *et al., Anal. Profiles Drug Subst.*, 1985, **14**, 273-323 (*rev, synth, pharmacol, anal*)
Ho, T.-I. *et al., Acta Cryst. C*, 1986, **42**, 1787-1789 (*cryst struct*)

p-Menthane-2,3-diol M-138

3-Methyl-6-(1-methylethyl)-1,2-cyclohexanediol. 3-Isopropyl-6-methyl-1,2-cyclohexanediol



(1*S*,2*R*,3*R*,4*R*)-*form*

$C_{10}H_{20}O_2$ 172.267

(1*S*,2*R*,3*R*,4*R*)-*form* [51745-19-8]
Oil. $[\alpha]_D$ +115.

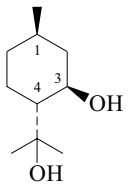
(1*R*,2*S*,3*S*,4*R*)-*form* [51745-21-2]
Isol. from peppermint oil. Oil. $[\alpha]_D$ +32.4.

Katsuhara, J. *et al., Kogyo Kagaku Zasshi*, 1966, **69**, 1170 (*isol*)
Seeman, J.I. *et al., J.O.C.*, 1974, **39**, 2444 (*synth*)

p-Menthane-3,8-diol, 8CI M-139

[42822-86-6]

[138663-70-4]
2-Hydroxy-α,α,4-trimethylcyclohexanemethanol, 9CI. Menthoglycol. Isopulegol hydrate. Cubebaol



(1*R*,3*R*,4*R*)-*form*

$C_{10}H_{20}O_2$ 172.267
Constit. of the roots of *Litsea cubeba* (mountain pepper).

(1*R*,3*R*,4*R*)-*form* [91739-72-9]
(-)-trans-*form*
Mp 67-70°. $[\alpha]_D^{20}$ -9.2 (c, 1 in $CHCl_3$).

(1*R*,3*S*,4*R*)-*form* [92471-23-3]
(+)-cis-*form*
Mp 62-65°. $[\alpha]_D^{20}$ +13.5 (c, 1 in $CHCl_3$).

(1*RS*,3*RS*,4*RS*)-*form* [3564-98-5]

[81176-88-7]
trans-*form*
Mp 60-61°.

▶OS9110000

(1*RS*,3*SR*,4*RS*)-*form* [3564-95-2]

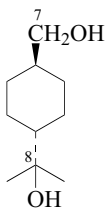
[81176-87-6]
cis-*form*
Mp 81-82.5°.

(1*SR*,3*RS*,4*SR*)-*form* [19956-48-0]
Mp 65-66°.

[91739-73-0, 107133-84-6, 140924-71-6]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 244C (*nmr*)
Barbier, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1897, **124**, 1309 (*synth*)
Grignard, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1928, **187**, 270-273 (*synth*)
Shishibori, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1170-1174 (*synth, ir*)
Chabudzinski, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1968, **42**, 283-287 (*synth*)
Nishimura, H. *et al., Agric. Biol. Chem.*, 1982, **46**, 319-320; 2601-2604 (*isol*)
Clark, B.C. *et al., J.O.C.*, 1984, **49**, 4557-4559 (*synth*)
Nishimura, H. *et al., Fragrance J.*, 1985, **13**, 160-162 (*rev, isol, props*)
Asakawa, Y. *et al., Phytochemistry*, 1988, **27**, 3861-3869 (*synth, ir, pmr, cmr*)
Chen, F. *et al., CA*, 1992, **116**, 67006p (*isol*)
Kočovský, P. *et al., J.O.C.*, 1999, **64**, 2765-2775 (*synth*)
Yuasa, Y. *et al., Org. Process Res. Dev.*, 2000, **4**, 159-161 (*isomers, synth, ir, pmr, cmr, ms*)

p-Menthane-7,8-diol M-140



$C_{10}H_{20}O_2$ 172.267

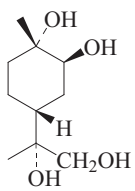
(1*RS*,4*RS*)-*form*
trans-*form*

7-O-*β*-D-*Glucopyranoside:* [217962-30-6]
$C_{16}H_{30}O_7$ 334.409
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{22}$ -23.1 (c, 0.8 in MeOH).

8-O-*β*-D-*Glucopyranoside:* [217962-31-7]
$C_{16}H_{30}O_7$ 334.409
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{22}$ +7.5 (c, 0.2 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1603-1606 (*isol, pmr, cmr*)

p-Menthane-1,2,8,9-tetrol M-141



(1*S*,2*S*,4*R*,8*R*)-*form*

$C_{10}H_{20}O_4$ 204.266

(1*S*,2*S*,4*R*,8*R*)-*form* [402593-46-8]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{22}$ +27 (c, 0.8 in MeOH).

2-O-*β*-D-*Glucopyranoside:* [402593-52-6]
$C_{16}H_{30}O_9$ 366.408
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{24}$ +17 (c, 0.7 in MeOH).

(1*S*,2*S*,4*R*,8*S*)-*form* [402593-45-7]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{22}$ +30 (c, 0.4 in MeOH).

2-O-*β*-D-*Glucopyranoside:* [402593-51-5]
Constit. of fruit of *Carum carvi* (caraway). Cryst. (MeOH). Mp 137-138°. $[\alpha]_D^{24}$ +22 (c, 1.3 in MeOH).

(1*R,2*R**,4*R**,8*S**)-*form*** [402593-49-1]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{21}$ -3 (c, 0.2 in MeOH).

9-O-*β*-D-*Glucopyranoside:* [402593-84-4]
$C_{16}H_{30}O_9$ 366.408
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{23}$ -15 (c, 0.2 in MeOH).

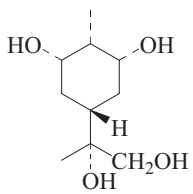
(1*R,2*R**,4*S**,8ξ)-*form*** [5581-31-7]
Amorph. powder. $[\alpha]_D^{23}$ -12 (c, 0.3 in MeOH).

(1*S,2*R**,4*R**,8*R**)-*form*** [402593-48-0]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{23}$ +26 (c, 0.1 in MeOH).

(1*S,2*R**,4*R**,8*S**)-*form*** [402593-47-9]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{23}$ +11 (c, 0.1 in MeOH).

Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1580-1582 (*Cnidium monnieri constit*)
Matsumura, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 66-72 (*Carum carvi constits*)

p-Menthane-2,6,8,9-tetrol M-142



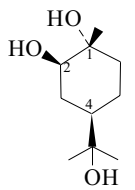
$C_{10}H_{20}O_4$ 204.266

(1α,2α,4β*H*,6α,8*R*)-*form* [402593-44-6]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{21}$ +4 (c, 1.6 in MeOH).

Matsumura, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 66-72 (*isol, pmr, cmr*)

p-Menthane-1,2,8-triol M-143

[58506-22-2]
4-(1-Hydroxy-1-methylethyl)-1-methyl-1,2-cyclohexanediol, 9CI



(1*R*,2*R*,4*R*)-*form*

$C_{10}H_{20}O_3$ 188.266

(1*R*,2*R*,4*R*)-*form* [93861-31-5]
Cryst. Mp 117°. $[\alpha]_D$ +2.5 (c, 0.42 in EtOH).

(1*R*,2*R*,4*S*)-*form* [103665-38-9]
Constit. of fruit of *Carum carvi* (caraway). Cryst. (MeOH). Mp 134-135°. $[\alpha]_D^{23}$ -25 (c, 0.2 in MeOH).

8-O-*β*-D-*Glucopyranoside:* [378254-09-2]
$C_{16}H_{30}O_8$ 350.408
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{23}$ -31 (c, 0.4 in MeOH).

(1*R*,2*S*,4*R*)-*form* [93861-32-6]
Cryst. ($CHCl_3$). Mp 141-143°. $[\alpha]_D$ +36.3 (c, 0.3 in EtOH).

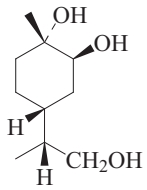
(1*S*,2*R*,4*R*)-*form* [93861-30-4]
Cryst. (CH_2Cl_2). Mp 81-82°. $[\alpha]_D$ +16.9 (c, 0.42 in EtOH).

(1*S*,2*S*,4*R*)-*form* [62014-81-7]
Cryst. ($CHCl_3$). Mp 141-142°. $[\alpha]_D$ +44.4 (c, 0.5 in EtOH).

[54145-82-3]

Carman, R.M. *et al., Aust. J. Chem.*, 1984, **37**, 2129 (*synth, bibl*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 584-588 (*1S,2S,4R-form, isol, pmr, cmr*)
Matsumara, T. *et al., Tetrahedron*, 2001, **57**, 8067-8074 (*isol, pmr, cmr*)

p-Menthane-1,2,9-triol M-144



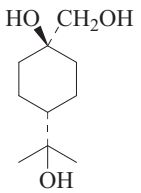
$C_{10}H_{20}O_3$ 188.266

(1*S*,2*S*,4*R*,8*R*)-*form* [378254-06-9]
Constit. of caraway fruits. Amorph. powder. $[\alpha]_D^{24}$ +25 (c, 0.2 in MeOH).

Matsumara, T. *et al., Tetrahedron*, 2001, **57**, 8067-8074 (*isol, pmr, cmr*)

p-Menthane-1,7,8-triol M-145

[145385-69-9]



(1*RS*,4*RS*)-*form*

$C_{10}H_{20}O_3$ 188.266
Prisms ($CHCl_3$). Mp 147-151°.

(1*RS*,4*RS*)-*form* [154843-72-8]
cis-*form*
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 137-139°.

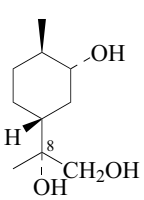
8-O-*β*-D-*Glucopyranoside:* [217962-29-3]
$C_{16}H_{30}O_8$ 350.408
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{22}$ -12.8 (c, 0.4 in MeOH).

(1*RS*,4*SR*)-*form* [154843-85-3]
trans-*form*
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 107-109°.

8-O-*β*-D-*Glucopyranoside:* [217962-28-2]
$C_{16}H_{30}O_8$ 350.408
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{22}$ -10 (c, 0.2 in MeOH).

Konda, Y. *et al., J. Nat. Prod.*, 1992, **55**, 1118 (*isol, pmr, cmr*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1603-1606 (*isol, pmr, cmr*)

p-Menthane-2,8,9-triol M-146



(1*R*,2*R*,4*R*,8*R*)-*form*

$C_{10}H_{20}O_3$ 188.266

(1*R*,2*R*,4*R*,8*R*)-*form* [212516-28-4]
Isol. from the fruiting body of *Flammulina velutipes* (velvet shank). $[\alpha]_D^{24}$ -5.3 (c, 2 in MeOH).

(1*R*,2*R*,4*R*,8*S*)-*form* [212516-26-2]

Isol. from the fruiting body of *Flammulina velutipes* (velvet shank). $[\alpha]_D^{24}$ -17 (c, 1 in MeOH).

(1*S*,2*R*,4*R*,8*R*)-*form* [378254-01-4]
Constit. of fruit of *Carum carvi* (caraway). Needles (MeOH). Mp 115-117°. $[\alpha]_D^{21}$ -35 (c, 0.4 in MeOH).

(1*S*,2*R*,4*R*,8*S*)-*form* [378254-00-3]
Constit. of fruit of *Carum carvi* (caraway). Cryst. (MeOH). Mp 119-122°. $[\alpha]_D^{25}$ -31 (c, 3.1 in MeOH).

2-O-β-D-Glucopyranoside: [378254-07-0]
$C_{16}H_{30}O_8$ 350.408
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{25}$ -46 (c, 1.8 in MeOH).

9-O-β-D-Glucopyranoside: [378254-08-1]
$C_{16}H_{30}O_8$ 350.408
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{21}$ -35 (c, 0.2 in MeOH).

(1*S*,2*S*,4*S*,8*R*)-*form* [378253-98-6]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{21}$ +14 (c, 0.2 in MeOH).

(1*S*,2*S*,4*S*,8*S*)-*form* [378253-99-7]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{21}$ +8 (c, 0.2 in MeOH).

(1*R,2*S**,4*R**,8*R**)-*form*** [378254-03-6]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{21}$ -30 (c, 0.4 in MeOH).

(1*R,2*S**,4*R**,8*S**)-*form*** [378254-02-5]
Constit. of fruit of *Carum carvi* (caraway). Needles (MeOH). Mp 123-126°. $[\alpha]_D^{21}$ -22 (c, 0.2 in MeOH).

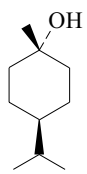
(1*S,2*S**,4*R**,8*R**)-*form*** [378254-05-8]
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{21}$ -13 (c, 0.1 in MeOH).

(1*S,2*S**,4*R**,8*S**)-*form*** [378254-04-7]
Constit. of fruit of *Carum carvi* (caraway). Needles (MeOH). Mp 130-133°. $[\alpha]_D^{21}$ -7 (c, 0.3 in MeOH).

Hirai, Y. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1364-1368 (*isol, synth, cd, ir, pmr, cmr, ms*)
Matsumara, T. *et al., Tetrahedron*, 2001, **57**, 8067-8074 (*isol, pmr, cmr*)

p-Menthan-1-ol M-147

[21129-27-1]
1-Methyl-4-(1-methylethyl)cyclohexanol, 9CI. 4-Isopropyl-1-methylcyclohexanol. Dihydro-β-terpineol



(1*RS*,4*RS*)-*form*

$C_{10}H_{20}O$ 156.267
Isol. from spearmint oil.

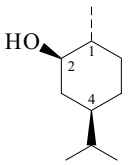
(1*RS*,4*RS*)-*form* [3901-95-9]
cis-*form*
Needles. Mp 41-43°.

(1*RS*,4*SR*)-*form* [3901-93-7]
trans-*form*
Bp_5 74°. n_D^{20} 1.4595.

Chabudzinski, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1963, **37**, 1571 (*synth*)
Tsukamoto, Y. *et al., Agric. Biol. Chem.*, 1975, **39**, 617 (*synth*)

p-Menthan-2-ol M-148

[60320-28-7]
2-Methyl-5-(1-methylethyl)cyclohexanol. 5-Isopropyl-2-methylcyclohexanol



(1*R*,2*R*,4*R*)-*form*

$C_{10}H_{20}O$ 156.267

(1*R*,2*R*,4*R*)-*form* [3858-43-3]
(-)-Carvomenthol
Oil. $[\alpha]_D^{20}$ -24.2.

3,5-Dinitrobenzoyl:
Cryst. (petrol). Mp 106-107°. $[\alpha]_D$ -52.1 (c, 2 in $CHCl_3$).

(1*R*,2*R*,4*S*)-*form* [1126-39-2] ***(-)-Isocarvomenthol***
Oil. Bp_{17} 106°. $[\alpha]_D^{16}$ -17.72.

3,5-Dinitrobenzoyl:
Yellow cryst. Mp 111°. $[\alpha]_D$ -26.7.

(1*R*,2*S*,4*R*)-*form* [3858-49-9] ***(+)-Neocarvomenthol***
Oil. $[\alpha]_D^{20}$ +37.5.

3,5-Dinitrobenzoyl:
Cryst. (petrol). Mp 128-129°. $[\alpha]_D$ +23 (c, 1.6 in $CHCl_3$).

(1*R*,2*S*,4*S*)-*form* [1126-41-6] ***(-)-Neoisocarvomenthol***
Oil. $[\alpha]_D^{17}$ -34.7.

3,5-Dinitrobenzoyl:
Yellow cryst. Mp 71-72°. $[\alpha]_D$ -16.

(1*S*,2*R*,4*R*)-*form* [3858-45-5]
[20752-34-5] ***(+)-Neoisocarvomenthol***
Oil. $[\alpha]_D^{17}$ +34.7.

3,5-Dinitrobenzoyl:
Cryst. Mp 102°. $[\alpha]_D$ -9 ($CHCl_3$).

(1*S*,2*R*,4*S*)-*form* [5563-78-0] ***(-)-Neocarvomenthol***
Oil. Bp_{18} 102°. $[\alpha]_D^{21}$ -41.7.

3,5-Dinitrobenzoyl:
Cryst. Mp 129°. $[\alpha]_D^{20}$ -22 ($CHCl_3$).

(1*S*,2*S*,4*R*)-*form* [3858-47-7] ***(+)-Isocarvomenthol***
Oil. $[\alpha]_D^{20}$ +19.3.

3,5-Dinitrobenzoyl:
Cryst. (petrol). Mp 110°. $[\alpha]_D$ +26 ($CHCl_3$).

(1*S*,2*S*,4*S*)-*form* [1845-59-6] ***(+)-Carvomenthol***
Oil. Bp_{14} 101.8-102°. $[\alpha]_D^{13}$ +27.69.

3,5-Dinitrobenzoyl:
Cryst. (EtOH/EtOAc). Mp 107°. $[\alpha]_D^{13}$ +52.8 ($CHCl_3$).

(1*RS*,2*RS*,3*RS*)-*form* [499-69-4] *(±)-Carvomenthol*
Flavouring ingredient.

(1*RS*,2*SR*,4*RS*)-*form* [1126-40-5] *(±)-Neocarvomenthol*
Oil. n_D^{20} 1.4637.

3,5-Dinitrobenzoyl:
Leaflets (EtOH). Mp 101°.

(1*RS*,2*RS*,4*SR*)-*form* [3127-80-8] *(±)-Isocarvomenthol*
Bp_{20} 110°. n_D^{18} 1.4669.

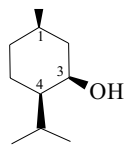
3,5-Dinitrobenzoyl:
Yellow prisms. Mp 85.5°.

[42846-32-2]

Abe, H. *et al., Phytochemistry*, 1971, **10**, 3330-3331 (*Carvomenthol, isol*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 1691-1694 (*synth*)
Noma, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1637-1642 (*synth*)
Brown, H.C. *et al., Tetrahedron*, 1975, **31**, 925-928 (*synth*)
Kartha, G. *et al., J.C.S. Perkin 2*, 1976, 717-723 (*cryst struct, pmr*)
Dauzonne, D. *et al., Org. Magn. Reson.*, 1981, **17**, 18-25 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 522

p-Menthan-3-ol M-149

[1490-04-6]
5-Methyl-2-(1-methylethyl)cyclohexanol. 2-Isopropyl-5-methylcyclohexanol



(1*R*,3*R*,4*R*)-*form*

$C_{10}H_{20}O$ 156.267
Found in many essential oils. Log P 3.23 (calc).
▶ GW0554000

(1*R*,3*R*,4*R*)-*form* [20752-34-5]
(+)-Neoisomenthol
Oil. Mp -8°. Bp 214.6°. $[\alpha]_D^{18}$ +3.8 (c, 6 in EtOH).

(1*R*,3*R*,4*S*)-*form* [2216-51-5]
(-)-Menthol. *Levomenthol, BAN, INN. Menthacamphor. Peppermint camphor. FEMA 2665*
Present in large amts. in peppermint oil (*Mentha piperita*), also in other *Mentha* spp.. Used in confectionery and perfumery. Flavouring agent. Cryst. (MeOH) with strong peppermint odour. Sl. sol. H_2O; v. sol. org. solvs. Mp 42.5-43°. Bp 216°. $[\alpha]_D^{20}$ -50 (c, 2 in $CHCl_3$). Log P 3.23 (calc). Exists in four cryst. modifications; Mp given is the highest. Component of Larylgan.
▶ Can cause hypersensitivity reactions and contact dermatitis. Gastrointestinal and CNS effects by ingestion. LD_{50} (rat, orl) 3300 mg/kg. OT0700000

Ac: [2623-23-6]

[89-48-5]
$C_{12}H_{22}O_2$ 198.305
Bp 228-230°. $[\alpha]_D^{20}$ -80 (c, 8 in C_6H_6).
▶ AI5900000

Chloroformyl: [7635-54-3] *Menthyl chloroformate*
$C_{11}H_{19}ClO_2$ 218.723

Chloromethyl ether: [26127-08-2]
$C_{11}H_{21}ClO$ 204.739
$Bp_{0.4}$ 72-74°. $[\alpha]_D^{25}$ -187.8 (c, 1.2 in CH_2Cl_2).

3-Methylbutanoyl: [16409-46-4] *Menthyl*

isovalerate. Validol. FEMA 2669
$C_{15}H_{28}O_2$ 240.385
Flavouring ingredient with a bitter, wood-like taste. Oil. Bp_{22} 140-146°.

2-Hydroxypropanoyl: [59259-38-0]
Menthyl lactate. FEMA 3748
$C_{13}H_{24}O_3$ 228.331
Flavouring ingredient. Cryst. Mp 38-40°.

4-Methylbenzenesulfonyl: [2230-82-2]
Menthyl tosylate
Cryst. Mp 92-93°. $[\alpha]_D^{20}$ -68.4 (c, 0.99 in $CHCl_3$).

(1*R*,3*S*,4*R*)-*form* [23283-97-8]

[15356-70-4] *(+)-Isomenthol*
Cryst. (MeOH). Mp 82.5°. Bp 218°. $[\alpha]_D^{20}$ +25.9 (c, 1.56 in $CHCl_3$).

Chloromethyl ether: [103128-76-3]
$C_{11}H_{21}ClO$ 204.739
$Bp_{0.4}$ 72-74°. $[\alpha]_D^{25}$ +187.8 (c, 1.2 in CH_2Cl_2) (96% ee).

(1*R*,3*S*,4*S*)-*form* [2216-52-6]

[490-99-3] *(+)-Neomenthol. FEMA 2666*
Constit. of Japanese peppermint oil. Flavouring ingredient. Oil. Mp -22°. Bp_{14} 83-84°. $[\alpha]_D^{10}$ +18.02 (neat).

(1*S*,3*R*,4*R*)-*form* [20747-49-3]

[490-99-3] *(-)-Neomenthol*
Oil. Bp_{10} 97.6°. $[\alpha]_D^{17}$ -20.7 (EtOH).

(1*S*,3*R*,4*S*)-*form* [20752-33-4]

[15356-70-4] *(-)-Isomenthol*
Cryst. (MeOH). Mp 82.5°.

(1*S*,3*S*,4*R*)-*form* [15356-60-2]

[1490-04-6] *(+)-Menthol*
Cryst. (MeOH). Mp 38-40°. $[\alpha]_D$ +48.3 (EtOH).

► OT0525000

(1*S*,3*S*,4*S*)-*form (-)-Neoisomenthol*
Isol. from geranium bourbon oil (*Pelargonium roseum*).

(1*RS*,3*RS*,4*RS*)-*form*

[491-02-1] *(±)-Neoisomenthol*
Mp 14°. Bp_6 81°. n_D^{17} 1.4676.

(1*RS*,3*RS*,4*SR*)-*form* [15356-20-4]

[89-78-1, 1490-04-6] *(±)-Menthol. Racementhol, BAN, INN*
Flavouring agent. Needles (petrol). Mp 34°. Bp 216°.

Ac: [29066-34-0]

[89-48-5]
Component of peppermint oil. Mp 228-229°. n_D^{20} 1.4470.

2-Aminobenzoyl: [134-09-8] ***Meradimate, USAN***. p-*Menth-3-yl anthranilate*
$C_{17}H_{25}NO_2$ 275.39
Mp 63-64°. $Bp_{0.33}$ 156°.

(1*RS*,3*SR*,4*RS*)-*form*

[3623-52-7, 15356-70-4] *(±)-Isomenthol*
Needles. Mp 53-54°. Bp 218.5-218.6°.

(1*RS*,3*SR*,4*SR*)-*form*

[490-99-3, 3623-51-6] *(±)-Neomenthol*
Plates (petrol). Mp 51°. Bp_{163} 212°.

[491-01-0, 16409-45-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 163A; 163B; 163C; 164A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 239B; 239C; 240B; 240C; 1207A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 239A; 239B; 239C; 239D; 240A (*ir*)
Rule, H.G. *et al., J.C.S.*, 1929, 401-409 (*meradimate, synth*)
U.S. Pat., 1939, 2 170 185, (*Givaudan-Delawanna*); *CA*, **34**, 226[8] (*meradimate, synth, use*)
Vitt, S.V. *et al., Tet. Lett.*, 1965, 2575 (*use*)
Katsuhara, J. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 617 (*synth, menthol*)
Hashimoto, A. *et al., Agric. Biol. Chem.*, 1970, **34**, 1843 (*synth, isomenthol*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 1695 (*synth, neoisomenthol*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Leffingwell, J.C. *et al., Cosmet. Perfum.*, 1974, **89**, 69 (*rev*)
Hasegawa, M. *et al., Anal. Biochem.*, 1975, **63**, 308 (*use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 471; 473 (*rev, tox, menthol*)
Yamaguchi, S. *et al., Tet. Lett.*, 1977, 89 (*abs config*)
Nakatani, Y. *et al., Synthesis*, 1978, 147 (*synth*)
Dauzonne, D. *et al., Org. Magn. Reson.*, 1981, **17**, 18 (*cmr*)
Tani, K. *et al., J.A.C.S.*, 1984, **106**, 5208 (*synth*)
Sardin, M. *et al., CA*, 1985, **103**, 162168h (*Ac*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 304-305
Kotha, S. *et al., Tetrahedron*, 1994, **50**, 3639 (*manuf*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 447; 450-451 (*esters*)
U.S. Pat., 1995, 5 445 815; *CA*, **123**, 237538c (*meradimate, use*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 343 (*bibl, synth*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1724
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1679-1684 (*esters*)
Hartung, J. *et al., Synthesis*, 1997, 1433-1438 (*tosylate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCF750; MCG000; MCG250; MCG750

p-Menthan-4-ol M-150

[470-65-5]
4-Methyl-1-(1-methylethyl)cyclohexanol. 1-Isopropyl-4-methylcyclohexanol



(1*RS*,4*RS*)-*form*

$C_{10}H_{20}O$ 156.267
Present in turpentine from *Pinus sylvestris* (Scotch pine).

(1*RS*,4*RS*)-*form* [3239-02-9]
cis-*form*
Cryst. Mp 52-53°.

Phenylurethane:
Cryst. Mp 131-141°.

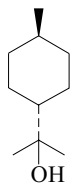
(1*RS*,4*SR*)-*form* [3239-03-0] trans-*form*
Oil.

Phenylurethane:
Cryst. Mp 99-100°.

Bowman, R.M. *et al., J.C.S.(C)*, 1966, 612 (*synth*)
Murphy, R. *et al., Aust. J. Chem.*, 1976, **29**, 617 (*synth*)

p-Menthan-8-ol M-151

[498-81-7]
α,α,4-Trimethylcyclohexanemethanol, 9CI. 1-(1-Hydroxy-1-methylethyl)-4-methylcyclohexane. ***Menthanol****. Dihydro-α-terpineol*



(1*RS*,4*RS*)-*form*

$C_{10}H_{20}O$ 156.267
Present in lemon and spearmint oils.

► Skin irritant. LD_{50} (rat, orl) >5000 mg/kg. OS9539000

Ac: [80-25-1] *Menthanyl acetate*
$C_{12}H_{22}O_2$ 198.305
Liq. d 0.94. Bp_{16} 104°. Props. presumably refer to an undefined mixt. of stereoisomers.

(1*RS*,4*RS*)-*form* [29789-01-3]
trans-*form*
Plates or needles with floral odour. Mp 35°. $Bp_{1.5}$ 63-65°.

Phenylurethane:
Long needles (petrol). Mp 115°.

4-Nitrobenzoyl:
Cryst. (EtOH/EtOAc). Mp 98.5-99.5°.

(1*RS*,4*SR*)-*form* cis-*form*
Mp 46-47° (25°). Bp_{30} 110°.

Phenylurethane:
Short needles. Mp 114°.

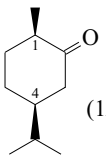
4-Nitrobenzoyl:
Cryst. (EtOH/EtOAc). Mp 88-88.5°.

[29789-01-3]

Perkin, W.H. *et al., J.C.S.*, 1905, **87**, 639 (*synth*)
Behal, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1910, **150**, 1763 (*Ac*)
Zeitschel, O. *et al., Ber.*, 1927, **60**, 1372 (*isol, synth*)
Keats, G.H. *et al., J.C.S.*, 1937, 2003 (*synth*)
Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 1505 (*synth*)
Von Rudloff, E. *et al., Can. J. Chem.*, 1963, **41**, 1; 2615 (*isol, synth, glc*)
Gollnick, K. *et al., Tetrahedron*, 1966, **22**, 123 (*synth, struct, ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 529 (*rev, use, tox*)
Carman, R.M. *et al., Aust. J. Chem.*, 1976, **29**, 133 (*synth, pmr*)
Simpson, R.F. *et al., Phytochemistry*, 1976, **15**, 328 (*isol*)
Hugel, H.M. *et al., Aust. J. Chem.*, 1977, **30**, 1287 (*synth*)
Dauzonne, D. *et al., Org. Magn. Reson.*, 1981, **17**, 18 (*cmr*)
Bazyl'chik, V.V. *et al., J. Chromatogr.*, 1982, **248**, 321 (*pmr, glc*)

p-Menthan-2-one M-152

[59471-80-6]
2-Methyl-5-(1-methylethyl)cyclohexanone. 5-Isopropyl-2-methylcyclohexanone. FEMA 3176



(1*R*,4*S*)-*form*

$C_{10}H_{18}O$ 154.252
Flavouring ingredient.

(1*R*,4*S*)-*form* [13163-74-1]
(-)-Isocarvomenthone
Oil. Bp 220-221°. $[\alpha]_D^{20}$ -1.4 ($CHCl_3$).

Semicarbazone:
Cryst. (petrol). Mp 105°.

(1*S*,4*S*)-*form* [13163-73-0] ***(-)-Carvomenthone***
Isol. from oils of *Tanacetum vulgare* (tansy). Oil. Bp 220°. $[\alpha]_D^{19}$ -27.95 (MeOH).

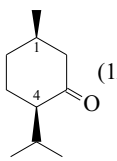
Semicarbazone:
Cryst. (EtOH). Mp 193°.

[499-70-7, 3901-91-5, 5206-83-7, 7065-48-7, 116562-19-7]

Simonson, J.L. *et al., J.C.S.*, 1922, 876 (*isol*)
Willhalm, B. *et al., J.C.S.*, 1965, 6478 (*ms*)
Barieux, J.-J. *et al., Bull. Soc. Chim. Fr.*, 1971, 3978 (*synth*)
Fringuelli, F. *et al., J.C.S.(C)*, 1971, 297 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 443
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1673-1674

p-Menthan-3-one M-153

[10458-14-7]
5-Methyl-2-(1-methylethyl)cyclohexanone. 2-Isopropyl-5-methylcyclohexanone



(1*R*,4*R*)-*form*

$C_{10}H_{18}O$ 154.252
► Skin irritant. LD_{50} (rat, orl) 2180 mg/kg.

(1*R*,4*R*)-*form* [1196-31-2]
(+)-Isomenthone
Found in American pennyroyal oil (*Hedeoma pulegioides*), *Mentha arvensis, Pelargonium tomentosum* and other essential oils. Oil. Bp 212°. $[\alpha]_D$ +95. $[\alpha]_D^{20}$ +73.68 (c, 0.855 in MeOH). n_D^{20} 1.4530.

Semicarbazone:
Cryst. Mp 264°.

(1*R*,4*S*)-*form* [14073-97-3] ***(-)-Menthone***
Occurs with menthol in many essential oils including peppermint and geranium oils. Used in flavour compositions. Liq. with peppermint odour. Sol. MeOH, hexane; poorly sol. H_2O, hexane. Mp -6°. Bp 207°. $[\alpha]_D^{20}$ -24.8. n_D^{23} 1.4490.

Semicarbazone:
Cryst. (EtOH). Mp 185-187°. $[\alpha]_D$ -64 (chloral hydrate).

(1*S*,4*R*)-*form* [3391-87-5] ***(+)-Menthone***
Found in some essential oils, e.g. those of *Barosma pulchellum, Mentha sachalinensis*. Oil. Bp 204°. $[\alpha]_D^{18}$ +24.85.

Semicarbazone:
Cryst. (EtOH). Mp 187-189°.

(1*S*,4*S*)-*form* [18309-28-9] ***(-)-Isomenthone***
Isol. from oils of *Mentha arvensis, Mentha pulegium, Hedeoma pulegioides* and others. Bp_7 79-80°. $[\alpha]_D^{20}$ -94.3.

(1*RS*,4*RS*)-*form* [36977-92-1]

[491-07-6] *(±)*-cis-*form. (±)-Isomenthone. Thymomenthone. FEMA 3460*
Flavouring ingredient. Spar. sol. H_2O. d_4^{19} 0.9. Bp 210° Bp_{20} 99.5-100°. n_D^{19} 1.4528.

Oxime:
$C_{10}H_{19}NO$ 169.266
Needles (EtOH). Mp 80°.

2,4-Dinitrophenylhydrazone:
Yellow leaflets or needles. Mp 145°.

(1*RS*,4*SR*)-*form* [1074-95-9]

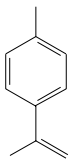
[89-80-5] ***(±)-Menthone***
Bp_{10} 82-83°. n_D^{20} 1.4508.

2,4-Dinitrophenylhydrazone:
Mp 141-142°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 436A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 672A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 521C (*ir*)
Barney, A.L. *et al., Ind. Eng. Chem.*, 1944, **36**, 85-87 (*(±)-Menthone, synth*)
Brown, H.C. *et al., J.A.C.S.*, 1961, **83**, 2952-2953 (*synth*)
Wellman, K.M. *et al., J.A.C.S.*, 1965, **87**, 66-72 (*1R,4S-form, cd*)
Willhalm, B. *et al., J.C.S.*, 1965, 6478-6485 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 545; 546 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037-1062 (*ir*)
Hibino, K. *et al., Tet. Lett.*, 1974, 1295-1298 (*1S,4R-form*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 315 (*rev, tox, Isomenthone*)
Liang, L.Y. *et al., Agric. Biol. Chem.*, 1989, **53**, 2517-2518 (*(+)-Isomenthone, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 405
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1475-1476
Eisenreich, W. *et al., Tet. Lett.*, 1997, **38**, 3889-3892 (*biosynth*)
Sagner, S. *et al., Chem. Comm.*, 1998, 221-222 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IKY000; MCE250; MCG275

p-Mentha-1,3,5,8-tetraene M-154

[1195-32-0]
1-Methyl-4-(1-methylethenyl)benzene, 9CI. p,α-*Dimethylstyrene, 8CI. 1-Methyl-4-isopropenylbenzene.* p-*Isopropenyltoluene. 2-(4-Methylphenyl)propene.* p-*Cymenene. FEMA 3144*



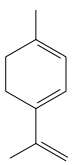
$C_{10}H_{12}$ 132.205
Occurs in *Chamaecyparis*, *Citrus*, *Eucalyptus*, *Juniperus* and *Ribes* spp. oils and juices. Flavouring ingredient. Mp -20°. Bp 184-185°.

Nitrosochloride:
Cryst. (MeOH). Mp 100-102°.

Perkin, W.H. *et al., J.C.S.*, 1905, **87**, 639-655 (*synth*)
Tiffeneau, M. *et al., Ann. Chim. (Paris)*, 1907, **10**, 193-198 (*synth*)
Birch, S.F. *et al., J.A.C.S.*, 1949, **71**, 1362-1369 (*synth*)
Attaway, J.A. *et al., Phytochemistry*, 1966, **5**, 1273-1279 (*isol*)

p-Mentha-1,3,8-triene M-155

[18368-95-1]
1-Methyl-4-(1-methylethenyl)-1,3-cyclohexadiene, 9CI. 1-Isopropenyl-4-methyl-1,3-cyclohexadiene

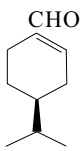


$C_{10}H_{14}$ 134.221
Isol. from *Petroselinum sativum* (Yugoslavian parsley). Bp_5 65°. n_D^{20} 1.5395.

Garnero, J. *et al., Bull. Soc. Chim. Fr.*, 1967, 4679 (*isol*)
Birch, A.J. *et al., Aust. J. Chem.*, 1969, **22**, 2037 (*synth*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1970, **53**, 770 (*synth*)

p-Menth-1-en-7-al M-156

[21391-98-0]
4-(1-Methylethyl)-1-cyclohexene-1-carboxaldehyde. 4-Isopropyl-1-cyclohexene-1-carboxaldehyde. ***Phellandral***



$C_{10}H_{16}O$ 152.236

(*S*)-*form*
Constit. of *Anethum sowa* (Indian dill). Oil. Bp 220-230°. $[\alpha]_D$ -139 ($CHCl_3$).

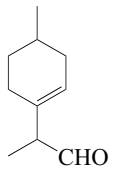
Semicarbazone:
Cryst. (MeOH). Mp 204-205°.

[536-58-3, 23963-70-4]

Frank, R.L. *et al., J.A.C.S.*, 1949, **71**, 3889 (*synth*)
Gillespie, D.T.C. *et al., J.C.S.*, 1955, 665
Stadler, P.A. *et al., Helv. Chim. Acta*, 1960, **43**, 1601 (*isol*)

p-Menth-3-en-9-al M-157

[71855-42-0]
α,4-Dimethyl-1-cyclohexene-1-acetaldehyde, 9CI

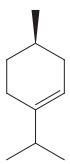


$C_{10}H_{16}O$ 152.236
Constit. of Spanish oregano (*Coridothymus capitatus*), *Origanum* spp. and blackberries.

Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 89-92 (*isol*)
Georgilopoulos, D.N. *et al., Food Chem.*, 1988, **28**, 141 (*isol*)

p-Menth-3-ene M-158

[500-00-5]
4-Methyl-1-(1-methylethyl)cyclohexene. 1-Isopropyl-4-methylcyclohexene. Menthomenthene



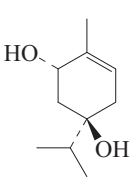
(*R*)-*form*

$C_{10}H_{18}$ 138.252
► LD_{50} (rat, orl) 21000 mg/kg. OS9800000
(*R*)-*form* [619-52-3]
Oil. Bp 168°. $[\alpha]_D$ +116.74.
(±)-*form*
Bp_{14} 55°.
(ξ)-*form*
Isol. from thyme and peppermint oil.

[22564-83-6]

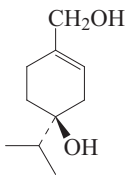
Thomas, A.F. *et al., Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Rodd's Chem. Carbon Compd. (2nd edn.), 1967, **2B**, 219 (*bibl*)
Sakota, N. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 485
Hutchins, R.O. *et al., J.O.C.*, 1975, **40**, 923 (*synth*)
Posner, G.H. *et al., J.O.C.*, 1976, **41**, 578 (*synth*)
Brieger, G. *et al., J.O.C.*, 1979, **44**, 1340 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCE500

p-Menth-1-ene-4,6-diol M-159



$C_{10}H_{18}O_2$ 170.251
(4*R*,6*S*)-*form* [360042-68-8]
Amorph. powder. $[\alpha]_D^{21}$ -20 (c, 0.2 in MeOH).
4-O-*β*-D-*Glucopyranoside:* [359875-78-8]
$C_{16}H_{28}O_7$ 332.393
Constit. of fruit of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{24}$ -29 (c, 1.8 in MeOH).
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*isol, pmr, cmr*)

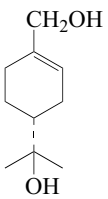
p-Menth-1-ene-4,7-diol M-160



$C_{10}H_{18}O_2$ 170.251
(*S*)-*form* [359875-83-5]
Amorph. powder. $[\alpha]_D^{21}$ +18 (c, 0.3 in MeOH).
4-O-*β*-D-*Glucopyranoside:* [359875-77-7]
$C_{16}H_{28}O_7$ 332.393
Constit. of fruit of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{24}$ -15 (c, 0.5 in MeOH).
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*isol, pmr, cmr*)

p-Menth-1-ene-7,8-diol M-161

[19894-91-8]
7-Hydroxyterpineol

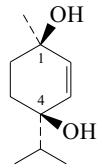


(*R*)-*form*

$C_{10}H_{18}O_2$ 170.251
(*R*)-*form*
8-O-*β*-D-*Glucopyranoside:* [217962-32-8]
$C_{16}H_{28}O_7$ 332.393
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{22}$ +7.5 (c, 0.2 in MeOH).
8-O-*[β*-D-*Apiofuranosyl-(1→6)-β*-D-*glucopyranoside]:* [217969-33-0]
$C_{21}H_{36}O_{11}$ 464.509
Amorph. powder. $[\alpha]_D^{22}$ -22.8 (c, 0.4 in MeOH).
(*S*)-*form*
Mp 130°. $[\alpha]_D^{23}$ -163.4 (EtOH).
8-O-*β*-D-*Glucopyranoside:* [231277-28-4]
Amorph. powder. $[\alpha]_D^{25}$ -50 (c, 1.9 in MeOH).
8-O-*[β*-D-*Apiofuranosyl-(1→6)-β*-D-*glucopyranoside]:*
Amorph. powder. $[\alpha]_D^{22}$ -35.7 (c, 0.5 in MeOH).
Sato, T. *et al., Nippon Kagaku Zasshi*, 1965, **86**, 252; 1967, **88**, 1005 (*synth*)
Tan, R.X. *et al., Phytochemistry*, 1991, **30**, 583 (*isol, pmr, cmr*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1595-1598; 1999, **47**, 639-642 (*glycosides*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1603-1606 (*glucoside*)

p-Menth-2-ene-1,4-diol M-162

[40735-19-1]
1-Methyl-4-(1-methylethyl)-2-cyclohexene-1,4-diol. 1-Isopropyl-4-methyl-2-cyclohexene-1,4-diol



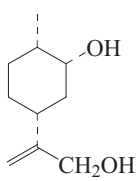
(1*RS*,4*RS*)-*form*

$C_{10}H_{18}O_2$ 170.251
(1*RS*,4*RS*)-*form*
cis-*form*
Mp 80°.
(1*RS*,4*SR*)-*form* [21473-37-0]

[10219-66-6]
trans-*form*
Isol. from peppermint oil and *Chenopodium ambroisioides*. Cryst. (Et_2O/hexane). Mp 101°. $Bp_{1.5}$ 75-77°. $[\alpha]_D^{24}$ -1.2 (c, 0.1 in MeOH). $[\alpha]_D^{25}$ -2.6 (c, 0.13 in $CHCl_3$).

Schenck, G.O. *et al., Annalen*, 1964, **674**, 93 (*synth*)
Katsuhara, J. *et al., Kogyo Kagaku Zasshi*, 1966, **69**, 1170 (*isol*)
Pierson, G.O. *et al., J.O.C.*, 1969, **34**, 3654 (*synth*)
Ahmed, A.A. *et al., J. Nat. Prod.*, 2000, **63**, 989-991 (*isol, pmr, cmr*)

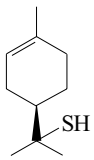
p-Menth-8-ene-2,10-diol M-163



$C_{10}H_{18}O_2$ 170.251
(1*S*,2*R*,4*R*)-*form* [402593-55-9]
Amorph. powder. $[\alpha]_D^{22}$ -11 (c, 0.3 in MeOH).
2-O-*β*-D-*Glucopyranoside:* [402593-53-7]
$C_{16}H_{28}O_7$ 332.393
Constit. of fruit of *Carum carvi* (caraway). Amorph. powder. $[\alpha]_D^{25}$ -26 (c, 0.9 in MeOH).
Matsumura, T. *et al., Chem. Pharm. Bull.*, 2002, **50**, 66-72 (*isol, pmr, cmr*)

p-Menth-1-ene-8-thiol M-164

[71159-90-5]
*α,α,4-Trimethyl-3-cyclohexene-1-methanethiol, 9CI. 4-(1-Mercapto-1-methylethyl)-1-methylcyclohexene. 8-Mercapto-*p*-menth-1-ene. FEMA 3700*



(*R*)-*form*

$C_{10}H_{18}S$ 170.318
Powerful flavour constit. of grapefruit juice detectable at 10^{-4} ppb (equiv. to 10^{-4} mg per ton of water). Opt. activity of natural enantiomer not known.

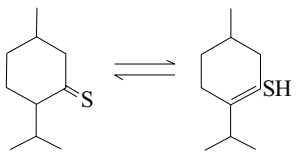
(*R*)-*form* [83150-78-1]
Oil. $[\alpha]_D^{20}$ +79.8 (c, 1.44 in $CHCl_3$) (Value corrected to 100% op is +82).

(*S*)-*form* [83150-77-0]
Oil. $[\alpha]_D^{20}$ -63.9 (c, 0.91 in $CHCl_3$).

Demole, E. *et al., Helv. Chim. Acta*, 1982, **65**, 1785 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 445 (*rev*)

p-Menth-3-ene-3-thiol, 8CI M-165

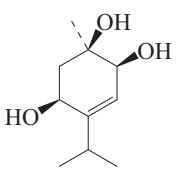
[25946-28-5]
5-Methyl-2-(1-methylethyl)cyclohexanethione, 9CI. 2-Isopropyl-5-methylcyclohexanethione. Thiomenthone



$C_{10}H_{18}S$ 170.318
Flavouring ingredient. Intensely red liq. with strong smell. Bp_{763} 215-216°. Dec. on standing, evolving H_2S.

Paquer, D. *et al., Bull. Soc. Chim. Fr.*, 1969, 3595-3601 (*synth*)
Paquer, D. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1981, **100**, 52-58 (*ms*)

p-Menth-3-ene-1,2,5-triol M-166

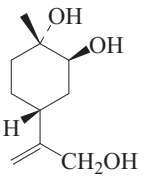


$C_{10}H_{18}O_3$ 186.25

(1β,2β,5β)-*form* [359875-80-2]
Constit. of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{22}$ +53 (c, 0.2 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*isol, pmr, cmr*)

p-Menth-8-ene-1,2,10-triol M-167



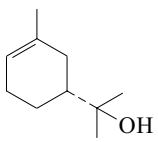
$C_{10}H_{18}O_3$ 186.25

(1*S*,2*S*,4*R*)-*form*
2-O-β-D-Glucopyranoside: [378254-11-6]
$C_{16}H_{28}O_8$ 348.392
Isol. from caraway fruit. Amorph. powder. $[\alpha]_D^{23}$ +7 (c, 0.1 in MeOH).

Matsumara, T. *et al., Tetrahedron*, 2001, **57**, 8067-8074 (*isol, pmr, cmr*)

m-Menth-1(6)-en-8-ol M-168

[29545-90-2]
α,α,3-Trimethyl-3-cyclohexene-1-methanol, 9CI. ***α*-Sylveterpineol**



$C_{10}H_{18}O$ 154.252

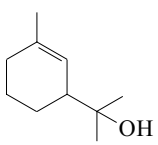
(*R*)-*form* [22625-86-1]
Constit. of oil from *Pinus sylvestris* (Scotch pine). Bp_1 65-66°. $[\alpha]_D^{26}$ +108.2 (c, 2.7 in C_6H_6). n_D^{20} 1.4846.

[25094-54-6, 29789-41-1]

Chabudzinski, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1961, **35**, 985 (*isol*)
Gollnick, K. *et al., Annalen*, 1969, **721**, 133 (*synth, config*)
Kaimal, K. *et al., J. Indian Chem. Soc.*, 1971, **48**, 759
Zutshi, S.K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 64 (*isol*)

m-Menth-1-en-8-ol M-169

[24220-40-4]
α,α,3-Trimethyl-2-cyclohexene-1-methanol, 9CI

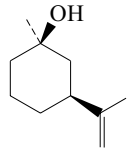


$C_{10}H_{18}O$ 154.252
Constit. of oil from *Pinus sylvestris* (Scotch pine). Bp_3 84°. $[\alpha]_D^{20}$ +46.2.

Chabudzinski, Z. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1961, **35**, 985 (*isol*)

m-Menth-8-en-1-ol M-170

[36386-54-6]
1-Methyl-3-(1-methylethenyl)cyclohexanol, 9CI



(1*R*,3*R*)-*form*

$C_{10}H_{18}O$ 154.252

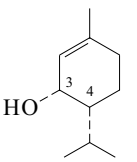
(1*R*,3*R*)-*form* [53538-30-0]
(-)-trans-*form*
Constit. of turpentine from *Pinus sylvestris* (Scotch pine). Mp 48-49°. $[\alpha]_D^{25}$ -0.2 (c, 4.6 in C_6H_6).

[6750-68-1, 22625-87-2]

Bardyshev, I.I. *et al., Khim. Prir. Soedin.*, 1968, **4**, 384; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 325
Gollnick, K. *et al., Annalen*, 1969, **721**, 133

p-Menth-1-en-3-ol M-171

[491-04-3]
3-Methyl-6-(1-methylethyl)-2-cyclohexen-1-ol, 9CI. 6-Isopropyl-3-methyl-2-cyclohexen-1-ol. ***Piperitol*****†**. *3-Carvomenthenol. FEMA 3179*



(3*R*,4*R*)-*form*

$C_{10}H_{18}O$ 154.252
Flavouring material with a pungent taste.

(3*R*,4*R*)-*form* [65733-27-9]
(-)-cis-*form*
Mp 30°. $[\alpha]_D$ -246 (C_6H_6).

(3*R*,4*S*)-*form* [25437-28-9]
(-)-trans-*form*
Isol. from essential oils of *Mentha* and *Eucalyptus* spp.. Oil. Bp_{15} 98°. $[\alpha]_D^{35}$ -25 (c, 2.1 in C_6H_6).

(3*S*,4*R*)-*form* [65733-28-0]
(+)-trans-*form*
Bp_{16} 101-104°. $[\alpha]_D^{16}$ +40.22 (+28).

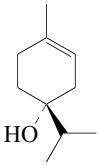
(3*S*,4*S*)-*form* [34350-53-3]
(+)-cis-*form*
Oil. Mp 11°. Bp_{15} 96°. $[\alpha]_D^{25}$ +218.3 (c, 2.1 in C_6H_6).

[16721-38-3, 16721-39-4, 75363-64-3, 75363-65-4]

Macbeth, A.K. *et al., J.C.S.*, 1952, 2852 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 297 (*occur*)
Prasad, R.S. *et al., Tetrahedron*, 1976, **32**, 1437 (*synth, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 446
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1676-1677

p-Menth-1-en-4-ol M-172

[562-74-3]
4-Methyl-1-(1-methylethyl)-3-cyclohexen-1-ol. 1-Isopropyl-4-methyl-3-cyclohexen-1-ol. 1-Terpinen-4-ol. 4-Carvomenthenol. Origanol. FEMA 2248



(*R*)-*form*

$C_{10}H_{18}O$ 154.252
Flavouring ingredient.
► Skin irritant. LD_{50} (rat, orl) 1300 mg/kg.
OT0175110

(*R*)-*form* [20126-76-5]
Oil. Bp 208-210°. $[\alpha]_D^{29}$ -36 (c, 1.44 in EtOH).

(*S*)-*form* [2438-10-0]
Occurs in many essential oils, e.g. lavender. Oil. Bp 208-210°. $[\alpha]_D^{11}$ +24.5.

(ξ)-*form*
(5-Isopropyl-2-methylphenyl) ether: [74638-20-3]
$C_{20}H_{30}O$ 286.456
Constit. of the essential oil of *Coridothymus capitatus* (Spanish oregano).

(±)-*form* [28219-82-1]
Liq. d^{24} 0.92. Bp 212-214°. n_D^{24} 1.4778.

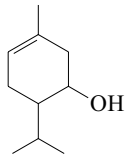
Ac: [4821-04-9]

[66686-66-6]
$C_{12}H_{20}O_2$ 196.289
$Bp_{1.3}$ 71-73°. n_D^{25} 1.4623.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 164B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 259B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 240B (*ir*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1965, **48**, 10 (*abs config*)
Verghese, J. *et al., Perfum. Essent. Oil Res.*, 1966, **57**, 694 (*rev*)
Suga, T. *et al., Can. J. Chem.*, 1969, **47**, 3682-3687 (***synth***)
Van Sydow, E. *et al., Arch. Mass Spectral Data*, 1970, **1**, 392-495 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 298 (*occur*)
Willson, C.W. *et al., J.O.C.*, 1973, **38**, 1684 (*synth*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1974, **57**, 2062 (*synth*)
Klein, E. *et al., Tet. Lett.*, 1978, 349-352 (*synth*)
Sendra, J.M. *et al., Phytochemistry*, 1980, **19**, 89 (*isopropylmethylphenyl ether*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 108
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 521-522
Ngo, K.S. *et al., Phytochemistry*, 1998, **47**, 1117-1123 (*pmr, cmr*)
Matsunaga, T. *et al., Biol. Pharm. Bull.*, 2000, **23**, 595-598 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBD825

p-Menth-1-en-5-ol M-173

[55708-42-4]
3-Methyl-6-(1-methylethyl)-3-cyclohexen-1-ol. 6-Isopropyl-3-methyl-3-cyclohexen-1-ol. p-*Menth-1(6)-en-3-ol. 1-Terpinen-5-ol*



$C_{10}H_{18}O$ 154.252
Isol. from *Piper nigrum* (pepper).

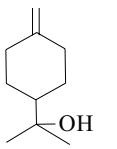
[29801-64-7, 71933-06-7]

Debrauwere, J. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 167 (*isol, pmr*)

p-Menth-1(7)-en-8-ol M-174

[17023-62-0]

[7299-42-5]
α,α-Dimethyl-4-methylenecyclohexanemethanol. δ-Terpineol



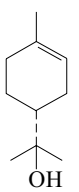
$C_{10}H_{18}O$ 154.252
Isol. from *Zanthoxylum piperitum* (Japanese pepper tree). Oil.

[8000-41-7, 8007-35-0, 62395-45-3]

Mitzner, B.M. *et al., J.O.C.*, 1966, **31**, 2022
Lawrence, B.M. *et al., Phytochemistry*, 1974, **13**, 2009 (*isol*)
Bull, S.D. *et al., Aust. J. Chem.*, 1992, **45**, 2077; 1993, **46**, 1869 (*synth, props, bibl*)

p-Menth-1-en-8-ol M-175

[98-55-5]
α,α,4-Trimethyl-3-cyclohexene-1-methanol, 9CI. 2-(4-Methyl-3-cyclohexenyl)-2-propanol. ***α-Terpineol****. Terpinol†. FEMA 3045*



(*R*)-*form*

$C_{10}H_{18}O$ 154.252
Flavouring agent.
► Flammable, fl. p. 43°. LD_{50} (mus, ims) 2000 mg/kg. LD_{50} (rat, orl) 5170 mg/kg.
WZ6700000

Cinnamoyl: [10024-56-3] *α-Terpinyl cinnamate. FEMA 3051*
$C_{19}H_{24}O_2$ 284.397
Flavouring ingredient with a heavy, fruity, somewhat spicy taste. Liq. $d^{15.5}$ 1.03. Bp 360°. n_D^{20} 1.5500.

2-Methylpropanoyl: [1334-93-6] *α-Terpinyl isobutyrate. FEMA 3050*
$C_{14}H_{24}O_2$ 224.342
Flavouring ingredient with a heavy, fruity-type flavour. Oil. Bp 242°.

2-Aminobenzoyl: [14481-52-8] *α-Terpinyl anthranilate. FEMA 3048*
$C_{17}H_{23}NO_2$ 273.374
Flavouring ingredient with a complex fruity odour and bitter taste. $d^{15.5}$ 1.06. Bp 365°. n_D^{20} 1.4830.

(*R*)-*form* [7785-53-7]
Cryst. Mp 37°. Bp_{15} 104°. $[\alpha]_D^{20}$ +100.5.

O-*β*-*D*-*Glucopyranoside:* [114673-99-3]
$C_{16}H_{28}O_6$ 316.394
Constit. of *Citrus* sp. and wine grapes (*Vitis vinifera*).

Formyl:
$C_{11}H_{18}O_2$ 182.262
d_4^{13} 0.99. $[\alpha]_D$ +88.32. n_D^{20} 1.4712.

(*S*)-*form* [10482-56-1]
Cryst. Mp 37°. Bp_{15} 104°. $[\alpha]_D^{20}$ -100.5.

O-*β*-*D*-*Glucopyranoside:* [89616-07-9]
Constit. of wine grapes (*Vitis vinifera*).

Ac: [58206-95-4]
$C_{12}H_{20}O_2$ 196.289
$[\alpha]_D^{20}$ -79.92. n_D^{20} 1.4657.

Propanoyl: [77889-76-0]
$C_{13}H_{22}O_2$ 210.316
d_4^{22} 0.95. $[\alpha]_D^{20}$ -75.12. n_D^{20} 1.4641.

(±)-*form* [2438-12-2]
Cryst. Mp 40-41°. Bp_{12} 99-100°.
► OT0175122

Formyl: [2153-26-6] *α-Terpineol formate. FEMA 3052*
Flavouring agent. d 0.99. Bp 213°.

Ac: [10581-37-0]

[80-26-2] *α-Terpineol acetate. FEMA 3047*
Flavouring agent. d 0.96. Bp 220°.

Propanoyl: [80-27-3] *α-Terpineol propanoate. FEMA 3053*
Flavouring agent. d 0.95. Bp 240°.

Butanoyl: [2153-28-8] *α-Terpineol butanoate. FEMA 3049*
$C_{14}H_{24}O_2$ 224.342
Flavouring agent. d 0.94. Bp 246°.

Pentanoyl: [14481-55-1]
$C_{15}H_{26}O_2$ 238.369
Prob. a flavouring agent. d 0.93. Bp 256°.

3-Methylbutanoyl: [1142-85-4] *Terpenyl isovalerate. FEMA 3054*
$C_{16}H_{26}O_2$ 250.38
Flavouring ingredient. Oily liq. Bp 248°.

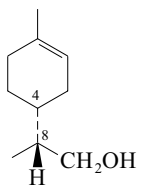
[7785-54-8, 7785-54-8, 8000-41-7, 8007-35-0, 39015-85-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 154B (*ir*)
Perkin, W.H. *et al., J.C.S.*, 1904, 654 (*synth*)
Fuller, A.T. *et al., J.C.S.*, 1924, **125**, 2304 (*esters*)
Freudenberg, K. *et al., Annalen*, 1955, **594**, 76 (*abs config*)
Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 188 (*Ac*)
Prelog, V. *et al., Annalen*, 1957, **603**, 1 (*synth*)
Mitzner, B.M. *et al., Am. Perfum. Cosmet.*, 1966, **81**, 25 (*ir*)
Beckey, H.D. *et al., Org. Mass Spectrom.*, 1968, **1**, 47 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 299 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Ackermann, I. *et al., Annalen*, 1989, 79 (*synth, glucosides*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1419
Pei, W. *et al., Chin. Chem. Lett.*, 1997, **8**, 19-20 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2743-2744; 2746-2753 (*esters*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1669; 1671-1678 (*use, esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBD750

p-Menth-1-en-9-ol M-176

[18479-68-0]
β,4-Dimethyl-3-cyclohexene-1-ethanol, 9CI. 2-(4-Methyl-3-cycohexen-1-yl)-1-propanol



(4*R*,8*R*)-*form*

$C_{10}H_{18}O$ 154.252
Constit. of *Vaccinium myrtillus* (bilberry) and tangerine oil.

Ac: [28839-13-6]
$C_{12}H_{20}O_2$ 196.289
Flavouring ingredient.

(4*R*,8*R*)-*form* [13835-30-8]
$Bp_{0.2}$ 64-69°. $[\alpha]_D^{25}$ +104 (neat).

(4*R*,8*S*)-*form* [13835-75-1]
$Bp_{0.25}$ 75-82°. $[\alpha]_D^{25}$ +97.3 (c, 1 in $CHCl_3$).

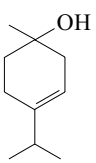
(4*S*,8*R*)-*form* [26462-90-8]
$Bp_{0.2}$ 75-80°. $[\alpha]_D^{25}$ -94 (c, 0.92 in $CHCl_3$).

(4*S*,8*S*)-*form* [26462-81-7]
$Bp_{0.15}$ 70-78°. $[\alpha]_D^{25}$ -103.1 (c, 4.8 in C_6H_6).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 164C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 258C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 240C (*ir*)
Schulte-Elte, K.H. *et al., Helv. Chim. Acta*, 1966, **49**, 2150
Pawson, B.A. *et al., J.A.C.S.*, 1970, **92**, 336 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 447 (*Ac*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1678 (*Ac*)

p-Menth-3-en-1-ol M-177

[586-82-3]
1-Methyl-4-(1-methylethyl)-3-cyclohexen-1-ol. 4-Isopropyl-1-methyl-3-cyclohexen-1-ol. Terpinen-1-ol. FEMA 3563



$C_{10}H_{18}O$ 154.252

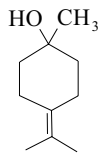
(±)-*form*
Oil. Bp 208-210°. n_D^{20} 1.4760.

(ξ)-*form*
Constit. of oregano (*Origanum vulgare*), lime peel (*Citrus aurantifolia*) and mandarin peel. Also present in grapefruit juice, cognac, wines, cocoa, black tea and cardamon. Flavouring agent.

Kováts, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2705 (*isol*)
Brieskorn, C.H. *et al., Planta Med. (Suppl.)*, 1967, 96 (*isol*)
Goryaev, M.I. *et al., CA*, 1969, **70**, 70998a (*isol*)
Accrombessi, G. *et al., Tetrahedron*, 1981, **37**, 3135 (*synth*)

p-Menth-4(8)-en-1-ol M-178

[586-81-2]
1-Methyl-4-(1-methylethylidene)cyclohexanol, 9CI. 4-Isopropylidene-1-methylcyclohexanol. ***γ*-Terpineol**



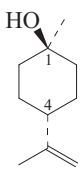
$C_{10}H_{18}O$ 154.252
Isol. from carrot oils, from the cinnamon tree (*Cinnamomum zeylanicum*) and Scotch pine (*Pinus sylvestris*). Cryst. (Et_2O). Mp 68-70°.

[8000-41-7, 8007-35-0, 62395-45-3]

Bayer, A. *et al., Ber.*, 1894, **27**, 436; 444 (*synth*)
Verghese, J. *et al., Indian Perfum.*, 1972, **16**, 35 (*rev*)

p-Menth-8-en-1-ol M-179

[138-87-4]
1-Methyl-4-(1-methylethenyl)cyclohexanol. 4-Isopropenyl-1-methylcyclohexanol. ***β*-Terpineol**. *FEMA 3564*



(1*RS*,4*RS*)-*form*

$C_{10}H_{18}O$ 154.252
Flavouring ingredient. Oil with hyacinth odour.

►OT0175130

(1*RS*,4*RS*)-*form* [7299-41-4]
cis-*form*
Mp 36°. $Bp_{1.5}$ 78°.

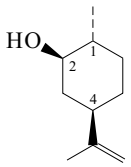
(1*RS*,4*SR*)-*form* [7299-40-3]
trans-*form*
Mp 32-33°. Bp_{10} 90°.

[1142-85-4, 8000-41-7, 8007-35-0, 62395-45-3]

Vig, O.P. *et al., J. Indian Chem. Soc.*, 1971, **48**, 993 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 736
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2744-2745

p-Menth-8-en-2-ol M-180

[17699-09-1]
2-Methyl-5-(1-methylethenyl)cyclohexanol. 5-Isopropenyl-2-methylcyclohexanol. FEMA 2379



(1*R*,2*R*,4*R*)-*form*

$C_{10}H_{18}O$ 154.252
Occurs in *Mentha* spp., *Piper longum* (long pepper), *Heracleum candicans* and other essential oils. Stereoisomeric mixt. used as flavour ingredient.

(1*R*,2*R*,4*R*)-*form* [20549-47-7]
(-)-Dihydrocarveol
Occurs in caraway oil. Oil. Bp_{10} 99-99.5°. $[\alpha]_D^{25}$ -34.15 (neat).

O-*β*-D-*Glucopyranoside:* [129829-12-5]
$C_{16}H_{28}O_6$ 316.394

Ac: [20777-49-5] *Dihydrocarveol acetate. FEMA 2380*
$C_{12}H_{20}O_2$ 196.289
Flavouring ingredient. Bp 232-234°. $[\alpha]_D^{25}$ -13.5 (neat). n_D^{20} 1.4590.

(1*R*,2*S*,4*R*)-*form* [20549-48-8]
(+)-Neodihydrocarveol
Viscous liq. Bp_{19} 107-107.9°. $[\alpha]_D^{25}$ +35.16 (neat).

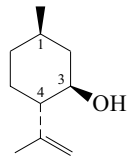
O-*β*-D-*Glucopyranoside:* [129742-32-1]
$C_{16}H_{28}O_6$ 316.394

[619-01-2, 18675-33-7, 18675-34-8, 18675-35-9, 22567-21-1, 22567-22-2, 36237-64-6, 38049-26-2, 51773-45-6, 53796-77-3, 53796-80-8]

Klages, A. *et al., Ber.*, 1899, **32**, 2550 (*Ac*)
Shishibori, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1170 (*synth*)
Ladwa, P.H. *et al., Indian J. Chem.*, 1968, **6**, 765 (*synth*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1972, **49**, 159 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 771 (*rev, tox, Dihydrocarveol*)
Shimizu, S. *et al., J. Essent. Oil Res.*, 1990, **2**, 81 (*isol, glucosides*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 163-164 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DKV150

p-Menth-8-en-3-ol M-181

[7786-67-6]
5-Methyl-2-(1-methylethenyl)cyclohexanol, 9CI. 2-Isopropenyl-5-methylcyclohexanol. FEMA 2962



(1*R*,3*R*,4*S*)-*form*

$C_{10}H_{18}O$ 154.252
Various stereoisomers occur in essential oils. Flavouring agent.
► LD_{50} (rat, orl) 1030 mg/kg. LD_{50} (rbt, skn) 3000 mg/kg. OT0190000

(1*R*,3*R*,4*S*)-*form* [89-79-2]
(-)-Isopulegol
Isol. from *Mentha pulegium* (European pennyroyal) and other essential oils. Oil. Bp_3 65-66°. $[\alpha]_D^{25}$ -22.5 (neat).

Ac: [89-49-6] *Isopulegol acetate. FEMA 2965*
$C_{12}H_{20}O_2$ 196.289
Flavouring agent. Bp_8 112-114°.

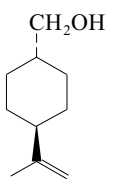
(1*R*,3*S*,4*S*)-*form* [20549-46-6]
(+)-Neoisopulegol
Oil. Bp_9 81-81.2°. $[\alpha]_D^{25}$ +32.3 (neat).

[21290-09-5, 29141-10-4, 50373-36-9, 59905-53-2, 59905-54-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 165B; 631D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 260A; 1000A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 241B; 661B (*ir*)
Shishibori, T. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1170 (*synth*)
Sakai, K. *et al., Tet. Lett.*, 1972, 4375 (*synth*)
Helmchen, G. *et al., Tet. Lett.*, 1974, 1527 (*abs config*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 823 (*rev, tox*)
Proenca da Cunha, A. *et al., Bol. Fac. Farm., Univ. Coimbra, Ed. Cient.*, 1976, **1**, 23-36; *CA*, **88**, 78955b (*occur*)
Koch, W.-G. *et al., Z. Naturforsch., C*, 1987, **42**, 159 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 422; 423 (*rev*)
Aggarwal, V.K. *et al., Tet. Lett.*, 1998, **39**, 1997-2000 (*synth*)
Kocovský, P. *et al., J.O.C.*, 1999, **64**, 2765-2775 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCE750

p-Menth-8-en-7-ol M-182

[18479-64-6]
4-(1-Methylethenyl)cyclohexanemethanol, 9CI. 1-Hydroxymethyl-4-isopropenylcyclohexane. ***Shisool***



(1*RS*,4*RS*)-*form*

$C_{10}H_{18}O$ 154.252

(1*RS*,4*RS*)-*form* [22451-48-5]
trans-*form*
Oil. Bp 225°.

3,5-Dinitrobenzoyl:
Mp 79.5°.

7-O-β-D-Glucopyranoside: [146763-94-2]
Perilloside C
$C_{16}H_{28}O_6$ 316.394
Constit. of *Perilla frutescens* (perilla). Needles. Mp 125.5-126.5°. $[\alpha]_D^{22}$ -32.3 (c, 0.6 in MeOH).

*3,4-Dihydroxycinnamoyl(*E-*):* [179694-78-1] **p-*Menth-8-en-7-yl caffeate***
$C_{19}H_{24}O_4$ 316.396
Constit. of *Perilla frutescens* var. *crispa*. Yellow cryst. Mp 155-156°. λ_{max} 217 (ϵ 15450); 236 (ϵ 9130); 245 (ϵ 9730) (EtOH).

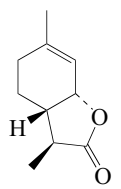
(1*RS*,4*SR*)-*form* [22521-57-9]
cis-*form*
Minor constit. of *Perilla* spp..

3,5-Dinitrobenzoyl:
Mp 73°.

7-O-β-D-Glucopyranoside: [153548-82-4]
Perilloside D
$C_{16}H_{28}O_6$ 316.394
Constit. of *Perilla frutescens* (perilla). Amorph. powder.

Iskenderov, M.A. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1937, **7**, 1429 (*synth*)
Kayahara, H. *et al., Agric. Biol. Chem.*, 1969, **33**, 86 (*synth*)
Fujita, Y. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 2637 (*isol*)
Fujita, T. *et al., Phytochemistry*, 1993, **34**, 1545 (*Perilloside C, Perilloside D*)
Tada, M. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1093 (*caffeate*)

p-Menth-1-en-9,3-olide M-183



$C_{10}H_{14}O_2$ 166.219
All 8 stereoisomers synthesised.

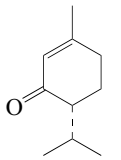
(3*R*,4*S*,8*S*)-*form* [182699-77-0]
Wine lactone
Constit. of wine. Cryst.. with intense sweet coconut-like odour. Mp 48-50°. $[\alpha]_D^{20}$ -13.1 (>99.9% e.e.). λ_{max} 207 (ϵ 4040) (no solvent reported).

[182699-78-1, 182699-79-2, 182699-80-5, 182699-81-6, 182699-82-7, 182699-83-8, 182699-84-9]

Guth, H. *et al., Helv. Chim. Acta*, 1996, **79**, 1559-1571 (*isol, synth, abs config*)
Bergner, E.J. *et al., Eur. J. Org. Chem.*, 2000, 419-423 (*synth*)

p-Menth-1-en-3-one M-184

[89-81-6]
3-Methyl-6-(1-methylethyl)-2-cyclohexen-1-one. 6-Isopropyl-3-methyl-2-cyclohexen-1-one. ***Piperitone****. 3-Carvomenthenone. FEMA 2910*



(*R*)-*form*

$C_{10}H_{16}O$ 152.236
Flavouring ingredient. Log P 2.5 (calc).
► Skin irritant. LD_{50} (rat, orl) 2450 mg/kg. OT0257000

(R)*-*form [4573-50-6]
Constit. of *Mentha* spp. and *Zanthoxylum piperitum* (Japanese pepper tree) oil. Mp -29°. Bp_{15} 110.5°. $[\alpha]_D^{20}$ -51.53.

(S)*-*form [6091-50-5]
Common constit. of *Mentha* spp. oils. Oil with camphoraceous odour. Bp_{20} 116-118.5°. $[\alpha]_D^{20}$ +49.13.

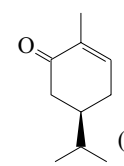
Semicarbazone:
Cryst. Mp 193-194°. $[\alpha]_D^{20}$ -216.8.

[6091-52-7]

Thomas, A.F. *et al., J.C.S.(B)*, 1967, 392 (*ms*)
Nagasawa, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 2083 (*abs config*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 863 (*rev, tox*)
Burbott, A.J. *et al., Phytochemistry*, 1983, **22**, 2227-2230 (*isol, uv, cd, abs config*)
Kuwahara, Y. *et al., Agric. Biol. Chem.*, 1987, **51**, 3441 (*isol*)
Garcez, F.R. *et al., Phytochemistry*, 1988, **27**, 1079 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 679
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2230-2231
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCF250

p-Menth-1-en-6-one M-185

[499-71-8]
2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-one. 5-Isopropyl-2-methyl-2-cyclohexen-1-one. ***Carvotanacetone****. Carvotagetone*



(*R*)-*form*

$C_{10}H_{16}O$ 152.236

(*R*)-*form* [33375-08-5]
Constit. of *Piper nigrum* (pepper) and *Cymbopogon nardus* (citronella). Also from *Tanacetum vulgare* (tansy). Oil. Bp 227-229°.

Semicarbazone:
Cryst. (EtOH). Mp 135°. $[\alpha]_D^{22}$ -114 ($CHCl_3$).

(*S*)-*form* [22567-12-0]
Oil. Bp 227-228°. $[\alpha]_D^{25}$ +49.5.

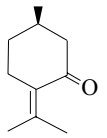
Semicarbazone:
Cryst. (EtOH). Mp 173-174°. $[\alpha]_D^{21}$ +114.7.

[2244-15-7, 43205-82-9]

Simonsen, J.L. *et al., J.C.S.*, 1922, 876 (*isol, struct*)
Sutherland, M.D. *et al., Aust. J. Chem.*, 1960, **13**, 357 (*isol*)
Org. Synth., 1973, **53**, 63 (*synth*)
Noma, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1637 (*synth*)
Debraumere, J. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 167 (*isol, struct*)

p-Menth-4(8)-en-3-one M-186

[15932-80-6]
5-Methyl-2-(1-methylethylidene)cyclohexanone. 2-Isopropylidene-5-methylcyclohexanone. ***Pulegone****. β-Pulegone*



(*R*)-*form*

$C_{10}H_{16}O$ 152.236
► LD_{50} (rat, orl) 470 mg/kg. Skin irritant.
OT0260000

(*R*)-*form* [89-82-7]
FEMA 2963
Occurs in oils of *Mentha* spp., *Hedeoma pulegioides* and many other essential oils. Fragrance and flavour ingredient. Oil with pleasant peppermint odour. d_4^{20} 0.94. Bp 224°. $[\alpha]_D^{20}$ +23 (c, 5 in EtOH).
► OT0261000

Semicarbazone:
Cryst. (EtOH). Mp 174°.

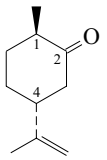
(*S*)-*form* [3391-90-0]
Oil. Bp_{22} 104-108°. $[\alpha]_D^{23}$ -22.5 (neat).

[3285-04-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 449A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 693B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 538D (*ir*)
Black, C. *et al., J.C.S.*, 1956, 2971 (*synth*)
Banthorpe, D.V. *et al., J.C.S. Perkin 1*, 1972, 1532 (*isol, biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 549 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Corey, E.J. *et al., J.O.C.*, 1976, **41**, 380 (*synth*)
Allen, K.G. *et al., Phytochemistry*, 1976, **15**, 101 (*biosynth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1407
Eisenreich, W. *et al., Tet. Lett.*, 1997, **38**, 3889-3892 (*biosynth*)
Bartoli, G. *et al., J.O.C.*, 2002, **67**, 9111-9114 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCF500

p-Menth-8-en-2-one M-187

[7764-50-3]
2-Methyl-5-(1-methylethenyl)cyclohexanone, 9CI. 5-Isopropenyl-2-methylcyclohexanone. ***Dihydrocarvone****. FEMA 3565*



(1*R*,4*R*)-*form*

$C_{10}H_{16}O$ 152.236
Flavouring agent with spearmint-like flavour.
► Skin irritant. LD_{50} (mus, scu) 2900 mg/kg.
PC8710000

(1*R*,4*R*)-*form* [5524-05-0]
Oil. Bp 221-222°. $[\alpha]_D$ +17.5.

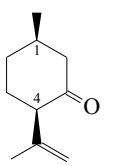
(1*S*,4*S*)-*form* [6909-25-7]
Constit. of caraway, dill and mint oils. Oil. Bp 220-221°. $[\alpha]_D$ -19.

[619-02-3, 3792-53-8, 5948-04-9, 53796-79-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 445A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 693C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 532B (*ir*)
Nigam, M.C. *et al., Can. J. Chem.*, 1965, **43**, 521 (*isol*)
Noma, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 735 (*synth*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1976, **53**, 50 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1980, **18**, 665 (*rev, tox*)
Verghese, J. *et al., Perfum. Flavor.*, 1980, **5**, 23 (*rev*)
Jirovetz, L. *et al., Ernaehrungsforschung*, 1994, **18**, 534-536; *CA*, **123**, 168090m (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 163 (*rev*)
Tumen, G. *et al., J. Essent. Oil Res.*, 1995, **7**, 175-176; 177-178 (*occur*)
Gabriels, S. *et al., Eur. J. Org. Chem.*, 1999, 1803-1809 (*1R,4R-form, synth, ir, pmr, cmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DKV175

p-Menth-8-en-3-one M-188

[529-00-0]
5-Methyl-2-(1-methylethenyl)cyclohexanone. 2-Isopropenyl-5-methylcyclohexanone. ***Isopulegone****. α-Pulegone*



(1*R*,4*R*)-*form*

$C_{10}H_{16}O$ 152.236

(1*R*,4*R*)-*form* [3391-89-7]
(+)-cis-*form. Isoisopulegone*
Oil. Bp_{10} 84°. $[\alpha]_D^{20}$ +144.36. n_D^{20} 1.4700.

Semicarbazone:
Cryst. (MeOH aq.). Mp 157.5-158.5°.

(1*R*,4*S*)-*form* [57129-09-6]

[29606-79-9] *(-)*-trans-*form. FEMA 2964*
Flavouring ingredient. Isol. from oil of American pennyroyal (*Hedeoma pulegioides*), *Mentha* spp. and others, usually with Pulegone. Oil. Bp_{13} 98-100°. $[\alpha]_D^{25}$ -7.9 (neat). $[\alpha]_D^{32}$ -13.5 (c, 1.04 in $CHCl_3$). n_D^{25} 1.4670.

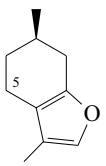
Semicarbazone:
Cryst. Mp 173-174° dec.

[3391-89-7, 17882-43-8, 52152-10-0]

Ohloff, G. *et al., Chem. Ber.*, 1962, **95**, 1400 (*synth, config*)
Watanabe, S. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 1546 (*synth, cd*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1976, **53**, 50 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 2964
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1502-1503

Menthofuran M-189

[494-90-6]
*4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran, 9CI. 3,9-Epoxy-*p*-mentha-3,8-diene. FEMA 3235*



$C_{10}H_{14}O$ 150.22

(*R*)-*form* [17957-94-7]
Constit. of peppermint oil (*Mentha piperita*) and other *Mentha* spp. as minor but essential organoleptic. Used in peppermint oil formulations. Oil. d_4^{15} 0.97. Bp_{18} 80°. $[\alpha]_D^{25}$ +92.5.

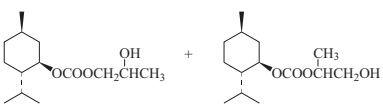
5-Oxo: See Evodone in *The Combined Chemical Dictionary.*

(±)-*form* [59553-66-1]
Oil.

Treibs, W. *et al., Ber.*, 1937, **70**, 85 (*abs config*)
Eastman, R.H. *et al., J.A.C.S.*, 1950, **72**, 5313 (*isol*)
Nigam, I.C. *et al., J. Pharm. Sci.*, 1964, **53**, 1008 (*occur*)
Tori, K. *et al., Tet. Lett.*, 1975, 4583 (*cmr*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1976, **53**, 50 (*synth*)
Tsuboi, S. *et al., J.O.C.*, 1980, **45**, 1517 (*synth*)
Juo, R.-R. *et al., J.O.C.*, 1985, **50**, 700 (*synth*)
Ho, T.L. *et al., Synth. Commun.*, 1989, **19**, 813 (*synth*)
Shishido, K. *et al., Heterocycles*, 1992, **33**, 73; 1993, **36**, 345 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1680

Menthol propylene glycol carbonate M-190

[156324-82-2]
2-Hydroxypropyl menthyl carbonate. 2-Hydroxypropyl 5-methyl-2-(1-methylethyl)cyclohexyl carbonate. Frescolate MPC. FEMA 3806

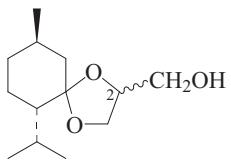


$C_{14}H_{26}O_4$ 258.357
Flavouring agent with cooling taste for chewing gum and candies. Liq. d_{25}^{25} 1.01. Bp 140-143°. $[\alpha]_D^{25}$ -62.2 (c, 10 in EtOH). CAS no., and possibly the phys. props. also, refer to the 2-propylene glycol isomer.

Ger. Pat., 1994, 4 226 043; *CA*, **121**, 83678t (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1026 (*props, use*)

Menthone 1,2-glyceryl ketal M-191

[63187-91-7]
9-Methyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decane-2-methanol, 9CI. 2-Hydroxymethyl-6-isopropyl-9-methyl-1,4-dioxaspiro[4.5]decane. Frescolat. Frescolat MGA. FEMA 3807. FEMA 3808

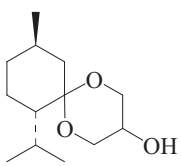


$C_{13}H_{24}O_3$ 228.331
Generally prepd. as a mixt. with Menthone 1,3-glyceryl ketal, M-192, to which phys. props. and synonyms refer. Flavour enhancer for chewing gum and other low moisture foods. Liq. with cool taste. Bp *ca.* 295° Bp_{20} 135°. $[\alpha]_D$ -24.6.

Svishchuk, A.A. *et al., Ukr. Khim. Zh. (Russ. edn.)*, 1977, **43**, 173-176; *CA*, **87**, 39667u (*synth*)
Eur. Pat., 1992, 485 170; *CA*, **118**, 123355g (*synth, ms, use, ir*)
Jacobs, P. *et al., Parfuem. Kosmet.*, 1999, **80**, 26; 28-31; *CA*, **131**, 23210f (*rev, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1027-1029 (*use*)

Menthone 1,3-glyceryl ketal M-192

[63187-41-7]
10-Methyl-7-(1-methylethyl)-1,5-dioxaspiro[5.5]undecan-3-ol, 9CI. 3-Hydroxy-7-isopropyl-10-methyl-1,5-dioxaspiro[5.5]undecane

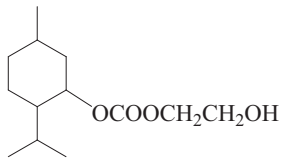


$C_{13}H_{24}O_3$ 228.331
Generally prepd. as a mixt. with Menthone 1,2-glycerol ketal, q.v. for props. and synonyms. Flavouring ingredient esp. for chewing gum.

Eur. Pat., 1992, 485 170; *CA*, **118**, 123355g (*use, synth, ms, ir*)
Jacobs, P. *et al., Parfuem. Kosmet.*, 1999, **80**, 26; 28-31; *CA*, **131**, 23210f
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1027-1028 (*props, use*)

Menthyl ethylene glycol carbonate M-193

[156324-78-6]
2-Hydroxyethyl 5-methyl-2-(1-methylethyl)cyclohexyl carbonate, 9CI. Menthol glycol carbonate. Frescolat MGC. FEMA 3805

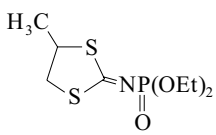


$C_{13}H_{24}O_4$ 244.33
Physiol. cooling agent used in foods. Strong mint flavorant used in chewing gum. Mp 51.5°. Bp_{10} 72°. The corresponding homologue derived from 1,2-propanediol (mixt. of regioisomers), known as Frescolate MPC (FEMA 3806) is also used.

Ger. Pat., 1994, 4 226 043; *CA*, **121**, 83678t (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1025-1026

Mephosfolan, BSI M-194

[950-10-7]
Diethyl (4-methyl-1,3-dithiolan-2-ylidene)-phosphoramidate, 9CI. P,P-*Diethyl cyclic propylene phosphonodithioimidocarbonate, 8CI. Cytrolane*



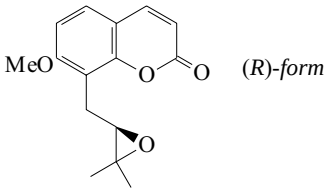
$C_8H_{16}NO_3PS_2$ 269.325
▶ JP1050000
(±)-*form*
Agricultural insecticide with contact and stomach action, now superseded. Yellow liq. Sol. Me_2CO, EtOH, C_6H_6, CH_2Cl_2, sl. sol. H_2O. $Bp_{0.001}$ 120°. n_D^{26} 1.5390. *S*-Oxides known.
▶ LD_{50} (rat, orl) 9 mg/kg. LD_{50} (rbt, skn) 28.7 mg/kg.

[99910-07-3, 99910-08-4, 99910-21-1]

U.K. Pat., 1961, 974 138; *CA*, **59**, 10066f (*synth*)
Ku, C.C. *et al., J. Agric. Food Chem.*, 1979, **27**, 1046 (*props, synth*)
Ku, C.C. *et al., ACS Symp. Ser.*, 1981, **158**, 97 (*metab*)
Abou-Donia, S.A. *et al., J. Chromatogr.*, 1982, **240**, 532 (*hplc*)
Gorder, G.W. *et al., Bioorg. Chem.*, 1985, **13**, 344; 353 (*synth, oxides, pmr, cmr, P-31 nmr*)
Pesticide Manual, 9th edn., 1991, No. 7910
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DHH400

Meranzin M-195

[489-53-2]
*8-[(3,3-Dimethyloxiranyl)methyl]-7-methoxy-2*H*-1-benzopyran-2-one, 9CI. Merangin. Osthole oxide. Merancin. Auraptent*



(*R*)-*form*

$C_{15}H_{16}O_4$ 260.289
The name Aurapten is more widespread in the lit., but Meranzin is used here to avoid confusion with Auraptene, A-491 (see Kariyone *et al*).
(*R*)-*form*
Constit. of orange peel oil. Needles (EtOH). Mp 98°. $[\alpha]_D$ +0.81 (EtOH). $[\alpha]_D$ +1.4 ($CHCl_3$).
(*S*)-*form*
Needles (EtOH). Mp 97-98°. $[\alpha]_{Hg}$ -1.48 ($CHCl_3$).

Bohme, H. *et al., Ber.*, 1939, **72**, 780 (*struct*)
Kariyone, T. *et al., Chem. Pharm. Bull.*, 1959, **1**, 119 (*nomencl*)
Bohlmann, F. *et al., Annalen*, 1968, **717**, 186 (*isol*)
Coates, R.M. *et al., Tetrahedron*, 1970, **26**, 1970 (*isol*)
Grundon, M.F. *et al., Phytochemistry*, 1975, **14**, 143 (*synth, abs config*)
Raj, K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 332 (*synth*)
Yamada, S.N. *et al., Tet. Lett.*, 1976, 2557 (*synth*)

Mercaptoacetaldehyde M-196

[4124-63-4]
$HSCH_2CHO$
C_2H_4OS 76.119Known only in soln. Readily dimerises to 1,4-Dithiane-2,5-diol, D-988.

Oxime:
C_2H_5NOS 91.134
Oil. Bp 123°.

Di-Et acetal: [53608-94-9] *2,2-Diethoxyethanethiol, 9CI. Mercaptoacetal*
$C_6H_{14}O_2S$ 150.241
Liq. with acetal odour. $Bp_{0.3}$ 81° $Bp_{0.12}$ 59-60°. n_D^{25} 1.4391. Dec. slowly on standing.

S-*Me:* [23328-62-3] *(Methylthio)acetaldehyde. FEMA 3206*
C_3H_6OS 90.146
Flavouring ingredient. Bp 129-134° Bp_{10} 35°.

S-*Me, 2,4-dinitrophenylhydrazone:*
Cryst. (EtOH aq.). Mp 131-131.5°.

S-*Me, semicarbazone:*
Mp 133.5-134°.

S-*Me, di-Me acetal:* [40015-15-4] *1,1-Dimethoxy-2-(methylthio)ethane, 9CI*
$C_5H_{12}O_2S$ 136.215
Bp_{10} 55°.

S-*Me, di-Et acetal:* [51517-03-4] *2-(Ethylthio)-1,1-dimethoxyethane, 9CI*
$C_7H_{16}O_2S$ 164.268
Bp_{11} 63-64°.

S-*Et:* [33672-79-6] *(Ethylthio)acetaldehyde*
C_4H_8OS 104.173
Bp_{10} 46.5°.

S-*Et, 2,4-dinitrophenylhydrazone:*
Mp 125.5-126°.

S-*Et, semicarbazone:*
Mp 93-93.5°.
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 444B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 347A (*ir*)
Hesse, G. *et al., Chem. Ber.*, 1952, **85**, 924; 933
Wick, E.H. *et al., J. Agric. Food Chem.*, 1961, **9**, 289 (*deriv, synth*)
Org. Synth., Coll. Vol., 4, 1963, 295
Gassman, P.G. *et al., J.A.C.S.*, 1974, **96**, 5495 (*deriv, synth*)
Mikolajczyk, M. *et al., Synthesis*, 1987, 659 (*synth, pmr, ms, bibl*)
Aurich, H.G. *et al., Annalen*, 1995, 1649 (*oxime*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 566 (*S-Me*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1864 (*S-Me*)

3-Mercaptobutanal M-197

[13638-74-9]
$H_3CCH(SH)CH_2CHO$
C_4H_8OS 104.173

(±)-*form*
Bp_{17} 71°.
2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 102-103°.
S-*Me:* [16630-52-7] *3-(Methylthio)butanal. FEMA 3374*
$C_5H_{10}OS$ 118.199
Flavouring ingredient. d^{20} 1. Bp_{11} 63-65°. n_D^{20} 1.4771.
Boustany, K. *et al., J. Chem. U.A.R.*, 1966, **9**, 317 (*synth, S-Me*)
Asinger, F. *et al., J. Prakt. Chem.*, 1967, **35**, 81 (*synth*)
Ger. Pat., 1987, 3 627 410; *CA*, **106**, 213492f (*synth, S-Me*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 570
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1865-1866

4-Mercaptobutanal, 9CI M-198

$HSCH_2CH_2CH_2CHO$
C_4H_8OS 104.173
Bp 97° Bp_{10} 97°. n_D^{20} 1.4515.
Di-Et acetal:4,4-Diethoxy-1-butanethiol
$C_8H_{18}O_2S$ 178.295
Bp_{10} 97°. n_D^{20} 1.4515.
S-*Me:* [42919-64-2] *4-(Methylthio)butanal. FEMA 3414*
$C_5H_{10}OS$ 118.199
Flavouring ingredient. Bp_{22} 76-78°.
S-*Me, di-Et acetal:1,1-Diethoxy-4-(methylthio)butane*
$C_9H_{20}O_2S$ 192.322
Bp_{10} 102-103°.
Bateman, L. *et al., J.C.S.*, 1958, 2834-2837 (*acetal*)
Speck, J.C. *et al., J.A.C.S.*, 1965, **87**, 4979-4980 (*S-Me, synth*)
U.S. Pat., 1975, 3 904 556; *CA*, **84**, 8859s (*S-Me, use, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 568 (*S-Me, use*)

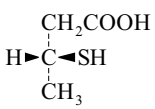
2-Mercaptobutanoic acid, 9CI M-199

[26473-48-3]
$H_3CCH_2CH(SH)COOH$
$C_4H_8O_2S$ 120.172

(±)-*form*
Oil. Sol. H_2O. Bp_{19} 118-122°.
S-*Me, Me ester:* [51534-66-8] *Methyl 2-(methylthio)butyrate. FEMA 3708*
$C_6H_{12}O_2S$ 148.226
Flavouring ingredient. Present in cheese. Insol. H_2O, sol. EtOH. Bp 153°. n_D^{23} 1.4610.
S-*Ph:* [120584-27-2]
$C_{10}H_{12}O_2S$ 196.27
Liq. Bp_1 100-140°.
Biilmann, E. *et al., Annalen*, 1905, **339**, 368
Iwai, K. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 242 (*S-Ph, synth, pmr*)
Parkes, K.E.B. *et al., J.C.S. Perkin 1*, 1988, 1119 (*S-Ph, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 525 (*S-Me Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1800 (*S-Me Me ester*)

3-Mercaptobutanoic acid, 9CI M-200

[26473-49-4]



(*R*)-*form*

$C_4H_8O_2S$ 120.172

(*R*)-*form*
Liq. $Bp_{0.15}$ 120-125°. $[\alpha]_D$ +101.5 (c, 0.62 in CH_2Cl_2).
S-*Me:* [141079-84-7] *3-(Methylthio)butanoic acid, 9CI*
$C_5H_{10}O_2S$ 134.199
Liq. Bp_{150} 70°. $[\alpha]_D$ -2.2 (c, 1.02 in EtOH).
S-tert-*Butyl:* [141079-85-8]
$C_8H_{16}O_2S$ 176.279
Liq. $Bp_{0.076}$ 40°. $[\alpha]_D$ -7.4 (c, 1.79 in EtOH).
S-*Ph:3-(Phenylthio)butanoic acid*
$C_{10}H_{12}O_2S$ 196.27
Oil. $Bp_{0.3}$ 160-165°. $[\alpha]_D$ -24.3 (c, 0.28 in CH_2Cl_2).
S-*Ph,* S-*oxide:3-(Phenylsulfinyl)butanoic acid*
$C_{10}H_{12}O_3S$ 212.269
Needles. Mp 130-131°. $[\alpha]_D$ +119.5 (c, 2.46 in MeOH). A single diastereoisomer obt. by fractional crystallisation and having $(R)_C(S)_S$-config..

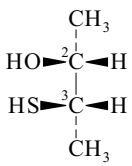
(±)-*form*
Liq. Spar. sol. H_2O. d_4^{20} 1.14. Bp_{10} 110-111° $Bp_{2.5}$ 87-88°. n_D^{20} 1.4782.
Et ester:
$C_6H_{12}O_2S$ 148.226
Liq. Bp_{50} 95-100°.
S-Me, Et ester:Ethyl 3-(methylthio)butanoate. FEMA 3836
$C_7H_{14}O_2S$ 162.252
Used in food flavouring of baked goods etc.. Liq.
Lovén, J.M. *et al., Ber.*, 1915, **48**, 1257
Johansson, H. *et al., CA*, 1917, **11**, 2577
Griesbeck, A. *et al., Helv. Chim. Acta*, 1987, **70**, 1326 (*synth, ir, pmr, cmr*)
Breitschuh, R. *et al., Synthesis*, 1992, 83 (*deriv, synth, pmr, cmr, ms*)
Hutchinson, J.H. *et al., J. Med. Chem.*, 1994, **37**, 1153 (*synth*)

4-Mercaptobutanoic acid, 9CI M-201

[13095-73-3]
$HSCH_2CH_2CH_2COOH$
$C_4H_8O_2S$ 120.172
Free acid spontaneously lactonises.
▶ ET5100000
Et ester: [70124-54-8]
$C_6H_{12}O_2S$ 148.226
Liq. $Bp_{1.3}$ 165°.
S-*Me:* [32391-97-2] *4-(Methylthio)butanoic acid, 9CI*
$C_5H_{10}O_2S$ 134.199
$Bp_{1.5}$ 107-109°.
S-*Me, Me ester:* [53053-51-3] *Methyl 4-(methylthio)butyrate. FEMA 3412*
$C_6H_{12}O_2S$ 148.226
Flavouring ingredient.
S-*Me, Et ester:* [22014-48-8] *Ethyl 4-(methylthio)butyrate. FEMA 3681*
$C_7H_{14}O_2S$ 162.252
Flavouring agent. Liq. with pungent sulfur odour. d^{23} 1. Bp_{15} 95°. n_D^{23} 1.4592.
S-*Ph:4-(Phenylthio)butanoic acid*
$C_{10}H_{12}O_2S$ 196.27
Cryst. (petrol). Mp 68-69°.
S-*Ph,* S,S-*dioxide:* [6178-52-5] *4-(Phenylsulfonyl)butanoic acid, 9CI*
$C_{10}H_{12}O_4S$ 228.268
Cryst. ($CHCl_3$). Mp 90-91°.
Reppe, W. *et al., Annalen*, 1955, **596**, 158 (*synth*)
Traynelis, V.J. *et al., J.O.C.*, 1961, **26**, 2728 (*deriv, synth*)
Truce, W.E. *et al., J.O.C.*, 1963, 964-967 (*S-Me*)
Kukalenko, S.S. *et al., Zh. Org. Khim.*, 1970, **6**, 680; *J. Org. Chem. USSR (Engl. Transl.)*, 1970, **6**, 682 (*deriv, synth*)
Danehy, J.P. *et al., J.O.C.*, 1971, **36**, 2530 (*synth*)
Thompson, C.M. *et al., J.O.C.*, 1989, **54**, 890 (*deriv, synth, pmr, cmr, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1990, **15**, 262 (*use, S-Ph, dioxide*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 254; 525 (*S-Me esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1017; 1799 (*S-Me esters*)

3-Mercapto-2-butanol, 9CI M-202

[54812-86-1]
FEMA 3502



(2*R*,3*S*)-*form*

$C_4H_{10}OS$ 106.188
Flavouring ingredient.
▶ Odour induces nausea.

(2*R*,3*S*)-*form*
(+)-erythro-*form*

Bp_{31} 73.5-74°. $[\alpha]_D^{25}$ +16. n_D^{25} 1.4783.
Hygroscopic.

(2*RS*,3*RS*)-*form*

(±)-threo-*form*
Bp_{10} 53°.

S-*Me:* [27022-36-2] *3-(Methylthio)-2-butanol*
$C_5H_{12}OS$ 120.215
Bp_{25} 78°.

Me ether:2-Mercapto-3-methoxybutane. 3-Methoxy-2-butanethiol
$C_5H_{12}OS$ 120.215
Bp_{100} 70°.

O,S-*Di-Me:* [37887-07-3] *2-Methoxy-3-(methylthio)butane*
$C_6H_{14}OS$ 134.242
Bp_{23} 63°.

(2*RS*,3*SR*)-*form* *(±)*-erythro-*form*
Bp_{10} 55-56°.

S-*Me:* [27022-37-3]
Bp_{21} 76°.

Me ether:
Bp_{15} 35-36.5°.

O,S-*Di-Me:* [37887-08-4]
Bp_{20} 58°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 423A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 345A (*ir*)
Price, C.C. *et al., J.A.C.S.*, 1953, **75**, 2396 (*synth, abs config, haz*)
Kondo, K. *et al., J.A.C.S.*, 1972, **94**, 5786 (*synth, pmr, ir, stereochem*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 451
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1684

4-Mercapto-1-butanol M-203

[14970-83-3]

$HSCH_2CH_2CH_2CH_2OH$

$C_4H_{10}OS$ 106.188
Liq. with unpleasant odour. Mp -99.2°. Bp_{20} 102-103° Bp_5 69-71° $Bp_{0.001}$ 38-43°.

S-*Me:* [20582-85-8] *4-(Methylthio)-1-butanol, 9CI. FEMA 3600*
$C_5H_{12}OS$ 120.215
Present in coffee. Flavouring ingredient. d^{22} 1. Bp_{20} 95-98° Bp_3 81-85°. n_D^{23} 1.4856.

Szarvasi, E. *et al., Bull. Soc. Chim. Fr.*, 1950, 463
Harding, J.S. *et al., J.C.S.*, 1954, 1536
Willems, J. *et al., Bull. Soc. Chim. Belg.*, 1955, **64**, 409
Goethals, E.J. *et al., Bull. Soc. Chim. Belg.*, 1965, **74**, 21 (*synth*)
Brown, H.C. *et al., J.A.C.S.*, 1968, **90**, 2902 (*S-Me*)
Harpp, D.N. *et al., J.O.C.*, 1976, **41**, 3987 (*S-Me*)
Robinson, P.L. *et al., Phosphorus Sulfur Relat. Elem.*, 1987, **31**, 59 (*synth, pmr, cmr*)
Köster, R. *et al., Annalen*, 1992, 835 (*synth, ir, ms, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 569 (*S-Me*)
Iglesias, L.E. *et al., Org. Prep. Proced. Int.*, 1996, **28**, 319 (*synth, pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1867 (*S-Me*)

4-Mercapto-2-butanol, 9CI M-204

3-Hydroxybutanethiol

$C_4H_{10}OS$ 106.188
Naturally occurring flavour volatile.

(*S*)-*form* [108861-09-2]

S-*Ph:* [110920-29-1] *4-(Phenylthio)-2-butanol, 9CI*
$C_{10}H_{14}OS$ 182.286
$[\alpha]_D^{23}$ +26.8 (c, 1.34 in $CHCl_3$) (96% ee).

(±)-*form* [30098-74-9]
Strong smelling mobile liq. d_4^{20} 1.02. Bp_{20} 88-92°. n_D^{20} 1.4840.

S-*Ac:* [140896-83-9]
$C_6H_{12}O_2S$ 148.226
Pale yellow liq. Bp_{55} 91-95°.

S-*Me:* [13296-23-6] *4-(Methylthio)-2-butanol, 9CI*
$C_5H_{12}OS$ 120.215
Formed during fermentation of white wines. Liq. Bp_{13} 88-91° $Bp_{0.6}$ 46-47°.

S-*Ph:* [149881-90-3]
Liq. Bp_2 105-106°.

[27998-52-3, 108861-08-1, 134641-08-0, 141041-27-2, 149883-16-9]

Huyser, E.S. *et al., J.O.C.*, 1966, **31**, 3366 (±-*form, S-Me, synth*)
Pihlaja, K. *et al., Acta Chem. Scand.*, 1970, **24**, 2257 (±-*form, synth*)
Allingham, Y. *et al., Org. Magn. Reson.*, 1971, **3**, 37 (±-*form, S-Ac, synth*)
Steadman, T.R. *et al., J. Agric. Food Chem.*, 1975, **23**, 1137 (±-*form, S-Me, synth*)
Ueno, Y. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 3615 (±-*form, S-Ph, synth, pmr*)
Brown, H.C. *et al., J.O.C.*, 1981, **46**, 930 (±-*form, S-Me deriv, synth*)
Fujisawa, T. *et al., Chem. Lett.*, 1987, 2227 (*R-form, S-form, S-Ph derivs, synth*)
Siedlecka, R. *et al., Synthesis*, 1994, 407 (±-*form, S-Ph, synth*)
Liu, H. *et al., J.O.C.*, 1995, **60**, 2022 (*S-form, S-Ph, synth, pmr, cmr, ir, ms, tlc*)

1-Mercapto-2-butanone M-205

[39861-37-5]

$H_3CCH_2COCH_2SH$

C_4H_8OS 104.173
Unstable liq. Undergoes ready dimerisation.

S-*Me:* [13678-58-5] *1-(Methylthio)-2-butanone. FEMA 3207*
$C_5H_{10}OS$ 118.199
Constit. of coffee concentrate. Flavouring agent. Liq. with mushroom odour with garlic undertone. d_4^{22} 1. Bp_8 52-53°. n_D^{20} 1.4700.

Tullio, B. *et al., Gazz. Chim. Ital.*, 1953, **83**, 1031-1036; 1956, **86**, 1168-1173 (*synth, dimer*)
Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628-694 (*S-Me, isol, synth*)
Shu, C.-K. *et al., J. Agric. Food Chem.*, 1985, **33**, 442-446 (*S-Me, formn, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 569 (*S-Me, use*)

3-Mercapto-2-butanone, 9CI M-206

[40789-98-8]
FEMA 3298

$H_3CCH(SH)COCH_3$

C_4H_8OS 104.173

(±)-*form*
Flavouring ingredient. d^{20} 1.02. Bp_{18} 50°. n_D^{20} 1.4694.

S-*Me:* [99315-41-0]

[53475-15-3] *3-(Methylthio)-2-butanone*
$C_5H_{10}OS$ 118.199
Bp_{20} 50-54°. n_D^{20} 1.4710.

S-*Ph:* [13023-53-5] *3-(Phenylthio)-2-butanone*
$C_{10}H_{12}OS$ 180.27
d_4^{22} 1.08. Bp_{15} 135°. n_D^{20} 1.5550 (1.5563).

S-*Ph, 2,4-dinitrophenylhydrazone:* [35875-07-1]
Yellow-orange powder (EtOH). Mp 101°.

Werner, E.G.G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1949, **68**, 509-519 (*S-Ph*)
Asinger, F. *et al., Annalen*, 1957, **610**, 25 (*synth, S-Me*)
Faller, P. *et al., Bull. Soc. Chim. Fr.*, 1962, 30-34 (*S-Ph*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 452
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1685

4-Mercapto-2-butanone, 8CI M-207

[34619-12-0]
2-Thiahexan-5-one. 2-Keto-4-butanethiol. FEMA 3357

$HSCH_2CH_2COCH_3$

C_4H_8OS 104.173
Flavouring ingredient. Oil. Bp_{15} 63-65°.

S-*Me:* [34047-39-7] *4-(Methylthio)-2-butanone, 8CI. FEMA 3375*
$C_5H_{10}OS$ 118.199
Flavouring ingredient. Bp_{55} 106° Bp_{16} 72-73°. n_D^{25} 1.4772.

S-*Me, 2,4-dinitrophenylhydrazone:*
Orange prisms (EtOH). Mp 100.5° (98.5-100°).

S-*Me, semicarbazone:*
Prisms ($CHCl_3$/petrol). Mp 127-128°.

S-*Me,* S-*oxide:4-Methylsulfinyl-2-butanone*
$C_5H_{10}O_2S$ 134.199
Cryst. (petrol). Mp 28-29°.

S-*Me,* S,S-*dioxide:* [68152-37-4] *4-Methylsulfonyl-2-butanone*
$C_5H_{10}O_3S$ 150.198
Cryst. (2-propanol). Mp 88-89°.

S-*Me,* S,S-*dioxide, oxime:*
$C_5H_{11}NO_3S$ 165.213
Needles (2-propanol). Mp 107-108°.

S-*Et:* [61224-82-6] *4-(Ethylthio)-2-butanone*
$C_6H_{12}OS$ 132.226
Oil. Bp_{17} 118-120°.

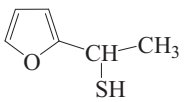
S-*Ph:* See 4-(Phenylthio)-2-butanone in *The Combined Chemical Dictionary.*

Cardwell, H.M.E. *et al., J.C.S.*, 1949, 715 (*S-Me, synth*)
Gill, N.S. *et al., J.A.C.S.*, 1952, **74**, 4923 (*synth, derivs*)
Böhme, H. *et al., Chem. Ber.*, 1953, **86**, 443 (*S,S-dioxide, synth*)
Pfister, K. *et al., J.A.C.S.*, 1955, **77**, 697 (*S-Me, synth*)
Murata, N. *et al., Kogyo Kagaku Zasshi*, 1956, **59**, 129 (*synth*)
Cain, M.E. *et al., J.C.S.*, 1962, 2959 (*derivs*)
McIntosh, J.M. *et al., Can. J. Chem.*, 1976, **54**, 1923 (*synth*)

Ozaki, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 734 (*S-Et*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 425; 570
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1522; 1868

2-(1-Mercaptoethyl)furan M-208

[96631-04-8]
α-Methyl-2-furanmethanethiol, 9CI



C_6H_8OS 128.195
Cysteine/cystine-derived Maillard product, present in model meat aroma systems. Characterised spectroscopically.

Krafft, G.A. *et al., Tet. Lett.*, 1985, **26**, 135-138 (*synth*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, ms, pmr*)
Hofmann, T. *et al., J. Agric. Food Chem.*, 1997, **45**, 898-906 (*occur, synth, ms, pmr*)

3-Mercaptohexanal M-209

$H_3CCH_2CH_2CH(SH)CH_2CHO$

$C_6H_{12}OS$ 132.226

(±)-*form*

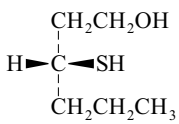
S-*Me:* [38433-74-8]

[149310-62-3] *3-(Methylthio)hexanal. FEMA 3877*
$C_7H_{14}OS$ 146.253
Flavouring ingredient. Bp_{10} 87-88°.

Winter, M. *et al., Helv. Chim. Acta*, 1976, **59**, 1613 (*synth, pmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1238

3-Mercapto-1-hexanol M-210

[51755-83-0]
FEMA 3850



(*R*)-*form*

$C_6H_{14}OS$ 134.242

(*R*)-*form* [90180-88-4]
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). $[\alpha]_D^{20}$ -6.18 (c, 10 in CCl_4). $[\alpha]_D^{20}$ -8.5 (c, 0.8 in $CHCl_3$).

O-*Ac:* [145937-71-9]
$C_8H_{16}O_2S$ 176.279
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). Characterised by pmr and ms.

S-*Me:* [90180-89-5] *3-(Methylthio)-1-hexanol*
$C_7H_{16}OS$ 148.269
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). Oil with weakly herbal odour. $[\alpha]_D^{20}$ -11.05 (c, 6.85 in CCl_4).

(*S*)-*form* [90180-90-8]
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). $[\alpha]_D^{20}$ +6.2 (c, 10 in CCl_4).

O-*Ac:* [145937-72-0]
$C_8H_{16}O_2S$ 176.279
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). Characterised by pmr and cmr.

O-*Butanoyl:* [136954-21-7]
$C_{10}H_{20}O_2S$ 204.333
Isol. from yellow passion fruit (*Passiflora edulis*). Flavouring ingredient. Characterised by pmr.

O-*Pentanoyl:*
$C_{11}H_{22}O_2S$ 218.36
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*).

O-*Hexanoyl:* [145937-76-4]

[136954-22-8, 145937-75-3]
$C_{12}H_{24}O_2S$ 232.386
Isol. from yellow passion fruit (*Passiflora edulis*). Flavouring ingredient. Characterised by pmr.

S-*Me:* [90180-91-9]
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). Oil with exotic, fruity odour. $[\alpha]_D^{20}$ +11.1 (c, 6.6 in CCl_4).

S-*Me,* O-*Ac:* [145937-78-6]

[51755-85-2]
$C_9H_{18}O_2S$ 190.306
Identified in volatile oil of *Passiflora edulis*. Flavouring ingredient.

S-*Me,* O-*butanoyl:* [145937-80-0]

[136954-23-9, 145937-79-7]
$C_{11}H_{22}O_2S$ 218.36
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). Characterised by pmr and ms.

S-*Me,* O-*hexanoyl:* [145937-82-2]

[136954-24-0, 145937-81-1]
$C_{13}H_{26}O_2S$ 246.413
Constit. of volatile oil of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). Characterised by pmr and ms.

(±)-*form*
Flavouring agent. Oil with intensely sulfurous odour. Bp_{10} 61-62° Bp 198°.

O-*Ac:* [136954-20-6] *3-Mercaptohexyl acetate. FEMA 3851*
$C_8H_{16}O_2S$ 176.279
Liq. d 0.994. Bp 186°.

O-*Butanoyl:3-Mercaptohexyl butyrate. FEMA 3852*
$C_{10}H_{18}O_2S$ 202.317
Flavouring agent. Liq. d 0.963. Bp 196°.

O-*Hexanoyl:3-Mercaptohexyl hexanoate. FEMA 3853*
$C_{12}H_{24}O_2S$ 232.386
Flavouring agent. Liq. d 0.945. Bp 280°.

S-*Me:*

[51755-66-9, 149403-20-3] *3-(Methylthio)-1-hexanol. FEMA 3438*
Flavouring ingredient. Bp_{10} 61-62°.

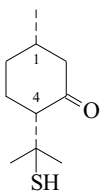
(ξ)-*form*
Isol. from yellow passion fruit (*Passiflora edulis*). Flavouring ingredient.

O,S-*Di-Ac:* [136954-25-1] S-*[1-[2-(Acetyloxy)ethyl]butyl] ethanethioate. 3-Acetylmercaptohexyl acetate. FEMA 3816*
$C_{10}H_{18}O_3S$ 218.316
Isol. from yellow passion fruit (*Passiflora edulis*). Flavouring ingredient. Characterised by pmr and ms.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 442C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 361C (*ir*)
Ger. Pat., 1974, 2 338 680; *CA*, **80**, 132786 (*synth*)
Winter, M. *et al., Helv. Chim. Acta*, 1976, **59**, 1613-1620 (*isol, pmr, ms, synth*)
Pickenhagen, W. *et al., Helv. Chim. Acta*, 1984, **67**, 947-952 (*synth*)
Heusinger, G. *et al., Tet. Lett.*, 1984, **25**, 507-510 (*R-form, S-form, S-Me, synth*)
Engel, K.H. *et al., J. Agric. Food Chem.*, 1991, **39**, 2249-2252 (*S-Me, Ac*)
Weber, B. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 426-428; 1994, **199**, 48-50 (*chiral glc, esters, synth, pmr*)
Weber, B. *et al., J. Agric. Food Chem.*, 1995, **43**, 2438-2441 (*esters*)
Werkhoff, P. *et al., J. Agric. Food Chem.*, 1998, **46**, 1076-1093 (*Passiflora constits*)
Bouchilloux, P. *et al., J. Agric. Food Chem.*, 1998, **46**, 3095-3099 (*O-Ac, occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 23; 1037-1040
van de Waal, M. *et al., Helv. Chim. Acta*, 2002, **85**, 1246-1260 (*Me ether*)

8-Mercapto-*p*-menthan-3-one, 8CI M-211

[38462-22-5]
2-(1-Mercapto-1-methylethyl)-5-methylcyclohexanone, 9CI. FEMA 3177



(1*S*,4*R*)-*form*

$C_{10}H_{18}OS$ 186.318
A mixt. of stereoisomers is used as a blackcurrant flavour.

(1*S*,4*R*)-*form* [35117-86-3]
(-)-cis-*form*
$[\alpha]_D^{20}$ -36 (neat).

S-*Ac:* [57129-12-1] *Menthone 8-thioacetate. FEMA 3809*
$C_{12}H_{20}O_2S$ 228.355
Flavour ingredient for various formulations (as mixt. with the *trans*-form). Present in Buchu leaf oil. $[\alpha]_D^{20}$ -34.1.

S-*Me:* [57129-15-4]
$C_{11}H_{20}OS$ 200.344
$[\alpha]_D^{20}$ -53.3.

(1*S*,4*S*)-*form* [35117-85-2] *(+)*-trans-*form*
$[\alpha]_D^{20}$ +21.5 (neat).

S-*Ac:* [57074-34-7]
Present in Buchu leaf oil. Flavouring ingredient. $[\alpha]_D^{20}$ +27.

S-*Me:* [57129-14-3]
$[\alpha]_D^{20}$ +29.2.

[33281-91-3, 33284-96-7, 34349-25-2, 34352-05-1, 94293-57-9]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 674A (*nmr*)
Sundt, E. *et al., Helv. Chim. Acta*, 1971, **54**, 1801 (*synth*)
Lamparsky, D. *et al., Parfums, Cosmet. Savons Fr.*, 1972, **2**, 465 (*isol*)
Kaiser, R. *et al., J. Agric. Food Chem.*, 1975, **23**, 943 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 444
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1674-1675

3-Mercapto-2-(mercaptomethyl)propanoic acid, 9CI M-212

[7634-96-0]
β,β′-Dimercaptoisobutyric acid. Dihydroasparagusic acid

$(HSCH_2)_2CHCOOH$

$C_4H_8O_2S_2$ 152.238
Isol. from asparagus *Asparagus officinalis*. Cryst. (petrol). Mp 59.5-60.5°.

S-*Ac:* [38146-83-7]
$C_6H_{10}O_3S_2$ 194.275
Constit. of asparagus*Asparagus officinalis*.

Jansen, E.F. *et al., J. Biol. Chem.*, 1948, **176**, 657 (*isol*)
Yanagawa, H. *et al., Synthesis*, 1973, 607 (*synth*)
Singh, R. *et al., J.A.C.S.*, 1990, **112**, 1190 (*synth, pmr*)

2-Mercapto-3-methyl-1-butanol M-213

$(H_3C)_2CHCH(SH)CH_2OH$

$C_5H_{12}OS$ 120.215

(±)-*form* [148154-24-9]
Bp_{13} 75-77°.

(ξ)-*form*
Substance found in beer causing unpleasant aftertaste.

Vegh, D. *et al., Coll. Czech. Chem. Comm.*, 1993, **58**, 404 (*synth*)

3-Mercapto-3-methyl-1-butanol, 9CI M-214

[34300-94-2]
FEMA 3854

$(H_3C)_2C(SH)CH_2CH_2OH$

$C_5H_{12}OS$ 120.215
Found in coffee volatiles, white wine and passion fruit. Flavouring agent for baked goods, meat products etc.. Mod. sol. H_2O (1%). d^{20} 0.999. Bp_{730} 186° Bp_{20} 87-89° Bp_{17} 85-90°. n_D^{20} 1.4725.

O-*Formyl:* [50746-10-6] *3-Mercapto-3-methylbutyl formate. FEMA 3855*
$C_6H_{12}O_2S$ 148.226
Present in coffee volatiles. Flavouring agent. Liq. Spar. sol. H_2O (0.1%). d 1.03. Bp 181° Bp_1 30-31°. n_D^{20} 1.4610.

O-*Ac:* [50746-09-3]
$C_7H_{14}O_2S$ 162.252
Present in passion fruit volatiles. Bp_1 39-40°. n_D^{20} 1.4616.

Me ether: [94087-83-9] *4-Methoxy-2-methyl-2-butanethiol, 9CI*
$C_6H_{14}OS$ 134.242
Present in blackcurrant buds/berries, virgin olive oil and Japanese green tea (Sen-cha). Liq. with blackcurrant-like odour.

Ger. Pat., 1973, 2 316 456; *CA*, **92**, 58054m (*synth, use, formate, O-Ac*)
Pihlaja, K. *et al., Org. Magn. Reson.*, 1979, **12**, 331-336 (*synth*)
Rigaud, J. *et al., Sci. Aliments*, 1986, **6**, 213-220; *CA*, **105**, 151683n (*Me ether, occur*)
Guth, H. *et al., Fett Wiss. Technol.*, 1991, **93**, 335-339 (*Me ether, occur, synth*)
Holscher, H. *et al., J. Agric. Food Chem.*, 1992, **40**, 655-658 (*occur, formyl*)
Guth, H. *et al., J. Am. Oil Chem. Soc.*, 1993, **70**, 513-518 (*Me ether, occur*)
Reiners, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 2754-2763 (*Me ether, occur, olive oil*)
Kumazawa, K. *et al., J. Agric. Food Chem.*, 1999, **47**, 5169-5172 (*Me ether, occur, green tea*)
Tominaga, T. *et al., J. Agric. Food Chem.*, 2000, **48**, 2874-2876 (*Ac, occur, ms*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1040-1041; 1053-1054 (*formyl, Me ether, use*)

3-Mercapto-2-methylpentanal, 9CI M-215

[227456-28-2]

$H_3CCH_2CH(SH)CH(CH_3)CHO$

$C_6H_{12}OS$ 132.226
Aroma constit. of cut raw onion. Viscous oil. Odour threshold 0.95 µg/L in H_2O.

Widder, S. *et al., J. Agric. Food Chem.*, 2000, **48**, 418-423 (*isol, synth*)

3-Mercapto-2-methylpentanol, 9CI M-216

[227456-27-1]

[227456-29-3, 227456-30-6, 227456-31-7, 227456-32-8]

$H_3CCH_2CH(SH)CH(CH_3)CH_2OH$

$C_6H_{14}OS$ 134.242
Aroma constit. of cut, raw onion. Powerful flavour compound. Liq. $Bp_{0.4}$ 44-46°. Bp data is for a 1:1 mixt. of diastereoisomers. Odour threshold 0.15 µg/L in H_2O as mixed isomers. Odour activity resides principally in the *threo*-diastereoisomers. All four diastereomers were obt. from onions and have been synthesised.

Eur. Pat., 1997, 924 198; *CA*, **131**, 44011g (*synth*)
Widder, S. *et al., J. Agric. Food Chem.*, 2000, **48**, 418-423; 424-427 (*isol, synth, struct, props, pmr, cmr, ms*)

4-Mercapto-4-methyl-2-pentanone, 9CI, 8CI M-217

[19872-52-7]

$(H_3C)_2C(SH)CH_2COCH_3$

$C_6H_{12}OS$ 132.226
Present in Sauvignon wines. Liq. with odour of cat urine. $Bp_{0.12}$ 55-58°.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH or petrol). Mp 102-103°.

S-*Ac:* [31539-83-0]
$C_8H_{14}O_2S$ 174.263
Liq. Bp_{20} 95°.

S-*Me:* [23550-40-5] *4-Methyl-4-(methylthio)-2-pentanone. Corps Cassis. FEMA 3376*
$C_7H_{14}OS$ 146.253
Flavouring ingredient with blackcurant aroma. Bp_{12} 84° Bp_{15} 78°. n_D^{13} 1.4750.

Foldi, Z. *et al., J.C.S.*, 1948, 1683-1685 (*synth*)
Asinger, A. *et al., Annalen*, 1957, **610**, 1-16 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 1971, **93**, 676-684 (*synth, nmr, ir*)
Ger. Pat., 1974, 2 338 680; *CA*, **80**, 132786x (*S-Me*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 573 (*S-Me*)
Darriett, P. *et al., Flavour Fragrance J.*, 1995, **10**, 385-392 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1871 (*S-Me*)
Tominaga, T. *et al., Flavour Fragrance J.*, 1997, **12**, 373-376 (*isol*)

3-[(2-Mercapto-1-methylpropyl)thio]-2-butanol M-218

[54957-02-7]

[57526-75-7, 57526-76-8, 57526-77-9, 57526-78-0]
α-Methyl-β-mercaptopropyl-α′-methyl-β′-hydroxypropyl sulfide. FEMA 3509

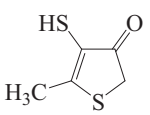
$H_3CCH(SH)CH(CH_3)SCH(CH_3)CH(OH)CH_3$

$C_8H_{18}OS_2$
Flavour ingredient for roast meat, poultry, soups and baked goods. $Bp_{0.4}$ 85-88°. No data on stereoisomers.

Ger. Pat., 1974, 2 417 385; *CA*, **82**, 123593w (*synth, use*)
U.S. Pat., 1975, 3 907 900; *CA*, **86**, 4927f (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 515 (*use*)

4-Mercapto-5-methyl-3(2*H*)-thiophenone, 9CI M-219

[26486-09-9]



$C_5H_6OS_2$ 146.234
Constit. of a synthetic roast meat-like odour produced from reaction of 4-Hydroxy-5-methyl-3(2*H*)-furanone, H-588 with H_2S. Characterised spectroscopically.

Ger. Pat., 1970, 1 932 800; *CA*, **72**, 90265d (*occur, use*)
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms, ir*)

9-Mercaptononanoic acid M-220

$HS(CH_2)_8COOH$

$C_9H_{18}O_2S$ 190.306

S-*Me, nitrile:* [58214-94-1] *9-(Methylthio)nonanenitrile, 9CI. 1-Cyano-8-(methylthio)octane*
Isol. from watercress (*Nasturtium officinale*). Liq. with a radish-like aroma.

Bp 278°. n_D^{20} 1.4764.

S-*Me, nitrile,* S-*oxide:* [75272-88-7] *9-(Methylsulfinyl)nonanenitrile. 8-Cyanooctyl methyl sulfoxide*
$C_{10}H_{19}NOS$ 201.332

S-*Et:*

[127705-22-0] *9-(Ethylthio)nonanoic acid. 10-Thialauric acid*
$C_{11}H_{22}O_2S$ 218.36Prepd. as Me ester.

Macleod, A.J. *et al., Phytochemistry*, 1977, **16**, 907 (*S-Me nitrile*)
Spencer, G.F. *et al., J. Sci. Food Agric.*, 1980, **31**, 359 (*ms, derivs*)
Lie Ken Jie, M.S.F. *et al., J.C.S. Perkin 2*, 1989, 2121 (*S-alkyl derivs*)
Christie, W.W. *et al., Biomed. Mass Spectrom.*, 1991, **20**, 629 (*ms, derivs*)
Repcak, M. *et al., Phytochemistry*, 1998, **47**, 1219-1221 (*isol, S-Me S-oxide nitrile*)

8-Mercaptooctanoic acid, 9CI M-221

$HS(CH_2)_7COOH$

$C_8H_{16}O_2S$ 176.279

Nitrile: [58214-93-0] *8-(Methylthio)octanenitrile, 9CI. 1-Cyano-8-(methylthio)-heptane*
$C_9H_{17}NS$ 171.306
Isol. from watercress (*Nasturtium officinale*). Liq. with a radish-like aroma. Bp 236°. n_D^{20} 1.4762.

MacLeod, A.J. *et al., Phytochemistry*, 1977, **16**, 907 (*isol, synth*)

4-Mercapto-2-oxobutanoic acid, 9CI M-222

[4273-28-3]

$HSCH_2CH_2COCOOH$

$C_4H_6O_3S$ 134.156

Only marginal stability in soln..No phys. props. reported.

S-*Me:* [583-92-6]

[51828-97-8] *4-(Methylthio)-2-oxobutanoic acid. α-Oxomethionine. FEMA 3881*
$C_5H_8O_3S$ 148.182
Found in provolone cheese. Flavouring agent. Oil or cryst. + $^1/_2H_2O$ (as Na salt). Mp >300° (as Na salt hemihydrate).

Szabo, J.L. *et al., J.A.C.S.*, 1948, **70**, 3667 (*synth, derivs*)
Yamada, S. *et al., J. Biochem. (Tokyo)*, 1957, **44**, 553-564 (*S-Me*)
Cooper, A.J. *et al., J. Biol. Chem.*, 1975, **250**, 527-532 (*pmr*)
Cooper, A.J.L. *et al., Arch. Biochem. Biophys.*, 1985, **239**, 556-566 (*synth, props*)
Nann, K.C. *et al., J. Labelled Compd. Radiopharm.*, 1994, **36**, 431-437 (*S-Me derivs, synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1245 (*S-Me*)

3-Mercapto-2-oxopropanoic acid M-223

[2464-23-5]
β-Mercaptopyruvic acid

$HSCH_2COCOOH$

$C_3H_4O_3S$ 120.129
Cryst. (Me_2CO/petrol). Mp 140-141°.

Na salt: [10255-67-1] *Sodium mercaptopyruvate. FEMA 3901*
Flavouring ingredient. Cryst. Mp 200° Mp 300°.

Parrod, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1942, **215**, 146 (*synth*)
Meister, A. *et al., J. Biol. Chem.*, 1954, **206**, 561 (*synth*)
Tanabe, S. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2843 (*synth*)
Pat. Coop. Treaty (WIPO), 1996, 96 10 927; *CA*, **125**, 56856a (*use*)

2-Mercapto-3-pentanone, 9CI M-224

[17042-24-9]

$H_3CCH_2COCH(SH)CH_3$

$C_5H_{10}OS$ 118.199
Aroma/flavour component of cooked meats. Maillard product from reaction of cysteine and ribose.

(±)-*form*
Bp_{15} 59-61°.

Asinger, F. *et al., Annalen*, 1957, **602**, 37-49 (*synth*)
Gough, T.E. *et al., Can. J. Chem.*, 1967, **45**, 2531-2535 (*conformn, pmr*)
Kerscher, R. *et al., J. Agric. Food Chem.*, 1998, **46**, 1954-1958 (*occur, bibl*)

3-Mercapto-2-pentanone, 9CI M-225

[67633-97-0]
FEMA 3300

$H_3CCH_2CH(SH)COCH_3$

$C_5H_{10}OS$ 118.199
Maillard product from reaction of cysteine and ribose. Aroma/flavour component of cookes meats. Flavouring agent. Odour threshold 0.7 μg/kg in H_2O.

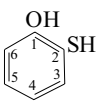
(±)-*form*
Bp_{11} 51-52°.

2,4-Dinitrophenylhydrazone:
Cryst. (MeOH). Mp 67°.

Asinger, F. *et al., Annalen*, 1964, **672**, 156-178 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 453 (*use*)
Kerscher, R. *et al., J. Agric. Food Chem.*, 1998, **46**, 1954-1958 (*occur, bibl*)

2-Mercaptophenol, 9CI M-226

[1121-24-0]
2-Hydroxybenzenethiol. 2-Hydroxythiophenol. o-Hydroxyphenyl mercaptan. Thiocatechol



C_6H_6OS 126.179
Oil. Mp 5-6°. $Bp_{0.15}$ 90°. Bp also given as 88-90°/8 mm.

Me ether: [7217-59-6] *2-Methoxybenzenethiol, 9CI. 2-Mercaptoanisole*
C_7H_8OS 140.206
Bp 218-219°.

► LD_{50} (rat, orl) 1740 mg/kg. DC1790000

S-*Me:* [1073-29-6] *2-(Methylthio)phenol, 9CI. 2-Hydroxythioanisole. FEMA 3210*
C_7H_8OS 140.206
Present in coffee. Flavouring agent. d_{25}^{25} 1.17. Bp 218-219° Bp_{22} 104-106°.

O,S-*Di-Me:* [2388-73-0] *1-Methoxy-2-(methylthio)benzene, 9CI*
$C_8H_{10}OS$ 154.232
Bp 237°.

Et ether: [54615-63-3] *2-Ethoxybenzenethiol, 9CI. 2-Mercaptophenetole*
$C_8H_{10}OS$ 154.232
Bp 226-227°.

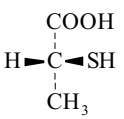
O,S-*Di-Et:* [85428-45-1] *1-Ethoxy-2-(ethylthio)benzene, 9CI*
$C_{10}H_{14}OS$ 182.286
Bp 248-250°.

Disulfide: See Bis(2-hydroxyphenyl) disulfide in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1175B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 419B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1091C (*ir*)
Haitinger, L. *et al., Monatsh. Chem.*, 1883, **4**, 170
Gattermann, L. *et al., Ber.*, 1899, **32**, 1136-1159 (*synth*)
Holt, H.S. *et al., J.A.C.S.*, 1924, **46**, 2333-2337 (*S-Me*)
U.S. Pat., 1969, 3 468 961; *CA*, **71**, 113938w (*synth*)
Fr. Pat., 1970, 2 036 086; *CA*, **75**, 63390 (*synth*)
U.S. Pat., 1972, 3 647 885; *CA*, **76**, 140178 (*synth*)
Hundscheid, F.J.A. *et al., Tetrahedron*, 1987, **43**, 5073-5088 (*Me ether, synth, pmr, cmr*)
Perez-Encabo, A. *et al., J.C.S. Perkin 1*, 1994, 629-642 (*di-Me, synth, ir, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 575 (*S-Me*)
Han, Y.S. *et al., Adv. Food Sci.*, 1996, **18**, 7-12 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1873 (*S-Me*)
Selassie, C.D. *et al., J.C.S. Perkin 2*, 1999, 2729-2733 (*S-Me, synth, pmr, cmr, ir, ms*)

2-Mercaptopropanoic acid, 9CI M-227

[79-42-5]
Thiolactic acid. FEMA 3180



(*R*)-*form*

$C_3H_6O_2S$ 106.145
Flavouring ingredient.

► UF5250000

(*R*)-*form* [33178-96-0]
Oil. Bp_{16} 95-100°. $[\alpha]_D^{23}$ +56.4 (c, 5 in EtOAc). Optically pure.

Me ester:
$C_4H_8O_2S$ 120.172
Yellow liq. Bp_{20} 78-80°. $[\alpha]_D^{25}$ +55.1 (c, 1.81 in $CHCl_3$).

Et ester: [103616-07-5]
$C_5H_{10}O_2S$ 134.199
Flavouring ingredient. Liq. Bp_{15} 75°. $[\alpha]_D^{22}$ +60.5 (c, 3 in $CHCl_3$). >98% e.e..

S-*Ac:*
$C_5H_8O_3S$ 148.182

Oil. $Bp_{0.3}$ 115° (bulb). $[\alpha]_D$ +136 (c, 1.06 in $CHCl_3$) (>98% op).

S-*Ac, Et ester:* [78560-77-7]
$C_7H_{12}O_3S$ 176.236
Oil. Bp_7 50°. $[\alpha]_{578}^{20}$ +137.5 (c, 3 in $CHCl_3$). Optically pure.

S-*Benzoyl:* [33179-02-1]
$C_{10}H_{10}O_3S$ 210.253
Needles (cyclohexane). Mp 62.5-63°. $[\alpha]_D^{23}$ +102 (c, 3.5 in $CHCl_3$).

(*S*)-*form* [57965-30-7]
Oil. $d^{19.2}$ 1.19. Bp_{15} 130° (bulb). $[\alpha]_D^{15}$ -45.47. $[\alpha]_D$ -54.3 (c, 5.76 in EtOAc) (95% op).

S-*Ac:*
$[\alpha]_D$ -135.5 (c, 4.35 in $CHCl_3$) (>98% op).

(±)-*form* [71563-86-5]
Oil with disagreeable odour. Sol. H_2O, EtOH, Et_2O. d_4^{15} 1.22. Mp *ca.* ° 10. Bp_{20} 110-115° Bp_{14} 98.5-99°. pK_{a1} 3.63; pK_{a2} 10.24 (20°).

Et ester: [66707-26-4] *FEMA 3279*
Flavouring ingredient. Liq. Spar. sol. H_2O.

Amide:
C_3H_7NOS 105.16
Mp 123-124°.

Anilide: [67201-68-7] *2-Mercapto*-N-*phenylpropanamide, 9CI*
$C_9H_{11}NOS$ 181.258
Cryst.

Nitrile: [100704-18-5] *2-Mercaptopropanenitrile. 2-Cyanoethyl mercaptan. 1-Cyano-2-mercaptoethane*
C_3H_5NS 87.145
Oil. Bp_6 57-59° $Bp_{0.18}$ 44-56°.

S-*Ac:* [6431-92-1]
Bp_3 55°.

S-*Me:* [58809-73-7] *2-(Methylthio)propanoic acid, 9CI*
$C_4H_8O_2S$ 120.172
Mp 17.3°. Bp_9 106.5°. Known also in opt. active forms.

S-*Me, Me ester:* [61366-76-5]
$C_5H_{10}O_2S$ 134.199
Mp 272°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 527C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 818B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 596C (*ir*)
Billmann, E. *et al., Annalen*, 1906, **348**, 120 (*synth*)
Mellander, A. *et al., Ark. Kemi, Sect. B*, 1936, **12**, 27; *Ark. Kemi, Sect. A*, 1937, **12**, 16 (*deriv*)
Eugster, C.H. *et al., Helv. Chim. Acta*, 1962, **45**, 1750 (*synth*)
Solladié-Cavallo, A. *et al., Bull. Soc. Chim. Fr.*, 1967, 517 (*synth, ir*)
Scopes, P.M. *et al., J.C.S.(C)*, 1971, 1671 (*cd, abs config*)
Fritz, J.S. *et al., Talanta*, 1972, **19**, 366 (*detn, Mo*)
Nacu, A. *et al., Rev. Roum. Chim.*, 1977, **28**, 1091 (*detn, Pd*)
Skiles, J.W. *et al., J. Med. Chem.*, 1986, **29**, 784 (*derivs*)
Strijtveen, B. *et al., J.O.C.*, 1986, **51**, 3664 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 245; 755
Brierer, D.E. *et al., J. Med. Chem.*, 1995, **38**, 2628 (*nitrile, synth, pmr, cmr*)
Tanabe, Y. *et al., J.C.S. Perkin 1*, 1995, 935 (*synth, pmr*)
Hof, R.P. *et al., J.C.S. Perkin 1*, 1995, 1247 (***synth***)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1006-1007; 1687
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFK250

3-Mercaptopropanoic acid, 9CI M-228

[107-96-0]
Thiohydracrylic acid
$HSCH_2CH_2COOH$
$C_3H_6O_2S$ 106.145
Cryst. Sol. H_2O, EtOH, Et_2O. d^{21} 1.22. Mp 16.8°. Bp_{13} 114-115.5° Bp_3 85-86°. n_D^{20} 1.4920. pK_{a1} 4.38; pK_{a2} 10.38 (25°).
▶ LD_{50} (rat, orl) 96 mg/kg. UF5270000

Me ester: [2935-90-2]
$C_4H_8O_2S$ 120.172
Bp_{20} 67-68°.

Et ester: [5466-06-8] *FEMA 3677*
$C_5H_{10}O_2S$ 134.199
Flavouring ingredient. Bp 162° . Bp_{10} 75-76°. n_D^{20} 1.4570.

Butyl ester: [16215-21-7]
$C_7H_{14}O_2S$ 162.252
Bp_{12} 101°. n_D^{20} 1.4570.

6-Methylheptyl ester: [30374-01-7]
$C_{11}H_{22}O_2S$ 218.36

Anilide: [10220-66-3] *3-Mercapto*-N-*phenylpropanamide, 9CI*
$C_9H_{11}NOS$ 181.258
Cryst.

Nitrile: [1001-58-7]
C_3H_5NS 87.145
Bp_3 40°.

S-*Me:* 3-(Methylthio)propanoic acid, M-689

S-*Ph:* See 3-(Phenylthio)propanoic acid in *The Combined Chemical Dictionary.*

[50727-77-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 527D; 670A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 818C; 1062A; 1062B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 596D; 728D; 729A (*ir*)
Billmann, E. *et al., Annalen*, 1906, **348**, 120 (*synth*)
Holmberg, B. *et al., Ark. Kemi, Sect. B*, No. 7, 1945, **21**, (*deriv*)
Cheney, L.C. *et al., J.A.C.S.*, 1945, **67**, 731 (*synth*)
Meyers, A.I. *et al., J.O.C.*, 1960, **25**, 1147 (*butyl ester*)
Danehy, J.P. *et al., J.O.C.*, 1967, **32**, 1491 (*synth*)
Traut, R.R. *et al., Biochemistry*, 1973, **12**, 3266 (*synth*)
Talipova, L.L. *et al., Zh. Anal. Khim.*, 1976, **31**, 106 (*detn, Re*)
Nacu, A. *et al., Rev. Roum. Chim.*, 1977, **28**, 1091 (*detn, Pd*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 246 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1007 (*Et ester*)
Org. Synth., 2000, **77**, 186-197 (*nitrile, synth, ir, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MCQ000

3-Mercapto-1-propanol, 9CI M-229

[19721-22-3]
$HOCH_2CH_2CH_2SH$
C_3H_8OS 92.162
Liq. with unpleasant odour. Bp_{14} 87° Bp_9 72-73°.

S-*Me:* [505-10-2] *3-(Methylthio)-1-propanol. 3-Hydroxypropyl methyl sulfide. FEMA 3415*
$C_4H_{10}OS$ 106.188
Widely distributed aroma constit. of foods and beverages e.g. wines, beers, stored apples, melon, pineapple, cheddar cheese, asparagus, tomato, shoyu, ham, roasted coffee, cooked clams, cooked shrimps, soy sauce etc.. d_4^4 1.03. Bp_{13} 89-90° Bp_6 72-72.5°. n_D^{20} 1.4832.

S-*Me,* O-*Ac:* [16630-55-0] *3-(Methylthio)propyl acetate. FEMA 3883*
$C_6H_{12}O_2S$ 148.226
Found in apple, melon, pineapple, beer, whisky and wine. Flavouring agent. Oil with fatty/ester odour. Bp_{14} 96°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 442A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 360B (*ir*)
Djerassi, C. *et al., J.A.C.S.*, 1953, **75**, 3704 (*synth*)
Harding, J.S. *et al., J.C.S.*, 1954, 1536 (*synth*)
Truce, W.E. *et al., J.O.C.*, 1961, **26**, 1463 (*S-alkyl derivs*)
Robinson, P.L. *et al., Phosphorus Sulfur Relat. Elem.*, 1987, **31**, 59 (*synth, pmr, cmr*)
Homatidou, V. *et al., Dev. Food Sci.*, 1990, **24**, 1011-1023 (*S-Me, detn, melon*)
Girard, B. *et al., Food Res. Int.*, 1995, **28**, 465-471 (*S-Me, apples*)
Iglesias, L.E. *et al., Org. Prep. Proced. Int.*, 1996, **28**, 319 (*synth, pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1874 (*S-Me, use, occur*)
Sekiwa, Y. *et al., J. Agric. Food Chem.*, 1997, **45**, 826-830 (*S-Me, detn, clams*)
Gomez-Plaza, E. *et al., Z. Lebensm.-Unters. - Forsch.*, 1999, **209**, 257-260 (*S-Me, detn, wine*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1251 (*S-Me S-Ac*)

1-Mercapto-2-propanone, 9CI M-230

[24653-75-6]
Acetonyl mercaptan. Mercaptoacetone. 2-Oxopropanethiol. FEMA 3856
H_3CCOCH_2SH
C_3H_6OS 90.146
Present in pork volatiles. Used in roast pork flavours. Solid with powerful, sweetish odour. Mp 112-114° (109-111°). Unstable above 0°.

S-*Me:* [14109-72-9] *1-(Methylthio)-2-propanone, 9CI. (Methylthio)acetone, 8CI. 2-Thia-4-pentanone. FEMA 3882*
C_4H_9OS 105.181
Present in roasted sesame seed oil, cooked beef liver and acid hydrolysed

soy protein. Flavouring agent. Pale yellow liq. with melon-like odour. d_4^{20} 1.02. Bp_{100} 90-92°. n_D^{25} 1.4713.

Hromatka, O. *et al., Monatsh. Chem.*, 1948, **78**, 29 (*synth*)
Asinger, F. *et al., Annalen*, 1963, **661**, 95 (*synth*)
Hancock, J.R. *et al., Can. J. Chem.*, 1983, **61**, 1472-1480 (*S-Me, synth, pmr, ms*)
Klein, R.F.X. *et al., J.O.C.*, 1986, **51**, 4644 (*synth*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1988, **53**, 1891-1899 (*S-Me, occur, ms*)
Ishibashi, H. *et al., Synth. Commun.*, 1989, **19**, 443-452 (*S-Me, synth, pmr*)
Werkhoff, P. *et al., Adv. Food Sci.*, 1996, **18**, 19-27 (*S-Me, occur, ms*)
Aaslyng, M.D. *et al., J. Agric. Food Chem.*, 1998, **46**, 5225-5231 (*S-Me, occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1044; 1249 (*S-Me, use*)

Mercenene M-231

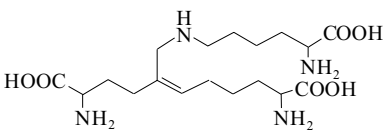
[8057-77-0]

Struct. unknown; the active principle is a low-MW species loosely bound to a protein or glycoprotein. Isol. from the common clam *Mercenaria mercenaria* and from *Mercenaria campechiensis*. Sol. H_2O; poorly sol. MeOH, hexane. λ_{max} 214 ; 234 ; 250 ; 274 (H_2O) (Berdy).

Schmeer, M.R. *et al., Ann. N.Y. Acad. Sci.*, 1966, **136**, 211-218 (*isol*)
Schmeer, M.R. *et al., Life Sci.*, 1966, **5**, 1169-1178 (*isol*)
Schmer, A.C. *et al., Natl. Cancer Inst. Monogr.*, 1969, **31**, 581-591 (*antitumour activity*)

Merodesmosine M-232

[17096-97-8]
2,10-Diamino-5-[[(5-amino-5-carboxypentyl)amino]methyl]-5-undecenedioic acid, 9CI



$C_{18}H_{34}N_4O_6$ 402.49
Aminoacid from reduced elastin.

[51510-36-2]

Starcher, B.C. *et al., Biochemistry*, 1967, **6**, 2425 (*isol, struct, ir, pmr, uv, ms*)
Paz, M.A. *et al., Biochem. Biophys. Res. Commun.*, 1971, **44**, 1518 (*ms*)

Mesentericin Y105 M-233

[169591-94-0]

[178668-22-9]

Peptide containing 36 amino acid residues and one disulfide bond. Prod. by *Leuconostoc mesenteroides* Y105 isol. from goat's milk. A non-lantibiotic bacteriocin. Mesentericin $Y105^{37}$ containing an additional Trp at the COOH terminus also produced.

Hechard, Y. *et al., J. Gen. Microbiol.*, 1992, **138**, 2725-2731 (*struct*)
Hechard, Y. *et al., NATO ASI Ser., Ser. H*, 1992, **65**, 421-426 (*struct*)
Fleury, Y. *et al., J. Biol. Chem.*, 1996, **271**, 14421-14429 (*Mesentericin $Y105^{37}$*)

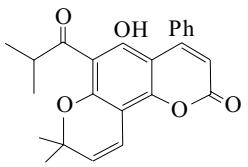
Mesenterocin 52 M-234

[148937-48-8]
Prod. by *Leuconostoc mesenteroides* FR52 from raw milk. Bacteriocin.

Mathieu, F. *et al., J. Appl. Bacteriol.*, 1993, **74**, 372-379 (*isol*)

Mesuagin M-235

[21721-08-4]
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-phenyl-2H,8H-benzo[1,2-b:3,4-b′]dipyran-2-one, 9CI. 5-Hydroxy-6-isobutyryl-8,8-dimethyl-4-phenyl-2H,8H-benzo[1,2-b:3,4-b′]dipyran-2-one, 8CI



$C_{24}H_{22}O_5$ 390.435
Constit. of seeds of *Mammea americana* (mamey). Pale-yellow cryst. (hexane). Mp 152-153°.

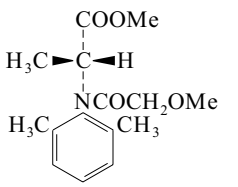
Ac: [21721-11-9]
Needles (C_6H_6/petrol). Mp 166-167°.

Me ether: [21721-10-8] ***Mesuarin***
$C_{25}H_{24}O_5$ 404.462
Cryst. (hexane). Mp 129-130°. λ_{max} 233 (ϵ 42660); 282 (ϵ 22400); 360 (ϵ 12600) (EtOH) (Berdy).

Chakraborty, D.P. *et al., J.O.C.*, 1969, **34**, 3784 (*isol, uv, ir, pmr, ms*)
Bala, K.R. *et al., Phytochemistry*, 1971, **10**, 1131 (*synth, uv*)
Bhattacharyya, P. *et al., Chem. Ind. (London)*, 1988, 239 (*isol*)

Metalaxyl, ANSI, BSI, ISO M-236

[57837-19-1]
Methyl N-*(2-methoxyacetyl)*-N-*(2,6-dimethylphenyl)alaninate, 9CI. Apron. Mefenoxam.* ***Metalaxyl-M, BSI, ISO.*** *Ridomil. CGA 48988*



(*R*)-*form*

$C_{15}H_{21}NO_4$ 279.335
► AY6910000
(R)-form [70630-17-0]
Oil. $[\alpha]_D^{20}$ -55 (c, 1.89 in Me_2CO).
(±)-form
Systemic agricultural fungicide. Cryst. solid. Sol. most org. solvs.; sl. sol. H_2O. Mp 71-72°.
► LD_{50} (rat, orl) 669 mg/kg.
U.K. Pat., 1974, 1 500 581; *CA*, **84**, 30713m
Urech, P.A. *et al., Phytiatr.-Phytopharm.*, 1978, **27**, 239 (*rev*)
Kerkenaar, A. *et al., Pestic. Biochem. Physiol.*, 1981, **15**, 71 (*activity*)
Fisher, D.J. *et al., Pestic. Sci.*, 1982, **13**, 330 (*activity*)
Ripley, B.D. *et al., J. Agric. Food Chem.*, 1985, **33**, 560 (*glc, ms*)
Gozzo, F. *et al., Pestic. Sci.*, 1985, **16**, 277 (*activity*)
Effenberger, F. *et al., Annalen*, 1986, 314 (*synth*)
Pesticide Manual, 11th edn., 1997, No. 470; No. 471
Pesticide Manual, 12th edn., 2000, No. 502 (*Metalaxyl-M*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MDM100

Metaphosphoric acid ($H_6P_6O_{18}$) M-237

[18694-07-0]
Cyclohexaphosphoric acid. Hexametaphosphoric acid
$H_6P_6O_{18}$
$H_6O_{18}P_6$ 479.879
The free acid is not a chem. entity but a mixt. of higher polyphosphoric acids.
Hexa-Na salt: Hexasodium metaphosphate ($P_6O_{18}^{6\ominus}$),
Hexa-NH_4 salt: Hexaammonium metaphosphate (P_6O_{18} See $^{6\ominus}$) in *The Combined Chemical Dictionary.*
Tri-Ca salt: [32280-49-2]

[10102-76-8]
$Ca_3O_{18}P_6$ 594.066
Used in food processing as a sequestrant. Cryst. + $9H_2O$. Loses $6H_2O$ at 110° and the remaining $3H_2O$ at 350°.

Tri-Ba salt:
White cryst. + $8H_2O$. Struct. contains 8- and 10-coordinate $Ba^{2\oplus}$.

Boulle, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1938, **206**, 507-508 (*Ca salt, synth*)
Huhti, A.L. *et al., Can. J. Chem.*, 1956, **34**, 789-797 (*struct*)
Thilo, E. *et al., Z. Anorg. Allg. Chem.*, 1957, **290**, 209-222 (*Ca salt, synth*)
Rzaigui, M. *et al., Acta Cryst. C*, 1992, **48**, 241-243 (*Ba salt*)
Rzaigui, M. *et al., J. Solid State Chem.*, 1994, **108**, 11-17 (*synth, ir, struct*)
Abid, S. *et al., Bull. Soc. Chim. Belg.*, 1995, **104**, 1-6 (*synth, ir, dta, cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 389-390 (*Ca salt*)

Metatartaric acid M-238

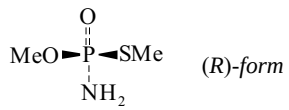
[39469-81-3]
E 353
The hemipolyactide of tartaric acid, formed by self-esterification. Used to stabilise fine wines by inhibiting potassium bitartrate crystal formn.. Pale yellow solid. Sol. H_2O. Slowly hydrolyses to tartaric acid.

Scazzola, E. *et al., CA*, 1960, **54**, 17787f (*synth, use*)
Fr. Pat., 1960, 1 203 111; *CA*, **55**, 19799b (*synth*)
Ingram, A.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 253-257 (*tox*)
Weger, B. *et al., Wein-Wiss.*, 1982, **37**, 193-207; *CA*, **98**, 87549f (*use*)

Methamidophos, BSI M-239

[10265-92-6]

O,S-*Dimethyl phosphoramidothioate, 9CI.* O,S-*Dimethyl amidothiophosphate. Filitox. Tamaron*



(*R*)-*form*

$C_2H_8NO_2PS$ 141.13

▶ LD_{50} (rat, orl) 7.5 mg/kg. LD_{50} (rat, skn) 50 mg/kg. Exp. teratogenic effects. Exp. and human neurotoxic effects. TB4970000

(*R*)-*form* [65960-95-4]

$[\alpha]_D$ +24 (c, 0.5 in $CHCl_3$).

(±)-*form* [115182-35-9]

Agricultural systemic insecticide and acaricide. Metab. of Acephate. Needles (petrol). Sol. H_2O, EtOH; mod. sol. $CHCl_3$, C_6H_6, Et_2O.

[65960-97-6]

Lubkowitz, J.A. *et al., J. Agric. Food Chem.*, 1974, **22**, 151 (*synth, ms, pmr*)
Holmstead, R.L. *et al., J. Assoc. Off. Anal. Chem.*, 1974, **57**, 1050 (*ms*)
Hall, C.R. *et al., J.C.S. Perkin 1*, 1979, 1646 (*stereochem*)
Thompson, C.M. *et al., J. Agric. Food Chem.*, 1982, **30**, 282; 1983, **31**, 696 (*synth, pmr, cmr, tox*)
Robinson, C.P. *et al., J. Appl. Toxicol.*, 1982, **2**, 217 (*tox*)
Schneider, P. *et al., J. Prakt. Chem.*, 1982, **324**, 1063 (*props*)
Agrochemicals Handbook, Royal Society of Chemistry, 1983, A265
Ripley, B.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 1084 (*glc*)
Miyazaki, A. *et al., J. Agric. Food Chem.*, 1988, **36**, 835 (*synth, resoln, activity*)
Solov'ev, V.N. *et al., Phosphorus, Sulfur, Silicon, Relat. Elem.*, 1991, **57**, 135 (*cryst struct*)
Pesticide Manual, 11th edn., 1997, No. 479
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1090
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTQ400

Methanedithiol, 9CI M-240

[6725-64-0]

Dimercaptomethane

$H_2C(SH)_2$

CH_4S_2 80.175

Component of mushroom and onion flavour. Liq. with powerful offensive odour. Bp_{80} 58°. n_D^{25} 1.5840.

Ca salt: [135778-01-7]
Solid.

S,S-*Dibenzoyl:Methylene thiobenzoate*
$C_{15}H_{12}O_2S_2$ 288.391
Long needles (EtOH). Mp 119-119.5°.

S-*Me,* S-*Ac:* [38634-59-2] S-*[(Methylthio)methyl]ethanethioate*
$C_4H_8OS_2$ 136.239
Liq. Bp_{11} 71-72°.

S,S-*Di-Me:* Bis(methylthio)methane, B-150

S,S-*Di-Et:* See Bis(ethylthio)methane in *The Combined Chemical Dictionary.*

S,S-*Di-Ph:* See Bis(phenylthio)methane in *The Combined Chemical Dictionary.*

S,S-*Divinyl:* See Bis(vinylthio)methane in *The Combined Chemical Dictionary.*

[105064-28-6]

Wheeler, H.L. *et al., J.A.C.S.*, 1902, **24**, 439 (*dibenzoyl*)
Bohme, H. *et al., Ber.*, 1941, **74**, 1667 (*S,S-di-Me*)
Cairns, T.L. *et al., J.A.C.S.*, 1952, **74**, 3982 (*synth*)
Dubs, P. *et al., Helv. Chim. Acta*, 1978, **61**, 2351 (*S-Me S-Ac*)
Adolfsson, L. *et al., Chem. Scr.*, 1980, **16**, 122 (*synth*)
Sinha, N.K. *et al., J. Agric. Food Chem.*, 1992, **40**, 842 (*isol, glc, ms*)

Methanesulfonothioic acid, 9CI M-241

[44059-82-7]

[1950-85-2]

$MeSO_2SH$

$CH_4O_2S_2$ 112.173

Hygroscopic cryst. (EtOH)(as Na salt). Mp 271-272° (Na salt).

Me ester: [2949-92-0] *Methyl methanethiosulfonate*
$C_2H_6O_2S_2$ 126.2
Isol. from cauliflower (*Brassica oleracea* var. *botrytis*). Detected in the aroma of caucas (*Allium victorialis*). Antimutagenic agent. Oil. $Bp_{4.5}$ 96-97° Bp_1 75-76°.

▶ PB2765000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 881A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1440A (*nmr*)
Bentley, M.D. *et al., J.O.C.*, 1972, **37**, 333-334 (*synth*)
Slusarchyk, W.A. *et al., J.O.C.*, 1973, **38**, 943-950 (*synth, use*)
Smith, D.J. *et al., Biochemistry*, 1975, **14**, 766-771 (*synth, use, Me ester*)
Currier, S.F. *et al., Biochemistry*, 1977, **16**, 1944-1948 (*synth, use, Me ester*)
Kenyon, G. *et al., Methods Enzymol.*, 1978, **47**, 407-430 (*synth, use, rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 243; 1986, **12**, 325 (*use*)
Shaked, Z. *et al., Biochemistry*, 1980, **19**, 4156-4166 (*synth*)
Nishimura, H. *et al., J. Agric. Food Chem.*, 1988, **36**, 563-566 (*occur, ester*)
Barbarella, G. *et al., J. Magn. Reson.*, 1990, **88**, 277-283 (*O-17 nmr, S-33 nmr*)
Machion, P.D. *et al., Synth. Commun.*, 1990, **20**, 365-370 (*synth, bibl*)
Nakamura, Y. *et al., Biol. Pharm. Bull.*, 1993, **16**, 207-209 (*isol, ester*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **5**, 3538-3541 (*Me ester, use*)
Org. Synth., 2000, **78**, 99-103 (*Me ester, synth, ir, pmr, cmr*)

Methanethiol, 9CI, 8CI M-242

[74-93-1]

Methyl mercaptan. Methyl thioalcohol. Mercaptomethane. FEMA 2716

MeSH

CH_4S 48.109

Flavouring agent. Isol. from higher plants, e.g. radish (*Raphanus sativus*), also present in orange juice, pineapple, strawberries, asparagus, wheatbread, gruyere cheese, hop oil, coffee, roasted filberts, cooked rice and other foods. Gas with odour of rotten cabbage. Sol. H_2O. d_4^{20} 0.87. Mp -123°. Bp 5.95°. pK_a 10.33 (25°). Forms a cryst. hydrate.

▶ Extremely flammable, fl. p. -18°, OES: long-term 0.5 ppm. PB4375000

Hg deriv.:
Mp 176°.

[7175-75-9, 17302-63-5]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 335B (*ir*)
Arndt, F. *et al., Ber.*, 1921, **54**, 2236 (*synth*)
Ellis, L.M. *et al., J.A.C.S.*, 1932, **54**, 1674 (*synth*)
Reid, E.E. *et al., Organic Chemistry of Bivalent Sulphur*, Chemical Publishing Co., 1958, **1**, 15 (*rev*)
Levy, F.J. *et al., Anal. Chem.*, 1961, **33**, 707 (*ms*)
Pettit, G.R. *et al., Can. J. Chem.*, 1964, **42**, 2537 (*pmr*)
Yang, S.F. *et al., Biochem. Biophys. Res. Commun.*, 1966, **24**, 739 (*biosynth*)
Taguchi, T. *et al., Tet. Lett.*, 1969, 3631 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MLE650
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0466
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 817

Methanol, 9CI, 8CI M-243

[67-56-1]

Methyl alcohol. Hydroxymethane. Wood alcohol. Carbinol

MeOH

CH_4O 32.042

For esters see the relevant acids. Present in various wines and spirits. Used as a solvent for the preparation of modified hop extracts and spice oleoresins. Liq. Misc. H_2O, most org. solvs.; part. misc. petrol. d_4^{20} 0.79. Mp -97.8°. Bp 64.7° Bp_{200} 34.8° Bp_{40} 5°. n_D^{20} 1.3287. pK_a -1.98 (base). Dissolves many inorg. salts. Combines with $CaCl_2$. Crit. point 242°/78.6 atm. Forms constant-boiling mixts. with nearly all common solvs..

▶ Highly flammable, fl. p. 10°, autoignition temp. 385°. Violent reaction with a range of materials. Effects of acute exposure in humans and non-human primates are optic neuropathy, metabolic acidosis and respiratory depression *via* ingestion, inhalation or skin absorption. Blindness may occur from ingestion of 4 ml. Chronic exposure to vapour concs. 1200-8300 ppm may also impair vision. Contact with liq. may damage eyes, prolonged or repeated skin contact causes dermatitis, erythema and scaling. OES: long-term 200 ppm; short-term 250 ppm (Sk). PC1400000

Na salt: See Sodium methoxide in *The Combined Chemical Dictionary.*

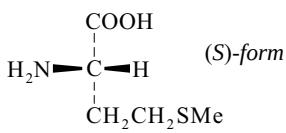
[811-98-3, 1455-13-6, 1849-29-2, 2143-68-2, 3315-60-4, 14742-26-8, 17836-08-7]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 163A (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 109B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 155B (*ir*)
Rodd's Chem. Carbon Compd. (2nd edn.), 1965, **1B**, 16 (*rev*)
Ger. Pat., 1970, 20 13 297; *CA*, **75**, 151351 (*manuf*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **15**, 398 (*rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 463
Gesser, H.D. *et al., Chem. Rev.*, 1985, **85**, 235 (*rev, manuf*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1103
Methanol: International Thermodynamic Tables of the Fluid State, (Eds. de Reuck, K.M. *et al*), IUPAC, 1993, (*thermodynamics*)
Fall, R. *et al., Trends Plant Sci.*, 1996, **1**, 9 (*rev, occur*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4528
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MGB150
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0462
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 818
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 3
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 320

Methionine, 9CI, INN M-244

[7005-18-7]
2-Amino-4-(methylthio)butanoic acid. S-*Methylhomocysteine*. *Met*



(*S*)-*form*

$C_5H_{11}NO_2S$ 149.213

(*R*)-*form* [348-67-4]
D-form
$[\alpha]_D^{25}$ +8.12 (H_2O). $[\alpha]_D$ -23.5 (1*M* HCl).
▶ LD_{50} (rat, ipr) 5223 mg/kg. PD0455000

Me ester: [21691-49-6]
$C_6H_{13}NO_2S$ 163.24
Mp 149-150° (as hydrochloride). $[\alpha]_D^{21}$ -26.3 (c, 5 in H_2O).

(*S*)-*form* [63-68-3]
L-form
Dietary supplement and nutrient. Plates. Mod. sol. H_2O (3.5 g/100 g at 25°). Mp 283° dec. $[\alpha]_D^{25}$ -14.9 (H_2O). $[\alpha]_D$ +34.6 (5*M* HCl). pK_{a1} 2.17; pK_{a2} 9.2 (20°, 0.15*M* $NaClO_4$). Log P -1.73 (calc). Isoelectric point 5.74. Appetising taste.
▶ LD_{50} (rat, orl) 36000 mg/kg. Exp. reprod. and teratogenic effects (v. large doses). PD0457000

S-*Oxide:* See Methionine sulfoxide in *The Combined Chemical Dictionary.*

S,S-*Dioxide:* [7314-32-1] *Methionine sulfone*
$C_5H_{11}NO_4S$ 181.212
$[\alpha]_D^{20}$ +29.7 (c, 1 in 1*M* HCl).

Me ester: [2491-18-1]

[10332-17-9]
Mp 150° (as hydrochloride). $[\alpha]_D^{19}$ +26.8 (c, 5 in H_2O) (hydrochloride). CAS no. refers to hydrochloride.

Et ester: [2899-36-7]

[3082-77-7]
$C_7H_{15}NO_2S$ 177.267
Mp 81-82° (as hydrochloride). $[\alpha]_D^{21}$ +18.7 (c, 2.2 in EtOH) (hydrochloride). CAS no. refers to hydrochloride.

Amide: [4510-08-1] *Methioninamide*
$C_5H_{12}N_2OS$ 148.229
Mp 43-44°. $[\alpha]_D^{19.5}$ -28.4 (c, 2.1 in DMF).

N-*Formyl:* [4289-98-9]
$C_6H_{11}NO_3S$ 177.224
Cryst. (EtOH/petrol). Mp 98-99°. $[\alpha]_D^{25}$ -10 (H_2O).

N-tert-*Butyloxycarbonyl:* See *tert*-Butyloxycarbonylmethionine in *The Combined Chemical Dictionary.*

(±)-*form* [59-51-8]
Racemethionine, USAN. *Petameth. FEMA 3301*
Flavouring ingredient; dietary supplement. Plates. Mp 281° dec. pK_{a1} 2.13; pK_{a2} 9.28 (25°).
▶ Exp. reprod. and teratogenic effects (v. large doses). PD0456000

S-*Oxide:* See Methionine sulfoxide in *The Combined Chemical Dictionary.*

S,S-*Dioxide:* [820-10-0]

[1118-85-0]
$C_5H_{11}NO_4S$ 181.212
Cryst. (H_2O). Mp 254° dec.

Me ester: [43189-32-8]
Mp 109-111° (as hydrochloride).

Et ester: [452-95-9]
Bp_{25} 112°.

N-*Formyl:* [4309-82-4]
Cryst. (EtOAc). Mp 99-100°.

N-*Ac:* *N*-Acetylmethionine,

N-*Benzoyl:* [4703-38-2]
$C_{12}H_{15}NO_3S$ 253.321
Cryst. (EtOH aq.). Mp 143-145°.

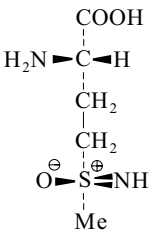
N-*(2,4-Dinitrophenyl):*
Cryst. (Et_2O/petrol). Mp 117-118°.

[3654-96-4, 56329-42-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 593A; 594B; 594C; 676D; 677A; 880A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 893C; 894A; 1075B; 1075C (*nmr*)
Org. Synth., 1934, **14**, 58 (*synth*)
Dekker, C.A. *et al., J. Biol. Chem.*, 1949, **180**, 155
Brenner, M. *et al., Helv. Chim. Acta*, 1951, **34**, 2085
Biochem. Prep., 1955, **4**, 80 (*oxide*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., Vol. 3, 1961, 2125 (*rev*)
Biemann, K. *et al., J.A.C.S.*, 1962, **84**, 3192 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Bruton, C.J. *et al., Biochem. J.*, 1968, **108**, 281-288 (*amide, biochem*)
Torii, K. *et al., Acta Cryst. B*, 1973, **29**, 2799 (*cryst struct*)
Richman, P.G. *et al., J. Biol. Chem.*, 1973, **248**, 6684
Clandinin, M.T. *et al., Phytochemistry*, 1974, **13**, 585 (*biosynth*)
Oguri, T. *et al., Chem. Pharm. Bull.*, 1975, **23**, 167 (*synth*)
Appel, R. *et al., Chem. Ber.*, 1983, **116**, 2037-2040 (*amide*)
Stipanuk, M.H. *et al., Annu. Rev. Nutr.*, 1986, **6**, 179 (*rev, metab*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 345
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MDT750
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 683
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 455
Dalhus, B. *et al., Acta Chem. Scand.*, 1996, **50**, 544-545 (*cryst struct, L-form*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1688-1691
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MDT730; MDT740; MDT750

Methionine sulfoximine M-245

[1982-67-8]
S-*(3-Amino-3-carboxypropyl)*-S-*methylsulfoximine, 9CI*. *2-Amino-4-(*S-*methylsulfonimidoyl)butanoic acid*



(*S*)$_C$,(*S*)$_S$ -*form*

$C_5H_{12}N_2O_3S$ 180.227
Found in flours treated with NCl_3 as a prod. of NCl_3 action on wheat proteins.

(*S*)$_C$(*S*)$_S$-*form* [15985-39-4]
Cnestine. Glabrin†
Mp 239°. $[\alpha]_D^{22}$ +34 (c, 2 in HCl).
▶ Neurotoxin, convulsive agent, potent glutamine synthetase inhibitor. Induces hypothermia in exp. animals.

(*S*)$_C$(*R*)$_S$-*form* [21752-31-8]
Mp 235°. $[\alpha]_D^{22}$ +39 (c, 2 in 1*M* HCl).

[21752-32-9]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 805C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 905A (*ir*)
Christensen, B.W. *et al., Chem. Comm.*, 1969, 169 (*cryst struct, abs config*)
Sugiyama, Y. *et al., Tet. Lett.*, 1983, **24**, 1471 (*isomers, synth*)
Chevrier, B. *et al., Acta Cryst. C*, 1986, **42**, 1632 (*cryst struct, bibl*)
Murakoshi, I. *et al., Chem. Pharm. Bull.*, 1993, **41**, 388 (*isol, abs config*)

Methomyl, BSI M-246

[16752-77-5]
Methyl N-*[[(methylamino)carbonyl]oxy]ethanimidothioate, 9CI*. S-*Methyl* N-*(methylcarbamoyloxy)thioacetimidate*. N-*[[(Methylamino)carbonyl]oxy]-2-(methylthio)ethanimine. Nudrin. Lannate*

MeNHCOON=C(CH_3)SMe

$C_5H_{10}N_2O_2S$ 162.212
Agricultural insecticide and nematocide. Cryst. solid. V. sol. Me_2CO, EtOH, MeOH, toluene; mod. sol. H_2O. Mp 78-79°. Coml. product is a mixt. of (*Z*)- and (*E*)-isomers.

▶ Cholinesterase inhibitor. Symptoms from occup. exposure incl. miosis, nausea, muscle weakness and other cholinergic effects. LD_{50} (rat, orl) 17 mg/kg. LC_{50} (rat, ihl) 77 ppm. OES: long-term 2.5 mg m^{-3} (Sk). AK2975000

(E)-form [19145-17-6]
Mp 43.5°.

S-*Oxide:* [55620-23-0]
$C_5H_{10}N_2O_3S$ 178.212
Cryst. Mp 72-73.5°.

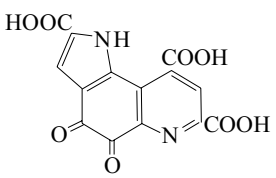
S,S-*Dioxide:* [55620-24-1]
$C_5H_{10}N_2O_4S$ 194.211
Cryst. (EtOH). Mp 107.5-109°.

[19145-10-9, 115809-61-5]

U.S. Pat., 1964, 3 576 834; *CA*, **75**, 19985v
Pease, H.L. *et al., J. Agric. Food Chem.*, 1968, **16**, 554 (*glc*)
Davies, J.H. *et al., J.C.S.(C)*, 1968, 431 (*synth, isomers*)
Roodhans, G.A. *et al., Meded. Fac. Landbouwwet., Rijksuniv. Gent*, 1968, **33**, 833 (*props, activity*)
Sim, G.A. *et al., J.C.S.(B)*, 1971, 752 (*cryst struct*)
Harvey, J. *et al., J. Agric. Food Chem.*, 1973, **21**, 769 (*metab, S-oxides*)
Takusagawa, F. *et al., J. Agric. Food Chem.*, 1977, **25**, 577 (*cryst struct*)
Thean, J.E. *et al., J. Assoc. Off. Anal. Chem.*, 1978, **61**, 15 (*hplc*)
Aranda, G. *et al., Bioorg. Chem.*, 1987, **15**, 346 (*pmr, cmr, S-oxide, bibl*)
Pesticide Manual, 11th edn., 1997, No. 483
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1163
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MDU600

Methoxatin M-247

[72909-34-3]
*4,5-Dihydro-4,5-dioxo-1*H*-pyrrolo[2,3-*f*]quinoline-2,7,9-tricarboxylic acid. Coenzyme PQQ. PQQ. Pyrroloquinolinequinone*



$C_{14}H_6N_2O_8$ 330.21
Believed to be a mammalian redox-cofactor vitamin (B group). Widely distributed in various foods such as vegetables and meat. Dark red solid. Sol. H_2O. λ_{max} 250 ; 332 (H_2O) (Berdy).

Tri-Me ester: [74447-88-4]
Orange-red solid. Mp 260-263° (>250°).

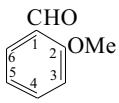
[122628-50-6]

Anthony, C. *et al., Biochem. J.*, 1967, **104**, 960 (*isol*)
Corey, E.J. *et al., J.A.C.S.*, 1981, **103**, 5599 (*synth*)
Gainor, J.A. *et al., J.O.C.*, 1982, **47**, 2833 (*synth*)
Buechi, G. *et al., J.A.C.S.*, 1985, **107**, 5555 (*synth*)
Hendrickson, J.B. *et al., J.O.C.*, 1985, **50**, 1688 (*synth*)
Itoh, S. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1907 (*bibl*)
Duine, J.A. *et al., FEMS Microbiol. Rev.*, 1986, **32**, 165 (*rev*)
MacKenzie, A.R. *et al., Tetrahedron*, 1986, **42**, 3259 (*synth, bibl*)
Ameyama, M. *et al., BioFactors*, 1988, **1**, 51 (*rev*)
Flückiger, R. *et al., Biochem. Biophys. Res. Commun.*, 1988, **153**, 353-358 (*occur*)
Houen, G. *et al., Tetrahedron*, 1989, **45**, 4235 (*use*)
Kumazawa, T. *et al., Biochim. Biophys. Acta*, 1992, **1156**, 62-66 (*occur*)
Itoh, S. *et al., J.C.S. Perkin 2*, 1992, 1245 (*uv, bibl*)
Martin, P. *et al., Helv. Chim. Acta*, 1993, **76**, 988; 1996, **79**, 658 (***synth***)
Itoh, S. *et al., Chem. Comm.*, 1995, 2077 (*ester, synth, pmr, cmr, uv*)
Itoh, S. *et al., Nat. Prod. Rep.*, 1995, **12**, 45-53 (*rev*)
Kasahara, T. *et al., Nature (London)*, 2003, **422**, 832 (*vitamin*)

2-Methoxybenzaldehyde, 9CI M-248

[135-02-4]

[50984-52-6]
o-*Anisaldehyde, 8CI. Salicylaldehyde methyl ether*



$C_8H_8O_2$ 136.15
Present in cinnamon (*Cinnamomum zeylanicum*). Flavouring ingredient. Cryst. with faint floral odour and spice-like flavour. Sol. H_2O. Mp 39°. Bp 243° $Bp_{1.5}$ 70-75°.

▶ Skin irritant. LD_{50} (rat, orl) 2500 mg/kg. Fl. p. 110°. BZ2610000

(E)-Oxime: [54582-20-6]
$C_8H_9NO_2$ 151.165
Mp 95°.

(Z)-Oxime: [54582-27-3]
$C_8H_9NO_2$ 151.165
Mp 101°. Unstable.

2,4-Dinitrophenylhydrazone:
Mp 249°.

Semicarbazone:
Mp 219°.

*Hydrate, di-Ac:*o-*Methoxybenzylidene diacetate*
$C_{12}H_{14}O_5$ 238.24
Prisms. Mp 75°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 105C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 934A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1285A (*ir*)
Brady, O.L. *et al., J.C.S.*, 1927, 894 (*oximes*)
Grammaticakis, P. *et al., Bull. Soc. Chim. Fr.*, 1940, 527 (*synth*)
Kocsis, E.A. *et al., Fresenius' Z. Anal. Chem.*, 1942, **124**, 45
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972,
Org. Synth., 1974, **54**, 42 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 855 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 455
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1691-1692
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 9th edn., Van Nostrand Reinhold*, 1996, AOT525

4-Methoxybenzaldehyde, 9CI M-249

[123-11-5]

[50984-52-6]
p-*Anisaldehyde, 8CI. Aubepine. FEMA 2670*

$C_8H_8O_2$ 136.15
Found in anise oil, fennel and vanilla. Flavouring ingredient. Liq. with a characteristic hawthorn odour and a pungent, anise-like flavour. d_4^{15} 1.12. Mp 0°. Bp 248° Bp_{210} 199-200° Bp_{12} 134-135°. pK_a 15.96 (25°,hydrate, 1% EtOH). Log P 1.78 (calc). Steam-volatile.

▶ Skin irritant. LD_{50} (rat, orl) 1510 mg/kg. BZ2625000

(E)-Oxime: [3717-21-3]

[3235-04-9] *α-Anisaldoxime*
$C_8H_9NO_2$ 151.165
Leaflets, needles. Mp 45° Mp 65°.

(Z)-Oxime: [3717-22-4]

[3235-04-9] *β-Anisaldoxime*
$C_8H_9NO_2$ 151.165
Needles (C_6H_6). Mp 133°.

Hydrazone: [5953-85-5]
$C_8H_{10}N_2O$ 150.18
Yellow leaflets. Mp 167°.

2,4-Dinitrophenylhydrazone: [1773-49-5]
Red leaflets (xylene). Mp 254°.

Semicarbazone: [6292-71-3]
Needles (EtOH), prisms (Me_2CO). Mp 168° Mp 209°.

Thiosemicarbazone: [4334-74-1]
$C_9H_{11}N_3OS$ 209.271
Cryst. (EtOH). Sol. DMF, EtOH.

Di-Me acetal: [2186-92-7] *1-(Dimethoxymethyl)-4-methoxybenzene. Dimethoxy(4-methoxyphenyl)methane*
$C_{10}H_{14}O_3$ 182.219
d^{15} 1.08. Bp 253°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 111B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 941A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1290C (*ir*)
Tiemann, F. *et al., Ber.*, 1877, **10**, 63 (*synth*)
Hinkel, L.E. *et al., J.C.S.*, 1932, 2793 (*synth*)
Niedzielski, E.L. *et al., J.A.C.S.*, 1941, **63**, 1492 (*synth*)
Birkinshaw, J.H. *et al., Biochem. J.*, 1955, **60**, 255 (*isol*)
Kotake, M. *et al., Annalen*, 1957, **607**, 153 (*isol*)
Dhami, K.S. *et al., Can. J. Chem.*, 1966, **44**, 2855 (*cmr*)
Bowie, J.H. *et al., J.C.S.(B)*, 1969, 89 (*ms*)
Org. Synth., 1971, **51**, 20 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn.,

Birkhäuser Verlag, Basel, 1972, no. 392 (*occur*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Thimmaiah, K.N. *et al., Indian J. Chem., Sect. A*, 1983, **22**, 690 (*deriv, detn, Pd, Cu*)
Salem, F.B. *et al., Analyst (London)*, 1985, **110**, 1125 (*use*)
Belcher, A. *et al., J. Chem. Ecol.*, 1988, **14**, 1367
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AOT500
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 456
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1692-1693
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOT530

Methoxybenzene, 9CI M-250

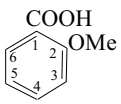
[100-66-3]
Anisole, 8CI. Phenol methyl ether. Methyl phenyl ether. FEMA 2097
PhOMe
C_7H_8O 108.14
Flavouring agent. Liq. with a pleasant aromatic odour. Mp -37.5°. Bp 155°. pK_a -6.51 (H_2SO_4 aq.).
▶ Flammable, fl. p. 52° (oc), autoignition temp. 475°. Skin irritant. LD_{50} (rat, orl) 3700 mg/kg. BZ8050000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1035A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 175A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 963A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 58 (*synth*)
Qureshi, M. *et al., Anal. Chem.*, 1963, **35**, 1592 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 41
Brieger, G. *et al., J. Chem. Eng. Data*, 1968, **13**, 581 (*props*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 243 (*rev, tox*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 45
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 178-179
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOX750

2-Methoxybenzoic acid, 9CI M-251

[579-75-9]

[1335-08-6]
o-*Anisic acid, 8CI. Salicylic acid methyl ether. FEMA 3943*



$C_8H_8O_3$ 152.149
Flavouring agent. Plates (H_2O). Mp 106°. pK_a 3.9 (25°, 0.1*M* $NaClO_4$ or H_2O). pK_a 5.52 (25°, 50% EtOH aq.). Log P 1.59 (calc).
▶ BZ4385000
Me ester: [606-45-1] *Methyl 2-methoxybenzoate. FEMA 2717*
$C_9H_{10}O_3$ 166.176
Present in the mushroom *Tramates graveolens*. Flavouring ingredient. Bp 245-246° Bp_{11} 127-127.5°.
▶ DH3549000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 188A; 297D; 444C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1065A; 1255B; 1339B; 1510C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1323C; 1366D; 1408A (*ir*)
v. Auwers, K. *et al., Annalen*, 1915, **408**, 212 (*synth*)
Dippy, J.F.J. *et al., J.C.S.*, 1937, 1426 (*synth*)
Brunet, J.-J. *et al., Tet. Lett.*, 1981, **22**, 1013 (*synth*)
Parvez, M. *et al., Acta Cryst. C*, 1987, **43**, 2243 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1793-1794 (*Me ester*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1049; 1152-1153
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOT750

3-Methoxybenzoic acid, 9CI M-252

[586-38-9]
m-*Anisic acid, 8CI. FEMA 3944*

$C_8H_8O_3$ 152.149
Flavouring ingredient for foods. Food additive listed in the EAFUS Food Additive Database (Jan. 2001). Needles (H_2O). Mp 110.5°. Bp_{10} 170-172°. pK_a 4.1 (25°). pK_a 5.37 (25°, 50% EtOH aq.). Log P 2.02 (calc).
▶ BZ4375000
Me ester: [5368-81-0]
$C_9H_{10}O_3$ 166.176
$Bp_{0.1}$ 80-81°.
Et ester: [10259-22-0]
$C_{10}H_{12}O_3$ 180.203
Bp_5 110°.
Chloride: [1711-05-3]
$C_8H_7ClO_2$ 170.595
Bp_{24} 148°.
Amide: [5813-86-5]
$C_8H_9NO_2$ 151.165
Mp 134°.
Nitrile: [1527-89-5] *1-Cyano-3-methoxybenzene. 3-Cyanoanisole*
C_8H_7NO 133.149
Mp 60°. Bp_{14} 113°.
Hydrazide: [5785-06-8]
$C_8H_{10}N_2O_2$ 166.179
Mp 93-95°.

[1335-08-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 192A; 343D; 369D; 447B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1070C; 1341B; 1392A; 1411C; 1514C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1325B; 1410C (*ir*)
Dippy, J.F.J. *et al., J.C.S.*, 1936, 644 (*synth*)
Grammaticakis, P. *et al., Bull. Soc. Chim. Fr.*, 1940, **7**, 527 (*synth*)
Korst, J.J. *et al., J.A.C.S.*, 1968, **90**, 439 (*synth*)
v. Meurs, F. *et al., J. Organomet. Chem.*, 1977, **142**, 299
Marco, J.A. *et al., Phytochemistry*, 1978, **17**, 1438 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 1049 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOU500

4-Methoxybenzoic acid, 9CI M-253

[100-09-4]

[1335-08-6]
p-*Anisic acid, 8CI. Umbellinic acid. Dragonic acid. Badianic acid. FEMA 3945*

$C_8H_8O_3$ 152.149
Flavouring agent. Food additive listed in the EAFUS Food Additive Database (Jan. 2001). Needles or prisms. Mp 184°. Bp 275-280°. pK_a 4.5 (25°).
▶ LD_{50} (mus, scu) 400 mg/kg. BZ4395000
Me ester: [121-98-2] *Methyl 4-methoxybenzoate. Methyl* p-*anisate. FEMA 2679*
$C_9H_{10}O_3$ 166.176
Flavouring ingredient. Flakes (EtOH or Et_2O) with a herbaceous, anise-like odour and sweet melon-like taste. Mp 48°. Bp 256° Bp_{20} 160°.
▶ BZ4925000
Et ester: [94-30-4] *Ethyl* p-*anisate. FEMA 2420*
$C_{10}H_{12}O_3$ 180.203
Flavouring ingredient. Liq. with a sweet, fruity, anise-like taste and odour. $d^{14.4}$ 1.11. Mp 7-8°. Bp 263°. $n_D^{18.5}$ 1.5245.
▶ BZ4697000
3-Methylbutyl ester: [27739-29-3] *3-Methylbutyl 4-methoxybenzoate. Isoamyl* p-*anisate*
$C_{13}H_{18}O_3$ 222.283
Food flavouring agent. d 1.06. Bp 312°. n_D^{19} 1.5091.
Ph ester: [4181-97-9]
$C_{14}H_{12}O_3$ 228.247
Mp 75-76°.
Chloride: [100-07-2] *4-Methoxybenzoyl chloride. Anisoyl chloride*
$C_8H_7ClO_2$ 170.595
Mp 22°. Bp_{35} 160-164° Bp_{14} 145°.
▶ Can explode in bottles at r.t. Storage at 5° recommended. Fl. p. >107°. Corrosive to all tissues. CA0270000
Amide: [3424-93-9] *4-Methoxybenzamide. Anisamide*
$C_8H_9NO_2$ 151.165
Needles or tablets (H_2O). Mp 163°. Bp 295°.
Anilide:
$C_{14}H_{13}NO_2$ 227.262
Leaflets (C_6H_6). Mp 171°.
Hydrazide: [3290-99-1]
$C_8H_{10}N_2O_2$ 166.179
Needles (H_2O). Mp 139-140°.
Nitrile: [874-90-8] *4-Methoxybenzonitrile. 1-Cyano-4-methoxybenzene. Anisonitrile*
C_8H_7NO 133.149
Mp 61-62°. Bp 256-257° (240°).
Anhydride: [794-94-5]
$C_{16}H_{14}O_5$ 286.284

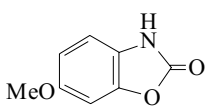
Mp 99°.

► BZ5300000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 196D; 298A; 347B; 371D; 450B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1079B; 1255C; 1345A; 1395A; 1519C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1328A; 1367A; 1413B (*ir*)
Rossel, A. *et al., Annalen*, 1869, **151**, 25 (*bibl*)
Radcliffe, L.G. *et al., Perfum. Essent. Oil Rec.*, 1922, **13**, 414 (*esters*)
Gilman, H. *et al., J.A.C.S.*, 1940, **62**, 346 (*synth*)
Sah, P.P.T. *et al., J. Chin. Chem. Soc. (Taipei)*, 1946, **13**, 77; *CA*, **41**, 5869 (*synth*)
Rabimi, T. *et al., J.O.C.*, 1965, **30**, 2486-2488 (*hydrazide*)
Cox, R.H. *et al., Spectrochim. Acta A*, 1969, **25**, 1189 (*nmr*)
Porcaro, P.J. *et al., Anal. Chem.*, 1972, **44**, 1865 (*use, chloride*)
Beistel, D.W. *et al., J. Phys. Chem.*, 1976, **80**, 2023 (*cmr*)
Brunet, J.-J. *et al., Tet. Lett.*, 1981, **22**, 1013 (*synth*)
Chatani, N. *et al., J.O.C.*, 1986, **51**, 4714 (*deriv, synth, pmr, ir*)
Suda, K. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3607-3611 (*N-benzylidene*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 217; 469; 1714-1715 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 948-949 (*esters*)
Ortiz-Marciales, M. *et al., Synth. Commun.*, 1998, **28**, 2807-2811 (*nitrile*)
Hwu, J.R. *et al., Synthesis*, 1998, 329-332 (*nitrile*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1050 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2743
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOV000; AOY250; AOV750

6-Methoxy-2(3*H*)-benzoxazolone, 9CI M-254

[532-91-2]
6-Methoxy-2-benzoxazolinone, 8CI. Coixol. MBOA



$C_8H_7NO_3$ 165.148
Isol. from roots of *Coix lacryma jobi* (Job's tears) and from seedlings of wheat, corn and rye. Pink cryst. (MeOH aq.). Sol. bases, EtOH, Et_2O, C_6H_6; fairly sol. H_2O; poorly sol. hexane. Mp 160-161° (154-155°). λ_{max} 229 ; 286 (H_2O) (Berdy).

► DM5275200

N-*Ac:* [62655-08-7]
$C_{10}H_9NO_4$ 207.185
Needles. Mp 147.5°.

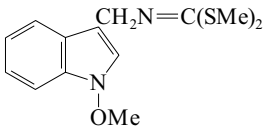
N-*Benzoyl:*
$C_{15}H_{11}NO_4$ 269.256
Needles. Mp 162-162.5°.

*5-Chloro:5-Chloro-6-methoxy-2(3*H*)-benzoxazolone. 5-Chloro-6-methoxy-2-benzoxazolinone*
$C_8H_6ClNO_3$ 199.593
Isol. from corn shoots and leaves.

Koyama, T. *et al., Yakugaku Zasshi*, 1955, **75**, 699
Virtanen, A.I. *et al., Suom. Kemistil. B*, 1956, **29**, 143; 171
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 452
Allen, E.H. *et al., J.O.C.*, 1971, **36**, 2004 (*synth*)
Richey, J.D. *et al., Agric. Biol. Chem.*, 1976, **40**, 2413 (*synth*)
Kubo, I. *et al., Experientia*, 1983, **39**, 355 (*isol, synth*)
Sicher, D. *et al., Synthesis*, 1989, 875 (*synth*)
Maleski, R.J. *et al., J. Het. Chem.*, 1991, **28**, 1937 (***synth***)
Bjostad, L.B. *et al., J. Chem. Ecol.*, 1992, **18**, 931
Hayashi, T. *et al., Phytochemistry*, 1994, **37**, 1611 (*isol, occur*)
Kato-Noguchi, H. *et al., Phytochemistry*, 1998, **49**, 433-435 (*5-chloro*)

Methoxybrassenin A M-255

[142449-74-9]

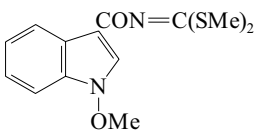


$C_{13}H_{16}N_2OS_2$ 280.414
Stress metabolite isol. from cabbage (*Brassica oleracea* var. *capitata*) inoculated with *Pseudomonas cichorii*. Gum. λ_{max} 205 (ϵ 25200); 220 (ϵ 23800); 290 (ϵ 3800) (MeOH) (Berdy).

Monde, K. *et al., Phytochemistry*, 1991, **30**, 3921-3922 (*isol, uv, ir, pmr, ms, struct*)

Methoxybrassenin B M-256

[142449-75-0]

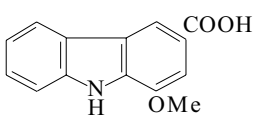


$C_{13}H_{14}N_2O_2S_2$ 294.398
Stress metabolite isol. from cabbage inoculated with *Pseudomonas cichorii*. Mp 73-74°.

Monde, K. *et al., Phytochemistry*, 1991, **30**, 3921-3922 (*isol, uv, ir, pmr, cmr, ms, struct*)

1-Methoxy-9*H*-carbazole-3-carboxylic acid, 9CI M-257

[3889-89-2]
Mukoeic acid. *Mukeic acid*



$C_{14}H_{11}NO_3$ 241.246
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6 or EtOAc). Mp 242°.

Picrate:
Mp 225-228°.

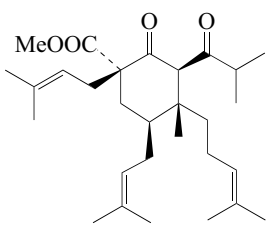
Me ester: [23523-94-6] ***Mukonine***
$C_{15}H_{13}NO_3$ 255.273
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. ($CHCl_3$/C_6H_6). Mp 198-200° (195°).

N-*Me, Me ester:*
Needles (C_6H_6/petrol). Mp 133°.

O-*De-Me, Me ester:* [182261-83-2] ***Clausine E***. *Clauszoline I*
$C_{14}H_{11}NO_3$ 241.246
Powder (Me_2CO). Mp 218-220°.

Choudhury, B.K. *et al., Phytochemistry*, 1971, **10**, 1967 (*isol, uv, ir, pmr, struct*)
Chakraborty, D.P. *et al., Phytochemistry*, 1978, **17**, 834 (*deriv*)
Knölker, H.-J. *et al., Tetrahedron*, 1993, **49**, 11221 (*synth, Mukoeic acid, Mukonine*)
Wu, T.-S. *et al., Phytochemistry*, 1996, **43**, 133 (*Clausine E*)
Ho, C. *et al., Chem. Pharm. Bull.*, 1997, **45**, 48-52 (*Clauszoline I*)
Knölker, H.J. *et al., Tet. Lett.*, 1997, **38**, 533 (*synth, Mukonine*)
Bringmann, G. *et al., Synthesis*, 1998, 1501-1505 (*synth, Mukoeic acid, Mukonine, Clausine E*)
Brenna, E. *et al., Tetrahedron*, 1998, **54**, 1585-1588 (*synth*)
Zempoalteca, A. *et al., Heterocycles*, 2002, **57**, 259-267 (*Mukonine, synth*)

2-(Methoxycarbonyl)-5-methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone M-258



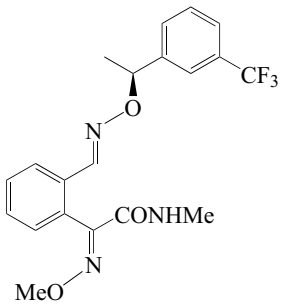
$C_{29}H_{46}O_4$ 458.68
Constit. of *Hypericum perforatum* (St. John's Wort). Viscous oil. $[\alpha]_D^{26}$ +95.5 (c, 1.1 in $CHCl_3$). λ_{max} 245 (log ϵ 2.83); 274 (log ϵ 2.7) ($CHCl_3$).

De(methoxycarbonyl):
$C_{27}H_{44}O_2$ 400.643
Constit. of *Hypericum perforatum* (St. John's Wort). Viscous oil. $[\alpha]_D^{26}$ +18.3 (c, 1.8 in $CHCl_3$). λ_{max} 245 (log ϵ 3.02); 265 (log ϵ 2.96) ($CHCl_3$).

Shan, M.D. *et al., J. Nat. Prod.*, 2001, **64**, 127-130

α-(Methoxyimino)-*N*-methyl-2-[[[1-[3-(trifluoromethyl)phenyl]ethoxy]imino]methyl]benzeneacetamide, 9CI M-259

[208195-95-3]
MA 20565



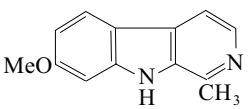
$C_{20}H_{20}F_3N_3O_3$ 407.392
Agricultural fungicide.

(*S*)-*form* [208195-96-4]
Cryst. (hexane/EtOAc). Mp 89-90°. $[\alpha]_D^{22}$ -42.7 (c, 1.00 in $CHCl_3$).

Pat. Coop. Treaty (WIPO), 1998, 9 823 582; *CA*, **129**, 40986q (*synth, isomers, activity*)
Tanaka, K. *et al., J.O.C.*, 2000, **65**, 432-437 (*synth*)

7-Methoxy-1-methyl-β-carboline M-260

[442-51-3]
*7-Methoxy-1-methyl-9*H*-pyrido[3,4-*b*]indole, 9CI.* ***Harmine****. Telepathine. Yageine. Banisterine*



$C_{13}H_{12}N_2O$ 212.251
Alkaloid from *Passiflora edulis* (passionfruit). Cryst. Mp 264-265° (257-259°). pK_a 7.61 (20°). Log P 3.12 (calc). λ_{max} 210 ; 240 ; 300 ; 338 (MeOH) (Berdy).

▶ Adverse gastrointestinal and CNS effects in humans by intramuscular route . LD_{50} (mus, scu) 243 mg/kg; LD_{50} (mus, ivn) 38 mg/kg. UV0175000

Hydrochloride: [343-27-1]
Dihydrate. Mp 268-270° dec Mp 321° (anhyd.).

▶ MG9450000

Picrate:
Mp 249-250° dec.

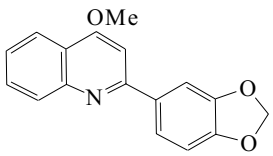
N-*Oxide:* [57498-78-9] ***Harmine*** **N-*oxide***
$C_{13}H_{12}N_2O_2$ 228.25
Needles (MeOH). Mp 226-227° dec.

N-*De-Me:* [6253-19-6] *7-Methoxy-9*H*-pyrido[3,4-*b*]indole, 9CI. 7-Methoxy-β-carboline.* ***Norharmine***
$C_{12}H_{10}N_2O$ 198.224
Needles (C_6H_6). Mp 213-215°. Sublimes.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 682C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 166B; 166C (*nmr*)
Späth, E. *et al., Ber.*, 1930, **63**, 120 (*synth*)
Ismailov, N.A. *et al., Farm. Farmakol*, 1938, **4**, 8 (*use*)
Doig, G.G. *et al., J.C.S.*, 1952, 3912 (*uv*)
Schlittler, E. *et al., Helv. Chim. Acta*, 1953, **36**, 996 (*synth*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, 695 (*use*)
Hashimoto, Y. *et al., Phytochemistry*, 1975, **14**, 1633 (*oxide*)
Hernandez, N.M.R. *et al., Rev. Cubana Farm.*, 1977, **11**, 249-255 (*activity*)
Shoemaker, D.W. *et al., J. Chromatogr.*, 1979, **174**, 159 (*glc, ms*)
Ross, S.A. *et al., Fitoterapia*, 1980, **6**, 309-312 (*activity*)
Al-Shamma, A. *et al., J. Nat. Prod.*, 1981, **44**, 745-747 (*activity*)
Siddiqui, S. *et al., Heterocycles*, 1989, **29**, 521 (*isol, uv, ir, pmr, ms, bibl, Norharmine*)
Ahmad, A. *et al., J. Ethnopharmacol.*, 1992, **35**, 289-294 (*activity*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1376
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HAI500

4-Methoxy-2-(3,4-methylenedioxyphenyl)quinoline M-261

[4179-37-7]
2-(1,3-Benzodioxol-5-yl)-4-methoxyquinoline, 9CI. ***Graveolinine***

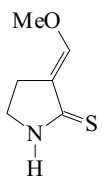


$C_{17}H_{13}NO_3$ 279.295
Alkaloid of *Ruta graveolens* (rue). Prisms (pentane/EtOAc). Mp 116-117°. Log P 3.97 (calc).

Goodwin, S. *et al., J.A.C.S.*, 1959, **81**, 6209 (*isol, ir, uv, struct*)
Chatterjee, A. *et al., Chem. Ind. (London)*, 1962, 1982 (*isol, ir, uv, synth*)
Reisch, J. *et al., Naturwissenschaften*, 1967, **54**, 200 (*synth*)

3-(Methoxymethylene)-2-pyrrolidinethione M-262

[104730-65-6]
Raphanusamide

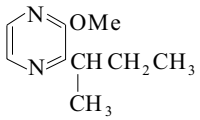


C_6H_9NOS 143.209
Originally assigned a 1,3-oxazepin-2-one struct. The 1997 *CA* Index Guide retains the erroneous nomencl.. Isol. from Japanese radish *Raphanus sativus*. Prisms (EtOAc/hexane). Mp 150-151°. λ_{max} 270 (ϵ 15800); 307 (ϵ 8200) (MeOH) (Derep).

Hasegawa, K. *et al., Plant Physiol.*, 1986, **81**, 976 (*isol*)
Harada, N. *et al., Tet. Lett.*, 1991, **32**, 6761 (*uv, ir, pmr, cmr, ms, cryst struct, bibl*)

2-Methoxy-3-(1-methylpropyl)pyrazine, 9CI M-263

[24168-70-5]
*2-*sec*-Butyl-3-methoxypyrazine, 8CI. 2-Methoxy-3-*sec*-butylpyrazine. FEMA 3433*



$C_9H_{14}N_2O$ 166.222
Volatile component of many vegetables, e.g. asparagus, carrot, celery, cucumber, parsnip, bell peppers and pea, also in ginger, galbanum oil and white wine. Flavouring ingredient.

(±)-*form*
Bp_{10} 78-83°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 842C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 404C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1560D (*ir*)
Bramwell, A.F. *et al., Tet. Lett.*, 1969, 3215
Murray, K.E. *et al., Chem. Ind. (London)*, 1970, 897
Murray, K.E. *et al., J. Sci. Food Agric.*, 1975, **26**, 973
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 459
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1698 (*occur*)

2-Methoxy-3-(2-methylpropyl)pyrazine, 9CI M-264

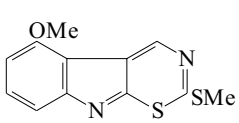
[24683-00-9]
2-Isobutyl-3-methoxypyrazine, 8CI. Galbazine. FEMA 3132

$C_9H_{14}N_2O$ 166.222
Occurs in petitgrain and galbanum oils, potent bell-pepper component. Fragrance and flavouring ingredient with powerful earthy flavour. Odour threshold 2 parts per trillion in water.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 842D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 405A (*nmr*)
Buttery, R.G. *et al., Chem. Ind. (London)*, 1969, 490-491 (*isol, synth, ir, pmr, ms*)
Murray, K.E. *et al., Chem. Ind. (London)*, 1970, 897-898 (*isol*)
Seifert, R.M. *et al., J. Agric. Food Chem.*, 1972, **20**, 135-137; *CA*, **76**, 44863g (*props, struct*)
Bramwell, A.F. *et al., J.C.S. Perkin 1*, 1972, 2004-2007 (*synth, pmr*)
Calabretta, P.J. *et al., Cosmet. Perfum.*, 1975, **90**, 74; 76; 79-80; *CA*, **83**, 183292c (*synth, use*)
Hawksworth, G.S. *et al., Xenobiotica*, 1975, **5**, 389-399; *CA*, **83**, 188835s (*metab*)

5-Methoxy-2-(methylthio)-1,3-thiazino[6,5-*b*]indole, 9CI M-265

[154933-74-1]
Dehydro-4-methoxycyclobrassinin



$C_{12}H_{10}N_2OS_2$ 262.356
Isol. from roots of the turnip *Brassica*

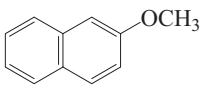
campestris ssp. *rapa* (Cruciferae) inoculated with *Pseudomonas cichorii*. Mp 142-143°.

Monde, K. *et al., Heterocycles*, 1994, **38**, 263 (*isol, uv, ir, pmr, cmr, ms, struct*)

2-Methoxynaphthalene, 9CI, 8CI M-266

[93-04-9]

Methyl 2-naphthyl ether. β-Naphthyl methyl ether. Nerolin. Yara yara



$C_{11}H_{10}O$ 158.199

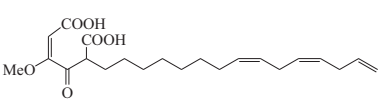
Flavouring ingredient. Plates (Et_2O) with an intensely sweet, floral odour and a sweet, strawberry taste. Mp 72°. Bp 274°.

Picrate:
Yellow cryst. ($CHCl_3$). Mp 113°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1060D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 218A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 994A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 58-60 (*synth*)
Wenkert, E. *et al., J.A.C.S.*, 1960, **82**, 4675-4680 (*synth*)
Baramki, G.A. *et al., Can. J. Chem.*, 1962, **40**, 441-444 (*synth*)
Bowie, J.H. *et al., J.C.S.(B)*, 1966, 785-789 (*pmr*)
Sterns, M. *et al., Aust. J. Chem.*, 1968, **21**, 2131-2133 (*cryst struct*)
Tulp, M.T.M. *et al., J. Chromatogr.*, 1977, **139**, 51-59 (*glc, ms*)
Tulp, M.T.M. *et al., Biomed. Mass Spectrom.*, 1978, **5**, 224-231 (*synth, ms*)
Seita, J. *et al., Org. Magn. Reson.*, 1978, **11**, 239-245 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 589
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1936-1937
Bolte, M. *et al., Acta Cryst. C*, 1998, **54**, 1862-1863 (*cryst struct, synth*)

3-Methoxy-4-oxo-5-(8,11,14-pentadecatrienyl)-2-hexenedioic acid M-267

2-Methoxy-3-oxo-1,12,15,18-nonadecatetraene-1,4-dicarboxylic acid



$C_{22}H_{32}O_6$ 392.491

Di-Me ester:
$C_{24}H_{36}O_6$ 420.545
Constit. of etiolated seedlings of *Sorghum bicolor* (sorghum). λ_{max} 233 (sh) (ϵ 5000); 268 (sh) (ϵ 2200) (EtOH).

Suzuki, Y. *et al., Phytochemistry*, 1998, **47**, 997-1001 (*isol, uv, pmr, cmr, ms*)

1-Methoxy-1-pentyloxyethane M-268

[73142-32-2]

1-(1-Methoxyethoxy)pentane. Acetaldehyde methyl pentyl acetal

$H_3C(CH_2)_4OCH(OMe)CH_3$

$C_8H_{18}O_2$ 146.229

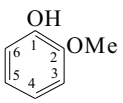
Detected in strawberry volatiles by gc-ms.

McFadden, W.H. *et al., J. Chromatogr.*, 1965, **18**, 10 (*isol*)
Safiev, O.G. *et al., Zh. Org. Khim.*, 1980, **16**, 1388; *CA*, **94**, 3438a

2-Methoxyphenol, 9CI M-269

[90-05-1]

Guaiacol. Catechol methyl ether. o-*Hydroxyanisole. FEMA 2532*



$C_7H_8O_2$ 124.139

Present in Parmesan cheese, tea and soybean. Flavouring ingredient. Prisms or needles. $d_4^{21.4}$ 1.13. Fp -3.2 (needles) Fp 28.2° Mp 32° (prisms). Bp_{24} 106.5° Bp 205°. Log P 1.32 (calc).

▶ Eye and skin irritant. Adverse CNS and gastrointestinal effects by ingestion accompanied by burning sensation in mouth and throat. LD_{50} (rat, orl) 725 mg/kg ; LD_{50} (mus, ivn) 900 mg/kg. SL7525000

Ac: [613-70-7] *Guaicyl acetate. 2-Acetoxyanisole. FEMA 3687*
$C_9H_{10}O_3$ 166.176
Flavouring ingredient. d_4^{25} 1.13. Bp_{22} 107° Bp_{13} 123-124°.

Benzoyl: [531-37-3]
$C_{14}H_{12}O_3$ 228.247
Mp 57-58°.

3,5-Dinitrobenzoyl:
Mp 141-142°.

Phenylacetyl: [4112-89-4] *Guaicyl phenylacetate. FEMA 2535*
$C_{15}H_{14}O_3$ 242.274
Flavouring ingredient. Viscous amber liq. with a woody, spicy, smoky flavour and honey-like taste. Mp 32°.

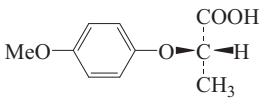
Me ether: 1,2-Dimethoxybenzene, D-735

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1072C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 247B; 1288B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1004C (*ir*)
Hirao, N. *et al., Nippon Kagaku Kaishi*, 1932, **53**, 488; *CA*, **27**, 276
Swiss Pat., 1947, 244 470; *CA*, **43**, 5802h (*phenylacetyl*)
Briggs, A.I. *et al., Trans. Faraday Soc.*, 1956, **52**, 35
Vas'kova, A.G. *et al., CA*, 1969, **75**, 94294x (*detn, Cu*)
Yamaguchi, R. *et al., Yakugaku Zasshi*, 1969, **89**, 804; *CA*, **71**, 108850g (*detn, NH_3*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 180 (*occur*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 697 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 308-309 (*phenylacetyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1244-1245; 1246-1247 (*phenylacetyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GKI000

2-(4-Methoxyphenoxy)propanoic acid, 9CI M-270

[13794-15-5]

[4276-75-9]



(*S*)-*form*

$C_{10}H_{12}O_4$ 196.202

(S)-form [4276-74-8]
Detected in Arabian coffee as a partial racemate (80% o.p.). Mp 65-66°. $[\alpha]_D^{20}$ -42.7 (c, 0.95 in EtOH).

Me ester:
Pale yellow liq. $[\alpha]_D^{20}$ -71.4 (c, 2.3 in Me_2CO).

(±)-form [4276-73-7]
Cryst. (hexane/EtOAc). Mp 86-88°.

Na salt: [150436-68-3]

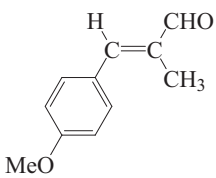
[150767-88-7] *FEMA 3773*
Sweet taste inhibitor for foodstuffs. Mp 190°.

Rathbone, E.B. *et al., J. Agric. Food Chem.*, 1989, **37**, 54-57; 58-60 (*S-form, synth, occur, coffee*)
Johnson, C. *et al., Chem. Senses*, 1994, **19**, 349-358 (*Na salt, use*)
Mathlouthi, M. *et al., J. Mol. Struct.*, 1994, **326**, 25-34 (*cryst struct*)
Camps, P. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 1877-1894 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1641 (*Na salt, use*)

3-(4-Methoxyphenyl)-2-methyl-2-propenal, 9CI M-271

[65405-67-6]

[119711-59-0]
p-*Methoxy-α-methylcinnamaldehyde. FEMA 3182*



(*E*)-*form*

$C_{11}H_{12}O_2$ 176.215

Flavouring ingredient.

(E)-form [75101-99-4]
$Bp_{0.15}$ 120°.

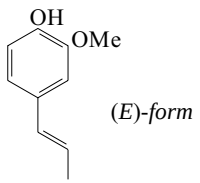
Thiosemicarbazone:
Mp 202°.

Dallacker, F. *et al., Annalen*, 1961, **643**, 67-82 (*synth*)
Untehalt, B. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1986, **319**, 666-671 (*E-form, synth*)
Tay, M.K. *et al., Tet. Lett.*, 1987, **28**, 1263-1266 (*E-form, synth*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 458 (*props, use*)

2-Methoxy-4-(1-propenyl)phenol, 9CI M-272

[97-54-1]
4-Hydroxy-3-methoxy-1-propenylbenzene. 5-(1-Propenyl)guaiacol. ***Isoeugenol.*** *FEMA 2468*



(*E*)-*form*

$C_{10}H_{12}O_2$ 164.204
Used in flavourings. Occurs in ylang-ylang and other essential oils. Sol. MeOH, Et_2O; fairly sol. H_2O. Normally isol. as a mixt. of *E*- and *Z*-forms.

▶ Skin irritant. LD_{50} (rat, orl) 1560 mg/kg. Fl. p. >74/>100°. SL7875000

(*E*)-*form* [5932-68-3]
Cryst. Mp 33°. Bp_{12} 140-141°. n_D^{20} 1.5790. pK_a 9.88 (25°). λ_{max} 260 (ϵ 15135) (EtOH).

▶ SL7876000

O-*β*-D-*Glucopyranoside:* [120442-72-0]
$C_{16}H_{22}O_7$ 326.346
Needles. Mp 170-174°. $[\alpha]_D^{25}$ -39.4 (c, 1 in Py).

Formyl: [7774-96-1] *Isoeugenol formate. FEMA 2474*
$C_{11}H_{12}O_3$ 192.214
Flavouring ingredient. Viscous liq. with warm, spicy odour. Bp 282°.

Ac: [5912-87-8]

[93-29-8] *Isoeugenol acetate. FEMA 2470*
$C_{12}H_{14}O_3$ 206.241
Flavouring ingredient. Cryst. with a weak rose-carnation, somewhat spicy odour and burning sweet taste. Mp 79°.

2-Methylbutanoyl: [76236-22-1]
$C_{15}H_{20}O_3$ 248.321
Oil.

3-Methylbutanoyl: [60958-23-8] ***Isoeugenol isovalerate***
$C_{15}H_{20}O_3$ 248.321

Benzoyl: [6379-74-4]
$C_{17}H_{16}O_3$ 268.312
Mp 102-103°.

Phenylacetyl: [120-24-1] *Isoeugenol phenylacetate. FEMA 2477*
$C_{18}H_{18}O_3$ 282.338
Flavouring ingredient. Viscous liq. with sweet spicy flavour.

Benzyl ether:

[120-11-6] *2-Methoxy-1-(phenylmethoxy)-4-(1-propenyl)benzene, 9CI. 1-(Benzyloxy)-2-methoxy-4-(1-propenyl)benzene. 1-(4-Benzyloxy-3-methoxyphenyl)-1-propene. Isoeugenol benzyl ether. FEMA 3698*
$C_{17}H_{18}O_2$ 254.328
Flavouring ingredient. Prisms (petrol) with a faint floral odour. Mp 58-60°.

1′,2′-Epoxide, 3-methylbutanoyl: [22678-68-8] ***Isoeugenoloxide isovalerate***
$C_{15}H_{20}O_4$ 264.321
Oil. $Bp_{0.01}$ 132°.

(*Z*)-*form* [5912-86-7]
Oil. Bp_{13} 133-135°. λ_{max} 258 (ϵ 13800); 291 (ϵ 3890) (EtOH).

▶ SL7877000

Phenylurethane:
Mp 118°.

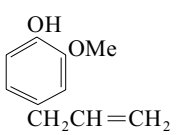
Benzoyl: [6380-30-9]
Mp 68° (59-61°).

[93-29-8, 61114-23-6, 92666-21-2, 119060-97-8, 128839-47-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1091B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 278C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1028B (*ir*)
Pond, F.J. *et al., J.A.C.S.*, 1897, **19**, 828 (*benzyl ether*)
Hirao, N. *et al., CA*, 1933, **27**, 5731 (*synth*)
Briggs, L.H. *et al., Tetrahedron*, 1958, **2**, 256 (*isol*)
Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1959, 1233 (*uv, ir*)
Von Rudloff, E. *et al., Can. J. Chem.*, 1964, **42**, 1890 (*isol*)
Aulin-Erdtman, G. *et al., Acta Chem. Scand.*, 1968, **22**, 1187 (*uv*)
Bohlmann, F. *et al., Chem. Ber.*, 1969, **102**, 1691 (*Isoeugenoloxide isovalerate*)
Fujita, S. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2251 (*isol, ir*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 815 (*rev, tox*)
Von Massow, F. *et al., J.C.S. Perkin 2*, 1976, 977 (*cmr*)
Andrieux, J. *et al., J.C.S. Perkin 1*, 1977, 359 (*synth*)
Hendriks, H. *et al., Phytochemistry*, 1977, **16**, 1853 (*Isoeugenol isovalerate*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 1141 (*2-methylbutanoyl*)
Nakano, K. *et al., Phytochemistry*, 1989, **28**, 301 (*1-glucoside*)
Giles, R.G.F. *et al., Aust. J. Chem.*, 1990, **43**, 777 (*benzyl ether*)
Purchase, R. *et al., Food Chem. Toxicol.*, 1992, **30**, 475 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 399-402
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1464-1471
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IKQ000

2-Methoxy-4-(2-propenyl)phenol, 9CI M-273

[97-53-0]
1-Allyl-4-hydroxy-3-methoxybenzene. 4-Allyl-2-methoxyphenol. 5-Allylguaiacol. ***Eugenol, USAN.*** *FEMA 2467*



$C_{10}H_{12}O_2$ 164.204
Very widespread occurrence in essential oils. Major component of clove oil. Also found in citrus and thyme oils. Present in apple, apricot, banana and cherry fruits. Flavouring agent. Oil with strong clove-like odour, and spicy pungent taste. Spar. sol. H_2O. d_4^{20} 1.07. Fp -9. Bp 248° Bp_{15} 128-130°. n_D^{20} 1.5400. pK_{a1} 10.19 (25°). Log P 2.4 (calc). Bp also given as 254°.

▶ Skin irritant. LD_{50} (rat, orl) 1930 mg/kg ; LD_{50} (mus, ipr) 365 mg/kg. SJ4375000

O-*β*-D-*Glucopyranoside:* [18604-50-7] ***Citrusin C***
$C_{16}H_{22}O_7$ 326.346
Constit. of leaves of white flowered perilla *Perilla frutescens* var. *forma viridis* and the leaves of Dalmatian sage (*Salvia officinalis*). Flavouring agent. Powder. Mp 130-131°. $[\alpha]_D^{22}$ -50.7 (c, 0.13 in MeOH).

O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:* [152041-15-1]
$C_{23}H_{26}O_{11}$ 478.452
Constit. of the leaves of clove *Syzygium aromaticum*. Needles (H_2O). Mp 207-208°. $[\alpha]_D^{25}$ -30.3 (c, 0.9 in Me_2CO).

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [585-90-0] ***Gein.*** *Eugenol vicanoside. Geoside*
$C_{21}H_{30}O_{11}$ 458.461
Isol. from roots of *Geum urbanum* (herb bennet). Mp 146-147° (monohydrate) Mp 183-184° (anhyd). $[\alpha]_D^{20}$ -55 (Me_2CO).

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [229333-98-6]
$C_{21}H_{30}O_{11}$ 458.461
Constit. of *Rosa damascena* (damask rose).

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [18604-54-1] ***Sasanquin.*** *Eugenol β-primeveroside*
$C_{21}H_{30}O_{11}$ 458.461
Isol. from leaves of *Camellia sasanqua* and *Camellia japonica*. Needles. V. sol. H_2O. Mp 200-201° (197-198°). $[\alpha]_D^{25}$ -82.5 (c, 1.7 in H_2O). Bitter taste.

Formyl: [10031-96-6] *Eugenyl formate. FEMA 2473*
$C_{11}H_{12}O_3$ 192.214
Flavouring ingredient. Bp 270°.

Ac: [93-28-7] *Aceteugenol. Eugenyl acetate. FEMA 2469*
$C_{12}H_{14}O_3$ 206.241
Flavouring agent. Found in oil of clove (*Syzygium aromaticum*), cinnamon leaf (*Cinnamomum verum*) and other essential oils. Liq. or plates (EtOH) with clove oil odour and a burning aromatic flavour. Mp 30-31°. Bp_{752} 280-281° Bp_{13} 163-164°.

▶ Skin irritant. LD_{50} (rat, orl) 1670 mg/kg. SJ4550000

Hexadecanoyl: ***Oryzarol.*** *Eugenol palmitate*
$C_{26}H_{42}O_3$ 402.616
Isol. from rice straw(*Oryza sativa*). Needles (EtOH). Mp 39-40°.

Benzoyl: [531-26-0] *FEMA 2471*
$C_{17}H_{16}O_3$ 268.312
Constit. of *Perilla frutescens* and the leaves of Dalmatian sage (*Salvia officinalis*). Flavouring agent. Cryst. (EtOH), with balsamic odour. Mp 69-70°. Bp

360°.

[8068-83-5, 18431-60-2, 18604-55-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1091A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 278A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1028A (*ir*)
Erdmann, F. *et al., J. Prakt. Chem.*, 1897, **56**, 143 (*synth*)
Naves, Y.-R. *et al., Helv. Chim. Acta*, 1948, **31**, 378 (*isol*)
Chaudhury, D.N. *et al., J.C.S.*, 1949, 2054 (*Gein*)
Tamari, K. *et al., CA*, 1963, **59**, 6717 (*Oryzarol*)
Yamada, T. *et al., Agric. Biol. Chem.*, 1967, **31**, 85; 1076 (*Sasanquin*)
Psenak, M. *et al., Planta Med.*, 1970, **19**, 154 (*Gein*)
Manito, P. *et al., J.C.S. Perkin 1*, 1974, 1727; 1975, 1548 (*biosynth*)
Khischies, M. *et al., Chem. Comm.*, 1975, 879 (*biosynth*)
Yamaguchi, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1169 (*pmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 545 (*rev, tox*)
Massow, F. *et al., J.C.S. Perkin 2*, 1976, 977 (*cmr*)
Bohlmann, F. *et al., Phytochemistry*, 1976, **15**, 1318 (*isol*)
Parks, C.R. *et al., CA*, 1981, **95**, 93943j (*Sasanquin*)
Wenkert, E. *et al., Synthesis*, 1983, 701 (*synth*)
IARC Monog., 1985, **36**, 75; *Suppl.*, **7**, 63 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EQR500; EQS000
Howes, A.J. *et al., Food Chem. Toxicol.*, 1990, **28**, 537 (*cytotoxicity*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1368
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 274-275
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1052-1058 (*occur, props, esters*)
Straubinger, M. *et al., Nat. Prod. Lett.*, 1999, **13**, 5-10 (*arabinofuranosylglucoside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EQR500; EQS000

2-Methoxy-5-(1-propenyl)phenol, 9CI M-274

[501-20-2]
Isochavibetol

$C_{10}H_{12}O_2$ 164.204

(*E*)-*form*
Cryst. (EtOH) with vanilla-carnation odour. Mp 96°. Bp_{19} 147°. pK_{a1} 9.9 (25°).

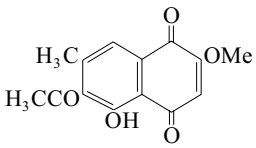
Et ether: [92-42-2] *2-Ethoxy-1-methoxy-4-(1-propenyl)benzene, 9CI. Isochavibetol ethyl ether*
$C_{12}H_{16}O_2$ 192.257
Isol. from the roots of *Trifolium pratense* (red clover).

[41243-66-7]

Funakubo, E. *et al., Nippon Kagaku Kaishi*, 1942, **63**, 1623; 1628; *CA*, **41**, 4122bc (*Et ether*)
Kovacs, J. *et al., Acta Chim. Acad. Sci. Hung.*, 1958, **16**, 141 (*synth*)
Fraishtat, P.D. *et al., Bioorg. Khim.*, 1978, **4**, 563; **5**, 1654 (*Et ether*)

2-Methoxystypandrone M-275

[85122-21-0]
6-Acetyl-5-hydroxy-2-methoxy-7-methyl-1,4-naphthoquinone

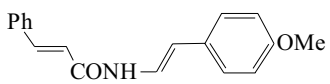


$C_{14}H_{12}O_5$ 260.246
Isol. from roots of *Polygonum cuspidatum* (Japanese knotweed). Brownish-red needles (C_6H_6/petrol). Mp 187°. May be identical with Orientalone from roots of *Rumex orientalis*. Orientalone was assigned the isomeric 3-methoxy struct. but the evidence is unconvincing λ_{max} 222 (ε 19500); 288 (ε 11200); 412 (ε 4300) (MeOH) (Berdy). λ_{max} 204 ; 288 ; 407 (EtOH) (Berdy).

Kimura, Y. *et al., Planta Med.*, 1983, **48**, 164 (*isol*)
Rauwald, H.W. *et al., Z. Naturforsch., C*, 1983, **38**, 17 (*isol*)
Hanumaiah, T. *et al., Phytochemistry*, 1985, **24**, 1811 (*isol*)
Hughes, A.B. *et al., J.C.S. Perkin 1*, 1989, 449 (*synth*)

N-4-Methoxystyrylcinnamide M-276

N-*[2-(4-Methoxyphenyl)ethenyl]-3-phenyl-2-propenamide, 9CI*



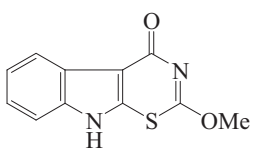
$C_{18}H_{17}NO_2$ 279.338

(*E,E*)-*form* [87596-53-0]
Alkaloid from the leaves of *Aegle marmelos* (bael fruit). Yellow needles (MeOH). Mp 191°.

Govindachari, T.R. *et al., Phytochemistry*, 1983, **22**, 755 (*isol, uv, ir, pmr, ms, struct*)

2-Methoxy-1,3-thiazino[6,5-*b*]indol-4(9*H*)-one, 9CI M-277

[156953-82-1]
Cyclobrassinone

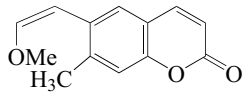


$C_{11}H_8N_2O_2S$ 232.262
The name cyclobrassinone is misleading.
Isol. from *Brassica oleracea* var. *gongylodes* (kohlrabi).

Gross, D. *et al., Z. Naturforsch., C*, 1994, **49**, 281-285 (*isol*)
Kutschy, P. *et al., Tetrahedron*, 2002, **58**, 9029-9039 (*synth*)

6-(2-Methoxyvinyl)-7-methyl-2*H*-1-benzopyran-2-one M-278

6-(2-Methoxyethenyl)-7-methyl-2H-1-benzopyran-2-one, 9CI. 6-(2-Methoxyvinyl)-7-methylcoumarin



$C_{13}H_{12}O_3$ 216.236

(*Z*)-*form* [195259-91-7]
Constit. of *Ficus carica* (fig). Mp 168-170°.

Yin, W. *et al., Zhongcaoyao*, 1997, **28**, 3-4; *CA*, **127**, 231892z (*isol*)

Methyl acetate, 9CI, 8CI M-279

[79-20-9]
FEMA 2676

$H_3CCOOMe$

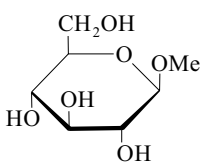
$C_3H_6O_2$ 74.079
Flavouring ingredient. Present in grape, banana and other fruits. Pleasant-smelling, volatile liq. Sol. H_2O, misc. EtOH, Et_2O. d_4^{20} 0.93. Mp -98.7°. Bp 56.3°. n_D^{20} 1.3614. Dissolves many metallic salts. Low acute tox..

▶ Eye and respiratory tract irritant. High vapour conc. narcotic. Highly flammable, fl. p. -9°, autoignition temp. 454/475°. OES: long-term 200 ppm; short-term 250 ppm. AI9100000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 600A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 898A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 607B (*ir*)
Mumford, S.A. *et al., J.C.S.*, 1950, 75 (*synth, props*)
Ger. Pat., 1968, 1 939 286; *CA*, **74**, 126332 (*manuf*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 859 (*rev, tox*)
Riddick, J.A. *et al., Tech. Chem. (N.Y.)*, 4th edn., Wiley-Interscience, 1986, **2**, 229 (*props*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 466
Kallies, B. *et al., J.C.S. Perkin 2*, 1996, 1397; 1403 (*struct, theory*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1706-1707
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 823
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFW100

Methyl β-D-glucopyranoside M-280

[709-50-2]



$C_7H_{14}O_6$ 194.184
Present in *Medicago sativa* (alfalfa). Mp

108-110°. $[\alpha]_D$ -34.2 (H_2O).

[3149-68-6, 7000-27-3, 84324-94-7]

Koenigs, W. *et al., Ber.*, 1901, **34**, 957 (*synth*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate*, Edwards Bros. Inc., Ann Arbor, 1943, 262 (*rev, derivs*)
Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1963, **256**, 1397 (*occur*)
Rao, V.S.R. *et al., J. Phys. Chem.*, 1963, **67**, 951 (*pmr*)
De Belder, A.N. *et al., Adv. Carbohydr. Chem.*, 1965, **20**, 219; 1977, **34**, 179 (*rev, derivs*)
Breitmaier, E. *et al., Chem. Ber.*, 1971, **104**, 1147 (*cmr*)
Lindberg, K.B. *et al., Acta Cryst. B*, 1976, **32**, 642 (*cryst struct, 6-Ac*)
Bock, K. *et al., Annu. Rep. NMR Spectrosc.*, (Webb, G.A. ed.), Acad. Press, London and New York, 1982, **13**, 41 (*pmr, cmr*)

Methyl glucosinolate M-281

[497-77-8]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)ethanimidate], 9CI. ***Glucocapparin***

$H_3CC(SGlc)=NOSO_3H$

$C_8H_{15}NO_9S_2$ 333.34

A mustard oil glycoside widely distributed in the Capparidaceae. Needles (aq. EtOH) (as K salt). Mp 207-209° (K salt). $[\alpha]_D^{22}$ -28 (c, 1.9 in H_2O).

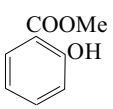
Tetra-Ac:
Cryst. (EtOH aq.) (as K salt). Mp 215-217° (K salt). $[\alpha]_D^{22}$ -29 (c, 2 in H_2O).

[15592-33-3]

Kjaer, A. *et al., Acta Chem. Scand.*, 1956, **10**, 335 (*isol, ir*)
Kjaer, A. *et al., Phytochemistry*, 1963, **2**, 29 (*isol*)
Benn, M.H. *et al., Can. J. Chem.*, 1964, **42**, 163 (*synth*)
Helboe, P. *et al., J. Chromatogr.*, 1980, **197**, 199-205 (*hplc*)
Eagles, J. *et al., Biomed. Mass Spectrom.*, 1981, **8**, 278 (*ms*)
Kokkonen, P. *et al., Rapid Commun. Mass Spectrom.*, 1989, **3**, 102-106 (*hplc, ms*)
Verkerk, R. *et al., Natural Toxicants in Food*, 1998, 29-53

Methyl 2-hydroxybenzoate, 9CI M-282

[119-36-8]
Methyl salicylate, 8CI. Oil of wintergreen. FEMA 2745



$C_8H_8O_3$ 152.149

Present in white wine, tea, porcini mushroom *Boletus edulis*, Bourbon vanilla, clary sage, red sage and fruits incl. cherry, apple, raspberry, papaya and plum. Found in leaves of *Gaultheria procumbens* (wintergreen). Flavouring agent. Oil with characteristic odour. $d_4^{18.5}$ 1.85. Mp -8.6°. Bp 223.3° Bp_{12} 101°. pK_a 9.87 (20°, 0.1*M* $NaClO_4$). Log P 2.44 (calc). Component of Theragesic.

► Mod. toxic orally. Fl. p. 96°, autoignition temp. 454°. Skin and eye irritant. Fatalities reported from ingestion. LD_{50} (rat, orl) 887 mg/kg. Exp. reprod. and teratogenic effects. VO4725000

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [490-67-5] ***Monotropitoside.*** *Monotropitin. Gaultherin*

$C_{19}H_{26}O_{12}$ 446.407

Prisms (Me_2CO). Mp 180°. $[\alpha]_D$ -58.2 (H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 295C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1251A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1363B (*ir*)
Tijmstra, S. *et al., Ber.*, 1905, **38**, 1375 (*synth*)
Robertson, A. *et al., J.C.S.*, 1931, 1881 (*Monotropitoside*)
Emery, E.M. *et al., Anal. Chem.*, 1960, **32**, 1495 (*ms*)
Hallas, G. *et al., J.C.S.*, 1965, 5770 (*synth*)
Towers, G.H.N. *et al., Phytochemistry*, 1966, **5**, 677 (*Monotropitoside*)
Scott, K.N. *et al., J. Magn. Reson.*, 1970, **2**, 361 (*pmr*)
Sântavý, F. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1825 (*uv*)
Scott, K.N. *et al., J.A.C.S.*, 1972, **94**, 8564 (*cmr*)
Bowie, J.H. *et al., Org. Mass Spectrom.*, 1974, **9**, 1006 (*ms*)
Wu, S.K. *et al., J. Macromol. Sci., Part A: Chem.*, 1985, **22**, 1121 (*uv*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MPI000
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Methyl isothiocyanate, BSI, ISO, JMAF M-283

[556-61-6]
Isothiocyanatomethane, 9CI. Methyl mustard oil. Trapex. MITC. MIT

MeNCS

C_2H_3NS 73.118

Isol. from mustard oil, present as glucoside (Methyl glucosinolate, M-281). Cryst. Mp 36°. Bp 119°. n_D 1.5258.

► Flammable, fl. p. 29°. Eye, skin and mucous membrane irritant. LD_{50} (rat, orl) 97 mg/kg. PA9625000

[8066-01-1, 49582-15-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 873D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1410A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 826C (*ir*)
Delépine, M. *et al., Bull. Soc. Chim. Fr.*, 1908, **3**, 642 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1955, **9**, 857; 1963, **17**, 2143 (*isol, ms*)
Org. Synth., Coll. Vol., 3, 1955, 599 (*synth*)
Mathias, A. *et al., Tetrahedron*, 1965, **21**, 1073 (*pmr*)
Attril, J.E. *et al., Anal. Lett.*, 1970, **3**, 59 (*use*)
Waterfield, M. *et al., Biochemistry*, 1970, **9**, 832 (*use*)
Anderson, D.W.W. *et al., J. Mol. Struct.*, 1972, **14**, 385 (*struct*)
Fairwell, T. *et al., Anal. Biochem.*, 1973, **53**, 115 (*use*)
Molina, P. *et al., Synthesis*, 1982, 596 (*synth*)
Durig, J.R. *et al., J. Mol. Struct.*, 1983, **100**, 241 (*ir, Raman*)
Giffard, M. *et al., J.C.S. Perkin 2*, 1985, 157 (*pmr, cmr, N-15 nmr*)
Giesselmann, G. *et al., Chem.-Ztg.*, 1990, **114**, 215 (*rev, synth, use, props*)
Pesticide Manual, 9th edn., 1991, No. 8390
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A274
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **5**, 3520-3522 (*use*)
Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, D.), Sheffield Academic Press/CRC, 1998, 29-53 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ISE000

Methyl α-linolenate hydroperoxides M-284

Methyl hydroperoxidooctadecatrienoates

$H_3CCH_2CH=CHCH_2CH=CHCH=CHCH(OOH)(CH_2)_7COOCH_3$ (9-isomer)

$C_{19}H_{32}O_4$ 324.459

Reaction with singlet oxygen produces the 9-, 10-, 12-, 13-, 15- and 16-hydroperoxides. Free radical autoxidn. produces the 9-, 12-, 13- and 16-hydroperoxides.. The 13-isomer is formed stereospecifically (13*S*-) by lipoxygenase which occurs in flax seed and cabbage leaves.

Frankel, E.N. *et al., J.O.C.*, 1961, **26**, 4663
Cobern, D. *et al., J.C.S.(C)*, 1966, 1897
Chan, H.W.-S. *et al., J. Am. Oil Chem. Soc.*, 1977, **54**, 100
Terao, J. *et al., J. Am. Oil Chem. Soc.*, 1977, **54**, 234
Frankel, E.N. *et al., Lipids*, 1977, **12**, 1055

Methyl 3-methyl-1-butenyl disulfide M-285

2-Methyl-5,6-dithia-3-heptene. FEMA 3865

$(H_3C)_2CHCH=CH\text{-}S\text{-}SMe$

$C_6H_{12}S_2$ 148.293

Flavouring ingredient. Pale yellow liq. with powerful odour. d 0.83. Synth. and props. not publ..

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1157 (*use*)

Methyl methylthio selenide M-286

[41884-42-8]
Methyl methanesulfenoselenoate, 9CI. 2-Thia-3-selenabutane

Me–Se–S–Me

C_2H_6SSe 141.095

Constit. of *Allium* sp..

Cai, X.-J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081 (*occur*)

Methyl (methylthio)methyl disulfide, 9CI M-287

[42474-44-2]
2,3,5-Trithiahexane

$MeS–S–CH_2–SMe$

$C_3H_8S_3$ 140.294

Found in essential oil of hops and in Camembert cheeses, cooked cabbage, broccoli and cauliflower. Sl. yellow liq. $Bp_{0.01}$ 32°. Readily disproportionates to Dimethyl disulfide, D-742 and Bis[(methylthio)methyl] disulfide, B-151.

S^5-*Oxide, (±)-:* [42474-27-1] *Methyl (methylsulfinyl)methyl disulfide, 9CI. 2,3,5-Trithiahexane 5-oxide*
$C_3H_8OS_3$ 156.294
Oil. Sol. H_2O. $Bp_{0.04}$ 98°. Config. of natural isolate not determined.

S^2,S^2-*Dioxide:* S-*Methylthiomethyl methanesulfonothioate*
$C_3H_8O_2S_3$ 172.293

S^3,S^3-*Dioxide:* S-*Methyl methylthiomethanesulfonothioate*
$C_3H_8O_2S_3$ 172.293

S^5,S^5-*Dioxide:* [42474-28-2] *Methyl (methylsulfonyl)methyl disulfide*
$C_3H_8O_2S_3$ 172.293
Sl. yellow oil.

Block, E. *et al., J.A.C.S.*, 1974, **96**, 3929-3944 (S^5-*oxides, synth, ir, pmr, ms*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1976, **24**, 829-832 (*isol*)
Dumont, J.P. *et al., Lait*, 1976, **56**, 595-599 (*isol*)
Dubs, P. *et al., Helv. Chim. Acta*, 1978, **61**, 2351-2359 (*synth, ir, pmr, ms*)
Moir, M. *et al., Phytochemistry*, 1980, **19**, 2201 (*isol, synth, spectra*)
Kubota, K. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 644-646 (*isol, bibl*)
Kouokam, J.C. *et al., Phytochemistry*, 2002, **60**, 403-407 (*oxides, isol*)

Methyl 3-(methylthio)-1-propenyl disulfide, 9CI M-288

2,3,7-Trithia-4-octene
$MeS^7CH_2CH{=}CHSSMe$
$C_5H_{10}S_3$ 166.332

(*E*)-*form*

7-Oxide: [104228-50-4]

[104228-67-3] *Methyl 3-(methylsulfinyl)-1-propenyl disulfide*
$C_5H_{10}OS_3$ 182.331
Constit. of *Allium sativum* (garlic) and *Allium ursinum* (ramsons). Oil.

(*Z*)-*form*

7-Oxide: [104229-00-7]
Constit. of *Allium sativum* (garlic) and *Allium ursinum* (ramsons). Oil.

Block, E. *et al., J.A.C.S.*, 1986, **108**, 7045-7055 (*synth, ir, pmr*)
Sendl, A. *et al., Planta Med.*, 1991, **57**, 361-362; 1992, **58**, 1-7 (*isol*)

Methyl 1-(methylthio)propyl disulfide M-289

[53897-66-8]
4-Ethyl-2,3,5-trithiahexane
$H_3CCH_2CH(^5SMe)$–S–S–Me
$C_5H_{12}S_3$ 168.348
Constit. of *Allium cepa* (onion) juice, *Allium fistulosum* (Welsh onion) and *Allium tuberosum* (Chinese chives). Bp_{13} 99-100°.

5-Oxide: [134018-95-4]

[132216-20-7, 132216-24-1, 139012-33-2, 139012-36-5] *Methyl 1-(methylsulfinyl)propyl disulfide*
$C_5H_{12}OS_3$ 184.347
Constit.of *Allium cepa* (onion) juice and *Allium tricoccum* (wood leek).

Dubs, P. *et al., Helv. Chim. Acta*, 1978, **51**, 2351-2359 (*synth, ir, pmr, ms*)
Morimitsu, Y. *et al., Phytochemistry*, 1990, **29**, 3435-3439 (*isol*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*deriv,synth,pmr,cmr*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol*)

Methyl phenyl disulfide, 9CI M-290

[14173-25-2]
FEMA 3872
Ph–S–S–Me
$C_7H_8S_2$ 156.272
Found in cocoa. Flavouring agent for baked goods, beverages and seasonings. Liq. with powerful odour. $Bp_{0.5}$ 86°. n_D^{25} 1.6135.

Armitage, D.A. *et al., J.C.S. Perkin 1*, 1972, 680 (*synth, pmr*)
Capozzi, G. *et al., Gazz. Chim. Ital.*, 1990, **120**, 421-426 (*synth, pmr, ms*)
Metzner, P. *et al., Synthesis*, 1994, 761-762 (*synth, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1204

Methyl phenyl sulfide, 8CI M-291

[100-68-5]
(Methylthio)benzene, 9CI. Thioanisole. Methylmercaptobenzene. FEMA 3873
PhSMe
C_7H_8S 124.206
Found in coffee. Flavouring agent for baked and meat products and seasonings. Food additive listed in the Food Additive Database (Jan. 2001). Oil with unpleasant odour. d_4^{25} 1.05. Fp -15. Bp 188° (194-196°) Bp_6 58-60°. n_D^{20} 1.5865.
▶ Irritant. LD_{50} (rat, orl) 891 mg/kg.
DA6200000

S-*Oxide:* See Methyl phenyl sulfoxide in *The Combined Chemical Dictionary.*

S,S-*Dioxide:* [3112-85-4] *Methyl phenyl sulfone. (Methylsulfonyl)benzene, 9CI*
$C_7H_8O_2S$ 156.205
Plates (H_2O). Mp 88°.
▶ WR6800000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1182A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 431B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1100A (*ir*)
Bourgeois, M.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1911, **30**, 407 (*synth*)
Knapp, W. *et al., Monatsh. Chem.*, 1930, **56**, 66 (*footnote, synth*)
Adv. Chem. Ser., 1955, **15**, 175 (***props***)
Org. Synth., Coll. Vol., 4, 1963, 674 (*deriv*)
Bowie, J.H. *et al., J.C.S.(B)*, 1966, 951 (*ms*)
Wladislaw, B. *et al., J.C.S.(B)*, 1971, 2037 (*ir, Raman*)
Baarschers, W.H. *et al., Can. J. Chem.*, 1973, **51**, 156 (*deriv, ms*)
Knauf, H. *et al., Z. Chem.*, 1973, **13**, 73 (*pmr*)
Buchanan, G.W. *et al., Can. J. Chem.*, 1974, **52**, 3895 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 660; **6**, 582
Jones, I.W. *et al., J.C.S. Perkin 2*, 1979, 217 (*uv*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Chaloner, P.A. *et al., Acta Cryst. C*, 1992, **48**, 717 (*cryst struct, sulfone*)
Page, P.C.B. *et al., Tetrahedron*, 1992, **48**, 5933 (*synth, nmr*)
Hachtel, J. *et al., Eur. J. Org. Chem.*, 2000, 1457-1465 (*S,S-dioxide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFC250

Methyl 1-propenyl disulfide M-292

[5905-47-5]
4,5-Dithia-2-hexene. FEMA 3576
$H_3CCH{=}CH{-}^4S{-}^5S{-}Me$
$C_4H_8S_2$ 120.239

(*E*)-*form* [23838-19-9]
Constit. of the essential oils of *Allium* spp.. Oil. Bp_{17} 55°.

4-Oxide: [134568-43-7]

[121955-53-1] S-*Methyl 1-propenesulfinothioate*
$C_4H_8OS_2$ 136.239
Constit. of *Allium* spp..

5-Oxide: [119052-99-2] S-*1-Propenyl methanesulfinothioate*
$C_4H_8OS_2$ 136.239
Constit. of onion (*Allium cepa*), garlic (*Allium sativum*) and other *Allium* spp..

(*Z*)-*form* [23838-18-8]
Constit. of the essential oils of *Allium* spp.. Pale yellow oil. Bp_{30} 69-70°.

4-Oxide: [136516-41-1]
Constit. of *Allium* spp..

5-Oxide: [119053-00-8]
Constit. of onion (*Allium cepa*), garlic (*Allium sativum*) and other *Allium* spp..

Wijers, H.E. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 519 (*synth*)
Bayer, T. *et al., Phytochemistry*, 1989, **28**, 2373 (*deriv, isol, pmr*)
Block, E. *et al., Pure Appl. Chem.*, 1993, **65**, 625-632 (*deriv, occur*)
Block, E. *et al., J.A.C.S.*, 1996, **118**, 2799 (*synth, pmr, cmr, ms*)

Methyl 2-propenyl disulfide M-293

[2179-58-0]
Allyl methyl disulfide. 4,5-Dithia-1-hexene. FEMA 3127
$H_2C{=}CHCH_2{-}^4S{-}^5S{-}Me$
$C_4H_8S_2$ 120.239
Constit. of the essential oils of *Allium* spp. Flavouring ingredient. Oil.

4-Oxide: [3736-98-9] S-*Methyl 2-propene-1-sulfinothioate*
$C_4H_8OS_2$ 136.239
Constit. of *Allium* spp..

5-Oxide: [104228-49-1] S-*2-Propenyl methanesulfinothioate. Allyl methanethiosulfinate*
$C_4H_8OS_2$ 136.239
Constit. of *Allium* spp.. Oil.

[41865-22-9]

Armitage, D.A. *et al., J.C.S. Perkin 1*, 1972, 680 (*synth*)
Baechler, R.D. *et al., Tet. Lett.*, 1978, 105 (*synth*)
Block, E. *et al., J.A.C.S.*, 1986, **108**, 7045-7055 (*deriv, synth, pmr*)
Devlin, M.T. *et al., J. Mol. Struct.*, 1990, **238**, 119 (*Raman, conformn*)
Block, E. *et al., Pure Appl. Chem.*, 1993, **65**, 625-632 (*occur*)

Methyl 2-propenyl pentasulfide M-294

[118023-99-7]
Allyl methyl pentasulfide
$H_2C{=}CHCH_2$-S-S-S-S-S-Me
$C_4H_8S_5$ 216.437
Isol. from garlic oil.

Ding, Z. *et al., CA*, 1989, **110**, 22443p (*isol*)

Methyl 2-propenyl selenide M-295

[93370-41-3]
3-(Methylseleno)-1-propene, 9CI. Allyl methyl selenide. 4-Selena-1-pentene
$MeSeCH_2CH{=}CH_2$
C_4H_8Se 135.067
Constit. of *Allium* sp..

Clarernbeau, M. *et al., Tet. Lett.*, 1984, **25**, 3629 (*use*)
Musorin, G.K. *et al., Zh. Org. Khim.*, 1992, **28**, 681 (*synth*)
Cai, X.-J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081 (*occur*)

Methyl 2-propenyl tetrasulfide, 9CI M-296

[90195-83-8]
Allyl methyl tetrasulfide
$H_2C{=}CHCH_2$-S-S-S-S-Me
$C_4H_8S_4$ 184.371
Isol. from garlic oil.

Zoghbi, M.G.B. *et al., J. Agric. Food Chem.*, 1984, **32**, 1009-1010 (*isol*)
Ding, Z. *et al., CA*, 1989, **110**, 22443p (*isol*)

Methyl 2-propenyl trisulfide, 9CI M-297

[34135-85-8]
Allyl methyl trisulfide. 4,5,6-Trithia-1-heptene
$H_2C{=}CHCH_2$–S–S–S–Me
$C_4H_8S_3$ 152.305
Constit. of *Allium sativum* (garlic oil) and other *Allium* spp.. Yellow oil. $Bp_{0.05}$ 28-30°.

Kameoka, H. *et al., Phytochemistry*, 1984, **23**, 155-158 (*isol*)
Mott, A.W. *et al., Synthesis*, 1984, 657-658 (*synth, pmr*)
Vernin, G. *et al., Planta Med.*, 1986, 96-101 (*isol*)

Methyl (1-propenylthio) selenide M-298

Methyl 1-propene-1-sulfenoselenoate, 9CI. 4-Thia-5-selena-2-hexene
Me–Se–S–CH=$CHCH_3$
C_4H_8SSe 167.133
Constit. of *Allium* sp..

[158634-81-2, 158634-84-5]

Cai, X.-J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081 (*occur*)

Methyl (2-propenylthio) selenide M-299

[158634-80-1]
Methyl 2-propene-1-sulfenoselenoate. Allylthio methyl selenide. 4-Thia-5-selena-1-hexene
Me-Se-S-$CH_2CH{=}CH_2$
C_4H_8SSe 167.133
Constit. of *Allium* sp..

Cai, X.-J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081 (*occur*)

Methyl 1-(1-propenylthio)propyl disulfide M-300

[126876-23-1]
4-Ethyl-2,3,5-trithia-6-octene
$H_3CCH{=}CH^5SCH(CH_2CH_3)$–S–SMe
$C_7H_{14}S_3$ 194.386
Constit. of *Allium cepa* (onion) oil and *Allium fistulosum* (Welsh onion).

(E)-form

5-Oxide:

[138898-86-9] *Methyl 1-(1-propenylsulfinyl)propyl disulfide*
$C_7H_{14}OS_3$ 210.385
Constit. of *Allium tricoccum* (wood leek).

Kuo, M.C. *et al., J. Agric. Food Chem.*, 1990, **38**, 1378-1381; 1992, **40**, 111-117 (*isol*)
Morimitsu, Y. *et al., J. Agric. Food Chem.*, 1992, **40**, 368-372 (*deriv, synth*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol, ms*)

Methyl 1-(2-propenylthio)propyl disulfide M-301

1-(Allylthio)propyl methyl disulfide. 4-Ethyl-2,3,5-trithia-7-octene
$H_2C{=}CHCH_2^5SCH(CH_2CH_3)$–S–SMe
$C_7H_{14}S_3$ 194.386

5-Oxide: Methyl 1-(2-propenylsulfinyl)propyl disulfide
$C_7H_{14}OS_3$ 210.385
Constit. of *Allium tricoccum* (wood leek).

Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*isol, ms*)

Methyl propyl disulfide, 8CI M-302

[2179-60-4]
2,3-Dithiahexane. FEMA 3201
$H_3CCH_2CH_2$-S-S-Me
$C_4H_{10}S_2$ 122.255
Constit. of chive (*Allium schoenoprasum*) and other *Allium* spp. Flavouring component of onion oil. Also present in cooked cabbage, French fried potato, cooked beef, roasted peanut, brussel sprouts and tomato. Bp_{43} 69-71°. n_D^{20} 1.5070.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 427C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 349A (*ir*)
Milligan, B. *et al., J.C.S.*, 1963, 6008 (*synth*)
Jacobsen, J.V. *et al., Arch. Biochem. Biophys.*, 1964, **104**, 473 (*ir, glc*)
Wahlroos, O. *et al., Acta Chem. Scand.*, 1965, **19**, 1327 (*isol*)
Harpp, D.N. *et al., J.O.C.*, 1979, **44**, 4140 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1847-1848 (*use, occur, props*)

Methyl propyl trisulfide, 9CI, 8CI M-303

[17619-36-2]
2,3,4-Trithiaheptane. FEMA 3308
$H_3CCH_2CH_2$–S–S–S–Me
$C_4H_{10}S_3$ 154.321
Volatile flavouring component of onion oil, leeks and other *Allium* spp. Also present in French fried potato and cocoa.

Carson, J.F. *et al., J.O.C.*, 1959, **24**, 175-179 (*synth, glc*)
Ger. Pat., 1971, 2 020 051; *CA*, **74**, 86571 (*synth*)
Wu, J.L.P. *et al., J. Chromatogr.*, 1981, **214**, 234 (*occur, hplc*)

Methyl 1-(propylthio)propyl disulfide M-304

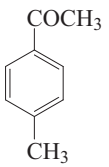
4-Ethyl-2,3,5-trithiaoctane
$H_3CCH_2CH_2$-^{5}S-$CH(CH_2CH_3)$-S-S-Me
$C_7H_{16}S_3$ 196.401

5-Oxide: Methyl 1-(propylsulfinyl)propyl disulfide
$C_7H_{16}OS_3$ 212.401
Constit. of *Allium* sp..

Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422

4′-Methylacetophenone, 8CI M-305

[122-00-9]
1-(4-Methylphenyl)ethanone, 9CI. Methyl p-*tolyl ketone.* p-*Acetyltoluene. FEMA 2677*



$C_9H_{10}O$ 134.177
Present in sour cherry, orange, grapefruit peel, blackcurrants, guava, peach, other fruits, celery, potato, tomato, pepper, parsley, smoked fish, cognac, Parmesan cheese and other foodstuffs. Flavouring ingredient. Needles with mild flowery odour and sweet, strawberry-like taste. d_4^{20} 1.01. Mp 28°. Bp_{736} 225° Bp_{11} 112.5°. pK_{a1} -5.47 (H_2SO_4 aq.).

▶ Fl. p. 92/96°. Human skin irritant. LD_{50} (rat, orl) 1400 mg/kg. AM9463000

Oxime: [2089-33-0]
$C_9H_{11}NO$ 149.192
Cryst. (petrol). Mp 88°.

▶ AM9472200

Semicarbazone: [3352-98-5]
Needles or plates (EtOH). Mp 205°.

Hydrazone:
$C_9H_{12}N_2$ 148.207
Yellow cryst. (EtOH). Mp 131-132°.

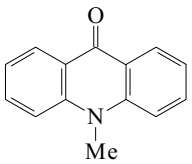
2,4-Dinitrophenylhydrazone: [1237-49-6]
Mp 205°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 25B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 818A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1244A (*ir*)
Noller, C.R. *et al., J.A.C.S.*, 1924, **46**, 1893

Dermer, O.C. *et al., J.A.C.S.*, 1941, **63**, 2881
Kosolapoff, G.M. *et al., J.A.C.S.*, 1947, **69**, 1651
Beckey, H.D. *et al., Org. Mass Spectrom.*, 1972, **6**, 923 (*ms*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 933 (*rev, tox*)
Ghersetti, S. *et al., Spectrosc. Lett.*, 1975, **8**, 391 (*ir*)
Shapiro, B.L. *et al., J. Phys. Chem. Ref. Data*, 1977, **6**, 919 (*nmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1065-1066 (*props, use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFW250

10-Methylacridone M-306

[719-54-0]
*10-Methyl-9(10*H*)-acridinone, 9CI. 10-Methyl-9-acridanone, 8CI.* N-*Methylacridone*



$C_{14}H_{11}NO$ 209.247
Constit. of the roots of *Citrus deliciosa* (Italian tangerine). Cryst. (MeOH). Mp 199-200°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 93A (*ir*)
Gilman, H. *et al., J.O.C.*, 1952, **17**, 860 (*synth*)
Schumann, D. *et al., Chem. Ber.*, 1969, **102**, 3192 (*ms*)
Chang, P.T.O. *et al., J. Nat. Prod.*, 1976, **39**, 134 (*isol, uv, ir, pmr, ms*)
Potescu, I.D. *et al., J. Prakt. Chem.*, 1976, **318**, 515 (*synth*)
Beak, P. *et al., J.A.C.S.*, 1976, **98**, 171 (*uv*)
Adams, J.H. *et al., J.C.S. Perkin 1*, 1977, 2173 (*synth*)
Grignon-Dubois, M. *et al., Synth. Commun.*, 1995, **25**, 2999 (*synth*)
El-Shafae, A.M. *et al., Pharmazie*, 1998, **53**, 640-643 (*cmr*)

2-(Methylamino)benzoic acid, 9CI M-307

[119-68-6]
N-*Methylanthranilic acid, 8CI*

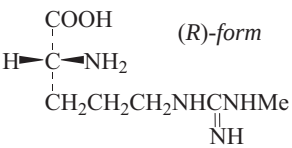


$C_8H_9NO_2$ 151.165
Isol. from grapefruit peel oil. Plates (EtOH or petrol). Mp 178-179° (175-182°). $Bp_{0.01}$ 80°. pK_{a1} 2; pK_{a2} 5.34 (22°, 0.1*M* KCl). Amphoteric. Sublimes.
► Eye irritant. CB3300000
Hydrochloride:
Needles. Mp 141°.
Me ester: [85-91-6] *Methyl* N-*methylanthranilate. FEMA 2718*
$C_9H_{11}NO_2$ 165.191
Constit. of mandarin peel oil (*Citrus madurensis*), petitgrain oil and other *citrus* spp. oils. Flavouring agent. Cryst. (petrol) with apple-like flavour at low conc. Mp 19°. Bp 256° Bp_{15} 130-131°.
► CB3500000
Me ester, hydrochloride:
Needles (EtOH). Mp 218°.
N-*(3-Phenylpropanoyl):2-[Methyl(3-phenylpropanoyl)amino]benzoic acid*
$C_{17}H_{17}NO_3$ 283.326
Prod. by the marine *Streptomyces* sp. B7747. Cryst. (Et_2O). Mp 107°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 189B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1066C (*nmr*)
Houben, J. *et al., Ber.*, 1906, **39**, 3235; 1909, **42**, 3194
Cosulich, D.B. *et al., J.A.C.S.*, 1948, **70**, 1922 (*synth*)
Tomita, K. *et al., Yakugaku Zasshi*, 1951, **71**, 1100; *CA*, **46**, 50456
Freifelder, M. *et al., J. Phys. Chem.*, 1965, **69**, 3645 (*pmr*)
Pant, L.M. *et al., Acta Cryst. B*, 1972, **28**, 647 (*cryst struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MGQ250
Biabani, M.A.F. *et al., J. Antibiot.*, 1998, **51**, 333-340 (*3-phenylpropanoyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MGQ000; MGQ250

N^G-Methylarginine M-308

N^5-*[Imino(methylamino)methyl]ornithine, 9CI.* N^5-*(Methylamidino)ornithine, 8CI.* N^G-*Monomethylarginine.* N^{ω}-*Methylarginine. 546C88*

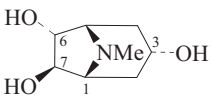


$C_7H_{16}N_4O_2$ 188.229
(R)-form [137694-74-7]
[137694-75-8]
D-form
$[\alpha]_D^{22}$ -9.5 (c, 0.1 in H_2O) (as monoacetate).
(S)-form [17035-90-4]
L-form. ***Targinine, INN***
Isol. from broad bean seeds. Amorph. solid. $[\alpha]_D^{20}$ +23 (c, 1 in 1*M* HCl).
[51827-02-2, 53308-83-1]

Baldwin, G.S. *et al., Biochem. J.*, 1971, **123**, 69 (*isol*)
Nakajima, T. *et al., Biochim. Biophys. Acta*, 1971, **230**, 212; **243**, 31 (*isol*)
Deibler, G.E. *et al., J. Biol. Chem.*, 1973, **248**, 2387 (*anal*)
Corbin, J.L. *et al., Anal. Biochem.*, 1974, **57**, 310 (*synth*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 2449 (*isol, synth, pmr, ir*)
Ferrario, F. *et al., Synth. Commun.*, 1991, **21**, 99 (***synth***)
Paik, W.K. *et al., Amino Acids*, 1993, **4**, 267 (*rev, biosynth, metab*)
Feldman, P.L. *et al., J. Med. Chem.*, 1993, **236**, 491-496 (*pharmacol*)
Joly, G.A. *et al., Biochem. Biophys. Res. Commun.*, 1994, **199**, 147-154 (*pharmacol*)
Bedarida, G.V. *et al., Horm. Metab. Res.*, 1994, **26**, 109-112 (*pharmacol*)
Zhang, W. *et al., Synth. Commun.*, 1994, **24**, 2789-2792 (*synth*)
Griffith, O.W. *et al., Methods Enzymol.*, 1996, **268**, 375-392 (*biochem, rev*)
Vallance, P. *et al., Methods Enzymol.*, 1996, **269**, 453-459 (*biochem, rev*)
Schwartz, S. *et al., Xenobiotica*, 1997, **27**, 1259-1271 (*pharmacokinet, metab*)
Hussein, Z. *et al., Clin. Pharmacol. Ther. (St. Louis)*, 1999, **65**, 1-9 (*pharmacol*)

8-Methyl-8-azabicyclo[3.2.1]octane-3,6,7-triol, 9CI M-309

3,6,7-Tropanetriol. 3,6,7-Trihydroxytropane



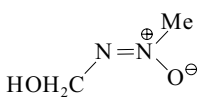
(1*R**,3*S**,6*R**,7*R**)-*form*

$C_8H_{15}NO_3$ 173.211
The alkaloids are named here as given in the lit., but the numbering of positions 6 and 7, which is irregular in the lit., has been corrected.Mp 169-170° (hydrate).
(1R,3S,6S,7R)-form [575-62-2]
(3α,6β,7β)-form. Teloidine
Mp 169-172° (hydrate). A *meso*-stereoisomer but 6-mono- and 3,6-disubstituted derivs are chiral. There is currently no data on abs. configs.
3,6-Di-O-*tigloyl:* [7159-86-6] ***3,6-Ditigloyloxytropan-7-ol***
$C_{18}H_{27}NO_5$ 337.415
Alkaloid present in *Cyphomandra betacea* (tree tomato). Mp 215° (as hydrobromide).
[21030-92-2, 62058-54-2]

Evans, W.C. *et al., Phytochemistry*, 1972, **11**, 3293 (*derivs*)
El-Imam, Y.M.A. *et al., Phytochemistry*, 1987, **26**, 2385-2389; 1988, **27**, 2181-2184 (*3-cinnamoyl, 3-benzoyl, 6-benzoyl, 3-tigloyl*)

Methylazoxymethanol M-310

[590-96-5]
(Methyl-ONN-*azoxy)methanol, 9CI. MAM*



$C_2H_6N_2O_2$ 90.082
► PC2625000
(Z)-form
$Bp_{0.6}$ 51°.
► Exp. carcinogen and teratogen. PC2625000
Ac: [592-62-1]
$C_4H_8N_2O_3$ 132.119
Bp 191° $Bp_{0.45}$ 49°.
► LD_{50} (rat, orl) 270 mg/kg. Possible human carcinogen. Exp. carcinogen and teratogen. PC2800000
O-*β-D-Glucopyranoside:* [14901-08-7] ***Cy-***

casin. *β-D-Glucosyloxyazoxymethane*
$C_8H_{16}N_2O_7$ 252.224
Alkaloid from seeds of the false sago *Cycas circinalis* and sago cycas *Cycas revoluta* (Cycadaceae). Carcinogen of significance in human nutrition; but in practice the toxin is present in the seeds of the plant and the pith is used as a food source. Mp 154° dec. (144-145° dec.). $[\alpha]_D^{18}$ -44 (c, 0.62 in H_2O). λ_{max} 218 (ϵ 7240); 275 (sh) (ϵ 50) (H_2O) (Derep).
▶ Carcinogenic. Exp. teratogen. LZ5950000

O-*β-D-Glucopyranoside, tetra*-O-*Ac:*
Mp 137°. $[\alpha]_D^{18}$ -27 (c, 1 in $CHCl_3$).

O-*[β-D-Xylopyranosyl-(1→6)-D-gluco-pyranoside]:* [6327-93-1] ***Macrozamin***
$C_{13}H_{24}N_2O_{11}$ 384.339
Prisms (EtOH aq.). Mp 202-203° dec. $[\alpha]_D^{23}$ -71.3 (c, 0.4 in H_2O). λ_{max} 217 (ϵ 7940); 275 (sh) (ϵ 50) (H_2O) (Derep).

O-*[β-D-Glucopyranosyl(1→3)-β-D-gluco-pyranoside]:* [2288-32-6] ***Neocycasin A***
$C_{14}H_{26}N_2O_{12}$ 414.366
Cryst. + $1H_2O$. Mp 162-163° dec. $[\alpha]_D^{29}$ -35.1. λ_{max} 217 (ϵ 7940); 275 (sh) (ϵ 50) (H_2O) (Derep).
▶ QO7500000

O-*[β-D-Glucopyranosyl-(1→4)-β-D-glu-copyranoside]:* ***Neocycasin E***
$C_{14}H_{26}N_2O_{12}$ 414.366
Mp 156-158° dec. $[\alpha]_D^{15}$ -29.2 (c, 0.9 in H_2O).

O-*[α-D-Glucopyranosyl(1→6)-β-D-gluco-pyranoside]:* [97673-88-6] ***Neocycasin B$_\alpha$***
$C_{14}H_{26}N_2O_{12}$ 414.366

O-*[β-D-Glucopyranosyl(1→6)-β-D-gluco-pyranoside]:* [2697-20-3] ***Neocycasin B***
$C_{14}H_{26}N_2O_{12}$ 414.366
λ_{max} 217 (ϵ 7940); 275 (sh) (ϵ 50) (H_2O) (Derep).

O-*[β-D-Glucopyranosyl(1→3)-β-D-gluco-pyranosyl(1→3)-β-D-glucopyranosyl(1→3)-β-D-glucopyranoside]:* [2288-31-5] ***Neocycasin C***
$C_{26}H_{46}N_2O_{22}$ 738.65

O-*[β-D-Glucopyranosyl(1→4)-β-D-gluco-pyranosyl(1→3)-β-D-glucopyranoside]:* [102770-23-0] *Neocycasin H*
$C_{20}H_{36}N_2O_{17}$ 576.508Artifact formed from Neocycasin A by enzymic tranglycosylation.

O-*[β-D-Glucopyranosyl(1→6)-β-D-gluco-pyranosyl(1→3)-β-D-glucopyranoside]:* [2288-28-0] ***Neocycasin G***
$C_{20}H_{36}N_2O_{17}$ 576.508

O-*[β-D-Glucopyranosyl(1→6)[β-D-gluco-pyranosyl(1→3)]-β-D-glucopyrano-side]:* [102770-22-9] *Neocycasin I*
$C_{20}H_{36}N_2O_{17}$ 576.508

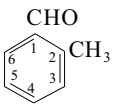
O-*[β-D-Glucopyranosyl(1→3)[β-D-xylo-pyranosyl(1→6)]-β-D-glucopyrano-side]:* [102770-21-8] ***Neocycasin J***
$C_{19}H_{34}N_2O_{16}$ 546.481

[106251-55-2]

Riggs, N.V. *et al., Chem. Ind. (London)*, 1956, 926 (*isol, uv, struct*)
Nagahama, T. *et al., Agric. Biol. Chem.*, 1961, **25**, 937 (*Neocycasin E*)
Korsch, B.H. *et al., Tet. Lett.*, 1964, 523 (*pmr, struct*)
Kobayashi, A. *et al., Arch. Biochem. Biophys.*, 1965, **110**, 373 (*isol*)
Palekar, R.S. *et al., Nature (London)*, 1965, **206**, 1363
IARC Monog., 1976, **10**, 131; *Suppl.*, **7**, 66 (*tox, rev, Ac*)
Baldwin, J.E. *et al., J.O.C.*, 1978, **43**, 2427 (*synth*)
Cannon, J.R. *et al., Aust. J. Chem.*, 1980, **33**, 2229 (*Macrozamin*)
Moretti, A. *et al., Phytochemistry*, 1981, **20**, 1415 (*occur*)
Yagi, F. *et al., Agric. Biol. Chem.*, 1983, **47**, 137; 1985, **49**, 1531; 2985 (*Neocycasins*)
Matsumoto, H. *et al., CRC Handb. Nat. Occurring Food Toxicants*, 1983, 39 (*rev*)
Zedeck, M.S. *et al., ACS Monogr.*, No. 182, 1984, (*rev*)
Hoffmann, G.R. *et al., Environ. Mutagen.*, 1984, **6**, 103 (*rev*)
Tate, M.E. *et al., Aust. J. Chem.*, 1995, **48**, 1059 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COU000; HMG000; MGS750

2-Methylbenzaldehyde M-311

[529-20-4]
o-*Toluic aldehyde.* o-*Tolualdehyde*



C_8H_8O 120.151
Component of FEMA 3068. Flavouring ingredient (see further under 4-Methylbenzaldehyde, M-313). Liq. d_4^{19} 1.04. Bp 197° Bp_6 68-72°.

Oxime: [14683-79-5]
C_8H_9NO 135.165
Needles (petrol). Mp 49°.

Oxime, O-*Ac:*
$C_{10}H_{11}NO_2$ 177.202
Mp 55-56°.

Hydrazone:
$C_8H_{10}N_2$ 134.18
Mp 97°.

Phenylhydrazone: [59473-50-6]
Mp 105-106°.

4-Nitrophenylhydrazone:
Red cryst. (EtOH). Mp 222°.

2,4-Dinitrophenylhydrazone: [1773-44-0]
Orange-red cryst. (EtOH). Mp 193-194°.

Semicarbazone:
Mp 212°.

Di-Et acetal:
$C_{12}H_{18}O_2$ 194.273
Oil. Bp_{37} 125°. n_D^{23} 1.4949.

[1334-78-7]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 103D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 104B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1283C (*ir*)
Post, H.W. *et al., J.O.C.*, 1940, **5**, 244-249 (*Di-Et acetal, synth*)
Org. Synth., Coll. Vol., 3, 1955, 818 (*synth*)
Staskun, B. *et al., J.C.S.*, 1964, 5880 (*synth*)
Org. Synth., 1971, **51**, 20 (*synth*)
Costa, L. *et al., J. Het. Chem.*, 1974, **11**, 943 (*synth*)
Scheiss, P. *et al., Helv. Chim. Acta*, 1976, **59**, 1745 (*pmr*)
Berry, J.M. *et al., J.C.S. Perkin 1*, 1997, 1147-1156 (*Di-Et acetal, synth, pmr*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1706 (*use*)

3-Methylbenzaldehyde M-312

[620-23-5]
m-*Toluic aldehyde.* m-*Tolualdehyde*

C_8H_8O 120.151
Flavouring ingredient. Component of FEMA 3068; see further under 4-Methylbenzaldehyde, M-313. $d_4^{21.4}$ 1.02. Bp 201° Bp_{17} 93-94°.
▶ Fl. p. 78°.

Hydrazone:
$C_8H_{10}N_2$ 134.18
Mp 71-72°.

Phenylhydrazone: [59670-13-2]
Mp 90°.

4-Nitrophenylhydrazone:
Mp 151-157°.

2,4-Dinitrophenylhydrazone: [2880-05-9]
Mp 211.5-212.5°.

Semicarbazone:
Mp 223-224°.

[1334-78-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 107A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 935B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1286C (*ir*)
Costa, L. *et al., J. Het. Chem.*, 1974, **11**, 943 (*synth*)
Watanabe, Y. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2490 (*synth*)
Schiess, P. *et al., Helv. Chim. Acta*, 1976, **59**, 1745 (*pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1706 (*use*)

4-Methylbenzaldehyde M-313

[104-87-0]

[3235-02-7]
p-*Toluic aldehyde.* p-*Tolualdehyde*

C_8H_8O 120.151
Component of FEMA 3068 together with the *o*- and *m*-isomers. Flavouring ingredient. Methylbenzaldehydes are present in roasted nuts, cooked beef, cider, tomato, coffee, tea and elderberry juice. Liq. with peppermint odour. $d_4^{16.7}$ 1.02. Bp 204-205° Bp_{10} 106°.
▶ Fl. p. 80°.

(E)-Oxime: [3717-15-5]
C_8H_9NO 135.165
Mp 79-80°.

(Z)-Oxime: [3717-16-6]

[3235-02-7]
Mp 108-110°.

Hydrazone: [52693-87-5]
$C_8H_{10}N_2$ 134.18
Mp 135°. Bp_{12} 148°.

Phenylhydrazone: [2829-25-6]

Mp 121°.

4-Nitrophenylhydrazone: [10477-83-5]
Dark red cryst. (EtOH). Mp 200.5°.

2,4-Dinitrophenylhydrazone: [2571-00-8]
Orange-yellow cryst. ($PhNO_3$). Mp 232.5-234.5°.

Semicarbazone:
Mp 234°.

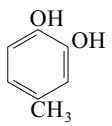
Di-Et acetal:1-(Diethoxymethyl)-4-methylbenzene
$C_{12}H_{18}O_2$ 194.273
Bp_{12} 116-119°.

[1334-78-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 109B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 938C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1288D (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 583 (*synth*)
Costa, L. *et al., J. Het. Chem.*, 1974, **11**, 943 (*synth*)
Schiess, P. *et al., Helv. Chim. Acta*, 1976, **59**, 1745 (*pmr*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1706 (*use*)

4-Methyl-1,2-benzenediol, 9CI M-314

[452-86-8]
3,4-Dihydroxytoluene. 4-Methylcatechol. Homopyrocatechol. Homocatechol



$C_7H_8O_2$ 124.139
Prisms (C_6H_6). Mp 65°. Bp 251° Bp_{20} 143-146°. pK_{a1} 9.7; pK_{a2} 12.95 (25°, 0.1*M* KCl). Sublimes.

► UX1915000

Di-Ac: [13287-30-4]
$C_{11}H_{12}O_4$ 208.213
Bp 260-264° Bp_{70} 160°.

1-Me ether: [1195-09-1] *2-Methoxy-5-methylphenol. Isocreosol*
$C_8H_{10}O_2$ 138.166
Mp 37-39°. Bp 223°. Steam-volatile.

► GP1770000

2-Me ether: [93-51-6] *2-Methoxy-4-methylphenol, 9CI. Creosol. 5-Methylguaiacol. 4-Hydroxy-3-methoxytoluene. Homoguaiacol. FEMA 2671*
$C_8H_{10}O_2$ 138.166
Flavouring ingredient. Constit. of ylang-ylang oil. Spar. sol. H_2O, sol. EtOH, Et_2O, C_6H_6, $CHCl_3$, AcOH. d_4^{25} 1.09. Mp 5.5°. Bp 221° Bp_{22} 113.5°. n_D^{25} 1.5353. pK_{a1} 10.28 (25°). Log P 1.82 (calc). Steam-volatile.

► Eye and skin irritant. LD_{50} (rat, orl) 740 mg/kg. GP1755000

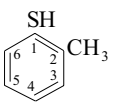
2-Me ether, 1-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [133137-60-7]
$C_{19}H_{28}O_{11}$ 432.424
Powder. $[\alpha]_D^{29}$ -100.3 (c, 0.1 in MeOH).

Di-Me ether: [494-99-5] *1,2-Dimethoxy-4-methylbenzene, 9CI. 3,4-Dimethoxytoluene, 8CI. 4-Methylveratrole. Homoveratrole*
$C_9H_{12}O_2$ 152.193
Cryst. (Et_2O). Mp 24°. Bp 219-221° Bp_5 90°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1101D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 276C; 296A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1027A; 1038A (*ir*)
Steinkopf, W. *et al., Ber.*, 1931, **64**, 990 (*isol, deriv*)
Karrer, P. *et al., Helv. Chim. Acta*, 1943, **26**, 800 (*deriv*)
Org. Synth., Coll. Vol., 4, 1963, 203 (*deriv*)
Highet, R.J. *et al., J.O.C.*, 1965, **30**, 902 (*pmr*)
Takai, H. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1303 (*nmr*)
Sammes, P.G. *et al., J.C.S. Perkin 1*, 1979, 1736 (*synth*)
Vickery, E.H. *et al., J.O.C.*, 1979, **44**, 4444 (*synth*)
Tsuchiya, T. *et al., Nippon Kagaku Kaishi*, 1979, 370 (*synth*)
Nishimura, H. *et al., Phytochemistry*, 1990, **29**, 3303 (*Me ether apiosylglucoside*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 459 (*2-Me ether*)
Bunnett, J.F. *et al., J.O.C.*, 1996, **61**, 8069-8073 (*Me ethers, synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1696-1697 (*2-Me ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DNE200; MEK250

2-Methylbenzenethiol, 9CI M-315

[137-06-4]
o-*Toluenethiol, 8CI.* o-*Thiocresol.* o-*Mercaptotoluene.* o-*Methylthiophenol. FEMA 3240*



C_7H_8S 124.206
Flavouring ingredient. Leaves or liq. Insol. H_2O; sol. common org. solvs. d_4^{20} 1.04. Mp 15°. Bp 194.3° Bp_{50} 106°. pK_a 6.64 (26°).

► LD_{50} (mus, ipr) 100 mg/kg. XT8750000

S-*Et:1-(Ethylthio)-2-methylbenzene. Ethyl* o-*tolyl sulfide*
$C_9H_{12}S$ 152.26
Bp 220°.

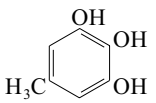
Disulfide: See 2,2′-Dimethyldiphenyl disulfide in *The Combined Chemical Dictionary.*

[34878-60-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1174B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 417B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1090B (*ir*)
Adv. Chem. Ser., 1955, **15**, 182; 326 (***props***)
Hirota, M. *et al., Tetrahedron*, 1969, 5953 (*pmr*)
Jones, I.W. *et al., J.C.S. Perkin 2*, 1973, 1125 (*uv*)
Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, (*detn, Te*)
Schroth, W. *et al., Z. Chem.*, 1977, **17**, 411 (*synth*)
Shagun, L.G. *et al., Zh. Org. Khim.*, 1978, **14**, 187 (*synth*)
Shaw, J.E. *et al., J.O.C.*, 1991, **56**, 3728 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 575
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2807-2808
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGP000

5-Methyl-1,2,3-benzenetriol, 9CI M-316

[609-25-6]
5-Methylpyrogallol, 8CI. 3,4,5-Trihydroxytoluene. 4,6-Dihydroxyorcinol



$C_7H_8O_3$ 140.138
Dark red cryst. (Me_2CO/C_6H_6). Mp 146°. Sublimes.

Tri-Ac:
$C_{13}H_{14}O_6$ 266.25
Cryst. Mp 101.5-102.5°.

1-Me ether:3-Methoxy-5-methyl-1,2-benzenediol
$C_8H_{10}O_3$ 154.165
Tablets. Mp 68°.

1,3-Di-Me ether: [6638-05-7] *2,6-Dimethoxy-4-methylphenol, 9CI. 2,6-Dimethoxy-*p*-cresol. FEMA 3704*
$C_9H_{12}O_3$ 168.192
Present in smoked fish and pork. Flavouring ingredient. Cryst. (EtOH). Mp 36°. Bp_{12} 145°.

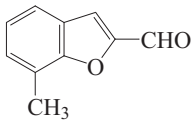
2,3-Di-Me ether: [1128-32-1] *2,3-Dimethoxy-5-methylphenol, 9CI*
$C_9H_{12}O_3$ 168.192
Mp 49-51°.

Tri-Me ether: [6443-69-2] *1,2,3-Trimethoxy-5-methylbenzene. 3,4,5-Trimethoxytoluene*
$C_{10}H_{14}O_3$ 182.219
Mp 35-37° (24-26°). Bp_5 117-118°. n_D^{20} 1.5230.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1050D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 203B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 982C (*ir*)
Koller, G. *et al., Monatsh. Chem.*, 1935, **65**, 367 (*synth*)
Goodwin, S. *et al., J.A.C.S.*, 1957, **79**, 179 (*synth*)
Packter, N.M. *et al., Biochem. J.*, 1966, **98**, 353
Simonart, P. *et al., Bull. Soc. Chim. Biol.*, 1966, **48**, 943 (*isol*)
Merz, A. *et al., Synthesis*, 1993, 797 (*tri-Me ether*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 497 (*1,3-di-Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1754-1755 (*1,3-di-Me ether*)

7-Methyl-2-benzofurancarboxaldehyde, 9CI M-317

[57897-70-8]



$C_{10}H_8O_2$ 160.172
Flavour enhancer for coffee. Pale yellow solid. Mp 58-59°.

U.S. Pat., 1977, 4 002 793, (*Firmenich*); *CA*, **86**, 171246p (*synth, use*)
Ansar, M. *et al., Eur. J. Med. Chem. (Chim. Ther.)*, 1996, **31**, 449-460 (*synth*)
Yoshimura, H. *et al., J. Med. Chem.*, 2000, **43**, 2929-2937 (*synth, pmr*)

4-Methylbenzoic acid, 9CI M-318

[99-94-5]

[25567-10-6]
p-*Toluic acid. Crithmic acid*



$C_8H_8O_2$ 136.15
Isol. from horseradish. Spar. sol. H_2O. Mp 181°. Bp 274-275°. pK_a 4.37. Sublimes. Steam-volatile.

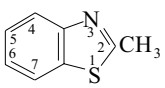
► LD_{50} (rat, orl) 400 mg/kg. XU1575000

[17264-54-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 193B; 294C; 344B; 370C; 381D; 448D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1072C; 1247C; 1248A; 1342A; 1393B; 1412A (*nmr*)
Org. Synth., Coll. Vol., 3, 1955, 822 (*synth*)
Kaiser, E.M. *et al., J.O.C.*, 1970, **36**, 1198 (*synth*)
Takwale, M.G. *et al., Acta Cryst. B*, 1971, **27**, 1152 (*cryst struct*)
Org. Synth., 1971, **51**, 96 (*synth*)
Yamamoto, O. *et al., Anal. Chem.*, 1972, **44**, 1794 (*pmr*)
Brunet, J.J. *et al., J.O.C.*, 1979, **44**, 2199 (*synth*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPX850; TGU000; TGQ250; TGT750

2-Methylbenzothiazole, 9CI M-319

[120-75-2]



C_8H_7NS 149.216
Known as an aroma constit. of tea leaves. Mp 14°. Bp 238° Bp_{15} 150-151°. pK_a 2.06 (H_2O). pK_a 8.63 (MeCN).

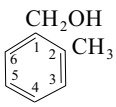
► LD_{50} (mus, ipr) 300 mg/kg. DL5600000

[14933-76-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 699D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 200B; 201B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1511B (*ir*)
Hofmann, A.W. *et al., Ber.*, 1880, **13**, 8-22; 1223-1238 (*synth*)
Mills, W.H. *et al., J.C.S.*, 1922, **121**, 455-466 (*N-Rt*)
Clark, L.M. *et al., J.C.S.*, 1928, 2313-2320 (*synth*)
Millard, B.J. *et al., Org. Mass Spectrom.*, 1968, **1**, 285 (*ms*)
Schweizer, E.E. *et al., J.O.C.*, 1978, **43**, 2972 (*synth*)
Sawhney, S.N. *et al., J.O.C.*, 1979, **44**, 1136 (*cmr*)
Peyronel, G. *et al., Spectrochim. Acta A*, 1981, **37**, 71 (*ir*)
Bowman, W.R. *et al., Tet. Lett.*, 1982, **23**, 5093 (*synth*)
Wanner, K.T. *et al., Annalen*, 1984, 1100 (*synth*)
Stefaniak, L. *et al., Org. Magn. Reson.*, 1984, **22**, 215 (*N-15 nmr*)
Kolb, B. *et al., J. Agric. Food Chem.*, 1985, **33**, 999 (*isol*)
Alyea, E.C. *et al., J. Het. Chem.*, 1985, **22**, 1325 (*synth*)
Stierle, A.A. *et al., Tet. Lett.*, 1991, **32**, 4847 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHI750

2-Methylbenzyl alcohol M-320

[89-95-2]
*2-Methylbenzenemethanol, 9CI. α-Hydroxy-*o*-xylene. 1-Hydroxymethyl-2-methylbenzene.* o-*Tolylmethanol*



$C_8H_{10}O$ 122.166
Needles (petrol/Et_2O). Mp 37-39°. Bp 219° $Bp_{0.75}$ 85-86.5°.

Ac: [17373-93-2]

[29759-11-3]
$C_{10}H_{12}O_2$ 164.204
Flavouring ingredient. Component of FEMA 2684. Liq. Bp_{753} 228-230°.

4-Nitrobenzoyl:
Mp 100-101°.

Me ether:1-(Methoxymethyl)-2-methylbenzene
$C_9H_{12}O$ 136.193
Unpleasant smelling oil. Mp 187-188°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1126C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 339B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1051A (*ir*)
CRC Atlas of Spectral Data and Physical Constants, M200 (*uv, ms*)
Org. Synth., Coll. Vol., 4, 1963, 582 (*synth*)
Bryant, D.R. *et al., J.O.C.*, 1969, **34**, 1106 (*Ac*)
Azzena, U. *et al., J.O.C.*, 1996, **61**, 4913 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1074-1075 (*Ac, use*)

3-Methylbenzyl alcohol M-321

[587-03-1]
*3-Methylbenzenemethanol, 9CI. α-Hydroxy-*m*-xylene. 1-Hydroxymethyl-3-methylbenzene.* m-*Tolymethanol*

$C_8H_{10}O$ 122.166
Oil. d^{17} 0.92. Mp -20°. Bp_{743} 217.5-219.5° Bp_{17} 110-112°.

Ac: [17369-57-2]

[29759-11-3]
$C_{10}H_{12}O_2$ 164.204
Component of FEMA 2684. Flavouring ingredient. Liq. Mp 226°.

4-Nitrobenzoyl:
Cryst. (petrol). Mp 111°.

Et ether: [64988-09-6] *1-(Ethoxymethyl)-3-methylbenzene*
$C_{10}H_{14}O$ 150.22
Bp_{740} 202°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1129D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 344A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1054C (*ir*)
CRC Atlas of Spectral Data and Physical Constants, M201 (*uv, ms, ir*)
Field, B.O. *et al., J.C.S.*, 1955, 1110 (*synth*)
Bryant, D.R. *et al., J.O.C.*, 1969, **34**, 1106 (*Ac*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1074-1075 (*Ac, use*)

4-Methylbenzyl alcohol M-322

[589-18-4]
*4-Methylbenzenemethanol, 9CI. α-Hydroxy-*p*-xylene. 1-Hydroxymethyl-4-methylbenzene.* p-*Tolylmethanol*

$C_8H_{10}O$ 122.166
Needles (heptane). Mp 61-62° (57-58°). Bp 217°.

► Skin irritant. LD_{50} (rat, orl) 1400 mg/kg. DO9370000

3,5-Dinitrobenzoyl:
Mp 117-118°.

Ac: [2216-45-7]

[29759-11-3]
$C_{10}H_{12}O_2$ 164.204
Component of FEMA 2684. Flavouring ingredient. $Bp_{0.5}$ 65-67°.

Et ether: [54191-22-9] *1-(Ethoxymethyl)-4-methylbenzene*
$C_{10}H_{14}O$ 150.22
d^{17} 0.93. Bp_{740} 203°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1132D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 348B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1057A (*ir*)
CRC Atlas of Spectral Data and Physical Constants, M202 (*uv, ms, ir*)
Mozingo, R. *et al., J.A.C.S.*, 1948, **70**, 229 (*synth*)
Watson, J.R. *et al., J. Chromatogr.*, 1970, **52**, 63
Fraser, R.R. *et al., J.A.C.S.*, 1972, **94**, 3253
Hilborn, J.W. *et al., J.A.C.S.*, 1994, **116**, 3337 (*acetate*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1074-1075 (*Ac, use*)

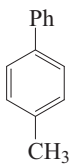
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHB250

4-Methylbiphenyl, 8CI M-323

[644-08-6]

[28652-72-4]

p-*Phenyltoluene. FEMA 3186*



$C_{13}H_{12}$ 168.238

Present in cocoa. Flavouring ingredient. Plates (MeOH or petrol). Mp 49-50°. Bp 267-268° Bp_{15} 134-136°.

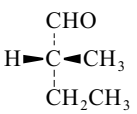
► LD_{50} (rat, orl) 2570 mg/kg. DV5460000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 950B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 32C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 873C (*ir*)
Sherwood, I.R. *et al., J.C.S.*, 1932, 1832 (*synth*)
Brown, D.A. *et al., J.C.S.(A)*, 1966, 1617 (*ir, pmr*)
Mostecky, J. *et al., Anal. Chem.*, 1970, **42**, 1132 (*glc*)
Bullpitt, M. *et al., J.O.C.*, 1976, **41**, 760 (*cmr*)
Korzeniowski, S.H. *et al., Tet. Lett.*, 1977, 1871 (*synth*)
Tius, M.A. *et al., Tet. Lett.*, 1981, 3335 (*synth*)
Hart, H. *et al., J.O.C.*, 1985, **50**, 3104 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1726-1727

2-Methylbutanal, 9CI M-324

[96-17-3]

2-Methylbutyraldehyde. FEMA 2691



(*R*)-form

$C_5H_{10}O$ 86.133

► Highly flammable, fl. p. 9° (oc). Eye and skin irritant. ES3400000

(*R*)-*form* [33204-48-7]
$[\alpha]_D^{20}$ -19.3 (c, 1.52 in Me_2CO).

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 135-137°. $[\alpha]_D$ +29.5 (AcOH).

(*S*)-*form* [1730-97-8]
Found in tea, coffee, peppermint oil (*Mentha piperita*). Bp 90-92°. $[\alpha]_D^{22}$ +34.5 (neat).

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 135-137°. $[\alpha]_D^{22}$ +34.7 (c, 2.9 in Me_2CO).

(±)-*form* [57456-98-1]
Flavouring agent. Insol. H_2O. Bp 92-93°.

Oxime:
$C_5H_{11}NO$ 101.148
Bp 149-151°.

2,4-Dinitrophenylhydrazone:
Orange prisms (EtOH). Mp 129-130°.

Semicarbazone:
Needles (EtOH aq.). Mp 103°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 466C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 728A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 552B (*ir*)
Karabatsos, G.J. *et al., J.A.C.S.*, 1965, **87**, 2864 (*pmr*)
Kirmse, W. *et al., Chem. Ber.*, 1971, **104**, 1800
Org. Synth., 1971, **51**, 31
Bott, K. *et al., Angew. Chem., Int. Ed.*, 1973, **12**, 851
Cainelli, G. *et al., Tet. Lett.*, 1973, 2491
Banno, K. *et al., Chem. Lett.*, 1976, 279
Enders, D. *et al., Tet. Lett.*, 1977, 191
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 739 (*rev, tox*)
Brown, H.C. *et al., J.A.C.S.*, 1985, **107**, 4980 (*synth*)
White, J.D. *et al., J.A.C.S.*, 1995, **117**, 1908 (*synth, ir, pmr, cmr*)
Shustov, G.V. *et al., J.O.C.*, 1998, **63**, 661-669 (*S-form, cd*)
Jauch, J. *et al., Tetrahedron*, 1999, **55**, 9787-9792 (*S-form, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MJX500

3-Methylbutanal, 9CI M-325

[590-86-3]

Isovaleraldehyde. 3-Methylbutyraldehyde. FEMA 2692

$(H_3C)_2CHCH_2CHO$

$C_5H_{10}O$ 86.133

Occurs in orange, bergamot, lemon, sandalwood, citronella, peppermint, eucalyptus and other oils. Also in apple, grape, peach cider, vinegar, wines, wheatbreads, scallops and ginger. Liq. with pungent, apple-like odour. Misc. EtOH, Et_2O; spar. sol. H_2O. Fp -51. Bp 92.5°.

► Highly flammable, fl. p. -5°. LD_{50} (rat, orl) 5600 mg/kg. ES3450000

Oxime: [626-90-4]
$C_5H_{11}NO$ 101.148
Cryst. Mp 48.5°. Bp 164-165°.

2,4-Dinitrophenylhydrazone: [2256-01-1]
Cryst. Mp 122-123°.

Di-Me acetal: [57094-35-6] *1,1-Dimethoxy-3-methylbutane*
$C_7H_{16}O_2$ 132.202
Liq. Bp 128°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 729A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 467A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 552D (*ir*)
Sabatier, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1913, **156**, 1730; 1914, **158**, 985 (*synth*)
Meyers, A.I. *et al., J.O.C.*, 1973, **38**, 36 (*synth*)
Larcheveque, M. *et al., Tet. Lett.*, 1975, 3851 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 379 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHX500

3-Methylbutanethioic acid, 9CI M-326

[60681-87-0]

$(H_3C)_2CHCH_2COSH \Leftrightarrow (H_3C)_2CHCH_2C(S)OH$

$C_5H_{10}OS$ 118.199

***SH*-form**

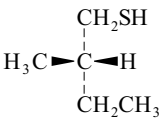
Me ester: [23747-45-7] S-*Methyl 3-methylthiobutyrate. Methanethiol isovalerate. FEMA 3864*
$C_6H_{12}OS$ 132.226
Prod. by micrococaceae and coryneform bacteria isolated from cheeses. Also in hop oil, honeydew melon, galbanum oil and (tentatively) cantaloupes. Flavouring ingredient. Liq. with catty, garlic-like odour. Bp 157°.

2,5-Dimethyl-3-furanyl ester: S-2,5-Dimethyl-3-furanyl 3-methylbutanethioate,
Dauphin, G. *et al., Org. Magn. Reson.*, 1979, **12**, 557-560 (*S-Me ester, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1156 (*S-Me ester, use*)
Lermusieau, G. *et al., J. Agric. Food Chem.*, 2001, **49**, 3867-3874 (*S-Me ester, occur, hops*)
Valero, E. *et al., J. Chromatogr. Sci.*, 2001, **39**, 222-228 (*S-Me ester, occur, glc*)

2-Methyl-1-butanethiol M-327

[1878-18-8]

1-Mercapto-2-methylbutane. FEMA 3303



(*S*)-form

$C_5H_{12}S$ 104.216

(*S*)-*form* [20089-07-0]
$[\alpha]_D^{25}$ +3.1.

S-*Me:* [22299-60-1] *2-Methyl-1-(methylthio)butane. Methyl 2-methylbutyl sulfide*
$C_6H_{14}S$ 118.243
Mp 137°. $[\alpha]_D^{25}$ +18.1.

(±)-*form*
Flavouring ingredient. d_4^{20} 0.85. Bp 119.1°. n_D^{20} 1.4477.

[15013-37-3, 31050-04-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 259A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 415B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 340B (*ir*)
Lanum, W.J. *et al., J. Chem. Eng. Data*, 1964, **9**, 272; 1969, **14**, 93 (*props*)
Polak, V. *et al., CA*, 1968, **69**, 43345h (*synth*)
Salvadori, P. *et al., Gazz. Chim. Ital.*, 1968, **98**, 1400 (*synth, deriv*)
Schlenk, W. *et al., Annalen*, 1973, 1156 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 477
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1727
Goldoni, F. *et al., Synth. Commun.*, 1998, **28**, 2237-2244 (*synth, pmr*)

3-Methyl-1-butanethiol, 9CI M-328

[541-31-1]

Isopentyl mercaptan. Isoamyl mercaptan. Isopentanethiol. Isoamyl thioalcohol. Thioisoamyl alcohol. 1-Mercapto-3-

methylbutane. FEMA 3858

$(H_3C)_2CHCH_2CH_2SH$

$C_5H_{12}S$ 104.216

Found in beer. Flavouring agent. d_4^{20} 0.84. Bp 116°. n_D^{20} 1.4412.

► Highly flammable, fl. p. 18°.

S-*Me:3-Methyl-1-(methylthio)butane. Isopentyl methyl sulfide*

$C_6H_{14}S$ 118.243

Bp 136-138°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 259B (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 415C (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 340C (*ir*)

Nord, F.F. *et al., Ber.*, 1919, **52**, 1207 (*synth*)

Vejdelek, Z.J. *et al., CA*, 1955, **49**, 336 (*synth*)

Obolentsev, R.D. *et al., CA*, 1960, **54**, 250 (*synth*)

Andersen, K.K. *et al., J. Chem. Ecol.*, 1975, **1**, 43 (*occur*)

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1081

3-Methyl-2-butanethiol, 9CI M-329

[2084-18-6]

[68716-68-7]
FEMA 3304

$H_3CCH(CH_3)CH(SH)CH_3$

$C_5H_{12}S$ 104.216

Flavour enhancer for meat products. Present in cooked beef. Formed from thermal degradation of 4-Hydroxy-2,5-dimethyl-3(2*H*)-furanone, H-407 in the presence of a sulfur source. Liq. with repulsive mercaptan-like odour. d_4^{20} 0.84. Bp 109.8° (118°). n_D^{20} 1.4446. Props. doubtless refer to a mixt. of diastereomers.

Lanum, W.J. *et al., J. Chem. Eng. Data*, 1969, **14**, 93-98 (*props*)

U.S. Pat., 1973, 3 713 848; *CA*, **78**, 122978f (*use*)

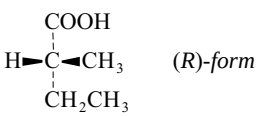
Makoto, U. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1837-1845 (*synth*)

Morishita, F. *et al., J. Chromatogr.*, 1982, **239**, 483-492 (*glc*)

Zheng, Y. *et al., J. Agric. Food Chem.*, 1997, **45**, 894-897 (*occur*)

2-Methylbutanoic acid, 9CI M-330

[116-53-0]
Ethylmethylacetic acid. Butane-2-carboxylic acid. FEMA 2695



(*R*)-*form*

$C_5H_{10}O_2$ 102.133

► EK7897000

(*S*)-*form* [1730-91-2]

Isol. from many essential oils and other biol. sources. Bp 177° Bp_{15} 76-78°.

Me ester: [10307-60-5]

Flavour component of apple and strawberry. Bp 115.5-116°. $[\alpha]_D$ +16.56 (H_2O).

(±)-*form* [600-07-7]

Present in angelica root oil and coffee. Flavouring agent, e.g. for Roquefort cheese. Oil with acrid odour and taste, becoming fruity on dilution. d_{17}^{24} 0.94. Bp 177° Bp_{21} 84°. n_D 1.4047.

Me ester: [53955-81-0] *FEMA 2719*

Flavouring agent. Present in apple, apricot, morello cherry, melon, strawberry, peas, baked potato and mint oils. Liq. with apple-like flavour on dilution. d 0.88. Bp 115°. n_D^{20} 1.3930. Chirality of natural form undetermined.

Et ester: [7452-79-1] *Ethyl 2-methylbutyrate. FEMA 2443*

$C_7H_{14}O_2$ 130.186

Found in many fruits, e.g.raw and cooked apple, apricot, orange, grapefruit. Flavouring agent. Used in fruit flavouring. Liq. with apple-like odour. d_4^{20} 0.87. Bp 133.5°. n_D^{20} 1.3964.

Isopropyl ester: [66576-71-4] *Isopropyl 2-methylbutanoate. FEMA 3699*

$C_8H_{16}O_2$ 144.213

Flavouring ingredient. Liq. d^{20} 0.8496. Bp_{100} 81-83°. n_D^{20} 1.3970.

Butyl ester: [15706-73-7] *Butyl 2-methylbutanoate. FEMA 3393*

$C_9H_{18}O_2$ 158.24

Flavouring agent.

2-Methylbutyl ester: [2445-78-5] *2-Methylbutyl 2-methylbutanoate. FEMA 3359*

$C_{10}H_{20}O_2$ 172.267

Flavouring ingredient. Present in essential oil of hops (*Humulus lupulus*) and odorous component of grapes *Vaccinium vitis-idaea*.

Hexyl ester: [10032-15-2] *Hexyl 2-methylbutanoate. FEMA 3499*

$C_{11}H_{22}O_2$ 186.294

Flavouring ingredient. Liq. with a sweet, fruity taste.

(ξ)-*form*

3-Methylbutyl ester: [27625-35-0] *3-Methylbutyl 2-methylbutanoate. Isoamyl 2-methylbutyrate. FEMA 3505*

Flavouring ingredient. Present in apple, strawberry, banana, cognac, cider, sherry, red wine, Roman chamomile oil, Scotch spearmint oil and sea buckthorn. Liq. with fruity odour. Bp_8 70-71°. n_D^{20} 1.4124.

[868-57-5, 86491-60-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 488B; 488C (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 760A; 760B; 914A; 1353A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 578C; 578D; 617D; 797C (*ir*)

Org. Synth., Coll. Vol., 1, 1932, 353; 361 (*synth*)

Freudenberg, K. *et al., Annalen*, 1955, **594**, 76 (*abs config*)

Brechbühler, S. *et al., J.O.C.*, 1967, **32**, 2641 (*abs config*)

Bestmann, H.J. *et al., Tet. Lett.*, 1974, 1275 (*synth*)

Korver, O. *et al., Tetrahedron*, 1974, **30**, 4041 (*cd, conformn*)

Eberson, L. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 186 (*synth*)

Meyers, A.I. *et al., J.A.C.S.*, 1976, **98**, 567 (*synth*)

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EMP600

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 482; 1088; **2**, 92; 353; 416 (*esters*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 350-351; 1008; 1333-1334; 1493-1494; 1736-1737; 1741; 1797 (*esters, occur, props, use*)

Kwon, D.Y. *et al., J. Agric. Food Chem.*, 2000, **48**, 524-530 (*Me ester, synth, isol*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EMP600

3-Methylbutanoic acid M-331

[503-74-2]
Isovaleric acid. Viburnum acid. Baldrianic acid. Phocenic acid. Isopropylacetic acid. Isopentanoic acid. FEMA 3102

$(H_3C)_2CHCH_2COOH$

$C_5H_{10}O_2$ 102.133

Flavouring agent. Simple esters are used in flavourings. Constit. of hops, cheese etc.; an important component of cheese aroma and flavour. Oil with disagreeable, rancid-cheese aroma, acid taste. Mod. sol. H_2O. d_4^{18} 0.93. Mp -37.6°. Bp 176.7° (183°). n_D^{15} 1.4064. pK_a 4.8.

► Skin and eye irritant. LD_{50} (rat, orl) 2000 mg/kg. Fl. p. 79°, autoignition temp. 416/418°. NY1400000

NH_4 salt: [7563-33-9] *Ammonium isovalerate. FEMA 2054*

Used in butter, nut and cheese flavouring. Deliquescent cryst.

Me ester: [556-24-1] *Methyl 3-methylbutanoate. Methyl isovalerate. FEMA 2753*

$C_6H_{12}O_2$ 116.16

Flavouring ingredient. Present in fruits of apple, banana, bilberry, wild blueberry, melon, pineapple, strawberry, and some Florida oranges. Also found in peas, peppermint oil and gruyere de comte cheese. Pungent apple-like odour; bitter flavour. Oil with a strong, pungent, apple-like odour and bitter flavour. Insol. in H_2O. d^{20} 0.88. Bp 116-117°. n_D^{20} 1.3927.

► Highly flammable, fl. p. 20°. NY1510000

Et ester: [108-64-5] *Ethyl 3-methylbutanoate. Ethyl isovalerate. FEMA 2463*

$C_7H_{14}O_2$ 130.186

Found in fruits and vegetables e.g. apple, banana, melon, strawberry, pineapple, blackberries and celery. Used in fruit aroma compositions. Flavouring ingredient. Liq. with fruity odour reminiscent of apple. Mp -99.3°. Bp 134.7°. n_D^{20} 1.3962.

► Flammable, fl. p. 25°. NY1504000

Propyl ester: [557-00-6] *Propyl 3-methylbutanoate. Propyl isovalerate. FEMA 2960*

$C_8H_{16}O_2$ 144.213

Used in fruit flavouring. Present in banana, jackfruit and gruyere de comte cheese. Liq. with a pineapple-like odour. Insol. in H_2O, sol. in EtOH. d_4^{20} 0.86. Bp 156°. n_D^{25} 1.4035. n_D^{20} 1.3955.

Isopropyl ester: [32665-23-9] *Isopropyl 3-methylbutanoate. Isopropyl isovalerate. FEMA 2961*

$C_8H_{16}O_2$ 144.213

Used in pineapple fruit flavouring. d^{17}

0.85. Bp 145°. n_D^{25} 1.3938.

2-Propenyl ester: [2835-39-4] *2-Propenyl 3-methylbutanoate. Allyl isovalerate. FEMA 2045*
$C_8H_{14}O_2$ 142.197
Flavouring ingredient. Liq. Bp 89-90°. n_D^{21} 1.4162.

2-Methylpropyl ester: [589-59-3] *2-Methylpropyl 3-methylbutanoate. Isobutyl isovalerate. FEMA 3369*
$C_9H_{18}O_2$ 158.24
Present in many plants. Flavouring ingredient. d^{20} 0.87. Bp 171°. n_D^{20} 1.4057.

Butyl ester: [109-19-3] *Butyl 3-methylbutanoate. Butyl isovalerate. FEMA 2218*
$C_9H_{18}O_2$ 158.24
Used in fruit flavouring. Present in apricot, banana, strawberries, Parmesan and gruyere de comte cheeses, white wine, olives, plums, jack fruit, cherimoga and lamb's lettuce. d_4^{20} 0.86. Bp 167°. n_D^{20} 1.4087.

tert-*Butyl ester:* [16792-03-3] tert-*Butyl 3-methylbutanoate.* tert-*Butyl isovalerate*
$C_9H_{18}O_2$ 158.24
Liq. Bp 154-157°.

2-Methylbutyl ester: [2445-77-4] *2-Methylbutyl 3-methylbutanoate. 2-Methylbutyl isovalerate. FEMA 3506*
$C_{10}H_{20}O_2$ 172.267
Flavouring ingredient. Liq.

3-Methylbutyl ester: [659-70-1] *3-Methylbutyl 3-methylbutanoate. Isopentyl isopentanoate. Isoamyl isovalerate. FEMA 2085*
$C_{10}H_{20}O_2$ 172.267
Constit. of banana fruit and tomatoes and alcoholic beverages e.g. cognac, cider. Flavouring agent. Liq. with a fruity odour and sweet apple-like flavour. Bp 190.5°.

▶ Flammable, fl. p. 24°. Skin irritant. LD_{50} (rbt, orl) 14000 mg/kg. NY1508000

Pentyl ester: [25415-62-7] *Pentyl 3-methylbutanoate. Amyl isovalerate*
$C_{10}H_{20}O_2$ 172.267
Used in food flavouring. Bp_{11} 78-80°.

Hexyl ester: [10032-13-0] *Hexyl 3-methylbutanoate. Caproyl isovalerate. FEMA 3500*
$C_{11}H_{22}O_2$ 186.294
Used in fruit flavouring. Odour of unripe fruit. Bp 215°. n_D^{20} 1.4210.

Nonyl ester: [7786-47-2] *Nonyl isovalerate. FEMA 2791*
$C_{14}H_{28}O_2$ 228.374
Flavouring ingredient. Liq. Bp 264°.

Benzyl ester: [103-38-8] *Benzyl 3-methylbutanoate. Benzyl isovalerate. FEMA 2152*
$C_{12}H_{16}O_2$ 192.257
Used in food flavouring. Liq. with a fruity odour reminiscent of apple or pineapple. d_4^{18} 1. Bp 246°. n_D^{18} 1.4906.

Chloride: [108-12-3]
C_5H_9ClO 120.578
Liq. Bp 114.5-115.5°.

Amide: [541-46-8] *3-Methylbutanamide*
$C_5H_{11}NO$ 101.148
Mp 131°.

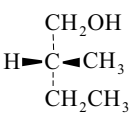
▶ EJ3650000

Nitrile: [625-28-5] *1-Cyano-2-methylpropane. Isobutyl cyanide*
C_5H_9N 83.133
Fp -101. Bp 130.5° (126-128°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 488A; 605D; 727A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 760C; 915C; 1192B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 578B; 619A; 769C (*ir*)
Gustak, E. *et al., Ark. Kemi*, 1952, **24**, 11-13; *CA*, **49**, 163e (*synth*)
Org. Synth., Coll. Vol., 3, 1955, 142-144 (*tert-butyl ester*)
Schmeltz, I. *et al., J. Assoc. Off. Agric. Chem.*, 1963, **46**, 779-784 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 689 (*occur*)
Batchelor, J.G. *et al., J. Magn. Reson.*, 1975, **20**, 19-38 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 841-843 (*rev, tox*)
Merck Index, 11th edn., 1989, Nos. 3772; 5121
Pirrung, M.C. *et al., J.O.C.*, 1994, **59**, 2423-2429 (*tert-butyl ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 27; 35; 482; 554; 606 (*NH_4 salt, esters*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 62; 89; 243; 352; 415; 424; 518; 702; 816 (*rev, free acid*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 93-94; 138-139; 271-272; 346-347; 1001-1002; 1332-1333; 1427-1428; 1492-1493; 1506-1507; 1735-1736; 1788-1789; 1848-1849; 1986; 2367 (*NH_4 salt, esters, occur, use*)
Dembitsky, V.M. *et al., Phytochemistry*, 2000, **54**, 965-967 (*isol, amide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ISU000; ISY000; ITB000; ITC000

2-Methyl-1-butanol, 9CI M-332

[137-32-6]
active-*Amyl alcohol*



(*R*)-*form*

$C_5H_{12}O$ 88.149

▶ Flammable, fl. p. 49°, autoignition temp. 340/385°. Eye, skin and mucous membrane irritant. EL5250000

(*S*)-*form* [1565-80-6]
Isol. from grapes, apples, tomatoes etc.. Bp 128°. $[\alpha]_D^{25}$ -5.8 (heptane). $[\alpha]_D^{20}$ -6.7 (c, 1 in EtOH).

(±)-*form* [34713-94-5]
d_0^0 0.83. Bp 128-129°. n_D^{20} 1.4092.

Ac: [624-41-9]

[129829-14-7] *FEMA 3644*
$C_7H_{14}O_2$ 130.186
Present in apple juice, flavouring ingredient. Liq. with an apple peel and banana odour. d_{20}^4 0.88. Bp 142°. n_D 1.4019.

[624-23-7, 1565-78-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 114D; 115B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 170C; 171A (*nmr*)
Milburn, A.H. *et al., J.C.S.*, 1954, 3344 (*S-form, isol*)
Hawthorne, M.F. *et al., J.O.C.*, 1958, **23**, 1788 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 939; **2**, 386
Rossi, R. *et al., Gazz. Chim. Ital.*, 1968, **98**, 1391 (*synth*)
Bieber, H. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 278 (*rev*)
Giacomelli, G. *et al., J.C.S. Perkin 1*, 1977, 1333 (*synth*)
Tius, M.A. *et al., Synthesis*, 1988, 36 (*synth, ms, ir, pmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 709 (*rev, bibl*)
Gaucher, A. *et al., Can. J. Chem.*, 1994, **72**, 1312 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 480 (*Ac*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1734-1735 (*Ac*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 108
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHS750

2-Methyl-2-butanol, 9CI M-333

[75-85-4]
tert-*Amyl alcohol. Ethyldimethylcarbinol.* tert-*Pentanol. Amylene hydrate, USAN.* tert-*Pentyl alcohol*
$(H_3C)_2C(OH)CH_2CH_3$
$C_5H_{12}O$ 88.149
Isol. from strawberry aroma. Liq. Mod. sol. H_2O. d_4^{20} 0.81. Mp -8.4°. Bp 102°. n_D^{20} 1.4052.

▶ Highly flammable, fl. p. 19°, autoignition temp. 435/437°. Liq. is severe eye irritant. High vapour conc. narcotic. LD_{50} (rat, orl) 1000 mg/kg. SC0175000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 125D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 189B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 182B; 268A (*ir*)
Kyriakides, L.P. *et al., J.A.C.S.*, 1914, **36**, 660 (*synth*)
Chastrette, M. *et al., J. Organomet. Chem.*, 1974, **71**, 11 (*synth*)
Bieber, H. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 278 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 709
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 167
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 831
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBV000

3-Methyl-1-butanol, 9CI M-334

[123-51-3]
Isopentyl alcohol, 8CI. Isoamyl alcohol. FEMA 2057
$(H_3C)_2CHCH_2CH_2OH$
$C_5H_{12}O$ 88.149
Major component of fusel oil. A common

constit. of plant oils, free and as esters. Present in many wines and spirits. Flavouring agent. Pungent liq. Spar. sol. H_2O. d_4^{15} 0.81. Mp -117.2°. Bp 132°. n_D^{20} 1.4055.

▶ Skin and human eye irritant. CNS depressant. OES: long-term 100 ppm; short-term 125 ppm. EL5425000

O-*β-D-Glucopyranoside:Isopentyl β-D-glucoside*
$C_{11}H_{22}O_6$ 250.291
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 86-88°. $[\alpha]_D^{23}$ -33 (c, 0.7 in MeOH).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [178275-89-3] *Isopentyl gentiobioside*
$C_{17}H_{32}O_{11}$ 412.433
Constit. of tomato cell cultures (*Lycopersicon esculentum*). $[\alpha]_D$ -41.5 (c, 0.01 in H_2O).

Formyl: [110-45-2] *3-Methylbutyl formate. Isopentyl formate*
$C_6H_{12}O_2$ 116.16
Used in plum food flavouring. d 0.88. Mp -93.5°. Bp 123-124°. n_D^{20} 1.3976.

Ac: [123-92-2] *Isopentyl acetate. Isoamyl acetate. FEMA 2055*
$C_7H_{14}O_2$ 130.186
Present in many fruit aromas, esp. banana. Used in banana flavouring. Liq. with strong fruity odour. d_4^{15} 0.88. Bp 142°. n_D^{21} 1.3999. n_D^{18} 1.4017.

▶ Flammable, fl. p. 23°, autoignition temp. 360/379°. OES: long-term 100 ppm; short-term 125 ppm. NS9800000

Propanoyl: [105-68-0] *3-Methylbutyl propanoate. Isoamyl propanoate. FEMA 2082*
$C_8H_{16}O_2$ 144.213
Used in food flavouring. Liq. with apricot/pineapple odour. d 0.87. Bp 160-161°.

▶ Low fl. p..

Butanoyl: [106-27-4] *Isoamyl butyrate. FEMA 2060*
$C_9H_{18}O_2$ 158.24
Present in fruit aromas, e.g. apricot, melon, mango etc. Also present in wines, eucalyptus oil and coconut oil. Used in fruit flavours. Liq. with strong fruity odour. Bp 178.5°. n_D^{20} 1.4106.

▶ ET5034000

2-Methylpropanoyl: [2050-01-3] *3-Methylbutyl 2-methylpropanoate. Isoamyl isobutyrate. FEMA 3507*
$C_9H_{18}O_2$ 158.24
Flavouring ingredient.

Benzoyl: [94-46-2] *3-Methylbutyl benzoate. Isoamyl benzoate. FEMA 2058*
$C_{12}H_{16}O_2$ 192.257
Present in sweet cherry, papaya, quince, cherimoya (*Annona cherimola*) vinegar, beer, cocoa. Flavouring agent. Liq. with fruity, pungent odour. d_4^{20} 0.99. Bp 261-262° Bp_4 96-98°. n_D^{20} 1.4949.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 115C; 602D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 171B; 902B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 162B; 609C (*ir*)
Kopp, *et al., Annalen*, 1855, **94**, 311 (*benzoyl*)
Hannotte, T. *et al., Bull. Soc. Chim. Belg.*, 1926, **35**, 92 (*formyl*)
Vogel, A.I. *et al., J.C.S.*, 1948, 624-644 (*formyl*)
Dolgov, B.N. *et al., Zh. Obshch. Khim.*, 1955, **25**, 1549-1557; *J. Gen. Chem. USSR (Engl. Transl.)*, 1955, **25**, 1503-1507 (*benzoyl*)
Brown, H.C. *et al., J.A.C.S.*, 1960, **82**, 1504 (*synth*)
Karpov, O.N. *et al., Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 2853-2857; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 2718-2721 (*formyl, propanoyl*)
Zanetta, J.P. *et al., J. Chromatogr.*, 1973, **76**, 91 (*use*)
Felker, P. *et al., Anal. Biochem.*, 1975, **67**, 245 (*use*)
Blackburn, T.F. *et al., Tet. Lett.*, 1975, 3041 (*synth*)
Debal, A. *et al., Synthesis*, 1976, 391 (*synth*)
Yamamoto, T. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1977, **26**, 515; *CA*, **88**, 181841k (*detn, Zr*)
Bieber, H. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 278 (*rev*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 785 (*rev, tox*)
Sandell, E.B. *et al., Photometric Determination of Traces of Metals, General Aspects*, Wiley, N.Y., 1978,
Goodrich, B.S. *et al., J. Chem. Ecol.*, 1990, **16**, 2091; 2107
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 709 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 483 (*2-methylpropanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1416-1422; 1426-1427 (*occur, esters*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1643-1646 (*isol, glucoside*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 118
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IHO850; IHP000; IHP400

3-Methyl-2-butanol, 9CI M-335

[598-75-4]
sec-*Isoamyl alcohol. Isopropylmethylcarbinol. FEMA 3703*

$C_5H_{12}O$ 88.149
Flavouring ingredient. Present in apple, cider, grape, honey, wine, orange juice and strawberry.

▶ Flammable, fl. p. 39°, autoignition temp. 343°.

(*R*)-*form* [1572-93-6]
$[\alpha]_D^{25}$ -1.91 (36% op).

(*S*)-*form* [1517-66-4]
Bp 110-112°. $[\alpha]_D^{20}$ +5.34 (EtOH).

Ac: [56640-64-3]
$C_7H_{14}O_2$ 130.186
Bp 128.5-129°.

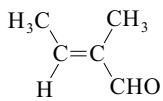
(±)-*form*
Liq. with a fruity fresh odour. Sl. sol. H_2O, misc. EtOH. Bp 113-114°.

Me ether:2-Methoxy-3-methylbutane
$C_6H_{14}O$ 102.176
Bp 81.2-81.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 122C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 183C; 184A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 173A; 173B (*ir*)
Stevens, P.G. *et al., J.A.C.S.*, 1932, **54**, 3732; 1933, **55**, 4237 (*abs config*)
Org. Synth., Coll. Vol., 2, 1943, 406 (*synth*)
Brown, H.C. *et al., J.A.C.S.*, 1959, **81**, 6423 (*synth*)
Cook, P.L. *et al., J.O.C.*, 1962, **27**, 3873 (*synth*)
Giacomelli, G. *et al., J.O.C.*, 1974, **39**, 1757 (*synth*)
Rahn, W. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1976, **357**, 1223 (*use*)
Meek, A.G. *et al., J.O.C.*, 1976, **41**, 323 (*synth*)
Koenig, W.A. *et al., J. Chromatogr.*, 1977, **133**, 141 (*use*)
Krishnamurphy, S. *et al., J.O.C.*, 1977, **47**, 2534 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 570 (*rev*)
White, J.D. *et al., J.O.C.*, 1988, **53**, 5909 (*synth, ir, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 478
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1728-1729

2-Methyl-2-butenal, 9CI M-336

[1115-11-3]
2,3-Dimethylacrolein. 2-Methylcrotonaldehyde


(*E*)-*form*

C_5H_8O 84.118

(*E*)-*form* [497-03-0]
Tiglic aldehyde. Tiglaldehyde. FEMA 3407
Isol. from chives (*Allium schoenoprasum*). Also present in onion, tomato, cheeses, Scotch, spearmint oil, tangerine peel oil, cooked chicken and other foods. Flavour ingredient. Liq. Spar. sol. H_2O. d_4^{20} 0.87. Bp 116.5-117.5° Bp_{119} 63.2-65°. n_D^{20} 1.4475. Readily oxidizes in air.

Oxime:
C_5H_9NO 99.132
Cryst. (Et_2O). Mp 43°.

2,4-Dinitrophenylhydrazone:
Red cryst. (EtOAc/Me_2CO). Mp 215.5-217.5° (222°).

Semicarbazone:
Needles (EtOH). Mp 219° (234°).

(*Z*)-*form* [6038-09-1] *Angelic aldehyde. Angelaldehyde*
Liq. Isom. to *E*-form after 2 weeks at r.t..

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 734C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 558D (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 279C (*ir*)
Wahlroos, O. *et al., Acta Chem. Scand.*, 1965, **19**, 1327 (*isol*)
Satsumabayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 1586 (*synth, ir*)
Botteghi, C. *et al., Tet. Lett.*, 1974, 4285 (*synth*)
Vögeli, U. *et al., Org. Magn. Reson.*, 1975, **7**, 617 (*synth, pmr, cmr, isom*)
Loewenthal, H.J.E. *et al., Synth. Commun.*, 1975, **5**, 201 (*synth*)
Eletti-Bianchi, G. *et al., J.O.C.*, 1976, **41**, 1648 (*synth*)

Kieczykowski, G.R. *et al., Tet. Lett.*, 1976, 597 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1729-1730 (*use, occur*)

3-Methyl-2-butenal, 9CI M-337

[107-86-8]
3-Methylcrotonaldehyde, 8CI. 3,3-Dimethylacrolein. Senecioaldehyde. Senecialdehyde. FEMA 3646

$(H_3C)_2C{=}CHCHO$

C_5H_8O 84.118
Present in blackberry, grape brandy, cocoa, currants, baked potato, tea, costmary and white bread. Flavouring ingredient. Liq. with almond odour. d_4^{20} 0.87. Bp 132-133°. n_D^{20} 1.4526. Readily oxidised.

Phenylhydrazone:
Reddish-violet cryst. Mp 161-162°.

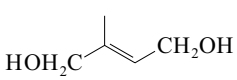
Semicarbazone:
Cryst. (MeOH). Mp 221-222°.

Di-Et acetal: [1740-74-5] *1,1-Diethoxy-3-methyl-2-butene*
$C_9H_{18}O_2$ 158.24
Bp 163-165°. Easily dec..

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 735B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 559A (*ir*)
Wittig, G. *et al., Tetrahedron, Suppl.*, No. 8, 1966, 347-358 (*synth*)
Meyers, A.I. *et al., J.A.C.S.*, 1969, **91**, 764-765 (*synth*)
Pauling, H. *et al., Helv. Chim. Acta*, 1976, **59**, 1233-1243 (*synth*)
Cainelli, G. *et al., J.A.C.S.*, 1976, **98**, 6737-6738 (*synth*)
Erman, M.B. *et al., Tet. Lett.*, 1976, 2981-2984 (*synth*)
Cardillo, G. *et al., Tetrahedron*, 1976, **32**, 107-108 (*synth, ir, pmr*)
Schuda, P.F. *et al., J.O.C.*, 1987, **52**, 1972-1979 (*synth, pmr, ir*)
Klusener, P.A.A. *et al., J.O.C.*, 1987, **52**, 5261-5266 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 479
Kubo, A. *et al., J. Nat. Prod.*, 1995, **58**, 1565-1569 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1730-1731
Schlosser, M. *et al., Chem. Eur. J.*, 1998, **4**, 1738-1743 (*synth, pmr*)
Picquet, M. *et al., Eur. J. Org. Chem.*, 2000, 2361-2366 (*synth, ir, pmr, cmr*)
Vani, P.V.S.N. *et al., Synth. Commun.*, 2001, **31**, 219-224 (*synth, pmr*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 967

2-Methyl-2-butene-1,4-diol M-338

[61842-14-6]



(*E*)-*form*

$C_5H_{10}O_2$ 102.133
Bp_7 127.5-128°.

(*Z*)-*form* [40560-13-2]
Liq. $Bp_{0.5}$ 100-101°.

1-O-*β*-D-*Glucopyranoside:* ***Ilicifolinoside A***
$C_{11}H_{20}O_7$ 264.275
Constit. of *Vitis vinifera* (wine grape). Oil. $[\alpha]_D$ -55.2 (MeOH).

4-O-*β*-D-*Glucopyranoside:*
$C_{11}H_{20}O_7$ 264.275
Constit. of *Vitis vinifera* (wine grape).

[30264-54-1, 40560-13-2, 53170-98-2, 53252-06-5, 57152-93-9, 59054-99-8, 70473-55-1, 104411-04-3, 132032-87-2]

Nicoletti, M. *et al., Planta Med.*, 1992, **58**, 472 (*1-glucoside*)
Messerer, M. *et al., Nat. Prod. Lett.*, 1995, **5**, 241 (*isol, glucosides*)
Zhu, N. *et al., Phytochemistry*, 1998, **47**, 265-268 (*Ilicifolinoside A*)

3-Methyl-2-butene-1-thiol, 9CI M-339

[5287-45-6]
Dimethylallyl mercaptan. 4-Mercapto-2-methyl-2-butene. Prenylthiol. FEMA 3896

$(H_3C)_2C{=}CHCH_2SH$

$C_5H_{10}S$ 102.2
Substance responsible for "sun-struck" flavour of beer. Found in coffee. Used in food flavourings. Liq. with leek-like aroma. Bp 125.5-127°.

S-*Ac:* [33049-93-3] S-*(3-Methyl-2-butenyl) ethanethioate.* S-*Prenyl thioacetate*
$C_7H_{12}OS$ 144.237
Flavouring ingredient. Bp_2 70-72°.

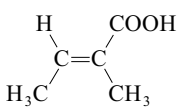
S-*(2-Methylpropanoyl):* [53626-94-1] S-*(3-Methyl-2-butenyl) 2-methylpropanethioate.* S-*Prenyl thioisobutyrate*
$C_9H_{16}OS$ 172.291
Constit. of buchu (*Agathosma*) spp.. Bp_{15} 100°. λ_{max} 206 (ε 6800); 234 (ε 5300) (no solvent reported).

S-*(3-Methylbutanoyl):* [75631-91-3] S-*(3-Methyl-2-butenyl) 3-methylbutanethioate.* S-*Prenyl thioisovalerate*
$C_{10}H_{18}OS$ 186.318
Bp_4 88-92°.

Kuroiwa, Y. *et al., Agric. Biol. Chem.*, 1961, **25**, 257 (*isol*)
Obota, Y. *et al., Nature (London)*, 1961, **190**, 635 (*isol, synth*)
Moore, C.G. *et al., Tetrahedron*, 1962, **18**, 205 (*synth*)
Rivett, D.E.A. *et al., Tet. Lett.*, 1974, 1253 (*isol, ester*)
Lui, K.-C. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 1019 (*synth*)
Campbell, W.E. *et al., Phytochemistry*, 1980, **19**, 1537 (*isol, esters*)

2-Methyl-2-butenoic acid M-340

[13201-46-2]



(*E*)-*form*

$C_5H_8O_2$ 100.117
Log P 1.19 (calc).

(*E*)-*form* [80-59-1]
Tiglic acid. *Cevadic acid. FEMA 3599*
Flavouring ingredient. Cryst. (H_2O) with a sweet, warm spicy odour. Mp 63.5-64°. Bp 198.5° $Bp_{11.5}$ 95-96°. pK_a 4.96 (18°).

▶ Skin irritant. GQ5430000

Me ester: [6622-76-0]
$C_6H_{10}O_2$ 114.144
Oil. Bp_{766} 139.4-139.6°.

▶ EM9254600

Et ester: [5837-78-5] *FEMA 2460*
$C_7H_{12}O_2$ 128.171
Flavouring ingredient. $d^{16.8}$ 0.92. Bp 156° Bp_{15} 55-57°. $n_D^{16.8}$ 1.4347.

Isopropyl ester: [1733-25-1] *Isopropyl tiglate. FEMA 3229*
$C_8H_{14}O_2$ 142.197
Flavouring ingredient.

2-Propenyl ester: [7493-71-2] *Allyl tiglate. FEMA 2043*
$C_8H_{12}O_2$ 140.182
Flavouring ingredient.

1-Ethylhexyl ester: [94133-92-3] *1-Ethylhexyl tiglate. FEMA 3676*
$C_{13}H_{24}O_2$ 212.331
Flavouring agent. Liq. Bp_{60} 94-96°. n_D^{20} 1.4450.

Benzyl ester: [37576-88-8] *Benzyl tiglate. FEMA 3330*
$C_{12}H_{14}O_2$ 190.241
Flavouring agent. Liq.

2-Phenylethyl ester: [55719-85-2] *Phenethyl tiglate. FEMA 2870*
$C_{13}H_{16}O_2$ 204.268
Flavouring ingredient. Liq. Bp 259°.

Amide: [6028-38-2]
C_5H_9NO 99.132
Cryst. Mp 73-74°.

(*Z*)-*form* [565-63-9] ***Angelic acid***
Constit. of *Angelica archangelica* (angelica). Monoclinic prisms with spicy odour (H_2O). Mp 45°. Bp 185° Bp_{10} 88-89°. Steam-volatile. Isomerises to (*E*)-form at Bp..

Me ester: [5953-76-4]
Bp 128°.

2-Methylpropyl ester: [7779-81-9] *Isobutyl angelate. FEMA 2180*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient. Liq. Bp 177°.

Amide:
Mp 127-128°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 499D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 777B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 584C (*ir*)
Buckles, R.E. *et al., Chem. Rev.*, 1955, **55**, 659 (*rev*)
Leete, E. *et al., Tet. Lett.*, 1967, 1727 (*biosynth*)
Myles, A. *et al., J. Med. Chem.*, 1968, **11**, 143 (*synth*)
Johns, S.R. *et al., Aust. J. Chem.*, 1969, **22**, 1315 (*isol*)
Vogeli, U. *et al., Org. Magn. Reson.*, 1975, **7**, 617 (*cmr*)
McGaw, B.A. *et al., Phytochemistry*, 1979, **18**, 1647 (*biosynth*)
Hill, R.K. *et al., J.A.C.S.*, 1980, **102**, 7344 (*biosynth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 837 (*rev, tox, E-form*)
Moats, R.A. *et al., J. Chem. Ecol.*, 1987, **13**, 451
Bartlett, R.J. *et al., J. Chem. Ecol.*, 1988, **14**, 1319
Begley, M.J. *et al., J.C.S. Perkin 1*, 1991, 1951 (*synth, pmr*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 33; 66; 237; 268; 388; 421; 479; 654
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 102; 273-274; 993-994; 1043-1044; 1444-1445; 1501; 1731-1732; 2170 (*esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGA700

3-Methyl-2-butenoic acid, 9CI M-341

[541-47-9]
3-Methylcrotonic acid, 8CI. 3,3-Dimethylacrylic acid. Senecioic acid. Isopropylideneacetic acid. FEMA 3187
$(H_3C)_2C{=}CHCOOH$
$C_5H_8O_2$ 100.117
Flavouring ingredient. Prisms (H_2O). Mp 70°. Bp 199° Bp_{40} 114°. Sublimes.
▶ Skin and severe eye irritant. LD_{50} (rat, orl) 3560 mg/kg. GQ5425000

Me ester: [924-50-5]
$C_6H_{10}O_2$ 114.144
Bp 135-138°.

Et ester: [638-10-8]
$C_7H_{12}O_2$ 128.171
Bp 154-155°.
▶ GQ5750000

2-Hydroxyethyl ester: [56500-42-6]
$C_7H_{12}O_3$ 144.17
Bp_{12} 85-88°.

3-Methylbutyl ester: [56922-73-7]
$C_{10}H_{18}O_2$ 170.251
Used in flavour industry. Bp_{22} 105-107°.

Benzyl ester: [37526-89-9]
$C_{12}H_{14}O_2$ 190.241
Liq. Bp_2 95-97°.

Chloride: [3350-78-5]
C_5H_7ClO 118.562
Bp 145-150°.

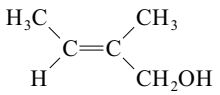
Amide: [4479-75-8]
C_5H_9NO 99.132
Mp 107-108°.
▶ GQ2320000

Nitrile: [4786-24-7] *1-Cyano-2-methylpropene*
C_5H_7N 81.117
Bp 140-142°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 500A; 642C; 732D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 983A; 983B; 1199C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 584D; 682B (*ir*)
U.S. Pat., 1951, 2 554 947; *CA*, **46**, 3069i (*2-hydroxyethyl ester, synth*)
Org. Synth., Coll. Vol., 3, 1955, 302 (*synth, bibl*)
Akahori, Y. *et al., Chem. Pharm. Bull.*, 1961, **9**, 921,936 (*isol*)
Collin, P.J. *et al., Aust. J. Chem.*, 1966, **19**, 317 (*pmr*)
Edwards, J.D. *et al., J.O.C.*, 1966, **31**, 2282 (*synth*)
Santi, R. *et al., J. Organomet. Chem.*, 1979, **182**, 117 (*synth*)
King, R.B. *et al., Tetrahedron*, 1986, **41**, 3235 (*deriv, synth, pmr, cmr, ir*)
Boehler, M.A. *et al., Tetrahedron*, 1991, **47**, 4519-4538 (*2-hydroxyethyl ester, pmr, cmr, ir*)
Perdue, R.E. *et al., Phytochemistry*, 1993, **34**, 1075 (*benzyl ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 490
Abarbri, M. *et al., Tet. Lett.*, 1995, **36**, 2469 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1745-1746
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHT500; MIP800

2-Methyl-2-buten-1-ol, 9CI M-342

[4675-87-0]



(*E*)-*form*

$C_5H_{10}O$ 86.133
Widespread nat. occurrence, e.g. in *Ochromonas danica*, in *Anthemis nobilis* (as acetate), in fruit juices and animal sources (unspecified stereochem.).

(*E*)-*form* [497-02-9]
Tiglic alcohol. Tiglyl alcohol
Found in Roman chamomile (*Anthemis nobilis*) (together with esters). Bp 122-127° (135°) Bp_{33} 66°.

O-*β*-D-*Glucopyranoside:*
$C_{11}H_{20}O_6$ 248.275
Occurs in fennel. Needles (MeOH). Mp 55-56°. $[\alpha]_D^{22}$ -15.8 (c, 0.2 in MeOH).

(*Z*)-*form* [19319-26-7]
Angelic alcohol. Angelyl alcohol
Bp 136-137° Bp_{25} 61-63°. n_D^{20} 1.4410.

Katzenellenbogen, J.A. *et al., J.A.C.S.*, 1976, **98**, 4925 (*synth, ir, pmr*)
Jarolim, V. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 3490 (*synth*)
Zaidlewicz, M. *et al., Synthesis*, 1979, 62 (*synth, pmr*)
Depezay, J.-C. *et al., Bull. Soc. Chim. Fr.*, 1981, 306 (*synth, ms, pmr*)
Smith, P.A.S. *et al., J.O.C.*, 1981, **46**, 3970 (*synth, ir, pmr*)
Bury, A. *et al., J.C.S. Perkin 1*, 1982, 645 (*synth, pmr*)
Ono, N. *et al., Tet. Lett.*, 1984, **25**, 5319 (*synth*)
Masami, Y. *et al., Tetrahedron*, 1984, **40**, 3481 (*synth, ir, pmr*)
Ashcroft, M.R. *et al., J. Organomet. Chem.*, 1985, **289**, 403 (*synth*)
Trost, B.M. *et al., J.A.C.S.*, 1985, **107**, 1293 (*synth, pmr*)
Kurth, M.J. *et al., J.O.C.*, 1985, **50**, 5769 (*synth*)
Simon, H. *et al., Angew. Chem., Int. Ed.*, 1987, **26**, 785 (*synth*)
Bicchi, C. *et al., J. Chromatogr.*, 1987, **411**, 237 (*glc, ms*)
Begley, M.J. *et al., J.C.S. Perkin 1*, 1991, 1951 (*synth, ir, pmr*)
Iyer, R.S. *et al., J.O.C.*, 1994, **59**, 6038 (*synth, pmr*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1643-1646 (*glucoside*)

2-Methyl-3-buten-2-ol M-343

[115-18-4]
Isoprenyl alcohol. 1,1-Dimethylallyl alcohol
$(H_3C)_2C(OH)CH{=}CH_2$
$C_5H_{10}O$ 86.133
The name Isoprenyl alcohol should be avoided as it is likely to be confused with 3-Methyl-2-buten-1-ol, M-344. Flavour ingredient. Present in ylang ylang, orange juice, lemon juice, pineapple and other fruits. Oil. Bp 98-99°.
▶ LD_{50} (rat, ipr) 1315 mg/kg. EM9472000

O-*β*-D-*Glucopyranoside:* [63026-02-8] *1,1-Dimethyl-2-propenyl glucoside. 1,1-Dimethylallyl glucoside.* ***Crenulatin***†
$C_{11}H_{20}O_6$ 248.275
Cryst. (Me_2CO). Mp 135-136°. $[\alpha]_D$ -25 (c,1 in Py).

4-Nitrobenzoyl:
Mp 115-115.5°.

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [76873-98-8]
$C_{16}H_{28}O_{10}$ 380.391
Amorph. powder. $[\alpha]_D^{22}$ -84 (c, 0.2 in MeOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 140A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 210A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 202C (*ir*)
Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1971, 886-888 (*isol*)
Meléndez, E. *et al., An. Quim.*, 1972, **68**, 1283-1294 (*synth, pmr*)
Olah, G.A. *et al., J.A.C.S.*, 1975, **97**, 1539-1546 (*cmr*)
Pinar, M.M. *et al., Phytochemistry*, 1977, **16**, 281-282 (*glucoside*)
Jakupovic, J. *et al., Phytochemistry*, 1991, **30**, 1941-1946 (*Crenulatin*)
Ahmed, A.A. *et al., J. Nat. Prod.*, 1996, **59**, 1171-1173 (*glucoside*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1732
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1939-1940 (*apiosylglucoside*)
Vani, P.V.S.N. *et al., Synth. Commun.*, 2001, **31**, 219-224 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHU100

3-Methyl-2-buten-1-ol M-344

[556-82-1]
Prenol. Isopentenol. Isopentenyl alcohol. Prenyl alcohol. FEMA 3647
$(H_3C)_2C{=}CHCH_2OH$
$C_5H_{10}O$ 86.133
Constit. of ylang-ylang and hop oils. Found in orange peel oil and various fruits e.g. orange, lemon, lime, grape, pineapple, purple passion fruit, loganberry etc. Flavouring ingredient. Oil. Bp 137-138°.
▶ Skin irritant. LD_{50} (rat, orl) 810 mg/kg. LD_{50} (rbt, skn) 3900 mg/kg. EM9472500

O-*β*-D-*Glucopyranoside:* [117861-55-9]
Prenyl glucoside
$C_{11}H_{20}O_6$ 248.275
Isol. from satsuma orange (*Citrus unshiu*). Needles (MeOH). Mp 68-70°. $[\alpha]_D^{21}$ -23.6 (c, 0.2 in MeOH).

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [175737-84-5]
$C_{16}H_{28}O_{10}$ 380.391
Constit. of purple passion fruit *Passiflora edulis*.

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [198832-70-1]
$C_{16}H_{28}O_{10}$ 380.391
Constit. of a wine grape (*Vitis vinifera*) and *Bupleurum falcatum*. Powder. $[\alpha]_D^{26}$ -66.2 (c, 2 in MeOH).

Ac: [1191-16-8] *Isopentenyl acetate*
$C_7H_{12}O_2$ 128.171
Constit. of ylang-ylang oil. Oil. Bp_{32} 54-

56°.
▶ Skin irritant. LD_{50} (rat, orl) 3000 mg/kg.
EM9473700

3,5-Dinitrobenzoyl:
Mp 71°.

3,4-Dihydroxy-E-*cinnamoyl:* [118971-61-2]
3-Methyl-2-butenyl caffeate
$C_{14}H_{16}O_4$ 248.278
Constit. of *Populus* spp..

3,4-Dihydroxy-Z-cinnamoyl: [119644-11-0]
$C_{14}H_{16}O_4$ 248.278
Constit. of *Populus* spp. Flavouring agent.

4-Hydroxy-3-methoxy-E-*cinnamoyl:*
[123022-25-3]
$C_{15}H_{18}O_4$ 262.305

Me ether: [22093-99-8] *1-Methoxy-3-methyl-2-butene*
$C_6H_{12}O$ 100.16
Liq. Bp 102-104°.

Et ether: [22094-00-4] *1-Ethoxy-3-methyl-2-butene, 9CI*
$C_7H_{14}O$ 114.187
Flavouring ingredient. Bp 124-125°.

[100884-13-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 139C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 209A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 201D (*ir*)
Boch, R. *et al., Nature (London)*, 1962, **195**, 1018-1020 (*Ac, isol*)
Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1971, 886-888 (*isol*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1975, 913-915 (*cmr*)
Wenkert, E. *et al., Org. Magn. Reson.*, 1975, **7**, 51-53 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 895 (*rev, tox*)
Hashimoto, T. *et al., Z. Naturforsch., C*, 1988, **43**, 470-472 (*synth, caffeate*)
Stuewe, H.T. *et al., Naturwissenschaften*, 1989, **76**, 426-427 (*synth, caffeate*)
English, S. *et al., Phytochemistry*, 1992, **31**, 1255-1260 (*ferulate*)
Amoros, M. *et al., J. Nat. Prod.*, 1994, **57**, 644-647 (*caffeate*)
Ramalingam, K. *et al., Synth. Commun.*, 1995, **25**, 743-752 (*ethers*)
Chassagne, D. *et al., Phytochemistry*, 1996, **41**, 1497-1500 (*6-arabinosylglucoside*)
Baltenweck-Guyot, R. *et al., J. Nat. Prod.*, 1997, **60**, 1326-1327 (*6-apiofuranosylglucoside*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1643-1646 (*Prenyl glucoside*)
Ono, M. *et al., Phytochemistry*, 1999, **51**, 819-823 (*6-apiofuranosylglucoside*)
Akita, H. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 2429-2439 (*Prenyl glucoside, synth*)
Vani, P.V.S.N. *et al., Synth. Commun.*, 2001, **31**, 219-224 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOQ350; MHU110

3-Methyl-3-buten-1-ol M-345

[763-32-6]
$H_2C{=}C(CH_3)CH_2CH_2OH$
$C_5H_{10}O$ 86.133
Constit. of ylang-ylang oil. Oil.

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [198832-72-3]
$C_{16}H_{28}O_{10}$ 380.391
Constit. of a wine from grapes *Vitis vinifera* cv. Gewurztraminer.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 139B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 209C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 201C (*ir*)
Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1971, 886-888 (*isol*)
Trost, B.M. *et al., J.A.C.S.*, 1975, **97**, 7152-7157 (*synth*)
Baltenweck-Guyot, R. *et al., J. Nat. Prod.*, 1997, **60**, 1326-1327 (*6-apiofuranosylglucoside*)

3-Methyl-3-buten-2-ol, 9CI M-346

[10473-14-0]
Isopropenylmethylcarbinol
$C_5H_{10}O$ 86.133
▶ Highly flammable, fl. p. 18°.
(S)-form [88376-46-9]
Bp 130°. $[\alpha]_D^{21}$ -5.6 (c, 8 in $CHCl_3$).
(±)-form [60041-32-9]
Bp 116-117° Bp_{60} 54.6-56.8°.

3,5-Dinitrobenzoyl:
Mp 110°.

Phenylurethane:
Cryst. (petrol). Mp 66-66.5°.

Ph ether: [62338-46-9] *2-Methyl-3-phenoxy-1-butene*
$C_{11}H_{14}O$ 162.231
Oil. $Bp_{0.025}$ 43°.

(ξ)-form
Constit. of orange, blackcurrant, grape and hops.

Lauchenauer, A. *et al., Helv. Chim. Acta*, 1951, **34**, 1514 (*synth*)
Green, M.B. *et al., J.C.S.*, 1957, 3262 (*synth*)
Hart, H. *et al., J.O.C.*, 1959, **24**, 1261 (*synth*)
Hartley, R.D. *et al., Chem. Ind. (London)*, 1967, 1601 (*isol*)
Crout, D.H.G. *et al., J.C.S. Perkin 1*, 1983, 2435 (*synth, resoln*)
Ryu, E.K. *et al., Synth. Commun.*, 1994, **24**, 1859 (*Ph ether*)
Feeder, N. *et al., J.C.S. Perkin 1*, 1999, 3413-3424 (*synth, pmr*)

3-Methyl-3-buten-2-one, 9CI M-347

[814-78-8]
Isopropenyl methyl ketone. Methyl isopropenyl ketone
$H_2C{=}C(CH_3)COCH_3$
C_5H_8O 84.118
Listed in the EAFUS Food Additive Database (Jan. 2001) but with no current reported use. Oil with a pleasant odour. Sl. sol. H_2O; v. sol. EtOH. d_{20}^{20} 0.86. Mp -54°. Bp 98-100° Bp_{70} 36-38°. n_D^{20} 1.4230. Q/e values for copolym., Q 1.03, e 0.64.
▶ Highly flammable, fl. p. 21°. Skin and severe eye irritant. LD_{50} (rat, orl) 180 mg/kg; LD_{50} (rbt, skn) 230 mg/kg.
EN0175000

Oxime: [20963-51-3]
C_5H_9NO 99.132
Plates. Mp 68°. Bp_{15} 102-104°.

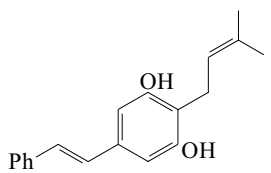
2,4-Dinitrophenylhydrazone: [5077-59-8]
Mp 189.5-191.5°.

Semicarbazone: [22633-27-8]
Mp 172.6-173.5°.

Thorne, N. *et al., J.C.S.*, 1956, 2587 (*synth*)
Hart, H. *et al., J.A.C.S.*, 1957, **79**, 931 (*synth*)
Watanabe, H. *et al., J. Polym. Sci.*, 1962, **62**, 574 (*polym*)
Cook, K.L. *et al., J.C.S. Perkin 1*, 1973, 529 (*synth*)
Chkir, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1975, **281**, 731 (*synth*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1989, **17**, 548 (*rev, polym*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1734
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1792
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKY500

2-(3-Methyl-2-butenyl)-5-(2-phenylethenyl)-1,3-benzenediol M-348

5-Cinnamyl-2-prenylresorcinol. 3,5-Dihydroxy-4-prenylstilbene. ***Chiricanin A***



$C_{19}H_{20}O_2$ 280.366
Amorph. yellow powder. Mp 107-111°.
λ_{max} 210 (4.22); 238 (4.02 sh); 315 (4.28) (MeOH).

Mono-Me ether: [64095-60-9] *3-Methoxy-2-(3-methyl-2-butenyl)-5-(2-phenylethenyl)phenol, 9CI. 5-Cinnamyl-3-methoxy-2-prenylphenol. 3-Hydroxy-5-methoxy-4-prenylstilbene.* ***Longistylin A***
$C_{20}H_{22}O_2$ 294.393
Isol. from leaves of *Cajanus cajan* (pigeon pea). Cryst. (hexane). Mp 75°.

Di-Me ether: [55051-76-8] ***3,5-Dimethoxy-4-prenylstilbene***
$C_{21}H_{24}O_2$ 308.419
Cryst. (hexane). Mp 84-86°.

Monodeoxy, Me ether: [64125-60-6] *3-Methoxy-4-prenylstilbene.* ***Longistylin C***
$C_{20}H_{22}O$ 278.393
Isol. from *Cajanus cajan* (pigeon pea). Cryst. ($CHCl_3$/hexane). Mp 99-100°.
▶ SL7760000

[64095-26-7]

Braz Filho, R. *et al., Phytochemistry*, 1975, **14**, 261; 1454 (*3,5-dimethoxy-4-prenylstilbene*)
Delle Monache, F. *et al., J. Nat. Prod.*, 1977, **40**, 201
Delle Monache, F. *et al., Phytochemistry*, 1978, **17**, 1812 (*isol*)
Marta, M. *et al., Gazz. Chim. Ital.*, 1979, **109**, 323 (*synth*)
Ioset, J.-R. *et al., J. Nat. Prod.*, 2001, **64**, 710-715 (*Chiricanin A*)

3-Methylbutyl glucosinolate M-349

[76265-22-0]
1-Thio-β-D-glucopyranoside 1-[4-methyl-N-(sulfooxy)pentanimidate], 9CI
$(H_3C)_2CHCH_2CH_2C(SGlc){=}NOSO_3H$

$C_{12}H_{23}NO_9S_2$ 389.447
Present in horseradish (*Armoracia lapathifolia*).

Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)

3-Methyl-1-butylamine M-350

[107-85-7]
3-Methyl-1-butanamine, 9CI. 1-Amino-3-methylbutane. Isoamylamine. Isopentylamine. FEMA 3219

$(H_3C)_2CHCH_2CH_2NH_2$

$C_5H_{13}N$ 87.164
Widespread in fungi and higher plants e.g. apple, banana, wine grape, swede, rhubarb, porcini (*Boletus edulis*). Protein degradn. product. Present in bread, apple, banana, white wine, cheeses, rye and ergot. Liq. Misc. H_2O. Bp 95° Bp 232°.

▶ Highly flammable, fl. p. < 21°, irritant.

N-*Ac:* [13434-12-3] N-*(3-Methylbutyl)acetamide.* N-*Isopentylacetamide.* N-*Isoamylacetamide*
$C_7H_{15}NO$ 129.202
Found in wines. Bp 238°.

N-*Me:* [4104-44-3]
$C_6H_{15}N$ 101.191
Bp_{759} 108-110°.

N-*Me; hydrochloride:* [2419-59-2]
Plates (Me_2CO). V. sol. H_2O, insol. Et_2O. Mp 181° (178°).

N-*Et:* [21035-52-9]
$C_7H_{17}N$ 115.218
Bp 127°.

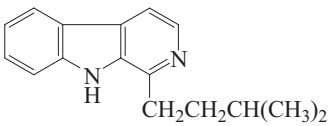
N-*Et; hydrochloride:*
Mp 205-206°.

N-*Propyl:* [78579-58-5] *3-Methyl*-N-*propylbutylamine, 9CI. Isopentylpropylamine*
$C_8H_{19}N$ 129.245
Bp 148-149° Bp_{200} 106-107°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 458C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 286D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 370C (*ir*)
Erickson, J.L.E. *et al., Ber.*, 1926, **59**, 2665 (*synth*)
Nicholas, H.O. *et al., J.A.C.S.*, 1926, **48**, 2174 (*synth*)
Campbell, K.N. *et al., J.A.C.S.*, 1944, **66**, 82 (*N-propyl*)
Dornow, A. *et al., Annalen*, 1954, **588**, 62 (*deriv*)
Cope, A.C. *et al., J.A.C.S.*, 1957, **79**, 4750 (*N-propyl*)
von Kamienski, E.S. *et al., CA*, 1958, **52**, 5551; 6502 (*occur*)
Richardson, M. *et al., Phytochemistry*, 1966, **5**, 23 (*biosynth*)
Demole, E. *et al., Helv. Chim. Acta*, 1972, **55**, 1866 (*isol, deriv*)
Eggert, H. *et al., J.A.C.S.*, 1973, **95**, 3710 (*cmr*)
Ger. Pat., 1976, 2 456 006; *CA*, **85**, 62631v (*synth*)
Heath, R.R. *et al., Experientia*, 1988, **44**, 82 (*isol, synth*)
Perkins, M.V. *et al., J.C.S. Perkin 1*, 1990, 1111 (*isol, bibl, deriv*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 748

1-(3-Methylbutyl)-β-carboline M-351

[40944-75-0]
*1-(3-Methylbutyl)-9*H*-pyrido[3,4-b]indole, 9CI. 1-Isopentyl-β-carboline*

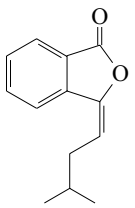


$C_{16}H_{18}N_2$ 238.332
λ_{max} 235 ; 288 ; 336 ; 350 (MeOH) (Berdy).

Tsuji, K. *et al., Yakugaku Zasshi*, 1973, **93**, 33-38; 1978, **98**, 898-903 (*isol*)

3-(3-Methylbutylidene)-1(3*H*)-isobenzofuranone, 9CI M-352

3-Isovalidenephthalide



(*E*)-*form*

$C_{13}H_{14}O_2$ 202.252
Minor odorous constit. of celery (*Apium graveolens*). Pale-yellow oil. Bp_7 170-172°. (*E*)- and (*Z*)-forms have been separated.

[56014-70-1, 56014-71-2]

Gold, H.J. *et al., J.O.C.*, 1963, **28**, 985 (*isol, ir, uv*)
Knight, D.W. *et al., J.C.S. Perkin 1*, 1975, 635 (*synth, ir, pmr*)

3-[(3-Methylbutyl)nitrosoamino]-2-butanone, 9CI M-353

[71016-15-4]
N-*Nitroso*-N-*(1-methyl-2-oxopropyl)-3-methyl-1-butanamine.* N-*Nitroso*-N-*(1-methylacetonyl)-3-methylbutylamine*
$(H_3C)_2CHCH_2CH_2N(NO)CH(CH_3)$-$COCH_3$

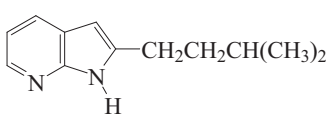
$C_9H_{18}N_2O_2$ 186.253
Isol. from mouldy corn of Linxian, China. Pale yellow oil.

▶ Exp. carcinogen and neoplastic agent.
EL8990000

Singer, G.M. *et al., J. Agric. Food Chem.*, 1987, **35**, 130 (*synth, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MHW350

2-(3-Methylbutyl)-1*H*-pyrrolo[2,3-*b*]pyridine M-354

[946-18-9]
2-Isopentyl-7-azaindole



$C_{12}H_{16}N_2$ 188.272

Constit. of chicken eggs. Cryst. Mp 150-151°.

Tsuji, K. *et al., Yakugaku Zasshi*, 1976, **96**, 475-478 (*isol*)
Landor, S.R. *et al., J.C.S. Perkin 1*, 1979, 2289-2293 (*synth*)

Methylcarbamodithioic acid, 9CI M-355

[144-54-7]
N-*Methylaminodithioformic acid. Methyldithiocarbamic acid. Metam, BSI, ISO. Metham. Zuvapin*

MeNHCSSH

$C_2H_5NS_2$ 107.2

Free acid not isol..pK_{a1} 2.89 (25°).

Na salt: [137-42-8] *Metham-sodium, BSI. Metam-sodium. Vapam. Sistam. SMDC. Monam. Carbam, JMAF. Karbation. Nematin. Carbam. Geort*
Cryst. + $2H_2O$. V. sol. H_2O.

▶ Skin and mucous membrane irritant. LD_{50} (rat, orl) 1700 mg/kg. LD_{50} (rbt, skn) 800 mg/kg. FC2100000

K salt: [137-41-7]
Antimicrobial agent used for control of microorganisms in sugar cane and sugar beet mills.

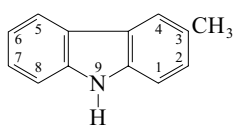
Me ester:
$C_3H_7NS_2$ 121.227
Bp_{20} 155-156°.

[6734-80-1]

Freund, M. *et al., Annalen*, 1895, **285**, 175
Delépine, M. *et al., Bull. Soc. Chim. Fr.*, 1908, **3**, 641; 1910, **7**, 896
U.K. Pat., 1954, 789 690; *CA*, **51**, 4638i; 11641e
Bunt, J.A. *et al., Meded. Fac. Landbouwwet., Rijksuniv. Gent*, 1977, **42**, 1529 (*activity*)
Miles, C.J. *et al., Anal. Chem.*, 1988, **60**, 220 (*hplc*)
Pesticide Manual, 9th edn., 1991, No. 8005
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A264
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2306 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VFU000; VFW009

3-Methyl-9*H*-carbazole, 9CI M-356

[4630-20-0]



$C_{13}H_{11}N$ 181.237
Plates (CH_2Cl_2/hexane). Mp 206-208°. Pale green soln. in H_2SO_4, which becomes deep green on addn. of HNO_3.

Picrate:
Mp 176°.

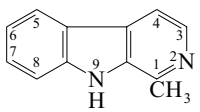
N-*Formyl:3-Methyl-9*H*-carbazole-9-carboxaldehyde. 9-Formyl-3-methyl-9*H*-carbazole*
$C_{14}H_{11}NO$ 209.247
Alkaloid from the roots of *Murraya koenigii* (curryleaf tree). Off-white solid. Mp 58-60°. λ_{max} 222 ; 267 ; 291 (sh) ; 315 (EtOH).

N-*(Ethoxycarbonyl):Ethyl 3-methyl-9*H-*carbazole-9-carboxylate. 9-Carbethoxy-3-methyl-9*H-*carbazole*
$C_{16}H_{15}NO_2$ 253.3
Alkaloid from the roots of *Murraya koenigii* (curryleaf tree). Needles (MeOH). Mp 122-123°. λ_{max} 229 ; 251 ; 262 ; 278 (sh) ; 287 ; 304 ; 315 (EtOH).

Campaigne, E. *et al., J.O.C.*, 1959, **24**, 478
Islam, A. *et al., Chem. Comm.*, 1972, 537 (*synth*)
Joshi, B.S. *et al., Indian J. Chem.*, 1974, **12**, 437 (*isol, uv*)
Roy, S. *et al., Phytochemistry*, 1974, **13**, 1017 (*isol, uv, ir*)
Åkermark, B. *et al., J.O.C.*, 1975, **40**, 1365 (*synth*)
Clancy, M.G. *et al., Chem. Comm.*, 1980, 1112 (*synth*)
Bhattacharyya, P. *et al., Chem. Comm.*, 1984, 1668 (*synth*)
Chowdhury, B.K. *et al., Phytochemistry*, 1987, **26**, 2138 (*isol*)
Luo, J.K. *et al., J. Het. Chem.*, 1989, **26**, 1213 (*synth, pmr*)
Chakrabarty, M. *et al., Phytochemistry*, 1997, **46**, 751-755 (*isol, derivs, pmr, cmr*)

1-Methyl-β-carboline M-357

[486-84-0]
*1-Methyl-9*H-*pyrido[3,4-*b*]indole, 9CI.* ***Harman****. Loturine. Passiflorine†. Zygofabagine. Aribine*



$C_{12}H_{10}N_2$ 182.224
Alkaloid from the may pop (*Passiflora incarnata*, Passifloraceae) and many other *Passiflora* spp. Mp 237-238° (228°). Log P 3.06 (calc).

▶ LD_{50} (mus, ipr) 50 mg/kg. UV0280000

Hydrochloride:
Mp 292-295°.

Picrate:
Mp 250-255°.

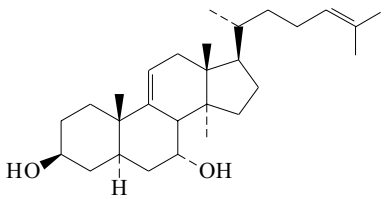
N-*Oxide:* [2506-09-4] ***Harmanine***
$C_{12}H_{10}N_2O$ 198.224
Detected in wines. Needles (EtOAc/MeOH); cryst (H_2O)(as picrate). Mp 182-184° subl Mp 239-248° (picrate).

N^a-*Formyl:*
Isol. from roots of *Panax ginseng* and *Codonopsis lanceolata* (todok). Struct. has now been shown to be identical with 1-Acetyl-β-carboline. Mp 89°.

N^b-*Me:* [6801-22-5] ***Melinonine F***
$C_{13}H_{13}N_2^{\oplus}$ 197.259
Poorly sol. hexane. Mp 288° dec. (as chloride).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 682A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 165B (*nmr*)
Bächli, E. *et al., Helv. Chim. Acta*, 1957, **40**, 1167-1187 (*Melinonine F, isol, uv, ir*)
Kametani, T. *et al., J.C.S.(C)*, 1968, 1006-1007 (*synth, pmr*)
Phillipson, J.D. *et al., J. Chromatogr.*, 1975, **105**, 163-178 (*tlc, glc, uv, ms*)
Han, B.H. *et al., Arch. Pharmacal Res.*, 1986, **9**, 21; *CA*, **105**, 57927y (*N^a-Formylharman, isol*)
Yomosa, K. *et al., Agric. Biol. Chem.*, 1987, **51**, 921-922 (*isol, bibl*)
Hardiman, J. *et al., Bioorg. Chem.*, 1987, **15**, 213-223 (*cryst struct*)
Bracher, F. *et al., Annalen*, 1993, 1335-1337 (*synth, pmr, cmr*)
Seki, H. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1169-1172 (*pmr, cmr*)
Rocca, P. *et al., Tetrahedron*, 1993, **49**, 3325-3342 (*synth*)
Dachriyanus, *et al., Aust. J. Chem.*, 2000, **53**, 221-224 (*oxide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPA050

14-Methylcholesta-9(11),24-diene-3,7-diol M-358

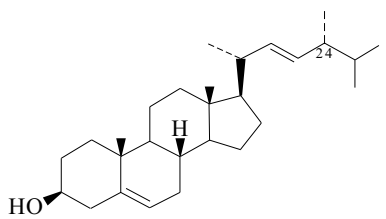


$C_{28}H_{46}O_2$ 414.67

(3β,5α,7α)-*form* [138523-61-2]
Constit. of the tubers of *Colocasia esculenta* (taro).

Ali, M. *et al., Indian J. Pharm. Sci.*, 1991, **53**, 98 (*isol, struct*)

24-Methylcholesta-5,22-dien-3-ol M-359



(3β,22*E*,24*R*)-*form*

$C_{28}H_{46}O$ 398.671

(3β,22*E*,24*R*)-*form* [474-67-9]

[2638-57-5]
Ergosta-5,22-dien-3-ol. ***Brassicasterol***
Constit. of *Brassica rapa* oil. Cryst. Mp 157-158° (148°). $[\alpha]_D^{19}$ -39.4. $[\alpha]_D^{19}$ -54 ($CHCl_3$). Prob. identical with Shakosterol isol. from a mollusc.

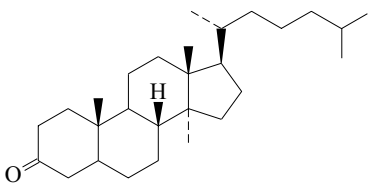
3-Ketone:Ergosta-5,22-dien-3-one. 24-Methylcholesta-5,22-dien-3-one. ***Brassicasterone***
$C_{28}H_{44}O$ 396.655

(3β,22*E*,24*S*)-*form* [17472-78-5]

[2638-57-5]
Crinosterol*. Campesta-5,22-dien-3-ol*
Cryst. (MeOH or Me_2CO). Mp 147-148°. $[\alpha]_D^{26}$ -47.2.

Bolker, H.I. *et al., Nature (London)*, 1967, **213**, 905 (*isol*)
Rubinstein, I. *et al., Phytochemistry*, 1974, **13**, 485; 1976, **15**, 195 (*isol, pmr*)
Sheikh, Y.M. *et al., Tetrahedron*, 1974, **30**, 4095 (*isol*)
Sheikh, Y.M. *et al., Steroids*, 1975, **26**, 129 (*synth*)
Kobayashi, M. *et al., Steroids*, 1975, **26**, 605 (*isol*)
Adler, J.H. *et al., Lipids*, 1976, **11**, 634 (*biosynth*)
Tsai, L.B. *et al., Phytochemistry*, 1976, **15**, 1131 (*biosynth*)
Wright, J.L.C. *et al., Can. J. Chem.*, 1978, **56**, 1898 (*cmr*)
Theobald, N. *et al., J.A.C.S.*, 1978, **100**, 7677 (*isol*)
Lang, R.W. *et al., Helv. Chim. Acta*, 1982, **65**, 407 (*synth*)
Anastasia, M. *et al., J.C.S. Perkin 1*, 1983, 379; 2365 (*synth*)
Seo, S. *et al., Chem. Comm.*, 1984, 1174 (*biosynth*)
Khripach, V.A. *et al., Khim. Prir. Soedin.*, 1992, **28**, 90; *Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 74 (*synth*)
Ulubelen, A. *et al., Phytochemistry*, 1997, **47**, 895-897 (*Brassicasterone*)

14-Methylcholestan-3-one M-360

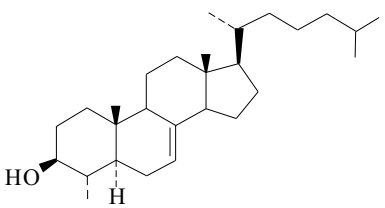


$C_{28}H_{48}O$ 400.687

(5α,14α)-*form* [54411-55-1]
Constit. of mature wheat straw (*Triticum aestivum*).

Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523 (*isol*)

4-Methylcholest-7-en-3-ol M-361



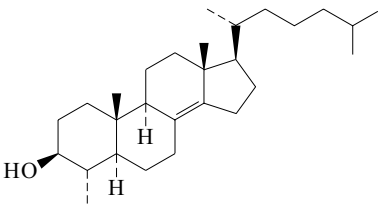
$C_{28}H_{48}O$ 400.687

(3β,4α,5α)-*form* [481-25-4]
Lophenol*. Methosterol*
Constit. of potato leaves (*Solanum tuberosum*). Cryst. (MeOH). Mp 149-151°. $[\alpha]_D$ +5 ($CHCl_3$).

Djerassi, C. *et al., J.A.C.S.*, 1958, **80**, 6284 (*struct*)
Schreiber, K. *et al., Tetrahedron*, 1964, **20**, 2575 (*isol*)
Scallen, T.J. *et al., J. Lipid Res.*, 1968, **9**, 120 (*ir*)
Sucrow, W. *et al., Chem. Ber.*, 1977, **110**, 1523 (*synth*)
Iida, T. *et al., Steroids*, 1977, **29**, 453 (*pmr*)

4-Methyl-8(14)-cholesten-3-ol M-362

[62014-96-4]



$C_{28}H_{48}O$ 400.687

(3β,4α,5α)-*form*

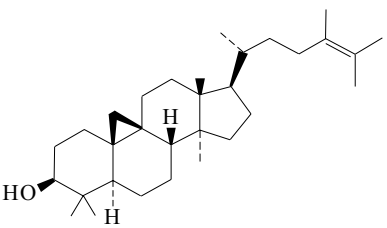
Constit. of *Capsicum annuum* seeds.

Ac:

Cryst. Mp 78-78.5°.

Matsumoto, T. *et al., Phytochemistry*, 1983, **22**, 2621

24-Methylcycloart-24-en-3-ol M-363



$C_{31}H_{52}O$ 440.751

3β-*form* [25692-13-1]

Cyclobranol

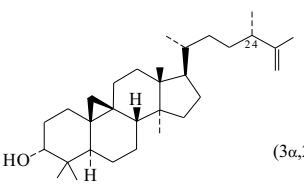
Constit. of rice bran. Cryst. Mp 156.5-157.5°. $[\alpha]_D$ +38.4 ($CHCl_3$).

Tachibara, K. *et al., CA*, 1970, **73**, 4058 (*isol*)

Itoh, T. *et al., Steroids*, 1975, **25**, 729; **26**, 93; 1976, **27**, 275 (*glc, pmr*)

24-Methylcycloart-25-en-3-ol M-364

24-Methyl-9,19-cyclolanost-25-en-3-ol



(3α,24*S*)-*form*

$C_{31}H_{52}O$ 440.751

(3β,24*S*)-*form* [511-61-5]

Cyclolaudenol

Found in opium. Cryst. (MeOH). Mp 125°. $[\alpha]_D$ +46 (c, 1.5 in $CHCl_3$).

Hexadecanoyl: [104109-19-5]

$C_{47}H_{82}O_2$ 679.164

Isol. from corn pollen (*Zea mays*).

[108864-87-5]

Berti, G. *et al., Bull. Soc. Chim. Fr.*, 1964, 2359 (*isol*)

Ghisalberti, E.L. *et al., Chem. Comm.*, 1969, 1401 (*biosynth*)

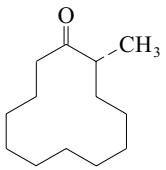
Ageta, H. *et al., Chem. Lett.*, 1982, 881 (*isol, struct*)

Govardhan, C. *et al., Phytochemistry*, 1984, **23**, 411 (*isol*)

Desoky, E.K. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 1113 (*isol, Ac*)

2-Methylcyclododecanone M-365

[16837-94-8]



(*R*)-*form*

$C_{13}H_{24}O$ 196.332

Isol. from Galbanum gum. Oil with musky odour.

Semicarbazone:

Mp 211-213°.

(*R*)-*form* [77857-75-1]

$[\alpha]_D^{25}$ +10.3 (c, 4.7 in $CHCl_3$) (80% ee).

2,4-Dinitrophenylhydrazone:

Cryst. (EtOH). Mp 178-179°.

(*S*)-*form* [77857-88-6]

$[\alpha]_D^{25}$ -3.16 (c, 4.7 in $CHCl_3$) (30% ee).

2,4-Dinitrophenylhydrazone:

Cryst. (EtOH). Mp 102-103°.

Spencer, T.A. *et al., J.A.C.S.*, 1967, **89**, 5727 (*synth*)

Posner, G.H. *et al., J.A.C.S.*, 1973, **95**, 7788

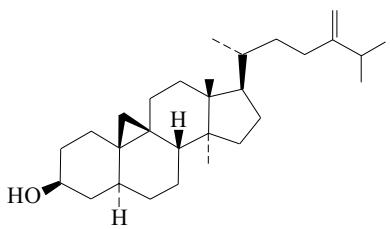
Kaiser, R. *et al., Helv. Chim. Acta*, 1978, **61**, 2671 (*isol*)

Meyers, A.I. *et al., J.A.C.S.*, 1981, **103**, 3088 (*pmr, ir, synth*)

Kruizinga, W.H. *et al., J.A.C.S.*, 1981, **103**, 5183 (*synth*)

14-Methyl-9,19-cycloergost-24(28)-en-3-ol M-366

14-Methyl-24-methylene-9,19-cyclocholestan-3-ol



$C_{29}H_{48}O$ 412.698

(3β,5α,9β,14α)-*form* [34443-88-4]

24-Methylenepollinasterol

Constit. of banana peel *Musa sapientium*. Cryst. (MeOH aq.). Mp 115-117°.

Ac:

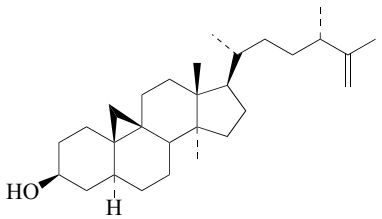
Cryst. (Me_2CO/MeOH). Mp 52-52.5°. $[\alpha]_D^{23}$ +28.

Knapp, F.F. *et al., Phytochemistry*, 1972, **11**, 3497 (*isol*)

Thompson, M.J. *et al., Phytochemistry*, 1978, **17**, 1053 (*isol*)

14-Methyl-9,19-cycloergost-25-en-3-ol, 9CI M-367

14,24-Dimethyl-9,19-cyclocholest-25-en-3-ol. 24-Methyl-28,29-dinorcycloart-25-en-3-ol



$C_{29}H_{48}O$ 412.698

(3β,5α)-*form* [62305-30-0]

Constit. of *Musa sapientum* (banana).

3-Ketone: [207850-21-3] *14-Methyl-9,19-cycloergost-25-en-3-one.* ***28-Norcyclomusalenone***

$C_{29}H_{46}O$ 410.682

Constit. of *Musa sapientum* (banana).

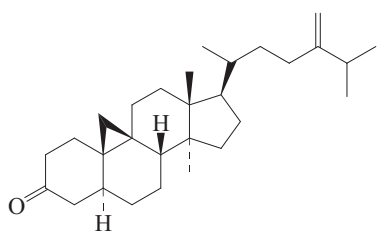
Chiu, P.-L. *et al., Phytochemistry*, 1976, **15**, 1907-1910 (*ms*)

Akihisa, T. *et al., Lipids*, 1986, **21**, 494-497 (*isol*)

14-Methyl-9,19-cycloergost-24(28)-en-3-one M-368

[149756-25-2]

24-Methylene-28,29-dinorcycloartan-3-one. ***24-Methylenepollinastanone****. 28-Norcycloeucalenone*



$C_{29}H_{46}O$ 410.682

Constit. of *Musa sapientum* (banana) fruit peel. Cryst. Mp 76-77° (65-67°). $[\alpha]_D^{22}$ +37 (c, 0.4 in $CHCl_3$).

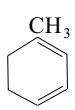
Akihisa, T. *et al., Phytochemistry*, 1998, **47**, 1107-1110 (*isol, pmr, cmr, ms*)

Koorbanally, N. *et al., Phytochemistry*, 2000, **54**, 93-97 (*isol, pmr, cmr, ms*)

1-Methyl-1,3-cyclohexadiene, 9CI M-369

[1489-56-1]

2,3-Dihydrotoluene



C_7H_{10} 94.156

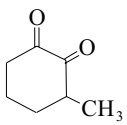
Flavouring ingredient. Liq. with a lime odour. d_4^{20} 0.84. Bp 108-110° (117°). n_D^{20} 1.4762.

Cargill, R.L. *et al., J.A.C.S.*, 1973, **95**, 4346 (*synth*)

Ruttimann, A. *et al., Helv. Chim. Acta*, 1975, **58**, 1450 (*synth*)
Gregson, R.P. etal. *et al., Aust. J. Chem.*, 1976, **29**, 2037 (*synth*)
Spangler, C.W. *et al., J.C.S. Perkin 1*, 1976, 1792 (*synth*)
Grob, C.A. *et al., Helv. Chim. Acta*, 1977, **60**, 482 (*synth*)
Eilbracht, P. *et al., Chem. Ber.*, 1986, **119**, 169 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1746-1747
U.S. Pat., 3 989 765; *CA*, **86**, 8581m (*use*)

3-Methyl-1,2-cyclohexanedione, 9CI M-370

[3008-43-3]
2-Hydroxy-3-methyl-2-cyclohexen-1-one. FEMA 3305



$C_7H_{10}O_2$ 126.155

Enolised α-diketone. Constit. of coffee. Flavouring ingredient. Cryst. (petrol). Sol. H_2O. Mp 64-65°. Bp 160-162° Bp_{12} 80-85°.

1-Oxime: [24863-57-8]
$C_7H_{11}NO_2$ 141.169
Mp 78-80°.

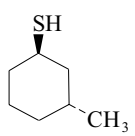
Dioxime: [18310-18-4] *3-Methylnioxime*
$C_7H_{12}N_2O_2$ 156.184
Cryst. (EtOH or C_6H_6). Sol. EtOH, C_6H_6; spar. sol. H_2O. Mp 165°. pK_{a1} 10.6 (25°).

1-Phenylhydrazone: [14192-51-9]
Mp 190-191°.

Banks, C.V. *et al., J.O.C.*, 1956, **21**, 547 (*synth*)
Giammarino, A.S. *et al., Tetrahedron*, 1963, **19**, 2051 (*isol*)
Cumper, C.W.N. *et al., J.C.S.*, 1965, 2067 (*synth*)
Giammarino, A.S. *et al., Nature (London)*, 1966, **210**, 1358 (*isol*)
Bassett, J. *et al., Analyst (London)*, 1967, **92**, 279 (*detn, Bi, Ni, Pd*)
Bassett, J. *et al., J.C.S.(A)*, 1969, 2873 (*synth*)
Plekhanov, N.A. *et al., Vestn. Mosk. Univ., Ser. 2: Khim.*, 1974, **15**, 492; *CA*, **82**, 77689g (*detn, Ni*)
Moriuchi, C.A. *et al., Synthesis*, 1989, 785 (*synth, ir, pmr, cmr*)
Matsumoto, K. *et al., J.A.C.S.*, 1990, **112**, 9614 (*synth*)

3-Methylcyclohexanethiol, 9CI M-371

[38699-50-2]



(1*R**,3*R**)-*form*

$C_7H_{14}S$ 130.254
Food flavour additive. Use supported only by patent information.

(1*R,3*R**)-*form***
(+)-trans-*form*
Bp 171°. $[\alpha]_{Hg}$ +5.5.

(1*R,3*S**)-*form***
(-)-cis-*form*
Bp 165°. $[\alpha]_{Hg}$ -2.24.

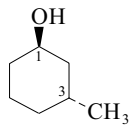
(±)-*form*
Bp 172-174°. Mixt. of diastereoisomers.

Mousseron, M. *et al., Bull. Soc. Chim. Fr.*, 1948, 84 (*synth, bibl*)
Yukawa, Y. *et al., CA*, 1952, **46**, 7061 (*synth*)
U.S. Pat., 1972, 3 677 772; *CA*, **77**, 112755w (*use*)

3-Methylcyclohexanol, 9CI M-372

[591-23-1]

[25639-42-3]
Hexahydro-m-*cresol*



(1*R*,3*R*)-*form*

$C_7H_{14}O$ 114.187
Isol. from oil of *Mentha pulegium* (European pennyroyal) (prob. as *trans*-form).
▶ Fl. p. *ca*. 70°, autoignition temp. 295°.
GW0200000

(1*R*,3*R*)-*form* [24965-94-4]
(-)(?)-trans-*form*

(1*RS*,3*RS*)-*form* [23068-71-5]

[7443-55-2]
(±)-trans-*form*
Bp 173-174° Bp_{20} 78-79°. In the early lit. referred to as the *cis*-form.

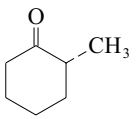
[25639-42-3]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 237A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 160B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 235B (*ir*)
Naves, Y.R. *et al., Helv. Chim. Acta*, 1943, **26**, 1992 (*isol*)
Goering, H.L. *et al., J.A.C.S.*, 1954, **76**, 5405 (*synth*)
Hückel, W. *et al., Annalen*, 1961, **645**, 115; 177 (*synth*)
Klein, J. *et al., J.O.C.*, 1967, **32**, 935 (*synth*)
Hill, R.K. *et al., J.O.C.*, 1967, **32**, 2330 (*config*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 1695 (*synth, resoln*)
Yamaguchi, S. *et al., Tet. Lett.*, 1977, 89 (*config*)
Brown, H.C. *et al., J.O.C.*, 1979, **44**, 1910 (*synth*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4649
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIQ750

2-Methylcyclohexanone, 9CI M-373

[583-60-8]

[1331-22-2]
FEMA 3946



(*R*)-*form*

$C_7H_{12}O$ 112.171
▶ Flammable, fl. p. 47°. LD_{50} (rat, orl) 2140 mg/kg. LD_{50} (rbt, skn) 1635 mg/kg. Eye and respiratory tract irritant. OES: long-term 50 ppm; short-term 75 ppm (sk).
GW1750000

(*R*)-*form* [22554-29-6]
$[\alpha]_D^{20}$ -12.19 (neat).

(*S*)-*form* [22554-27-4]
Bp 166.5-168°. $[\alpha]_D^{25}$ +12.3 (MeOH). $[\alpha]_D^{25}$ +14.2 ($CHCl_3$).

(±)-*form* [24965-84-2]
Flavouring ingredient. Oil with peppermint odour. d_4^{20} 0.93. Fp -13.9. Bp 165-166° Bp_{20} 89-90°. n_D^{20} 1.4483.

Oxime: [1122-26-5]
$C_7H_{13}NO$ 127.186
Cryst. Mp 43°. Bp_{13} 112-113°.
▶ GW1802000

2,4-Dinitrophenylhydrazone:
Cryst. (MeOH/EtOAc). Mp 137.4-138°.

Semicarbazone:
Cryst. Mp 191°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 433A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 669B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 518A (*ir*)
Fell, B. *et al., Tet. Lett.*, 1968, 1003 (*synth*)
Meyers, A.I. *et al., J.A.C.S.*, 1976, **98**, 3032 (*synth*)
Cheer, C.J. *et al., Tet. Lett.*, 1976, 3877 (*abs config*)
Whitesell, J.K. *et al., J.O.C.*, 1977, **42**, 377 (*synth*)
Hashimoto, S. *et al., Tet. Lett.*, 1978, 578 (*synth*)
Kergomard, A. *et al., Tet. Lett.*, 1978, 5197 (*synth*)
Matsumoto, K. *et al., J.A.C.S.*, 1990, **112**, 9614 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1104
Abraham, R.J. *et al., J.C.S. Perkin 2*, 2001, 302-307 (*cmr*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4782
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 837
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIR500

3-Methylcyclohexanone, 9CI M-374

[591-24-2]

[1331-22-2]
Hedeomol. FEMA 3947

$C_7H_{12}O$ 112.171
▶ Forms explosive peroxide with H_2O_2 + HNO_3. Eye and respiratory tract irritant.
GW1750100

(*R*)-*form* [13368-65-5]
Isol. from oil of *Hedeoma pulegioides* (American pennyroyal), *Mentha* spp. and other oils. Bp 169° Bp_{12} 68-70°.

Oxime:
$C_7H_{13}NO$ 127.186
Cryst. Mp 43-44°. Bp 216-217° Bp_{18} 110°.

Semicarbazone:

Plates (MeOH). Mp 180°. $[\alpha]_D^{23.5}$ -27 (EtOH).

(*S*)-*form* [24965-87-5]
Bp 164-168° Bp_{15} 65°.

Semicarbazone:
Mp 181°. $[\alpha]_D^{27}$ +30.5.

(±)-*form* [625-96-7]
Flavouring ingredient for candies etc. Oil with acetone-like odour. d_4^{20} 0.91. Fp -73.5. Bp 169° Bp_{15} 60-60.2°. n_D^{20} 1.4457.

Picrate:
Plates. Mp 155°.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 153-155° (164-165°).

Semicarbazone:
Plates (MeOH). Mp 185-186°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 433C; 433D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 670A; 670B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 518D; 519A (*ir*)
Barrowcliff, M. *et al., J.C.S.*, 1907, **91**, 875 (*isol*)
Adams, R. *et al., J.A.C.S.*, 1942, **64**, 2087 (*synth*)
Eisenbraun, E.J. *et al., J.A.C.S.*, 1955, **77**, 3383 (*abs config*)
Hückel, W. *et al., Annalen*, 1961, **645**, 177 (*synth*)
Ohloff, G. *et al., Chem. Ber.*, 1962, **95**, 1400 (*synth*)
Krechmer, R.A. *et al., J.O.C.*, 1972, **37**, 2744 (*synth*)
Fristad, W.E. *et al., J.O.C.*, 1978, **43**, 1620 (*synth*)
Mérour, J.Y. *et al., J. Organomet. Chem.*, 1979, **168**, 337 (*synth*)
Thurkauf, A. *et al., J.O.C.*, 1987, **52**, 5466 (*synth*)
Freedman, J.B. *et al., J.A.C.S.*, 1988, **110**, 689 (*spectra*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1105
Abraham, R.J. *et al., J.C.S. Perkin 2*, 2001, 302-307 (*cmr*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4782
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2660
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIR600

4-Methylcyclohexanone, 9CI M-375

[589-92-4]

[1331-22-2]
FEMA 3948

$C_7H_{12}O$ 112.171
Flavouring for baked goods and candies. Oil with acetone-like odour. d_4^{20} 0.91. Fp -40.6. Bp 170°. n_D^{20} 1.4451.

▶ Detonates with HNO_3 at 75°. LD_{50} (rat, orl) 800 mg/kg. Eye and respiratory tract irritant. GW1750200

Oxime: [4994-13-2]
$C_7H_{13}NO$ 127.186
Cryst. Mp 37-39°. Bp_{14} 114°.

2,4-Dinitrophenylhydrazone: [5138-32-9]
Orange cryst. (EtOH aq.). Mp 133-134°.

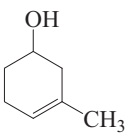
Semicarbazone: [5439-97-4]
Prisms (MeOH). Mp 197°.

Enol acetate: [22422-17-9] *1-Acetoxy-4-methylcyclohexene*
$C_9H_{14}O_2$ 154.208
Bp_{38} 99-100° Bp_3 53-56°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 434A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 670C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 519B (*ir*)
Skita, A. *et al., Ber.*, 1923, **56**, 1016 (*synth*)
Machinskaya, I.V. *et al., CA*, 1954, **48**, 6383 (*synth*)
Benkeser, R.A. *et al., J.A.C.S.*, 1958, **80**, 5414 (*synth*)
Draper, A.L. *et al., J.O.C.*, 1962, **27**, 2727 (*synth*)
Kwart, H. *et al., J.O.C.*, 1973, **38**, 2011 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1106
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4782
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2661
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIR625

3-Methyl-3-cyclohexen-1-ol M-376

[53783-91-8]



$C_7H_{12}O$ 112.171

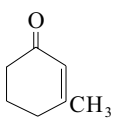
(±)-*form*
Bp_{14} 80°.

(ξ)-*form*
Constit. of oil of *Thymus vulgaris* (thyme).

Mitsui, S. *et al., J. Catal.*, 1975, **36**, 119-124 (*synth*)
Reddy, M.V.B. *et al., Phytochemistry*, 1988, **47**, 1515-1520 (*occur*)
Harris, N.J. *et al., J.A.C.S.*, 1994, **116**, 6121-6129 (*synth, pmr, cmr*)
Kocovsky, P. *et al., J.O.C.*, 1999, **64**, 2765-2775 (*pmr*)

3-Methyl-2-cyclohexen-1-one, 9CI M-377

[1193-18-6]
Seudenone. FEMA 3360



$C_7H_{10}O$ 110.155
Flavouring ingredient. Light-sensitive liq. Misc. H_2O. d^{20} 0.97. Mp -21°. Bp 200-202° Bp_{12} 78-79°. n_D^{20} 1.4947. Steam-volatile.

▶ GW7340000

Oxime: [2607-95-6]
$C_7H_{11}NO$ 125.17
Bp_3 93-95°.

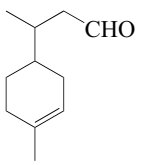
2,4-Dinitrophenylhydrazone: [3234-76-2]
Mp 177-178°.

[88693-90-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 447C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 691B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 535D (*ir*)
Rabe, P. *et al., Ber.*, 1912, **45**, 2924-2927 (*isol*)
Natelson, S. *et al., J.A.C.S.*, 1939, **61**, 1001-1002 (*synth*)
Torri, J. *et al., Tet. Lett.*, 1973, 3251-3254 (*uv*)
Torri, J. *et al., Bull. Soc. Chim. Fr.*, 1974, 1633-1637 (*cmr*)
Pitman, G.B. *et al., Environ. Entomol.*, 1974, **3**, 886-887 (*biosynth*)
Ager, D.J. *et al., Chem. Comm.*, 1978, 177-178 (*synth*)
Helferty, P.H. *et al., Org. Magn. Reson.*, 1983, **21**, 352-356 (*cmr*)
Bestmann, H.J. *et al., Chem. Ber.*, 1985, **118**, 2640-2658; 1993, **126**, 725-731 (*synth*)
Robinson, P.L. *et al., J.O.C.*, 1985, **50**, 3860-3863 (*synth, pmr*)
Ponaras, A.A. *et al., J.O.C.*, 1988, **53**, 1110-1112 (*synth*)
Cahiez, G. *et al., Tet. Lett.*, 1989, **30**, 3541-3544 (*synth*)
Boykin, D.W. *et al., Magn. Reson. Chem.*, 1990, **28**, 305-310 (*O-17 nmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 493
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1748-1749
Chong, B.-D. *et al., J.O.C.*, 1997, **62**, 9323-9325 (*synth*)
Barbot, F. *et al., Synthesis*, 1998, **28**, 3279-3289 (*ir, pmr, cmr, ms*)

3-(4-Methyl-3-cyclohexenyl)-butanal M-378

[6784-13-0]
β,4-Dimethyl-3-cyclohexene-1-propanal, 9CI. Limonene aldehyde



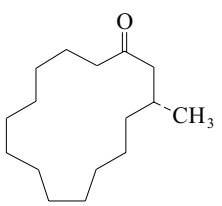
Flavouring ingredient.

(±)-*form*
Bp_{10} 111-112°.

Kogami, K. *et al., Yakugaku Zasshi*, 1973, **22**, 316; *CA*, **79**, 92400n (*synth*)
Eur. Pat., 1980, 8 459; *CA*, **93**, 94891m (*synth*)
Ger. Pat., 1980, 2 849 742; *CA*, **93**, 86613a (*synth*)

3-Methylcyclopentadecanone M-379

[541-91-3]
Muscone. FEMA 3434



(*R*)-*form*

$C_{16}H_{30}O$ 238.412
Flavouring ingredient.

▶ Skin irritant. GY0950000

(*R*)-*form* [10403-00-6]
d_4^{17} 0.92. $Bp_{0.5}$ 130°. $[\alpha]_D^{17}$ -13.9. n_D^{17} 1.4802.

Semicarbazone:
Mp 134°.

(*S*)-*form* [63975-98-4]
$[\alpha]_D$ +13.83.

Semicarbazone:
Mp 132.2-132.8°.

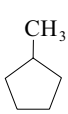
(±)-*form* [956-82-1]
$Bp_{0.8}$ 132-134°.

Semicarbazone:
Mp 134.5°.

Rodd's Chem. Carbon Compd. (2nd edn.), 1968, **2B**, 416 (*rev, bibl*)
Stork, G. *et al., J.A.C.S.*, 1975, **97**, 1264 (*synth, bibl*)
Fischli, A. *et al., Helv. Chim. Acta*, 1976, **59**, 2443; 1977, **60**, 925 (*synth, bibl*)
Gray, R.W. *et al., Helv. Chim. Acta*, 1977, **60**, 1969 (*synth*)
Shono, T. *et al., Tet. Lett.*, 1977, 2667 (*synth*)
Torii, S. *et al., J.O.C.*, 1979, **44**, 2303 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 749 (*rev, tox*)
Bernandinelli, M. *et al., Helv. Chim. Acta*, 1982, **65**, 1310 (*cryst struct*)
Sakane, S. *et al., Tet. Lett.*, 1983, **24**, 943 (*synth, bibl*)
Abad, A. *et al., Chem. Ind. (London)*, 1985, 29 (*synth*)
Jaechachoonhakit, S. *et al., Chem. Lett.*, 1986, 911 (*synth*)
Bienz, S. *et al., Helv. Chim. Acta*, 1987, **70**, 2146; 1988, **71**, 1704 (*synth, ir, pmr, cmr*)
Suginome, M. *et al., Tet. Lett.*, 1987, **28**, 3963 (*synth*)
Deprés, J.-P. *et al., Tetrahedron*, 1989, **45**, 2989 (*synth*)
Rautenstrauch, V. *et al., Helv. Chim. Acta*, 1990, **73**, 896 (*synth*)
Ogawa, T. *et al., Chem. Comm.*, 1991, 1438 (*synth*)
Tanaka, K. *et al., Chem. Comm.*, 1991, 1630 (*synth*)
Mhaskar, S.Y. *et al., J. Am. Oil Chem. Soc.*, 1992, **69**, 837 (*synth*)
Ballini, R. *et al., Annalen*, 1995, 1381 (*synth, pmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 493
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1749-1750
Kamat, V.P. *et al., Tetrahedron*, 2000, **56**, 4397-4403 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIT625

Methylcyclopentane, 9CI, 8CI M-380

[96-37-7]



C_6H_{12} 84.161
Isol. from *Helianthus annuus* (sunflower). Liq. d_4^{21} 0.75. Fp -139.8. Bp 72-72.2°. n_D^{21} 1.4088.

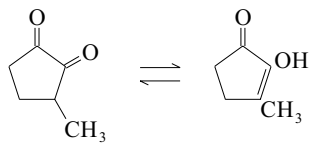
► Highly flammable, fl. p. -29°, autoignition temp. 258/361°. GY4640000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 34D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 47C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 50A (*ir*)
Adv. Chem. Ser., 1955, **15**, 360 (***props***)
Lipnick, R.L. *et al., J.A.C.S.*, 1974, **96**, 2941 (*pmr*)
Bernard, M. *et al., Ullmanns Encykl. Tech. Chem., 4. Aufl.*, 1975, **9**, 680 (*rev*)
Takahashi, S. *et al., Chem. Comm.*, 1976, 839 (*synth*)
Bowen, R.D. *et al., Org. Mass Spectrom.*, 1977, **12**, 453 (*ms*)
Schneider, H.J. *et al., Tetrahedron*, 1982, **38**, 2327 (*cmr*)
Liu, Q. *et al., CA*, 1988, **109**, 134804t (*isol*)
Pham-Delegue, M.H. *et al., J. Chem. Ecol.*, 1989, **15**, 329 (*isol*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2311
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MIU500

3-Methyl-1,2-cyclopentanedione, 9CI M-381

[765-70-8]

[3250-08-6]
Cyclotene. Corylone. FEMA 2700. 2-Hydroxy-5-methyl-2-cyclopenten-1-one



$C_6H_8O_2$ 112.128
Enolised α-diketone. Enol-form predominates in non-polar solvs. and solid state. Constit. of coffee aroma, roast barley and many other foods. Important flavouring ingredient. Cryst. + $2H_2O$ with caramel odour and sweet liquorice taste. Mp 78-79° (hydrate) Mp 106.5-107° (anhyd.).

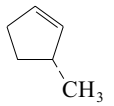
Enol-*form* [80-71-7]
2-Hydroxy-3-methyl-2-cyclopenten-1-one
► GY7298000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 446C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 689B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 541D (*ir*)
Gianturco, M.A. *et al., Tetrahedron*, 1963, **19**, 2051-2059 (*isol*)
Sato, K. *et al., J.O.C.*, 1967, **32**, 339-346; 1973, **38**, 551 (*synth, bibl*)
Rojas, J. *et al., Microchem. J.*, 1982, **27**, 433-444; 445-453 (*synth, use*)
dos Santos, M.L. *et al., Synth. Commun.*, 1991, **21**, 1783-1788 (*synth*)
Wild, H. *et al., Chimia*, 1992, **46**, 399-402 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1750 (*occur, use*)
Fayle, S.E. *et al., Acta Cryst. C*, 1998, **54**, 404-405 (*cryst struct*)

3-Methylcyclopentene, 9CI M-382

[1120-62-3]

[27476-50-2]



(*R*)-*form*

C_6H_{10} 82.145
Constit. of the flowers of *Jasminum sambac* (Arabian jasmine).

(*R*)-*form* [39750-38-4]
Liq. Bp 67°. $[\alpha]_D^{25}$ +174.5 (neat). $[\alpha]_D^{25}$ +167.4 (c, 5.23 in $CHCl_3$) (97% ee).

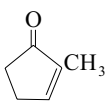
(*S*)-*form* [39750-39-5]
Liq. Bp 60-64°. $[\alpha]_D$ -166.6 (c, 5.14 in $CHCl_3$) (97% ee).

(±)-*form* [39750-75-9]
d_4^{20} 0.76. Bp 66.5-67°. n_D^{20} 1.4207.

Zelinsky, N. *et al., Ber.*, 1902, **35**, 2491 (*synth*)
Adv. Chem. Ser., 1955, **15**, 417 (***props***)
Hückel, W. *et al., Annalen*, 1961, **649**, 13 (*synth*)
Brown, H.C. *et al., J.A.C.S.*, 1964, **86**, 397 (*synth*)
Wilke, G. *et al., Angew. Chem., Int. Ed.*, 1966, **5**, 151; 1972, **11**, 1023 (*synth*)
Schurig, V. *et al., Angew. Chem.*, 1977, **89**, 113 (*synth, resoln*)
Schurig, V. *et al., Isr. J. Chem.*, 1977, **15**, 96 (*resoln*)
Sliwka, H.R. *et al., Helv. Chim. Acta*, 1984, **67**, 434 (*synth, abs config, pmr, bibl*)
Zhu, L. *et al., Zhiwu Xuebao*, 1984, **26**, 189 (*isol*)
Nugent, W.A. *et al., J.A.C.S.*, 1995, **117**, 8992 (*synth, pmr, cmr*)

2-Methyl-2-cyclopenten-1-one, 9CI M-383

[1120-73-6]



C_6H_8O 96.129
Present in bread aroma. d_4^{16} 0.98. Bp 157° Bp_{15} 54°. n_D^{15} 1.4762.

Oxime:
C_6H_9NO 111.143
Plates (H_2O). Mp 128°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 687B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 535C (*ir*)
Merour, J.Y. *et al., J. Organomet. Chem.*, 1973, **51**, C24 (*synth*)
Fischli, F. *et al., Helv. Chim. Acta*, 1975, **58**, 564 (*synth, nmr*)
Ho, T.-L. *et al., Chem. Ind. (London)*, 1982, 371 (*synth, bibl*)
Disanayaka, B. *et al., Synthesis*, 1983, 952 (*synth*)
Schow, S.R. *et al., J.A.C.S.*, 1986, **108**, 2662 (*synth, pmr*)
Hua, D.Y. *et al., J.O.C.*, 1988, **53**, 507 (*synth, pmr*)

3-Methyl-2-cyclopenten-1-one, 9CI M-384

[2758-18-1]
FEMA 3435

C_6H_8O 96.129
Flavouring ingredient. Liq. with unpleasant odour. Sol. H_2O. d^{26} 0.98. Bp 157-158° Bp_{10} 55.5°. n_D^{25} 1.4860.

Oxime:
C_6H_9NO 111.143
Plates. Mp 127°.

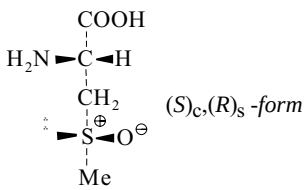
Semicarbazone:
Plates. Mp 230°.

2,4-Dinitrophenylhydrazone:
Mp 182-183°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 411B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 446A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 533D (*ir*)
Acheson, R.M. *et al., J.C.S.*, 1952, 1127 (*synth*)
Al-Jallo, H.N.A. *et al., J.C.S.(B)*, 1966, 73 (*ir*)
Cottee, F.J. *et al., J.C.S.(B)*, 1968, 326 (*nmr*)
Toder, B.H. *et al., Synth. Commun.*, 1975, **5**, 435
Janssen, C.G.M. *et al., Synthesis*, 1982, 389 (*deriv*)
Bestmann, H.J. *et al., Chem. Ber.*, 1993, **126**, 725 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 494
Karpinski, M.L. *et al., Org. Prep. Proced. Int.*, 1995, **27**, 569 (*synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1751-1752
Morales-Morales, D. *et al., Can. J. Chem.*, 2001, **79**, 823-829 (*synth, pmr, cmr*)

S-Methylcysteine sulfoxide M-385

3-(Methylsulfinyl)alanine, 9CI. ***Methiin***



$(S)_C,(R)_S$ *-form*

$C_4H_9NO_3S$ 151.186

$(S)_C(R)_S$-*form* [3226-62-8]
Mp 165° dec. $[\alpha]_D$ -202 (c, 0.4 in H_2O).

N-*Ac:*
Mp 168-169° (as dicyclohexylammonium salt). $[\alpha]_D$ -251 (c, 1.5 in H_2O).

$(S)_C(S)_S$-*form* [32726-14-0]

[6853-87-8]
Constit. of onion (*Allium cepa*), other *Allium* spp. and *Brassica* spp.. Potential nutriceutical. Mp 163° dec. $[\alpha]_D$ +204 (c, 0.4 in H_2O).

N-*Ac:*
Mp 166-167° (as dicyclohexylammonium salt). $[\alpha]_D$ +138 (c, 1.5 in H_2O).

Barnsley, E.A. *et al., Tetrahedron*, 1968, **24**, 3747 (*synth, abs config*)
Meese, C.O. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1990, **323**, 957
Meese, C.O. *et al., Z. Naturforsch., C*, 1990, **45**, 1171 (*pmr*)
Kubec, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 428-433 (*occur*)
Handbook of Nutraceuticals and Functional Foods, (ed. Wildman, R.E.C.), CRC Press, 2001, 169-191

2-Methyldecane M-386

[6975-98-0]
Isoundecane
$H_3C(CH_2)_7CH(CH_3)_2$
$C_{11}H_{24}$ 156.311
Constit. of *Angelica* spp., *Cicer arietinum* (chickpea). d_4^{20} 0.74. Bp 190° Bp_{10} 74-75°. n_D^{20} 1.4152.
▶Autoignition temp. 500°.
Francis, A.W. *et al., Ind. Eng. Chem.*, 1943, **35**, 442
Streif, A.J. *et al., Anal. Chem.*, 1955, **27**, 411
Mathis, C. *et al., Phytochemistry*, 1964, **3**, 115 (*isol*)
Mann, G. *et al., Tetrahedron*, 1967, **23**, 3393 (*conformn, props*)
Lehmkuhl, H. *et al., Annalen*, 1975, 145; 1176 (*synth*)

3-Methyldecane M-387

[13151-34-3]
$C_{11}H_{24}$ 156.311

(*S*)-*form* [54964-06-6]
d^{25} 0.74. Bp 190-191°. $[\alpha]_D^{25}$ +8.78 (neat). n_D^{25} 1.4161.

(ξ)-*form*
Aroma constit. of milled chickpeas (*Cicer arietinum*) and dry-cured ham. Also present in common rue (*Ruta graveolens*) and coconut flesh (*Cocos nucifera*).
Francis, A.W. *et al., Ind. Eng. Chem.*, 1943, **35**, 442 (*props*)
Brown, H.C. *et al., J.A.C.S.*, 1961, **83**, 1001 (*synth*)
Lardicci, L. *et al., Ann. Chim. (Rome)*, 1962, **52**, 652 (*synth*)
Netzel, D.A. *et al., Fuel*, 1981, **60**, 307 (*cmr*)
Christen, P. *et al., Pharm. Acta Helv.*, 1987, **62**, 158 (*isol*)
Bagneres, A.G. *et al., Biochem. Syst. Ecol.*, 1991, **19**, 25 (*isol, ants*)
Berdague, J.L. *et al., J. Agric. Food Chem.*, 1991, **39**, 1257-1261 (*occur, food*)

4-Methyldecane M-388

[2847-72-5]
$H_3C(CH_2)_5CH(CH_3)CH_2CH_2CH_3$
$C_{11}H_{24}$ 156.311

(±)-*form*
d_4^{20} 0.74. Bp 187° Bp_{12} 71-72°. n_D^{20} 1.4175.

(ξ)-*form*
Also isol. from aroma volatiles of chick pea (*Cicer arietinum*), coconut flesh (*Cocos nucifera*), cooked beef and wheat.
Letsinger, R.L. *et al., J.A.C.S.*, 1948, **70**, 3342; 1950, **72**, 849 (*synth*)
Mann, G. *et al., Tetrahedron*, 1967, **23**, 3393 (*conformn, props*)
Lehmkuhl, H. *et al., Annalen*, 1975, 145 (*synth*)
Netzel, D.A. *et al., Fuel*, 1981, **60**, 307 (*cmr*)
Lipshutz, B.H. *et al., J.O.C.*, 1984, **49**, 3928 (*synth*)
Leod, G.M. *et al., J. Food Sci.*, 1987, **52**, 42-45; 56 (*occur, beef*)
Rembold, H. *et al., J. Agric. Food Chem.*, 1989, **37**, 659-662 (*occur, chickpea*)
Bagneres, A.G. *et al., Biochem. Syst. Ecol.*, 1991, **19**, 25 (*isol, ants*)

8-Methyldecanoic acid M-389

[5601-60-5]
$H_3CCH_2CH(CH_3)(CH_2)_6COOH$
$C_{11}H_{22}O_2$ 186.294

(±)-*form*
Mp -11.6°. $Bp_{0.5}$ 111-112° Bp_{25} 175°.

Me ester:
$C_{12}H_{24}O_2$ 200.32
Bp_{22} 129-132° $Bp_{1.95}$ 88°.

(ξ)-*form*
Volatile cooked meat component. Occurs in mutton flavours.
Weitkamp, A.W. *et al., J.A.C.S.*, 1945, **67**, 447-454 (*occur*)
Nunn, J.R. *et al., J.C.S.*, 1951, 1740-1744 (*synth*)
Laneele, M.A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1968, **266**, 1901 (*isol*)
Wong, E. *et al., J. Agric. Food Chem.*, 1975, **23**, 495-498 (*occur*)

9-Methyldecanoic acid, 9CI M-390

[1119-63-7]
9-Methylcapric acid
$(H_3C)_2CH(CH_2)_7COOH$
$C_{11}H_{22}O_2$ 186.294
Trace fatty acid found in aroma of cooked mutton. Bp_{23} 174-174.5° Bp_3 122-124°.
Levene, P.A. *et al., J. Biol. Chem.*, 1916, **27**, 449
Laneele, M.A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1968, **266**, 1901 (*isol*)
Wong, E. *et al., J. Agric. Food Chem.*, 1975, **23**, 495-498 (*occur*)
Takahashi, M. *et al., Yakugaku Zasshi*, 1976, **96**, 1000 (*synth*)
Kaga, H. *et al., Synthesis*, 1989, 864 (*synth, ir, pmr*)

3-Methyl-3-decenoic acid, 8CI M-391

$H_3C(CH_2)_5CH{=}C(CH_3)CH_2COOH$
$C_{11}H_{20}O_2$ 184.278

(*E*)-*form* [24404-64-6]
$Bp_{0.001}$ 90-95°.

Me ester: [24404-63-5]
$C_{12}H_{22}O_2$ 198.305
Bp_{11} 113-115°.

(*Z*)-*form* [22882-87-7]
Constit. of the fragrance oil of cassie (*Acacia farnesiana*). $Bp_{0.001}$ 90-94°.
Demole, E. *et al., Helv. Chim. Acta*, 1969, **52**, 24; 933 (*synth*)

3-Methyl-4-decenoic acid, 8CI M-392

$H_3C(CH_2)_4CH{=}CHCH(CH_3)CH_2COOH$
$C_{11}H_{20}O_2$ 184.278

(*E*)-*form* [22882-86-6]
Oil.

(*Z*)-*form* [24404-67-9]
Occurs in fragrance of the oil of cassie (*Acacia farnesiana*). Oil.
Demole, E. *et al., Helv. Chim. Acta*, 1969, **52**, 24; 933 (*isol, synth*)

3-Methyl-3-decen-1-ol, 8CI M-393

$H_3C(CH_2)_5CH{=}C(CH_3)CH_2CH_2OH$
$C_{11}H_{22}O$ 170.294

(*E*)-*form* [24404-65-7]
Oil.

(*Z*)-*form* [24404-66-8]
Occurs in fragrance oil of cassie (*Acacia farnesiana*). $Bp_{0.001}$ 53-56°.
Demole, E. *et al., Helv. Chim. Acta*, 1969, **52**, 24; 933 (*isol, synth*)

3-Methyl-4-decen-1-ol, 8CI M-394

$H_3C(CH_2)_4CH{=}CHCH(CH_3)CH_2CH_2OH$
$C_{11}H_{22}O$ 170.294

(±)-(*E*)-*form* [24404-71-5]

Constit. of nutmeg oil. Oil.

Ac: [78335-40-7]
$C_{13}H_{24}O_2$ 212.331
Constit. of nutmeg oil.

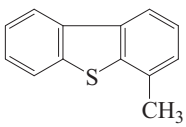
(±)-(*Z*)-*form* [24404-72-6]
Oil.

Demole, E. *et al., Helv. Chim. Acta*, 1969, **52**, 933 (*synth*)
Schenk, H.P. *et al., J. Chromatogr.*, 1981, **204**, 391-395 (*isol*)
Kang, S.H. *et al., Nat. Prod. Lett.*, 1996, **9**, 13-20 (*synth*)

4-Methyldibenzothiophene M-395

[7372-88-5]

[30995-64-3]



$C_{13}H_{10}S$ 198.288
Constit. of the rhizomes of rhubarb (*Rheum palmatum*) and starfruit aroma. Needles (MeOH). Mp 66.5°.

Gilman, H. *et al., J.O.C.*, 1938, **3**, 108-119 (*synth*)
Omata, A. *et al., Agric. Biol. Chem.*, 1987, **51**, 3421-3422 (*isol*)
Katritzky, A.R. *et al., J. Het. Chem.*, 1990, **27**, 1737-1740 (*synth, pmr*)
Katritzky, A.R. *et al., Magn. Reson. Chem.*, 1990, **28**, 914-917 (*pmr, cmr*)
Macleod, G. *et al., Phytochemistry*, 1990, **29**, 165-172 (*isol*)
Meille, V. *et al., Tetrahedron*, 1996, **52**, 3953-3960 (*synth, pmr*)
Ichinose, H. *et al., CA*, 1999, **131**, 225909b (*isol*)
Katsumata, H. *et al., Geochem. J.*, 2001, **35**, 37-48 (*occur*)

2-Methyl-3,5-dinitrobenzoic acid, 9CI M-396

[28169-46-2]
*3,5-Dinitro-*o*-toluic acid, 8CI. 4,6-Dinitro-*o*-toluic acid (incorr.)*



$C_8H_6N_2O_6$ 226.145
Needles (H_2O). Mp 205-206°.

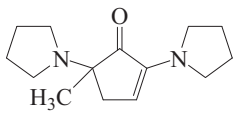
Amide: [148-01-6] *2-Methyl-3,5-dinitrobenzamide, 9CI.* ***Dinitolmide, BAN, INN.*** *Abilene. Coccidine. Salcostat. Whitsyn T. Zamix. Zoalene. Zoamix*
$C_8H_7N_3O_5$ 225.16
Poultry feed additive. Coccidiostat. Needles (EtOH aq.). Mp 181°. Log P 0.63 (calc).

▶ Has exploded on drying in bulk. Dust explosion hazard. LD_{50} (rat, orl) 600 mg/kg. ACGIH TLV: long-term 5 mg m^{-3}. XS4200000

McGookin, A. *et al., J. Soc. Chem. Ind., London*, 1940, **59**, 92-94 (*synth, esters, amide*)
Peterson, E.H. *et al., Poultry Sci.*, 1960, **39**, 739-745 (*amide*)
Joyner, L.P. *et al., Res. Vet. Sci.*, 1960, **1**, 363-370 (*amide*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 617
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 541
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DUP300

5-Methyl-2,5-di-1-pyrrolidinyl-2-cyclopenten-1-one M-397

[97826-64-7]

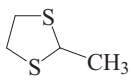


$C_{14}H_{22}N_2O$ 234.341
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*synth, ms, pmr, ir*)

2-Methyl-1,3-dithiolane, 9CI, 8CI M-398

[5616-51-3]
Acetaldehdye ethylene thioacetal. FEMA 3705



$C_4H_8S_2$ 120.239
Maillard product from cysteine and glucose degradation. Flavouring ingredient; present in boiled beef volatiles. Liq. with burnt, alliaceous odour. Bp_{18} 75°.

Seebach, D. *et al., Synthesis*, 1969, 17-19 (*synth*)
Garbusov, V. *et al., Nahrung*, 1976, **20**, 235-241 (*occur*)
Hoppman, A. *et al., Annalen*, 1977, 1547-1556 (*synth, pmr, cmr*)
Pihlaja, K. *et al., Org. Mass Spectrom.*, 1988, **23**, 770-776 (*ms*)
Tai, C.-Y. *et al., J. Agric. Food Chem.*, 1997, **45**, 3586-3589 (*occur*)

2-(Methyldithio)propanoic acid, 9CI M-399

[58847-92-0]
MeS-S-CH(CH$_3$)COOH
$C_4H_8O_2S_2$ 152.238

Et ester: [23747-43-5] *FEMA 3834*
$C_6H_{12}O_2S_2$ 180.292
Flavouring agent for baked goods and seasonings. Liq. Bp 105°.

Chloride: [58847-93-1]
$C_4H_7ClOS_2$ 170.683
Bp_{55} 100-122°.

Netherlands Pat., 1969, 6 812 899; *CA*, **71**, 61421a (*Et ester, synth, use*)
Von Dubs, P. *et al., Helv. Chim. Acta*, 1976, **59**, 1307-1311 (*Et ester, synth*)
U.S. Pat., 1976, 3 932 660; *CA*, **84**, 135317p (*chloride*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 565 (*Et ester*)

2-Methyldodecane M-400

[1560-97-0]
$H_3C(CH_2)_9CH(CH_3)_2$
$C_{13}H_{28}$ 184.364
Constit. of *Cicer arietinum* (chickpea) and *Humulus lupulus* (hops). Bp 229° $Bp_{10.5}$ 103°. n_D^{20} 1.4241.

Petrov, A.A. *et al., CA*, 1960, **54**, 1257c (*synth*)
Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1670 (*isol*)
Mann, G. *et al., Tetrahedron*, 1967, **23**, 3393 (*synth*)
Schlenk, W. *et al., Annalen*, 1973, 1179 (*synth*)
Rembold, H. *et al., J. Agric. Food Chem.*, 1989, **37**, 659 (*isol*)

3-Methyldodecane M-401

[17312-57-1]
$C_{13}H_{28}$ 184.364

(*S*)-*form*
Bp_{16} 108-109°. $[\alpha]_D$ +7.6 (neat). n_D^{20} 1.4244.

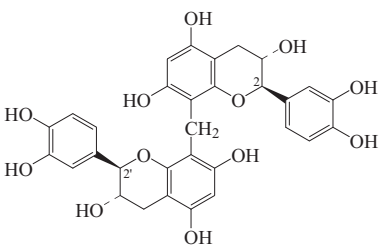
(±)-*form*
Bp 230° Bp_{15} 111°. n_D^{20} 1.4262.

(ξ)-*form*
Constit. of chick pea (*Cicer arietinum*) and coconut.

[55194-17-7]

Petrov, A.A. *et al., CA*, 1960, **65**, 1257c (*synth*)
Lardicci, L. *et al., Ann. Chim. (Rome)*, 1962, **52**, 652 (*synth*)
Mann, G. *et al., Tetrahedron*, 1967, **23**, 3393 (*synth*)
Schlenk, W. *et al., Annalen*, 1973, 1179 (*synth*)
Rembold, H. *et al., J. Agric. Food Chem.*, 1989, **37**, 659 (*isol*)

8,8′-Methylenebis[3,3′,4′,5,7-pentahydroxyflavan] M-402



$C_{31}H_{28}O_{12}$ 592.555

(2*R*,2′*R*,3*S*,3′*S*)-*form* [81555-08-0]
8,8′-Methylenebiscatechin. Di(8-catechinyl)methane
Constit. of cacao liquor, *Theobroma cacao*.

Kiatgrajai, P. *et al., J.O.C.*, 1982, **47**, 2913-2917 (*synth*)
Hatano, T. *et al., Phytochemistry*, 2002, **59**, 749-758 (*isol*)

Methylenebutanedioic acid, 9CI M-403

[97-65-4]
Methylenesuccinic acid, 8CI. 2-Propene-1,2-dicarboxylic acid. Itaconic acid
$H_2C{=}C(COOH)CH_2COOH$
$C_5H_6O_4$ 130.1
Isol. from plants, e.g. roots of *Vicia faba*. Hygroscopic cryst. or needles ($MeNO_2$). Mod. sol. H_2O, EtOH, Me_2CO; spar. sol.

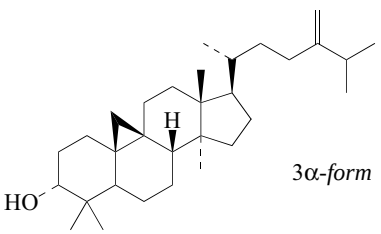
Et_2O, C_6H_6, $CHCl_3$, hexane. Mp 167-168° (162-164° dec.). pK_{a1} 3.68; pK_{a2} 5.14 (25°, 0.1*M* $NaClO_4$). V. low toxicity. Interconverts with citraconic and mesaconic acids (see 2-Methyl-2-butenedioic acid) under strongly basic conds. or on htg. Q/e values for polym., Q 0.78, e 1.07.

[2287-83-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 504B; 646C; 716D; 744A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 786C; 997A; 1176C; 1214B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 692B (*ir*)
Sadtler Standard C-13 NMR Spectra, 6812 (*cmr*)
Org. Synth., Coll. Vol., 2, 1943, 368 (*synth*)
Pfeifer, V.F. *et al., Ind. Eng. Chem.*, 1952, **44**, 2975 (*manuf*)
Jones, E.R.H. *et al., J.C.S.*, 1954, 1865 (*synth*)
Chiusoli, G.P. *et al., Angew. Chem.*, 1960, **72**, 74 (*synth*)
Coïc, Y. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 914 (*isol*)
Harlow, R.L. *et al., Acta Cryst. B*, 1973, **29**, 2965 (*cryst struct*)
Dallinga, J.W. *et al., Org. Mass Spectrom.*, 1984, **19**, 10 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **14**, 952 (*rev*)

24-Methylenecycloartan-3-ol M-404

[1449-09-8]
24-Methylene-9,19-cyclolanostan-3-ol, 9CI



$C_{31}H_{52}O$ 440.751

3β-*form*

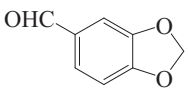
Constit. of rice bran oil. Cryst. (MeOH). $[\alpha]_D^{14.5}$ +48.8 (c, 0.26 in $CHCl_3$).

4-Hydroxy-3-methoxycinnamoyl: ***Oryzanol C***
$C_{41}H_{60}O_4$ 616.923
From rice bran oil. Cryst. ($CHCl_3$/MeOH). Mp 193-194°. $[\alpha]_D$ +36 (c, 1.87 in $CHCl_3$).

Ohta, G. *et al., Chem. Pharm. Bull.*, 1960, **8**, 5; 9 (*Oryzanol C*)
Cocker, W. *et al., J.C.S.*, 1965, 1692 (*synth*)
Alpin, R.T. *et al., J.C.S.(B)*, 1966, 1078 (*ms*)
Malhotra, H.C. *et al., J. Biol. Chem.*, 1972, **247**, 6243 (*biosynth*)
Lenton, J.R. *et al., Phytochemistry*, 1975, **14**, 1523 (*biosynth*)
Itoh, T. *et al., Steroids*, 1976, **27**, 275 (*pmr*)
De Pascual Teresa, J. *et al., Phytochemistry*, 1987, **26**, 1767 (*pmr, cmr*)
Seo, S. *et al., J.C.S. Perkin 1*, 1988, 2407 (*biosynth*)
Guo, D. *et al., Tet. Lett.*, 1996, **37**, 6823 (*biosynth*)
Böhme, F. *et al., Phytochemistry*, 1997, **45**, 1041-1044 (*ms*)
Ohtsu, H. *et al., Phytochemistry*, 1998, **49**, 1761-1768 (*3α-form*)

3,4-Methylenedioxybenzaldehyde M-405

[120-57-0]
1,3-Benzodioxole-5-carboxaldehyde, 9CI. Piperonal, 8CI. Heliotropin. Piperonyl aldehyde. Protocatechuic aldehyde methylene ether. FEMA 2911



$C_8H_6O_3$ 150.134
Flavouring agent used in cherry and vanilla flavours. Cryst. (H_2O) with floral odour and bittersweet taste. Mp 37°. Bp 263° Bp_{15} 140°.

▶ Skin irritant. CNS depressant. LD_{50} (rat, orl) 2700 mg/kg. TO1575000

(E)-Oxime: [20747-41-5]
$C_8H_7NO_3$ 165.148
Cryst. (MeOH). Mp 146°.

(Z)-Oxime: [20747-42-6]
Needles (H_2O). Mp 112°.

2,4-Dinitrophenylhydrazone:
Red or purplish-red cryst. Mp 271°.

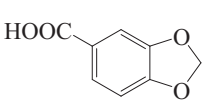
Semicarbazone:
Leaflets. Mp 237°.

Di-Me acetal: [59259-90-4]
$C_{10}H_{12}O_4$ 196.202
$Bp_{0.05}$ 84°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 956B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 119A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1299D (*ir*)
Ciamician, G. *et al., Ber.*, 1890, **23**, 1159; *Gazz. Chim. Ital.*, 1890, **20**, 571
Brady, O.L. *et al., J.C.S.*, 1931, 756
Sasaki, Y. *et al., Chem. Pharm. Bull.*, 1967, **15**, 599 (*nmr*)
Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 2418 (*uv*)
Perjessi, A. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 3302 (*ir*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Knudsen, R.D. *et al., J.O.C.*, 1975, **40**, 2878 (*derivs*)
Napolitano, E. *et al., J.O.C.*, 1983, **48**, 3653 (*deriv, ir, pmr*)
Torii, S. *et al., J.O.C.*, 1984, **49**, 1830 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PIW250
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

3,4-Methylenedioxybenzoic acid M-406

[94-53-1]
1,3-Benzodioxole-5-carboxylic acid, 9CI. Piperonylic acid. Heliotropic acid



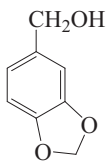
$C_8H_6O_4$ 166.133
Isol. from *Piper longum* (long pepper). Needles (EtOH), cryst. (H_2O). Mp 229°. pK_a 4.5 (25°, 5% EtOH). Sublimes in prisms.

▶ DF4912765

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1111A; 1349B; 1533C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 212C; 457B (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 538 (*synth*)
Briggs, L.H. *et al., J.C.S.*, 1950, 2376 (*isol*)
Dobrowsky, A. *et al., Monatsh. Chem.*, 1955, **86**, 325 (*synth*)
Byrne, M.M. *et al., J.C.S.(B)*, 1968, 809
Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 2418 (*uv*)

3,4-Methylenedioxybenzyl alcohol M-407

[495-76-1]
1,3-Benzodioxole-5-methanol, 9CI. Piperonyl alcohol, 8CI. Piperonol



$C_8H_8O_3$ 152.149
Needles (petrol). Mp 58°. Bp_5 156-158° (Bp_{10} 150-151°).

Ac: [326-61-4] *Piperonyl acetate. FEMA 2912*
$C_{10}H_{10}O_4$ 194.187
Flavouring agent. Present in endive (*Cichorium endiva*). Cryst. (CCl_4 or petrol) or liq. with sweet, floral flavour at low conc., bitter at high levels. d_4^{18} 1.24. Mp 51°. Bp_{14} 153-154°.

▶ Skin irritant. LD_{50} (rat, orl) 2100 mg/kg. AI9050000

2-Methylpropanoyl: [5461-08-5] *Piperonyl isobutyrate. FEMA 2913*
$C_{12}H_{14}O_4$ 222.24
Flavouring ingredient, not reported in nature. Liq. with intense, sweet, plum-like flavour. $Bp_{0.07}$ 99° $Bp_{0.005}$ 91-92°. n_D^{25} 1.5068.

Benzoyl: [5469-06-7]
$C_{15}H_{12}O_4$ 256.257
Needles (EtOH). Mp 66°.

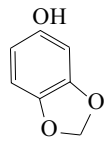
Me ether: [86633-25-2] *5-(Methoxymethyl)-1.3-benzodioxole. 4-Methoxymethyl-1,2-methylenedioxybenzene*
$C_9H_{10}O_3$ 166.176
Liq. $Bp_{0.02}$ 75°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1142A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 364B; 1203B (*nmr*)
Barger, G. *et al., J.C.S.*, 1908, **93**, 563
Palfray, L. *et al., Bull. Soc. Chim. Fr.*, 1947, **14**, 676
Shepard, E.R. *et al., J.O.C.*, 1952, **17**, 568 (*synth*)
Gertler, S.I. *et al., J.O.C.*, 1959, **24**, 327-329 (*esters, synth*)
Napolitano, E. *et al., J.O.C.*, 1983, **48**, 3653 (*deriv, ir, pmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PIX000

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 681 (*isobutyrate*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2233-2234 (*isobutyrate*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1508; 1509 (*Ac, isobutyrate, use, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

3,4-Methylenedioxyphenol, 8CI M-408

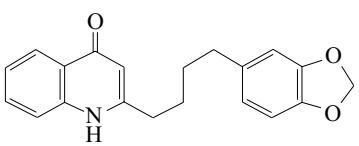
[533-31-3]
1,3-Benzodioxol-5-ol, 9CI. 1,2,4-Benzenetriol methylene ether. ***Sesamol***



$C_7H_6O_3$ 138.123
Isol. from sesame oil. Cryst. ($CHCl_3$/petrol). Mp 65.8°. Bp_{13} 135-140°.
► Exp. carcinogen (high oral doses). SM0890000
4-Methylbenzenesulfonyl:
$C_{14}H_{12}O_5S$ 292.312
Needles. Mp 86-87°.
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 280A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1092B (*ir*)
Böeseken, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1936, **55**, 815
Suarez, C.C. *et al., Anal. Chem.*, 1952, **24**, 668 (*isol*)
Takata, Y. *et al., Yakugaku Zasshi*, 1954, **74**, 693; *CA*, **48**, 10652h
Haslam, E. *et al., J.C.S.*, 1955, 827
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MJU000

2-[4-(3,4-Methylenedioxyphenyl)butyl]-4(1*H*)-quinolinone M-409

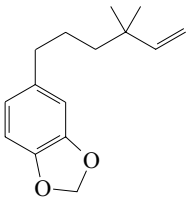
[17889-77-9]



$C_{20}H_{19}NO_3$ 321.375
Alkaloid from *Ruta graveolens* (rue). Cryst. (MeOH). Mp 224°.
Novák, I. *et al., Pharmazie*, 1965, **20**, 654 (*isol, ir, pmr, ms, struct*)
Reisch, J. *et al., Naturwissenschaften*, 1967, **54**, 517 (*synth*)

6-[(3,4-Methylenedioxy)phenyl]-3,3-dimethyl-1-hexene, 8CI M-410

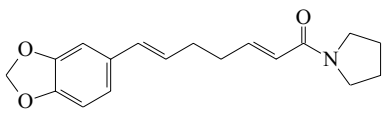
[30310-56-6]
5-(4,4-Dimethyl-5-hexenyl)-1,3-benzodioxole, 9CI



$C_{15}H_{20}O_2$ 232.322
Constit. of *Ruta graveolens* (rue). Oil. n_D^{22} 1.5135.
Reisch, J. *et al., Tet. Lett.*, 1970, 4305 (*isol, ir, uv, pmr*)

1-[7-(3,4-Methylenedioxyphenyl)-2,6-heptadienoyl]pyrrolidine M-411

1-[7-(1,3-Benzodioxol-5-yl)-1-oxo-2,6-heptadienyl]pyrrolidine, 9CI. 7-(3,4-Methylenedeoxyphenyl)-2,6-heptadienoic acid pyrrolidide

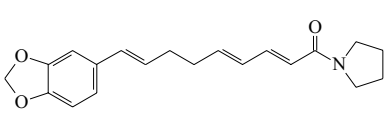


(2*E*,6*E*)-*form*

$C_{18}H_{21}NO_3$ 299.369
(2*E*,6*E*)-*form* [112448-68-7]
Piperamide-C7:2 (2*E*,6*E*). *Sarmentosine*†
Constit. of the fruits of pepper (*Piper nigrum*) and cha-plu (*Piper sarmentosum*) (Piperaceae). Mp 77.5-79.5°.
2,3-Dihydro: [117137-66-3] *1-[7-(1,3-Benzodioxol-5-yl)-1-oxo-6-heptenyl]pyrrolidine, 9CI. 1-[7-(3,4-Methylenedioxyphenyl)-6-heptenoyl]-pyrrolidine. 7-(3,4-Methylenedioxyphenyl)-6-heptenoic acid pyrrolidide.*
Piperamide-C7:1 (6*E*)
$C_{18}H_{23}NO_3$ 301.385
Constit. of pepper fruits (*Piper nigrum*). Oil.
Likhitwitayawuid, K. *et al., Tetrahedron*, 1987, **43**, 3689 (*Sarmentosine*)
Kiuchi, F. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2452 (*isol, uv, ir, pmr, ms, struct*)
Strunz, G.M. *et al., Phytochemistry*, 1995, **39**, 731 (*synth, Sarmentosine*)
Bari, S.S. *et al., J. Indian Chem. Soc.*, 1996, **73**, 520 (*synth, Sarmentosine*)

1-[9-(3,4-Methylenedioxyphenyl)-2,4,8-nonatrienoyl]pyrrolidine M-412

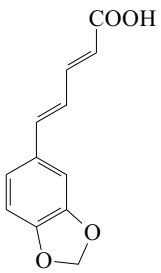
1-[9-(1,3-Benzodioxol-5-yl)-1-oxo-2,4,8-nonatrienyl]pyrrolidine, 9CI. 9-(3,4-Methylenedioxyphenyl)-2,4,8-nonatrienoic acid pyrrolidide



$C_{20}H_{23}NO_3$ 325.407
(2*E*,4*E*,8*E*)-*form* [117137-68-5]
Piperamide-C9:3 (2*E*,4*E*,8*E*)
Constit. of pepper fruits (*Piper nigrum*, Piperaceae). Yellow needles. Mp 105-106°.
4,5-Dihydro: [117137-67-4] *1-[9-(1,3-Benzodioxol-5-yl)-1-oxo-2,8-nonadienyl]-pyrrolidine, 9CI. 1-[9-(3,4-Methylenedioxyphenyl)-2,8-nonadienoyl]pyrrolidine. 9-(3,4-Methylenedioxyphenyl)-2,8-nonadienoic acid pyrrolidide.* ***Piperamide-C9:2 (2*E*,8*E*)***. *Brachyamide B*
$C_{20}H_{25}NO_3$ 327.422
Constit. of pepper fruits (*Piper nigrum*). Oil.
2,3,4,5-Tetrahydro: [62510-52-5] *1-[9-(1,3-Benzodioxol-5-yl)-1-oxo-8-nonenyl]pyrrolidine, 9CI. 1-[9-(3,4-Methylenedioxyphenyl)-8-nonenoyl]pyrrolidine. 9-(3,4-Methylenedioxyphenyl)-8-nonenoic acid pyrrolidide.* ***Piperamide-C9:1 (8*E*)***. *Tricholein*
$C_{20}H_{27}NO_3$ 329.438
Constit. of pepper (*Piper nigrum*). Oil.
Singh, J. *et al., Phytochemistry*, 1976, **15**, 2018 (*Piperamide-C9:1*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 560 (*Piperamide-C9:1*)
Kiuchi, F. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2452 (*isol, uv, ir, pmr, cmr, ms, struct*)
Koul, S.K. *et al., Phytochemistry*, 1988, **27**, 3523 (*Piperamide-C9:2*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419 (*synth*)

5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoic acid M-413

[5285-18-7]
5-(1,3-Benzenedioxol-5-yl)-2,4-pentadienoic acid, 9CI. ***Piperic acid, 8CI****. Piperinic acid. Piperonic acid*



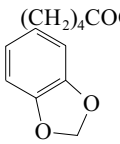
(*E*,*E*)-*form*

$C_{12}H_{10}O_4$ 218.209
Obt. from black pepper (*Piper nigrum*), from *Minthostachys verticillata*, peppermint (*Mentha piperita*) and others.
(E,E)-form [136-72-1]
Needles (EtOH). Mp 216°. pK_a 5.7 (50% MeOH aq.).
Me ester: [6190-46-1]
$C_{13}H_{12}O_4$ 232.235
Yellow plates (MeOH). Mp 146°.
(2*E*,4*Z*)-*form* [495-87-4] *Isochavicinic acid. Isochavicic acid*
Cryst. (EtOH). Mp 143°. pK_a 5.5 (50% MeOH aq.).
(2*Z*,4*E*)-*form* [495-88-5] *Isopiperinic acid*
Cryst. (C_6H_6). Mp 153° (138°). pK_a 5.35 (50% MeOH aq.).
(Z,Z)-form [495-89-6] *Chavicinic acid. Chavicic acid*
Cryst. (C_6H_6). Mp 129-130° (120°). pK_a 5.9 (50% MeOH aq.).
Ladenburg, A. *et al., Ber.*, 1894, **27**, 2958

Zetzsche, F. *et al., Ber.*, 1940, **73**, 114
Grewe, R. *et al., Chem. Ber.*, 1970, **103**, 3752 (*synth, stereochem, uv, ir, pmr*)
De Cleyn, R. *et al., Bull. Soc. Chim. Belg.*, 1972, **81**, 529 (*bibl*)
Banerji, A. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 546-549 (*ester, synth, cmr*)

5-(3,4-Methylenedioxyphenyl)pentanoic acid M-414

[41917-45-7]
1,3-Benzodioxole-5-pentanoic acid, 9CI. Piperhydronic acid. Tetrahydropiperinic acid



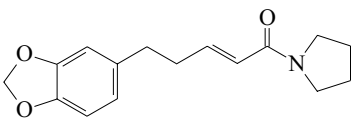
$C_{12}H_{14}O_4$ 222.24
Isol. from fruits of *Piper longum* (long pepper). Tablets or platelets (EtOH). Mp 100-101° (90-91°).

Et ester:
$C_{14}H_{18}O_4$ 250.294
Bp_1 155°.

Gokhale, V.G. *et al., CA*, 1949, **43**, 1085 (*isol*)
Viswanathan, N. *et al., Helv. Chim. Acta*, 1975, **58**, 2026 (*synth*)

1-[5-(3,4-Methylenedioxyphenyl)-2-pentenoyl]pyrrolidine M-415

5-(3,4-Methylenedioxyphenyl)-2-pentenoic acid pyrrolidide

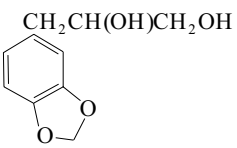


$C_{16}H_{19}NO_3$ 273.331
(*E*)-*form* [117137-65-2]
Piperamide-C5:1 (2E)
Constit. of pepper fruits (*Piper nigrum*, Piperaceae). Oil.

Kiuchi, F. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2452; 2647 (*isol, uv, ir, pmr, ms, struct*)
Alecio, A.C. *et al., J. Nat. Prod.*, 1998, **61**, 637-639 (*isol, pmr, cmr*)

3-(3,4-Methylenedioxyphenyl)-1,2-propanediol M-416

3-(1,3-Benzodioxol-5-yl)-1,2-propanediol, 9CI. 5-(2,3-Dihydroxypropyl)-1,2-methylenedioxybenzene. ***Safrolglycol***

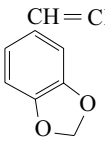


$C_{10}H_{12}O_4$ 196.202
(+)-*form* [36150-22-8]
Constit. of the wood of Sassafras root. Needles (cyclohexane). Mp 79°. $[\alpha]_D^{20}$ +10 (c, 0.25 in $CHCl_3$).

Rosenmund, K.W. *et al., Ber.*, 1923, **56**, 1265 (*synth*)
Höke, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1972, **305**, 33 (*pmr, uv, ir, ms*)

3-(3,4-Methylenedioxyphenyl)propenal M-417

[14756-00-4]
3-(1,3-Benzodioxol-5-yl)-2-propenal, 9CI. 3,4-Methylenedioxycinnamaldehyde, 8CI. 3-(3,4-Methylenedioxyphenyl)acrolein. Piperonylideneacetaldehyde. Piperonylacrolein



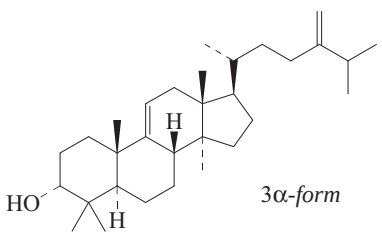
$C_{10}H_8O_3$ 176.171
Isol. from *Sassafras albidum* (sassafras). Pale-yellow needles (CH_2Cl_2/petrol). Mp 84-85°. $Bp_{0.1}$ 110-112°.

Oxime: [97476-41-0]
$C_{10}H_9NO_3$ 191.186
Needles (C_6H_6), plates (EtOH) or needles (C_6H_6). Mp 155° Mp 191° Mp 195° (trimorph.).

Phenylhydrazone:
Yellow needles (EtOH). Mp 163-164°.

Ikeda, T. *et al., CA*, 1942, **36**, 6754 (*isol*)
Coates, J. *et al., J.C.S. Perkin 1*, 1974, 37 (*synth*)
Dallacker, F. *et al., Chem. Ber.*, 1975, **108**, 95 (*synth, uv*)
Vig, O.P. *et al., Indian J. Chem.*, 1975, **13**, 1015 (*synth*)
Sethi, M.L. *et al., Phytochemistry*, 1976, **15**, 1773 (*isol*)
Kulkarni, M.G. *et al., Tet. Lett.*, 1990, **31**, 4497 (*synth*)
Parsons, I.C. *et al., Phytochemistry*, 1993, **33**, 479 (*isol, pmr*)

24-Methylenelanost-9(11)-en-3-ol M-418



$C_{31}H_{52}O$ 440.751
3α-*form* [264192-27-0]
3β-*form* [52222-75-0]
Constit. of shea butter. Cryst. Mp 178.5-179.5°. $[\alpha]_D^{20}$ +60 (c, 0.92 in $CHCl_3$).

Itoh, T. *et al., Lipids*, 1975, **10**, 454 (*isol*)
Itoh, T. *et al., Steroids*, 1976, **27**, 275 (*pmr*)
Yuan, J. *et al., Zhongguo Yaowu Huaxue Zazhi*, 1999, **9**, 216-217; *CA*, **132**, 290993j (*isol, pmr, cmr*)

3-Methylene-2-octanone, 9CI M-419

[63759-55-7]
3-Pentyl-3-buten-2-one. FEMA 3725
$H_2C{=}C(COCH_3)(CH_2)_4CH_3$
$C_9H_{16}O$ 140.225
Flavouring ingredient. Pale yellow liq. Bp_{40} 90-92°.

Shono, T. *et al., J.A.C.S.*, 1979, **101**, 984-987 (*synth, pmr*)
Paterson, I. *et al., Tetrahedron*, 1988, **44**, 4207-4219 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 642 (*use*)

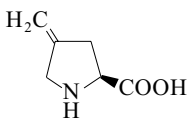
2-Methylene-4-oxopentanedioic acid M-420

γ-Methylene-α-ketoglutaric acid. 2-Methylene-4-oxoglutaric acid
$H_2C{=}C(COOH)CH_2COCOOH$
$C_6H_6O_5$ 158.11
Isol. from *Arachis hypogaea* (peanuts).

Towers, G.H.N. *et al., J.A.C.S.*, 1954, **76**, 1959
Fowden, L. *et al., Biochem. J.*, 1955, **59**, 228
Winter, H.C. *et al., Phytochemistry*, 1987, **26**, 2477 (*occur*)

4-Methylene-2-pyrrolidinecarboxylic acid M-421

4-Methyleneproline, 9CI



(*S*)-*form*

$C_6H_9NO_2$ 127.143
(*S*)-*form* [20309-87-9]
L-form
Cryst. (EtOH aq.). Mp 243-245°. $[\alpha]_D^{25}$ -50.9 (c, 0.44 in H_2O).

N-*Benzyloxycarbonyl, dicyclohexylamine salt:*
Mp 160-161°. $[\alpha]_D^{19}$ -5.5 (c, 2 in $CHCl_3$).

(±)-*form* [2370-38-9]
Present in loquat seeds (*Eriobotrya japonica*). Mp 224-245° (225°) dec.

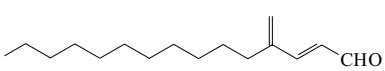
Hydrochloride:
Plates (EtOH/EtOAc). Mp 217-218°.

N-*Benzyloxycarbonyl, dicyclohexylamine salt:*
Mp 139°.

Bethell, M. *et al., J.C.S.*, 1965, 3850 (*synth*)
Gray, D.O. *et al., Phytochemistry*, 1972, **11**, 745 (*isol, struct*)
Manfré, F. *et al., J.O.C.*, 1992, **57**, 2060 (*synth, pmr*)

4-Methylene-2-tetradecenal, 9CI M-422

4-Decyl-2,4-pentadienal



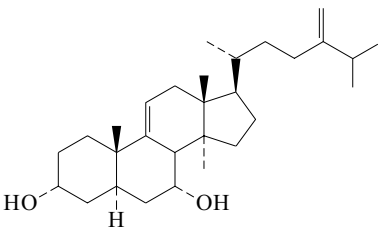
$C_{15}H_{26}O$ 222.37
(*E*)-*form* [85769-28-4]
α-Triticene
Constit. of *Triticum aestivum* (wheat). Oil. Sol. MeOH, Et_2O; poorly sol. hexane. λ_{max} 276 (ε 10000) (EtOH) (Derep).

Spendley, P.J. *et al., Phytochemistry*, 1982, **21**,

2403

14-Methylergosta-9(11),24(28)-dien-3,7-diol M-423

14-Methyl-24-methylenecholest-9(11)-ene-3,7-diol

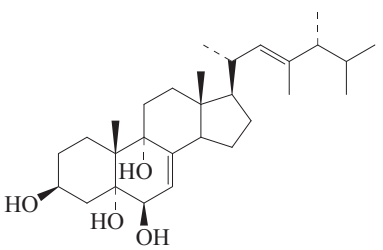


$C_{29}H_{48}O_2$ 428.697

(3α,5α,7α)-*form* [138504-34-4]
Constit. of the tubers of *Colocasia esculenta* (taro).
Ali, M. *et al., Indian J. Pharm. Sci.*, 1991, **53**, 98 (*isol, struct*)

23-Methylergosta-7,22-diene-3,5,6,9-tetrol M-424

23,24-Dimethylcholesta-7,22-diene-3,5,6,9-tetrol

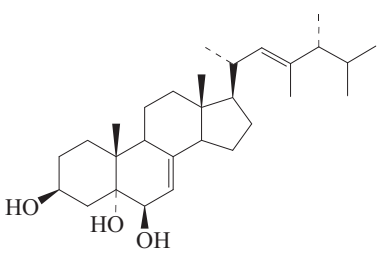


$C_{29}H_{48}O_4$ 460.696

(3β,5α,6β,9α,22*E*,24*R*)-*form* [243449-55-0]
Constit. of *Lentinula edodes* (shiitake). Amorph. powder.
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 847-851 (*isol, pmr*)

23-Methylergosta-7,22-diene-3,5,6-triol M-425

23,24-Dimethylcholesta-7,22-diene-3,5,6-triol

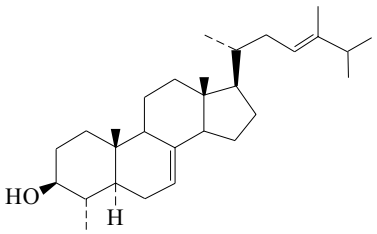


$C_{29}H_{48}O_3$ 444.696

(3β,5α,6β,22*E*,24*R*)-*form* [243449-54-9]
Constit. of *Lentinula edodes* (shiitake). Amorph. powder. $[\alpha]_D^{23}$ -15.9 (c, 0.06 in $CHCl_3$).
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1999, **47**, 847-851 (*isol, pmr, cmr*)

4-Methylergosta-7,23-dien-3-ol, 9CI M-426

4,24-Dimethylcholesta-7,23-dien-3-ol

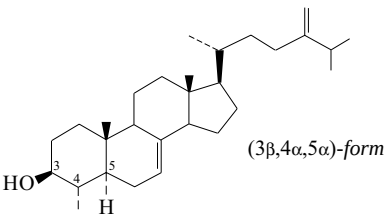


$C_{29}H_{48}O$ 412.698

(3β,4α,5α,23*E*)-*form* [79683-95-7]
Constit. of *Zea mays* (sweet corn) germ oil.
Itoh, T. *et al., Phytochemistry*, 1981, **20**, 1353 (*isol*)
Scheid, F. *et al., Phytochemistry*, 1982, **21**, 1959 (*isol*)

4-Methylergosta-7,24(28)-dien-3-ol, 9CI M-427

4-Methyl-24-methylenecholest-7-en-3-ol



(3β,4α,5α)-*form*

$C_{29}H_{48}O$ 412.698

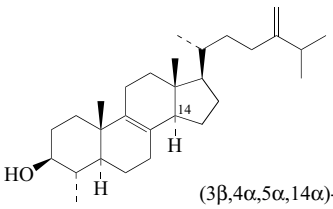
(3β,4α,5α)-*form* [1176-52-9]
24-Methylenelophenol. Gramisterol. Gramisterin
Constit. of sugar, potatoes, grapefruit, peas (*Pisum sativum*). Cryst. Mp 172-173°. $[\alpha]_D^{19}$ +6 (c, 1.4 in $CHCl_3$).

(3β,4β,5α)-*form* [21490-25-5]
Isol. from Marigold (*Calendula officinalis*) flowers. Mp 151°.

(3β,4α,5α,20*S*)-*form*
20-Epi-24-methylenelophenol
Cryst. (EtOH). Mp 176-178°. $[\alpha]_D$ +3 (c, 0.8 in $CHCl_3$).
Schreiber, K. *et al., Tetrahedron*, 1964, **20**, 2575 (*isol*)
Osske, G. *et al., Tetrahedron*, 1965, **21**, 1559 (*isol*)
Pyrek, J.St. *et al., Chem. Comm.*, 1969, 107 (*isol*)
Lenton, J.R. *et al., Phytochemistry*, 1975, **14**, 1523 (*biosynth*)
Della Greca, M. *et al., Phytochemistry*, 1990, **29**, 1797 (*isol, pmr*)

4-Methylergosta-8,24(28)-dien-3-ol M-428

4-Methyl-24-methylenecholest-8-en-3-ol



(3β,4α,5α,14α)-*form*

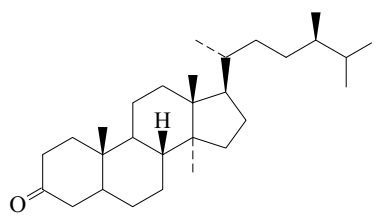
$C_{29}H_{48}O$ 412.698

(3β,4α,5α,14α)-*form* [17757-07-2]
4α-Methylfecosterol
Minor constit. of yeast and constit. of wheat germ oil (*Triticum aestivum*). Cryst. (Me_2CO/MeOH). Mp 143-145°. $[\alpha]_D^{29}$ +55 (c, 3 in $CHCl_3$).

(3β,4α,5α,14β)-*form* [224566-30-7]
Triticusterol
Constit. of wheat germ oil (*Triticum aestivum*). Needles. Mp 107-109°. $[\alpha]_D^{25}$ +118.6 (c, 0.6 in $CHCl_3$).
Barton, D.H.R. *et al., Chem. Comm.*, 1968, 17 (*isol*)
Barton, D.H.R. *et al., J.C.S.(C)*, 1970, 775 (*biosynth*)
Stanković, S. *et al., Phytochemistry*, 1985, **24**, 2466 (*isol*)
Akihisa, T. *et al., J.C.S. Perkin 1*, 1999, 497-500 (*isol, pmr, cmr*)

14-Methylergostan-3-one M-429

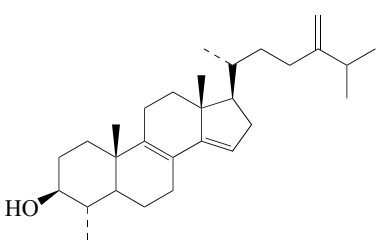
14,24-Dimethylcholestan-3-one



$C_{29}H_{50}O$ 414.713

(5α,14α,24*R*)-*form* [151676-47-0]
Constit. of mature wheat straw (*Triticum aestivum*). Cryst. (EtOH). Mp 152-155°.
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523 (*isol, pmr*)

4-Methylergosta-8,14,24(28)-trien-3-ol M-430



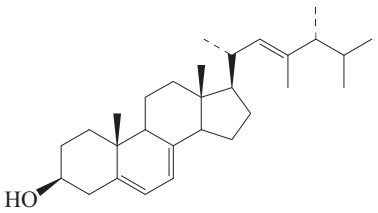
$C_{29}H_{46}O$ 410.682

(3β,4α,5α)-*form* [74635-33-9]
Constit. of wheat germ oil (*Triticum*

aestivum). Needles. Mp 124-126°. λ_{max} 248 (EtOH).

Akihisa, T. *et al., J.C.S. Perkin 1*, 1999, 497-500 (*isol, pmr, cmr*)

23-Methylergosta-5,7,22-trien-3-ol M-431



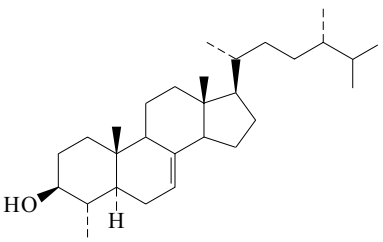
$C_{29}H_{46}O$ 410.682

(3β,22*E*,24*R*)-*form* [276864-97-2]
Constit. of *Lentinula edodes* (shiitake). Amorph. powder. $[\alpha]_D^{27}$ -78.9 (c, 0.04 in $CHCl_3$).

Ohnuma, N. *et al., Chem. Pharm. Bull.*, 2000, **48**, 749-751 (*isol, pmr, cmr*)

4-Methylergost-7-en-3-ol M-432

4,24-Dimethylcholest-7-en-3-ol



$C_{29}H_{50}O$ 414.713

(3β,4α,5α,24*R*)-*form* [33903-17-2]
24α-Methyllophenol
Isol. from seeds of *Phaseolus vulgaris* (kidney bean) and other plants. Mp 140-141° (as acetate).

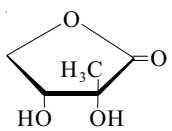
[1106-35-0, 81275-83-4, 81445-17-2]

Conner, A.H. *et al., Phytochemistry*, 1981, **20**, 2543 (*isol, pmr*)

Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219 (*isol, pmr, ms*)

2-*C*-Methyl-1,4-erythronolactone M-433

3,4-Dihydroxy-3-methyldihydro-2(3H)-furanone, 9CI



$C_5H_8O_4$ 132.116

D-*form* [18465-71-9]
Constit. of *Trifolium incarnatum* (crimson clover) and *Phaseolus vulgaris* (kidney bean). $[\alpha]_D$ -58.6 ($CHCl_3$).

2,3-Di-Ac: [74831-17-7] *2,3-Di*-O-*acetyl-2*-C-*methyl-D-1,4-erythronolactone*
$C_9H_{12}O_6$ 216.19
Mp 87-88°. $[\alpha]_D$ -9 (c, 0.9 in $CHCl_3$).

3-O-*(3,4-Dihydroxycinnamoyl):* [144881-15-2] *3*-O-*Caffeoyl-2*-C-*methyl-D-1,4-erythronolactone*
$C_{14}H_{14}O_7$ 294.26
Pale yellow solid. $[\alpha]_D^{25}$ -93.3 (c, 0.8 in MeOH).

2,3-O-*Isopropylidene:2,3*-O-*Isopropylidene-2*-C-*methyl-D-1,4-erythronolactone*
$C_8H_{12}O_4$ 172.18
Mp 40-41°. $[\alpha]_D$ -99 (c, 0.85 in $CHCl_3$).

2-Benzyl:2-O-*Benzyl-2*-C-*methyl-D-1,4-erythronolactone*
$C_{12}H_{14}O_4$ 222.24
$[\alpha]_D^{22}$ -21.8 (c, 1.2 in $CHCl_3$).

Ishizu, A. *et al., Acta Chem. Scand.*, 1967, **21**, 424 (*isopropylidene*)

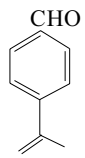
De Pascual Teresa, J. *et al., Tet. Lett.*, 1980, 1359 (*isol, di-Ac, isopropylidene*)

Yoshimura, J. *et al., Carbohydr. Res.*, 1982, **101**, 343 (*di-Ac, benzyl*)

Ono, H. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1970-1973 (*isol, pmr, cmr*)

4-(1-Methylethenyl)benzaldehyde, 9CI M-434

[10133-50-3]
4-Isopropenylbenzaldehyde. p-*Mentha-1,3,5,8-tetraen-7-al*



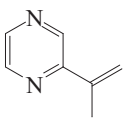
$C_{10}H_{10}O$ 146.188
Constit. of Roman chamomile oil (*Anthemis nobilis*). Oil. $Bp_{0.01}$ 100°.

Semicarbazone:
Cryst. (2-propanol). Mp 240-242°.

Thomas, A.F. *et al., Helv. Chim. Acta*, 1981, **64**, 2393

(1-Methylethenyl)pyrazine, 9CI M-435

[38713-41-6]
Isopropenylpyrazine, 8CI. FEMA 3296



$C_7H_8N_2$ 120.154
Flavouring ingredient. Present in roasted sesame seed, roasted coffee beans, roasted peanut, Oolong tea, cooked beef, fried chicken, roasted cocoa beans, tortilla chips and fermented soybeans. Maillard product.

Lu, G. *et al., J. Agric. Food Chem.*, 1997, **45**, 233-236 (*formn*)

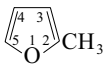
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1998, **46**, 2764-2769 (*glc, ms, occur*)

Chung, H.Y. *et al., J. Agric. Food Chem.*, 1999, **47**, 2690-2696 (*glc, occur, soybean*)

2-Methylfuran, 9CI M-436

[534-22-5]

[27137-41-3]
α-Methylfuran. Silvan. Sylvan



C_5H_6O 82.102
Maillard product. Spar. sol. H_2O. d_4^{20} 0.83. Bp 63-63.5°. n_D^{20} 1.4332. Turns yellow in air. Dec. by strong NaOH.

▶ Eye irritant. Highly flammable, fl. p. -30°. LD_{50} (rat, orl) 167 mg/kg. LU2625000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 14B (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 580A (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1450B (*ir*)

Harries, C. *et al., Ber.*, 1898, **31**, 37 (*synth*)

Schniepp, L.E. *et al., J.A.C.S.*, 1947, **69**, 672 (*synth*)

Pascal, Y. *et al., Bull. Soc. Chim. Fr.*, 1965, 2211 (*pmr*)

Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)

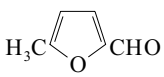
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 682

Kiewiet, A. *et al., Org. Magn. Reson.*, 1974, **6**, 461 (*cmr*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKH000

5-Methyl-2-furancarboxaldehyde, 9CI M-437

[620-02-0]
5-Methylfurfural. 2-Formyl-5-methylfuran. FEMA 2702



$C_6H_6O_2$ 110.112
Isol. from brown algae and other plant sources, doubtless as a secondary prod. from saccharides. Flavouring ingredient. Oil with sweet spicy odour and caramel-like flavour. d_4^{18} 1.11. Bp 187° Bp_{12} 79-81°. n_D^{20} 1.5263.

▶ LD_{50} (rat, orl) 2200 mg/kg. LT7032500

*Oxime(*E-*):* [57784-58-4]
$C_6H_7NO_2$ 125.127
Prisms (petrol). Mp 51-52°.

*Oxime(*Z-*):* [57784-53-9]
$C_6H_7NO_2$ 125.127
Needles (petrol). Mp 112°.

Phenylhydrazone:
Mp 147-148°.

Thiosemicarbazone: [6823-95-6] *5-Methyl-2-furancarboxaldehyde thiosemicarbazone*
$C_7H_9N_3OS$ 183.234
Cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 584C (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 25B (*nmr*)

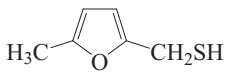
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1458C (*ir*)

Fromherz, K. *et al., Ber.*, 1907, **40**, 404

Reichstein, T. *et al., Helv. Chim. Acta*, 1930, **13**, 346
Org. Synth., 1934, **14**, 62
Grigg, R. *et al., Tetrahedron*, 1965, **21**, 3441 (*ms*)
Mas'ko, L.I. *et al., Zh. Anal. Khim.*, 1975, **30**, 315 (*detn, Pd*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 751 (*rev, tox*)
Comins, D.L. *et al., J.O.C.*, 1987, **52**, 104 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 501
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1761-1762

5-Methyl-2-furanmethanethiol, 9CI M-438

[59303-05-8]
5-Methyl-2-furfurylmercaptan. 2-(Mercaptomethyl)-5-methylfuran

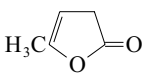


C_6H_8OS 128.195
Cysteine-derived Maillard product. Constit. of coffee, roasted sesame and yeast-extract volatiles. Bp_3 70°. n_D^{20} 1.5258.

Kipnis, F. *et al., J.A.C.S.*, 1949, **71**, 2270 (*synth*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1981, **29**, 1078-1082 (*synth, ms, occur*)
Schieberle, P. *et al., Food Chem.*, 1996, **55**, 145-152 (*occur*)
Hofmann, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1998, **207**, 229-236

5-Methyl-2(3*H*)-furanone, 9CI M-439

[591-12-8]
4-Hydroxy-3-pentenoic acid γ-lactone. α-Angelica lactone. Δ^2-Angelica lactone. Angelic lactone. FEMA 3293



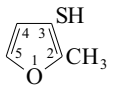
$C_5H_6O_2$ 98.101
Flavouring for baked goods, milk and meat produts. Cryst. with sweet, hebaceous odour. Sl. sol. H_2O. Mp 18°. Bp 167-170° Bp_{12} 53°. Readily isom. to 5-Methyl-2(5*H*)-furanone.

► LD_{50} (mus, orl) 2800 mg/kg. LU5075000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 701C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1147B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 754A (*ir*)
Kuehl, F.A. *et al., J.C.S.*, 1950, 2213 (*synth*)
Wineburg, J.P. *et al., J. Het. Chem.*, 1975, **12**, 749 (*synth, pmr*)
Lambert, C. *et al., Tet. Lett.*, 1984, **25**, 5323 (*synth*)
Guntrum, E. *et al., Synthesis*, 1986, 921 (*synth, ir, cmr*)
Boykin, D.W. *et al., Heterocycles*, 1989, **29**, 301 (*O-17 nmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 91
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKH250

2-Methyl-3-furanthiol, 9CI M-440

[28588-74-1]
3-Mercapto-2-methylfuran. FEMA 3188



C_5H_6OS 114.168
Occurs in chicken, beef and tunafish. Formed by thermal treatment of cysteine-ribose mixtures. Organoleptic compd. with beef broth aroma. Well patented. Odour threshold 0.0025 ng/L in air, 0.007μg/kg in H_2O.

► LD_{50} (mus, orl) 100 mg/kg. LU6235000

S-*Me:* [63012-97-5] *2-Methyl-3-(methylthio)furan. Dimethylthiofuran. FEMA 3949*
C_6H_8OS 128.195
Occurs in coffee and cooked beef aromas. Compd. with intense roasted meat aroma.

S-*Ph:* [105621-16-7] *2-Methyl-3-(phenylthio)furan*
$C_{11}H_{10}OS$ 190.265
Oil. $Bp_{0.9}$ 100-110°.

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1454A (*ir*)
U.S. Pat., 1977, 4 020 175; *CA*, **87**, 135020y (*synth, deriv*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249 (*tox*)
Tressel, R. *et al., J. Agric. Food Chem.*, 1981, **29**, 1078
MacLeod, G. *et al., Chem. Ind. (London)*, 1986, 175 (*isol, deriv*)
Gasser, U. *et al., Z. Lebensm.-Unters. -Forsch.*, 1988, **186**, 489; 1990, **190**, 3 (*occur*)
McDougal, P.G. *et al., J.O.C.*, 1989, **54**, 91 (*deriv, synth, pmr, ir, ms*)
Kerscher, R. *et al., J. Agric. Food Chem.*, 1998, **46**, 1954-1958 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1163 (*S-Me*)

5-Methyl-2-furanthiol, 9CI M-441

[60965-60-8]
2-Mercapto-5-methylfuran

C_5H_6OS 114.168
Oil. $Bp_{1.7}$ 72-73°.

S-*Me:* [13678-59-6] *2-Methyl-5-(methylthio)furan, 9CI. FEMA 3366*
C_6H_8OS 128.195
Constit. of roasted coffee aroma. Flavouring agent. Yellow oil. d_4^{20} 1.06. Bp_{50} 80° (Kugelrohr). n_D^{20} 1.5170.

Cederlund, B. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 198 (*synth, ir, pmr*)
Eugster, C.H. *et al., Helv. Chim. Acta*, 1981, **64**, 2636 (*S-Me, synth, uv, ir, pmr*)

5-Methyl-3-furanthiol, 9CI M-442

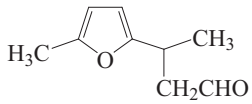
[56078-97-8]
4-Mercapto-2-methylfuran

C_5H_6OS 114.168
Cysteine-derived Maillard product. Component of meat aroma model systems. Possesses a green, meaty-herbaceous odour. Characterised spectroscopically.

Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms, ir*)

3-(5-Methyl-2-furanyl)butanal M-443

[31704-80-0]
β,5-Dimethyl-2-furanpropanal. FEMA 3307



$C_9H_{12}O_2$ 152.193
Flavouring ingredient. d_4^{20} 1. Bp_2 60-61°. n_D^{20} 1.4709.

2,4-Dinitrophenylhydrazone:
Orange platelets (EtOH). Mp 103-104°.

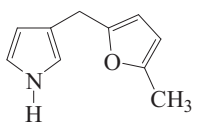
Ethylene acetal: [222528-23-6] *2-[2-(5-Methyl-2-furanyl)propyl]-1,3-dioxolane*
$C_{11}H_{16}O_3$ 196.246
Liq. with intense floral, lilac-note odour. Bp_2 90°. n_D^{20} 1.4786.

Propylene acetal: [222528-26-9] *2-[2-(5-Methyl-2-furanyl)propyl]-1,3-dioxane*
$C_{12}H_{18}O_3$ 210.272
Liq. with weak floral, lilac-note odour. $Bp_{1.5}$ 75°. n_D^{20} 1.4797.

Yurev, Y.K. *et al., Zh. Obshch. Khim.*, 1963, **33**, 1150-1156; *J. Gen. Chem. USSR (Engl. Transl.)*, 1963, **33**, 1132-1137 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 504 (*use*)
Nowicki, J. *et al., J. Cosmet. Sci.*, 1999, **50**, 99-104 (*acetals, props*)

3-[(5-Methyl-2-furanyl)-methyl]-1*H*-pyrrole M-444

[118248-37-6]
3-(5-Methylfurfuryl)pyrrole. 2-Methyl-5-(3-pyrrolylmethyl)furan

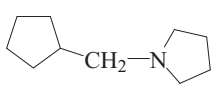


$C_{10}H_{11}NO$ 161.203
Putative proline-derived Maillard product formed in model reactions with 1-pyrroline and 5-methylfurfural. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **13**, 405-410 (*occur, ms, ir, pmr*)

1-[(5-Methyl-2-furanyl)-methyl]pyrrolidine, 10CI M-445

[61480-99-7]
5-Methyl-2-(N-pyrrolidinomethyl)furan. 1-(5-Methylfurfuryl)pyrrolidine

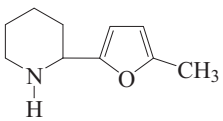


$C_{10}H_{15}NO$ 165.235
Proline-derived Maillard product. Constit. of roasted, dried squid aroma. Oil. $Bp_{2.8}$ 72-74° Kugelrohr.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*occur, ms*)
Kawai, T. *et al., J. Agric. Food Chem.*, 1991, **39**, 770-777 (*occur, squid*)
Heaney, H. *et al., Tetrahedron*, 1997, **53**, 2941-2958; 1977, 13361-13372 (*synth, pmr, cmr*)

2-(5-Methyl-2-furanyl)piperidine, 9CI M-446

[97073-18-2]
2-Methyl-5-(2-piperidinyl)furan

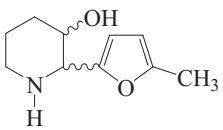


$C_{10}H_{15}NO$ 165.235
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*ms*)
Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*synth, ir, ms, pmr*)

2-(5-Methyl-2-furanyl)-3-piperidinol, 9CI M-447

2-(3-Hydroxy-2-piperidinyl)-5-methylfuran



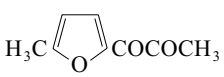
$C_{10}H_{15}NO_2$ 181.234
Proline-derived Maillard product.

[118248-24-1, 118248-25-2]

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, ms*)

1-(5-Methyl-2-furanyl)-1,2-propanedione, 9CI M-448

[1197-20-2]

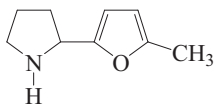


$C_8H_8O_3$ 152.149
Minor constit. of coffee aroma. Bp_6 96°. n_D^{23} 1.5320. λ_{max} 296 (log ϵ 3.98) (no solent reported).

Gianturco, M.A. *et al., Tetrahedron*, 1964, **20**, 2951

2-(5-Methyl-2-furanyl)pyrrolidine M-449

[118248-27-4]
2-Methyl-5-(2-pyrrolidinyl)furan

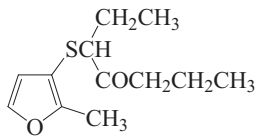


$C_9H_{13}NO$ 151.208
Putative proline-derived Maillard product formed in model reactions with 1-pyrroline and ascorbic acid. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*synth, occur, ms*)

3-[(2-Methyl-3-furanyl)thio]-4-heptanone, 9CI M-450

[61295-41-8]
FEMA 3570

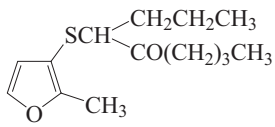


$C_{12}H_{18}O_2S$ 226.339
Meat flavouring ingredient. Liq. with roast meat odour. d_4^{25} 1.04. $Bp_{0.3}$ 85-86°. n_D^{20} 1.4986.

Ger. Pat., 1976, 2 600 707; *CA*, **86**, 29610k (*synth, use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)

4-[(2-Methyl-3-furanyl)thio]-5-nonanone, 9CI M-451

[61295-50-9]
FEMA 3571

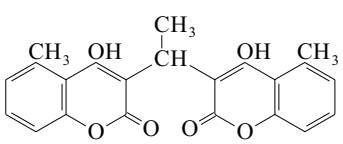


$C_{14}H_{22}O_2S$ 254.393
Flavouring ingredient. Liq. with meat-like odour. d^{25} 1.01. $Bp_{0.25}$ 102-103°. n_D^{20} 1.4926.

Ger. Pat., 1976, 2 600 707; *CA*, **86**, 29610k (*synth, use*)
Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-62; 64-66; 68-70 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 505 (*use, props*)

11-Methylgerberinol M-452

[173559-76-7]
3,3′-Ethylidenebis(4-hydroxy-5-methyl-2H-1-benzopyran-2-one)

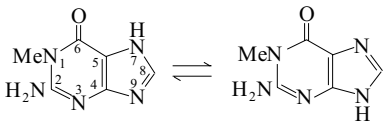


$C_{22}H_{18}O_6$ 378.381
Constit. of *Diospyros kaki* (Japanese persimmon). Cryst. (EtOAc). Mp 218° (210-217°). λ_{max} 246 (ϵ 13200); 295 (ϵ 25700); 305 (ϵ 21900); 320 (ϵ 13200) (EtOH).

Paknikar, S.K. *et al., Phytochemistry*, 1996, **41**, 931-933 (*isol, synth, uv, ir, pmr*)

1-Methylguanine, 8CI M-453

[938-85-2]
2-Amino-1,7-dihydro-1-methyl-6H-purin-6-one, 9CI



7H-form *9H-form*

$C_6H_7N_5O$ 165.154
Present in Chinese cabbage (*Brassica chinensis*), and other plants. Plates or needles (AcOH aq.). Mp 350°.

Traube, W. *et al., Ber.*, 1913, **46**, 3845 (*synth*)
Dunn, D.B. *et al., Biochem. J.*, 1959, **72**, 294; 1963, **88**, 34P (*isol*)
Pfleiderer, W. *et al., Annalen*, 1961, **647**, 167 (*synth*)
Elion, G.B. *et al., J.O.C.*, 1962, **27**, 2478 (*synth*)
Rice, J.M. *et al., J.A.C.S.*, 1967, **89**, 2719 (*ms*)
Le Breton, P.R. *et al., J.A.C.S.*, 1990, **112**, 2138 (*synth, pmr, uv, cmr*)

2-Methylheneicosane, 9CI M-454

Isodocosane
$H_3C(CH_2)_{18}CH(CH_3)_2$
$C_{22}H_{46}$ 310.605
Found in orange oil (*Citrus sinensis*) and hops (*Humulus lupulus*).

Steibl, M. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 2522 (*synth*)
Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807 (*isol*)

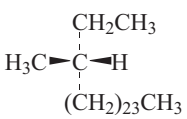
8-Methyl-3-hentriacontene M-455

[239091-55-5]
$H_3C(CH_2)_{22}CH(CH_3)(CH_2)_3CH=CHCH_2CH_3$
$C_{32}H_{64}$ 448.858
Constit. of the fruit of the famine food *Momordica dioica*.

Ali, M. *et al., Indian J. Pharm. Sci.*, 1998, **60**, 287-289

3-Methylheptacosane, 9CI M-456

[14167-66-9]



(*R*)-form

$C_{28}H_{58}$ 394.766
(R)-form
Cryst. (EtOH). Mp 43°. $[\alpha]_D^{26}$ -3.6 (c, 1.06 in $CHCl_3$).
(S)-form
Cryst. (EtOH). Mp 43°. $[\alpha]_D^{24}$ +3.7 (c, 0.95 in $CHCl_3$).

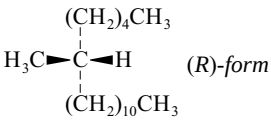
(ξ)-*form*
Isol. from hop oil (*Humulus lupulus*) and orange oil (*Citrus sinensis*).

[55194-24-6]

Mold, J.D. *et al., Biochemistry*, 1963, **2**, 605 (*isol*)
Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807 (*isol*)
Marukawa, K. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 305-314 (*synth*)

6-Methylheptadecane M-457

[26741-13-9]



(*R*)-*form*

$C_{18}H_{38}$ 254.498
Isol. from the oil of *Ruta graveolens* (rue).

(*R*)-*form* [55194-50-8]
Bp_{10} 166°.

Calvin, M. *et al., Chem. Comm.*, 1970, 1490 (*isol*)
Schlenk, W. *et al., Annalen*, 1973, 1179 (*synth*)
Tattje, D.H.E. *et al., Pharm. Weekbl.*, 1978, **113**, 1169 (*isol*)

16-Methylheptadecanoic acid, 9CI M-458

[2724-58-5]
Isostearic acid. Isooctadecanoic acid
$(H_3C)_2CH(CH_2)_{14}COOH$
$C_{18}H_{36}O_2$ 284.481
Found in meats, liver and fats. Mp 69.5°.

Amide:
$C_{18}H_{37}NO$ 283.496
Mp 107.3°.

[30399-84-9]

Fordyce, C.R. *et al., J.A.C.S.*, 1933, **55**, 3368-3372 (*synth*)
Abrahamsson, S. *et al., Acta Cryst. B*, 1972, **28**, 2562 (*cryst struct*)
Rawdah, T.N. *et al., Meat Sci.*, 1994, **37**, 149-155 (*occur*)

6-Methyl-3,5-heptadien-2-one, 9CI M-459

[1604-28-0]
FEMA 3363
$(H_3C)_2C{=}CHCH{=}CHCOCH_3$
$C_8H_{12}O$ 124.182
Flavouring ingredient. Isol. from lavender oil (*Lavendula officinalis* hybrid).

(*E*)-(?)-*form* [16647-04-4]
Bp_{12} 89°. n_D^{20} 1.5265.

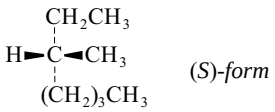
Oxime:
$C_8H_{13}NO$ 139.197
Cryst. (EtOH). Mp 114-115°.

Semicarbazone:
Needles (MeOH). Mp 192° dec.

Lacey, R.N. *et al., J.C.S.*, 1954, 827 (*synth, uv*)
U.K. Pat., 1955, 741 047; *CA*, **50**, 16839 (*synth*)
Stadler, P.A. *et al., Helv. Chim. Acta*, 1960, **43**, 1601 (*isol*)
Heck, R.F. *et al., J.A.C.S.*, 1963, **85**, 3383 (*synth*)
Schirmann, J.-P. *et al., Bull. Soc. Chim. Fr.*, 1967, 3896 (*synth*)
Saucy, G. *et al., Helv. Chim. Acta*, 1967, **50**, 1158 (*synth*)
Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1976, 1941 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 506
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1768-1769

3-Methylheptane, 9CI M-460

[589-81-1]



(*S*)-*form*

C_8H_{18} 114.23
Constit. of *Cicer arietinum* (chickpea), *Jasminum sambac* (Arabian jasmine) and other plant spp..

► Highly flammable, fl.p. -23°.

(*S*)-*form* [6131-25-5]
Bp 118-119°. $[\alpha]_D$ +9.34 (neat).

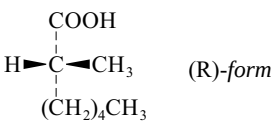
(±)-*form*
d_{15}^{15} 0.72. Bp 120-122°. n_D^{25} 1.4022.

[111002-96-1]

Hohenlohe-Oehringen, K. *et al., Monatsh. Chem.*, 1962, **93**, 586 (*synth*)
Dvoretzky, I. *et al., Anal. Chem.*, 1963, **35**, 545 (*synth*)
Lardicci, L. *et al., J.O.C.*, 1966, **31**, 1534 (*synth*)
Mann, G. *et al., Tetrahedron*, 1967, **23**, 3375 (*conform, props*)
Beierbeck, H. *et al., Can. J. Chem.*, 1977, **55**, 771 (*cmr*)
Consiglio, G. *et al., Tetrahedron*, 1986, **42**, 2043 (*synth*)

2-Methylheptanoic acid, 9CI M-461

[1188-02-9]
Amylmethylacetic acid. FEMA 2706



(R)-*form*

$C_8H_{16}O_2$ 144.213

(*R*)-*form* [159345-59-2]
Liq. Bp_{13} 121-122°. $[\alpha]_D^{25}$ -15.6 (neat) (86% ee).

Chloride:
$C_8H_{15}ClO$ 162.659
Liq. Bp_{727} 179.5-182°.

(*S*)-*form* [116454-37-6]
$[\alpha]_D^{20}$ +4.1 (neat).

(±)-*form* [128441-06-5]
Flavouring ingredient. Mp 15°. Bp_{13} 121-122°.

[13751-83-2]

Karrer, P. *et al., Helv. Chim. Acta*, 1930, **13**, 1292-1308 (*synth*)
Levene, P.A. *et al., J. Biol. Chem.*, 1941, **140**, 255-257 (*resoln, config*)
Adkins, H. *et al., J.A.C.S.*, 1950, **72**, 4550-4553 (*synth*)
Senn, W.L. *et al., Anal. Chim. Acta*, 1964, **31**, 441 (*pmr*)
Taylor, E.C. *et al., Tetrahedron*, 1967, **23**, 77-85 (*synth*)
Knapp, S. *et al., Synth. Commun.*, 1980, **10**, 837-842 (*synth*)
Fujisawa, T. *et al., Tet. Lett.*, 1980, **21**, 2181-2184 (*synth*)
Hayashi, T. *et al., Chem. Lett.*, 1987, 2037-2040 (*synth*)
Douglass, S.K. *et al., J. Chem. Ecol.*, 1993, **19**, 11-27 (*synth*)
Karl, V. *et al., Chirality*, 1994, **6**, 420-426 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 507
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1770

6-Methylheptanoic acid, 9CI M-462

[929-10-2]
Isooctanoic acid. Isocaprylic acid
$(H_3C)_2CH(CH_2)_4COOH$
$C_8H_{16}O_2$ 144.213
Present in hop oil (*Humulus lupulus*) as the Me ester. Liq. Mp 0°. Bp 232° (220° dec.) Bp_{14} 126-127°.

► Fl.p. 132° (oc), autoignition temp. 392°.

Me ester: [2519-37-1]
$C_9H_{18}O_2$ 158.24
Liq. Bp_{10} 73°.

Et ester: [62337-58-0]
$C_{10}H_{20}O_2$ 172.267
Liq. Bp 200.3°.

Chloride: [70767-37-2]
$C_8H_{15}ClO$ 162.659
Liq. Bp_9 73°.

Amide: [2979-83-1]
$C_8H_{17}NO$ 143.228
Plates. Mp 114°.

Nitrile: [138808-37-4] *1-Cyano-5-methylhexane*
$C_8H_{15}N$ 125.213
Liq. Bp 194°.

Wilkinson, S. *et al., Nature (London)*, 1963, **200**, 1008-1009 (*isol*)
Just, G. *et al., Can. J. Chem.*, 1968, **46**, 3381-3389 (*amide, synth, ir, pmr*)
Markgraf, J.H. *et al., J.O.C.*, 1977, **42**, 2631-2632 (*Me ester, Et ester, synth, ir*)
Crawforth, J.M. *et al., J.C.S. Perkin 1*, 1998, 1721-1726 (*synth, chloride, ir, pmr, cmr*)

4-Methyl-2-heptanol, 9CI M-463

[56298-90-9]
$H_3CCH_2CH_2CH(CH_3)CH_2CH(OH)CH_3$
$C_8H_{18}O$ 130.23
Constit. of *Osmanthus fragrans* (sweet osmanthus). Liq. Bp 168°. Config. of nat. prod. or of synthetic material not detd..

[111675-75-3, 147249-39-6, 147331-64-4, 147331-65-5, 147331-66-6, 147331-67-7]

Clarke, L. *et al., Ber.*, 1907, **40**, 352-355 (*synth*)
Alberty, R.A. *et al., J. Phys. Chem. Ref. Data*, 1987, **16**, 391-417 (*thermodyn*)
Ding, D. *et al., J. Essent. Oil Res.*, 1989, **1**, 295-297 (*occur*)

5-Methyl-3-heptanol, 9CI M-464

[18720-65-5]
active-*Amylethylcarbinol*
$H_3CCH_2CH(CH_3)CH_2CH(OH)CH_2CH_3$
$C_8H_{18}O$ 130.23

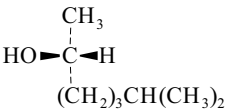
Liq. with odour of peppermint. Bp 167-168° Bp_{28} 70-72°.

[82749-48-2, 82749-49-3, 84709-54-6, 84709-55-7, 147331-68-8, 147331-69-9]

Powell, S.G. *et al., J.A.C.S.*, 1931, **53**, 765-768 (*synth*)
Vasi, I.G. *et al., J. Inst. Chem. (India)*, 1982, **54**, 19-21 (*synth*)
Brunner, H. *et al., J. Organomet. Chem.*, 1988, **346**, 413-424 (*synth*)

6-Methyl-2-heptanol, 9CI M-465

[4730-22-7]



(*R*)-*form*

$C_8H_{18}O$ 130.23

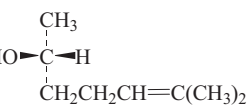
(±)-*form* [87187-86-8]
Liq. Bp_{22} 82-85°.

Ac:Isooctyl acetate. Fructurol
$C_{10}H_{20}O_2$ 172.267
Fruit food flavouring. Trace component of pummelo (*Citrus grandis*) oil and cheese aroma. Oily liq. Poorly documented.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 187B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 178A (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 75E (*ir*)
Doering, W.v.E. *et al., J.A.C.S.*, 1952, **74**, 2997-2999 (*abs config*)
Canonica, L. *et al., Farmaco, Ed. Sci.*, 1959, **14**, 122-136 (*synth*)
Finkbeiner, H.L. *et al., J.O.C.*, 1962, **27**, 3395-3400 (*synth*)
Levsen, K. *et al., Org. Mass Spectrom.*, 1977, **12**, 131-135 (*ms*)
Sawamura, M. *et al., J. Agric. Food Chem.*, 1988, **36**, 567-569 (*Ac, occur, pummelo*)

6-Methyl-5-hepten-2-ol, 9CI M-466

[1569-60-4]
Sulcatol



(*R*)-*form*

$C_8H_{16}O$ 128.214

(*R*)-*form* [58917-27-4]
Occurs in lemongrass oil. Bp 178-180° Bp_{20} 85-86°. $[\alpha]_D^{25}$ -14.5 (c, 1.3 in EtOH) (100% ee).

4-Nitrobenzoyl: [69891-45-8]
Light yellow cryst. (MeOH). Mp 54-55°. $[\alpha]_D^{22}$ -61.2 (c, 5.02 in $CHCl_3$).

(*S*)-*form* [58917-26-3]
Bp_{20} 85-86°. $[\alpha]_D^{23}$ +17.4 (neat).

4-Nitrobenzoyl: [69891-43-6]
Light yellow cryst. (MeOH). Mp 54-55°. $[\alpha]_D^{22}$ +61.4 (c, 5.01 in $CHCl_3$).

(±)-*form* [4630-06-2]
Flavouring ingredient. d^{20} 0.86. Bp 174-176° Bp_{34} 91°. n_D^{20} 1.4505.

Ac: [19162-00-6]
$C_{10}H_{18}O_2$ 170.251
Bp_9 78°.

Me ether: [99347-48-5] *6-Methoxy-2-methyl-2-heptene*
$C_9H_{18}O$ 142.241
Bp 163-164° Bp_9 50°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 143B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 215B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 209D (*ir*)
Mori, K. *et al., Tetrahedron*, 1975, **31**, 3011; 1981, **37**, 1341 (*synth*)
Breitholle, E.G. *et al., J.O.C.*, 1978, **43**, 1964 (*synth*)
Linstrumelle, G. *et al., Tet. Lett.*, 1978, 4069 (*synth*)
Johnson, B.D. *et al., Can. J. Chem.*, 1979, **57**, 233 (*synth*)
Fetizon, M. *et al., J.C.S. Perkin 1*, 1979, 1407 (*synth*)
Marfat, A. *et al., J.O.C.*, 1979, **44**, 3888 (*synth*)
Takano, S. *et al., Chem. Lett.*, 1982, 1913 (*synth*)
Takano, S. *et al., Heterocycles*, 1983, **20**, 1363 (*synth*)
Keinan, E. *et al., J.A.C.S.*, 1986, **108**, 162 (*synth*)
Mori, K. *et al., Annalen*, 1987, 271 (*synth*)
Belan, A. *et al., J.O.C.*, 1987, **52**, 256
Stokes, T.M. *et al., Tet. Lett.*, 1987, **28**, 2091 (*resoln*)
Sugai, T. *et al., Agric. Biol. Chem.*, 1990, **54**, 1577 (*synth*)
Sarma, B.K. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 615 (*synth*)
Davies, S.G. *et al., Tetrahedron: Asymmetry*, 1996, **7**, 1005 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1770-1771
Arnone, A. *et al., Eur. J. Org. Chem.*, 1999, 117-128 (*synth*)
Nakamura, K. *et al., J.C.S. Perkin 1*, 2000, 3205-3211 (*S-form, synth, pmr, ir*)
Fantin, G. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 2367-2373 (*resoln, R-form*)

3-Methyl-3-hepten-2-one, 9CI M-467

[39899-08-6]
$H_3CCH_2CH_2CH{=}C(CH_3)COCH_3$
$C_8H_{14}O$ 126.198
Geom. isom. not detd.. Constit. of the oil of *Glycyrrhiza glabra* (licorice). Bp 170-176° Bp_{15} 68-69°.

2,4-Dinitrophenylhydrazone:
Mp 137°.

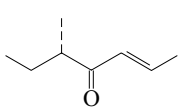
Semicarbazone:
Cryst. (EtOH). Mp 166-168°.

[75343-94-1]

Powell, S.G. *et al., J.A.C.S.*, 1938, **60**, 1914 (*synth*)
Andreeva, L.K. *et al., CA*, 1991, **114**, 163481 (*synth*)

5-Methyl-2-hepten-4-one M-468

[81925-81-7]



Filbertone. FEMA 3761
$C_8H_{14}O$ 126.198

(*S,E*)-*form* [122440-59-9]
[102322-83-8]
Principal flavour constit. of hazelnuts. Flavouring ingredient. Liq. Bp_{20} 70° (Kugelrohr). $[\alpha]_D^{22}$ +37.3 (c, 2.5 in Me_2CO). The (*S*)-enantiomer predominates in the nat. prod., however the enantiomeric excess depends on the conditions during isol. The two enantiomers have different odour characteristics.

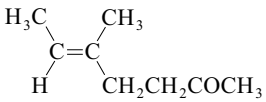
(±)-*form*
Bp 170°.

[103070-07-1]

Stutsman, P.S. *et al., J.A.C.S.*, 1939, **61**, 3303 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 508
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1772-1773
Blanch, G.P. *et al., J. Agric. Food Chem.*, 1998, **46**, 4283-4286 (*isol, glc, isomers*)
Zarbin, P.H.G. *et al., J. Braz. Chem. Soc.*, 1998, **9**, 583-585 (*S,E-form, synth*)
Jauch, J. *et al., Tetrahedron*, 1999, **55**, 9787-9792 (*S,E-form, synth, nmr, ms*)

5-Methyl-5-hepten-2-one, 9CI M-469

[10339-67-0]



(*E*)-*form*

$C_8H_{14}O$ 126.198
Constit. of *Daucus carota* (carrot). Bp_{45} 84°.

2,4-Dinitrophenylhydrazone:
Orange needles (MeOH). Mp 75-76°.

(*E*)-*form* [25524-99-6]
Liq.

Semicarbazone: [25525-00-2]
Cryst. (MeOH aq.). Mp 121-123°.

(*Z*)-*form* [25525-01-3]
Oil. Bp_{61} 95-96°.

Lanchenauer, A. *et al., Helv. Chim. Acta*, 1951, **34**, 1514-1523 (*synth*)
Wakabayashi, N. *et al., Tet. Lett.*, 1969, 3253-3256 (*synth*)
Kueh, J.S.H. *et al., J.C.S. Perkin 1*, 1981, 1052-1057 (*synth*)
Wender, P.A. *et al., Tetrahedron*, 1981, **37**, 4445-4450 (*synth, pmr*)
Pinilla, M.G. *et al., J. Essent. Oil Res.*, 1995, **7**, 433-435 (*isol*)
Trehan, J.R. *et al., J. Indian Chem. Soc.*, 1997, **74**, 500-501 (*synth*)

6-Methyl-5-hepten-2-one, 9CI M-470

[110-93-0]
Sulcatone. FEMA 2707
$H_3CCOCH_2CH_2CH{=}C(CH_3)_2$
$C_8H_{14}O$ 126.198
Present in Ceylon citronella oil, lemongrass oil and palmarosa oil. Product of 1,3,6,10-Farnesatetraene, F-6 oxidation in stored apples affected by superficial scald. Flavouring ingredient. d^{20} 0.86. Mp -67°. Bp 172-174° (161-162°) Bp_{10} 58.5°.

► Fl. p. 57°. MJ9700000

Oxime: [22418-73-1]
$C_8H_{15}NO$ 141.213
Bp_{12} 99°.

2,4-Dinitrophenylhydrazone: [6147-43-9]
Mp 78°.

Semicarbazone: [16769-68-9]
Mp 135° approx.

[409-02-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 415D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 646B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 501B (*ir*)
Birkinshaw, J.H. *et al., Biochem. J.*, 1950, **47**, 55 (*isol*)
Mousseron, M. *et al., Bull. Soc. Chim. Fr.*, 1963, 376 (*synth*)
Saucy, G. *et al., Helv. Chim. Acta*, 1967, **50**, 2091 (*synth*)
Sato, K. *et al., J.O.C.*, 1970, **35**, 565 (*synth*)
Boccara, N. *et al., Bull. Soc. Chim. Fr.*, 1972, 1448 (*synth*)
Ishihara, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 439 (*synth, bibl*)
Dennison, N.R. *et al., Aust. J. Chem.*, 1975, **28**, 1339 (*synth*)
Savoia, D. *et al., J.O.C.*, 1978, **43**, 2907 (*synth*)
Whitten, W.K. *et al., J. Chem. Ecol.*, 1980, **6**, 49
McKenzie, T.C. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 435 (*synth*)
Kim, J.H. *et al., J. Nat. Prod.*, 1989, **52**, 63 (*biosynth*)
Micha, S.H. *et al., Eur. J. Entomol.*, 1993, **90**, 439
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 507
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1771-1772
Mir, N.A. *et al., J. Agric. Food Chem.*, 1999, **47**, 7-11 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKK000

2-Methylhexacosane, 9CI M-471

[1561-02-0]
Isoheptacosane
$H_3C(CH_2)_{23}CH(CH_3)_2$
$C_{27}H_{56}$ 380.739
Isol. from hop oil (*Humulus lupulus*) and orange oil (*Citrus sinensis*). Cryst. (EtOAc). Mp 49-50.5°.

Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807 (*isol*)
Streibl, M. *et al., Fette, Seifen, Anstrichm.*, 1968, **70**, 543 (*synth*)
Tsuda, Y. *et al., Phytochemistry*, 1981, **20**, 505 (*isol, synth*)

25-Methyl-1-hexacosanol M-472

[75382-95-5]
$(H_3C)_2CH(CH_2)_{23}CH_2OH$
$C_{27}H_{56}O$ 396.739
Isol. from hazelnut oil.

Garcia Olmeda, R. *et al., CA*, 1980, **93**, 20285lj (*isol*)
Bradshaw, S.A. *et al., CA*, 1991, **115**, 1578445v (*isol*)

11-Methylhexadecanoic acid, 9CI M-473

[17001-25-1]
11-Methylpalmitic acid
$H_3C(CH_2)_4CH(CH_3)(CH_2)_9COOH$
$C_{17}H_{34}O_2$ 270.454

(±)-*form*
Constit. of butter fat. Cryst. (Me_2CO). Mp 18.5-19°. $Bp_{0.4}$ 187-188°.

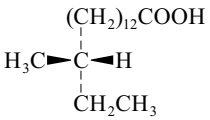
Et ester:
$C_{19}H_{38}O_2$ 298.508
Liq. $Bp_{0.7}$ 160°.

Amide:
$C_{17}H_{35}NO$ 269.47
Cryst. (EtOAc). Mp 71-71.5°.

Weitzel, G. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1951, **287**, 65; **288**, 189 (*synth*)
Ryhage, R. *et al., J. Dairy Res.*, 1967, **34**, 115 (*chromatog, ms*)
Dobner, B. *et al., Z. Chem.*, 1987, **27**, 63 (*synth*)
Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630 (*isol*)

14-Methylhexadecanoic acid, 9CI M-474

[5918-29-6]
14-Methylpalmitic acid



(*S*)-*form*

$C_{17}H_{34}O_2$ 270.454

(*S*)-*form* [5746-59-8]
Occurs in several animal fats. Mp 39.5-40°. $[\alpha]_D^{29}$ +5.2 (c, 14 in Me_2CO).

Me ester:
$C_{18}H_{36}O_2$ 284.481
Liq. Bp_2 156.5°. $[\alpha]_D^{27}$ +4.49.

Anilide:
$C_{23}H_{39}NO$ 345.567
Cryst. Mp 61.3-61.6°.

(±)-*form* [73641-04-0]
Cryst. (Me_2CO). Mp 39-40°.

Me ester: [2490-49-5]
Liq. $Bp_{1.8}$ 156°.

Et ester:
$C_{19}H_{38}O_2$ 298.508
Liq. Bp_2 169-174°.

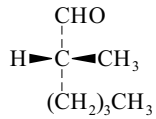
Amide:
$C_{17}H_{35}NO$ 269.47
Mp 89-90°.

[73641-07-3]

Velick, S.F. *et al., J. Biol. Chem.*, 1945, **160**, 473 (*synth, resoln, derivs*)
Velick, S.F. *et al., J.A.C.S.*, 1947, **69**, 2321 (*cryst struct*)
Sobotka, H. *et al., J.A.C.S.*, 1950, **72**, 5139 (*ir*)
Cason, J. *et al., J.O.C.*, 1951, **16**, 1187 (*ester*)
Milburn, A.H. *et al., J.C.S.*, 1954, 3344 (*amide, anilide*)
Campbell, I.M. *et al., J. Lipid Res.*, 1969, **10**, 593 (*ms*)
Silvins, J.R. *et al., Chem. Phys. Lipids*, 1980, **26**, 67 (*synth*)
Wolff, R.L. *et al., Lipids*, 1997, **32**, 971-973 (*isol, occur*)

2-Methylhexanal, 9CI M-475

[925-54-2]



(*R*)-*form*

$C_7H_{14}O$ 114.187

(*R*)-*form* [132151-88-3]
$[\alpha]_D^{25}$ -19.7 (c, 5.8 in $CHCl_3$) (99% ee).

(±)-*form* [72590-78-4]
Minor component of the essential oil of lemon balm, *Melissa officinalis*. Liq. Bp 141° Bp_{60} 132°.

2,4-Dinitrophenylhydrazone: [23546-53-4]
Solid. Mp 112-113.5° (122-126°).

Semicarbazone: [1070-43-5]
Solid. Mp 94.5-95.5°.

[66875-71-6]

Green, M.B. *et al., J.C.S.*, 1957, 3262 (*synth*)
Normant, H. *et al., Bull. Soc. Chim. Fr.*, 1959, 459 (*synth*)
Stork, G. *et al., J.A.C.S.*, 1963, **85**, 2178 (*synth*)
Vandenbroucke, W. *et al., J.C.S. Perkin 2*, 1972, 123 (*synth*)
Org. Synth., 1974, **54**, 46 (*synth*)
Skotnicki, J.S. *et al., J. Med. Chem.*, 1977, **20**, 1551 (*synth, ir, pmr*)
Goering, H.L. *et al., J.O.C.*, 1981, **46**, 5250 (*synth*)
Overman, L.E. *et al., J.A.C.S.*, 1984, **106**, 5360 (*synth, R-form*)
Nykanen, I. *et al., Dev. Food Sci.*, 1985, **10**, 329; *CA*, **103**, 121905c (*isol*)
Fox, D.N.A. *et al., J.A.C.S.*, 1991, **113**, 2652 (*synth, R-form*)
Goldstein, S.W. *et al., J.O.C.*, 1992, **57**, 1179 (*synth, pmr, R-form*)

5-Methyl-2,3-hexanedione, 9CI M-476

[13706-86-0]
Acetylisovaleryl. Isobutyl methyl diketone. Isobutylmethylglyoxal. FEMA 3190
$H_3CCOCOCH_2CH(CH_3)_2$
$C_7H_{12}O_2$ 128.171
Constit. of coffee and American potato chips. Flavour ingredient. Oil with oily-buttery odour and sweet taste. d_4^{22} 0.91. Bp 138°. n_D^{20} 1.4119.
▶ Skin irritant. MO3200000

2-Oxime: [20396-48-9]
$C_7H_{13}NO_2$ 143.185
Needles (EtOH aq.). Mp 64-65°.

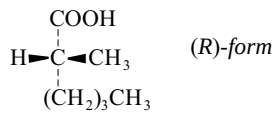
3-Oxime: [59303-00-3]
$C_7H_{13}NO_2$ 143.185
Leaflets. Mp 42°. Sublimes.

Dioxime: [71081-15-7] *Isobutylmethylglyoxime*
$C_7H_{14}N_2O_2$ 158.2
Leaflets (EtOH aq.). Mp 171-172°.

Hoy, K.L. *et al., J.O.C.*, 1958, **23**, 967 (*synth*)
Tischenko, I.G. *et al., CA*, 1960, **54**, 1286 (*synth*)
Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*isol*)
Coutrot, P. *et al., Synthesis*, 1975, 118 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKL300

2-Methylhexanoic acid, 9CI M-477

[4536-23-6]
2-Methylcaproic acid. Hexane-2-carboxylic acid. FEMA 3191



(*R*)-*form*

$C_7H_{14}O_2$ 130.186

(*R*)-*form* [51703-97-0]
Oil. Bp_5 105°. $[\alpha]_D^{20}$ -24.3 (neat). $[\alpha]_D^{20}$ -19.7 (c, 0.5 in CH_2Cl_2).

4-Nitrophenyl ester:
$Bp_{0.01}$ 138°. $[\alpha]_D$ -55 (heptane). $[\alpha]_D$ -148 (neat).

(*S*)-*form* [49642-51-5]
Oil. Bp_5 105°. $[\alpha]_D^{29}$ +19 (neat).

(±)-*form* [22160-12-9]
Flavouring ingredient. Oil. d_4^{20} 0.96. Bp 215-216° Bp_5 72°. n_D^{20} 1.4193. pK_a 5.04 (0.1*M* KCl).

Me ester: [2177-81-3]

[118628-17-4]
$C_8H_{16}O_2$ 144.213
Bp 159-160°.

Chloride: [41693-47-4]

[111555-10-3]
$C_7H_{13}ClO$ 148.632
Bp_9 45-48°.

Amide: [20923-63-1]
$C_7H_{15}NO$ 129.202
Needles (H_2O). Mp 70-72.5°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 763A (*nmr*)
Levering, D.R. *et al., J.O.C.*, 1958, **23**, 1836-1839 (*synth*)
Nicolaus, B.J.R. *et al., J.O.C.*, 1961, **26**, 1076-1084 (*synth*)
Creger, P.L. *et al., J.A.C.S.*, 1970, **92**, 1397-1398 (*synth*)
Meyers, A.I. *et al., J.A.C.S.*, 1976, **98**, 567-576 (*synth, abs config*)
Larcheveque, M. *et al., Tet. Lett.*, 1978, 3961-3964 (*synth*)
Baker, R. *et al., J.C.S. Perkin 1*, 1988, 85-97 (*R-form, synth*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1993, **65**, 155-163 (*cmr*)
Karl, V. *et al., Chirality*, 1994, **6**, 420-426 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 510
Uemura, T. *et al., J.O.C.*, 1996, **61**, 5510-5516 (*S-form, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1775

5-Methylhexanoic acid, 9CI M-478

[628-46-6]
Isoamylacetic acid. Isoheptanoic acid. 5-Methylcaproic acid. FEMA 3572
$(H_3C)_2CHCH_2CH_2CH_2COOH$
$C_7H_{14}O_2$ 130.186
Present in heated pork, strawberry and tea. Liq. with a fermented cheese odour. d^{19} 0.92. Bp 216°. n_D^{19} 1.4209.

S-*Benzylthiouronium salt:*
Cryst. (MeOH). Mp 149.5°.

Me ester: [2177-83-5]
$C_8H_{16}O_2$ 144.213
Isol. from hop oil (*Humulus lupulus*). Liq. d^{15} 0.88. Bp 166-167.5°. n_D 1.4214.

Et ester: [10236-10-9]
$C_9H_{18}O_2$ 158.24
Bp 181-182°.

Nitrile: [19424-34-1] *1-Cyano-4-methylpentane*
$C_7H_{13}N$ 111.186
Bp 178-180°.

Crombie, L. *et al., J.C.S.*, 1958, 4417-4435 (*synth*)
Goerner, G.L. *et al., J.O.C.*, 1959, **24**, 1561-1563 (*synth*)
Ritter, J.J. *et al., J.O.C.*, 1962, **27**, 622-623 (*synth*)
Larcheveque, M. *et al., Tet. Lett.*, 1975, 3851-3854 (*synth*)
Barabas, A. *et al., Tetrahedron*, 1978, **34**, 2191-2194 (*cmr*)
Yokoyama, M. *et al., Synthesis*, 1982, 591-592 (*nitrile, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 510
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1776

5-Methyl-2-hexanone, 9CI M-479

[110-12-3]
Isoamyl methyl ketone
$(H_3C)_2CHCH_2CH_2COCH_3$
$C_7H_{14}O$ 114.187
Volatile component in fruit pulp of papaya (*Carica papaya*), black tea aroma and in cooked beef and egg aroma. d^{17} 0.82. Bp 144°.

► Flammable. Eye and skin irritant (slight). LD_{50} (rat, orl) 4760 mg/kg. OES: long-term 50 ppm; short-term 75 ppm (current): short-term 100 ppm (Sk) (proposed). MP3850000

Oxime: [624-44-2]
$C_7H_{15}NO$ 129.202
Oil. Bp 195-196°.

► MP4025000

2,4-Dinitrophenylhydrazone:
Orange cryst. Mp 95°.

Semicarbazone:
Cryst. (EtOH). Mp 142-143°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 636A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 408C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 490D (*ir*)
Mick, W. *et al., J. Agric. Food Chem.*, 1984, **32**, 924 (*occur*)
Schreier, P. *et al., Z. Lebensm.-Unters. -Forsch.*, 1985, **180**, 297 (*occur*)
Coleman, W.M. *et al., Appl. Spectrosc.*, 1987, **41**, 1159 (*ir*)
Milovanovic, J.N. *et al., J.C.S. Perkin 2*, 1988, 533 (*synth*)
Jansen, J.F. *et al., Tet. Lett.*, 1988, **29**, 3593 (*synth*)
Umane, K. *et al., J. Agric. Food Chem.*, 1990, **38**, 461 (*occur*)
Marshall, A. *et al., J. Am. Soc. Mass Spectrom.*, 1991, **2**, 292 (*ms*)
Kennedy, G.L. *et al., Toxicol. Lett.*, 1991, **56**, 317 (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKW450; MKW500
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 845

5-Methyl-3-hexen-2-one, 9CI M-480

[5166-53-0]
Isobutylideneacetone. FEMA 3409
$H_3CCOCH{=}CHCH(CH_3)_2$
$C_7H_{12}O$ 112.171

► LD_{50} (rat, orl) 1680 mg/kg. LD_{50} (rbt, skn) 450 mg/kg. MP8750000

(*E*)-*form* [1821-29-0]
Flavouring ingredient. d^{22} 0.84. Bp_{50} 77.5°. n_D^{22} 1.4395. The (*Z*-)-form was erroneously reported in the earlier lit.(1930).

2,4-Dinitrophenylhydrazone:
Mp 170.5°.

Semicarbazone:
Mp 126°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 415A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 645C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 500C (*ir*)
Heilmann, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1956, **242**, 2008 (*synth*)
Sturtz, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 2477 (*synth*)
Sheikh, Y.M. *et al., Org. Mass Spectrom.*, (Suppl.), 1970, **4**, 273 (*ms*)
Karlsson, K. *et al., Acta Chem. Scand.*, 1972, **26**, 2837; 3839 (*occur*)
Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1975, 1363 (*synth*)
Jaxa-Chamiec, A.A. *et al., J.C.S. Perkin 1*, 1980, 170 (*synth*)
Grayson, D.H. *et al., J.C.S. Perkin 1*, 1986, 2137 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 512
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1778
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKM250

5-Methyl-5-hexen-2-one, 9CI M-481

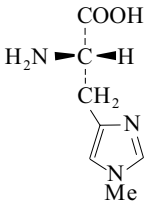
[3240-09-3]
4-Acetyl-2-methyl-1-butene. Methallylacetone. FEMA 3365
$H_2C{=}C(CH_3)CH_2CH_2COCH_3$
$C_7H_{12}O$ 112.171
Flavouring ingredient. d_{25}^{25} 0.85. Bp 148-149°. n_D^{25} 1.4279.

Semicarbazone: [14775-47-4]
Mp 136.5-137.5°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 646A (*nmr*)
Kimel, W. *et al., J.A.C.S.*, 1943, **65**, 1992 (*synth*)
Org. Synth., 1967, **47**, 87 (*synth*)
Rosini, G. *et al., Tetrahedron*, 1985, **41**, 4633 (*synth, ir, pmr*)
McKenzie, T.C. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 435 (*synth*)
Bloodworth, A.J. *et al., J.C.S. Perkin 1*, 1990, 2951 (*synth, pmr*)
Baeckström, P. *et al., J.O.C.*, 1991, **56**, 3358 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 513
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1779

1-Methylhistidine, 9CI M-482

2-Amino-3-(1-methyl-4-imidazolyl)propanoic acid. N^{τ}*-Methylhistidine. 3-Methylhistidine*†



$C_7H_{11}N_3O_2$ 169.183

Frequently referred to as 3-methylhistidine in biochemical papers due to the long-standing difference in the numbering of histidine.

(*S*)-*form* [332-80-9]

L-form

Protein metabolite; formed mainly by methylation of histidine residues in muscle actin and myosin. Urinary excretion levels used as an index of muscle protein breakdown. Plates (DMF aq.). Mp 248-250° dec. $[\alpha]_D^{20}$ -24.7 (c, 2.8 in H_2O). pK_{a2} 6.56; pK_{a3} 8.73 (25°, 0.1*M* KCl).

Hydrochloride:

Plates (DMF aq.). Mp 251-252° dec. $[\alpha]_D^{22}$ +6.9 (c, 2.0 in H_2O). $[\alpha]_D$ +9.4 (c, 2.0 in *M* HCl).

Hydrochloride (1:2): [69614-06-8]

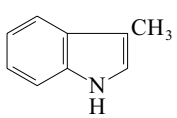
Prisms. Mp 258-259°. $[\alpha]_D^{20}$ +12.9 (c, 2 in *M* HCl).

Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2763 (*synth*)
Cocks, D.H. *et al., Nature (London)*, 1964, **202**, 184 (*isol*)
Anon, *et al., Eur. J. Biochem.*, 1972, **27**, 201-207 (*nomencl*)
Barlos, K. *et al., Annalen*, 1989, 387 (*synth*)
Betto, P. *et al., J. Chromatogr.*, 1992, **584**, 256-260 (*detm, hplc, use, bibl*)
Jain, R. *et al., Tetrahedron*, 1996, **52**, 5363-5370 (*synth, pmr*)
Dunnett, M. *et al., J. Chromatogr., B: Biomed. Appl.*, 1997, **688**, 47-55 (*hplc*)
Garlick, P.J. *et al., J. Nutr.*, Suppl. 2, 1998, **128**, 3565-3595 (*rev*)
Colombani, P.C. *et al., Int. J. Sport Nutr.*, 1999, **9**, 181-201 (*biochem*)

3-Methyl-1*H*-indole, 9CI M-483

[83-34-1]

β-Methylindole. Scatole. Skatole. FEMA 3019



C_9H_9N 131.177

A major contributor to boar taint in meat products from uncastrated male pigs. Flavouring ingredient. Leaflets (petrol) with faecal odour at high levels becoming warm and fruity at low concns. Mp 95°. Bp_{755} 265-266°. pK_{a1} -4.55; pK_{a2} 16.6 (25°,acid, KOH aq.).

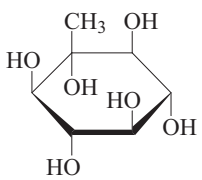
► LD_{50} (rat, orl) 3450 mg/kg. Exp. pneumotoxic and splenotoxic. Ruminants are particularly sensitive. NM0350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 653D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 122A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1497D (*ir*)
Fischer, E. *et al., Annalen*, 1886, **236**, 126 (*synth*)
Andrisano, R. *et al., Gazz. Chim. Ital.*, 1957, **87**, 949 (*uv*)
Stowe, B.B. *et al., Prog. Chem. Org. Nat. Prod.*, 1959, **17**, 254 (*occur*)
Safe, S. *et al., Org. Mass Spectrom.*, 1972, **6**, 33 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 863 (*rev, tox*)
Ito, Y. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 73 (*synth*)
Carlson, J.R. *et al., J. Toxicol., Toxin Rev.*, 1986, **5**, 217 (*rev*)
Yost, G.S. *et al., Chem. Res. Toxicol.*, 1989, **2**, 273 (*tox, rev*)
Tsuji, Y. *et al., J.O.C.*, 1990, **55**, 580 (*synth, pmr, cmr*)
Bray, T.M. *et al., Annu. Rev. Pharmacol. Toxicol.*, 1994, **34**, 91 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 726
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2513-2514
Baek, C. *et al., J. Agric. Food Chem.*, 1997, **45**, 2332-2340 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MKV750

1-*C*-Methyl-*scyllo*-inositol M-484

[564-92-1]

Mytilitol



$C_7H_{14}O_6$ 194.184

Isol. from blue mussels. Cryst. (H_2O). Mp 266-268°.

Hexa-Ac:

$C_{19}H_{26}O_{12}$ 446.407

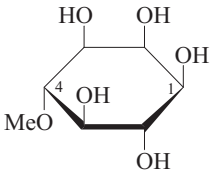
Mp 186-188°.

Posternak, T. *et al., Helv. Chim. Acta*, 1944, **27**, 457-468 (*synth*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1957, **11**, 506-511 (*isol*)
Angyal, S.J. *et al., Aust. J. Chem.*, 1974, **27**, 1075-1086 (*pmr*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 1633-1640 (*synth*)

4-*O*-Methyl-*myo*-inositol M-485

[484-69-5]

Ononitol



D-*form*

$C_7H_{14}O_6$ 194.184

D-*form* [6090-97-7]

Isol. from *Vigna catjang and Medicago sativa* (alfalfa). Mp 167-168°. $[\alpha]_D^{23}$ +5.5 (c, 11.2 in H_2O).

*Penta-Ac:1,2,3,5,6-Penta-*O*-acetyl-4-O-methyl-*myo*-inositol*

$C_{17}H_{24}O_{11}$ 404.37

Mp 121°. $[\alpha]_D^{23}$ -11.1 (c, 0.8 in $CHCl_3$).

L-*form* [166734-75-4] *6-O-Methyl-D-*myo*-inositol, 9CI. 1-O-Methyl-L-*myo*-inositol*

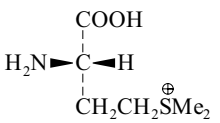
Mp 168-169°. $[\alpha]_D$ -5.7 (c, 2.0 in H_2O).

Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci.*, 1955, **241**, 983-985 (*isol*)
Post, G.G. *et al., J.A.C.S.*, 1962, **84**, 478-480 (*synth, D-form*)
Kindl, H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1966, **345**, 257 (*biosynth*)
Pietrusiewicz, K.M. *et al., Synth. Commun.*, 1995, **25**, 1863-1867 (*synth, D-form, L-form*)

S-Methylmethionine M-486

[13065-25-3]

(3-Amino-3-carboxypropyl)dimethylsulfonium(1+), 9CI, 8CI



$C_6H_{14}NO_2S^{\oplus}$ 164.248

(*S*)-*form* [6708-35-6]

Isol. from cabbage leaves and other fruits and vegetables.

Chloride: [1115-84-0] S-*Methylmethionyl chloride.* ***Vitamin U****. Cabagin U. Epadyn U. Vitas U. MMSC*

$C_6H_{14}ClNO_2S$ 199.701

Vitamin. Mp 139° dec.

► WR7440000

Bromide: [33515-32-1] *Ardesyl*

$C_6H_{14}BrNO_2S$ 244.152

Needles. Mp 134° dec.

(±)-*form* [44901-24-8]

Chloride: [3493-12-7] *FEMA 3445*

Flavouring ingredient for fish products. Cryst. (MeOH aq.). Mp 137-138°.

Iodide: [34236-06-1]

$C_6H_{14}INO_2S$ 291.153

Plates (Me_2CO/MeOH aq.). Mp 156-157°.

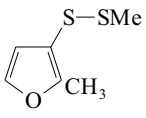
[2766-51-0, 3493-10-5, 3493-11-6, 3493-12-7, 4727-40-6, 7329-84-2, 27347-80-4, 41844-44-4, 63889-27-0, 71267-08-8]

Szabo, Z. *et al., Arzneim.-Forsch.*, 1960, **10**, 123
Fr. Pat., 1965, 1 394 705; *CA*, **63**, 8482 (*synth*)
Klee, W.A. *et al., Biochemistry*, 1967, **6**, 988 (*conformn*)
Ger. Pat., 1967, 1 239 697; *CA*, **67**, 73866 (*synth*)
Bukin, V.N. *et al., CA*, 1974, **80**, 48355; 56501 (*synth, rev, props*)
Del Re, G. *et al., Acta Cryst. B*, 1977, **33**, 3289 (*cryst struct*)

Harina, B.M. *et al., J.A.C.S.*, 1978, **100**, 4897 (*cmr*)
Lever, O.W. *et al., J. Pharm. Sci.*, 1984, **73**, 1241 (*synth*)
Baldwin, J.E. *et al., Tet. Lett.*, 1987, **28**, 3605 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 34
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 127-128 (*chloride*)

2-Methyl-3-(methyldithio)furan, 9CI M-487

[65505-17-1]
Methyl 2-methyl-3-furanyl disulfide. FEMA 3573



$C_6H_8OS_2$ 160.261
Occurs in coffee and whisky aroma. Also reported in hydrogenated vegetable oil. Flavour ingredient. Liq. with roast meat odour. d_4^{20} 1.2. Bp_{36} 37°. n_D^{20} 1.5718.
▶ JO1975000

Huber, U.A. *et al., Helv. Chim. Acta*, 1993, **76**, 2528
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 524 (*props, use*)

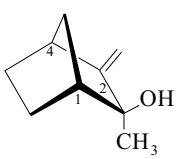
2-Methyl-2-(methyldithio)propanal, 9CI M-488

[67952-60-7]
2-(Methyldithio)isobutyraldehyde. FEMA 3866
MeS-S-C(CH_3)$_2$CHO
$C_5H_{10}OS_2$ 150.265
Meat-like flavouring for seasonings etc.. Liq. Bp_1 46°.

Blank, I. *et al., Dev. Food Sci.*, 1994, **35**, 271-276 (*glc, detn*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1158 (*use*)

2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol, 9CI M-489

2-Methyl-3-methylene-2-norbornanol

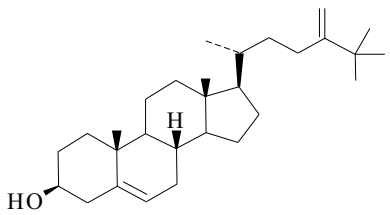


$C_9H_{14}O$ 138.209
(1*R,2*S**,4*S**)-*form*** [59300-40-2]
exo-*form*
Flavouring ingredient. Constit. from oil of the famine food *Santalum album* (sandalwood). Bp_{10} 70°. n_D^{20} 1.4975.

Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*synth*)

25-Methyl-24-methylenecholest-5-en-3-ol M-490

25-Methyl-5,24(28)-ergostadien-3-ol, 9CI

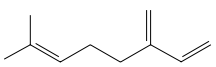


$C_{29}H_{48}O$ 412.698
3β-*form* [89702-24-9]
25-Methyl-24-methylenecholesterol
Constit. of seeds of Indian mustard (*Brassica juncea*), sunflower (*Helianthus annuus*) and French beans (*Phaseolus vulgaris*). Cryst. (EtOH). Mp 158.5-160°.

Matsumoto, T. *et al., Phytochemistry*, 1983, **22**, 2619; 1984, **23**, 921; 1988, **27**, 629; 3231 (*isol*)

7-Methyl-3-methylene-1,6-octadiene M-491

[123-35-3]
Myrcene. *β-Myrcene. FEMA 2762*

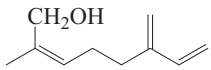


$C_{10}H_{16}$ 136.236
Found in many essential oils, e.g. hop oil. Flavouring agent. Oil. Bp 116° $Bp_{8.5}$ 51-51.5°. λ_{max} 226 (ϵ 16100) (MeOH) (Berdy).
▶ Skin and eye irritant. LD_{50} (rat, orl) >5000 mg/kg. RG5365000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 41B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 33A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 46C (*ir*)
Wrolstad, R.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 507 (*ir*)
Beckley, H.D. *et al., Org. Mass Spectrom.*, 1968, **1**, 47 (*ms*)
Waller, G.R. *et al., Phytochemistry*, 1968, **7**, 213 (*biosynth*)
Vig, O.P. *et al., Indian J. Chem.*, 1969, **7**, 450; 1975, **13**, 1244 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 32 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 615 (*rev, tox*)
Harris, R.K. *et al., Org. Magn. Reson.*, 1977, **9**, 483 (*pmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MRZ150
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

2-Methyl-6-methylene-2,7-octadien-1-ol, 9CI M-492

[57072-58-9]
8-Myrcenol



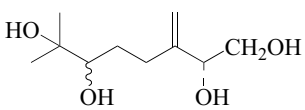
(*Z*)-*form*

$C_{10}H_{16}O$ 152.236
(*Z*)-*form* [38228-40-9]
Constit. of the essential oil of *Thymus vulgaris* (thyme). Isol. by glc λ_{max} 222 (ϵ 17000) (EtOH).
O-*(3-Phenylpropanoyl):* [139906-48-2]
$C_{19}H_{24}O_2$ 284.397
(ξ)-*form*
O-*β-D-Glucopyranoside:* [261915-20-2]
$C_{16}H_{26}O_6$ 314.378
Viscous oil. $[\alpha]_D$ -21.5 (c, 0.25 in MeOH).

Granger, R. *et al., Phytochemistry*, 1972, **11**, 2301-2305 (*isol, pmr*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1975, **52**, 161-163 (*synth*)
Zdero, C. *et al., Phytochemistry*, 1991, **30**, 3669-3677 (*3-phenylpropanoyl*)
Garg, S.N. *et al., Fitoterapia*, 1999, **70**, 472-474 (*glucoside*)

7-Methyl-3-methylene-1,2,6,7-octanetetrol M-493

3,7-Dimethyl-3(10)-octene-1,2,6,7-tetrol



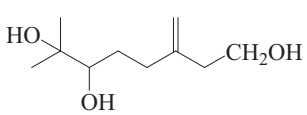
(2*R*,6ξ)-*form*

$C_{10}H_{20}O_4$ 204.266
(2*R*,6ξ)-*form*
2-O-*β-D-Glucopyranoside:* [219814-32-1]
$C_{16}H_{30}O_9$ 366.408
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{25}$ -51.4 (c, 0.3 in MeOH).
(2*S*,6ξ)-*form* [231281-06-4]
Syrup. $[\alpha]_D^{23}$ -25.3 (c, 0.3 in MeOH).
2-O-*β-D-Glucopyranoside:* [231281-05-3]
Needles (MeOH). Mp 69-70°. $[\alpha]_D^{25}$ -8.5 (c, 2 in MeOH).
(2*R,3*R**)-*form*** [152969-28-3]
(2*R,3*S**)-*form*** [152969-29-4]
(2ξ,6ξ)-*form* [217449-59-7]
Constit. of *Foeniculum vulgare* (fennel). Syrup. Mixt. of diastereoisomers.

Kitajima, J. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1667-1669; 1999, **47**, 639-642 (*isol, pmr, cmr*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1748-1751 (*isol, pmr, cmr*)
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 584-588 (*Glehnia littoralis constit*)

7-Methyl-3-methylene-1,6,7-octanetriol M-494

[240495-78-7]



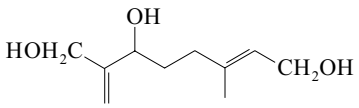
$C_{10}H_{20}O_3$ 188.266
Constit. of *Foeniculum vulgare* (fennel).

Amorph. powder. $[\alpha]_D^{23}$ -23 (c, 0.1 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 805-808 (*isol, pmr, cmr*)

6-Methyl-2-methylene-6-octene-1,3,8-triol M-495

[139051-31-3]

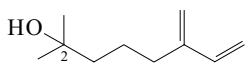


$C_{10}H_{18}O_3$ 186.25
Constit. of *Artemisia dracunculus* (tarragon).

Jakupovic, J. *et al., Planta Med.*, 1991, **57**, 450 (*isol, pmr*)

2-Methyl-6-methylene-7-octen-2-ol, 9CI M-496

[543-39-5]
Myrcenol



$C_{10}H_{18}O$ 154.252
Isol. from lavender oil and other plant oils. Liq. with lemon-like odour. Bp_{15} 105-106° Bp_5 78°. n_D^{20} 1.4731.

▶ Skin irritant. LD_{50} (rat, orl) 5300 mg/kg. RH3580000

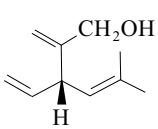
Ac: [1118-39-4] *7-Acetoxy-7-methyl-3-methylene-1-octene. Myrcenyl acetate*
Liq. with woody cologne-like odour. $Bp_{0.5}$ 53°.

▶ Skin irritant. LD_{50} (rat, orl) 6300 mg/kg. RH3585000

Houlihan, W.J. *et al., J.A.C.S.*, 1959, **81**, 4692-4694 (*struct, uv, ir*)
U.S. Pat., 1965, 3 176 022; *CA*, **62**, 16316 (*synth, uv, ir*)
Freeman, S.K. *et al., Appl. Spectrosc.*, 1969, **23**, 610-615 (*Raman*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1972, **49**, 163-166; 1973, **50**, 329-332 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 617 (*rev*)
Dorn, H. *et al., CA*, 1985, **103**, 119978k (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAW500; MLO250

5-Methyl-2-methylene-3-vinyl-4-hexen-1-ol M-497

3-Ethenyl-5-methyl-2-methylene-4-hexen-1-ol, 9CI. ***Neolyratol****. Lavendulol*



$C_{10}H_{16}O$ 152.236

(*S*)-*form* [90823-34-0]
Oil. $[\alpha]_D^{26}$ +78.7 (c, 1.6 in $CHCl_3$).

Ac: [79507-87-2]
$C_{12}H_{18}O_2$ 194.273
Constit. of *Artemisia vulgaris* (mugwort).

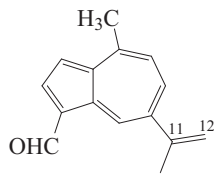
(ξ)-*form*

2-Methylbutanoyl: [86575-92-0]
$C_{15}H_{24}O_2$ 236.353
Oil. $[\alpha]_D^{24}$ +22.6 (c, 0.4 in $CHCl_3$).

Näf-Müller, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1424 (*Ac*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 2691-2697 (*isol, ester*)
Epstein, W.W. *et al., J.O.C.*, 1984, **49**, 2748

4-Methyl-7-(1-methylethenyl)-1-azulenecarboxaldehyde M-498

[85-33-6]
7-Isopropenyl-4-methyl-1-azulenecarboxaldehyde. 1-Formyl-7-isopropenyl-4-methylazulene. 1,3,5,7,9,11-Guaiahexaen-15-al. ***Lactaroviolin****. Delicial*



$C_{15}H_{14}O$ 210.275
Guaiane numbering shown. Constit. of mushroom *Lactarius deliciosus*. Violet-red cryst. (petrol). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. Mp 58°. λ_{max} 242 (ϵ 33900); 315 (ϵ 30900); 398 (ϵ 12600); 527 (ϵ 912) (EtOH) (Berdy).

15-Alcohol: [113393-59-2] *4-Methyl-7-(1-methylethenyl)-1-azulenemethanol, 9CI.* ***Deterrol***
$C_{15}H_{16}O$ 212.291
Isol. from the mushroom *Lactarius deterrimus*. Deep blue needles. Mp 100-101°. λ_{max} 239 (ϵ 21900); 290 (ϵ 46800); 370 (ϵ 7600) (EtOH).

15-Alcohol, octadecanoyl: [52898-98-3] *Deterrol stearate*
$C_{33}H_{50}O_2$ 478.757
Isol. from the mushrooms *Lactarius* spp..

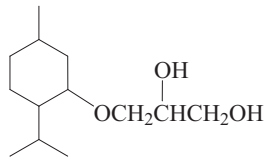
▶ Mutagenic.

11,12-Dihydro: [24687-70-5] ***11,12-Dihydrolactaroviolin****. 1-Formyl-7-isopropyl-4-methylazulene*
$C_{15}H_{16}O$ 212.291
Isol. from the mushroom *Lactarius deterrimus*. Cryst. Mp 59-60°.

Heilbronner, E. *et al., Helv. Chim. Acta*, 1954, **37**, 2018-2039 (*struct*)
Sörm, F. *et al., Coll. Czech. Chem. Comm.*, 1955, **20**, 227-240 (*struct*)
Meache, D. *et al., Helv. Chim. Acta*, 1967, **50**, 1178-1191 (*pmr*)
Koul, S.K. *et al., Phytochemistry*, 1985, **24**, 181-182 (*11,12-dihydro*)
Bergendorff, O. *et al., Phytochemistry*, 1988, **27**, 97-100 (*isol, uv, ir, pmr, cmr*)
Anke, H. *et al., Food Chem. Toxicol.*, 1989, **27**, 393-397 (*pharmacol*)

3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-1,2-propanediol, 9CI M-499

[87061-04-9]
3-Menthyloxy-1,2-propanediol



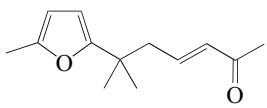
$C_{13}H_{26}O_3$ 230.347
Physiol. cooling agent used in food and beverages.

[165893-34-5, 193144-00-2, 207792-35-6]

Eur. Pat., 1983, 80 148; *CA*, **99**, 122707a (*synth*)
Erukulla, R.V. *et al., J.C.S. Perkin 1*, 1995, 2199-2100 (*synth*)
Japan. Pat., 1995, 07 82 200; *CA*, **123**, 286337v (*use*)

6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one M-500

[77822-40-3]



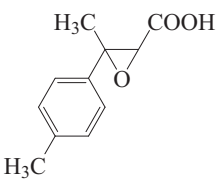
$C_{13}H_{18}O_2$ 206.284

(*E*)-*form* [77822-41-4]
Constit. of lavender, prunes, green and black tea and spinach leaves.

Naf, R. *et al., Flavour Fragrance J.*, 1997, **12**, 377-380 (*isol, synth*)

3-Methyl-3-(4-methylphenyl)oxiranecarboxylic acid, 9CI M-501

[60860-43-7]
Methyl-p-*tolylglycidic acid*



$C_{11}H_{12}O_3$

Et ester: [74367-97-8]

[36553-42-1, 36553-43-2] *FEMA 3757*
$C_{13}H_{16}O_3$ 220.268
Flavouring ingredient. Liq. with fruity odour. d_4^{20} 1.08. $Bp_{4.5}$ 135-140° (mixed isomers). n_D^{25} 1.5041. Fruity odour associated with the *cis*-isomer only. Mosandl incorr. describes the starting material for the synthesis as 4-methylbenzaldehyde.

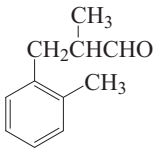
[60860-43-7]

Kulkarni, B.D. *et al., Synthesis*, 1976, 454-455 (*synth*)
Bansal, R.K. *et al., Gazz. Chim. Ital.*, 1980, **110**, 109-112 (*Et ester, synth, pmr, ms*)

Mosandl, A. *et al., Z. Lebensm.-Unters. - Forsch.*, 1983, **177**, 41-47 (*Et ester, props, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 255 (*use*)

2-Methyl-3-(2-methylphenyl)-propanal M-502

[57918-84-0]
α,2-Dimethylbenzenepropanal, 9CI



$C_{11}H_{14}O$ 162.231

(±)-*form*
Component of FEMA 2748 together with *m*- and *p*-isomers. Flavouring ingredient for baked goods, confectionery and non-alcoholic beverages. No phys. props. reported to *CA*, **135**.

Chalk, A.J. *et al., J.O.C.*, 1976, **41**, 1206-1209 (*synth*)
U.S. Pat., 1978, 4 070 374; *CA*, **86**, 120957q (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1253 (*use*)

2-Methyl-3-(4-methylphenyl)-propanal M-503

[41496-43-9]
*α,4-Dimethylbenzenepropanal, 9CI. α,4-Dimethylhydrocinnamaldehyde. 2-Methyl-3-(*p*-tolyl)propionaldehyde. FEMA 2748*

$C_{11}H_{14}O$ 162.231

(±)-*form*
Flavouring ingredient; coml. material FEMA 2748 contains some *ortho*- and a trace of *meta*-isomer. Bp_{10} 112-114° $Bp_{6.5}$ 108-109°.

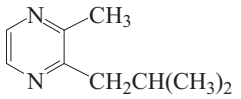
2,4-Dinitrophenylhydrazone:
Mp 73-74°.

Semicarbazone:
Mp 154°.

Terent'eva, I.V. *et al., Dokl. Akad. Nauk SSSR*, 1952, **86**, 555-558; *CA*, **48**, 615a (*synth*)
Scriabine, I. *et al., Bull. Soc. Chim. Fr.*, 1961, 1194-1198 (*synth*)
Ger. Pat., 1979, 2 851 024; 1994, 4 236 887; *CA*, **91**, 107808a; **121**, 82711m (*synth, use*)
Virgilio, J.A. *et al., Org. Prep. Proced. Int.*, 1982, **14**, 9-20 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 578
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1876-1877

2-Methyl-3-(2-methylpropyl)-pyrazine, 9CI M-504

[13925-06-9]
2-Isobutyl-3-methylpyrazine, 8CI. FEMA 3133



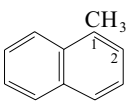
$C_9H_{14}N_2$ 150.223
Present in seed oils of red pepper and pumpkin. Also present in coffee aroma and baked or chipped potatoes. Flavouring ingredient. Bp_{10} 74°.

Flament, I. *et al., Helv. Chim. Acta*, 1967, **50**, 694-705 (*isol, synth, ms*)
Takken, H.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 638-642 (*props, occur*)
U.S. Pat., 1976, 3 989 713; *CA*, **86**, 43556d (*synth, use*)
Stofberg, J. *et al., Perfum. Flavor.*, 1984, **9**, 53-56; 58-59; 62; 65-72; 78-83 (*use*)
Buchbauer, G. *et al., Ernaehrung (Vienna)*, 1998, **22**, 246-249 (*detn, pumpkin oil*)
Jung, M.Y. *et al., J. Agric. Food Chem.*, 1999, **47**, 1700-1704 (*detn, pepper oil*)

1-Methylnaphthalene, 9CI, 8CI M-505

[90-12-0]

[1321-94-4]
FEMA 3193



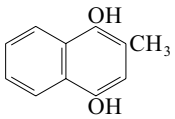
$C_{11}H_{10}$ 142.2
Flavouring ingredient. Oil with an earthy, phenolic odour. d^{20} 1.02. Fp -22. Bp 244° (241°) Bp_{12} 110°. n_D^{20} 1.6174.
▶ Fl. p. 82°, autoignition temp. 529°. LD_{50} (rat, orl) 1840 mg/kg. QJ9630000

Picrate:
Orange-red cryst. (EtOH). Mp 141-142°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 956B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 41A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 877D (*ir*)
Ger. Pat., 1927, 509 149; *CA*, **25**, 711 (*synth*)
Gilman, H. *et al., J.A.C.S.*, 1940, **62**, 1843 (*synth*)
Adv. Chem. Ser., 1955, **15**, 204 (***props***)
Hahn, R.C. *et al., J.A.C.S.*, 1969, **91**, 3558 (*uv*)
Poponova, R.V. *et al., Zh. Org. Khim.*, 1971, **7**, 2032 (*ms*)
Wilson, N.K. *et al., J. Magn. Reson.*, 1974, **15**, 31 (*nmr*)
Seita, J. *et al., Org. Magn. Reson.*, 1978, **11**, 239 (*cmr*)
Frycka, J. *et al., J. Chromatogr.*, 1979, **170**, 459 (*glc*)
Dowdy, D. *et al., Chem. Ind. (London)*, 1985, 338 (*purifn*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 529
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1804-1805
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3344
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MMB750

2-Methyl-1,4-naphthalenediol, 9CI, 8CI M-506

[481-85-6]
*1,4-Dihydroxy-2-methylnaphthalene. 2-Methyl-1,4-naphthoquinol. **Menadiol, BAN**. Protrombrovit*



$C_{11}H_{10}O_2$ 174.199
Cryst. (AcOH or toluene). Mp 177-178° (160°). Easily oxid. to 2-Methyl-1,4-naphthoquinone, M-508.
▶ QJ5075000

Bis(dihydrogen phosphate): [84-98-0]
$C_{11}H_{12}O_8P_2$ 334.158
Prothrombogenic vitamin. Cryst.

Bis(dihydrogen phosphate), tetra-Na salt: [131-13-5]

[6700-42-1] *Menadiol sodium diphosphate. Kappadione. Synkayvite*
Listed in the EAFUS Food Additive Database (Jan. 2001) but with no reported uses. Hexahydrate.

▶ LD_{50} (rat, ipr) 231 mg/kg. QJ5150000

Di-O-sulfate: [29520-22-7] *Menadiol disulfate. Menadiol sodium sulfate, INN*
$C_{11}H_{10}O_8S_2$ 334.327
Synthetic vitamin K analogue; prothrombogenic agent.

Di-O-sulfate, di-K salt: [1612-30-2] *Potassium menaphthosulfate, BAN. Menadiol potassium sulfate, INN. Vikastab*
Vitamin K analogue.

1-Ac: [2211-27-0]
$C_{13}H_{12}O_3$ 216.236
Mp 122-123°.

Di-Ac: [573-20-6] ***Acetomenaphthone, BAN**. Acetomenadione. Menadiol diacetate. Kapilin. Kappaxan. Kayvite. Vitamin K_4. Many other names*
$C_{15}H_{14}O_4$ 258.273
Synthetic vitamin. Cryst. (EtOH or AcOH). Mp 113°. Log P 2.68 (calc).
▶ QJ5250000

Dibutanoyl: [53370-44-8] ***Menadiol dibutyrate**. Karan. Karanum*
$C_{19}H_{22}O_4$ 314.38
Prothrombogenic vitamin. Mp *ca.* ° 53. Log P 4.8 (calc).
▶ LD_{50} (mus, orl) 12 g/kg. QJ5255000

Bis(3-carboxypropanoyl): [60539-13-1] ***Menadiol disuccinate**. Kapathrom*
$C_{19}H_{18}O_8$ 374.346
Prothrombogenic vitamin. Cryst. (EtOH aq.). Mp 177°. Log P 2.02 (calc).

*Bis(x-sulfobenzoyl):**Menadiol bissulfobenzoate**. K-Thrombyl inj.*
$C_{25}H_{18}O_{10}S_2$ 542.543
Prothrombogenic vitamin.

*1-(Trimethylammonioacetyl):**Menadiol trimethylammonioacetate**. Hemodal (T)*
$C_{16}H_{20}NO_5^{\oplus}$ 274.339Marketed as chloride.

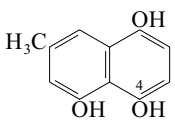
Di-Me ether:1,4-Dimethoxy-2-methylnaphthalene
$C_{13}H_{14}O_2$ 202.252

Bp_{14} 170-171°.

Fries, K. *et al., Ber.*, 1921, **54**, 2912 (*synth*)
Sah, P.P.T. *et al., Ber.*, 1940, **73**, 762; *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1940, **59**, 461 (*Acetomenadione*)
Fieser, L.F. *et al., J.A.C.S.*, 1940, **62**, 228 (*synth*)
Ger. Pat., 1943, 734 220, (*E Merck*); *CA*, **38**, 1252 (*Dibutyrate*)
Buu-Hoi, Ng.Ph. *et al., J.C.S.*, 1956, 1743 (*synth*)
Su, Y.-Z. *et al., Cancer Treat. Rep.*, 1987, **71**, 619 (*pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 3512
Dikow, A. *et al., Histochemistry*, 1990, **94**, 217 (*phosphate, synth, use*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1393
Fiorentini, D. *et al., Free Radical Res.*, 1997, **26**, 419
Ciuffreda, P. *et al., Tetrahedron*, 2000, **56**, 317-321 (*1-Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MMC250

7-Methyl-1,4,5-naphthalenetriol M-507

[60548-88-1]
1,5,8-Trihydroxy-3-methylnaphthalene



$C_{11}H_{10}O_3$ 190.198
Mp 112-113°.

4-O-β-D-Glucopyranoside: [29868-44-8]
Rossoliside
$C_{17}H_{20}O_8$ 352.34
Beige powder.

4-O-[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{22}H_{28}O_{12}$ 484.456
Isol. from callus cultures of *Diospyros kaki* (Japanese persimmon). Off-white powder. $[\alpha]_D^{17}$ -128.5 (c, 0.4 in DMSO).

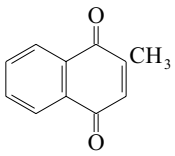
Tri-Ac: [33471-51-1]
$C_{17}H_{16}O_6$ 316.31
Cryst. ($CHCl_3$/MeOH). Mp 175.5-176.5°.

Tri-Me ether:1,4,5-Trimethoxy-7-methylnaphthalene
$C_{14}H_{16}O_3$ 232.279
Needles or plates (petrol). Mp 112-113°.

Cooke, R.G. *et al., Aust. J. Chem.*, 1952, **5**, 760; 1953, **6**, 53 (*isol*)
Laatsch, H. *et al., Annalen*, 1980, 1321 (*synth, derivs*)
Brockmann, H. *et al., Annalen*, 1983, 433 (*synth*)
Budzianowski, J. *et al., Phytochemistry*, 1995, **40**, 1145 (*Rossoliside*)
Gondo, M. *et al., Phytochemistry*, 1999, **51**, 879-881 (*4-xylosylglucoside*)

2-Methyl-1,4-naphthoquinone M-508

[58-27-5]
*2-Methyl-1,4-naphthalenedione, 9CI. **Menadione, BAN, USAN**. Vitamin K_3. Kanone. Kappaxin. Kayquinone. Thyloquinone. Many other names*



$C_{11}H_8O_2$ 172.183
Prothrombogenic vitamin (synthetic). Bright yellow cryst. (petrol, AcOH aq. or EtOH). Insol. H_2O; spar. sol. EtOH. Mp 104-105°. Log P 2.19 (calc). Dec. in light. Steam-volatile.

▶ Skin and respiratory tract irritant. Alcoholic soln. has vesicant props. LD_{50} (mus, orl) 500 mg/kg. LD_{50} (mus, ipr) 125 mg/kg. Exp. teratogenic effects. QL9100000

4-Oxime:
$C_{11}H_9NO_2$ 187.198
Platelets (EtOH). Mp 165-170° dec.

Dioxime:
$C_{11}H_{10}N_2O_2$ 202.212
Mp 166-168°.

[6147-37-1]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 85B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 79C (*ir*)
Fieser, L.F. *et al., J. Biol. Chem.*, 1940, **133**, 391 (*synth*)
Moore, M.B. *et al., J.A.C.S.*, 1941, **63**, 2049 (*synth*)
Gaertner, R. *et al., J.A.C.S.*, 1954, **76**, 6150 (*synth*)
Hahn, I. *et al., Pharmazie*, 1956, **11**, 91 (*pharmacol*)
Weygand, F. *et al., Chem. Ber.*, 1957, **90**, 1879 (*synth*)
Tanaka, T. *et al., Pharm. Bull.*, 1957, **5**, 82 (*synth*)
Rappoport, H. *et al., J.A.C.S.*, 1966, **88**, 1226 (*ms*)
Kim, J.Y. *et al., Tet. Lett.*, 1972, 3079
Konishi, T. *et al., Chem. Pharm. Bull.*, 1973, **21**, 220 (*metab*)
Kobayashi, M. *et al., Tet. Lett.*, 1976, 619 (*nmr*)
Altinkurt, O. *et al., Arzneim.-Forsch.*, 1980, **30**, 41; 286 (*activity*)
Torii, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1673 (*synth*)
Rohtagi, B.K. *et al., J. Nat. Prod.*, 1984, **47**, 901 (*isol*)
Rao, A.V.R. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 233 (*synth*)
Meyerson, M.L. *et al., Spectrochim. Acta A*, 1985, **41**, 1263 (*ir*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3774 (*anal, bibl*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1813
Ashnagar, A. *et al., J.C.S. Perkin 1*, 1988, 559 (*synth*)
Juan, C.C. *et al., Biochem. Biophys. Res. Commun.*, 1993, **190**, 907 (*pharmacol*)
Wu, F.Y.-H. *et al., Oncogene*, 1993, **8**, 2237 (*pharmacol*)
Adam, W. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 2475 (*synth*)
Hu, O.Y-P. *et al., J. Chromatogr., B: Biomed. Appl.*, 1995, **666**, 299 (*hplc*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1393
Villemin, D. *et al., Synth. Commun.*, 2002, **32**, 1501-1515 (*synth, uv, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MMD500

4-Methylnonacosane M-509

[125208-64-2]
$H_3C(CH_2)_{24}CH(CH_3)CH_2CH_2CH_3$
$C_{30}H_{62}$ 422.82
Constit. of *Papaver somniferum* (opium poppy). Mp 56°.

Bhakuni, R.S. *et al., J. Indian Chem. Soc.*, 1992, **69**, 889 (*isol*)

2-Methyl-3-nonacosanone M-510

[117596-98-2]
$H_3C(CH_2)_{25}COCH(CH_3)_2$
$C_{30}H_{60}O$ 436.803
Constit. of the seed coats of *Prunus amygdalus* (almond).

Joshi, B.C. *et al., Herba Pol.*, 1987, **33**, 163-166 (*isol*)

28-Methyl-27-nonacosenoic acid M-511

[194345-53-4]
$(H_3C)_2C{=}CH(CH_2)_{25}COOH$
$C_{30}H_{58}O_2$ 450.787
Constit. of *Piper retrofractum* (Javanese long pepper). Cryst. ($CHCl_3$/MeOH). Mp 104°.

Pande, A. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 377-379 (*isol, ir, pmr, ms*)

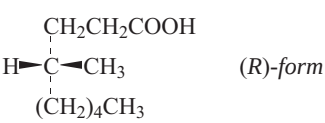
3-Methyl-2,4-nonanedione, 9CI M-512

[113486-29-6]
$H_3CCOCH(CH_3)CO(CH_2)_4CH_3$
$C_{10}H_{18}O_2$ 170.251
Exists as a 65:35 mixt. of keto and enol tautomers. The major contributor to light-induced flavour reversion in soybean oil and to off-flavour development in dried parsley and spinach. Present in green tea aroma. Oil. Odour variously descr. as lard-like, straw-like or fruity.

Masur, M. *et al., Org. Mass Spectrom.*, 1987, **22**, 493-500 (*ms*)
Mansanetz, C. *et al., Z. Lebensm.-Unters. -Forsch.*, 1988, **206**, 108-113; 114-120 (*occur, parsley, spinach*)
Guth, H. *et al., Fat Sci. Technol.*, 1989, **91**, 225-230 (*occur, soybean oil, ms, pmr, synth*)
Guth, H. *et al., Lebensm.-Wiss. Technol.*, 1990, **23**, 59-65; 513-522 (*occur, soybean oil*)
Guth, H. *et al., J. Am. Oil Chem. Soc.*, 1999, **76**, 145 (*bibl*)

4-Methylnonanoic acid, 9CI M-513

[45019-28-1]



(R)-form

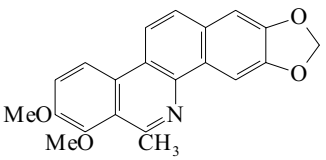
$C_{10}H_{20}O_2$ 172.267
(R)-form [124918-65-6]
$Bp_{0.25}$ 89°. $[\alpha]_D^{25}$ -1.34 (neat).
(±)-form [124842-68-8]
FEMA 3574
Found in cooked meats; flavouring ingredient. d^{20} 0.9. Bp_{70} 150°. n_D^{20} 1.4276.

[124918-66-7]

Weitzel, G. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1951, **287**, 65-89 (*synth*)
Canceill, J. *et al., Bull. Soc. Chim. Fr.*, 1975, 2066-2072 (*synth*)
Carpita, A. *et al., Gazz. Chim. Ital.*, 1989, **119**, 99-105 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 531
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1808
Anasaka, K. *et al., Tet. Lett.*, 1997, **38**, 6853-6856 (*resoln*)

8-Methylnorchelerythrine M-514

[154490-59-2]
1,2-Dimethoxy-13-methyl-[1,3]benzodioxolo[5,6-c]phenanthridine, 9CI



$C_{21}H_{17}NO_4$ 347.37
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Prisms ($CHCl_3$/MeOH). Mp 198-200°.

Chen, I.-S. *et al., J. Nat. Prod.*, 1994, **57**, 1206 (*isol, uv, ir, pmr, ms, struct*)

2-Methyloctacosane M-515

[1560-98-1]
$H_3C(CH_2)_{25}CH(CH_3)_2$
$C_{29}H_{60}$ 408.793
Present in hop and orange oil. Liq.

Mold, J.D. *et al., Biochemistry*, 1963, **2**, 605
Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1670
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807

16-Methyloctadecanoic acid, 9CI M-516

[17001-28-4]
16-Methylstearic acid. Anteisononadecanoic acid
$H_3CCH_2CH(CH_3)(CH_2)_{14}COOH$
$C_{19}H_{38}O_2$ 298.508

(±)-*form*
Mp 49.9-50.6°.

Me ester: [2490-16-6]
$C_{20}H_{40}O_2$ 312.535
$Bp_{1.2}$ 176°.

Amide:
$C_{19}H_{39}NO$ 297.523
Mp 93.2°.

(ξ)-*form*
Occurs in butterfat and Baltic salmon.

Me ester:

[59992-30-2, 73641-06-2]

Cason, J. *et al., J.A.C.S.*, 1944, **66**, 46
Abrahamsson, S. *et al., Acta Cryst.*, 1958, **11**, 270 (*cryst struct*)
Fischmeister, I. *et al., Ark. Kemi*, 1963, **20**, 353 (*ir*)
Silvius, J.R. *et al., Chem. Phys. Lipids*, 1980, **26**, 67
Jensen, N.J. *et al., Lipids*, 1986, **21**, 362 (*ms*)

17-Methyloctadecanoic acid, 9CI M-517

[2724-59-6]
17-Methylstearic acid. Isononadecanoic acid
$H_3CCH(CH_3)(CH_2)_{15}COOH$
$C_{19}H_{38}O_2$ 298.508

(±)-*form*
Mp 67.3-67.8°. $Bp_{0.3}$ 180°.

Me ester:
$C_{20}H_{40}O_2$ 312.535
Mp 26-27.5°. $Bp_{1.5}$ 171-172° (lit. gives a pressure range).

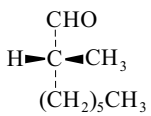
Amide:
$C_{19}H_{39}NO$ 297.523
Mp 100.2-101.3°.

(ξ)-*form*
Occurs in Baltic salmon.

Cason, J. *et al., J.A.C.S.*, 1942, **64**, 1106
Weitzel, G. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1951, **287**, 310 (*synth*)
Golovnya, R.V. *et al., Prikl. Biokhim. Mikrobiol.*, 1978, **14**, 609 (*ms*)

2-Methyloctanal, 9CI M-518

[7786-29-0]
FEMA 2727



(*R*)-*form*

$C_9H_{18}O$ 142.241
►Skin irritant. RG7914000

(*R*)-*form* [49642-49-1]
$[\alpha]_D$ +15.5 (neat).

(*S*)-*form* [55352-42-6]
$[\alpha]_D$ -12.6 (neat).

(±)-*form* [72598-55-1]
Flavouring ingredient. Oil. d 0.84. Bp_{20} 82-83°. n_D^{24} 1.4233.

Bott, K. *et al., Angew. Chem., Int. Ed.*, 1973, **12**, 851 (*synth*)
Botteghi, C. *et al., Tet. Lett.*, 1974, 4285 (*synth*)
Meyers, A.I. *et al., J.O.C.*, 1978, **43**, 892 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 533
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1811
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MNC175

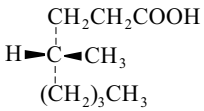
2-Methyloctane, 9CI M-519

[3221-61-2]
Isononane
$H_3C(CH_2)_5CH(CH_3)_2$
C_9H_{20} 128.257
Major constit. of oil of *Hypericum perforatum* (St. John's Wort). d_4^{20} 0.71. Mp -80.1°. Bp 142.8°. n_D^{20} 1.4029.
►Autoignition temp. 220°.

Whitmore, F. *et al., J.A.C.S.*, 1938, **60**, 2571 (*synth*)
Mathis, C. *et al., Phytochemistry*, 1964, **3**, 115; 133 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MNC250

4-Methyloctanoic acid, 9CI M-520

[54947-74-9]
4-Methylcaprylic acid. FEMA 3575



(*R*)-*form*

$C_9H_{18}O_2$ 158.24

(*R*)-*form*
Bp_{25} 166-172°. $[\alpha]_D$ -1.53 (c, 1.114 in $CHCl_3$) (*ca.* 95% ee).

(*S*)-*form*
$[\alpha]_D$ +1.45 (c, 1.106 in $CHCl_3$) (*ca.* 95% ee).

(±)-*form*
Flavouring ingredient. d^{20} 0.91. Bp_{10} 140-142° Bp_2 110.5-111.5°. n_D^{20} 1.4335.

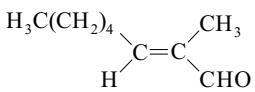
S-*Benzylthiouronium salt:*
Needles. Mp 135°.

Et ester: [56196-53-3]
$C_{11}H_{22}O_2$ 186.294
Bp_7 140° Bp_2 108°.

Levene, P.A. *et al., J.O.C.*, 1936, **1**, 76 (*abs config*)
Weitzel, G. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1951, **287**, 65 (*synth*)
Linstead, R.P. *et al., J.C.S.*, 1953, 1538 (*synth*)
Kenyon, J. *et al., J.C.S.*, 1953, 2129 (*synth*)
Wynberg, H. *et al., J.A.C.S.*, 1960, **82**, 1447 (*synth*)
Sonnet, P.E. *et al., Org. Prep. Proced. Int.*, 1990, **22**, 203 (*synth*)
Gries, G. *et al., Z. Naturforsch., C*, 1994, **49**, 363 (*Et ester, isol, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 534
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1812-1813
Pesticide Manual, 12th edn., 2000, No. 310 (*Et ester*)

2-Methyl-2-octenal M-521

[73757-27-4]
FEMA 1814



$C_9H_{16}O$ 140.225
Flavouring ingredient.

(*E*)-*form* [49576-57-0]
Bp_{14} 125° (Bp_{20} 98-101°).

Chamberlin, A.R. *et al., Synthesis*, 1979, 44 (*synth, pmr*)
Tamura, R. *et al., J.O.C.*, 1986, **51**, 4368 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 535
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1813-1814

7-Methyl-3-octen-2-one, 9CI M-522

[33046-81-0]
FEMA 3868
$(H_3C)_2CHCH_2CH_2CH{=}CHCOCH_3$

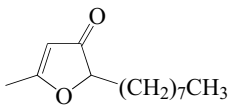
$C_9H_{16}O$ 140.225
Found in skimmed milk powder. Flavouring agent for a variety of foods, esp. for fried food taste. Bp_{10} 73-77°. Bp data is for a 7:3 mixt. of *E:Z*-isomers.

Liedtke, R.J. *et al., J.O.C.*, 1972, **37**, 776-789 (*ms*)
Pat. Coop. Treaty (WIPO), 1981, 81 00 802; *CA*, **95**, 113767k (*synth, use*)
U.S. Pat., 1982, 4 337 277; *CA*, **95**, 113767k (*use, synth, pmr*)
Shiratsuchi, H. *et al., J. Agric. Food Chem.*, 1994, **42**, 984-988 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1178 (*use*)

5-Methyl-2-octyl-3(2*H*)-furanone, 9CI M-523

[57877-72-2]

[59462-24-7]
Cepanone

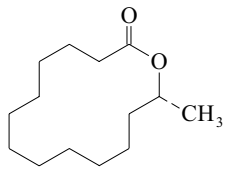


$C_{13}H_{22}O_2$ 210.316
Constit. of *Allium cepa* (shallot) flavour and other *Allium* spp..

Schreyen, L. *et al., J. Agric. Food Chem.*, 1976, **24**, 336-341; 1147-1152 (*isol*)
Galetto, W.G. *et al., J. Agric. Food Chem.*, 1976, **24**, 854-856 (*synth*)

14-Methyloxacyclotetradecan-2-one, 9CI M-524

[27198-63-6]
13-Tetradecanolide



(*R*)-*form*

$C_{14}H_{26}O_2$ 226.358
(*R*)-*form*
Constit. of *Ferula galbaniflua* (galbanum). Oil. $[\alpha]_D^{20}$ -38.2 (c, 2 in $CHCl_3$).
(*S*)-*form* [102849-50-3]
$[\alpha]_D^{22}$ +34 (c, 1.6 in $CHCl_3$).
(±)-*form*
Bp 5° 91.

Kaiser, R. *et al., Helv. Chim. Acta*, 1978, **61**, 2671 (*synth, isol, pmr, ms*)
Sims, R.J. *et al., Tet. Lett.*, 1983, **24**, 253 (*synth*)
Bestmann, H.J. *et al., Synthesis*, 1994, 1257 (*R-form, synth, pmr, cmr*)
Kraft, P. *et al., Annalen*, 1995, 1409 (*synth, ir, pmr, cmr, ms*)

11-Methyl-7-oxatetracyclo[6.3.1.0^{1,6}.0^{4,11}]dodecane M-525

[28344-11-8]
*Hexahydro-5*a*-methyl-3*H*-1,6:3,8*a*-dimethano-1*H*-cyclopent[*c*]oxepin, 8CI*

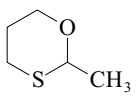


$C_{12}H_{18}O$ 178.274
Flavouring ingredient. Isol. from oil of the famine food *Santalum album* (sandalwood). Mp 178-180°.

Kretschmar, H.C. *et al., Tet. Lett.*, 1970, 37 (*isol, pmr, struct, synth*)
Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*isol*)

2-Methyl-1,3-oxathiane, 9CI M-526

[19134-37-3]



$C_5H_{10}OS$ 118.199
(±)-*form*
d_4^{20} 1.05. Bp_{24} 66-70° Bp_{16} 55-56°.
(ξ)-*form*
Constit. of the buds of Chinese chives (*Allium tuberosum*).

[59324-11-7, 107697-90-5, 107697-95-0, 109577-10-8]

Pagani, G. *et al., Gazz. Chim. Ital.*, 1967, **97**, 1770 (*synth*)
Pihlaja, K. *et al., Acta Chem. Scand.*, 1970, **24**, 2257 (*synth*)
Pihlaja, K. *et al., Org. Mass Spectrom.*, 1971, **5**, 763 (*ms*)
Pihlaja, K. *et al., Org. Magn. Reson.*, 1979, **12**, 331 (*pmr, conformn*)
Fuji, K. *et al., J.O.C.*, 1985, **50**, 657 (*synth, pmr*)
Deger, W. *et al., J. Chromatogr.*, 1986, **366**, 385 (*glc, resoln*)
Yi, Y. *et al., CA*, 1992, **117**, 86672 (*isol*)
Turyanskaya, A.M. *et al., Zh. Org. Khim.*, 1992, **28**, 79; *J. Org. Chem. USSR (Engl. Transl.)*, 1992, **28**, 65 (*pmr, cmr, conformn*)

Methyloxirane, 9CI M-527

[75-56-9]
Propylene oxide. 1,2-Epoxypropane



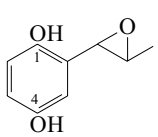
(*R*)-*form*

C_3H_6O 58.08
Etherification agent for food starch.
► Extremely flammable, fl. p. -37°, autoignition temp. 449°. Forms explosive mixtures with air. Eye, skin and respiratory tract irritant. Vesicant. Probable human carcinogen. LD_{50} (rat, orl) 380 mg/kg. Exp. carcinogen and teratogen. Exp. reprod. effects. ACGIH TLV: long-term 20 ppm. TZ2975000
(*R*)-*form* [15448-47-2]
Liq. Bp 36.5-38°. $[\alpha]_D^{25}$ +14 (c, 0.5 in Et_2O). $[\alpha]_D^{22}$ +18 (c, 5.73 in CCl_4).
(*S*)-*form* [16088-62-3]
Liq. Bp 35°. $[\alpha]_D^{24}$ -20.2 (c, 0.44 in CCl_4). $[\alpha]_D$ -16.6 (c, 5.69 in Et_2O).
(±)-*form* [16033-71-9]
Liq. Misc. H_2O, EtOH, Et_2O. d^0 0.86. Mp -111.9°. Bp 35°. n_D^{20} 1.3670. Vp 445 mmHg (25°).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 228B; 228C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 363B; 363C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 300D; 301A (*ir*)
Abderhalden, E. *et al., Ber.*, 1918, **51**, 1318 (*synth*)
Fickett, W. *et al., J.A.C.S.*, 1951, **73**, 5063 (*synth, abs config*)
Ghirardelli, R.G. *et al., J.A.C.S.*, 1973, **95**, 4987 (*synth*)
Golding, B.T. *et al., J.C.S. Perkin 1*, 1973, 1214 (*synth, glc*)
van der Sande, C.C. *et al., J.A.C.S.*, 1975, **97**, 4617
Davies, S.G. *et al., J.C.S. Perkin 2*, 1975, 861 (*cmr*)
Schurig, V. *et al., Angew. Chem., Int. Ed.*, 1978, 937 (*synth, abs config*)
Pirkle, W.H. *et al., J.O.C.*, 1978, **43**, 3803 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 246 (*rev*)
Pogany, G.A. *et al., Chem. Ind. (London)*, 1979, 16 (*handling*)
IARC Monog., 1985, **36**, 227; *Suppl.* 7, 328; *Suppl.* 6, 482 (*rev, tox*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 541 (*synth*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1986, **6**, 225
Simon, E.S. *et al., J.O.C.*, 1987, **52**, 4042 (*synth*)
Alkylene Oxides and Their Polymers; Surfactant Science Series, Vol. 35, (Eds. Bailey, F.E. *et al*), Dekker, New York, 1991,
Rossen, K. *et al., Synth. Commun.*, 1993, **23**, 1071 (***synth, enantiomers***)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4333-4336 (*use*)
Cotterill, A.S. *et al., J.C.S. Perkin 1*, 1995, 1215 (*synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2356-2357
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 426
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1151
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1077
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PNL600
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, II; 348 (*tox*)

2-(3-Methyl-2-oxiranyl)-1,4-benzenediol M-528

2-(1,2-Epoxypropyl)-1,4-benzenediol. 1-(2,5-Dihydroxyphenyl)-1,2-epoxypropane. 1-(2,5-Dihydroxyphenyl)-2-methyloxirane



$C_9H_{10}O_3$ 166.176

Diangeloyl: [159516-21-9]
$C_{19}H_{22}O_5$ 330.38
Cryst. (hexane). Mp 56°. $[\alpha]_D^{20}$ +0.1 (c, 9

in $CHCl_3$).

1-O-(2,3-Epoxy-2-methylbutanoyl), 4-angeloyl: [159390-96-2]
$C_{19}H_{22}O_6$ 346.379
Cryst. (hexane). Mp 74-75°. $[\alpha]_D^{20}$ +0.1 (c, 4.5 in $CHCl_3$).

4-Me ether, 1-O-(2-methylpropanoyl): [97164-70-0] *Epoxypseudoisoengenol isobutanoate*
$C_{14}H_{18}O_4$ 250.294
Oil. $[\alpha]_{436}^{23}$ +56 (c, 0.8 in $CHCl_3$). *trans*-Isomer.

4-Me ether, 1-O-(2-methylbutanoyl): [97180-28-4]

[125028-84-4, 263560-83-4] *Epoxypseudoisoeugenol 2-methylbutanoate.* ***Thellungianin G. EPB***
$C_{15}H_{20}O_4$ 264.321
Constit. of *Pimpinella anisum* (aniseed).

4-Me ether, 1-angeloyl: [101627-36-5]
$C_{15}H_{18}O_4$ 262.305
Oil. $[\alpha]_D^{20}$ +2.1 (c, 5.4 in $CHCl_3$).

4-Me ether, 1-O-tigloyl: [97164-71-1]

[115016-19-8, 115016-20-1]
$C_{15}H_{18}O_4$ 262.305

4-Me ether, 1-O-(2,3-epoxy-2-methylbutanoyl): [159390-97-3]
$C_{15}H_{18}O_5$ 278.304

[159516-20-8]

Martin, R. *et al., Planta Med.*, 1985, **51**, 198-202 (*isol, synth, pmr, cmr*)
Reichling, J. *et al., Z. Naturforsch., C*, 1985, **40**, 465-468 (*isol*)
Bottini, A.T. *et al., Phytochemistry*, 1986, **25**, 207-211 (*isol*)
Dev, V. *et al., J. Nat. Prod.*, 1987, **50**, 968-971 (*synth*)
Macias, M.J. *et al., Phytochemistry*, 1994, **37**, 539 (*isol, ir, pmr, cmr*)
Kemmerer, B. *et al., Phytochemistry*, 1996, **42**, 397-403 (*EPB, biosynth, synth*)

3-Methyl-2-oxobutanoic acid M-529

[759-05-7]
2-Oxoisopentanoic acid. α-Ketoisovaleric acid. Dimethylpyruvic acid. Ketovaline. FEMA 3869

$(H_3C)_2CHCOCOOH$

$C_5H_8O_3$ 116.116
Flavouring ingredient for use in butter-type flavours. Found in banana, bread, cheeses, asparagus, beer and cocoa. Cryst. Mp 31°. Bp 170.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 551B; 684C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 863B; 1095C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 741B (*ir*)
Bouveault, L. *et al., Bull. Soc. Chim. Fr.*, 1901, 1031 (*synth, derivs*)
Arfin, S.M. *et al., J. Biol. Chem.*, 1969, **244**, 2250 (*biosynth*)
Cooper, A.J.C. *et al., J. Biol. Chem.*, 1975, **250**, 527 (*pmr, bibl*)
Singh, J. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 501 (*synth*)
Hata, H. *et al., Synthesis*, 1991, 289 (*synth*)
Pat. Coop. Treaty (WIPO), 1996, 96 10 927; *CA*, **125**, 56856a (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1180 (*use*)

2-Methyl-6-oxo-2,4-heptadienoic acid M-530

$H_3CCOCH{=}CHCH{=}C(CH_3)COOH$

$C_8H_{10}O_3$ 154.165

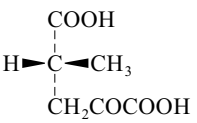
(2E,4E)-form

[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:
$C_{20}H_{30}O_{13}$ 478.449
Constit. of saffron (*Crocus sativus*).
λ_{max} 283 (MeOH) (per-Ac).

Straubinger, M. *et al., J. Agric. Food Chem.*, 1997, **45**, 1678-1681 (*isol, ester*)

2-Methyl-4-oxopentanedioic acid M-531

[55601-64-4]
2-Methyl-4-oxoglutaric acid



(R)-form

$C_6H_8O_5$ 160.126
Constit. of *Tamarindus indica* (tamarind). Config. not determined.

Di-Et ester: [107987-03-1]
Oil.

Di-Et ester, 2,4-dinitrophenylhydrazone: [14200-24-9]
Mp 75.5°.

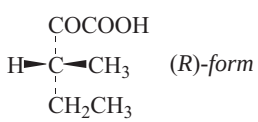
(R)-form [111768-22-0]

[42998-61-8, 97474-86-7]

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1955, **9**, 553 (*isol*)
Mukherjee, D. *et al., Biochem. Physiol. Pflanz.*, 1974, **166**, 429 (*isol*)
Righini-Tapie, A. *et al., J. Appl. Chem.*, 1984, **6**, 361 (*synth*)
Winter, H.C. *et al., Phytochemistry*, 1987, **26**, 2477 (*isol*)
Dowd, P. *et al., Tetrahedron*, 1988, **44**, 2137 (*synth, ester*)
Shono, T. *et al., J.O.C.*, 1990, **55**, 5037 (*synth, ester*)

3-Methyl-2-oxopentanoic acid, 9CI M-532

[1460-34-0]
3-Methyl-2-oxovaleric acid, 8CI. Ketoisoleucine. FEMA 3870



(R)-form

$C_6H_{10}O_3$ 130.143
Flavouring ingredient. Aroma constit. of cocoa, Fontina cheese and cooked white asparagus. Also present in beer, dough preferment and pumpkin sap.

(R)-form [61748-89-8]
$[\alpha]_D^{23}$ -36.3 (c, 1.0 in H_2O) (as Na salt).

Me ester: [3682-42-6] *FEMA 3713*
$C_7H_{12}O_3$ 144.17
Flavouring ingredient. Liq. $[\alpha]_D$ -20.5 (c, 4.9 in $CHCl_3$). n_D^{20} 1.4155. The FEMA number refers to material of unspecified stereochem..

(S)-form [24809-08-3]
$[\alpha]_D^{23}$ +34.1 (c, 1.0 in H_2O) (as Na salt).

Me ester: [91797-34-1]
Oil. $[\alpha]_D$ +25.5 (c, 4.0 in $CHCl_3$).

(±)-form [39748-49-7]
Flavouring ingredient for foods. Bp_{12} 75-80°.

Na salt: [66872-74-0]

[3715-31-9]
Mp 204-206°.

Rosculet, G. *et al., Proc. Am. Soc. Brew. Chem.*, 1969, 127-138 (*detn, beer*)
Armstrong, F.B. *et al., Biochim. Biophys. Acta*, 1977, **498**, 282-293 (*R-form, S-form*)
Ney, K.H. *et al., Fette, Seifen, Anstrichm.*, 1978, **80**, 249-251 (*Fontina cheese, detn*)
Ney, K.H. *et al., Gordian*, 1985, **85**, 90-92 (*occur, cocoa*)
Hata, H. *et al., Synthesis*, 1991, 289 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 537; 1182 (*Me ester, use*)
PCT Int. Appl., 1996, 9 610 927; *CA*, **125**, 56856a (*use*)
Podebrad, F. *et al., J. High Resol. Chromatogr.*, 1997, **20**, 355-362 (*anal*)
Hagelstein, P. *et al., J. Plant Physiol.*, 1997, **150**, 23-30 (*metab*)
Harding, J.R. *et al., J.C.S. Perkin 1*, 2000, 3406-3416 (*resoln, Me ester, synth, ir, pmr, cmr, ms*)
Ding, Z. *et al., CA*, **113**, 197732w (*Me ester, isol*)

4-Methyl-2-oxopentanoic acid, 9CI M-533

[816-66-0]
2-Oxoisocaproic acid. Isobutylglyoxylic acid. Isopropylpyruvic acid. Ketoisocaproic acid. Ketoleucine. KICA

$(H_3C)_2CHCH_2COCOOH$

$C_6H_{10}O_3$ 130.143
Found in bananas, asparagus, cheese, wine and cocoa. Constit. of *Trigonella caerulea* (sweet trefoil). Flavouring ingredient. Liq. Mp 10-11° (-1.5°). Bp_{15} 84-85°.

Na salt: [4502-00-5]
Solid. Mp 295-300° dec.

Oxime:
$C_6H_{11}NO_3$ 145.158
Cryst. (Et_2O). Mp 153-155°.

2,4-Dinitrophenylhydrazone:
Cryst. Mp 155-156°.

Semicarbazone:
Cryst. (EtOH aq.). Mp 205°.

Me ester: [3682-43-7]
$C_7H_{12}O_3$ 144.17
Liq. Bp_{11} 110°.

Amide:
$C_6H_{11}NO_2$ 129.158
Cryst. (C_6H_6). Mp 60°.

Nitrile: [66582-16-9]
C_6H_9NO 111.143
Bp 145-150°.

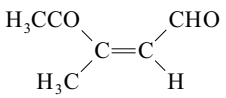
[51828-95-6, 63614-97-1, 98849-83-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 862B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1385C (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 816D (*ir*)
Collins, R.P. *et al., J. Nat. Prod.*, 1966, **29**, 245 (*isol*)
Poisel, H. *et al., Chem. Ber.*, 1978, **111**, 3136 (*synth*)
Nimitz, J.S. *et al., J.O.C.*, 1981, **46**, 211 (*synth*)
Ramage, R. *et al., J.C.S. Perkin 1*, 1984, 1531 (*synth, ir*)
Ney, K.H. *et al., Gordian*, 1986, **86**, 9; *CA*, **105**, 5347q (*isol*)
Kozlowski, R. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 75 (*synth*)
Blanchot, V. *et al., Synthesis*, 1990, 755 (*synth*)
PCT Int. Appl., 1996, 96 10 927; *CA*, **125**, 56856a (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1183

3-Methyl-4-oxo-2-pentenal M-534

3-Acetylcrotonaldehyde



$C_6H_8O_2$ 112.128

(*Z*)-*form* [58921-44-1]
Syoyualdehyde
Odoriferous constit. of soya. Bp_6 71-100°.

Nakajima, M. *et al., Nippon Kagaku Kaishi*, 1949, **70**, 47; *CA*, **45**, 7015
Rice, K.C. *et al., J. Het. Chem.*, 1975, **12**, 1325 (*synth, pmr*)

2-Methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid, 9CI M-535

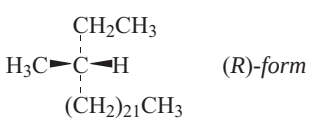
[15214-89-8]
2-Acrylamido-2-methyl-1-propanesulfonic acid, 8CI
$H_2C{=}CHCONHC(CH_3)_2CH_2SO_3H$
$C_7H_{13}NO_4S$ 207.25
FDA approved for use in polymer components of food-contact paper and board adhesives. Cryst. (MeOH). Mp 185.5-186°.

[5165-97-9]

U.S. Pat., 1970, 3 506 707; *CA*, **72**, 132053r (*synth*)
Salamone, J.C. *et al., J. Polym. Sci., Polym. Symp.*, 1978, **64**, 229-243 (*synth*)
Salamone, J.C. *et al., J. Polym. Sci., Polym. Lett. Ed.*, 1979, **15**, 487-491 (*synth*)
Food Chem. News, 2002, **43(47)**, 21 (*use*)

3-Methylpentacosane, 9CI M-536

[6902-54-1]



(R)-form

$C_{26}H_{54}$ 366.713

(*R*)-*form*
Cryst. (EtOH). Mp 36°. $[\alpha]_D^{24}$ -4.1 (c, 1 in $CHCl_3$).

(*S*)-*form*
Cryst. (EtOH). Mp 36°. $[\alpha]_D^{27}$ +4.2 (c, 1 in $CHCl_3$).

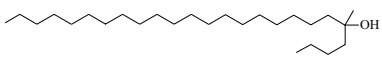
(ξ)-*form*
Isol. from hop oil (*Humulus lupulus*) and orange oil (*Citrus sinensis*). Bp 248-10°.

[55194-22-4]

Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807 (*isol*)
Streibl, M. *et al., Fette, Seifen, Anstrichm.*, 1968, **70**, 543; *CA*, **70**, 30318x (*synth*)

5-Methyl-5-pentacosanol, 9CI M-537

Grandiflorol



$C_{26}H_{54}O$ 382.712
Isol. from leaves of *Sesbania grandiflora* (agati). Mp 83-84°. $[\alpha]_D$ -20 ($CHCl_3$).

Tiwari, R.D. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1964, **297**, 310

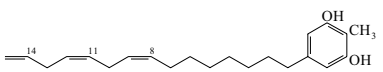
14-Methylpentadecanoic acid, 9CI M-538

[4669-02-7]
Isopalmitic acid
$(H_3C)_2CH(CH_2)_{12}COOH$
$C_{16}H_{32}O_2$ 256.428
Occurs in butterfat. Mp 61.8-62.4°.

Amide:
$C_{16}H_{33}NO$ 255.443
Mp 102°.

Fordyce, C.R. *et al., J.A.C.S.*, 1933, **55**, 3370 (*synth*)
Fujii, K. *et al., Eur. J. Biochem.*, 1970, **17**, 552 (*ms*)

2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-benzenediol M-539



$C_{22}H_{32}O_2$ 328.494

(*Z,Z*)-*form* [50423-15-9]
Constit. of cashew nut shell oil (*Anacardium occidentale*).

14,15-Dihydro: [50423-14-8] *2-Methyl-5-(8,11-pentadecadienyl)-1,3-benzenediol, 9CI*
$C_{22}H_{34}O_2$ 330.509
Isol. from *Anacardium occidentale* (cashew nut) shell oil.

11,12,14,15-Tetrahydro: [50423-13-7] *2-Methyl-5-(8-pentadecenyl)-1,3-benzenediol*
$C_{22}H_{36}O_2$ 332.525
Isol. from *Anacardium occidentale* (cashew nut) shell oil.

8,9,11,12,14,15-Hexahydro: See 2-Methyl-5-pentadecyl-1,3-benzenediol in *The Combined Chemical Dictionary.*

Tyman, J.H.P. *et al., J.C.S. Perkin 1*, 1973, 1639 (*isol, struct, synth, ir, pmr, ms*)
Tyman, J.H.P. *et al., Chem. Soc. Rev.*, 1979, **8**, 499
Kubo, I. *et al., J. Agric. Food Chem.*, 1986, **34**, 970 (*isol*)

14-Methyl-6-pentadecenoic acid M-540

[127486-79-7]
$(H_3C)_2CH(CH_2)_6CH{=}CH(CH_2)_4COOH$
$C_{16}H_{30}O_2$ 254.412

(*Z*)-*form* [123739-73-1]
Isol. from the freshwater mussel *Unio tumidus*.

Zimmerman, M.P. *et al., Lipids*, 1990, **25**, 383 (*isol*)
Harvey, D.J. *et al., Spectroscopy (Ottawa)*, 1990, **8**, 211 (*ms, struct*)
Stefanov, K. *et al., J. Nat. Prod.*, 1992, **55**, 979 (*isol, struct*)
Hassarajani, S.A. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 429 (*synth, ir, pmr*)

2-Methyl-3,4-pentadienoic acid M-541

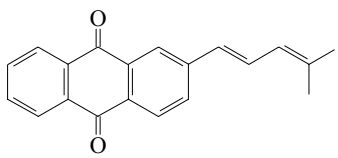
$H_2C{=}C{=}CHCH(CH_3)COOH$
$C_6H_8O_2$ 112.128

Et ester: [60523-21-9] *FEMA 3678*
$C_8H_{12}O_2$ 140.182
Flavouring ingredient. Liq. Bp_{43} 85°.

Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Kimura, M. *et al., Bull. Chem. Soc. Jpn.*, 1995, **68**, 1689-1705 (*Et ester, synth, pmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 249 (*use*)
Takeoka, G.R. *et al., Lebensm.-Wiss. Technol.*, 1998, **31**, 443-448 (*glc, props*)

2-(4-Methyl-1,3-pentadienyl)anthraquinone M-542

[150900-95-1]
2-(4-Methyl-1,3-pentadienyl)-9,10-anthracenedione, 9CI



$C_{20}H_{16}O_2$ 288.345
Isol. from the hairy root culture of *Sesamum indicum* (sesame). Oil.

1′,2′-Dihydro: [71308-16-2] *2-(4-Methyl-3-pentenyl)anthraquinone*
$C_{20}H_{18}O_2$ 290.361
Isol. from the hairy root culture of *Sesamum indicum* (sesame). Oil.

Japan. Pat., 1993, 93 238 981; *CA*, **120**, 86099 (*pmr, cmr, isol*)
Ogasawara, T. *et al., Phytochemistry*, 1993, **33**, 1095 (*isol, pmr, cmr*)

2-Methylpentanal, 9CI M-543

[123-15-9]
2-Methylvaleraldehyde. FEMA 3413
$H_3CCH_2CH_2CH(CH_3)CHO$
$C_6H_{12}O$ 100.16
▶ Highly flammable, fl.p. 17°, autoignition temp. 199°. YV4150000

(±)-*form*
Flavouring ingredient. Liq. with an ethereal fruity odour. Bp 116°. n_D^{20} 1.4120.

2,4-Dinitrophenylhydrazone:

Cryst. (AcOH). Mp 103°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 467C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 730A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 553C (*ir*)
Curphey, T.L. *et al., Chem. Comm.*, 1967, 510 (*synth*)
Pfeffer, P.E. *et al., Tet. Lett.*, 1970, 699 (*synth*)
Org. Synth., 1971, **51**, 39 (*synth*)
Ho, T.-L. *et al., Synth. Commun.*, 1974, **4**, 147 (*synth*)
Koster, R. *et al., Annalen*, 1976, 1116 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 537
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1818-1819
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 828

4-Methyl-2,3-pentanedione, 9CI M-544

[7493-58-5]
Acetylisobutyryl. Isopropyl methyl diketone. Isopropylmethylglyoxal. FEMA 2730
$H_3CCOCOCH(CH_3)_2$
$C_6H_{10}O_2$ 114.144
Flavouring ingredient. Present in beer, malt, krill and coffee. Yellow liq. with pungent odour. Spar. sol. H_2O. Bp 115-116°.

Dioxime: [4775-87-5] *Isopropylmethylglyoxime*
$C_6H_{12}N_2O_2$ 144.173
Needles (C_6H_6). Mp 155-158° (123-124°).

Disemicarbazone:
Mp 223° dec.

2,4-Dinitrophenylhydrazone:
Mp 115-117°.

Pauly, H. *et al., Ber.*, 1900, **33**, 503 (*synth*)
U.S. Pat., 1945, 2 393 593; *CA*, **40**, 2466 (*synth*)
Meister, H. *et al., Annalen*, 1969, **724**, 128 (*synth*)

4-Methylpentanethioic acid M-545

$(H_3C)_2CHCH_2CH_2COSH \Leftrightarrow (H_3C)_2CHCH_2CH_2C(S)OH$
$C_6H_{12}OS$ 132.226

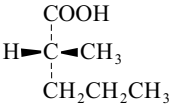
SH-form

Me ester: [61122-71-2] S-*Methyl 4-methylpentanethioate. FEMA 3867*
$C_7H_{14}OS$ 146.253
Found in fish oil, hop oil and beer. Flavouring agent. Pale yellow liq.

Pickett, J.A. *et al., Proc. Anal. Div. Chem. Soc.*, 1976, **13**, 215-217 (*S-Me ester, anal, occur, hop oil*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1160 (*S-Me ester, use*)

2-Methylpentanoic acid, 9CI M-546

[97-61-0]
2-Methylvaleric acid. FEMA 2754



(*R*)-*form*

$C_6H_{12}O_2$ 116.16
▶ Fl.p. 107° (oc), autoignition temp. 378°. Skin and eye irritant. LD_{50} (rat, orl) 2040 mg/kg. YV7700000

(*R*)-*form* [49642-47-9]
Bp_{15} 96°. $[\alpha]_D$ -18.4 (neat).

Et ester: [151526-65-7]
$C_8H_{16}O_2$ 144.213
Bp_4 78-80°. $[\alpha]_D^{25}$ -7.91.

Amide: [34241-21-9]
$C_6H_{13}NO$ 115.175
Mp 78°. $[\alpha]_D^{25}$ -5.79 (EtOH aq.).

Nitrile:2-Cyanopentane
$C_6H_{11}N$ 97.16
Bp_2 30-32°. $[\alpha]_D^{25}$ -13.77.

(*S*)-*form* [1187-82-2]
Bp_7 100°. $[\alpha]_D^{16}$ +17.15 (neat).

Et ester: [28959-02-6]
Bp_4 78-80°. $[\alpha]_D^{25}$ +5.67 (Et_2O).

Chloride: [25548-83-8]
$C_6H_{11}ClO$ 134.605
Bp_{15} 45-48°. $[\alpha]_D^{25}$ +4.06.

Amide: [34241-22-0]
Cryst. (H_2O). Mp 78°. $[\alpha]_D^{25}$ +5.79 (EtOH aq.).

(±)-*form* [22160-39-0]
Flavouring ingredient. d_4^0 0.94. Bp 192-193.6°. n_D^{20} 1.4136. pK_a 4.78 (25°).

Me ester: [2177-77-7] *FEMA 3707*
$C_7H_{14}O_2$ 130.186
Flavouring ingredient. Pale yellow liq. d^{20} 0.88. $Bp_{0.2}$ 45°. n_D^{20} 1.4012.

Et ester: [39255-32-8] *FEMA 3488*
Flavouring ingredient. Bp 153°.

Chloride: [5238-27-7]
Bp 140-140.8°.

Amide: [6941-49-7]
Mp 79.6°.

[6339-13-5]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 761C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 579D (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 288A (*ir*)
Ställberg-Sterhagen, S. *et al., Ark. Kemi*, No. 15, 1947, **23A**, (*abs config*)
Smith, L.I. *et al., J.A.C.S.*, 1957, **79**, 2962 (*synth*)
Falbe, J. *et al., Chem. Ber.*, 1964, **97**, 3088 (*synth*)
Goering, H.L. *et al., J.A.C.S.*, 1965, **87**, 1748 (*abs config*)
White, D.R. *et al., Chem. Comm.*, 1974, 988 (*synth*)
Riley, R.G. *et al., Tetrahedron*, 1974, **30**, 1171 (*synth*)
Meyers, A.I. *et al., J.A.C.S.*, 1976, **98**, 567 (*synth*)
Helmchen, G. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 63 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 763 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 250; 525; 582
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1009-1010; 1798-1799; 1882-1883
de Jesus, P.C. *et al., Synth. Commun.*, 1998, **28**, 2893-2901 (*resoln*)
Morrone, R. *et al., Eur. J. Org. Chem.*, 2001, 1441-1443 (*R-form, resoln*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4921
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MQJ750

3-Methylpentanoic acid, 9CI M-547

[105-43-1]
3-Methylvaleric acid. FEMA 3437
$C_6H_{12}O_2$ 116.16

(*R*)-*form* [16958-25-1]
Bp 198° Bp_{10} 90°. $[\alpha]_D$ -8.4 (c, 1 in CH_2Cl_2).

(*S*)-*form* [1730-92-3]
Bp 199°. $[\alpha]_D^{24}$ +6.44 (c, 1.27 in $CHCl_3$).

Me ester: [39616-77-8]
$C_7H_{14}O_2$ 130.186
Bp 142°. $[\alpha]_D$ +5.68 (1.22 in $CHCl_3$). n_D^{18} 1.4044.

Chloride:
$C_6H_{11}ClO$ 134.605
Bp 118-128°. $[\alpha]_D^{24}$ +6.23 (c, 1.23 in $CHCl_3$). n_D^{18} 1.4236.

Amide: [53254-70-9]
$C_6H_{13}NO$ 115.175
Cryst. (C_6H_6/heptane). Mp 125.7-126°. $[\alpha]_D^{23}$ +8.35 (c, 5.04 in C_6H_6/heptane).

Dimethylamide: [398453-86-6]
$C_8H_{17}NO$ 143.228
Bp_{17} 95°. $[\alpha]_D^{25}$ +13.36 (neat).

(±)-*form* [22160-40-3]
Flavouring ingredient. d_4^0 0.94. Fp -41.6. Bp 197.2-197.8° Bp_1 63°. n_D^{20} 1.4159. pK_a 4.77 (25°).

Et ester: [5870-68-8] *FEMA 3679*
$C_8H_{16}O_2$ 144.213
Flavouring ingredient. Bp 157-158°. n_D^{20} 1.4088.

Chloride: [51116-72-4]
Bp 142.5-143°.

Amide: [65137-49-7]
Needles. Mp 124.9°.

[2177-78-8, 28977-69-7, 39616-78-9, 61892-69-1, 68070-12-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 489B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 762B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 580A (*ir*)
Org. Synth., 1931, **11**, 76 (*synth*)
Wiberg, K.B. *et al., J.A.C.S.*, 1956, **78**, 1640 (*synth*)
Djerassi, C. *et al., J.A.C.S.*, 1959, **81**, 2789 (*abs config*)
Narayanan, C.S. *et al., Tetrahedron*, 1964, **20**, 963 (*isol*)
Hill, R.K. *et al., J.A.C.S.*, 1974, **96**, 4201 (*synth*)
Meyers, A.I. *et al., J.A.C.S.*, 1976, **98**, 2290 (*synth*)
Hara, S. *et al., Tet. Lett.*, 1978, 2891 (*synth*)
Menicagli, R. *et al., J. Het. Chem.*, 1979, **16**, 667 (*synth*)
Mori, K. *et al., Annalen*, 1991, 775 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 249; 538
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1010; 1820-1821

Belzecki, C. *et al., Synth. Commun.*, 2000, **30**, 2245-2252 (*R-form, synth, pmr*)
Aronica, L.A. *et al., Eur. J. Org. Chem.*, 2001, 4321-4329 (*S-form, synth, pmr, cmr, dimethylamide*)

4-Methylpentanoic acid, 9CI M-548

[646-07-1]
4-Methylvaleric acid. Isocaproic acid. Isohexanoic acid. Isobutylacetic acid. FEMA 3463

$(H_3C)_2CHCH_2CH_2COOH$

$C_6H_{12}O_2$ 116.16

Found in bananas and lime oil. Oil, with sour penetrating odour. d_4^{20} 0.92. Mp -33°. Bp 199.1° $Bp_{2.5}$ 69°. n_D^{20} 1.4144.

▶ Fl.p. 89°. Eye and skin irritant. NR2975000

NH_4 salt:
Mp 102°.

Me ester: [2412-80-8] *Methyl 4-methylpentanoate. FEMA 2721*
$C_7H_{14}O_2$ 130.186
Present in pineapple. Flavouring ingredient with a sweet, pineapple-like flavour. Bp 142-143°.

Et ester:
$C_8H_{16}O_2$ 144.213
Bp 160-164° Bp_{10} 50-53°.

Chloride: [38136-29-7]
$C_6H_{11}ClO$ 134.605
Bp 143.8-148.6°.

Amide: [1119-29-5] *4-Methylpentanamide*
$C_6H_{13}NO$ 115.175
Mp 120-121°.

Nitrile: [542-54-1] *1-Cyano-3-methylbutane. Isopentyl cyanide*
$C_6H_{11}N$ 97.16
Bp 156-157°.

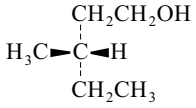
▶ LD_{50} (mus, orl) 488 mg/kg. YV8588000

Anhydride:
$C_{12}H_{22}O_3$ 214.304
Bp_{19} 139°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 762C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 580C (*ir*)
Curtius, T. *et al., J. Prakt. Chem.*, 1930, **125**, 152 (*synth*)
Haagen-Smit, A.J. *et al., J.A.C.S.*, 1945, **67**, 1646 (*isol*)
Milburn, A.H. *et al., J.C.S.*, 1954, 3344 (*synth*)
Sisido, K. *et al., J.A.C.S.*, 1959, **81**, 5817 (*synth*)
Brannock, K.C. *et al., J.O.C.*, 1964, **29**, 818 (*synth*)
Hara, S. *et al., Tet. Lett.*, 1978, 2891 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 528 (*Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1802-1803 (*Me ester*)
Dembitsky, V.M. *et al., Phytochemistry*, 2000, **54**, 965-967 (*isol, amide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IKT000; MNJ000

3-Methyl-1-pentanol, 9CI M-549

[589-35-5]
FEMA 3762



(*S*)-*form*

$C_6H_{14}O$ 102.176

▶ Flammable, fl. p. 54°, autoignition temp. 310°.

(*S*)-*form* [42072-39-9]
Bp 154° Bp_{25} 72°. $[\alpha]_D^{22}$ +7.4 (c, 1.4 in MeOH). n_D^{25} 1.4182.

(±)-*form* [20281-83-8]
Flavouring ingredient. d_4^{24} 0.82. Bp 151-152° Bp_8 51-52.5°. n_D^{23} 1.4112.

3,5-Dinitrobenzoyl:
Mp 38°.

1-Naphthylurethane:
Mp 58°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 116C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 172C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 163C (*ir*)
Levene, P.A. *et al., J. Biol. Chem.*, 1931, **91**, 77 (*synth, resoln*)
Pino, P. *et al., J.O.C.*, 1959, **24**, 1399 (*synth*)
Bailey, W.J. *et al., J.O.C.*, 1961, **26**, 3193 (*synth*)
Rossi, R. *et al., Tetrahedron*, 1985, **41**, 627 (*synth*)
Fuganti, C. *et al., J.C.S. Perkin 1*, 1988, 3061 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 539
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1822-1823
Roeder, M. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 841-853 (*S-form, synth, cmr*)

4-Methyl-2-pentanone, 9CI M-550

[108-10-1]
Isobutyl methyl ketone. Isopropylacetone. Hexone. MIBK. FEMA 2731

$(H_3C)_2CHCH_2COCH_3$

$C_6H_{12}O$ 100.16

Present in orange, lemon, concord grape, vinegar, cheeses, cooked beef, roasted peanut and other foodstuffs. Flavouring ingredient. Misc. organic solvs.; Sol. H_2O (2%). d_4^{20} 0.8. Bp 116.8°. n_D^{17} 1.3969.

▶ Highly flammable, fl. p. 17°. Camphor-like odour detectable at 100 ppm. Explosion during hot evaporation attributed to peroxide formn. Skin, eye and respiratory tract irritant. High conc. narcotic. LD_{50} (rat, orl) 2080 mg/kg. Exp. teratogen. OES: long-term 50 ppm; short-term 75 ppm (sk); short-term 100 ppm (sk, revised). SA9275000

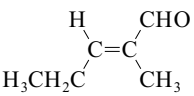
Semicarbazone:
Mp 134°.

2,4-Dinitrophenylhydrazone:
Mp 95°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 633C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 407A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 489A (*ir*)
Law, H.O. *et al., J.C.S.*, 1912, **101**, 1547 (*synth*)
Grignard, V. *et al., Ann. Chim. (Paris)*, 1928, **9**, 13 (*synth*)
Fuge, E.T.J. *et al., J. Phys. Chem.*, 1952, **56**, 1013 (*synth*)
Morrison, G.H. *et al., Solvent Extr. Anal. Chem.*, Wiley, New York, 1957, (*use*)
Zolotov, Y.A. *et al., Extraction of Halide Metal Complexes (in Russian)*, Izdat.Nauka, Moscow, 1973, (*use*)
Sandell, E.B. *et al., Photometric Determination of Traces of Metals, General Aspects*, Wiley, New York, 1978, (*use*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 907 (*rev*)
Ejchart, A. *et al., Org. Magn. Reson.*, 1980, **13**, 368 (*cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1104
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4747
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HFG500
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2341
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 861
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 337

2-Methyl-2-pentenal, 9CI M-551

[623-36-9]
3-Ethyl-2-methylacraldehyde. 2-Propylidenepropionaldehyde. FEMA 3194



(*E*)-*form*

$C_6H_{10}O$ 98.144

Constit. of onion (*Allium cepa*) and chive leaves (*Allium schoenoprasum*). Also found in fruits of cranberry, guava, grape, plum, in mustard, cognac, black tea, coffee, roasted peanuts, walnut and other foodstuffs. Flavouring ingredient. Liq. with pungent odour. n_D 1.4465.

▶ Eye and skin irritant. LD_{50} (rat, orl) 4290 mg/kg. SB2100000

(*E*)-*form* [14250-96-5]
Bp_{25} 38-39°.

2,4-Dinitrophenylhydrazone: [1572-64-1]
Carmine cryst. Mp 160°.

(*Z*)-*form* [16958-22-8] Characterised spectroscopically.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 736A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 559D (*ir*)
Grignard, V. *et al., Bull. Soc. Chim. Fr.*, 1910, **7**, 642 (*synth*)
v. Auwers, K. *et al., Ber.*, 1925, **58**, 1979 (*synth*)
Häusermann, M. *et al., Helv. Chim. Acta*, 1951, **34**, 1482 (*synth*)
Green, M.B. *et al., J.C.S.*, 1957, 3262 (*synth*)
Virtanen, A.I. *et al., Acta Chem. Scand.*, 1961, **15**, 1280; 1965, **19**, 1327 (*isol*)
Jewell, A. *et al., J.O.C.*, 1968, **33**, 3382 (*synth, nmr, uv, ir*)
Büchi, G. *et al., J.A.C.S.*, 1972, **94**, 9128 (*synth*)
Woo, E.P. *et al., J.O.C.*, 1986, **51**, 3704 (*synth, pmr, cmr*)
Mordini, A. *et al., J.O.C.*, 1994, **59**, 4784 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MNJ750

2-Methyl-4-pentenal M-552

[5187-71-3]

[61866-32-8, 131102-19-7]

$H_2C{=}CHCH_2CH(CH_3)CHO$

$C_6H_{10}O$ 98.144

Constit. of *Actinidia chinensis* (kiwi fruit), *Phaseolus lunatus* (butter bean), *Psidium guajava* (guava) and other plant spp..

(±)-*form* [114031-12-8]
Bp 118° Bp_{45} 45°.

2,4-Dinitrophenylhydrazone: [5497-66-5]
Cryst. (MeOH). Mp 104-105° (102-103°).

Weiss, F. *et al., Bull. Soc. Chim. Fr.*, 1965, 3215 (*synth*)
Montgomery, L.K. *et al., J.A.C.S.*, 1967, **89**, 923 (*synth*)
Block, E. *et al., J.A.C.S.*, 1986, **108**, 7045 (*synth*)
Liu, S.H. *et al., J. Agric. Food Chem.*, 1989, **37**, 496 (*isol*)
Tatsuka, K. *et al., J. Agric. Food Chem.*, 1990, **38**, 2176 (*isol*)
Lin, N.H. *et al., J.A.C.S.*, 1996, **118**, 9062 (*synth*)

4-Methyl-2-pentenal, 9CI M-553

[5362-56-1]
FEMA 3510

$(H_3C)_2CHCH{=}CHCHO$

$C_6H_{10}O$ 98.144

Flavouring ingredient.

(*E*)-*form* [24502-08-7]
Bp 182°.

2,4-Dinitrophenylhydrazone: [5362-53-8]
Red-orange cryst. (H_2O). Mp 188°.

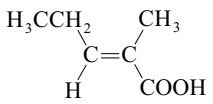
Semicarbazone:
Mp 176°.

(*Z*)-*form* [22597-48-4]
Bp_{115} 75°.

Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1966, 717; 1975, 1363 (*synth*)
Nakanishi, K. *et al., Tet. Lett.*, 1968, 1105 (*deriv*)
Dabrowski, J. *et al., J. Mol. Struct.*, 1969, **3**, 227 (*ir, struct*)
Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 541
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1825

2-Methyl-2-pentenoic acid, 9CI M-554

[3142-72-1]
3-Ethyl-2-methylacrylic acid. 2-Pentene-2-carboxylic acid. FEMA 3195



(*E*)-*form*

$C_6H_{10}O_2$ 114.144

Flavouring ingredient.

(*E*)-*form* [16957-70-3]
Mp 24.1°. Bp_{10} 106.5°.

Me ester: [1567-14-2]
$C_7H_{12}O_2$ 128.171
d 0.92. Bp_{15} 46-47°. n_D^{20} 1.4380.

(S)-1-Methylbutyl ester: [80510-15-2] ***Dominicalure 1***
$C_{11}H_{20}O_2$ 184.278
Liq. $[\alpha]_D$ +14.2 (c, 1.265 in Et_2O) (= 98% op).

(*Z*)-*form* [1617-37-4]
Bp_{10} 94-94.4°.

Me ester: [1567-13-1]
Bp 143°. n_D^{24} 1.4351.

[89301-90-6, 134176-70-8, 134732-07-3]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 778B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 585A (*ir*)
Goldberg, A.A. *et al., J.C.S.*, 1928, 2355 (*synth*)
McGreer, D.E. *et al., Can. J. Chem.*, 1963, **41**, 726 (*Me esters*)
Chan, K.C. *et al., J.O.C.*, 1968, **33**, 3382 (*synth*)
Williams, H.J. *et al., J. Chem. Ecol.*, 1981, **7**, 759 (*Dominicalure 1, isol, synth, activity*)
Moiseenkov, A.M. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1990, 595 (*synth, pmr*)
Lin-Yu, L. *et al., J. Chem. Ecol.*, 1990, **16**, 1921 (*Dominicalure 1, synth, pmr, ir, ms*)
Morgan, B. *et al., J.O.C.*, 1992, **57**, 3231 (*deriv*)
Rossi, R. *et al., Synth. Commun.*, 1993, **23**, 143 (*synth, Dominicalure 1*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 542
Palaty, J. *et al., J. Med. Chem.*, 1995, **38**, 3398 (*synth, pmr, ir*)
Razkin, J. *et al., J. Chem. Ecol.*, 1996, **22**, 673 (*synth, Dominicalure 1*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1825-1826

2-Methyl-3-pentenoic acid, 9CI M-555

[37674-63-8]
2-Pentene-4-carboxylic acid. FEMA 3464

$C_6H_{10}O_2$ 114.144

Flavouring ingredient. Bp_{740} 198-199°.

Et ester: [1617-23-8]

[16489-03-5, 58625-89-1] *Ethyl 2-methyl-3-pentenoate. FEMA 3456*
$C_8H_{14}O_2$ 142.197
Flavouring agent. Bp_{50} 85-91°. Stereochem. not known.

Hexyl ester:

[58625-94-8, 58625-95-9] *Hexyl 2-methyl-3-pentenoate*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Component of FEMA 3693 together with the 4-methyl isomer. Characterised spectroscopically as a 40:60 mixt. of *E*:*Z*-isomers.

(*S*,*E*)-*form* [71048-90-3]
$[\alpha]_D^{23}$ +63.6. The (±)-(*E*)- and (±)-(*Z*)-forms have been prepd. but their constants have not been publ..

[55894-36-5, 55894-37-6, 71011-55-7, 71048-89-0]

Fichter, F. *et al., Ber.*, 1904, **37**, 1616 (*synth*)
U.S. Pat., 1976, 3 931 293; *CA*, 121186h (*synth, hexyl ester, pmr*)
Bunnell, C.A. *et al., J.A.C.S.*, 1977, **99**, 5184 (*synth, resoln*)
Corey, E.J. *et al., Tet. Lett.*, 1979, 335 (*synth*)
Van der Veen, R.H. *et al., J.O.C.*, 1985, **50**, 342 (*synth, pmr*)
Girard, C. *et al., Tet. Lett.*, 1989, **30**, 7399 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 250; **2**, 542
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1011; 1826-1827 (*Et ester*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 790 (*FEMA 3693*)

2-Methyl-4-pentenoic acid, 9CI M-556

[1575-74-2]
Methylallylacetic acid. FEMA 3511

$C_6H_{10}O_2$ 114.144

(*S*)-*form* [20626-61-3]
$[\alpha]_D^{25}$ +10.5 (c, 1 in $CHCl_3$).

Me ester:
$C_7H_{12}O_2$ 128.171
$[\alpha]_D^{25}$ +17.38 (neat).

(±)-*form* [53729-46-7]
Flavouring ingredient. Sl. sol. H_2O; misc. EtOH. Bp 188-189° Bp_6 77-79°. n_D^{20} 1.4263.

Me ester: [20459-96-5]
Bp 137.5°.

Et ester: [53399-81-8]

[105999-68-6] *FEMA 3489*
$C_8H_{14}O_2$ 142.197
Flavouring agent. Insol. H_2O; misc. EtOH. d 0.87. Bp 153-155°. n_D^{20} 1.4180 (1.4128).

Hexyl ester: [58031-03-1] *Hexyl 2-methyl-4-pentenoate*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Component of FEMA 3693 used for flavouring chewing gum, confectionery and beverages. Bp_4 88° (lit. gives a pressure range). See also 2-Methyl-3-pentenoic acid, M-555.

Ställberg-Stenhagen, S. *et al., Ark. Kemi, Sect. B*, no. 9, 1947, **24**, (*abs config*)
Ställberg-Stenhagen, S. *et al., Acta Chem. Scand.*, 1956, **10**, 1360 (*abs config*)
Riley, R.G. *et al., Tetrahedron*, 1974, **30**, 1171 (*synth, resoln*)
Kurata, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 538 (*synth*)
U.S. Pat., 1976, 3 966 799; *CA*, **85**, 159453b (*hexyl ester, synth, use, pmr, ir, ms*)
Sato, T. *et al., Chem. Lett.*, 1980, 571 (*synth*)
Rossi, R. *et al., Chim. Ind. (Milan)*, 1981, **63**, 303 (*synth, resoln*)
Evans, D.A. *et al., Pure Appl. Chem.*, 1981, **53**, 1109 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 251; 543
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1011-1012; 1827
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 790 (*FEMA 3693*)
Heuger, G. *et al., Eur. J. Org. Chem.*, 2002, 1848-1854 (*synth, pmr, cmr*)

4-Methyl-2-pentenoic acid, 9CI M-557

[10321-71-8]
3-Isopropylacrylic acid

$(H_3C)_2CHCH{=}CHCOOH$

$C_6H_{10}O_2$ 114.144

Isol. from hops. pK_a 4.7 (25°).

(*E*)-*form* [16666-43-6]
Bp_3 78° $Bp_{0.1}$ 60-64°.

Me ester: [20515-15-5]
$C_7H_{12}O_2$ 128.171
Oil. Bp_{150} 100°.

Et ester: [15790-86-0]
$C_8H_{14}O_2$ 142.197
Bp 153° Bp_{17} 66°.

Chloride: [40794-19-2]
C_6H_9ClO 132.589
Bp_{25} 61-62°.

(*Z*)-*form* [1775-44-6]
Mp -19°. $Bp_{0.4}$ 69-70°.

Et ester: [15790-85-9]
Mp 147°.

Power, F.B. *et al., J.C.S.*, 1913, **103**, 1267 (*isol*)
Gibson, T.W. *et al., J.O.C.*, 1972, **37**, 1148 (*synth*)
Org. Synth., 1973, **53**, 123 (*synth*)
Pirrung, M.C. *et al., J.O.C.*, 1994, **59**, 2430 (*synth, pmr*)
Barrett, A.G.M. *et al., J.O.C.*, 1997, **62**, 4653-4664 (*Me ester, synth*)

4-Methyl-3-penten-2-one, 9CI M-558

[141-79-7]
Isopropylideneacetone. Mesityl oxide. FEMA 3368

$(H_3C)_2C{=}CHCOCH_3$

$C_6H_{10}O$ 98.144
Flavouring ingredient. Constit. of *Capsicum* spp., *Osmanthus fragrans* (sweet osmanthus) and other plants. Liq. with odour of honey. Spar. sol. H_2O. d_4^{25} 0.85. Mp -41.5° (-59°). Bp 130-131° Bp_{37} 50°. n_D^{13} 1.4484. pK_a 0.25 (25°, 0.2*M* $HClO_4$).
▶ Flammable, fl. p. 31°, autoignition temp. 340°. Eye, skin and respiratory tract irritant. High capour conc. narcotic. Contact with liq. can damage eyes. Prolonged or repeated exposure can injure liver, kidneys, and lungs, and cause dermatitis. LD_{50} (rat, orl) 1120 mg/kg. OES: long-term 15 ppm; short-term 25 ppm. SB4200000

E-*Oxime:* [28052-09-7]
$C_6H_{11}NO$ 113.159
Bp 184-187° Bp_{10} 85°. Unstable isomer, sepd. with difficulty from the *Z*-form.

Z-Oxime: [28052-10-0]
$C_6H_{11}NO$ 113.159
Cryst. (H_2O). Mp 49°. Bp_{13} 102°. Stable isomer.

4-Nitrophenylhydrazone: [88903-27-9]
Orange needles (EtOH aq.). Mp 207°.

2,4-Dinitrophenylhydrazone: [964-83-0]
Carmine cryst. (EtOH). Mp 200°.

[2158-24-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 414D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 644C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 500B (*ir*)
Wilson, F.J.W. *et al., J.C.S.*, 1923, **123**, 394 (*deriv*)
v. Auwers, K. *et al., Ber.*, 1924, **57**, 446 (*oxime*)
Allen, C.F.H. *et al., J.A.C.S.*, 1930, **52**, 2958 (*deriv*)
Org. Synth., Coll. Vol. 1, 1932, 345 (*synth*)
Klein, F.G. *et al., Ind. Eng. Chem.*, 1956, **48**, 1278 (*synth*)
Dhara, S.C. *et al., Mikrochim. Acta*, 1965, 931 (*detn, U*)
Dhond, P.V. *et al., Anal. Chim. Acta*, 1972, **59**, 161 (*detn, Ge*)
Sato, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1176 (*oxime*)
Sandell, E.B. *et al., Photometric Determination of Traces of Metals*, Wiley, New York, 1977, (*use*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **13**, 916 (*rev*)
Rao, T.P. *et al., Talanta*, 1982, **29**, 227 (*detn, Zn, Cd, Pd*)
Bell, V.A. *et al., J. Catal.*, 1983, **79**, 286 (*cmr*)
Baeckström, P. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 442 (*purifn*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 543
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1827-1829
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4752
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 312
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 862
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MDJ750

4-Methyl-4-penten-2-one, 9CI M-559

[3744-02-3]
Isopropenylacetone. 3-Acetylisobutene

$H_2C{=}C(CH_3)CH_2COCH_3$

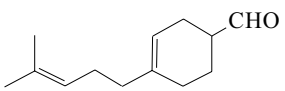
$C_6H_{10}O$ 98.144
Listed in the EAFUS Food Additive Database (Jan 2001) but with no current reported uses. Bp 121°.

Semicarbazone:
Cryst. Mp 192°.

v. Braun, J. *et al., Annalen*, 1912, **386**, 303 (*synth*)
Gillard, R.D. *et al., Org. Prep. Proced. Int.*, 1974, **6**, 131 (*synth*)

4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde, 9CI M-560

[37677-14-8]



$C_{13}H_{20}O$ 192.3
Used in flavouring formulations. $Bp_{1.6}$ 108°.

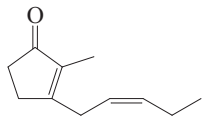
Semicarbazone:
Mp 140-141.5°.

Ohloff, G. *et al., Annalen*, 1957, **606**, 100 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, (Suppl.), 1976, **14**, 803; *CA*, **91**, 216602z (*rev*)
Ger. Pat., 1978, 2 730 176; *CA*, **88**, 152126a (*synth*)
U.S. Pat., 1978, 4 068 012; *CA*, **88**, 177629j (*use*)

2-Methyl-3-(2-pentenyl)-2-cyclopenten-1-one M-561

[11050-62-7]

[8029-70-7, 39346-90-2]
Isojasmone. FEMA 3552



(Z)-*form*

$C_{11}H_{16}O$
Flavouring ingredient. Confused with 2-Hexyl-2-cyclopenten-1-one in some literature.

(*Z*)-*form*
Liq. with odour similar to 3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one, M-562. Bp_5 140° (kugelrohr).

U.K. Pat., 1973, 1 306 017; *CA*, **78**, 122965z (*use*)
Weyerstahl, P. *et al., Flavour Fragrance J.*, 1996, **11**, 141-144 (*Z-form, synth, pmr, cmr, props*)

3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one M-562

[68043-00-5]
Jasmone

$C_{11}H_{16}O$ 164.247

(*Z*)-*form* [488-10-8]
Occurs in peppermint oil, green tea and bergamot oranges (*Citrus bergamia*). Oil. Bp_{12} 134-135°. n_D^{22} 1.4979. Low oral tox..
▶ GY7301000

Semicarbazone:
Cryst. (MeOH or EtOH). Mp 209.5-210°.

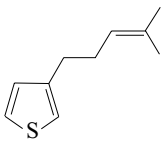
[6261-18-3]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 689A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 534A (*ir*)
Birch, A.J. *et al., Aust. J. Chem.*, 1973, **26**, 2671 (*synth*)
McMurry, J.E. *et al., J.O.C.*, 1973, **38**, 4367 (*synth*)
Ellison, R.A. *et al., Synthesis*, 1973, 397 (*synth, rev*)
Pattenden, G. *et al., J.C.S. Perkin 1*, 1974, 1603 (*synth*)
Joulain, D. *et al., Parfums, Cosmet., Aromes*, 1975, 33 (*synth, rev*)
Bulat, J.A. *et al., Can. J. Chem.*, 1976, **54**, 3869 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 845 (*rev, tox*)
Bazulkis, P. *et al., J.O.C.*, 1977, **42**, 2362
Sato, T. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 505 (*synth*)
Takahashi, T. *et al., Chem. Lett.*, 1981, 1189 (*synth*)
Furuhata, A. *et al., Agric. Biol. Chem.*, 1982, **46**, 1757 (*synth*)
Watanabe, S. *et al., Aust. J. Chem.*, 1982, **35**, 1739 (*synth*)
Yoshida, T. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 3931 (*synth*)
Piers, E. *et al., Can. J. Chem.*, 1982, **60**, 1256 (*synth*)
Ogura, F. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 1691 (*synth*)
Mikolajczyk, M. *et al., Z. Naturforsch., B*, 1986, **41**, 263 (*synth*)
Ohta, S. *et al., Heterocycles*, 1987, **26**, 141 (*synth*)
Welsh, S.C. *et al., J.O.C.*, 1987, **52**, 1440 (*synth*)
Billington, D.C. *et al., J. Chem. Res., Miniprint*, 1988, 2601 (*synth*)
Mathew, J. *et al., Chem. Comm.*, 1990, 684 (*synth*)

Sarkar, A.K. *et al., J. Chem. Res., Synop.*, 1992, 418 (*synth*)
Tsukasa, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1181 (*synth, bibl*)
Islam, M.S. *et al., Tet. Lett.*, 1996, **37**, 5735 (*synth*)

3-(4-Methyl-3-pentenyl)thiophene M-563

[62469-65-2]



$C_{10}H_{14}S$ 166.287
Constit. of hops. Oil. Bp_3 95°.

Peppard, T.L. *et al., Chem. Ind. (London)*, 1979, 552 (*isol, struct*)
Elvidge, J.A. *et al., J.C.S. Perkin 1*, 1982, 1089 (*isol, synth*)
Weyerstahl, P. *et al., Annalen*, 1995, 1849 (*synth, ms, pmr, cmr*)

3-Methylpentyl glucosinolate M-564

1-Thio-β-D-glucopyranose 1-[4-methyl-N-(sulfooxy)hexanimidate]
$H_3CCH_2CH(CH_3)CH_2CH_2C(SGlc)=NOSO_3H$

$C_{13}H_{25}NO_9S_2$ 403.474
Constit. of *Raphanus sativus* (radish) and *Wasabia japonica* (Japanese horseradish).

Fahey, J.W. *et al., Phytochemistry*, 2001, **56**, 5-51 (*rev*)

4-Methylpentyl glucosinolate M-565

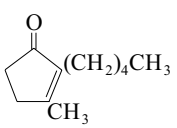
$(H_3C)_2CHCH_2CH_2CH_2C(SGlc)=NOSO_3H$

$C_{13}H_{25}NO_9S_2$ 403.474
Present in radish (*Raphanus sativus*).

Kjaer, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1715 (*occur*)

3-Methyl-2-pentyl-2-cyclopentenone, 9CI M-566

[1128-08-1]
Dihydrojasmone. Tetrahydropyrethrone. FEMA 3763



$C_{11}H_{18}O$ 166.263
Flavouring ingredient. Identified in bergamot orange oil (*Citrus bergamia*). Oil. d_4^{18} 0.92. Bp_{22} 140-147° Bp_{12} 115-117°. n_D^{20} 1.4767.
▶ Skin irritant. LD_{50} (rat, orl) 2500 mg/kg. GY7302000

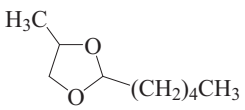
Semicarbazone:
Cryst. (C_6H_6). Mp 177-178°.
4-Nitrophenylhydrazone:
Cryst. (MeOH). Mp 118-119°.

Staudinger, H. *et al., Helv. Chim. Acta*, 1924, **7**, 257 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 523 (*rev, tox*)
Bakuzis, P. *et al., J.O.C.*, 1977, **42**, 2362 (*synth*)
Rohela, R.C. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 436 (*synth*)
Padmanabhan, S. *et al., Synth. Commun.*, 1980, **10**, 503 (*synth*)
Fujisawa, T. *et al., Chem. Lett.*, 1981, 55 (*synth*)
Takahashi, T. *et al., Chem. Lett.*, 1981, 1189 (*synth*)
Brown, H.C. *et al., Synthesis*, 1983, 886 (*synth*)
Liu, S.-H. *et al., Tet. Lett.*, 1983, **24**, 439 (*synth*)
Sato, F. *et al., Tet. Lett.*, 1983, **24**, 1041 (*synth*)
Cameron, A.G. *et al., Tet. Lett.*, 1984, **25**, 2267 (*synth*)
Mikolajczyk, M. *et al., Tet. Lett.*, 1984, **25**, 2489 (*synth*)
Anand, R.C. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 673 (*synth*)
Hendrickson, J.B. *et al., J.O.C.*, 1985, **50**, 2110 (*synth*)
Chattopodhyay, A. *et al., Chem. Ind. (London)*, 1986, 491 (*synth*)
Ohta, S. *et al., Heterocycles*, 1987, **26**, 141 (*synth*)
Pecunioso, A. *et al., J.O.C.*, 1988, **53**, 2614 (*synth*)
Antonioletti, R. *et al., Gazz. Chim. Ital.*, 1991, **121**, 233 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DLQ600

4-Methyl-2-pentyl-1,3-dioxolane, 9CI, 8CI M-567

[1599-49-1]

[26563-74-6, 26563-75-7]
Hexanal propylene glycol acetal. FEMA 3630

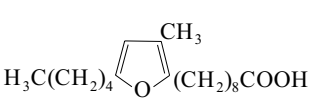


$C_9H_{18}O_2$
Flavouring ingredient. Liq. Bp_{10} 68°. Bp data is for 4:1 *cis:trans* mixt..

Rommelaere, Y. *et al., Bull. Soc. Chim. Belg.*, 1970, **79**, 11-14 (*synth, pmr*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Welch, R.C. *et al., J. Agric. Food Chem.*, 1980, **28**, 870-872 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 544 (*use*)

3-Methyl-5-pentyl-2-furannonanoic acid, 9CI M-568

[57818-39-0]
10,13-Epoxy-11-methyl-10,12-octadecadienoic acid. F_2 Acid

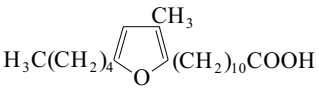


$C_{19}H_{32}O_3$ 308.46
Component of F acid fraction present in beef blood serum.

Glass, R.L. *et al., Lipids*, 1977, **12**, 828 (*occur*)
Hasma, H. *et al., Lipids*, 1978, **13**, 905 (*occur, ms, nmr*)
Lie Ken Jie, M.S.F. *et al., Chem. Phys. Lipids*, 1981, **28**, 99 (*cmr*)
Puchta, V. *et al., Annalen*, 1988, 25 (*occur*)
Batna, A. *et al., Annalen*, 1991, 861 (*biosynth*)
Tsukasa, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 511 (*synth*)

3-Methyl-5-pentyl-2-furanundecanoic acid, 9CI M-569

[57818-37-8]
F_5 Acid. F_5 Furan fatty acid

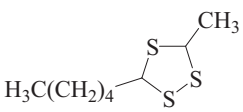


$C_{21}H_{36}O_3$ 336.514
Constit. of fats of the liver and gonads of fishes, e.g. pike (*Esox lucius*).

Glass, R.L. *et al., Lipids*, 1974, **9**, 1004; 1975, **10**, 695; 1977, **12**, 828
Scheinkönig, J. *et al., Annalen*, 1991, 451 (*biosynth*)
Marson, C.M. *et al., Tet. Lett.*, 1998, **39**, 333-334 (*synth*)
Bach, T. *et al., Eur. J. Org. Chem.*, 1999, 2045-2057 (*synth, pmr, cmr, ms*)

3-Methyl-5-pentyl-1,2,4-trithiolane M-570

[101517-93-5]



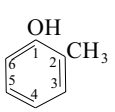
$C_8H_{16}S_3$ 208.412
Component of fried food model systems. Constit. of various cooked meat aromas. Characterised spectroscopically.

Zhang, Y. *et al., J. Agric. Food Chem.*, 1989, **37**, 1016-1020 (*occur, ms*)
Werkhoff, P. *et al., CA*, 1995, **122**, 313271g (*occur, meat aroma*)

2-Methylphenol, 9CI M-571

[95-48-7]

[1319-77-3]
o-*Cresol, 8CI.* o-*Hydroxytoluene.* o-*Cresylic acid. FEMA 3480*



C_7H_8O 108.14
Flavouring ingredient. Cryst. d_4^{20} 1.05. Mp 30°. Bp 191-192° Bp_{76} 120° Bp_6 70°. pK_a 10.32 (25°). Log P 1.97 (calc). Steam-volatile.
▶ Fl. p. 81°, autoignition temp. 555°. Corrosive and irritating to all tissues. Prolonged or repeated exposure can damage liver and kidneys, and cause adverse CNS and cardiovascular effects. Systemic effects produced by skin absorption (which is rapid), inhalation of vapours (at elevated temperatures) and by ingestion. LD_{50} (rat, orl) 121 mg/kg. LD_{50} (rat, skn) 620 mg/kg.

GO6300000

Picrate:
Orange needles. Mp 88°.

Ac: [533-18-6] o-*Tolyl acetate*
$C_9H_{10}O_2$ 150.177
Liq. Bp 208°.

2-Methylpropanoyl: [36438-54-7] *2-Methylphenyl 2-methylpropanoate.* o-*Tolyl isobutyrate. FEMA 3753*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient.

Me ether: [578-58-5] *1-Methoxy-2-methylbenzene. Methyl* o-*tolyl ether. 2-Methoxytoluene.* o-*Methylanisole. FEMA 2680*
$C_8H_{10}O$ 122.166
Flavouring ingredient. Liq. with a fruity nut-like flavour at low levels. $d^{15.5}$ 0.99. Bp 171-172°. $n_D^{15.3}$ 1.5199.

Trifluoromethyl ether: [42908-77-0] *1-Methyl-2-(trifluoromethoxy)benzene, 9CI.* o-*Trifluoromethoxytoluene*
$C_8H_7F_3O$ 176.138
Volatile liq. Bp 104° Bp_{100} 58-60°. n_D^{20} 1.4255.

Et ether: [614-71-1] *1-Ethoxy-2-methylbenzene. Ethyl* o-*tolyl ether. 2-Ethoxytoluene*
$C_9H_{12}O$ 136.193
Liq. Bp 184°.

1,1,2,2-Tetrafluoroethyl ether: [42145-66-4] *1-Methyl-2-(1,1,2,2-tetrafluoroethoxy)-benzene*
$C_9H_8F_4O$ 208.155
Bp_{14} 58-60°.

Ph ether: [3991-61-5] *Phenyl* o-*tolyl ether. 2-Methyldiphenyl ether. 2-Phenoxytoluene*
$C_{13}H_{12}O$ 184.237
Needles. Mp 22°. Bp_{738} 267°.

[1319-77-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1037B; 1069B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 178A; 243B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 965A; 1001B (*ir*)
Brückner, H. *et al., Z. Anorg. Allg. Chem.*, 1928, **75**, 289 (*purifn*)
Adv. Chem. Ser., 1955, **15**, 274 (***props***)
Yamazaki, M. *et al., CA*, 1966, **67**, 776 (*isol*)
Kotanigawa, T. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 1961 (*synth*)
Bois, C. *et al., Acta Cryst. B*, 1972, **28**, 25 (*cryst struct*)
Ger. Pat., 1973, 2 150 955; *CA*, **78**, 18377u (*tetrafluoroethyl ether*)
Mathey, F. *et al., Tet. Lett.*, 1973, 2253-2256 (*trifluoromethyl ether, synth, pmr, F-19 nmr*)
Fujio, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2127 (*pmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 113 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 132
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 469 (*Me ether*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 760 (*2-methylpropanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 734-735
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1715-1716 (*Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2811-2812 (*2-methylpropanoyl*)
Castagnetti, E. *et al., Eur. J. Org. Chem.*, 2001, 691-695 (*trifluoromethyl ether, synth, pmr*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2597
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 189
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 345
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNX000

3-Methylphenol, 9CI M-572

[108-39-4]

[1319-77-3]
m-*Cresol, 8CI.* m-*Hydroxytoluene.* m-*Cresylic acid. Metacresol, USAN. FEMA 3530*

C_7H_8O 108.14
Flavouring ingredient. d_4^{22} 1.04. Mp 11-12°. Bp 202° Bp_6 80°. n_D^{20} 1.5400. pK_a 10.09 (25°). Steam-volatile.

▶ Fl. p. 86°, autoignition temp. 558°. Corrosive and irritating to all tissues. Prolonged or repeated exposure can damage liver and kidneys and cause adverse CNS and cardiovascular effects. Systemic effects produced by skin absorption (which is rapid), inhalation of vapours (at elevated temperatures) and by ingestion. LD_{50} (rat, orl) 242 mg/kg. LD_{50} (rbt, skn) 2050 mg/kg. OES: long-term 5 ppm (Sk).
GO6125000

[1319-77-3, 3019-89-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1040C; 1056D; 1073B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 181A; 211B; 248B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 968C; 987D; 1005B (*ir*)
Ger. Pat., 1927, 541 037; *CA*, 1947, **26**, 541 037 (*purifn*)
U.K. Pat., 1928, 309 865; *CA*, **24**, 626 (*synth*)
Brückner, H. *et al., Z. Anorg. Allg. Chem.*, 1928, **75**, 289 (*purifn*)
Darzens, G. *et al., C. R. Hebd. Seances Acad. Sci.*, 1931, **192**, 1657 (*purifn*)
Adv. Chem. Ser., 1955, **15**, 275 (***props***)
Bois, C. *et al., Acta Cryst. B*, 1973, **29**, 1011 (*cryst struct*)
Fujio, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2127 (*pmr*)
Matsuo, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1399 (*cmr*)
Millefiori, S. *et al., Spectrochim. Acta A*, 1977, **33**, 21 (*uv*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A8**, 25 (*rev*)
Li, L. *et al., Int. J. Mass Spectrom. Ion Processes*, 1991, **110**, 103 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 133 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 131
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 733-734
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2597
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 189
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 345
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNW750

4-Methylphenol, 9CI M-573

[106-44-5]

[1319-77-3]
p-*Cresol, 8CI.* p-*Hydroxytoluene.* p-*Cresylic acid. Taurylic acid. FEMA 2337*

C_7H_8O 108.14
Present in blackcurrant buds, asparagus, cooked cured pork, black tea, fermented tea, yellow passion fruit juice, malt, peated malt, kumazasa (*Sasa albo-marginata*), lamb's lettuce, squid and cuttlefish. Flavouring ingredient. Cryst. d_4^{20} 1.03. Mp 36°. Bp 202.5° Bp_{11} 90°. pK_a 10.27 (25°). Steam-volatile.

▶ Fl. p. 86°, autoignition temp. 558°. Corrosive and irritating to all tissues. Prolonged or repeated exposure can damage liver and kidneys, and cause adverse CNS and cardiovascular effects. Systemic effects produced by skin absorption (which is rapid), inhalation of vapours (at elevated temperatures) and ingestion. LD_{50} (rat, orl) 207 mg/kg. LD_{50} (rbt, skn) 301 mg/kg.
GO6475000

Ac: [140-39-6] p-*Tolyl acetate. Narceol. FEMA 3073*
$C_9H_{10}O_2$ 150.177
Present in essential oils of wallflower, cananga and ylang-ylang. Flavouring ingredient. Liq. with floral odour and honey-like flavour. Bp 212-213°. Steam-volatile.

▶ LD_{50} (rat, orl) 1900 mg/kg. LD_{50} (rbt, skn) 2100 mg/kg. AJ7570000

2-Methylpropanoyl: [103-93-5] *4-Methylphenyl 2-methylpropanoate.* p-*Tolyl isobutyrate. FEMA 3075*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient. Liq. d^{25} 1.01. Bp 237°.

3-Methylbutanoyl: [55066-56-3] *4-Methylphenyl 3-methylbutanoate.* p-*Tolyl isovalerate. FEMA 3387*
$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient.

Octanoyl: [59558-23-5] *4-Methylphenyl octanoate.* p-*Tolyl caprylate. FEMA 3733*
$C_{15}H_{22}O_2$ 234.338
Flavouring ingredient. d_4^{24} 0.96. Bp_{12} 175°.

Dodecanoyl: [10024-57-4] *4-Methylphenyl dodecanoate.* p-*Tolyl laurate. FEMA 3076*
$C_{19}H_{30}O_2$ 290.445
Flavouring ingredient with a mild, floral, sweet odour and taste. Liq.

Benzoyl: [614-34-6] p-*Tolyl benzoate*
$C_{14}H_{12}O_2$ 212.248
Cryst. Mp 71-72°.

▶ DH7050000

Me ether: [104-93-8] *1-Methoxy-4-methyl-*

benzene. Methyl p-*tolyl ether. 4-Methoxytoluene. FEMA 2681*
$C_8H_{10}O$ 122.166
Isol. from ylang-ylang, cananga and other essential oils. Also present in tomato and Camembert cheese. Flavouring ingredient. Liq. with pungent ylang-ylang odour. Bp 175-176°.

▶ Skin irritant. LD_{50} (rat, orl) 1920 mg/kg. BZ8780000

Trifluoromethyl ether: [706-27-4] *1-Methyl-4-(trifluoromethoxy)benzene, 9CI*
$C_8H_7F_3O$ 176.138
d 1.18. Mp 134-135°. Bp_{100} 79°.

Et ether: [622-60-6] *1-Ethoxy-4-methylbenzene. Ethyl* p-*tolyl ether. 4-Ethoxytoluene*
$C_9H_{12}O$ 136.193
Liq. Bp 188-189°.

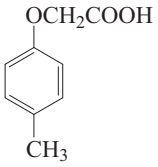
Ph ether: [1706-12-3] *Phenyl* p-*tolyl ether. 4-Methyldiphenyl ether. 4-Phenoxytoluene*
$C_{13}H_{12}O$ 184.237
Liq. Bp_{745} 277-278°.

[1121-70-6, 22113-51-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1042C; 1075D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 184B; 185A; 1244B; 1287A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 970C; 971B; 1008A; 1379D (*ir*)
U.K. Pat., 1928, 308 220; *CA*, **24**, 130 (*synth*)
Brückner, H. *et al., Z. Anorg. Allg. Chem.*, 1928, **75**, 289 (*purifn*)
U.S. Pat., 1929, 1 778 858; *CA*, **25**, 115 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 175 (*synth*)
Adv. Chem. Ser., 1955, **15**, 276 (***props***)
Naves, Y.-R. *et al., Helv. Chim. Acta*, 1959, **42**, 1692 (*isol, deriv*)
Sheppard, W.A. *et al., J.O.C.*, 1964, **29**, 1 (*trifluoromethyl ether*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 389 (*rev, tox*)
Flood, P.F. *et al., J. Chem. Ecol.*, 1989, **15**, 2207
Rasmussen, L.E.L. *et al., J. Chem. Ecol.*, 1990, **16**, 2167
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 133 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 758-762 (*esters*)
Haga, N. *et al., J.O.C.*, 1996, **61**, 735 (*Ph ether, synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 735; 1716; 2810-2815 (*occur, props, derivs*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2597
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 189
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 345
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNX250; MGP000; TGX100; MNR250

(4-Methylphenoxy)acetic acid, 9CI M-574

[940-64-7]
(p-Tolyloxy)acetic acid, 8CI



$C_9H_{10}O_3$ 166.176
Needles (H_2O). Mp 136-137°.

Me ester: [38768-63-7]
$C_{10}H_{12}O_3$ 180.203
Bp 257°.

Et ester: [67028-40-4] *Ethyl 4-methylphenoxyacetate. FEMA 3157*
$C_{11}H_{14}O_3$ 194.23
Flavouring ingredient. Bp_{740} 266-267°.

Chloride: [15516-47-9]
$C_9H_9ClO_2$ 184.622
Mp 23°. Bp_{20} 135°.

Amide: [35368-57-1]
$C_9H_{11}NO_2$ 165.191
Cryst. (C_6H_6). Mp 126-127°.

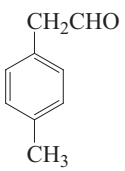
Hydrazide: [36304-39-9]
$C_9H_{12}N_2O_2$ 180.206
Mp 136°.

Nitrile: [33901-44-9]
C_9H_9NO 147.176
Needles. Mp 40°. Bp_{28} 148-149°.

Higginbotham, L. *et al., J.C.S.*, 1920, **117**, 1534-1542 (*synth*)
Gopalakrishnan, T. *et al., Acta Cryst. B*, 1981, **37**, 2085-2087 (*cryst struct*)
Kumar, S.V. *et al., Z. Kristallogr.*, 1982, **161**, 45-51 (*cryst struct*)
Deshmukh, J.G. *et al., Synth. Commun.*, 1986, **16**, 479-483 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 269 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1044 (*Et ester*)

(4-Methylphenyl)acetaldehyde M-575

[104-09-6]
4-Methylbenzeneacetaldehyde, 9CI. p-*Tolylacetaldehyde, 8CI. FEMA 3071*



$C_9H_{10}O$ 134.177
Flavouring ingredient with bitter almond odour and flavour. Needles. Mp 40°. Bp 221-222° Bp_{10} 96°.

Oxime: [66444-17-5]
$C_9H_{11}NO$ 149.192
Prisms (Et_2O). Mp 126-126.5°.

Semicarbazone: [16742-19-1]
Cryst. (EtOH). Mp 208°.

Ried, W. *et al., Annalen*, 1961, **642**, 121 (*synth*)
Lethbridge, A. *et al., J.C.S. Perkin 1*, 1973, 35 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 877 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 757
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2808-2809

2-Methyl-4-phenylbutanal M-576

[40054-82-8]

[186895-72-7]
α-Methylbenzenebutanal, 9CI. FEMA 2737
$PhCH_2CH_2CH(CH_3)CHO$
$C_{11}H_{14}O$ 162.231

(±)-*form*
Flavouring ingredient. d_{20}^{20} 0.95. $Bp_{2.4}$ 134-136° $Bp_{0.4}$ 54-57° $Bp_{0.15}$ 53-55°. n_D^{20} 1.5059.
Köster, R. *et al., Annalen*, 1976, 1116-1134 (*synth, pmr, ir, ms*)
Coutrot, P. *et al., J. Chem. Res., Miniprint*, 1977, 3401-3416; *J. Chem. Res., Synop.*, 1977, 308 (*synth*)
Chatani, N. *et al., J.A.C.S.*, 1986, **108**, 7361-7373 (*synth, ir, pmr*)
Miwa, K. *et al., Synlett*, 1994, 109 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 548 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1838 (*use*)
Hoffmann, R.W. *et al., Synthesis*, 2002, 207-212 (*synth, pmr, cmr*)

3-Methyl-2-phenylbutanal M-577

[2439-44-3]
α-(1-Methylethyl)benzeneacetaldehyde, 9CI. FEMA 2738
$(H_3C)_2CHCHPhCHO$
$C_{11}H_{14}O$ 162.231

(±)-*form* [107847-15-4]
Flavouring ingredient. Liq. Bp 238° Bp_{15} 107-112°.
Lodge, E.P. *et al., J.A.C.S.*, 1987, **109**, 3353 (*synth, ir, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 549
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1838-1839

2-Methyl-4-phenyl-2-butanol, 8CI M-578

[103-05-9]
α,α-Dimethylbenzenepropanol, 9CI. Dimethylphenylethylcarbinol. FEMA 3629
$PhCH_2CH_2C(CH_3)_2OH$
$C_{11}H_{16}O$ 164.247
Flavouring ingredient. Needles or liq. with lily-like odour. Mp 29-30°. Bp 238° Bp_{17} 128° Bp_3 71-94°. n_D^{21} 1.5077.

▶ LD_{50} (rat, orl) 2200 mg/kg. LD_{50} (rbt, skn) 3500 mg/kg. EL5785000

Phenylurethane:
Cryst. (petrol). Mp 139.1-140.1°.

Ac: [103-07-1] *3-Acetoxy-3-methyl-1-phenylbutane. Phenyl*-tert-*amyl acetate. Centifolia. FEMA 2735*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. Liq. with a jasmine and hyacinth-like odour. d_{20}^{20} 0.98. Bp_{12} 125-126° Bp 275°. n_D^{20} 1.4890.

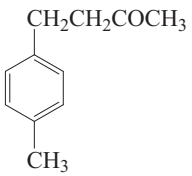
2-Methylpropanoyl: [10031-71-7] *FEMA 2736*
$C_{15}H_{22}O_2$ 234.338

Flavouring ingredient with a fruit juice flavour. Liq. Bp 250°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1155C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 390B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1076D (*ir*)
Kinzerskaya, K.N. *et al., Zh. Prikl. Khim. (Leningrad)*, 1940, **13**, 222; *J. Appl. Chem. USSR (Engl. Transl.)*, 1940, **13**, 226 (*Ac, synth*)
Oki, M. *et al., Tetrahedron*, 1961, **16**, 139-145 (*pmr*)
Warrick, P. *et al., J.A.C.S.*, 1962, **84**, 4095-4100 (*synth*)
Kochi, J.K. *et al., J.O.C.*, 1963, **28**, 1960-1968 (*synth*)
Nicolas, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1967, **265**, 1044-1047 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 537 (*rev, tox*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl. No. 1, 1978, **16**, 721 (*Ac, rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 546-547
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1834-1835; 1836-1837
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEC250

4-(4-Methylphenyl)-2-butanone, 9CI M-579

[7774-79-0]
*4-*p*-Tolyl-2-butanone. FEMA 3074*

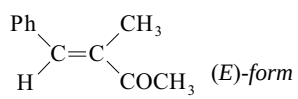


$C_{11}H_{14}O$ 162.231
Flavouring ingredient. Oily liq. with intense sweet fruity flavour. $Bp_{0.6}$ 69°.

Yamashita, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 835-838 (*synth*)
Cabello, J.A. *et al., J.O.C.*, 1986, **51**, 1786-1790 (*synth*)

3-Methyl-4-phenyl-3-buten-2-one, 9CI, 8CI M-580

[1901-26-4]
3-Benzylidene-2-butanone. FEMA 2734



(*E*)-*form*

$C_{11}H_{12}O$ 160.215
►EN0214000
(*E*)-*form* [42968-14-9]
Flavouring ingredient. Needles with a camphor-like odour. Mp 38-39°. Bp_{12} 130° Bp_1 88-93°.

Oxime:
$C_{11}H_{13}NO$ 175.23
Mp 104°.

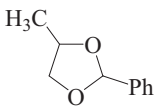
Phenylhydrazone:
Mp 105°.
(*Z*)-*form* [53793-27-4]
Pale-yellow oil.

Hightower, L.E. *et al., J.O.C.*, 1970, **35**, 1881 (*synth, nmr, ir*)
Rocquet, F. *et al., Bull. Soc. Chim. Fr.*, 1974, 888 (*synth, config*)
Eagen, M.C. *et al., J.O.C.*, 1974, **39**, 911 (*synth, nmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 547
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1835-1836

4-Methyl-2-phenyl-1,3-dioxolane, 9CI, 8CI M-581

[2568-25-4]

[5932-73-0, 25687-62-1, 25687-67-6, 51591-49-2, 71275-64-4, 71275-65-5, 188663-13-0]
Benzaldehyde propylene glycol acetal. FEMA 2130

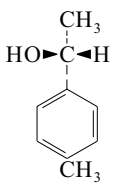


$C_{10}H_{12}O_2$ 164.204
Reported in port wine. Flavouring ingredient for beverages and candies. Artifact in benzaldehyde-based artificial flavours. Stabiliser for aspartame in chewing-gum formulations. Liq. with mild almond odour. d_4^{20} 1.07. $Bp_{0.25}$ 70°. Bp data is for a 3:2 mixt. of *cis*/*trans* isomers.

Piantadosi, C. *et al., J.A.C.S.*, 1958, **80**, 6613-6617 (*synth*)
Heydanek, M.G. *et al., J. Food Sci.*, 1976, **41**, 145-147 (*glc, occur*)
Grindley, T.B. *et al., Carbohydr. Res.*, 1979, **74**, 7-30 (*pmr, cmr*)
Sidhaghatta, D. *et al., J.O.C.*, 1979, **44**, 3082-3084 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 95; 113S-114S (*tox, props, rev*)
U.S. Pat., 1994, 5 277 919; *CA*, **120**, 132792r (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 130 (*use*)

1-(4-Methylphenyl)ethanol M-582

[536-50-5]
*α,4-Dimethylbenzenemethanol, 9CI. α,4-Dimethylbenzyl alcohol, 8CI. 1-*p*-Tolylethanol. Methyl-*p*-tolylcarbinol. 4-(1-Hydroxyethyl)toluene. FEMA 3139*



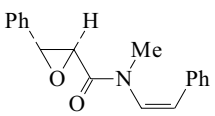
$C_9H_{12}O$ 136.193
►LD_{50} (rat, orl) 2800 mg/kg. DO4565000
(*R*)-*form* [42070-92-8]
Liq. Bp_{10} 101.5°. $[\alpha]_D^{22}$ +56 (liq.).
(*S*)-*form* [51154-54-2]
$[\alpha]_D^{25}$ -50.7 (c, 0.1 in $CHCl_3$).
(±)-*form* [5788-09-0]
Isol. from rhizomes of *Curcuma domestica*. Thick oil with an odour reminiscent of menthol. Bp 219° Bp_8 102°.

Phenylurethane:
Mp 94.5-95°.
(ξ)-*form*
Isol. from rhizomes of *Curcuma domestica*.

Dieterle, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1933, **271**, 337 (*isol*)
Overberger, C.G. *et al., J.A.C.S.*, 1952, **74**, 4848 (*synth*)
Wiberg, K.R. *et al., J.A.C.S.*, 1955, **77**, 277 (*synth*)
Protiva, M. *et al., Coll. Czech. Chem. Comm.*, 1962, **27**, 2102 (*synth*)
Cervinka, O. *et al., Coll. Czech. Chem. Comm.*, 1973, **28**, 441; 3299 (*synth, pmr*)
Schwarz, H. *et al., Tetrahedron*, 1973, **29**, 1735 (*ms*)
Vigneron, J.P. *et al., Tetrahedron*, 1976, **32**, 939 (*synth*)
Mathre, D.J. *et al., J.O.C.*, 1993, **58**, 2880 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 174
Akakabe, Y. *et al., J.C.S. Perkin 1*, 1995, 1295 (*S-form*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 848-849
Kuwano, R. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 485-496 (*S-form, synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGZ000

N-Methyl-*N*-(2-phenylethenyl)-3-phenyl-2-oxiranecarboxamide M-583

[173220-67-2]
SB 204900



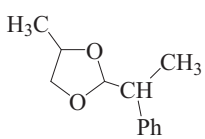
Relative configuration

$C_{18}H_{17}NO_2$ 279.338
Isol. from leaves of *Clausena lansium* (wampee). Mp 59-60°. $[\alpha]_D^{25}$ +14 (c, 1.0 in $CHCl_3$).

Milner, P.H. *et al., J. Nat. Prod.*, 1996, **59**, 400 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Stefanuti, I. *et al., Tet. Lett.*, 2000, **41**, 3735-3738 (*synth*)

4-Methyl-2-(1-phenylethyl)-1,3-dioxolane, 9CI M-584

[67634-23-5]
Hydratropic aldehyde propylene glycol acetal



$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Poorly documented.

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1351 (*use*)

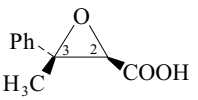
5-Methyl-2-phenyl-2-hexenal, 8CI M-585

[21834-92-4]
α-(3-Methylbutylidene)benzeneacetaldehyde, 9CI. FEMA 3199
$(H_3C)_2CHCH_2CH{=}CPhCHO$
$C_{13}H_{16}O$ 188.269
Constit. of various plant spp. and cooked foods e.g. cocoa beans and roasted peanut. Flavouring ingredient. $Bp_{6.7}$ 96-100°.

Stoffelsma, J. *et al., J. Agric. Food Chem.*, 1968, **16**, 1000-1004; *CA*, **70**, 2551z (*occur*)
Ger. Pat., 1969, 1 921 500; *CA*, **72**, 66381z (*synth*)
Waller, G.R. *et al., J. Agric. Food Chem.*, 1971, **19**, 1025-1027; *CA*, **75**, 108669n (*occur*)
Raspotnig, G. *et al., J. Insect Physiol.*, 1998, **44**, 413-417 (*isol*)

3-Methyl-3-phenyloxiranecarboxylic acid, 9CI M-586

[5669-15-8]
2,3-Epoxy-3-phenylbutanoic acid. α,β-Epoxy-β-methylhydrocinnamic acid. β-Methyl-β-phenylglycidic acid



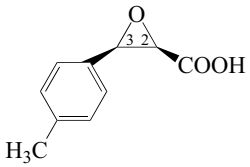
(2*R*,3*S*)-*form*

$C_{10}H_{10}O_3$ 178.187
(2*R*,3*S*)-*form*
(-)-trans-*form*
Et ester:
Bp_2 84°. $[\alpha]_D^{25}$ -85.6.
(2*S*,3*R*)-*form* *(+)*-trans-*form*
Et ester:
Bp_2 84°. $[\alpha]_D^{25}$ +128.8.
(2*RS*,3*SR*)-*form* *(±)*-trans-*form*
Et ester: [77-83-8] *Phenylmethylglycidic ester. Strawberry aldehyde. Aldehyde C_{16} (misleading). Fraise pure. Fraeseol. FEMA 2444*
$C_{12}H_{14}O_3$ 206.241
Fragrance used in food. Liq. with strawberry odour and taste. Bp_3 111-114°. Bp refers to a mixture of (±)-*cis*- and *trans*-forms. The two isomers have been sepd. by glc; the *cis*-form has the stronger fragrance.
► MW5250000

Org. Synth., Coll. Vol., 3, 1955, 727 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 96 (*tox, rev*)
Kraus, G.A. *et al., Tet. Lett.*, 1977, 4575 (*synth*)
Mosandl, A. *et al., Z. Lebensm.-Unters.-Forsch.*, 1977, **163**, 255; *CA*, **87**, 134862n
Abidi, S.L. *et al., J.O.C.*, 1979, **44**, 433 (*resoln, abs config*)
Domagalu, J.M. *et al., J.O.C.*, 1979, **44**, 3168 (*synth, pmr, abs config*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ENC000

3-(4-Methylphenyl)oxiranecarboxylic acid, 9CI M-587

[81476-88-2]



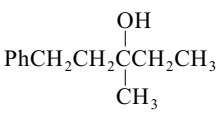
(2*R*,3*R*)-*form*

$C_{10}H_{10}O_3$ 178.187
Esters used in perfumery and flavouring. No phys. props. reported. CAS no. refers to Na salt.
(2*R*,3*R*)-*form*
Et ester: [143614-97-5]
$C_{12}H_{14}O_3$ 206.241
Cryst. (diisopropyl ether). Mp 66°.
(2*S*,3*R*)-*form* [136778-52-4]
Me ester: [132633-82-0]
$C_{11}H_{12}O_3$ 192.214
Mp 50°. $[\alpha]_D^{20}$ +209 (c, 0.2 in MeOH) (100% op).
(2*RS*,3*SR*)-*form* *(±)*-trans-*form*
Et ester: [87314-60-1]
Bp_{16} 160-164°.
[136778-53-5]

Banzal, R.K. *et al., Gazz. Chim. Ital.*, 1980, **110**, 109 (*Et ester, ms*)
Marcello, J.A. *et al., J.A.C.S.*, 1982, **104**, 3441 (*synth, Na salt*)
Svoboda, J. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 822 (*Me ester, synth*)
Murray, R.W. *et al., J.C.S. Perkin 2*, 1990, 349 (*Et ester, synth, pmr*)
Eur. Pat., 1991, 417 785; *CA*, **115**, 230541y (*Me ester, resoln*)
Pat. Coop. Treaty (WIPO), 1992, 92 09 589; *CA*, **117**, 251589c (*Et ester, chiral synth*)

3-Methyl-1-phenyl-3-pentanol M-588

[10415-87-9]
Ethylmethylphenethylcarbinol. α-Ethyl-α-methylbenzenepropanol. FEMA 2883



$C_{12}H_{18}O$ 178.274
► SA7624000
(±)-*form* [7321-45-1]
Flavouring ingredient. Liq. with fruity odour. Bp 254° Bp_{12} 132-133°. n_D^{20} 1.5100.
Ac:
$C_{14}H_{20}O_2$ 220.311

Klages, A. *et al., Ber.*, 1904, **37**, 2301 (*synth*)
Pines, H. *et al., J.A.C.S.*, 1957, **79**, 4958 (*synth*)
Amoore, J.E. *et al., J. Food Sci.*, 1966, **31**, 118; *CA*, **64**, 11645d
Montgomery, F.C. *et al., J.O.C.*, 1976, **41**, 2368 (*synth*)
Wrobel, D. *et al., Chem. Ber.*, 1982, **115**, 1694 (*pmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 644
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2191-2192
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PFR200

4-Methyl-1-phenyl-2-pentanol M-589

[7779-78-4]
α-(2-Methylpropyl)benzeneethanol, 9CI. Benzylisobutylcarbinol. FEMA 2208
$(H_3C)_2CHCH_2CH(OH)CH_2Ph$
$C_{12}H_{18}O$ 178.274
► DA0513300
(±)-*form*
Flavouring ingredient. Cryst. (C_6H_6). Mp 129°. Bp 250°.
Ac:
$C_{14}H_{20}O_2$ 220.311Poorly documented.

Petyunin, P.A. *et al., CA*, 1944, **38**, 950[9] (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 396
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1457-1458

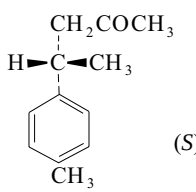
4-Methyl-1-phenyl-2-pentanone, 9CI M-590

[5349-62-2]
Benzyl isobutyl ketone. Isopropylphenylacetone. FEMA 2740
$(H_3C)_2CHCH_2COCH_2Ph$
$C_{12}H_{16}O$ 176.258
Flavouring ingredient. Yellow liq. with a sweet, woody, spicy odour. d^4 0.97. Bp 250.5° Bp_{15} 122°.
Phenylhydrazone:
Mp 67°.
Semicarbazone: [32508-82-0]
Mp 80°.

Ivanoff, D. *et al., Bull. Soc. Chim. Fr.*, 1932, **51**, 1334 (*synth*)
Sund, E.H. *et al., J. Chem. Eng. Data*, 1970, **15**, 200 (*synth*)
Dran, R.B. *et al., C. R. Hebd. Seances Acad. Sci.*, 1971, **272**, 1664 (*synth*)
Decock, P. *et al., Bull. Soc. Chim. Fr.*, 1973, 2889 (*uv*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 551
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1840-1841

4-(4-Methylphenyl)-2-pentanone, 9CI M-591

[451-25-2]
4-p-Tolyl-2-pentanone. Curcumone



(*S*)-*form*

$C_{12}H_{16}O$ 176.258
(*S*)-*form* [69657-27-8]
Isol. from rhizomes of *Curcuma longa*

(turmeric). Bp_{10} 120°. $[\alpha]_D^{30}$ +48.21 (neat). Artifact.

(±)-*form* [65075-32-3]
Bp_{12} 130°.

Semicarbazone:
Mp 144-145°.

Oxime:
Bp_{10} 160-161°.

Gandhi, R.P. *et al., Tetrahedron*, 1959, **7**, 236 (*synth*)
Banno, K. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 2284 (*synth*)
Hansson, A.T. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 483 (*synth*)
Ho, T.L. *et al., Synth. Commun.*, 1981, **11**, 579 (*synth*)
John, T.K. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 35 (*synth*)

4-Methyl-2-phenyl-2-pentenal, 8CI M-592

[26643-91-4]
α-(2-Methylpropylidene)benzeneacetaldehyde, 9CI. FEMA 3200

$(H_3C)_2CHCH{=}CPhCHO$

$C_{12}H_{14}O$ 174.242

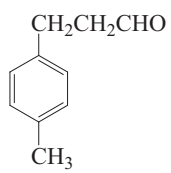
Present in aroma volatiles of roast filbert, tea, peppermint and krill seasoning. Ingredient of cocoa and chocolate-type flavours.. Liq. with cocoa aroma. $Bp_{0.7}$ 82-87°.

Ger. Pat., 1969, 1 921 560; *CA*, **72**, 66387z (*synth, use*)
Coleman, E.C. *et al., J. Agric. Food Chem.*, 1981, **29**, 42-48 (*glc, occur, potato*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 551 (*use*)
Baek, H.H. *et al., J. Food Sci.*, 1998, **63**, 234-237 (*glc, occur, chicory*)

2-(4-Methylphenyl)propanal M-593

[99-72-9]

[122091-53-6, 122091-55-8]
α,4-Dimethylbenzeneacetaldehyde, 9CI. p-*Methylhydratropaldehyde, 8CI.* p-*Methylhydratropic aldehyde. 2-*p-*Tolylpropionaldehyde. FEMA 3078*



$C_{10}H_{12}O$ 148.204
Occurs in parsley oil.

(±)-*form* [33596-66-6]
Used in caraway food flavouring. Oil with peppermint-like odour. d_4^{20} 0.98. Bp_{15} 125° Bp_{10} 92-93° Bp_6 92°. n_D^{25} 1.5122. Enantiomers prepared but not characterised.

Semicarbazone:
Cryst. (EtOH). Mp 158°.

Dutta, P.S. *et al., J. Indian Chem. Soc.*, 1941, **18**, 233-237 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 607 (*rev, props, use*)
Strubell, W. *et al., J. Prakt. Chem.*, 1977, **10**, 349-350 (*synth*)
Bokel, H.H. *et al., Tetrahedron*, 1980, **36**, 651-654 (*synth*)
Bansal, R.K. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 121-124 (*synth*)
MacLeod, A.J. *et al., Phytochemistry*, 1985, **24**, 2623-2627 (*occur*)
Takano, S. *et al., Chem. Comm.*, 1988, 1538-1540 (*chiral synth*)
Svoboda, J. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 822-832 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 762
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2815-2816

2-Methyl-1-phenyl-2-propanol M-594

[100-86-7]
α,α-Dimethylbenzeneethanol, 9CI. α,α-Dimethylphenethyl alcohol, 8CI. Benzyldimethylcarbinol. FEMA 2393

$(H_3C)_2C(OH)CH_2Ph$

$C_{10}H_{14}O$ 150.22
Flavouring ingredient. Present in cocoa. Needles or oil with floral-herbaceous odour. Mp 24°. Bp 214-216° Bp_1 58°. n_D^{20} 1.5170 (supercooled liq.).

► LD_{50} (rat, orl) 1280 mg/kg. SG8050000

Ac: [151-05-3] *FEMA 2392*
$C_{12}H_{16}O_2$ 192.257
Flavouring agent. Liq. with flowery, woody odour. Mp 30°. Bp_{10} 102-103°. n_D^{20} 1.4923 (supercooled liq.).

► Skin irritant. LD_{50} (rat, orl) 3300 mg/kg. SG8100000

Butanoyl: [10094-34-5] *FEMA 2394*
$C_{14}H_{20}O_2$ 220.311
Flavouring agent. Liq. with fruity, herbal odour and plum-like flavour. Bp_3 96°.

► n_D^{20} 1.4880. ET0130000

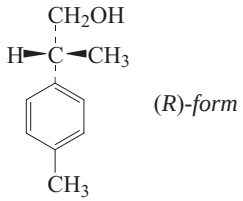
Benzoyl: [19284-03-8]
$C_{17}H_{18}O_2$ 254.328
$Bp_{0.15}$ 105°.

Formyl: [10058-43-2] *α,α-Dimethylphenethyl formate. FEMA 2395*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient with a spicy taste. Liq.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 386A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1074C (*ir*)
Cekovic, Z. *et al., Tetrahedron*, 1967, **23**, 3095 (*synth*)
Hansen, H.J. *et al., J.O.C.*, 1977, **42**, 3011
Dube, M.F. *et al., Tetrahedron*, 1980, **36**, 1753 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DQQ200
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 187-188 (*props, esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 867; 868; 869 (*props, esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEL750; DQQ200; BEL850

2-(4-Methylphenyl)-1-propanol M-595

[4371-50-0]
β,4-Dimethylbenzeneethanol, 9CI. p-*Cymen-9-ol, 8CI. 2-(*p-*Tolyl)-1-propanol*



(R)-form

$C_{10}H_{14}O$ 150.22
Volatile component of apricots.

(*R*)-*form* [122091-54-7]
Liq. $[\alpha]_D^{24}$ +14.01 (c, 1.26 in $CHCl_3$) (>98% ee).

(*S*)-*form* [93922-51-1]
Liq. $[\alpha]_D^{24}$ -14.05 (c, 1.22 in $CHCl_3$) (>98% ee).

Ac: [145621-76-7]
$C_{12}H_{16}O_2$ 192.257
$[\alpha]_D$ -6.5 (c, 0.93 in $CHCl_3$).

(±)-*form* [75316-56-2]
Liq. Bp_5 102°.

4-Methylbenzenesulfonyl:

[23430-44-6]
$C_{17}H_{20}O_3S$ 304.409
Cryst. Mp 49-50°.

DePuy, C.H. *et al., J.O.C.*, 1970, **35**, 2746-2750 (*synth*)
Bokel, H.H. *et al., Tetrahedron*, 1980, **36**, 651-654 (*synth, ir, pmr, ms*)
Gharpure, M.M. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 1214-1215 (*synth*)
Takano, S. *et al., Chem. Comm.*, 1988, 1538-1540 (*R-form, S-form, synth*)
Matsumoto, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1721-1726; 1993, **41**, 1459-1461 (*synth, resoln, ir, pmr, Ac*)
Kinoshita, T. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 816-823 (*synth*)
Chen, A. *et al., J.O.C.*, 1999, **64**, 9704-9710 (*R-form, synth*)

2-(4-Methylphenyl)-2-propanol M-596

[1197-01-9]
*α,α,4-Trimethylbenzenemethanol, 9CI. α,α,4-Trimethylbenzyl alcohol, 8CI. Dimethyl-*p-*tolylcarbinol. α-Hydroxy-*p-*cymene.* p-*(Hydroxyisopropyl)toluene. 8-*p-*Cymenol.* p-*Mentha-1,3,5-trien-8-ol. FEMA 3242*

$C_{10}H_{14}O$ 150.22
Occurs in essential oils, e.g. *Citrus reticulata* and various fresh fruits. Flavouring ingredient. d^{20} 0.98. Mp 9°. Bp_{75} 145° Bp_{16} 112°. n_D^{20} 1.5173.

Phenylurethane:
Mp 119-120°.

*Me ether:1-(1-Methoxy-1-methylethyl)-4-methylbenzene. 8-Methoxy-*p-*cymene. 8-Methoxy-*p-*mentha-1,3,5-triene*
$C_{11}H_{16}O$ 164.247
Isol. from lime (*Citrus aurantifolia*) oil. Liq. d^{20} 0.93. Bp_9 90-94°. n_D^{20} 1.4958.

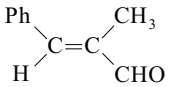
Et ether:
$Bp_{0.5}$ 63-63.5°.

McBay, H.C. *et al., J.O.C.*, 1954, **19**, 869 (*synth*)
Marayama, K. *et al., Nippon Kagaku Kaishi*, 1960, **81**, 1883; *CA*, **56**, 3385 (*synth*)

Oki, M. *et al., Bull. Chem. Soc. Jpn.*, 1963, **36**, 1 (*pmr*)
Kugler, E. *et al., Helv. Chim. Acta*, 1963, **46**, 1480 (*isol*)

2-Methyl-3-phenyl-2-propenal, 9CI M-597

[101-39-3]
α-Methylcinnamaldehyde, 8CI. 2-Methyl-3-phenylacrolein. FEMA 2697



(*E*)-*form*

$C_{10}H_{10}O$ 146.188
Present in peppermint oil (*Mentha piperita*). Flavour ingredient. Yellow oil with cinnamon-like odour and spicy flavour.
▶ Skin irritant. LD_{50} (rat, orl) 2050 mg/kg. GD6600000

(*E*)-*form* [15174-47-7]
trans-*form*
Bp_{100} 150° Bp_4 97-99°.

Semicarbazone:
Cryst. (EtOH aq.). Mp 209-210°.

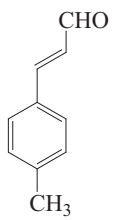
4-Nitrophenylhydrazone:
Violet needles. Mp 203°.

(*Z*)-*form* [66051-14-7] cis-*form*Unstable, easily isomerises to (*E*)-form.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 927A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 102B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1281B (*ir*)
v. Auwers, K. *et al., Ber.*, 1912, **45**, 2764 (*synth*)
Satsumabayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 1586 (*synth, ir*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Corey, E.J. *et al., Tet. Lett.*, 1976, 7 (*synth*)
Sato, T. *et al., J.A.C.S.*, 1977, **99**, 5827 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MIO000
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

3-(4-Methylphenyl)-2-propenal, 9CI M-598

[1504-75-2]
p-*Methylcinnamaldehyde, 8CI. 3*-p-*Tolylacrolein. FEMA 3640*



$C_{10}H_{10}O$ 146.188
Flavouring ingredient. Yellow leaflets (EtOH aq.). Mp 41.5°. Bp_{25} 154°.

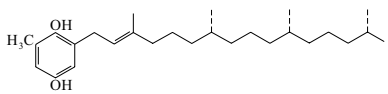
Oxime:
$C_{10}H_{11}NO$ 161.203
Mp 136°.

Semicarbazone:
Needles (EtOH). Mp 210°.

Meyers, A.I. *et al., J.A.C.S.*, 1969, **91**, 764 (*synth*)
Meyers, A.I. *et al., J.O.C.*, 1973, **38**, 36 (*synth*)
Lutskii, A.E. *et al., Zh. Strukt. Khim.*, 1973, **4**, 566 (*ir*)
Savin, G.I. *et al., Zh. Org. Khim.*, 1975, **11**, 1169 (*pmr*)
Bellassoued, M. *et al., J.O.C.*, 1993, **58**, 2517 (*synth, pmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 489
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1743

2-Methyl-6-phytylhydroquinone M-599

[54432-31-4]
2-Methyl-6-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-benzenediol, 9CI. 6-Phytyltoluquinol



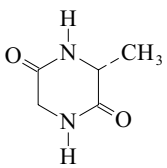
$C_{27}H_{46}O_2$ 402.659
Precursor of tocopherol synth. in spinach chloroplasts.

[75513-85-8]

Inoue, S. *et al., J.C.S. Perkin 1*, 1974, 2097 (*synth*)
Soll, J. *et al., Phytochemistry*, 1980, **19**, 215 (*biosynth*)
Marshall, P.S. *et al., Phytochemistry*, 1985, **24**, 1705 (*biosynth, metab*)

3-Methyl-2,5-piperazinedione, 9CI M-600

3-Methyl-2,5-dioxopiperazine. Glycylalanine anhydride. Methyldiacipiperazine. Cyclo(alanylglycyl). Alanylglycine anhydride



(*R*)-*form*

$C_5H_8N_2O_2$ 128.13

(*R*)-*form* [88547-15-3]
D-*form*
Cryst. Mp 247.5-249.5°. $[\alpha]_D^{25}$ +3.56 (H_2O).

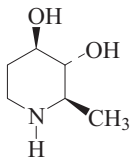
(*S*)-*form* [4526-77-6]
L-*form*
Present in roasted cocoa beans. Cryst. with a bitter taste. Mp 247° dec. $[\alpha]_D^{20}$ -5 (H_2O). Sublimes.

(±)-*form* [6062-46-0]
Needles (EtOH aq.). Sol. H_2O, hot EtOH, spar. sol. Me_2CO. Mp 244°. Reacts neutral. Tasteless.

Heimrod, G.O. *et al., Ber.*, 1914, **47**, 344 (*synth*)
Abderhalden, E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1925, **145**, 308 (*synth*)
Birkofer, L. *et al., Annalen*, 1962, **659**, 190 (*synth*)
Pickenhagen, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1078-1086 (*occur*)
Chu, D.T.W. *et al., J. Med. Chem.*, 1991, **34**, 168 (*synth, pmr*)

2-Methyl-3,4-piperidinediol, 9CI M-601

3,4-Dihydroxy-2-methylpiperidine



$C_6H_{13}NO_2$ 131.174

(2*R*,3*R*,4*R*)-*form* [197449-09-5]
6-Deoxyfagomine
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ -11.1 (c, 0.1 in H_2O).

Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*6-deoxyfagomine, isol, pmr, cmr, ms*)

2-Methylpropanal, 9CI M-602

[78-84-2]
Isobutanal. Isobutyraldehyde. FEMA 2220
$(H_3C)_2CHCHO$
C_4H_8O 72.107
Found in tea, beer, sake, brandy, fresh fruits (apple, banana, cherry etc.), breads, cooked pork, and spearmint oil. Flammable liq. with pungent odour. Misc. most org. solvs.; mod. sol. H_2O. d_4^{20} 0.79. Fp -65.9. Bp 63-64°. n_D^{20} 1.3725. Forms azeotrope with water Bp 59° (contains 6% H_2O).
▶ Highly flammable, fl. p. -40°/-25°, autoignition temp. 196°. Severe eye and skin irritant. LD_{50} (rat, orl) 960 mg/kg. NQ4025000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 466B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 727B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 551C (*ir*)
U.K. Pat., 1930, 354 388; *CA*, **26**, 5310 (*synth*)
Roberts, J.D. *et al., J.O.C.*, 1974, **39**, 1017 (*cmr*)
Loeffler, C.E. *et al., Encycl. Chem. Process. Des.*, 1977, **5**, 358
Harrison, A.G. *et al., J.C.S. Perkin 2*, 1981, 1544 (*ms*)
Ullmanns Encykl. Tech. Chem., 5th edn., VCH, Weinheim, 1985, **A4**, 447 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, IJS000
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 736 (*rev*)
Piart-Goypiron, A. *et al., Spectrochim. Acta A*, 1991, **47**, 363 (*ir, Raman*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IJS000; IJT000

2-Methylpropane, 9CI, 8CI M-603

[75-28-5]
Isobutane. E943b
$(H_3C)_3CH$
C_4H_{10} 58.123
Propellant/aerating agent used in foods. Gas. Sol. EtOH, Et_2O, $CHCl_3$, spar. sol. H_2O. Fp -145. Bp -10.2°.

► An asphyxiant. Extremely flammable, fl. p. -81°, autoignition temp. 460°. TZ4300000

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 9C (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 9C (*ir*)
Coffin, C.C. *et al., J.A.C.S.*, 1920, **50**, 1427 (*synth*)
Wagner, C.D. *et al., J.A.C.S.*, 1950, **72**, 5786 (*synth*)
Weiss, M.J. *et al., J. Chem. Phys.*, 1968, **48**, 4386 (*ms*)
Pretsch, E. *et al., Helv. Chim. Acta*, 1969, **52**, 2133 (*pmr*)
Olah, G.A. *et al., J.A.C.S.*, 1972, **94**, 3551 (*pmr*)
Hays, G.E. *et al., Encycl. Chem. Process. Des.*, (McKetta, J.J. *et al*, Eds.), Dekker, N.Y., 1977, 245 (*rev*)
Pitkänen, M. *et al., Org. Magn. Reson.*, 1984, **22**, 543 (*cmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 240
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1188
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1440-1441
Low, L.K. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 273 (*rev, tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 748
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MOR750

2-Methyl-1-propanethiol, 9CI M-604

[513-44-0]
Isobutanethiol. Isobutyl mercaptan. 1-Mercaptoisobutane. Thioisobutyl alcohol. 1-Mercapto-2-methylpropane. FEMA 3874
$(H_3C)_2CHCH_2SH$
$C_4H_{10}S$ 90.189
Food additive listed in the EAFUS Food Additive Database (Jan. 2001). Found in guava, milk, cooked beef, cooked pork and beer. Flavouring ingredient. Mobile liq. with heavy skunk odour. Sl. sol. H_2O; v. sol. EtOH, Et_2O. Fp -79. Bp 88°.

► An eye irritant. LD_{50} (rat, ipr) 917 mg/kg. LD_{50} (rat, orl) 7168 mg/kg. TZ7630000

S-*Ac:* [2432-37-3]
$C_6H_{12}OS$ 132.226
Bp 148-150°.

3,5-Dinitrobenzoyl:
Mp 63-64°.

S-*Me:* [5008-69-5] *2-Methyl-1-(methylthio)propane, 9CI. Isobutyl methyl sulfide*
$C_5H_{12}S$ 104.216
Bp 110-112°.

S-*Me,* S-*oxide(±):* [26547-93-3] *2-Methyl-1-(methylsulfinyl)propane. Isobutyl methyl sulfoxide*
$C_5H_{12}OS$ 120.215
$Bp_{0.2}$ 45-46° $Bp_{0.05}$ 48-55°.

S-*Et:* [1613-45-2] *1-(Ethylthio)-2-methylpropane*
$C_6H_{14}S$ 118.243
Bp 132-134°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 258A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 415A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 339B (*ir*)
Vogel, A.I. *et al., J.C.S.*, 1943, 21 (*synth*)
Leaver, D. *et al., J.C.S.*, 1957, 39 (*synth*)
Van de Graaf, B. *et al., J.A.C.S.*, 1977, **99**, 6810 (*ms*)
Lucien, J. *et al., Ind. Eng. Chem. Prod. Res. Dev.*, 1978, **17**, 354 (*synth*)
Milkolajczyk, M. *et al., Synthesis*, 1978, 758 (*synth*)
Hwang, D.-R. *et al., J.O.C.*, 1985, **50**, 1264 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1209
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IIX000

2-Methylpropanoic acid, 9CI M-605

[79-31-2]
Isobutyric acid, 8CI. FEMA 2222
$(H_3C)_2CHCOOH$
$C_4H_8O_2$ 88.106
Present in apple, morello cherry, guava fruit, wine grapes, pineapple, crispbread, other breads, cheeses, wines, scallop and several essential oils, e.g. Roman chamomile. Acid and simple esters used as flavouring agents. Liq. with pungent rancid odour. d_4^{15} 0.95. Fp -47. Bp 153.5-154.5° Bp_{35} 118-119°. n_D^{20} 1.3930. pK_a 4.79 (4.85).

► Fl. p. 56°, autoignition temp. 481°. Corrosive and irritating to skin, eyes and mucous membranes. LD_{50} (rat, orl) 280 mg/kg. NQ4375000

Me ester: [547-63-7] *Methyl 2-methylpropanoate. Methyl isobutyrate. FEMA 2694*
$C_5H_{10}O_2$ 102.133
Found in various fruits, e.g. apple, banana, kumquat peel, wild blueberry, strawberry. Also present in French fried potato, dill herb and Russian champagnes. Flavouring agent. Liq. d_4^0 0.91. Bp 93°.

► Highly flammable, fl. p. 13° (oc). NQ5425000

Et ester: [97-62-1] *Ethyl 2-methylpropanoate, 9CI. Ethyl isobutyrate. FEMA 2428*
$C_6H_{12}O_2$ 116.16
Present in many fruits, e.g. apple, banana, orange, wine grape, strawberry, nectarine. Flavouring agent. Liq. with fruity odour. d_4^{20} 0.87. Bp 110°.

► Highly flammable, fl. p. 13°. Skin irritant. LD_{50} (mus, ipr) 800 mg/kg. NQ4675000

Propyl ester: [644-49-5] *Propyl 2-methylpropanoate. Propyl isobutyrate. FEMA 2936*
$C_7H_{14}O_2$ 130.186
Used in fruit flavouring. Liq. d^{20} 0.86. Bp_{752} 134°. n_D^{20} 1.3955.

Isopropyl ester: [617-50-5] *Isopropyl 2-methylpropanoate. Isopropyl isobutyrate. FEMA 2937*
$C_7H_{14}O_2$ 130.186
Used in fruit flavouring. d 0.85. Bp 121°.

Butyl ester: [97-87-0] *Butyl 2-methylpropanoate. Butyl isobutyrate. FEMA 2188*
$C_8H_{16}O_2$ 144.213
Present in various fruits, e.g. apple, apricot, guava fruit, melon. Also present in provolone cheese, hop oil, honey, white wine and apple brandy. Flavouring agent. Liq. with fruity odour and sweet, pineapple-like taste. d_4^{20} 0.86. Bp 155°. n_D^{20} 1.4025.

2-Methylpropyl ester: [97-85-8] *Isobutyl isobutyrate. FEMA 2189*
$C_8H_{16}O_2$ 144.213
Present in apricot, banana, melon, strawberry and other fruits. Also present in olive, myrtle berry or leaf, hop oil and white wines. Flavouring agent. Liq. with pineapple-like taste. Mp -81°. Bp 147-148°. n_D^{20} 1.3980.

► NQ5250000

Hexyl ester: [2349-07-7] *Hexyl 2-methylpropanoate. Caproyl isobutyrate*
$C_{10}H_{20}O_2$ 172.267
Flavouring ingredient. Liq. Bp 199°.

Heptyl ester: [2349-13-5] *Heptyl 2-methylpropanoate. Heptyl isobutyrate. FEMA 2550*
$C_{11}H_{22}O_2$ 186.294
Present in hop oil. Flavouring ingredient. Liq. with herbaceous, woody odour. d_{15}^{15} 0.86. Bp_{10} 98°. n_D^{20} 1.4190.

Dodecyl ester: [6624-71-1] *Dodecyl 2-methylpropanoate. Lauryl isobutyrate. FEMA 3452*
$C_{16}H_{32}O_2$ 256.428
Flavouring agent. d_4^{20} 0.85. n_D^{20} 1.4332.

Benzyl ester: [103-28-6] *Phenylmethyl 2-methylpropanoate. Benzyl isobutyrate. FEMA 2141*
$C_{11}H_{14}O_2$ 178.23
Present in Scotch spearmint oil, beer, hybrid passion fruit and cherimoya. Flavouring agent. Liq. with strawberry-like taste. d_{25}^{25} 1. Bp 229°.

► LD_{50} (rat, orl) 2850 mg/kg. NQ4550000

[996-30-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 487C; 605A; 605B; 711D; 726D; 748A; 838B; 912A (*ir, pmr*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 759B; 911B; 911C; 912A; 1166B; 1189A; 1219C; 1352A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 577D; 616A; 616B; 617A; 761C; 768C; 777D; 796B (*ir, pmr*)
Sabatier, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1911, **152**, 1046 (*Et ester*)
Lippincott, S.B. *et al., Ind. Eng. Chem.*, 1939, **31**, 118 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1023; 1978, **16**, 741 (*rev, tox*)
Ger. Pat., 1975, 2 432 527; *CA*, **82**, 156983 (*synth, Et ester*)
Caswell, L.R. *et al., J.O.C.*, 1976, **41**, 3312 (*uv*)
Ger. Pat., 1978, 2 701 354; *CA*, **89**, 146431 (*manuf*)
Olah, G.A. *et al., Synthesis*, 1978, 929 (*synth, Et ester*)
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Marr, D.H. *et al., Org. Magn. Reson.*, 1980, **13**, 28 (*cmr*)
Maccoll, A. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1988, **86**, 227 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ELS000

Attygalle, A.B. *et al., Tet. Lett.*, 1991, **32**, 4849 (*biosynth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 208; 352; 701 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 270; 345; 907-908; 999; 1282; 1331-1332; 1454; 1463; 1649; 1785; 2367 (*occur, props, esters*)
Russell, G.A. *et al., Acta Chem. Scand.*, 1998, **52**, 528-532 (*anilide*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 751
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ELS000; IIW000; IJU000; IJV000; IJW000; IJX000; MKX000

2-Methyl-1-propanol M-606

[78-83-1]

[35296-72-1]

Isobutyl alcohol, 8CI. Isobutanol. FEMA 2179

$(H_3C)_2CHCH_2OH$

$C_4H_{10}O$ 74.122

Present in fusel oil, wines and spirits and produced by fermentation of carbohydrates. Used in the manuf. of flavouring essences. Liq. Misc. EtOH, Et_2O; spar. sol. H_2O. Fp -108. Bp 108.1°.

▶ Flammable, fl. p. 25°, autoignition temp. 408°. Eye, skin and respiratory tract irritant. Causes adverse CNS effects if ingested. LD_{50} (rat, orl) 2460 mg/kg. OES: long-term 50 ppm; short-term 75 ppm. NP9625000

Formyl: [542-55-2] *2-Methylpropyl formate, 9CI. Isobutyl formate, 8CI. Tetryl formate. FEMA 2197*
$C_5H_{10}O_2$ 102.133
Found in brandy, rum, beer, and vinegar. Used in fruit flavouring. Liq. with raspberry odour. Misc. EtOH, Et_2O; v. spar. sol. H_2O. Fp -95. Bp 98.2°.

▶ Highly flammable, fl. p. 5°, autoignition temp. 320°. LQ8650000

Ac: [110-19-0] *2-Methylpropyl acetate, 9CI. Isobutyl acetate, 8CI. FEMA 2175*
$C_6H_{12}O_2$ 116.16
Found in fruits, brandies and fortified wines. Used in flavouring agents. Liq. Sol. EtOH; prac. insol. H_2O. d 0.87. Fp -98.85. Bp 118°.

▶ Eye, respiratory tract and skin irritant. High conc. narcotic. Highly flammable, fl. p. 17°, autoignition temp. 420°. AI4025000

Butanoyl: [539-90-2] *2-Methylpropyl butanoate. Isobutyl butyrate. FEMA 2187*
$C_8H_{16}O_2$ 144.213
Found in bananas. Used in food flavouring. Liq. with apple/pineapple odour. d_4^{20} 0.86. Bp 157-158°. n_D^{20} 1.4045 (1.4030).

Benzoyl: [120-50-3] *2-Methylpropyl benzoate. Isobutyl benzoate. FEMA 2185*
$C_{11}H_{14}O_2$ 178.23
Used in perfumery and food flavouring. Present in banana, sweet cherry, papaya, beer, cider and cocoa. d 1. Bp 242°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 114C; 599D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 170A; 896B; 900C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 161B; 606A; 608D (*ir*)
U.K. Pat., 1928, 324 897; *CA*, **24**, 3802 (*manuf*)
Hückel, W. *et al., J. Prakt. Chem.*, 1933, **136**, 15 (*synth*)
Birkinshaw, J.H. *et al., Biochem. J.*, 1950, **47**, 55 (*isol*)
Mackenzie, S.L. *et al., J. Chromatogr.*, 1975, **111**, 413 (*use*)
Harrison, A.G. *et al., Can. J. Chem.*, 1976, **54**, 2029 (*ms*)
Konno, C. *et al., Tetrahedron*, 1976, **32**, 325 (*cmr*)
Loeffler, C.E. *et al., Encycl. Chem. Process. Des.*, (eds. McKetta, J.J. *et al*), Dekker, N.Y., 1977, 358 (*rev*)
Siezen, R.J. *et al., J. Chromatogr.*, 1977, **130**, 151 (*use*)
Nishishita, T. *et al., Org. Mass Spectrom.*, 1977, **12**, 16 (*ms*)
Sandell, E.B. *et al., Photometric Determination of Traces of Metals*, Wiley, New York, 1977, (*use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 795 (*rev, tox*)
Molnar-Perl, I. *et al., Chromatographia*, 1983, **17**, 493 (*use*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, IIJ000; IIL000
Shiota, M. *et al., J. Agric. Food Chem.*, 1993, **41**, 2056-2062 (*butanoyl, detn, glc*)
Food Chemicals Codex, 4th edn., National Academy Press, 1996, 514-515; 665 (*butanoyl, props, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1441; 1443; 1445; 1450 (*use, occur, esters*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 46; 247 (*tox, rev*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 866
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IIJ000; IIL000; IIR000; MRI775

2-Methyl-1-propenethiol M-607

[5954-69-8, 68860-48-0]

Isobutene-1-thiol. Thioisobutyraldehyde. 2-Methylpropanethial. 1-Mercapto-2-methylpropene

$(H_3C)_2C{=}CHSH \Leftrightarrow (H_3C)_2CHC(S)H$

C_4H_8S 88.173

Tautomeric system. Enethiol form more stable. Volatile flavour component of *Allium* spp.. Bp 94-95°. n_D^{20} 1.4825. Stable in soln. at r.t..

[74635-29-3, 74635-30-6]

Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1970, **89**, 593 (*synth, pmr*)
Block, E. *et al., Tet. Lett.*, 1980, **21**, 1277 (*isom, pmr, oxide*)
Vedejs, E. *et al., J.A.C.S.*, 1988, **110**, 5452 (*synth*)
Valleé, Y. *et al., Synth. Commun.*, 1993, **23**, 1267 (*synth, pmr, cmr*)

2-Methyl-2-propen-1-ol, 9CI M-608

[513-42-8]

Methallyl alcohol. Isopropenylcarbinol

$H_2C{=}C(CH_3)CH_2OH$

C_4H_8O 72.107

Bp 114°. Forms azeotrope with water contg. 40.2% H_2O, Bp 92°.

▶ Flammable, fl.p. 33°. Skin irritant. UD5250000

Ac: [820-71-3]
$C_6H_{10}O_2$ 114.144
Bp 124°.

Butanoyl: [7149-29-3] *2-Methylallyl butyrate. FEMA 2678*
$C_8H_{14}O_2$ 142.197
Flavouring ingredient. Liq. Bp 168°.

Me ether: [22418-49-1] *3-Methoxy-2-methyl-1-propene*
$C_5H_{10}O$ 86.133
Bp_{773} 68°. n_D^{20} 1.3964.

Et ether: [24309-28-2] *3-Ethoxy-2-methyl-1-propene*
$C_6H_{12}O$ 100.16
Bp 87-88.5°.

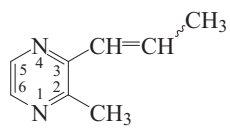
Ph ether: [5820-22-4] *2-Methyl-3-phenoxy-1-propene*
$C_{10}H_{12}O$ 148.204
Bp 175-176°. n_D^{20} 1.5140.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 138D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 207C; **2**, 207B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 201A; 985A (*Ph ether*)
Schales, O. *et al., Ber.*, 1937, **70**, 116-121 (*synth*)
Ryan, J.D. *et al., J.A.C.S.*, 1940, **62**, 3469 (*props*)
Canceill, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. B*, 1967, **265**, 918-920 (*ir*)
Krenmayr, P. *et al., Monatsh. Chem.*, 1975, **106**, 925-939 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 468 (*butanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1713-1714 (*butanoyl*)
Werkhoven, T.M. *et al., Eur. J. Org. Chem.*, 2000, 2113-2117 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IMW000

2-Methyl-3-(1-propenyl)pyrazine, 9CI M-609

[115610-67-8]

[55138-65-3]



$C_8H_{10}N_2$ 134.18

Claimed food uses are not well documented. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, pmr, ir*)

2-Methyl-3-(2-propenyl)pyrazine, 9CI M-610

[55138-62-0]

2-Allyl-3-methylpyrazine

$C_8H_{10}N_2$ 134.18

Volatile constit. of Korean salt-fermented shrimp paste (*Acetes chinensis*) and extrusion cooked wheat flour.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Cha, Y.J. *et al., J. Food Sci.*, 1995, **60**, 19-24 (*occur, shrimp*)
Farouk, K. *et al., Nahrung*, 2000, **44**, 188-192 (*occur*)

2-Methyl-5-(1-propenyl)pyrazine, 9CI M-611

[108653-51-6]

[18217-82-8, 55138-66-4]

$C_8H_{10}N_2$ 134.18
Maillard product. Constit. of okra pods, roasted green tea, roast peanut, coffee and cooked beef. Characterised spectroscopically.

Bondarovich, H.A. *et al., J. Agric. Food Chem.*, 1967, **15**, 1093-1099 (*occur, coffee, ms, ir, uv*)
Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, pmr, ir*)
Ames, J.M. *et al., Phytotherapia*, 1990, **29**, 1201-1207 (*occur, okra*)

2-Methyl-5-(2-propenyl)pyrazine, 9CI M-612

[55138-63-1]
2-Allyl-5-methylpyrazine

$C_8H_{10}N_2$ 134.18
Volatile constit. of roasted peanuts. Tentatively identified in white bread crust aroma. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Folkes, D.J. *et al., Prog. Food Nutr. Sci.*, 1981, **5**, 369-376 (*occur, bread*)

2-Methyl-6-(1-propenyl)pyrazine, 9CI M-613

[104638-11-1]

[18217-81-7, 55138-67-5]

$C_8H_{10}N_2$ 134.18
Constit. of okra pods, coffee, roasted sesame, roasted green tea and cooked beef. Characterised spectroscopically.

Bondarovich, H.A. *et al., J. Agric. Food Chem.*, 1967, **15**, 1093-1099 (*occur, coffee, ir, ms, uv*)
Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, pmr, ir*)
Shimoda, M. *et al., J. Agric. Food Chem.*, 1997, **45**, 3193-3196 (*occur, sesame*)

2-Methyl-6-(2-propenyl)pyrazine, 9CI M-614

[55138-64-2]

[80840-36-4]
2-Allyl-6-methylpyrazine

$C_8H_{10}N_2$ 134.18
Tentatively identified in white bread crust aroma. Possesses an earthy odour. Characterised spectroscopically.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, pmr, ir*)
Folkes, D.J. *et al., Prog. Food Nutr. Sci.*, 1981, **5**, 369-376 (*occur, bread*)

2-Methylpropyl glucosinolate M-615

[38226-91-4]
*1-Thio-β-D-glucoside 1-[3-methyl-*N*-(sulfooxy)butanimidate], 9CI. Isobutyl glucosinolate*

$(H_3C)_2CHCH_2C(SGlc)=NOSO_3H$

$C_{11}H_{21}NO_9S_2$ 375.42
Present in *Conringia orientalis* (hare's ear mustard) and seeds of *Brassica oleracea* (cabbage).

Underhill, E.W. *et al., Phytochemistry*, 1972, **11**, 2085 (*occur*)
Kjaer, A. *et al., Phytochemistry*, 1979, **18**, 1565 (*occur*)
Macleod, A.J. *et al., Phytochemistry*, 1989, **28**, 1405 (*occur*)

1-Methylpropyl 3-(methylthio)-2-propenyl disulfide, 9CI M-616

sec-*Butyl 3-(methylthio)allyl disulfide. 8-Methyl-2,6,7-trithia-3-decene*

$MeSCH=CHCH_2-S-S-CH(CH_3)CH_2CH_3$

$C_8H_{16}S_3$ 208.412

(+)-*form*
Constit. of *Ferula assa-foetida* (asafoetida). Oil. $Bp_{0.001}$ 90°. $[\alpha]_D^{25}$ +35.3 (c, 1.5 in $CHCl_3$). λ_{max} 207 (ε 7080); 256 (ε 11750) (MeOH).

[56019-34-2, 56019-36-4]

Naimie, H. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1166-1177 (*isol*)
Meijer, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 242 (*synth*)

1-Methylpropyl 1-propenyl disulfide, 9CI M-617

[36687-96-4]

[24351-70-0, 24351-71-1]
6-Methyl-4,5-dithia-2-octene

$H_3CCH=CH-S-S-CH(CH_3)CH_2CH_3$

$C_7H_{14}S_2$ 162.32

(-)-*form*
Constit. of *Ferula assa-foetida* (asafoetida). Oil. $[\alpha]_D^{25}$ -15.9 (c, 1.25 in EtOH). Usually obt. as a mixture of *E*/*Z* isomers. The opt. rotn. refers to a sample from *F. asafoetida* λ_{max} 210 (ε 7080); 228 (ε 500); 280 (ε 790) (MeOH).

Naimie, H. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1166-1177 (*isol*)
Min, Z. *et al., Planta Med.*, 1987, **53**, 300-302 (*isol*)

2-Methyl-1-propylamine M-618

[78-81-9]
2-Methyl-1-propanamine, 9CI. Isobutylamine, 8CI. Valamine†

$(H_3C)_2CHCH_2NH_2$

$C_4H_{11}N$ 73.138
Found in various foodstuffs. Liq. Misc. H_2O, EtOH, Et_2O. d_4^{20} 0.74. Fp -84.6. Bp 68-69°. n_D^{20} 1.3970. pK_a 10.48 (25°).
▶ Highly flammable, fl. p. -9°, autoignition temp. 378°. Very irritating to eyes, skin and mucous membranes. A vesicant. Inhalation can cause headache and dryness of nose and throat. LD_{50} (rat, orl) 228 mg/kg. NP9900000

Hydrochloride: [5041-09-8]
Cryst. (EtOH/Et_2O). Mp 177-178° (168-171°).

Hydrobromide: [74098-36-5]
Mp 138°.

N-*Formyl:* [6281-96-5] N-*(2-Methylpropyl)formamide, 9CI*. N-*Isobutylformamide*
$C_5H_{11}NO$ 101.148
Oil. Bp_{10} 115°.

N-*Ac:* [1540-94-9] N-*(2-Methylpropyl)acetamide, 9CI*. N-*Isobutylacetamide. Acetylisobutylamine*
$C_6H_{13}NO$ 115.175
Found in wine. Liq. with faint smell. Sol. H_2O. Bp_{20} 125°.

N-*Benzoyl:* [5705-57-7] N-*(2-Methylpropyl)benzamide, 9CI*. N-*Isobutylbenzamide*
$C_{11}H_{15}NO$ 177.246
Needles. Mp 55-57°. Bp 295-296°.
▶ CV5416000

N-*Me:* [625-43-4]
$C_5H_{13}N$ 87.164
Liq. Bp 76-78°.

N-*Me; hydrochloride:*
Sol. H_2O. Mp 179°.

N,N-*Di-Me:* [7239-24-9] N,N,*2-Trimethyl-1-propanamine, 9CI*
$C_6H_{15}N$ 101.191
Mp 82-85°. n_D^{20} 1.3928.

N-*Et:* [13205-60-2]
$C_6H_{15}N$ 101.191
Liq. Bp 97-98°. n_D^{25} 1.3985.

N-*Et; hydrochloride:*
Mp 209° dec.

N-*Propyl:* [39190-66-4] *2-Methyl*-N-*propyl-1-propylamine, 9CI*. N-*Propylisobutylamine. Isobutylpropylamine*
$C_7H_{17}N$ 115.218
Found in foodstuffs. Liq. with odour resembling fusel oil. Spar. sol. H_2O. Bp 123-125° (120°).

N-*Propyl, hydrochloride:*
Plates (EtOH/Et_2O). Mp 135°.

N-*Isopropyl:* [39099-24-6]
$C_7H_{17}N$ 115.218
Liq. Bp 95-96°.

N-*Butyl:* [20810-06-4]
$C_8H_{19}N$ 129.245
Liq. Bp 150-151°.

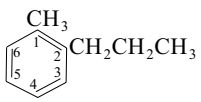
N-*Ph:* See *N*-(2-Methyl-1-propyl)aniline in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 285B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 369A (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 243D (*nmr*)
Taipale, K.A. *et al., CA*, 1925, **19**, 3478 (*synth*)
Brown, R. *et al., J.C.S.*, 1946, 781 (*synth*)
Dornow, A. *et al., Annalen*, 1954, **588**, 62 (*derivs*)
Cope, A.C. *et al., J.A.C.S.*, 1957, **79**, 4720 (*derivs*)
Feeney, J. *et al., J.C.S.*, 1961, 1123 (*pmr*)
Traynelis, V.J. *et al., J.O.C.*, 1961, **26**, 686 (*N,N-Di-Me*)
Fr. Pat., 1967, 1 468 354; *CA*, **67**, 81798 (*manuf*)
Becker, B.F. *et al., Chem. Ber.*, 1975, **108**, 3292 (*pmr*)
Curphey, T.J. *et al., J.O.C.*, 1975, **40**, 607 (*N-alkyl derivs*)

Faure, R. *et al., Org. Magn. Reson.*, 1980, **14**, 20 (*cmr*)
Potier, J. *et al., J. Raman Spectrosc.*, 1984, **15**, 186 (*ir*)
Harrison, A.G. *et al., Can. J. Chem.*, 1986, **64**, 1652 (*ms*)
Smirnov, Y.D. *et al., Zh. Org. Khim.*, 1992, **28**, 461; *J. Org. Chem. USSR (Engl. Transl.)*, 1992, **28**, 374 (*N-alkyl derivs*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IIM000
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 195

1-Methyl-2-propylbenzene, 9CI M-619

[1074-17-5]
o-*Propyltoluene, 8CI*

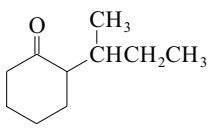


$C_{10}H_{14}$ 134.221
Found in cotton plant volatiles. Liq. d_4^{29} 0.88. Bp_{14} 65-68°.

Claus, A. *et al., Ber.*, 1880, **13**, 897 (*synth*)
v. Auwers, K. *et al., Annalen*, 1919, **419**, 111 (*synth*)
Kuhn, R. *et al., Ber.*, 1932, **65**, 48 (*synth*)
Adv. Chem. Ser., 1955, **15**, 29 (***props***)
Thompson, P.A. *et al., Phytochemistry*, 1975, **14**, 2087 (*isol*)
Parham, W.E. *et al., Synthesis*, 1976, **2**, 116 (*synth*)

2-(1-Methylpropyl)cyclohexanone M-620

[14765-30-1]
2-sec-*Butylcyclohexanone. Freskomenthe. FEMA 3261*



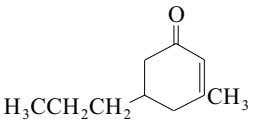
$C_{10}H_{18}O$ 154.252
Stereochem. not defined. Flavouring ingredient. Oil with peppermint odour. d^{20} 0.92. Bp_3 66-70°. n_D 1.4603.
► GW1804000

Oxime:
$C_{10}H_{19}NO$ 169.266
Bp_4 116-118°.

Booth, H. *et al., Tetrahedron*, 1967, **23**, 2421 (*synth*)
Posner, G.H. *et al., J.A.C.S.*, 1973, **95**, 7788 (*synth, pmr, ms*)
Pelosi, P. *et al., Chem. Senses Flavour*, 1978, **3**, 331; *CA*, **90**, 69887v
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 82
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 334-335
U.S. Pat., 3 124 614; *CA*, **60**, 14405

3-Methyl-5-propyl-2-cyclohexen-1-one, 9CI M-621

[3720-16-9]
Celery ketone. FEMA 3577



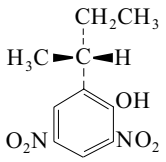
$C_{10}H_{16}O$ 152.236
Celery flavour ingredient.

(±)-form
$d_4^{22.3}$ 0.93. Bp 242-244° Bp_{12} 120-122°.

Horning, E.C. *et al., J.A.C.S.*, 1947, **69**, 1907-1908 (*azine*)
Whitmore, W.F. *et al., J.O.C.*, 1948, **13**, 31-37 (*synth*)
Leraux, Y. *et al., Ann. Chim. (Paris)*, 1972, **7**, 39-52 (*synth, ir, pmr*)
Cosse-Barbi, A. *et al., Bull. Soc. Chim. Fr.*, 1972, 3321-3332 (*uv*)
Ger. Pat., 1978, 2 654 850; *CA*, **89**, 108357y (*synth*)

2-(1-Methylpropyl)-4,6-dinitrophenol, 9CI M-622

Dinoseb, ANSI, BSI, ISO, WSSA. 2-sec-*Butyl-4,6-dinitrophenol. Premerge. Aretit. Ivosit*



(R)-form

$C_{10}H_{12}N_2O_5$ 240.215

(R)-form
Mp 29-30°. $[\alpha]_D^{23}$ -11.9 (c, 6 in C_6H_6).

(S)-form
Mp 30-31°. $[\alpha]_D^{23}$ +13.7 (c, 6 in C_6H_6).

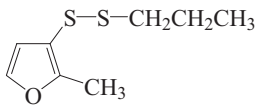
(±)-form [88-85-7]
Acaricide and weed killer. Cryst. (pentane) (technical grade usually liq.). Mp 40-41°. pK_a 4.62.
► LD_{50} (rat, orl) 58 mg/kg. Severe eye irritant. LD_{50} (rat, orl) 25 mg/kg. LD_{50} (rat, skn) 80 mg/kg. Exp. reprod. and teratogenic effects. SJ9800000

Ac: [2813-95-8] *Dinoseb acetate, ANSI, BSI, ISO, WSSA. DNBPA, JMAF*
$C_{12}H_{14}N_2O_6$ 282.252
Postemergence herbicide. Oil or cryst. Mp 26-27°. Slowly hyd. by H_2O.
► Eye and skin irritant. LD_{50} (rat, orl) 48.5-60 mg/kg. AF7140000

U.K. Pat., 1951, 650 906; *CA*, **45**, 9561
Hawthorne, F. *et al., J.A.C.S.*, 1952, **74**, 5859 (*synth, resoln*)
Lane, J.R. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1967, **5**, 385 (*rev*)
Anderson, B.S. *et al., Can. J. Spectrosc.*, 1974, **19**, 37 (*ir*)
Schmetz, H. *et al., Fresenius' Z. Anal. Chem.*, 1974, **270**, 356 (*tlc*)
Ohlrogge, A.J. *et al., Adv. Chem. Ser.*, 1977, **159**, 79 (*rev*)
Cessna, A.J. *et al., J. Agric. Food Chem.*, 1978, **26**, 289
Dangerous Prop. Ind. Mater. Rep., 1989, **9**, 74 (*tox, rev*)
Meyer, A. *et al., Fresenius' Z. Anal. Chem.*, 1989, **332**, 898 (*hplc*)
Riley, J.S. *et al., J. Am. Soc. Mass Spectrom.*, 1991, **2**, 69 (*ms*)
Pesticide Manual, 9th edn., 1991, 5190
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A159
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACE500; BRE500
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1203

2-Methyl-3-(propyldithio)furan, 9CI M-623

[61197-09-9]
2-Methyl-3-furyl propyl disulfide. FEMA 3607

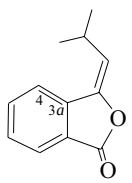


$C_8H_{12}OS_2$ 188.314
Meat flavouring ingredient. d_4^{25} 1.1. $Bp_{1.4}$ 75.5-79°. n_D^{20} 1.5364.

Ger. Pat., 1976, 2 604 340; *CA*, **86**, 16530j (*synth, use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)

3-(2-Methylpropylidene)-1(3*H*)-isobenzofuranone M-624

3-Isobutylidenephthalide



$C_{12}H_{12}O_2$ 188.226

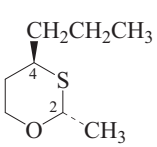
(E)-form [56014-69-8]
Odorous constit. of celery. Pale-yellow oil. Bp_5 83.5°.

3a,4-Dihydro: [66983-88-8] *3-(2-Methylpropylidene)-3a,4-dihydro-1(3*H*)-isobenzofuranone. 3-Isobutylidene-3a,4-dihydrophthalide. 6-(1-Hydroxy-3-methyl-1-butenyl)-1,3-cyclohexadiene-1-carboxylic acid γ-lactone*
$C_{12}H_{14}O_2$ 190.241
Odorous constit. of celery. Pale yellow oil. Bp_{10} 164°. $n_D^{27.5}$ 1.5092.

Gold, H.J. *et al., J.O.C.*, 1963, **28**, 985
Knight, D.W. *et al., J.C.S. Perkin 1*, 1975, 635

2-Methyl-4-propyl-1,3-oxathiane, 9CI M-625

[67715-80-4]
Oxane. FEMA 3578



(2R,4R)-form

$C_8H_{16}OS$ 160.28
Isol. from juice of passion fruit *Passiflora edulis*. Important organoleptic compd. Flavouring and fragrance agent with

blackcurrant aroma. Bp_{12} 85-86°. The isolate from passion fruit consisted of a mixt. of *cis*- and *trans*-isomers, *ca*. 10:1, of so-far undetd. chirality. Four sulfoxides have been synth..

(2*R*,4*R*)-*form* [90243-48-4]
(-)-trans-*form*
$[\alpha]_D^{20}$ +119.4 (CCl_4).

(2*R*,4*S*)-*form* [90243-46-2]
(-)-cis-*form*
Less powerful odorant than the (2*S*,4*R*)-form, with fresher, more ester-type odour and taste. $[\alpha]_D^{20}$ -56.07 (CCl_4).

(2*S*,4*R*)-*form* [90243-47-3]
(+)-cis-*form*
Powerful odorant and flavourant characteristic of passion fruit and similar fruits. $[\alpha]_D^{20}$ +56.12 (CCl_4).

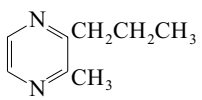
(2*S*,4*S*)-*form* [90243-45-1]
(+)-trans-form
$[\alpha]_D^{20}$ -117.6 (CCl_4).

[59323-76-1, 59324-17-3, 94669-62-2, 94669-63-3, 107436-63-5, 107436-64-6, 107436-65-7, 107436-66-8]

Ger. Pat., 1976, 2 534 162; *CA*, **85**, 37096s
Winter, M. *et al., Helv. Chim. Acta*, 1976, **59**, 1613-1620 (*isol, synth, pmr, ms*)
Pickenhagen, W. *et al., Helv. Chim. Acta*, 1984, **67**, 947-952 (*synth*)
Mosandl, A. *et al., Annalen*, 1985, 1185-1189 (*synth, ir, pmr, cmr, ms*)
Singer, G. *et al., Annalen*, 1987, 451-453 (*oxides*)
Kuentzel, H. *et al., Sulfur Lett.*, 1989, **10**, 181-186 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 556
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1849

2-Methyl-3-propylpyrazine, 9CI M-626

[15986-80-8]



$C_8H_{12}N_2$ 136.196
Flavour component of cooked foods. Bp_{763} 189-190° Bp_{10} 71-72°. n_D^{20} 1.4970.

Flament, I. *et al., Helv. Chim. Acta*, 1967, **50**, 1754 (*synth*)
Bramwell, A.F. *et al., J.C.S.(C)*, 1971, 1627 (*synth, pmr*)
Heynes, K. *et al., Chem. Ber.*, 1981, **114**, 240 (*synth*)
Yamagami, C. *et al., J. Pharm. Sci.*, 1991, **80**, 772 (*props*)
Liu, S.-Y. *et al., Life Sci.*, 1994, **55**, 1317 (*pharmacol*)

2-Methyl-5-propylpyrazine M-627

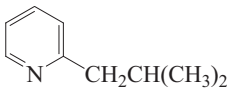
[29461-03-8]

$C_8H_{12}N_2$ 136.196
Constit. of roasted peanut, cocoa, yeast extract, roasted sesame, cooked pork, coffee aroma, roasted chicory and roasted wheat germ.

Friedel, P. *et al., J. Agric. Food Chem.*, 1971, **19**, 530-532 (*occur, coffee, ms, ir*)
U.S. Pat., 1972, 3 881 025; *CA*, **78**, 109541p (*synth, ms*)
Baek, H.H. *et al., J. Food Sci.*, 1998, **63**, 234-237 (*occur, chicory*)

2-(2-Methylpropyl)pyridine M-628

[6304-24-1]
2-Isobutylpyridine. FEMA 3370



$C_9H_{13}N$
Flavouring ingredient. d_4^{20} 0.9. Bp 181° Bp_{55} 110-111°. n_D^{20} 1.4831.

[67423-99-8]

Mariella, R.P. *et al., J.A.C.S.*, 1947, **69**, 2670-2674 (*synth*)
Ohta, A. *et al., Heterocycles*, 1977, **6**, 1881-1887 (*pmr*)
Dietrich, W. *et al., J. Prakt. Chem.*, 1977, **319**, 799-806 (*synth*)
Heckman, R.A. *et al., Tob. Int.*, 1981, **183**, 83-89 (*anal*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 556 (*use*)

3-(2-Methylpropyl)pyridine, 9CI M-629

[14159-61-6]
3-Isobutylpyridine, 8CI. FEMA 3371

$C_9H_{13}N$
Flavouring ingredient. Bp_{19} 85.5-87.5°. n_D^{20} 1.4912.

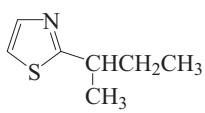
Picrate: [29209-57-2]
Cryst. (EtOH). Mp 114°.

N-*Oxide:* [29071-72-5]
$C_9H_{13}NO$ 151.208
No phys. props. reported.

Miller, A.D. *et al., J.O.C.*, 1957, **22**, 168-170 (*synth*)
Jankovsky, M. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 2797-2801 (*N-oxide*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 557 (*use*)

2-(1-Methylpropyl)thiazole, 9CI M-630

[18277-27-5]
2-sec-Butylthiazole. FEMA 3372



$C_7H_{11}NS$ 141.237

(±)-*form*
Flavouring ingredient. Liq. with raw, green, herbaceous odour. Bp 172°.

(ξ)-*form*
Flavour enhancer for tomato products.

Vernin, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 846-856 (*synth*)
U.S. Pat., 1972, 3 660 112; *CA*, **77**, 33120g (*use*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264-269 (*synth, ms, props*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 557 (*use*)

2-(2-Methylpropyl)thiazole, 9CI M-631

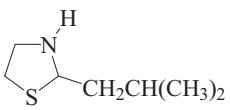
[18640-74-9]
2-Isobutylthiazole, 8CI

$C_7H_{11}NS$ 141.237
Tomato volatile and flavouring ingredient. Liq. with tomato leaf odour. Liq. with tomato leaf odour. d_4^{25} 1. Bp 180° (172°) Bp_{10} 66°. n_D^{25} 1.4939.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 109B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1492C (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1232D (*ir*)
Cottet, R. *et al., Bull. Soc. Chim. Fr.*, 1967, 4499-4502 (*synth, ir, pmr, uv*)
Viani, R. *et al., Helv. Chim. Acta*, 1969, **52**, 887-891 (*isol*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1971, **19**, 524-529; *CA*, **75**, 18920n (*isol*)
Tabacchi, R. *et al., Helv. Chim. Acta*, 1974, **57**, 324-336 (*ms*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264-269; *CA*, **80**, 120827y (*synth, ms, props*)
Dubs, P. *et al., Synthesis*, 1974, 294-295 (*synth, ir, pmr, ms*)
Dirinck, P. *et al., J. Sci. Food Agric.*, 1976, **27**, 499-508 (*isol*)
Burger, B.V. *et al., Z. Naturforsch., C*, 1988, **43**, 731-736 (*isol*)

2-(2-Methylpropyl)thiazolidine, 9CI M-632

[696-70-8]
2-Isobutylthiazolidine. Tetrahydro-2-(2-methylpropyl)thiazole



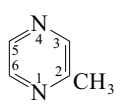
$C_7H_{15}NS$ 145.268

(±)-*form*
Flavouring ingredient. d_{20}^{20} 1.05. Mp 125° (as hydrochloride). $Bp_{0.5}$ 72-76°. n_D^{20} 1.5231.

Jondeur, R. *et al., Bull. Soc. Chim. Fr.*, 1964, 2493-2499 (*synth*)
U.S. Pat., 1971, 3 617 310; *CA*, **76**, 71314k (*use*)
Yasuhara, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 2273-2274 (*synth, pmr, ms*)

Methylpyrazine, 9CI, 8CI M-633

[109-08-0]
FEMA 3309



$C_5H_6N_2$ 94.116
Flavouring agent. Present in many foods, e.g. bakery products, dairy products, meats, baked or French fried potato, roasted barley, cocoa, coffee, tea, roasted filbert, roasted pecan, peanut, soy pro-

ducts, rum and whisky. Liq. with disagreeable picoline-like odour. Misc. H_2O, EtOH, Et_2O. d_4^{20} 1.03. Bp 136-137°. n_D^{20} 1.4953. pK_{a1} 1.41; pK_{a2} -4.89 (25°, H_2O).

▶ Emits highly toxic fumes when heated to dec. Flammable, fl. p. 50° (oc).
UQ3675000

Picrate:
Yellow prisms (EtOH). Mp 133°.

Methiodide: [34260-05-4]
Leaflets and needles (EtOH). V. sol. H_2O. Mp 129-130°.

1-Oxide: [31396-35-7]
$C_5H_6N_2O$ 110.115
Mp 93-95°.

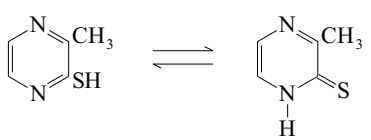
4-Oxide: [25594-37-0]
$C_5H_6N_2O$ 110.115
Mp 69-71°.

1,4-Dioxide: [32046-26-7]
$C_5H_6N_2O_2$ 126.115
Cryst. (MeOH). Mp 230-231°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 397C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 840A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1555D (*ir*)
Jones, R.G. *et al., J.A.C.S.*, 1950, **72**, 3539 (*synth*)
Kitchen, L.J. *et al., J.A.C.S.*, 1951, **73**, 1838 (*synth*)
Cox, R.H. *et al., J. Phys. Chem.*, 1968, **72**, 1646 (*pmr*)
Uchimaru, F. *et al., J. Het. Chem.*, 1971, **8**, 99 (*ms*)
Sanyal, N.K. *et al., J. Mol. Spectrosc.*, 1979, **78**, 335 (*uv*)
Matsuo, M. *et al., Org. Magn. Reson.*, 1980, **13**, 172 (*cmr*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MOW750

3-Methyl-2-pyrazinethiol M-634

[5271-25-0]
3-Methyl-2(1H)-pyrazinethione. 2-Mercapto-3-methylpyrazine



$C_5H_6N_2S$ 126.182
NH-form predominates.Orange solid (H_2O). Mp 180-182° dec.

SH-form

S-*Me:* [2882-20-4] *2-Methyl-3-(methylthio)pyrazine*
$C_6H_8N_2S$ 140.209
Constit. of coffee aroma and flavouring agent FEMA 3208, as mixt. with regioisomers. Bp_{23} 103-104°.

[67952-65-2]

Fr. Pat., 1965, 1 391 212; *CA*, **62**, 16270g (*deriv, synth*)
Cullen, J. *et al., J.C.S.(C)*, 1966, 495-497 (*synth, ir, uv*)
Friedel, P. *et al., J. Agric. Food Chem.*, 1971, **19**, 530-532 (*deriv, spectra*)
Kolor, M.G. *et al., Org. Mass Spectrom.*, 1971, **5**, 959-966 (*deriv, ms*)
Bourguignon, J. *et al., J. Het. Chem.*, 1980, **17**, 257-264 (*deriv, synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1164-1165 (*FEMA 3208*)

5-Methyl-2-pyrazinethiol M-635

5-Methyl-2(1H)-pyrazinethione. 2-Mercapto-5-methylpyrazine

$C_5H_6N_2S$ 126.182

SH-form

S-*Me:* [2884-13-1] *2-Methyl-5-(methylthio)pyrazine*
$C_6H_8N_2S$ 140.209
Flavouring ingredient with roasted almond/hazelnut flavour. Component of FEMA 3208 together with regioisomers. Prepd. synthetically only as regioisomeric mixt..

Fr. Pat., 1965, 1 391 212; *CA*, **62**, 16270g (*S-Me, synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1164-1165 (*S-Me, use, props*)

6-Methyl-2-pyrazinethiol M-636

6-Methyl-2(1H)-pyrazinethione. 2-Mercapto-6-methylpyrazine

$C_5H_6N_2S$ 126.182

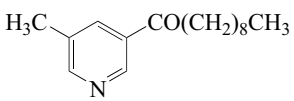
SH-form

S-*Me:* [2884-14-2] *2-Methyl-6-(methylthio)pyrazine*
$C_5H_6N_2S$ 126.182
Flavouring ingredient with roasted almond-hazelnut aroma. Component of FEMA 3208, together with regioisomers. Prepd. synthetically only as a regioisomeric mixt..

Fr. Pat., 1965, 1 391 212; *CA*, **62**, 16270g (*S-Me, synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1164-1165 (*S-Me, use, props*)

1-(5-Methyl-3-pyridinyl)-1-decanone M-637

[194345-50-1]
3-Decanoyl-5-methylpyridine



$C_{16}H_{25}NO$ 247.38
Constit. of *Piper retrofractum* (Javanese long pepper). Cryst. ($CHCl_3$). Mp 208°.

Pande, A. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 377-379 (*isol, ir, pmr, ms*)

1-Methylpyrrole, 9CI M-638

[96-54-8]



C_5H_7N 81.117
Maillard product. Bp 112-113°. pK_a -2.9.

▶ Highly flammable, fl. p. 16°. UX9640000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 1B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 565D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1445B (*ir*)
Derval, P. *et al., J. Mol. Struct.*, 1968, **2**, 73 (*ir*)
Lipmaa, E. *et al., Org. Magn. Reson.*, 1972, **4**, 153 (*nmr*)
Butler, R.N. *et al., Can. J. Chem.*, 1973, **51**, 2315 (*pmr*)
Ger. Pat., 1973, 2 255 570; *CA*, **79**, 106069 (*use*)
Heaney, H. *et al., J.C.S. Perkin 1*, 1973, 499 (*synth*)
Begtrup, M. *et al., J.C.S. Perkin 2*, 1978, 99 (*cmr*)
Lash, T.D. *et al., J. Het. Chem.*, 1991, **28**, 1671 (*synth*)
Diez-Barra, E. *et al., J. Het. Chem.*, 1994, **31**, 1715 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPB000

2-Methylpyrrole, 9CI M-639

[636-41-9]

C_5H_7N 81.117
Maillard product. Liq. Fp -35.6. Bp 147-148°. pK_a -0.21.

N-*Ac:* [38207-11-3]
C_7H_9NO 123.154
Insol. H_2O. Bp 197°.

N-*Methoxycarbonyl:*
$C_7H_9NO_2$ 139.154
Bp_{21} 63-65°. n_D^{20} 1.4930.

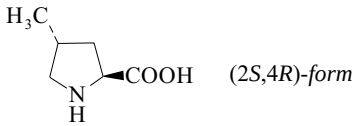
N-*Me:* [600-29-3] *1,2-Dimethyl-1H-pyrrole, 9CI*
C_6H_9N 95.144
Oil. Bp 138°. n_D^{25} 1.4893. n_D^{25} 1.4913.

N-*Ph:* [50691-32-2] *2-Methyl-1-phenyl-1H-pyrrole*
$C_{11}H_{11}N$ 157.215
d_4^{20} 1.03. Bp_{14} 118-119° Bp_4 100°. n_D^{20} 1.5820.

Rapoport, H. *et al., J.O.C.*, 1949, **14**, 664 (*N-Me*)
Elming, N. *et al., Acta Chem. Scand.*, 1952, **6**, 867 (*N-Ph*)
Doyle, F.P. *et al., J.C.S.*, 1958, 4458 (*N-Me*)
Achamatowitz, O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1961, **35**, 497 (*N-Me*)
Gabel, N.W. *et al., J.O.C.*, 1962, **27**, 301 (*deriv*)
Chiang, Y. *et al., J.A.C.S.*, 1963, **85**, 2763 (*pmr*)
Budzikiewicz, H. *et al., J.C.S.*, 1964, 1949 (*ms*)
Jones, R.A. *et al., Spectrochim. Acta*, 1965, **21**, 295 (*ir*)
Marey, T. *et al., C. R. Hebd. Seances Acad. Sci.*, 1971, **272**, 850 (*uv*)
Groves, J.K. *et al., Can. J. Chem.*, 1971, **49**, 2427 (*synth*)
Tsuchiya, T. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1516 (*N-Ph*)
Cushley, R.J. *et al., Can. J. Chem.*, 1975, **53**, 148 (*N-Me*)
Ernst, L. *et al., Angew. Chem.*, 1976, **88**, 335 (*cmr*)
Cowherd, F.G. *et al., Can. J. Chem.*, 1977, **55**, 2919 (*N-Ph*)
Lash, T.D. *et al., J.O.C.*, 1999, **64**, 7973-7982 (*synth, ir, pmr, cmr*)

4-Methyl-2-pyrrolidinecarboxylic acid M-640

4-Methylproline, 9CI



(2*S*,4*R*)-*form*

$C_6H_{11}NO_2$ 129.158

(2*R*,4*R*)-*form* [31137-95-8]
D-cis-*form*
Mp 238-239° dec. $[\alpha]_D^{20}$ +85.2 (c, 1.68 in H_2O). $[\alpha]_D$ +47.9 (c, 1.28 in 3*M* HCl).

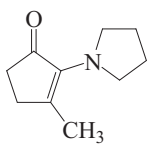
(2*S*,4*R*)-*form* [23009-50-9]
L-trans-*form*
Constit. of young apple fruit and perry. Needles (EtOH/Et_2O). Mp 239-240° dec. $[\alpha]_D^{18}$ -56.6 (c, 1.03 in H_2O). $[\alpha]_D^{20}$ -23.9 (c, 1.54 in 3*M* HCl).

(2*S*,4*S*)-*form* [6734-41-4]
L-cis-*form*
Cryst. (EtOH/Et_2O). $[\alpha]_D^{18}$ -83 (c, 0.53 in H_2O). $[\alpha]_D$ -43 (c, 0.51 in 3*M* HCl).

Dalby, J.S. *et al., J.C.S.*, 1962, 4387 (*synth*)
Moody, C.M. *et al., J.C.S. Perkin 1*, 1997, 3519-3530 (*synth, pmr, ir, cmr*)
Wang, Q. *et al., Tetrahedron*, 1998, **54**, 15759-15780 (*2S,4R-form, synth, ir, pmr, cmr*)

3-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, 9CI M-641

[41357-00-0]



$C_{10}H_{15}NO$ 165.235
Proline-derived Maillard product, present in dark malt. Pale yellow oil. Reported as virtually tasteless with long-lasting cooling effect by Ottinger *et al* and as bitter tasting by Tressl *et al*.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*synth, ms, pmr, ir*)
Ottinger, H. *et al., J. Agric. Food Chem.*, 2001, **49**, 1336-1344 (*synth, pmr, cmr*)

5-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, 9CI M-642

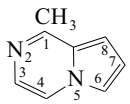
[4933-43-1]

$C_{10}H_{15}NO$ 165.235
Proline-derived Maillard product. Constit. of dark malt. Pale yellow oil. Bp 104-105°. Virtually tasteless with long-lasting cooling effect.

Cone, E.J. *et al., J.O.C.*, 1972, **32**, 4436-4439 (*synth, pmr, ms*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137; 1993, **41**, 547-553 (*occur, synth, ir, ms, pmr*)
Ottinger, H. *et al., J. Agric. Food Chem.*, 2001, **49**, 1336-1344 (*occur, synth, pmr, cmr*)

1-Methylpyrrolo[1,2-*a*]pyrazine, 9CI M-643

[64608-59-9]



$C_8H_8N_2$ 132.165
Maillard product. Bp_{10} 110-112°.

Flament, I. *et al., Helv. Chim. Acta*, 1977, **60**, 1872

3-Methylpyrrolo[1,2-*a*]pyrazine, 9CI M-644

[64608-61-3]

$C_7H_7N_3$ 133.152
Component of roast beef aroma. Mp 76-81°.

Flament, I. *et al., Helv. Chim. Acta*, 1977, **60**, 1872

4-Methylpyrrolo[1,2-*a*]pyrazine, 9CI M-645

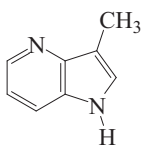
[64608-60-2]

$C_8H_8N_2$ 132.165
Component of roast beef aroma. Dark oil. Bp_{15} 140°.

Flament, I. *et al., Helv. Chim. Acta*, 1977, **60**, 1872
Cobb, J. *et al., Magn. Reson. Chem.*, 1986, **24**, 231 (*cmr*)
Minguez, J.M. *et al., J.O.C.*, 1996, **61**, 4655 (*synth, ir, pmr*)

3-Methyl-1*H*-pyrrolo[3,2-*b*]pyridine, 9CI M-646

[25796-94-5]
4-Azaskatole



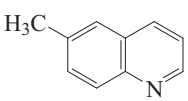
$C_8H_8N_2$ 132.165
Cryst. (C_6H_6). Mp 228-230°. λ_{max} 225 (ϵ 21950); 292 (ϵ 6950) (MeOH) (Berdy).

Kelly, A.H. *et al., J.C.S.(C)*, 1970, 303-307 (*synth*)
Wakabayashi, K. *et al., Yakugaku Zasshi*, 1978, **98**, 898-903 (*isol*)
Fontan, R. *et al., Heterocycles*, 1981, **16**, 1473-1474 (*synth*)

6-Methylquinoline M-647

[91-62-3]

[27601-00-9]
p-*Toluquinoline. FEMA 2744*



$C_{10}H_9N$ 143.188
Flavouring ingredient. Liq. with blossom odour. d_4^{20} 1.07. Fp -22. Bp_{745} 258° Bp_{100} 181°. pK_a 5.22 (25°).
▶ Fl. p. >107°. Skin irritant. LD_{50} (rat, orl) 1260 mg/kg. VC0550000

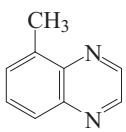
Picrate:
Yellow powder. Spar. sol. org. solvs. Mp 229°.

N-*Me:1,6-Dimethylquinolinium(1+)*
$C_{11}H_{12}N^{\oplus}$ 158.223
Yellow needles (EtOH) (as iodide). Mp 214-216° (iodide).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 422C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1565D (*ir*)
Capps, J.D. *et al., J.A.C.S.*, 1947, **69**, 176 (*synth*)
Lachowicz, A. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1967, **41**, 1543 (*ir*)
Draper, P.M. *et al., Can. J. Chem.*, 1968, **46**, 1487 (*ms*)
Lanum, W.J. *et al., J. Chem. Eng. Data*, 1969, **14**, 93 (*props*)
Tamura, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2982 (*synth*)
Johns, S.R. *et al., Aust. J. Chem.*, 1976, **29**, 1617 (*cmr*)
Takahashi, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4630 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 560
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1854-1855
Cho, C.S. *et al., J. Het. Chem.*, 1999, **36**, 1175-1178 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPF800

5-Methylquinoxaline, 9CI M-648

[13708-12-8]
FEMA 3203



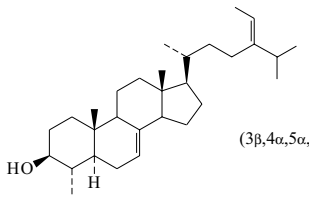
$C_9H_8N_2$ 144.176
Present in coffee. Flavouring ingredient. Pale yellow cryst. Mp 20-21° (hydrate 49-50°). Bp_{15} 120°. Forms hydrate in moist air.

1-Oxide:
$C_9H_8N_2O$ 160.175
Hydrated needles (petrol). Mp 131-132°.

1,4-Dioxide:
$C_9H_8N_2O_2$ 176.174
Cryst. (EtOH). Mp 192-194°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 468B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1574A (*ir*)
Lundquist, J.K. *et al., J.C.S.*, 1953, 2816
Brignell, P.J. *et al., J.C.S.(B)*, 1967, 1241 (*pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 561
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1855-1856

4-Methylstigmasta-7,24(28)-dien-3-ol, 9CI M-649



(3β,4α,5α,24*E*)-*form*

$C_{30}H_{50}O$ 426.724

(3β,4α,5α,24*E*)-*form* [39006-52-5]
Epicitrostadienol
Constit. of marigold flowers. Cryst. (MeOH).

(3β,4α,5α,24*Z*)-*form* [474-40-8]
α_1-Sitosterol. Citrostadienol. 24-Ethylidenelophenol
Constit. of potatoes (*Solanum tuberosum*), garden peas (*Pisum sativum*), citrus oils and other plants. Cryst. (Et_2O/EtOH). Mp 162-164°. $[\alpha]_D$ +24 (c, 1 in $CHCl_3$). α_1-Sitosterol was not homogeneous.

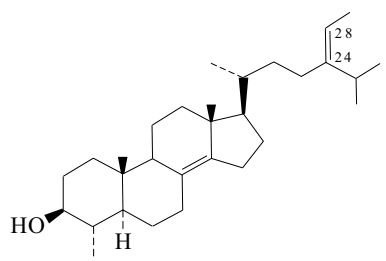
(3β,4β,5α,24*Z*)-*form* [21490-23-3]
Constit. of *Calendula officinalis* (pot marigold). Cryst. Mp 165°. $[\alpha]_D$ +6 ($CHCl_3$).

[11040-28-1]

Mazur, Y. *et al., J.A.C.S.*, 1958, **80**, 1008; 6293; 6296
Schreiber, K. *et al., Tetrahedron*, 1964, **20**, 2575
Bates, R.B. *et al., Tet. Lett.*, 1968, 6163 (*struct*)
St. Pyrek, J. *et al., Chem. Comm.*, 1969, 107 (*isol*)
Brooks, C.J.W. *et al., Steroids*, 1972, **20**, 487 (*ms*)
Lenton, J.R. *et al., Phytochemistry*, 1975, **14**, 1523 (*biosynth*)
Sucrow, W. *et al., Chem. Ber.*, 1977, **110**, 1523 (*synth*)
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1977, **51**, 951 (*isol, pmr*)

4-Methylstigmasta-8(14),24(28)-dien-3-ol, 9CI M-650

24-Ethylidene-4-methylcholest-8(14)-en-3-ol



$C_{30}H_{50}O$ 426.724

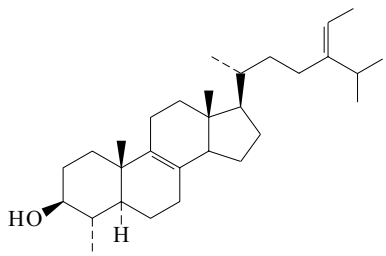
(3β,4α,5α,24*Z*)-*form* [78285-84-4]
Constit. of *Phaseolus vulgaris* (kidney bean).

24,28-Dihydro: [78340-86-0] *4α-Methyl-5α-stigmast-8(14)-en-3β-ol, 9CI*
$C_{30}H_{52}O$ 428.74

[123086-81-7]

Kokke, W.C.M.C. *et al., Phytochemistry*, 1981, **20**, 127 (*isol*)
Bohlin, L. *et al., Phytochemistry*, 1981, **20**, 2397 (*deriv*)
Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219 (*isol*)

4-Methylstigmasta-8,24(28)-dien-3-ol M-651



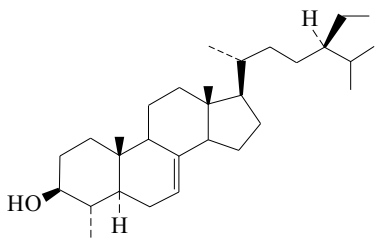
$C_{30}H_{50}O$ 426.724

(3β,4α,5α,24*Z*)-*form* [71418-13-8]
Constit. of *Phaseolus vulgaris* (kidney bean) and *Rubus fruticosus* (blackberry). Mp 130-132° (as acetate).

[71418-14-9]

Schmitt, P. *et al., Phytochemistry*, 1987, **26**, 2709 (*isol*)
Akihisa, T. *et al., Phytochemistry*, 1989, **28**, 1219 (*isol*)

4-Methylstigmast-7-en-3-ol M-652



$C_{30}H_{52}O$ 428.74

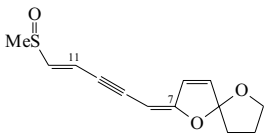
(3β,4α,5α,24*R*)-*form* [36735-29-2]
24-Ethyllophenol
Isol. from tomato (*Lycopersicon esculentum*) and numerous vegetable oils. Cryst. (Me_2CO/MeOH). Mp 175.5-176.5°.

Ac:
Cryst. (Me_2CO/MeOH). Mp 153-155°.

[33903-18-3, 65437-62-9, 77610-47-0]

Panosyan, A.G. *et al., Khim. Prir. Soedin.*, 1977, **13**, 353; 1980, **16**, 781; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 300; 1980, **16**, 554 (*isol*)
Itoh, T. *et al., Fette, Seifen, Anstrichm.*, 1978, **80**, 382
Itoh, T. *et al., Phytochemistry*, 1980, **19**, 2491
Itoh, T. *et al., Yukagaku*, 1981, **30**, 586 (*hplc*)

2-(5-Methylsulfinyl-2-pentyn-4-enylidene)-1,6-dioxaspiro[4.4]non-3-ene M-653



(7*E*,11*E*)-*form*

$C_{13}H_{14}O_3S$ 250.318

(7*E*,11*E*)-*form* [124460-81-7]
Isol. from *Chrysanthemum coronarium* (chop-suey greens). Yellowish oil. $[\alpha]_D^{24}$ -9 (c, 0.1 in $CHCl_3$).

(7*Z*,11*E*)-*form* [124442-14-4]
Isol. from *Chrysanthemum coronarium* (chop-suey greens). Yellowish oil. $[\alpha]_D^{24}$ -7 (c, 0.05 in $CHCl_3$).

Sanz, J.F. *et al., Annalen*, 1990, 303

[3-(Methylsulfinyl)-1-propenyl] 2-propenyl disulfide M-654

4,5,9-Trithia-1,6-decadiene 9-oxide. ***10-Devinylajoene***

$MeS(O)CH_2CH{=}CH{-}S{-}S{-}CH_2CH{=}CH_2$

$C_7H_{12}OS_3$ 208.369

(*Z*)-*form* [72869-75-1]
Isol. from garlic oil (*Allium sativum*). Oil.

Yoshida, H. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1015-1017 (*isol, pmr, cmr, ms*)

2-Methyltetracosane M-655

[1560-78-7]
Isopentacosane

$(H_3C)_2CH(CH_2)_{21}CH_3$

$C_{25}H_{52}$ 352.686

Found in hop (*Humulus lupulus*) and orange (*Citrus sinensis*) oils. Mp 56°.

Levene, P.A. *et al., J. Biol. Chem.*, 1922, **52**, 227
Streibl, M. *et al., Fette, Seifen, Anstrichm.*, 1968, **70**, 543 (*glc*)
Howard, R.W. *et al., J. Chem. Ecol.*, 1978, **4**, 233 (*glc, ms*)
Tsuda, Y. *et al., Phytochemistry*, 1981, **20**, 505 (*isol, synth*)

2-Methyltetradecane M-656

[1560-95-8]
Isopentadecane

$(H_3C)_2CH(CH_2)_{11}CH_3$

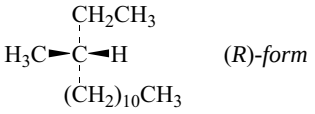
$C_{15}H_{32}$ 212.418

Constit. of *Humulus lupulus* (hops) and *Theobroma* sp.. d_4^{20} 0.77. Fp -8.3. $Bp_{1.5}$ 78°. n_D^{20} 1.4304.

Lunshof, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1947, **66**, 348 (*synth*)
Feldhues, M. *et al., Tetrahedron*, 1985, **41**, 4195 (*synth, pmr, ms*)
Baldwin, J.E. *et al., Tetrahedron*, 1986, **42**, 4235 (*synth*)
Ueyama, Y. *et al., Flavour Fragrance J.*, 1991, **6**, 63 (*isol*)
Garcia Martinez, A. *et al., Tetrahedron*, 1994, **50**, 13231 (*synth, ir, pmr, cmr, ms*)

3-Methyltetradecane M-657

[18435-22-8]



(*R*)-*form*

$C_{15}H_{32}$ 212.418

Constit. of *Ruta graveolens* (rue) and *Zea mays* (sweet corn).

(*R*)-*form* [55253-05-9]

$Bp_{0.4}$ 87-88°. $[\alpha]_D^{23}$ -6.5 (neat).

(*S*)-*form*

Bp_{15} 137°. $[\alpha]_D^{25}$ +6.5 (neat).

(±)-*form*

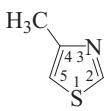
Bp_{10} 133°.

Lardicci, L. *et al., Ann. Chim. (Rome)*, 1962, **52**, 652 (*synth*)
Schlenk, W. *et al., Annalen*, 1973, 1179 (*synth*)
Thompson, A.C. *et al., Phytochemistry*, 1974, **13**, 2029 (*isol*)
Feldhues, M. *et al., Tetrahedron*, 1985, **41**, 4195 (*synth, pmr, ms*)
Brown, C.A. *et al., J.O.C.*, 1986, **51**, 162 (*synth, cmr*)
Ueyama, Y. *et al., Flavour Fragrance J.*, 1991, **6**, 63 (*isol*)
Nascimento, R.R. *et al., J. Chem. Ecol.*, 1993, **19**, 1993 (*occur*)

4-Methylthiazole, 9CI M-658

[693-95-8]

FEMA 3716



C_4H_5NS 99.156

Flavouring ingredient. Present in asparagus, cooked beef, cooked pork, pork liver, coffee, roast barley, roast peanut and cooked shrimp. Liq. with nutty, green odour. Misc. H_2O. d_4^{25} 1.11. Bp 130-133° Bp_{59} 70-71°. n_D^{20} 1.5234. pK_a 3.15 (25°).

► XJ5096000

Picrate:

Mp 181°.

N-*Me:*

$C_5H_8NS^{\oplus}$ 114.191

Cryst. (EtOH/Et_2O) (as iodide). Mp 117-118.5° (iodide).

N-*Et:*

$C_6H_{10}NS^{\oplus}$ 128.218

Cryst. (EtOH/Et_2O) (as iodide). Mp 169-171° (iodide).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 510D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 643A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1491D (*ir*)
Bergen, G. *et al., Acta Chem. Scand.*, 1966, **20**, 2593 (*pmr*)
Vincent, E.J. *et al., Bull. Soc. Chim. Fr.*, 1966, 3524 (*nmr*)
Colebourne, N. *et al., J.C.S.(C)*, 1967, 685 (*synth*)
Gisele, D. *et al., Spectrochim. Acta A*, 1967, **23**, 2669 (*ir, Raman*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511 (*ms*)
Galy, J.P. *et al., Can. J. Chem.*, 1978, **56**, 46 (*cmr*)
Amato, J.S. *et al., Heterocycles*, 1984, **22**, 1947 (*synth*)
Bordwell, F.G. *et al., J.A.C.S.*, 1991, **113**, 985 (*deriv, synth*)
Pavlik, J.W. *et al., J.O.C.*, 1993, **58**, 3407 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1861-1862 (*occur, props*)

5-Methylthiazole, 9CI M-659

[3581-89-3]

C_4H_5NS 99.156

Food flavouring ingredient. Bp 141°. pK_a 3.12 (25°).

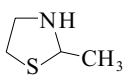
Picrate:

Mp 170°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 108C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1492A (*ir*)
Bergen, G. *et al., Acta Chem. Scand.*, 1966, **20**, 2593 (*pmr*)
Vincent, E.J. *et al., Bull. Soc. Chim. Fr.*, 1966, 3524 (*nmr*)
Vernin, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 846 (*synth*)
Colebourne, N. *et al., J.C.S.(C)*, 1967, 685 (*synth*)
Gisele, D. *et al., Spectrochim. Acta A*, 1967, **23**, 2669 (*ir, Raman*)
Tabacchi, R. *et al., Helv. Chim. Acta*, 1974, **57**, 324 (*ms*)
Galy, J.P. *et al., Can. J. Chem.*, 1978, **56**, 46 (*cmr*)
Amato, J.S. *et al., Heterocycles*, 1984, **22**, 1947 (*synth*)
Pavlik, J.W. *et al., J.O.C.*, 1993, **58**, 3407 (*synth*)

2-Methylthiazolidine, 9CI M-660

[24050-16-6]



C_4H_9NS 103.188

► LD_{50} (mus, ipr) 250 mg/kg. XJ6061000

(±)-*form*

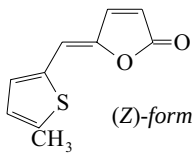
Used as aroma additive for food. Liq. Bp_{36} 76-78° Bp_5 37°.

(ξ)-*form*

Surzur, J.-M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1969, **268**, 2109 (*synth*)
Hillers, S. *et al., CA*, 1969, **71**, 70554y (*synth*)
Asinger, F. *et al., Monatsh. Chem.*, 1970, **101**, 1298 (*synth*)
Yasuhara, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 2273 (*synth, ms, pmr*)
Barbry, D. *et al., J.C.S. Perkin 2*, 1990, 133 (*pmr, cmr, N-15 nmr*)
Sirugue, D. *et al., J. Chem. Ecol.*, 1992, **18**, 2261 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPR000

5-[(5-Methyl-2-thienyl)methylene]-2(5*H*)-furanone, 9CI M-661

5-(5-Methyl-2-thienyl)-2,4-pentadien-4-olide



(*Z*)-*form*

$C_{10}H_8O_2S$ 192.238

(*E*)-*form* [35304-91-7]

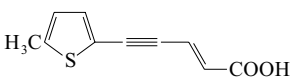
Needles. Mp 105° approx. Appears to isomerise on heating.

(*Z*)-*form* [5705-62-4]

Minor constit. of the roots of *Chamaemelum nobile* (Roman chamomile). Yellow cryst. (petrol). Mp 117°.

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 1226 (*isol, uv, ir, pmr, struct, synth*)
Yamada, K. *et al., Tetrahedron*, 1971, **27**, 5445 (*synth, uv, pmr*)
Negishi, E. *et al., Heterocycles*, 1997, **46**, 209-214 (*synth, pmr, cmr*)

5-(5-Methyl-2-thienyl)-2-penten-4-ynoic acid M-662



(E)-*form*

$C_{10}H_8O_2S$ 192.238

(*E*)-*form*

Me ester:

Yellowish cryst. (petrol). Mp 49°.

(*Z*)-*form* [23050-78-4]

Me ester:

$C_{11}H_{10}O_2S$ 206.265

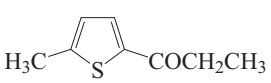
Isol. from roots of *Artemisia vulgaris* (mugwort) *and Anthemis nobilis* (Roman chamomile). Light yellow oil. λ_{max} 338 (Et_2O).

Bohlmann, F. *et al., Chem. Ber.*, 1962, **95**, 1733; 1963, **96**, 584; 588 (*isol, uv, ir, struct, synth*)
Schulte, K.E. *et al., Phytochemistry*, 1966, **5**, 949 (*biosynth*)

1-(5-Methyl-2-thienyl)-1-propanone, 9CI M-663

[59303-13-8]

2-Methyl-5-propanoylthiophene



$C_8H_{10}OS$ 154.232

Flavouring ingredient. Mp 31°. $Bp_{4.5}$ 93-94°.

Semicarbazone:

Cryst. (C_6H_6/EtOH). Mp 203-204°.

Farrar, M.W. *et al., J.A.C.S.*, 1950, **72**, 3695-3698 (*synth*)
U.S. Pat., 1976, 3 931 246; *CA*, **84**, 180019d (*use*)

Methylthio 2-(propanoyloxy)-propanoate M-664

S-*Methyl-2-(propionyloxy)propanethioate. Propionyllactic acid thiomethyl ester. FEMA 3790*

$H_3CCH_2COOCH(CH_3)COSMe$

$C_7H_{12}O_3S$ 176.236

Flavouring ingredient. Colourless to pale pink liq. d_4^{20} 1.1. $Bp_{4.5}$ 76°.

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1250 (*use, props*)

(Methylthio)acetic acid M-665

[2444-37-3]

Methylmercaptoacetic acid. S-*(Methylthio)glycolic acid. Dimethyl sulfide carboxylic acid*

$MeSCH_2COOH$

$C_3H_6O_2S$ 106.145

d_{20}^{20} 1.22. Bp_{27} 130-131°. n_D^{20} 1.4950.

Et ester: [4455-13-4] *FEMA 3835*
$C_5H_{10}O_2S$ 134.199
Found in melon, durian and other fruits. Flavouring agent. Liq. with fruity odour. Bp_{25} 70-72°.

Larsson, E. *et al., Ber.*, 1930, **63**, 1347 (*synth*)
Mathias, E. *et al., Chem. Comm.*, 1981, 569 (*synth, ir, pmr, cmr, haz*)
Takagi, T. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 1299 (*cmr*)

1-(Methylthio)-1-butene, 9CI M-666

[32951-19-2]

1-Buten-1-yl methyl sulfide, 8CI. 2-Thia-3-hexene. FEMA 3820

$H_3CCH_2CH{=}CHSMe$

$C_5H_{10}S$ 102.2

Food flavouring ingredient. Present in roasted peanuts. Liq. with unpleasant odour. Bp 123-126°. n_D^{25} 1.4809. Bp refers to a mixt. of *cis*- and *trans*- isomers.

Parham, W.E. *et al., J.O.C.*, 1968, **33**, 4150-4154 (*synth, pmr*)
Ho, C.T. *et al., J. Food Sci.*, 1981, **47**, 127-133 (*occur, peanuts*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 180 (*use*)

4-(Methylthio)-3-butenyl glucosinolate M-667

[28463-23-2]

1-Thio-β-D-glucopyranose 1-[5-(methylthio)-N-*(sulfooxy)-4-pentenimidate], 9CI.* ***Glucoraphasatin****. Glucodehydroerucin*

$MeSCH{=}CHCH_2CH_2C(SGlc){=}NOSO_3H$

$C_{12}H_{21}NO_9S_3$ 419.497

S-*Oxide:* [28463-24-3] *4-(Methylsulfinyl)-3-butenyl glucosinolate.* ***Glucoraphenin***
$C_{12}H_{21}NO_{10}S_3$ 435.497
Needles +1H_2O(EtOH) (as tetra-Ac, K salt). Mp 155-156° (tetra-Ac, K salt). $[\alpha]_D^{27}$ -23.5 (c, 1.5 in H_2O) (tetra-Ac, K salt).

6′-(4-Hydroxy-3,5-dimethoxycinnamoyl), S-*oxide:* [76653-80-0] ***6-Sinapoylglucoraphenin***
$C_{23}H_{31}NO_{14}S_3$ 641.694
Isol. from radish (*Raphanus sativus*) cotyledons.

Schultz, O.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1955, **288**, 525 (*isol*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1959, **13**, 851 (*isol*)
Gmelin, R. *et al., Phytochemistry*, 1970, **9**, 569 (*isol*)
Wendisch, D. *et al., Z. Naturforsch., C*, 1980, **35**, 907 (*isol*)

4-(Methylthio)butyl glucosinolate M-668

[21973-56-8]

[15592-37-7]
1-Thio-β-D-glucopyranose 1-[5-(methylthio)-N-*(sulfooxy)pentanimidate], 9CI.* ***Glucoerucin***

$MeSCH_2CH_2CH_2CH_2C(SGlc){=}NOSO_3H$

$C_{12}H_{23}NO_9S_3$ 421.513
Isol. from seeds of salad rocket (*Eruca sativa*) and Brussels sprouts (*Brassica oleracea* var. *gemmifera*). Mp 153-154° (as K salt). $[\alpha]_D^{25}$ -21.5 (c, 0.55 in H_2O) (K salt).

S-*Oxide:* [21414-41-5] *4-(Methylsulfinyl)-butyl glucosinolate.* ***Glucoraphanin***
$C_{12}H_{23}NO_{10}S_3$ 437.512
Isol. from radish (*Raphanus sativus*) and *Brassica* sp. seeds or tops.

S-*Oxide,* L-*proline salt:*
$C_{17}H_{32}N_2O_{12}S_3$ 552.644
Powder. $[\alpha]_D^{20}$ -44 (c, 16.3 in H_2O). λ_{max} 225 (H_2O).

S,S-*Dioxide:* [74542-16-8]

[11025-51-7, 22149-26-4] *4-(Methylsulfonyl)-butyl glucosinolate.* ***Glucoerysolin***
$C_{12}H_{23}NO_{11}S_3$ 453.512
Needles (EtOH aq.) (as K salt). Mp 161-163° (K salt). $[\alpha]_D^{28}$ -19.1 (c, 0.75 in H_2O) (K salt).

Tetra-Ac:
Mp 150-151° dec. (as K salt). $[\alpha]_D^{26}$ -14.9 (c, 0.51 in H_2O).

Tetra-Ac, S,S-*dioxide:* [23614-86-0]
Cryst. (EtOH) (as K salt). Mp 155-156° (K salt). $[\alpha]_D^{28}$ -17.1 (c, 0.86 in H_2O) (K salt).

*6′-*O-*Benzoyl:****6′-O-Benzoylglucoerucin***
$C_{19}H_{27}NO_{10}S_3$ 525.621

*6′-*O-*Benzoyl,* S-*oxide:****6′-O-Benzoylglucoraphanin***
$C_{19}H_{27}NO_{11}S_3$ 541.62

S-*De-Me:1-Thio-β-D-glucopyranose 1-[*N-*(sulfooxy)-5-thiopentanimidate], 9CI. 4-Mercaptobutyl glucosinolate*
$C_{11}H_{21}NO_9S_3$ 407.486
Isol. from the leaves of *Eruca sativa* (rocket).

Schneider, W. *et al., Annalen*, 1912, **392**, 1 (*Glucoerysolin, isol*)
Schmidt, H. *et al., Helv. Chim. Acta*, 1948, **31**, 1017 (*Glucoraphanin*)
Gmelin, R. *et al., Acta Chem. Scand.*, 1968, **22**, 2875 (*Glucoerysolin*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Heaney, R.K. *et al., J. Sci. Food Agric.*, 1980, **31**, 785-793 (*isol*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*cmr*)
Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, D.H.), CRC Press, 1998, 29-53 (*rev, occur*)
Fréchard, A. *et al., Fitoterapia*, 2002, **73**, 177-178 (*S-oxide proline salt*)
Reichelt, M. *et al., Phytochemistry*, 2002, **59**, 663-671 (*isol, pmr, cmr*)
Bennett, R.N. *et al., Phytochemistry*, 2002, **61**, 25-30 (*Mercaptobutyl glucosinolate*)

2-(Methylthio)ethyl glucosinolate M-669

[27303-30-6]

[10593-29-0]
1-Thio-β-D-glucopyranose 1-[3-(methylthio)-N-*(sulfooxy)propanimidate], 9CI*

$MeSCH_2CH_2C(SGlc){=}NOSO_3H$

$C_{10}H_{19}NO_9S_3$ 393.459
Present in horseradish (*Armoracia lapathifolia*).

S-*Oxide:2-(Methylsulfinyl)ethyl glucosinolate*
$C_{10}H_{19}NO_{10}S_3$ 409.459

Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)
Reichelt, M. *et al., Phytochemistry*, 2002, **59**, 663-671 (*S-oxide*)

1-(Methylthio)ethyl 2-propenyl disulfide, 9CI M-670

[195203-59-9]

Allyl 1-(methylthio)ethyl disulfide

$H_3CCH(SMe)$-S-S-$CH_2CH{=}CH_2$

$C_6H_{12}S_3$ 180.359
Constit. of the essential oil of *Allium tuberosum* (Chinese chives).

Lopes, D. *et al., Flavour Fragrance J.*, 1997, **12**, 237-239 (*isol*)

1-(Methylthio)-1-hexanethiol, 9CI M-671

[53897-65-7]

$H_3C(CH_2)_4CH(SMe)SH$

$C_7H_{16}S_2$ 164.335
Component of an allium-like organoleptic mixt. prod. from hexanal, H_2S and MeSH. Characterised spectroscopically.

Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*formn, isol, ms*)

6-(Methylthio)hexyl glucosinolate M-672

[74542-17-9]

1-Thio-β-glucopyranose 1-[7-(methylthio)-N-*(sulfooxy)heptanimidate], 9CI*

$MeS(CH_2)_6C(SGlc){=}NOSO_3H$

$C_{14}H_{27}NO_9S_3$ 449.567
Present in *Arabidopsis thaliana* and other crucifers.

S-*Oxide:* [33049-17-1] *6-(Methylsulfinyl)-hexyl glucosinolate.* ***Glucohesperalin****. Glucohesperin*
$C_{14}H_{27}NO_{10}S_3$ 465.566
Present in seeds of *Hesperis matronalis* (sweet rocket).

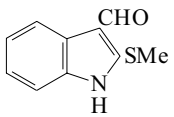
S,S-*Dioxide:* [74542-18-0] *6-(Methylsulfo-*

nyl)hexyl glucosinolate
$C_{14}H_{27}NO_{11}S_3$ 481.565
Present in crucifers.

Daxenbichler, M.E. *et al., J.O.C.*, 1961, **26**, 4168 (*isol*)
Christensen, B.W. *et al., Acta Chem. Scand.*, 1963, **17**, 846 (*Glucohesperalin*)
Hogge, L.R. *et al., J. Chromatogr. Sci.*, 1986, **26**, 551 (*isol*)

2-(Methylthio)-1*H*-indole-3-carboxaldehyde, 9CI M-673

[113866-44-7]
3-Formyl-2-(methylthio)indole. ***Brassicanal A***



$C_{10}H_9NOS$ 191.253
Alkaloid from Chinese cabbage (*Brassica campestris* ssp. *pekinensis*) inoculated with *Pseudomonas cichorii*. Mp 210-213°.

Monde, K. *et al., Chem. Lett.*, 1990, 209 (*isol, uv, pmr, struct*)
Pedras, M.S.C. *et al., Chem. Comm.*, 1998, 1565-1566 (*synth*)

(Methylthio)methanol M-674

[81898-54-6]
Hydroxymethyl methyl sulfide
$MeSCH_2OH$
C_2H_6OS 78.135
Stable liq. Bp_{13} 41°.

Ac: [16437-69-7]
$C_4H_8O_2S$ 120.172
Bp_{12} 48-49°. n_D^{20} 1.4550.

Butanoyl: [74758-93-3] *Methylthiomethyl butyrate. FEMA 3879*
$C_6H_{12}O_2S$ 148.226
Flavouring agent esp. for seasonings. Liq. with metallic, fruity odour. d 0.95.

Hexanoyl: [74758-91-1] *Methylthiomethyl hexanoate. FEMA 3880*
$C_8H_{16}O_2S$ 176.279
Flavouring agent for baked goods, seasonings etc. Liq. d 0.98.

p-*Nitrobenzoyl:*
Mp 50-52°.

Dossena, A. *et al., J.C.S. Perkin 1*, 1981, 2737 (*acetate*)
Jones, J.H. *et al., Synth. Commun.*, 1986, **16**, 1607 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1241-1243

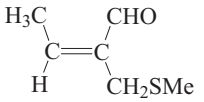
Methylthiomethyl 2-methylbutanethiolate M-675

$H_3CCH_2CH(CH_3)COSCH_2SMe$
$C_7H_{14}OS_2$ 178.319
Isol. from hop oil. Oil with intense cabbage/onion aroma. Bp_{10} 70°.

Bertz, S.H. *et al., Tet. Lett.*, 1980, 3151 (*synth*)
Moir, M. *et al., Tet. Lett.*, 1980, 1085 (*isol, synth*)

2-[(Methylthio)methyl]-2-butenal, 9CI M-676

[40878-72-6]
FEMA 3601



(*E*)-*form*

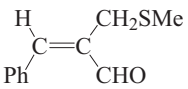
$C_6H_{10}OS$ 130.21
Flavour component of potato crisps and other snack foods, krill seasoning, roasted coffee and yeast extracts. Liq. with odour resembling cooked cabbage/onion. Bp_5 77°. Obt. as a mixt. of (*E*)- and (*Z*)-forms.

[80756-15-6]

Dekimpe, N.G. *et al., J. Agric. Food Chem.*, 1996, **44**, 3598 (*synth, pmr, cmr, ms, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1241

2-(Methylthiomethyl)-3-phenyl-2-propenal, 9CI M-677

[65887-08-3]



(*E*)-*form*

$C_{11}H_{12}OS$ 192.281
Flavouring ingredient. Viscous yellow liq. $Bp_{3.8}$ 151°. n_D^{20} 1.6221. No data on geom. isomers.

U.S. Pat., 1977, 4 064 279; *CA*, **88**, 150954v (*synth, use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 574 (*use, props*)

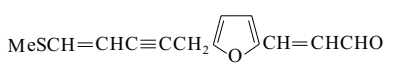
5-(Methylthio)-2-[(methylthio)methyl]-2-pentenal, 9CI M-678

[59902-01-1]
2,8-Dithianon-4-ene-4-carboxaldehyde. 4-Formyl-2,8-dithianon-4-ene. FEMA 3483
$MeSCH_2CH_2CH{=}C(CHO)CH_2SMe$
$C_8H_{14}OS_2$ 190.33
Flavouring ingredient and antioxidant. Present in tomato juice and hydrolysed vegetable protein. Liq. with sweet, meaty, hydrolysed vegetable protein taste.

Sims, R.J. *et al., J. Am. Oil Chem. Soc.*, 1977, **54**, 4-7 (*props*)
U.S. Pat., 1977, 4 064 279; *CA*, **88**, 150 954 (*synth, ms, use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 488 (*use*)

5-[5-(Methylthio)-4-penten-2-ynyl]-2-furanacrolein, 8CI M-679

4,7-Epoxy-12-methylthio-2,11-dodecadien-9-ynal



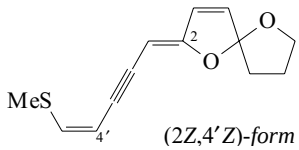
$C_{13}H_{12}O_2S$ 232.303

(2E,11Z)-form [24948-23-0]
Constit. of *Chrysanthemum coronarium* (chop-suey greens). Mp 41.5°.

Semicarbazone:
Mp 173°.

Bohlmann, F. *et al., Chem. Ber.*, 1964, **97**, 1179; 1969, **102**, 4209 (*synth*)

2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene, 9CI M-680



(2Z,4′Z)-*form*

$C_{13}H_{14}O_2S$ 234.318

(2Z,4′Z)-form
Isol. from above-ground parts of *Chrysanthemum coronarium* (chop-suey greens). Oil.

S,S-*Dioxide:*
Cryst. (Et_2O). Mp 98.5°. $[\alpha]_{Hg}^{20}$ -6.1 (c, 3.3 in $CHCl_3$).

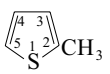
(2Z,4′E)-form
Isol. from *Chrysanthemum coronarium* (chop-suey greens). Yellowish cryst. (petrol). Mp 71°. $[\alpha]_{Hg}^{20}$ +1.2 (c, 7.3 in $CHCl_3$).

S-*Oxide:* ***2-[(5-Methylsulfinyl)-4-penten-2-ynylidene]-1,6-dioxaspiro[4.4]non-3-ene***
$C_{13}H_{14}O_3S$ 250.318
Isol. from *Chrysanthemum coronarium* (chop-suey greens). λ_{max} 338 (Et_2O).

Bohlmann, F. *et al., Chem. Ber.*, 1964, **97**, 1179; 1965, **98**, 2605 (*isol, uv, ir, pmr, struct, synth*)

2-Methylthiophene M-681

[554-14-3]
α-*Thiotolene*



C_5H_6S 98.168
Maillard product; present in roast beef and coffee aromas. d^{20} 1.02. Bp 110-112°. n_D^{20} 1.5203.

▶ Highly flammable, fl. p. 8°. Ignites on contact with HNO_3. LD_{50} (rat, orl) 3200 mg/kg. XM9625000

S-*Oxide:*
C_5H_6OS 114.168Short-lived synth. intermed. not isolated.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 43C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 591D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1466D (*ir*)
Adv. Chem. Ser., 1955, **15**, 184 (***props***)
Schulte, K.E. *et al., Chem. Ber.*, 1962, **95**, 1943 (*synth*)
Mathis, C.T. *et al., J. Phys. Chem.*, 1964, **68**, 571 (*pmr*)
Weigert, F.J. *et al., J.A.C.S.*, 1968, **90**, 3543 (*cmr*)
Nguyen, D.T. *et al., Z. Chem.*, 1973, **13**, 57 (*synth*)

Gronowitz, S. *et al., Chem. Scr.*, 1975, **7**, 111 (*nmr*)
Torsell, K. *et al., Acta Chem. Scand., Ser. B*, 1976, **B30**, 353 (*oxide, synth, use*)
Larock, R.C. *et al., Tet. Lett.*, 1981, **22**, 2443 (*synth*)
Larock, R.C. *et al., J. Organomet. Chem.*, 1982, **225**, 31 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPV000
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1764

3-Methylthiophene M-682

[616-44-4]
β-Thiotolene

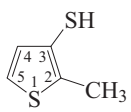
C_5H_6S 98.168
Maillard product, present in roast coffee aroma. d^{20} 1.03. Mp -69°. Bp 115°. n_D^{20} 1.5204.

▶ LD_{50} (mus, orl) 1800 mg/kg. XM9800000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 44B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 592B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1467C (*ir*)
Adv. Chem. Ser., 1955, **15**, 185 (***props***)
Reddy, G.S. *et al., J.A.C.S.*, 1961, **83**, 5020 (*nmr*)
Org. Synth., Coll. Vol., 4, 1963, 671 (*synth*)
Mathis, C.T. *et al., J. Phys. Chem.*, 1964, **68**, 571 (*pmr*)
Laszlo, P. *et al., Bull. Soc. Chim. Fr.*, 1966, 558 (*cmr*)
Poirer, Y. *et al., Bull. Soc. Chim. Fr.*, 1966, 1049; 1054 (*synth*)
Minoru, A. *et al., J. Mol. Spectrosc.*, 1972, **43**, 226 (*ir*)
Archer, W.J. *et al., J.C.S. Perkin 2*, 1982, 295 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPV250

2-Methyl-3-thiophenethiol, 9CI M-683

[2527-76-6]
3-Mercapto-2-methylthiophene



$C_5H_6S_2$ 130.234
Cysteine-derived Maillard product. Component of yeast extracts and meat flavour model systems. Possesses a meat-like, sulfury odour. Characterised spectroscopically. Odour threshold 0.0032-0.0128 ng/L in air.

Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms, ir*)
Werkhoff, P. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1991, **131**, 30-57 (*occur*)
Hofmann, T. *et al., J. Agric. Food Chem.*, 1995, **43**, 2187-2194 (*occur*)
Ames, J.M. *et al., J. Agric. Food Chem.*, 2001, **49**, 1885-1894 (*occur*)

5-Methyl-2-thiophenethiol M-684

[3920-28-3]
2-Mercapto-5-methylthiophene

$C_5H_6S_2$ 130.234
Bp_{13} 72-73°. n_D^{20} 1.5904.

S-*Me:2-Methyl-5-(methylthio)thiophene*
$C_6H_8S_2$ 144.261
Component of thermally degraded thiamine flavours. Bp_{12} 56-57°. n_D^{20} 1.5190.

Cederlund, B. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 198-202 (*synth, S-Me, pmr*)
Guentert, M. *et al., CA*, 1992, **117**, 169713e (*S-Me, occur*)

5-Methyl-3-thiophenethiol, 9CI M-685

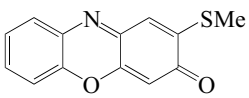
[2634-17-5]
3-Mercapto-5-methylthiophene

$C_5H_6S_2$ 130.234
Cysteine-derived Maillard product. Component of meat flavour model systems. Possesses a green, meaty, herbaceous odour. Characterised spectroscopically.

Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms, ir*)
Hincelin, O. *et al., Food Chem.*, 1992, **44**, 381-389 (*occur*)

2-(Methylthio)-3*H*-phenoxazin-3-one, 9CI M-686

[115695-20-0]



$C_{13}H_9NO_2S$ 243.286
Isol. from cultures of the mushroom *Calocybe gambosa* (St George's mushroom).

Kuchen, A. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 363-365

1-(Methylthio)-5-phenyl-1-penten-3-yne M-687

[5-(Methylthio)-4-penten-2-ynyl]benzene, 9CI
$PhCH_2C{\equiv}CCH{=}CHSMe$
$C_{12}H_{12}S$ 188.293

(Z)-form
Isol. from roots of *Chrysanthemum coronarium* (chop-suey greens). Light-yellow oil. $Bp_{0.1}$ 110°. λ_{max} 274 (ϵ 18400); 281 (ϵ 18400) (Et_2O).

Bohlmann, F. *et al., Chem. Ber.*, 1963, **96**, 226; 1964, **97**, 1179 (*isol, uv, ir, pmr, struct*)

3-(Methylthio)propanal, 9CI M-688

[3268-49-3]
3-(Methylthio)propionaldehyde, 8CI. Methylmercaptoaldehyde. MMP. Methional. FEMA 2747
$MeSCH_2CH_2CHO$
C_4H_8OS 104.173
Flavouring ingredient. Present in concord grape, asparagus, baked potato, wheat bread, other breads, Swiss cheese, cocoa, roasted filbert, roasted peanut and other foodstuffs. Liq. with powerful onion/meat-like odour and meat/soup-like taste. d^{20} 1.14. Bp 165-175° Bp_{14} 61°. n_D^{25} 1.4813.

▶ LD_{50} (rat, orl) 4400 mg/kg. UE2285000

2,4-Dinitrophenylhydrazone: [7372-49-8] Cryst. (MeOH) or yellow-orange needles (EtOH). Mp 122-123° (120.5°).

Di-Me acetal: [13214-29-4] *1,1-Dimethoxy-3-(methylthio)propane*
$C_6H_{14}O_2S$ 150.241
$Bp_{0.9}$ 73°.

Di-Et acetal: [16630-61-8] *1,1-Diethoxy-3-(methylthio)propane*
$C_8H_{18}O_2S$ 178.295
Bp_{12} 91° $Bp_{0.7}$ 68-74°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 748B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 571A (*ir*)
Catch, J.R. *et al., J.C.S.*, 1947, 1609 (*synth*)
Pierson, E. *et al., J.A.C.S.*, 1949, **70**, 1450 (*di-Et acetal*)
Mapson, L.W. *et al., Biochem. J.*, 1969, **111**, 413-418 (*biosynth*)
Boustany, K.S. *et al., Chimia*, 1969, **23**, 331-333 (*ir*)
Ichikawa, T. *et al., J.O.C.*, 1970, **35**, 344-346 (*di-Me acetal*)
Courtrot, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1975, **281**, 131-133 (*synth*)
Yoshifuji, M. *et al., Chem. Lett.*, 1979, 723-726 (*di-Et acetal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1875 (*occur, props*)

3-(Methylthio)propanoic acid, 9CI M-689

[646-01-5]
$MeSCH_2CH_2COOH$
$C_4H_8O_2S$ 120.172
Pale yellow oil or flaky solid (hexane). Mp 20.5-21.5°. Bp_{13} 131-133°.

Me ester: [13532-18-8] *FEMA 2720*
$C_5H_{10}O_2S$ 134.199
Isol. from pineapple (*Ananas comosus*), melon, naranjila fruit (*Solanum quitoense*) and white wine. Flavouring ingredient. Oil with sweet pineapple flavour at high dilutions. Bp 170-180° Bp_{100} 106-108°.

Et ester: [13327-56-5] *FEMA 3343*
$C_6H_{12}O_2S$ 148.226
Isol. from pineapple (*Ananas comosus*), melon, passion fruit and other fruits. Also present in alcoholic beverages and Parmesan cheese. Flavouring ingredient. Oil. Bp_{18} 88°.

[14090-35-8, 71922-81-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 670C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1064C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 729C (*ir*)
Haagen-Smit, A.J. *et al., J.A.C.S.*, 1945, **67**, 1646-1650; 1651-1652 (*isol, synth*)
Adlerová, E. *et al., Coll. Czech. Chem. Comm.*, 1959, **24**, 1208 (*synth*)
Connell, D.W. *et al., Aust. J. Chem.*, 1964, **17**, 130-140 (*occur*)
Rodin, J.O. *et al., J. Food Sci.*, 1966, **31**, 721-725; *CA*, **65**, 19225d (*isol*)
Langler, R.F. *et al., Can. J. Chem.*, 1979, **57**, 3193-3199 (*Me ester, ir, pmr, ms*)
Perraux, D. *et al., Physiol. Plant Pathol.*, 1982, **20**, 313-319 (*isol*)

Doi, J.T. *et al., J.O.C.*, 1986, **51**, 1026-1029 (*synth, pmr*)
Cadamuro, S. *et al., Synthesis*, 1986, 1070-1073 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1018; 1801 (*esters, use, occur*)

3-(Methylthio)-1-propene, 9CI M-690

[10152-76-8]
Allyl methyl sulfide, 8CI. Methyl 2-propenyl sulfide
$H_2C{=}CHCH_2SMe$
C_4H_8S 88.173
Constit. of garlic volatiles. Potential nutriceutical. Oil. d^{20} 0.88. Bp 91-93°. n_D^{20} 1.4712.

S-*Oxide, (+)-form:* [21632-71-3] *3-(Methylsulfonyl)-1-propene, 9CI. Allyl methyl sulfoxide*
C_4H_8OS 104.173
$[\alpha]_D^{24}$ +4.9 (c, 2.14 in EtOH).

S,S-*Dioxide:3-(Methylsulfonyl)-1-propene. Allyl methyl sulfone*
$C_4H_8O_2S$ 120.172
Bp_1 135°.

[21892-75-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 269B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 432B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 353C (*ir*)
Obermeyer, J. *et al., Ber.*, 1887, **20**, 2925 (*synth*)
Challenger, F. *et al., Biochem. J.*, 1949, **44**, 89 (*synth*)
Axelrod, M. *et al., J.A.C.S.*, 1968, **90**, 4835 (*oxide, synth, pmr*)
Baechler, R.D. *et al., Tet. Lett.*, 1978, **2**, 105 (*oxide, synth*)
Laakso, I. *et al., Planta Med.*, 1989, **55**, 257-261 (*isol*)
Culshaw, P.N. *et al., J.C.S. Perkin 2*, 1991, 1201 (*dioxide, pmr*)

3-(Methylthio)propyl glucosinolate M-691

[26888-03-9]
1-Thio-β-D-glucopyranose 1-[4-(methythio)-N-(sulfooxy)butanimidate], 9CI. ***Glucoibervirin***
$MeSCH_2CH_2CH_2C(SGlc){=}NOSO_3H$
$C_{11}H_{21}NO_9S_3$ 407.486

S-*Oxide:* [554-88-1] *3-(Methylsulfinyl)-propyl glucosinolate.* ***Glucoiberin***
$C_{11}H_{21}NO_{10}S_3$ 423.486
Isol. from seeds of *Brassica oleracea* and other crucifers. Needles (EtOH aq.). Mp 142-144° dec. (as K salt). $[\alpha]_D^{20}$ -55.3 (c, 4.9 in H_2O).

S-*Oxide, tetra-Ac:*
Needles + $1H_2O$ (EtOH aq.) (as K salt). Mp 145-147° dec. (K salt). $[\alpha]_D^{23}$ -16.6 (c, 2.0 in H_2O).

S,S-*Dioxide:* [554-86-9] *3-(Methylsulfonyl)propyl glucosinolate.* ***Glucocheirolin***
$C_{11}H_{21}NO_{11}S_3$ 439.485
Isol. from seeds of many crucifers. Cryst. (EtOH aq.) (as K salt). Mp 168° (K salt). $[\alpha]_D$ -18.5 (c, 3.45 in H_2O).

S,S-*Dioxide, tetra-Ac:*
$C_{19}H_{29}NO_{15}S_3$ 607.634
Mp 193-194° (as K salt). $[\alpha]_D$ -18 (c, 1.0 in H_2O).

[15592-34-4, 15592-36-6, 27303-31-7]

Schneider, W. *et al., Ber.*, 1913, **46**, 2634 (*isol*)
Schultz, O.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1954, **287**, 404 (*isol*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1955, **9**, 1143; 1959, **13**, 851 (*isol*)
Gmelin, R. *et al., Arzneim.-Forsch.*, 1966, **16**, 123; *CA*, **64**, 18023f (*isol*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*cmr*)
Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, D.H.), CRC Press, 1998, 29-53 (*rev, occur*)
Jaki, B. *et al., J. Nat. Prod.*, 2002, **65**, 517-522 (*Glucoiberin*)

1-(Methylthio)propyl 1-propenyl disulfide M-692

[37399-26-1]

[56019-32-0, 56019-35-3]
3-Ethyl-2,4,5-trithia-6-octene
$H_3CCH_2CH(^2SMe)–S–S–CH{=}CHCH_3$
$C_7H_{14}S_3$ 194.386
$Bp_{0.001}$ 68-70°.

2-Oxide:

[132216-22-9, 132216-25-2, 132216-26-3, 132240-37-0, 134053-76-2, 134053-77-3, 134053-78-4, 134053-79-5, 134107-57-6, 134107-58-7] *1-(Methylsulfinyl)propyl 1-propenyl disulfide*
$C_7H_{14}OS_3$ 210.385
Constit. of *Allium cepa* (onion) and *Allium tricoccum* (wood leek). Oil. Numerous stereoisomers have been identified.

(-)-*form*
Constit. of *Ferula assa-foetida* (asafoetida). Oil. Sol. MeOH, hexane; poorly sol. H_2O. $[\alpha]_D^{25}$ -8.4 (c, 0.2 in Me_2CO). λ_{max} 210 (ε 10000) (MeOH) (Berdy).

Naimie, H. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1166-1177 (*isol*)
Meijer, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 242 (*synth*)
Morimitsu, Y. *et al., Phytochemistry*, 1990, **29**, 3435-3439
Morimitsu, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 889-890
Morimitsu, Y. *et al., J. Agric. Food Chem.*, 1992, **40**, 368-372
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol, ms*)

1-(Methylthio)propyl 2-propenyl disulfide M-693

Allyl 1-(methylthio)propyl disulfide. 3-Ethyl-2,4,5-trithia-7-octene
$H_3CCH_2CH(^2SMe)–S–S–CH_2CH{=}CH_2$
$C_7H_{14}S_3$ 194.386

2-Oxide:1-(Methylsulfinyl)propyl 2-propenyl disulfide
$C_7H_{14}OS_3$ 210.385
Constit. of *Allium tricoccum* (wood leek).

Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*isol, ms*)

1-(Methylthio)propyl propyl disulfide M-694

[126876-22-0]
3-Ethyl-2,4,5-trithiaoctane
$H_3CCH_2CH(^2SMe)–S–S–CH_2CH_2CH_3$
$C_7H_{16}S_3$ 196.401
Constit. of *Allium fistulosum* (Welsh onion).

2-Oxide: [132216-21-8] *1-(Methylsulfinyl)propyl propyl disulfide*
$C_7H_{16}OS_3$ 212.401
Constit. of *Allium cepa* (onion) juice and *Allium tricoccum* (wood leek).

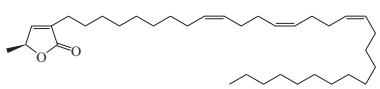
Kuo, M.C. *et al., J. Agric. Food Chem.*, 1992, **40**, 111-117 (*isol*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol, ms*)

25-Methyl-10-triacontanone M-695

[151454-16-9]
$H_3C(CH_2)_4CH(CH_3)(CH_2)_{14}CO(CH_2)_8CH_3$
$C_{31}H_{62}O$ 450.83
Constit. of the tubers of *Colocasia esculenta antiquorum*. Mp 73-74°.

Ali, M. *et al., J. Indian Chem. Soc.*, 1992, **69**, 887 (*isol*)

5-Methyl-3-(9,13,17-triacontatrienyl)-2(5*H*)-furanone M-696



$C_{35}H_{60}O_2$ 512.858
(5*S*,9′*Z*,13′*Z*,17′*Z*)-*form* [206131-74-0] ***Chatenaytrienin 2***
Constit. of *Annona muricata* (soursop).

9′,10′-Dihydro: [206131-77-3] *5-Methyl-3-(13,17-triacontadienyl)-2(5*H*)-furanone.* ***Muricadienin***
Constit. of *Annona muricata* (soursop).

Gleye, C. *et al., Phytochemistry*, 1998, **47**, 749-754 (*isol, pmr, cmr, ms*)

5-Methyl-3-(11,15,19-triacontatrienyl)-2(5*H*)-furanone M-697

$C_{35}H_{60}O_2$ 512.858
(5*S*,11′*Z*,15′*Z*,19′*Z*)-*form* [206131-73-9] ***Chatenaytrienin 1***
Constit. of *Annona muricata* (soursop).

19′,20′-Dihydro: [185502-80-1] *5-Methyl-3-(11,15-triacontadienyl)-2(5*H*)-furanone, 9CI.* ***Muridienin 1***
$C_{35}H_{62}O_2$ 514.874
Constit. of *Annona muricata* (soursop). Oil. $[\alpha]_D$ +11 (c, 0.1 in MeOH). λ_{max} 210 (log ε 3.6) (MeOH).

Gleye, C. *et al., Tet. Lett.*, 1996, **37**, 9301-9304 (*Muridienin 1*)
Gleye, C. *et al., Phytochemistry*, 1998, **47**, 749-754 (*Chatenaytrienin 1*)

2-Methyltricosane M-698

[1928-30-9]
$H_3C(CH_2)_{20}CH(CH_3)_2$

$C_{24}H_{50}$ 338.659
Minor constit. of hops (*Humulus lupulus*). Mp 42°.

Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1654; 1670 (*glc, ir*)

3-Methyltricosane, 9CI M-699

[13410-45-2]

$H_3C(CH_2)_{19}CH(CH_3)CH_2CH_3$

$C_{24}H_{50}$ 338.659
Isol. from hop oil (*Humulus lupulus*) and orange oil (*Citrus sinensis*). Bp_{10} 233°. n_D^{50} 1.4375.

[55194-20-2]

Wollrab, V. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1670 (*isol*)
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807 (*isol*)
Streibl,, M. *et al., Fette, Seifen, Anstrichm.*, 1968, **70**, 543 (*synth*)

12-Methyltridecanoic acid, 9CI M-700

[2724-57-4]
Isomyristic acid. Aseonostatin P1. Aseanostatin P1

$(H_3C)_2CH(CH_2)_{10}COOH$

$C_{14}H_{28}O_2$ 228.374
Occurs in Baltic salmon and sperm whale. Mp 53°. Bp_2 158°.

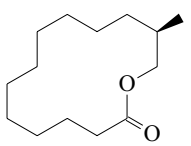
Et ester:
$C_{16}H_{32}O_2$ 256.428
Bp_5 140-142°.

Amide:
$C_{14}H_{29}NO$ 227.389
Mp 107°.

Fordyce, C.R. *et al., J.A.C.S.*, 1933, **55**, 3371 (*synth*)
Tyrrell, D. *et al., Lipids*, 1968, **3**, 368 (*ir, ms*)
Goodrich, B. *et al., Aust. J. Chem.*, 1971, **24**, 153
Carballeira, N. *et al., J.O.C.*, 1986, **51**, 2751 (*synth*)
Ishida-Okawara, A. *et al., J. Antibiot.*, 1991, **44**, 524 (*Aseonostatin*)

12-Methyl-13-tridecanolide M-701

[57092-32-7]
13-Methyloxacyclotetradecan-2-one



(*R*)-form

$C_{14}H_{26}O_2$ 226.358
Constit. of root of *Angelica archangelica* (angelica).

(R)-form
Liq. $[\alpha]_D^{25}$ +14.7 (c, 1.4 in $CHCl_3$).

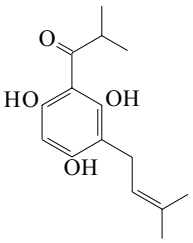
(S)-form
$[\alpha]_D^{22}$ -15.5 (c, 0.3 in $CHCl_3$).

(±)-form
Yellow oil with musk-like odour. $Bp_{0.005}$ 100°.

Taskinen, J. *et al., Acta Chem. Scand., Ser. B*, 1975, **29**, 637 (*isol, ir, ms, pmr*)
Stanchev, S. *et al., Helv. Chim. Acta*, 1987, **70**, 1389 (*synth, ir, pmr, cmr, ms*)
Kraft, P. *et al., Annalen*, 1994, 1161; 1995, 1409 (*synth, ir, pmr, cmr, ms*)

2-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-propanone M-702

[35932-36-6]
2-(2-Methylpropanoyl)-4-prenylphloroglucinol



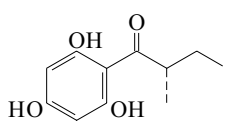
$C_{15}H_{20}O_4$ 264.321
Constit. of *Helichrysum* spp. Also found in hops. Yellow prisms (C_6H_6). Mp 166°.

4''-Acetoxy:
$C_{17}H_{22}O_6$ 322.357
Mp 140°.

Drawert, F. *et al., Phytochemistry*, 1976, **15**, 1695 (*isol*)
Meikle, T. *et al., J.C.S. Perkin 1*, 1978, 1303 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 348 (*isol*)
Cann, M.R. *et al., Chem. Ind. (London)*, 1982, 779 (*pmr*)
Kuhnke, J. *et al., Tet. Lett.*, 1985, **26**, 3955 (*synth*)
Jakupovic, J. *et al., Phytochemistry*, 1986, **25**, 1133 (*isol*)
Mathekga, A.D.M. *et al., Phytochemistry*, 2000, **53**, 93-96 (*acetoxy*)

2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone M-703

*(2-Methylbutyryl)phloroglucinol. **Multifidol***



$C_{11}H_{14}O_4$ 210.229

(S)-form [125074-06-8]
Cryst. Mp 116-118°. λ_{max} 229 (log ε 3.66); 287 (log ε 3.81) (MeOH).

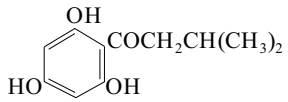
2-O-β-D-Glucopyranoside: [124960-73-2]
$C_{17}H_{24}O_9$ 372.371
Cryst. Mp 139-140°. λ_{max} 225 (log ε 3.97); 287 (log ε 4.2) (MeOH).

2-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [467437-62-3]
$C_{22}H_{32}O_{13}$ 504.487
Constit. of the leaves and branches of *Phyllanthus emblica* (emblic). Amorph. yellow powder. $[\alpha]_D^{18}$ -60.3 (c, 0.3 in MeOH). λ_{max} 285 (log ε 4.02); 320 (sh) (log ε 3.55) (MeOH).

Kosasi, S. *et al., Phytochemistry*, 1989, **28**, 2439-2441 (*isol, pmr, cmr*)
Zhang, Y.-J. *et al., Chem. Pharm. Bull.*, 2002, **50**, 841-843 (*isol, pmr, cmr*)

3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone, 9CI M-704

[26103-97-9]
2′,4′,6′-Trihydroxy-3-methylbutyrophenone, 8CI. 2,4,6-Trihydroxyisovalerophenone. Phlorisovalerophenone



$C_{11}H_{14}O_4$ 210.229
Constit. of *Humulus lupulus* (hops). Mp 95° (monohydrate) Mp 145° (anhyd.).

2,4-Dinitrophenylhydrazone:
Mp 196°.

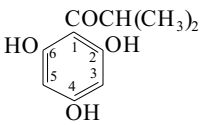
2-Me ether: [478-48-8]
$C_{12}H_{16}O_4$ 224.256
Mp 132°.

4-Me ether:
$C_{12}H_{16}O_4$ 224.256
Mp 96-97°.

Kenny, T.S. *et al., J.C.S.*, 1939, 1601 (*synth*)
Orth, W.A. *et al., Annalen*, 1963, **663**, 74
Zuurbier, K.W.M. *et al., Phytochemistry*, 1995, **38**, 77 (*isol, biosynth*)

2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-propanone, 9CI M-705

[35458-21-0]
2′,4′,6′-Trihydroxy-2-methylpropiophenone, 8CI. 2,4,6-Trihydroxyisobutyrophenone. Phlorisobutyrophenone



$C_{10}H_{12}O_4$ 196.202
Pale yellow cryst. Mp 197° (177-178°). Lower Mp's including hydrate formation have been reported.

2-O-β-Glucopyranoside: [17004-75-0]
$C_{16}H_{22}O_9$ 358.344
Constit. of hops (*Humulus lupulus*). Mp 118°. $[\alpha]_D$ -59.8.

2-Me ether: [102092-19-3] *1-(2,4-Dihydroxy-6-methoxyphenyl)-2-methyl-1-propanone, 9CI. 2′,4′-Dihydroxy-6′-methoxy-2-methylpropiophenone. **Robustaol B***
$C_{11}H_{14}O_4$ 210.229
Oil.

4-Me ether: [42541-62-8] *2′,6′-Dihydroxy-4′-methoxy-2-methylpropiophenone*
$C_{11}H_{14}O_4$ 210.229
Oil.

Tri-Me ether: [480-25-1] *2-Methyl-1-(2,4,6-trimethoxyphenyl)-1-propanone. 2,4,6-Trimethoxyisobutyrophenone. **Conglomerone***
$C_{13}H_{18}O_4$ 238.283
Mp 62-62.5°.

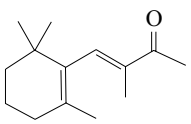
Riedl, W. *et al., Annalen*, 1954, **585**, 38-42 (*synth*)
Baigent, D.R. *et al., Aust. J. Chem.*, 1973, **27**, 2065-2066 (*4-Me ether, synth*)

Amer, M.I. *et al., J.C.S. Perkin 1*, 1983, 1075-1082 (*synth*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 174-176 (*isol*)
Mizobuchi, S. *et al., Agric. Biol. Chem.*, 1985, **49**, 719-724 (*synth*)
Qin, G. *et al., Huaxue Xuebao*, 1986, **44**, 151; *CA*, **104**, 203867 (*Robustaol B*)
Jakupovic, J. *et al., Phytochemistry*, 1986, **25**, 1133-1142 (*isol*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317-331 (*synth*)
Tada, M. *et al., J. Med. Chem.*, 1992, **35**, 1209-1212 (*synth*)
Bloor, S.J. *et al., J. Nat. Prod.*, 1992, **55**, 43-47 (*2-Me ether, 4-Me ether, synth*)
Howard, G.A. *et al., J.C.S.*, 1995, 174-181 (*synth*)
Zuurbier, K.W.M. *et al., Phytochemistry*, 1995, **38**, 77-82 (*biosynth*)

3-Methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one, 9CI, 8CI M-706

[79-89-0]

[1322-70-9]
3-Methyl-β-ionone. β-iso-*Methylionone. δ-Methylionone. FEMA 2713*



$C_{14}H_{22}O$ 206.327

Considerable confusion over the struct. and nomenclature of this and closely-related isomeric compds. given in the lit. under the various synonyms. It appears that some of the structs./names reported are erroneous. Flavouring ingredient. Liq. with floral odour and berry-like flavour. Bp_2 105-106° ($Bp_{3.1}$94°). n_D^{25} 1.4969.

Semicarbazone:
Cryst. (EtOH). Mp 183-184°.

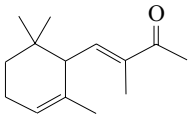
2,4-Dinitrophenylhydrazone:
Mp 148-149°.

[7784-98-7]

Köster, H. *et al., Chem. Ber.*, 1947, **80**, (*synth*)
Lusskin, R.M. *et al., J.A.C.S.*, 1949, **71**, 2412 (*uv*)
Beets, M.G.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1950, **69**, 307; 736 (*props, struct, synth, uv*)
Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1951, 249 (*synth*)
Naves, Y.R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 1308 (*ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 561 (*use*)

3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, 9CI M-707

[127-51-5]
3-Methyl-α-ionone. Isomethyl-α-ionone. Cetone Alpha. FEMA 2714



(*E*)-*form*

$C_{14}H_{22}O$ 206.327

(±)-(*E*)-*form* [97306-52-0]

[15789-90-9]
Flavouring ingredient. Liq. with a fine violet and orris-like odour. Bp_2 103-104° (105-110°).

2,4-Dinitrophenylhydrazone:
Mp 163.5-164°.

Semicarbazone:
Cryst. (EtOH). Mp 202°.

2-Alcohol: [70172-00-8] *3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-ol, 9CI. 3-Methyl-α-ionol. Isomethyl-α-ionol*
$C_{14}H_{24}O$ 208.343

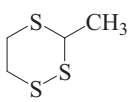
2-Alcohol, Ac: [68555-61-3] *3-Methyl-α-ionyl acetate. α-Isomethylionyl acetate. FEMA 3845*
$C_{16}H_{26}O_2$ 250.38
Flavouring ingredient for candies etc.. Liq. with soft violet-vetiver odour. Bp_1 90°.

(±)-(*Z*)-*form* [13743-21-0]
$Bp_{0.03}$ 69°.

Köster, H. *et al., Chem. Ber.*, 1947, **80**, 248 (*synth*)
Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1951, 247 (*synth*)
Lecomte, J. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1956, **53**, 462; *CA*, **50**, 11824h (*ir*)
Becker, J. *et al., Helv. Chim. Acta*, 1974, **57**, 2679
Ford, R.A. *et al., Food Cosmet. Toxicol.*, 1988, **26**, 383 (*2-alcohol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1476-1477
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 894-895 (*3-Methyl-α-ionyl acetate*)

3-Methyl-1,2,4-trithiane, 9CI M-708

[43040-01-3]
FEMA 3718



$C_4H_8S_3$

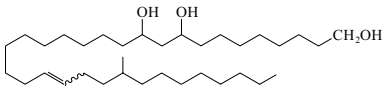
Cysteine derived Maillard product. Flavouring ingredient. Present in aroma of cooked beef, roasted sesame seed oil, yeast extracts and durian fruit (*Durio zibethinus*).

(±)-*form*
Liq. d_4^{20} 1.62. n_D^{20} 1.6168.

Werkhoff, P. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1991, **13**, 30-57 (*occur, yeast*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 579 (*use*)
Naef, R. *et al., Flavour Fragrance J.*, 1996, **11**, 295-300 (*occur, durian*)
Mottram, D.S. *et al., Dev. Food Sci.*, 1998, **40**, 483-492 (*occur*)
Kleipool, R.J.C. *et al., CA*, **81**, 63593p (*synth*)

25-Methyl-21-tritriacontene-1,9,11-triol M-709

[151454-19-2]

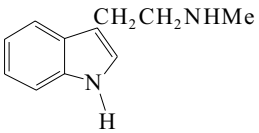


$C_{34}H_{68}O_3$ 524.909
Constit. of the tubers of *Colocasia esculenta* (taro). Mp 83-84°.

Ali, M. *et al., J. Indian Chem. Soc.*, 1992, **69**, 887 (*isol*)

N-Methyltryptamine M-710

[61-49-4]
N-*Methyl-1*H-*indole-3-ethanamine, 9CI. 3-(2-Methylaminoethyl)indole.* ***Dipterine***



$C_{11}H_{14}N_2$ 174.245
Prisms (petrol). Mp 90° (87-88°).
▶ NM0450000

Hydrochloride:
Mp 180°.

Methiodide:
Cryst. (MeOH). Mp 208-209°.

Picrate:
Red needles. Mp 193-195° (190°).

N^b-*Ac:* ***N^b-Acetyl-N^b-methyltryptamine***
$C_{13}H_{16}N_2O$ 216.282
Alkaloid from stems of *Limonia acidissima* (wood apple). Amorph.

N^b-*Hydroxy:* [57383-99-0] ***N^b-Hydroxy-N^b-methyltryptamine***
$C_{11}H_{14}N_2O$ 190.244
Prisms (C_6H_6). Mp 100-101°.

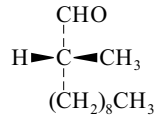
N^b-*(3-Methylbutanoyl):* ***Methylmadugin***
$C_{16}H_{22}N_2O$ 258.363
Oil. λ_{max} 224 ; 274 (sh) ; 283 ; 292 (Et_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 661A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 132A (*nmr*)
Yurashevskii, N.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1940, **10**, 1781; *CA*, **35**, 4016 (*isol, struct*)
Cohen, L.A. *et al., J.A.C.S.*, 1960, **82**, 2184 (*synth, pmr*)
Fitzgerald, J.S. *et al., Aust. J. Chem.*, 1965, **18**, 433 (*isol, struct*)
Nakagawa, M. *et al., J.A.C.S.*, 1975, **97**, 6496 (*N-Hydroxy-N-methyltryptamine*)
Grina, J.A. *et al., J.O.C.*, 1982, **47**, 2648 (*isol, uv, pmr, ms*)
Zarga, M.H.A. *et al., J. Nat. Prod.*, 1986, **49**, 901 (*deriv*)
Thompson, A.C. *et al., J. Agric. Food Chem.*, 1987, **35**, 361 (*N-Hydroxy-N-methyltryptamine*)
Riemer, B. *et al., Phytochemistry*, 1997, **45**, 337 (*Methylmadugin*)

2-Methylundecanal, 9CI M-711

[110-41-8]
2-Methylnonylacetaldehyde. Aldehyde

MNA. FEMA 2749



(*R*)-*form*

$C_{12}H_{24}O$ 184.321Enantiomers show little difference in odour props..

►YQ1509000

(*R*)-*form*

$Bp_{9.75}$ 114°. $[\alpha]_D^{25}$ -13.7 (neat) (96% ee).

(*S*)-*form* [128871-20-5]

Bp_{10} 115°. $[\alpha]_D^{25}$ +13.7 (neat).

(±)-*form* [135026-96-9]

Flavouring ingredient. Liq. with ambergris-like fatty odour. Bp 171° Bp_{10} 114°. n_D^{20} 1.4321.

►Fl. p. 69°.

Semicarbazone: [16742-16-8]

Mp 86°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 469C (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 733A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 556A (*ir*)

Wright, R.H. *et al., Am. Perfum. Cosmet.*, 1968, **83**, 43; *CA*, **69**, 91487c

Khulesza, J. *et al., Riechst., Aromen, Koerperpflegem.*, 1969, **19**, 8; *CA*, **71**, 49162j (*synth*)

Shutikova, L.A. *et al., CA*, 1974, **74**, 12552x (*synth*)

Groenewegen, F. *et al., Tet. Lett.*, 1979, 2817

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MQI550

Enders, D. *et al., Annalen*, 1990, 1107 (*synth, pmr, cmr*)

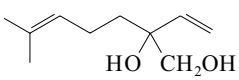
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 580

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1878-1879

6-Methyl-2-vinyl-5-heptene-1,2-diol M-712

[73510-11-9]

3-Hydroxymethyl-7-methyl-1,6-octadien-3-ol



$C_{10}H_{18}O_2$ 170.251

Oil.

1-O-β-D-Glucopyranoside: ***Unshuoside A***

$C_{16}H_{28}O_7$ 332.393

Constit. of *Citrus unshiu* (satsuma mandarin). Amorph. powder. $[\alpha]_D$ -5 (c, 0.45 in MeOH).

Ishida, T. *et al., J. Pharm. Sci.*, 1981, **70**, 406

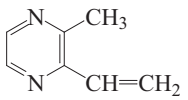
Coll, J.C. *et al., Aust. J. Chem.*, 1989, **42**, 1983 (*isol, pmr, cmr*)

Yoshikawa, K. *et al., Nat. Med. (Tokyo)*, 1996, **50**, 176; *CA*, **125**, 81942h (*Unshuoside A*)

2-Methyl-3-vinylpyrazine, 8CI M-713

[25058-19-9]

2-Ethenyl-3-methylpyrazine, 9CI



$C_7H_8N_2$ 120.154

Flavouring ingredient with a fresh, hazelnut, earthy note. Bp_{13} 66-67°.

U.S. Pat., 3 989 713; *CA*, **86**, 43556d (*synth, use*)

2-Methyl-5-vinylpyrazine, 8CI M-714

[13925-08-1]

2-Ethenyl-5-methylpyrazine, 9CI

$C_7H_8N_2$ 120.154

Aroma constit. of raw or cooked asparagus, baked or chipped potato, wheat bread, fried chicken, pork liver, cooked beef, cocoa, roasted coffee, roasted filbert, roasted peanut, popcorn, sukiyaki and roasted sesame seed oil. Bp_{12} 65-66°. Removed from GRAS list, formerly FEMA 3211.

Goldman, I.M. *et al., Helv. Chim. Acta*, 1967, **50**, 694-705 (*isol, synth, ms*)

Oser, B.L. *et al., Food Technol. (Chicago)*, 1984, **38**, 66-68 (*GRAS status*)

Stofberg, J. *et al., Perfum. Flavor.*, 1984, **9**, 53-56; **9(4)**, 58-59; 62; 65-72; 76-83 (*use*)

Boulton, A.J. *et al., J. Chem. Res., Miniprint*, 1989, 559-568 (*synth, pmr*)

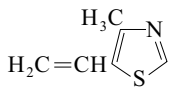
Shimoda, M. *et al., J. Agric. Food Chem.*, 1996, **44**, 3909 (*glc, occur, sesame oil*)

Buttery, R.G. *et al., J. Agric. Food Chem.*, 1997, **45**, 837-843 (*glc, occur, popcorn*)

4-Methyl-5-vinylthiazole, 8CI M-715

[1759-28-0]

5-Ethenyl-4-methylthiazole. FEMA 3313



C_6H_7NS 125.194

Meat flavouring ingredient. Found in grape wine distillate, garlic, cooked pork, cocoa, roasted filbert and yellow passion fruit. d_{25}^{25} 1.09. Bp_{25} 78-80° Bp_{19} 78-82° (lit. gives a pressure range).

►LD_{50} (mus, orl) 400 mg/kg. XJ5104000

Picrate:

Needles (AcOH). Mp 162-163°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 643B (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 111A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1493C (*ir*)

Buchman, E.R. *et al., J.A.C.S.*, 1945, **67**, 395-399 (*synth*)

Bachmann, G.B. *et al., J.A.C.S.*, 1949, **71**, 1985-1988 (*synth*)

Murav'eva, K.M. *et al., Zh. Obshch. Khim.*, 1963, **33**, 3723-3725; *J. Gen. Chem. USSR (Engl. Transl.)*, 1963, **33**, 3655-3657 (*synth*)

Schilling, C.L. *et al., Macromolecules*, 1968, **1**, 445-451 (*pmr*)

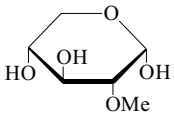
Fr. Pat., 1974, 2 329 309; *CA*, **82**, 170885c (*synth*)

Strauss, C.R. *et al., Chem. Ind. (London)*, 1978, 232-233 (*occur*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 583 (*rev*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1884 (*rev*)

2-*O*-Methylxylose M-716



α-D-Pyranose-*form*

$C_6H_{12}O_5$ 164.158

D-*form* [7434-28-8]

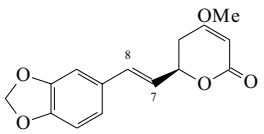
Isol. from hydrol. of *Prunus domestica* (plum) polysaccharides. Mp 137-138°. $[\alpha]_D$ -21 → +34 (2 hr.) (H_2O).

Ehrenthal, I. *et al., J.A.C.S.*, 1954, **76**, 5509 (*D-form, β-D-Me pyr*)

Andrews, P. *et al., Chem. Ind. (London)*, 1956, 1278 (*D-form, isol*)

Methysticin M-717

*6-[2-(1,3-Benzodioxol-5-yl)ethenyl]-5,6-dihydro-4-methoxy-2*H*-pyran-2-one. 4-Methoxy-6-(3,4-methylenedioxystyryl)-5,6-dihydropyran. Kaurain (obsol.)*†



(*R*)-*form*

$C_{15}H_{14}O_5$ 274.273Log P 1.2 (uncertain value) (calc).

(*R*)-*form* [495-85-2]

Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Cryst. (MeOH). Mp 139-140.5°. $[\alpha]_D^{28}$ +95 (c, 1 in Me_2CO).

►LD_{50} (mus, ipr) 530 mg/kg. UQ0517000

7,8-Dihydro: [19902-91-1] ***Dihydromethysticin***. *ψ-Methysticin. Pseudomethysticin*

$C_{15}H_{16}O_5$ 276.288

Isol. from *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Prisms (MeOH). Mp 117-118°. $[\alpha]_D$ +21 (MeOH). Log P 1.51 (uncertain value) (calc). Has (*S*)-config..

►UQ0516000

(±)-*form*

Cryst. (MeOH). Mp 132-134°.

7,8-Dihydro: [3155-57-5]

Needles (2-propanol). Mp 110-111°.

[583-18-6]

Borsch, W. *et al., Ber.*, 1929, **62**, 360 (*Dihydromethysticin*)

Klohs, M.W. *et al., J. Med. Chem.*, 1959, **1**, 95 (*isol*)

Klohs, M.W. *et al., J.O.C.*, 1959, **24**, 1829 (*synth*)

Beak, P. *et al., J.O.C.*, 1962, **27**, 3715 (*pmr*)

Snatzke, G. *et al., Tet. Lett.*, 1968, 1797 (*abs config*)

Engel, P. *et al., Verh. Schweiz. Naturforsch. Ges.*, 1971, **151**, 613 (*cryst struct*)

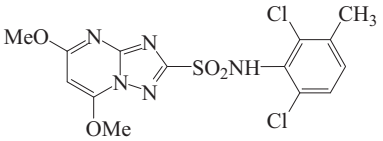
Achenbach, H. *et al., Chem. Ber.*, 1973, **106**, 2648 (*pmr*)

Franca, N.C. *et al., Phytochemistry*, 1973, **12**, 1182 (*Dihydromethysticin*)

Ranjith, H. *et al., Phytochemistry*, 2002, **59**, 429-433 (*isol, pmr, cmr, bibl*)

Metosulam, ANSI, BSI M-718

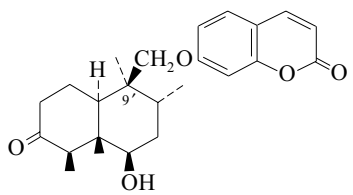
[139528-85-1]
N-*(2,6-Dichloro-3-methylphenyl)-5,7-dimethoxy[1,2,4]triazolo[1,5-*a*]pyrimidine-2-sulfonamide, 9CI. DE 511. XDE 511. XRD 511*



$C_{14}H_{13}Cl_2N_5O_4S$ 418.259
Selective post-emergence herbicide used on cereals against broad-leaved weeds. Cryst. (DMF aq.). Mp 224-226° (210-211.5°). pK_a 4.8.
► LD_{50} (rat, orl) >5000 mg/kg.
U.S. Pat., 1985, 4 818 273; *CA*, **103**, 196117f (*synth, use*)
Kleschick, W.A. *et al., ACS Symp. Ser.*, 1992, **504**, 17-25 (*synth, activity, sar*)
Shankar, R.B. *et al., J. Het. Chem.*, 1993, **30**, 169-172 (*synth, ir, pmr, cmr*)
Snel, M. *et al., Meded. - Fac. Landbouwkd. Toegepaste Biol. Wet. (Univ. Gent)*, 1993, **58**, 845-852 (*rev*)
Timchalk, C. *et al., J. Appl. Toxicol.*, 1997, **17**, 9-21 (*pharmacokinetics*)
Pesticide Manual, 11th edn., 1997, No. 495
Parnell, J.S. *et al., J. Agric. Food Chem.*, 1998, **46**, 152-156 (*occur, anal*)

Microlobin M-719

[89803-98-5]

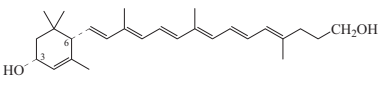


$C_{24}H_{30}O_5$ 398.498
Cryst. (EtOAc/hexane). Mp 150-151°. $[\alpha]_D^{20}$ +49 (c, 0.5 in $CHCl_3$).

9′-Epimer: [94898-76-7] ***Kamolonol***
$C_{24}H_{30}O_5$ 398.498
Constit. of *Ferula assa-foetida* (asafoetida). $[\alpha]_D^{20}$ +17 ($CHCl_3$).
Nabiev, A.A. *et al., Khim. Prir. Soedin.*, 1983, **19**, 700; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 664 (*Microlobin*)
Hofer, G. *et al., Monatsh. Chem.*, 1984, **115**, 1207 (*Kamolonol*)

α-Micropteroxanthin M-720

11′,12′-Dihydro-10′-apo-ϵ-carotene-3,10′-diol



(3*R*,6*S*)-*form*

$C_{27}H_{40}O_2$ 396.612

(3R,6S)-form [148044-84-2]
α-Micropteroxanthin B
Isol. from integuments of black bass, *Micropterus salmoides*. λ_{max} 353 ; 372 ; 394 (Et_2O).

(3S,6S)-form [148151-51-3]
α-Micropteroxanthin A
Isol. from integuments of black bass, *Micropterus salmoides*. λ_{max} 353 ; 372 ; 394 (Et_2O).

Δ^5-Isomer: [148031-80-5] *11′,12′-Dihydro-10′-apo-β-carotene-3,10′-diol.* ***β-Micropteroxanthin***
$C_{27}H_{40}O_2$ 396.612
Isol. from integuments of black bass *Micropterus salmoides*. λ_{max} 377 ; 395 (Et_2O).

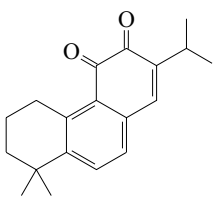
Δ^5-Isomer, 7,8-didehydro: [148031-76-9] *7,8-Didehydro-11′,12′-dihydro-10′-apo-β-carotene-3,10′-diol.* ***7,8-Dehydro-β-micropteroxanthin***
$C_{27}H_{38}O_2$ 394.596
Isol. from integuments of black bass *Micropterus salmoides*. λ_{max} 383 ; 404 (Et_2O).
Yamashita, E. *et al., Nippon Suisan Gakkaishi*, 1992, **58**, 2277-2282

Millefolide M-721

$C_{15}H_{22}O_3$ 250.337
Sesquiterpene monocyclic lactone contg. conjugated methylene, OH and CO groups. Isol. from *Achillea millefolium* (yarrow) flower heads. Fibrous needles (diisopropyl ether). Mp 138-140°. $[\alpha]_D^{20}$ +107.2 (c, 1.36 in $CHCl_3$). Readily polymerises.
Hochmannova, J. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1826

Miltirone M-722

[27210-57-7]
5,6,7,8-Tetrahydro-8,8-dimethyl-2-(1-methylethyl)-3,4-phenanthrenedione, 9CI. 5,6,7,8-Tetrahydro-2-isopropyl-8,8-dimethyl-3,4-phenanthraquinone. 20-Nor-5,7,9,13-abietatetraene-11,12-dione. Rosmariquinone

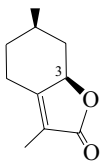


$C_{19}H_{22}O_2$ 282.382
Constit. of roots of *Salvia miltiorrhiza* (Chinese sage). Also present in leaves of rosemary (*Rosmarinus officinalis*). Antioxidant. Red needles (petrol). Mp 100°. λ_{max} 230 (ϵ 15800); 260 (ϵ 19000); 370 (ϵ 2000); 480 (ϵ 2250) (EtOH) (Derep). λ_{max} 260 (ϵ 35480); 362 (ϵ 2290); 436 (ϵ 3311) (MeOH) (Berdy).

1,2-Didehydro: [116064-77-8] *1,5,7,9,13-Abietapentaene-11,12-dione.* ***1,2-Didehydromiltirone***
$C_{19}H_{20}O_2$ 280.366
Red cryst. (hexane). Mp 71-75°.
Hayashi, T. *et al., Chem. Comm.*, 1970, 299 (*isol*)
Nasipuri, D. *et al., J.C.S. Perkin 1*, 1973, 285-287 (*synth*)
Romanova, A.S. *et al., Khim. Prir. Soedin.*, 1977, **13**, 414-415; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 350-351 (*isol*)
Chang, H.M. *et al., J.O.C.*, 1990, **55**, 3537-3543 (*Didehydromiltirone*)
Lee, J. *et al., J.O.C.*, 1990, **55**, 5013-5016 (*synth, ir, pmr, cmr, ms*)
Luis, J.G. *et al., J.C.S. Perkin 1*, 1996, 2207-2211 (*synth*)
Majetich, G. *et al., J.O.C.*, 1997, **62**, 6928-6951 (*synth*)
Hall, C.A. *et al., J. Agric. Food Chem.*, 1998, **46**, 1303-1310 (*synth, bibl*)

Mintlactone M-723

[38049-04-6]
*5,6,7,7*a*-Tetrahydro-3,6-dimethyl-2(4*H*)-benzofuranone, 9CI.* p-*Menth-4(8)-en-9,3-olide*

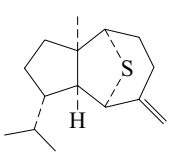


$C_{10}H_{14}O_2$ 166.219
Constit. of oil of peppermint. Flavouring ingredient. Oil. $[\alpha]_D^{20}$ -51.8 (c, 10 in EtOH).

3-Epimer: [75684-66-1] ***Isomintlactone***
$C_{10}H_{14}O_2$ 166.219
Present in peppermint oil. Flavour component. Cryst. Mp 77-79°. $[\alpha]_D^{25}$ +76.9 (c, 5 in EtOH).
Takahashi, K. *et al., Agric. Biol. Chem.*, 1980, **44**, 1535 (*isol*)
Tsuboi, S. *et al., J.O.C.*, 1980, **45**, 1517 (*synth*)
Fujita, T. *et al., J. Chem. Technol. Biotechnol.*, 1985, **35A**, 57 (*synth*)
Cory, R.M. *et al., Tet. Lett.*, 1990, **31**, 6789 (*synth*)
Akhita, A. *et al., Phytochemistry*, 1991, **30**, 485 (*biosynth*)
Shishido, K. *et al., Tet. Lett.*, 1992, **33**, 4589 (*synth*)
Chavan, S.P. *et al., Tet. Lett.*, 1992, **33**, 4605 (*synth*)
Carda, M. *et al., Tetrahedron*, 1992, **48**, 9789 (*synth*)
Chavan, S.P. *et al., Tetrahedron*, 1993, **49**, 6429 (*synth*)
Crisp, G.T. *et al., Tetrahedron*, 1995, **51**, 5831 (*synth*)
Lohray, B. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 226 (*synth*)
Tanyeli, C. *et al., Synth. Commun.*, 1997, **27**, 3471-3476 (*synth*)
Ferraz, H.M.C. *et al., J.O.C.*, 2000, **65**, 2606-2607 (*synth*)

Mintsulfide M-724

[72445-42-2]

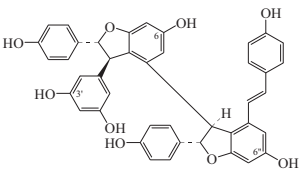


$C_{15}H_{24}S$ 236.421

Constit. of *Mentha piperita* oil. Cryst. (MeOH). Mp 64°. $[\alpha]_D^{25}$ -64.2 (c, 10 in hexane).

Yoshida, T. *et al., Chem. Comm.*, 1979, 512 (*cryst struct*)
Takahashi, K. *et al., Agric. Biol. Chem.*, 1981, **45**, 129 (*isol, synth*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr*)

Miyabenol C M-725



(E)-form

$C_{42}H_{32}O_9$ 680.709

(E)-form [109605-83-6]
Pale brown solid. $[\alpha]_D^{23}$ +69 (c, 0.07 in MeOH). λ_{max} 285 (MeOH) (Berdy).

(Z)-form [168037-22-7]
cis-*Miyabenol C*
Constit. of the fruit of *Foeniculum vulgare* (fennel). Yellowish powder. $[\alpha]_D^{28}$ +98.5 (c, 1 in MeOH).

3′-O-β-D-Glucopyranoside: [168010-10-4] ***Foeniculoside I***
$C_{48}H_{42}O_{14}$ 842.851
Constit. of the fruit of *Foeniculum vulgare* (fennel). Pale yellow powder. $[\alpha]_D^{23}$ +46.8 (c, 0.9 in MeOH).

6-O-β-D-Glucopyranoside: [168010-11-5] ***Foeniculoside II***
$C_{48}H_{42}O_{14}$ 842.851
Constit. of the fruit of *Foeniculum vulgare* (fennel). Brown powder. $[\alpha]_D^{28}$ +89.1 (c, 0.9 in MeOH). λ_{max} 285 (log ϵ 4.53) (MeOH).

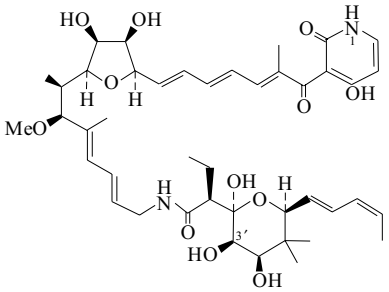
3′,6-Di-O-β-D-glucopyranoside: [168010-12-6] ***Foeniculoside III***
$C_{54}H_{52}O_{19}$ 1004.993
Constit. of the fruit of *Foeniculum vulgare* (fennel). Pale yellow powder. $[\alpha]_D^{23}$ +41.9 (c, 1 in MeOH).

3′,6,6″-Tri-O-β-D-glucopyranoside: [168010-13-7] ***Foeniculoside IV***
$C_{60}H_{62}O_{24}$ 1167.135
Constit. of the fruit of *Foeniculum vulgare* (fennel). Brown powder. $[\alpha]_D^{23}$ +40.7 (c, 0.8 in MeOH). λ_{max} 285 (log ϵ 4.53) (MeOH).

Suzuki, K. *et al., Agric. Biol. Chem.*, 1987, **51**, 1003-1008 (*Miyabenol C*)
Kawabata, J. *et al., Phytochemistry*, 1991, **30**, 649-653; 1995, **40**, 1507-1510 (*abs config*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 868-871 (*Foeniculosides*)

Mocimycin, 9CI, INN M-726

[50935-71-2]
Kirromycin. Delvomycin. MYC 8003. Antibiotic MYC 8003



$C_{43}H_{60}N_2O_{12}$ 796.953

A general term for Mocimycin, 1-Methylmocimycin and their derivs. is Elfamycins. Animal growth promoter used in poultry breeding. Yellow powder. $[\alpha]_D^{22}$ -60 (c, 1 in MeOH). Log P 1.03 (uncertain value) (calc). λ_{max} 233 (ϵ 15000); 276 (ϵ 6000); 286 (ϵ); 327 (ϵ 5000) (EtOH) (Derep).

▶ LD_{50} (mus, ipr) 500 mg/kg. QA2805000

1-Me: [12704-90-4] *1-Methylmocimycin, 9CI.* ***Goldinodox****. Goldinomycin. Aurodox. X 5108. Antibiotic X 5108*
$C_{44}H_{62}N_2O_{12}$ 810.98
Poultry growth promoter. Yellow amorph. solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -82.8 (c, 0.52 in EtOH). pK_a 6.1. λ_{max} 219 (E1%/1cm 680); 232 (E1%/1cm 660); 327 (E1%/1cm 415) (pH 7 buffer) (Berdy). λ_{max} 207 (E1%/1cm 500); 234 (E1%/1cm 610); 336 (E1%/1cm 388) (HCl) (Berdy). λ_{max} 219 (E1%/1cm 680); 230 (E1%/1cm 650); 327 (E1%/1cm 410) (NaOH) (Berdy).

▶ LD_{50} (mus, orl) >4000 mg/kg; LD_{50} (mus, scu) 1320 mg/kg. QA2809000

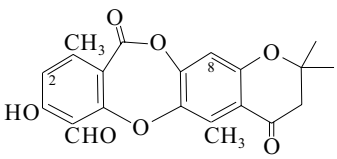
5,6-Dihydro: [61994-74-9] ***5,6-Dihydromocimyin C***
$C_{43}H_{62}N_2O_{12}$ 798.969
Sol. $CHCl_3$, bases, THF, EtOH, MeOH, dioxan, EtOAc, Me_2CO, butyl acetate; fairly sol. C_6H_6, CCl_4; poorly sol. Et_2O, H_2O, acids, hexane. Mp 123° dec. $[\alpha]_D^{20}$ -85 (MeOH aq.). λ_{max} 234 (ϵ 65000); 268 (ϵ 25000); 338 (ϵ 14000) (MeOH/HCl) (Derep). λ_{max} 235 (ϵ 62000); 277 (ϵ 25000); 308 (ϵ 29000) (MeOH/NaOH) (Derep). λ_{max} 234 (ϵ 63000); 267 (ϵ 23000); 291 (ϵ 19000); 333 (ϵ 18000) (MeOH aq.) (Derep). λ_{max} 233 (ϵ 65000); 268 (ϵ 25000); 338 (ϵ 14000) (MeOH-HCl) (Berdy).

3′-Deoxy, 1-Me: [66170-37-4] ***Heneicomycin****. 30-Deoxy-1-methylmocimycin, 9CI. Antibiotic A 21A*
$C_{44}H_{62}N_2O_{11}$ 794.981
Sol. MeOH, butanol, $CHCl_3$, Me_2CO, EtOH. λ_{max} 233 (ϵ 64300); 270 (sh) (ϵ 16000); 290 (sh) (ϵ 15000); 330 (ϵ 30800) (MeOH/HCl) (Derep). λ_{max} 224 (ϵ 64300); 318 (ϵ 34800) (MeOH/NaOH) (Derep). λ_{max} 233 (ϵ 50000); 325 (ϵ 22000) (H_2O pH 7) (Derep). λ_{max} 231 (E1%/1cm 722); 322 (E1%/1cm 328) (MeOH-HCl) (Berdy).

Maehr, H. *et al., J.A.C.S.*, 1973, **95**, 8449 (*struct, uv, ir, ms, pmr*)
Vos, C. *et al., Tet. Lett.*, 1973, 2823; 5173 (*struct, ir, uv, nmr, ms*)
Maehr, H. *et al., J.A.C.S.*, 1974, **96**, 4034 (*cryst struct, abs config*)
Ger. Pat., 1976, 2 621 615; *CA*, **86**, 119248 (*deriv*)
Frost, B.M. *et al., J. Antibiot.*, 1979, **32**, 626 (*Heneicomycin*)
Maehr, H. *et al., Can. J. Chem.*, 1980, **58**, 501 (*bibl, derivs*)
Wolf, H. *et al., Antibiotics (N.Y.)*, 1983, **6**, 71 (*rev*)
Dolle, R.E. *et al., J.A.C.S.*, 1985, **107**, 1695 (*Goldinodox*)
Dewey, R.S. *et al., J. Antibiot.*, 1991, **44**, 838 (*pmr, cmr, ms, Heneicomycin*)
Beretta, G. *et al., J. Antibiot.*, 1993, **46**, 1175 (*isol, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 183

Mollicellin A M-727

[68455-06-1]



$C_{21}H_{18}O_7$ 382.369

Depsidone numbering shown. Prod. by *Chaetomium* spp. and mutagenic mycotoxin. No phys. props. reported.

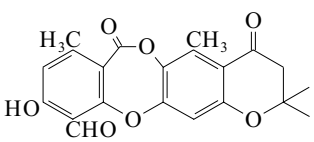
▶ Mutagen.

2-Chloro, 8-hydroxy: [68455-12-9] ***Mollicellin F***
$C_{21}H_{17}ClO_8$ 432.813
Prod. by *Chaetomium* spp. and mycotoxin.

Stark, A.A. *et al., Appl. Environ. Microbiol.*, 1978, **36**, 412 (*isol, props*)

Mollicellin B M-728

[68455-07-2]



$C_{21}H_{18}O_7$ 382.369

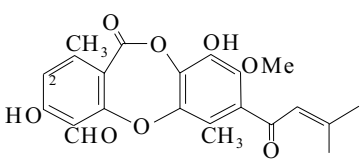
Prod. by *Chaetomium* spp. and mutagenic mycotoxin. No phys. props. reported.

▶ Mutagen.

Stark, A.A. *et al., Appl. Environ. Microbiol.*, 1978, **36**, 412 (*isol, props*)

Mollicellin C M-729

[68436-82-8]



$C_{22}H_{20}O_8$ 412.395

Depsidone antibiotic. Prod. by *Chaetomium* spp. and mutagenic mycotoxin. No phys. props. reported.

▶ Mutagen. HP3081950

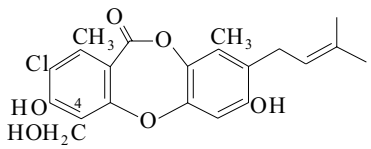
2-Chloro: [68455-10-7] ***Mollicellin E***
$C_{22}H_{19}ClO_8$ 446.84
Prod. by *Chaetomium* spp. and mutagenic mycotoxin.

▶ Mutagen. HP3081900

Stark, A.A. *et al., Appl. Environ. Microbiol.*, 1978, **36**, 412 (*isol, props*)

Mollicellin D M-730

[68455-11-8]



$C_{21}H_{21}ClO_6$ 404.846
Prod. by *Chaetomium* spp. and mycotoxin. No phys. props. reported.

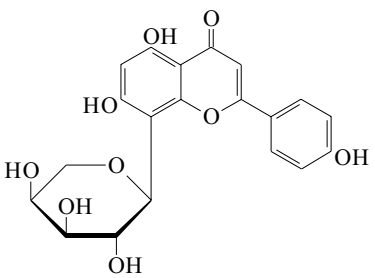
Dechloro, 4-aldehyde: [68455-09-4] ***Mollicellin H***
$C_{21}H_{20}O_6$ 368.385
Prod. by *Chaetomium* spp. and mutagenic mycotoxin.

▶ Mutagen.

Stark, A.A. *et al., Appl. Environ. Microbiol.*, 1978, **36**, 412 (*isol, props*)

Mollupentin M-731

[38642-55-6]
*8-α-L-Arabinopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one. 8-Arabinopyranosyl-4′,5,7-trihydroxyflavone. 8-Arabinopyranosylapigenin. 8-Arabinosylapigenin*



$C_{20}H_{18}O_9$ 402.357

7-Me ether: [66274-25-7] *8-Arabinopyranosyl-4′,5-dihydroxy-7-methoxyflavone.* ***Molludistin***
$C_{21}H_{20}O_9$ 416.384
Isol. from *Ocimum sanctum* (holy basil). Mp 260-261°.

*7-Me ether, 2″-*O*-α-L-rhamnopyranoside:*
$C_{27}H_{30}O_{13}$ 562.526
Isol. from *Gnetum africanum* and *Avena sativa* (oats).

*7-Me ether, 2″-*O*-β-D-glucopyranoside:* [70521-82-3]
$C_{27}H_{30}O_{14}$ 578.526

*7-Me ether, 2″-*O*-D-xyloside:* [101843-07-6]
$C_{26}H_{28}O_{13}$ 548.499

*2″-*O*-α-L-Rhamnopyranoside:* [146177-28-8]
$C_{26}H_{28}O_{13}$ 548.499

[62459-25-0]

Chopin, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1972, **274**, 1840 (*synth*)
Chopin, J. *et al., Phytochemistry*, 1977, **16**, 2041; 1978, **17**, 299; 1979, **18**, 2059 (*isol, Molludistin, 2″-rhamnoside*)
Jay, M. *et al., Phytochemistry*, 1979, **18**, 184 (*2″-glucoside*)
Nair, A.G.R. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 979 (*Molludistin*)
Wirasutisna, K.R. *et al., Phytochemistry*, 1986, **25**, 558 (*2″-xyloside*)
Hoffmann-Bohm, K. *et al., Planta Med.*, 1992, **58**, 544 (*2″-rhamnoside*)

Molt-inhibiting hormone M-732

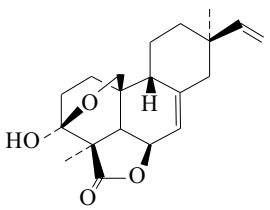
[131571-33-0]
Crustacean molt-inhibiting hormone

Peptide. Struct. consists of a chain of 71 AA residues including 6 cysteines.

Chang, E.S. *et al., Biochem. Biophys. Res. Commun.*, 1990, **171**, 818 (*isol, struct*)

Momilactone B M-733

[51415-08-8]
3β,20-Epoxy-3α-hydroxy-7,15-pimaradien-19,6β-olide



$C_{20}H_{26}O_4$ 330.423
Constit. of *Oryza sativa* (rice). Cryst. (CH_2Cl_2/EtOH). Mp 242° dec. $[\alpha]_D$ -185 ($CHCl_3$). λ_{max} 225 (EtOH) (Berdy).

Kato, T. *et al., J.C.S. Perkin 1*, 1977, 250 (*struct*)
Kato, T. *et al., Phytochemistry*, 1977, **16**, 45 (*isol*)
Orsini, F. *et al., Tet. Lett.*, 1977, 1085 (*struct*)
Koga, J. *et al., Tetrahedron*, 1995, **51**, 7907 (*cmr*)

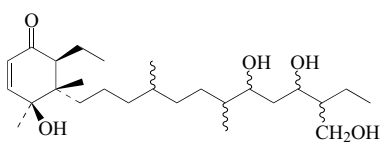
Momordin a M-734

Protein consisting of 250 AA residues. For full struct. see ref.. Constit. of the seeds of *Momordica charantia* (bitter melon). λ_{max} 280 (H_2O) (Berdy).

Minami, Y. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1470; 1993, **57**, 1141 (*isol, struct*)

Momordol M-735

[189156-42-1]



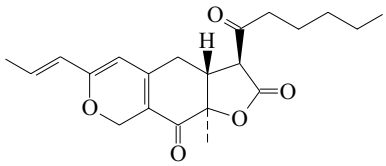
Relative Configuration

$C_{26}H_{48}O_5$ 440.662
Constit. of *Momordica charantia* (bitter melon). Oil. $[\alpha]_D^{27}$ +37 (c, 0.1 in $CHCl_3$). λ_{max} 215 (EtOH).

Begum, S. *et al., Phytochemistry*, 1997, **44**, 1313-1320 (*isol, uv, ir, pmr, cmr, ms*)

Monascin M-736

[21516-68-7]
Monascoflavin

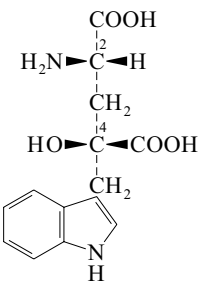


$C_{21}H_{26}O_5$ 358.433
Fungal pigment from *Monascus* spp. which infests rice and other foodstuffs. Food colourant. Yellow plates. Mp 144°. $[\alpha]_D^{20}$ +540 (c, 1.25 in $CHCl_3$). λ_{max} 232 (ε 19054); 288 (ε 1259); 392 (ε 20417) (EtOH) (Berdy).

Kurono, M. *et al., Chem. Pharm. Bull.*, 1963, **11**, 359 (*biosynth*)
Chen, F.C. *et al., J.C.S.(C)*, 1971, 3577-3579
Whalley, W.B. *et al., J.C.S. Perkin 1*, 1976, 1366 (*abs config*)
Lin, T.F. *et al., J. Ind. Microbiol.*, 1992, **9**, 173-179 (*derivs*)
Martinkova, L. *et al., Food Addit. Contam.*, 1999, **16**, 15-24; *CA*, **130**, 251401d (*activity*)

Monatin M-737

*4-Hydroxy-4-(1*H*-indol-3-ylmethyl)glutamic acid, 9CI. 2-Amino-4-hydroxy-5-(3-indolylmethyl)pentanedioic acid*



(2*S*,4*S*)-*form*

(2*S*,4*S*)-*form* [146142-94-1]
Constit. of the roots of *Schlerochiton ilicifolius*. High intensity sweetener. Cryst. + $^1/_4H_2O$ (EtOH/AcOH). Mp 216-220° efferv. $[\alpha]_D$ -7.6 (c, 1 in 1*M* HCl).

(2*RS*,4*RS*)-*form* [136440-36-3]
Cryst. Mp 212-214°.

[136440-37-4]

Vleggaar, R. *et al., J.C.S. Perkin 1*, 1992, 3095-3098 (*isol, pmr, cmr, struct*)
Holzapfel, C.W. *et al., Synth. Commun.*, 1994, **24**, 3197-3211 (*synth, pmr, cmr*)
Nakamura, K. *et al., Org. Lett.*, 2000, **2**, 2967-2970; 4269 (*synth*)
Oliviera, D.J. *et al., Tet. Lett.*, 2001, **42**, 6793-6796 (*synth*)

Monellin M-738

[9062-83-3]

Protein consisting of two non-covalently associated polypeptide chains. The A-chain contains 44 amino acid residues and the B-chain of 50 residues. Their

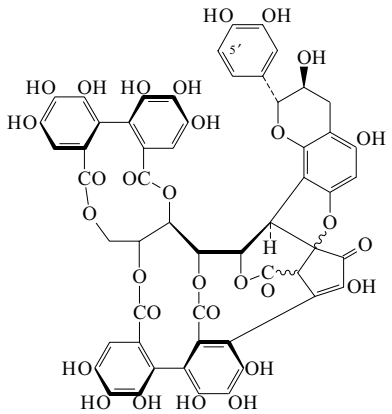
structs. have been determined. Isol. from the fruit of the serendipity berry (*Dioscoreophyllum cumminsii*). Intensely sweet compd..

[130453-08-6, 131571-28-3]

Wlodawer, A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1975, **72**, 398 (*cryst struct*)
Kohmura, M. *et al., Agric. Biol. Chem.*, 1990, **54**, 1521; 2219 (*synth, struct, bibl*)
Ota, M. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2043-2045 (*synth*)

Mongolicain A M-739

[115518-27-9]



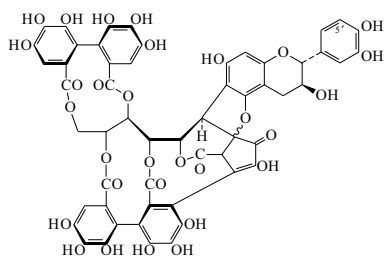
$C_{55}H_{36}O_{30}$ 1176.871
Pale brown amorph. powder + $3H_2O$. $[\alpha]_D^{18}$ -148.4 (c, 0.86 in MeOH).

5′-Hydroxy: [145826-26-2] ***Psidinin A***
$C_{55}H_{36}O_{31}$ 1192.871
Constit. of the bark of *Psidium guajava* (guava). Pale brown powder + $5H_2O$. $[\alpha]_D^{26}$ -146.6 (c, 1 in MeOH).

Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 857; 1990, **38**, 2151 (*struct, cd, pmr, cmr, abs config*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2092 (*Psidinin A*)

Mongolicain B M-740

[115518-28-0]



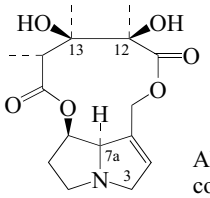
$C_{55}H_{36}O_{30}$ 1176.871
Pale brown amorph. powder + $5H_2O$. $[\alpha]_D^{18}$ -64.7 (c, 0.9 in MeOH).

5′-Hydroxy: [145826-27-3] ***Psidinin B***
$C_{55}H_{36}O_{31}$ 1192.871
Constit. of the bark of *Psidium guajava* (guava). Pale brown powder + $6H_2O$. $[\alpha]_D^{21}$ -27.2 (c, 1 in MeOH).

Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 857; 1990, **38**, 2151 (*struct, cd, pmr, cmr, abs config*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2092 (*Psidinin B*)

Monocrotaline M-741

[315-22-0]
14,19-Dihydro-12,13-dihydroxy-20-norcrotalanan-11,15-dione, 9CI



Absolute configuration

$C_{16}H_{23}NO_6$ 325.361
Cyclic ester of retronecine (see 2,3,5,7*a*-Tetrahydro-1-hydroxy-1*H*-pyrrolizine-7-methanol) with Monocrotalic acid. Hepatotoxin. Causative agent of much seneciosis, e.g. accidental poisoning by *S.* by weed residues in bread, and characterised by venoocculosive disease. Prisms (EtOH). Mp 202-203° (197-198° dec.). $[\alpha]_D^{26}$ -54.7 ($CHCl_3$). Log P -1.44 (uncertain value) (calc). λ_{max} 217 (ε 20500) (MeOH) (Berdy).

▶ Exp. carcinogen. Possible human carcinogen. LD_{50} (rat, orl) 66 mg/kg. Hepatotoxic. QB3140000

Hydrochloride:
Prisms (MeOH/$CHCl_3$). Mp 184° dec. $[\alpha]_D^{28}$ -38.4 (H_2O).

Methiodide:
Prisms (MeOH/$CHCl_3$). Mp 205° dec. $[\alpha]_D^{28}$ +23.4 (c, 3.1 in MeOH).

N-*Oxide:* [35337-98-5] ***Monocrotaline* N-*oxide***
$C_{16}H_{23}NO_7$ 341.36

▶ RC1295000

O^{13}-*Ac:* [520-55-8] ***Spectabiline***†. *Acetylmonocrotaline*
$C_{18}H_{25}NO_7$ 367.398
Prisms (EtOH). Mp 185.5-186°. $[\alpha]_D^{20}$ +121 (c, 1.7 in $CHCl_3$). $[\alpha]_D^{20}$ +143 (c, 1.38 in EtOH). Spectabiline is also a synonym for Lemobiline.

▶ RC1260000

O^{13}-*(2-Methylbutanoyl):* [24583-56-0] ***Grahamine***†
$C_{21}H_{31}NO_7$ 409.478
Mp 163°. $[\alpha]_D^{20}$ +100 (c, 1.05 in EtOH).

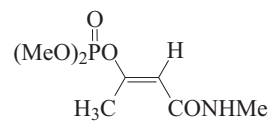
12,13-Cyclic acetaldehyde acetal: [64595-67-1] ***Monocrotaline***
$C_{18}H_{25}NO_6$ 351.399
Cryst. (Et_2O). Mp 160-161° dec. $[\alpha]_D$ +125.2 (EtOH). Prob. artifact.

*3,7*a*-Didehydro:* [23291-96-5] *Dehydromonocrotaline. Monocrotaline pyrrole*
$C_{16}H_{21}NO_6$ 323.345
Needles (petrol). Mp 85-90° dec. $[\alpha]_D^{18}$ +109.4 (c, 1.1 in EtOH).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 681B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1080C (*nmr*)
Neal, W.M. *et al., J.A.C.S.*, 1935, **57**, 2560 (*isol*)
Adams, R. *et al., J.A.C.S.*, 1939, **61**, 2815; 2819; 1950, **72**, 158 (*struct*)
Culvenor, C.C.J. *et al., Aust. J. Chem.*, 1957, **10**, 474; 1958, **11**, 97 (*Spectabiline*)
Neuner-Jehle, M. *et al., Monatsh. Chem.*, 1965, **96**, 321 (*ms*)
Atal, C.K. *et al., Aust. J. Chem.*, 1969, **22**, 1773 (*Grahamine*)
Simanek, V. *et al., Coll. Czech. Chem. Comm.*, 1969, **34**, 1832 (*uv*)
Culvenor, C.C.J. *et al., Aust. J. Chem.*, 1970, **23**, 1853-1857 (*Dehydromonocrotaline*)
Robins, D.J. *et al., J.C.S.(C)*, 1970, 1334; 1386 (*config*)
Culvenor, C.C.J. *et al., J.C.S.(C)*, 1971, 3653 (*cd*)
Willette, R.E. *et al., J. Pharm. Sci.*, 1972, **61**, 122 (*Monocrotaline N-oxide*)
Robins, D.J. *et al., J.C.S. Perkin 1*, 1974, 2082 (*biosynth*)
IARC Monog., 1976, **10**, 291; *Suppl.* 7, 67 (*rev, tox*)
Rajagopalan, T.R. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 455 (*Monocrotalinine*)
Stoeckli-Evans, H. *et al., Acta Cryst. B*, 1979, **35**, 231 (*cryst struct*)
Matsumoto, T. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 3329 (*synth, abs config*)
Mody, N.V. *et al., J. Nat. Prod.*, 1979, **42**, 417 (*cmr*)
Jones, A.J. *et al., Aust. J. Chem.*, 1982, **35**, 1173 (*cmr*)
Wang, S. *et al., CA*, 1982, **97**, 19843o (*cryst struct, Spectabiline*)
Molyneux, R.J. *et al., Phytochemistry*, 1982, **21**, 439 (*cmr*)
Mackay, M.F. *et al., Acta Cryst. C*, 1984, **40**, 473-476 (*cryst struct, Dehydromonocrotaline*)
Mattocks, A.R. *et al., Chemistry and Toxicology of Pyrrolizidine Alkaloids*, 1986, (*tox, rev*)
Vedejs, E. *et al., J.O.C.*, 1987, **52**, 3937 (*synth*)
Niwa, H. *et al., Tet. Lett.*, 1988, **29**, 5139 (*synth*)
Jackson, G.E. *et al., Spectrosc. Lett.*, 1990, **23**, 971 (*pmr, cmr*)
Niwa, H. *et al., Tetrahedron*, 1992, **48**, 10531 (*synth*)
Yan, C.C. *et al., Toxicol. Appl. Pharmacol.*, 1994, **127**, 58-63 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MRH000

Monocrotophos, BSI, ISO, JMAF M-742

[2157-98-4]
*Dimethyl 1-methyl-3-(methylamino)-3-oxo-1-propenyl phosphate, 9CI. Dimethyl phosphate, ester with 3-hydroxy-*N*-methylcrotonamide, 8CI. Dimethyl 1-methyl-2-methylcarbamoylvinyl phosphate. Nuvacron. Azodrin. Alphate. Parryfos. Cerophos. Apadrin. Croton 36*



(*E*)-*form*

$C_7H_{14}NO_5P$ 223.165
The (*E*)-isomer is the major constit. of the technical prod..

(*E*)-*form* [6923-22-4]
Agricultural insecticide with both systemic and contact action. Cryst. Sol. H_2O, Me_2CO; insol. hexane. Mp 54-55°.

▶ LD_{50} (rat, orl) 8 mg/kg. LD_{50} (rat, skn) 112 mg/kg. LC_{50} (rat, ihl) 63 mg m^{-3} (4 h exposure). Human neurotoxic effects.

ACGIH TLV 0.25 mg m^{-3} (sk).
TC4375000

(*Z*)-*form* [919-44-8]
No phys. props. reported.
►TC4981100
Menzer, R.E. *et al., J. Agric. Food Chem.*, 1965, **13**, 102 (*ir*)
U.S. Pat., 1965, 3 400 177; *CA*, **70**, 87064r (*synth*)
Babad, H. *et al., Anal. Chim. Acta*, 1968, **41**, 259 (*pmr*)
Ross, R.T. *et al., Anal. Chim. Acta*, 1970, **52**, 139 (*P nmr*)
Beynon, K.I. *et al., Residue Rev.*, 1973, **47**, 55 (*metab, rev*)
Szalontai, G. *et al., J. Chromatogr.*, 1976, **124**, 9 (*hplc*)
Busch, K.L. *et al., Appl. Spectrosc.*, 1978, **32**, 388 (*ms*)
Stan, H.-J. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 483 (*ms*)
Stan, H.-J. *et al., J. Chromatogr.*, 1983, **279**, 173 (*glc*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A284
Pesticide Manual, 11th edn., 1997, No. 502
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 1012
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MRH209

Monoethyl carbonate, 9CI M-743

[13932-53-1]
Ethyl hydrogen carbonate. Ethyl carbonate†
EtOCOOH
$C_3H_6O_3$ 90.079
Found in wines. Unstable at ordinary temps. Fp -61.

Chloride: See Ethyl chloroformate in *The Combined Chemical Dictionary.*

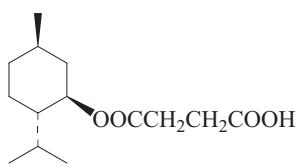
Amide: Ethyl carbamate, E-261

Hempel, W. *et al., Ber.*, 1898, **31**, 2997 (*synth*)
Faurholt, C. *et al., Z. Phys. Chem. (Leipzig)*, 1927, **126**, 227 (*props*)
Berenblum, I. *et al., Biochem. Pharmacol.*, 1959, **2**, 168 (*pharmacol*)
Kozenko, E.M. *et al., CA*, 1960, **54**, 21629 (*isol*)
Patrick, T.B. *et al., J.O.C.*, 1973, **38**, 2828 (*synth*)

Monomenthyl succinate M-744

[188709-97-9]

[75363-56-3, 77341-68-5]
Mono[5-methyl-2-(1-methylethyl)cyclohexyl] butanedioate, 9CI. FEMA 3810

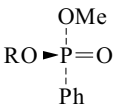


$C_{14}H_{24}O_4$ 256.341
Flavouring ingredient with a cooling, minty taste. Cryst. (hexane). Sol. H_2O. Mp 61.5-62.5°. $[\alpha]_D$ -65.

Jobloner, H. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1980, **18**, 2933-2940 (*use, synth*)
Shimizu, T. *et al., Synlett*, 1995, 650-652 (*synth*)
Gerard, M. *et al., Perfum. Flavor.*, 1998, **23(5)**, 49-52 (*use, props*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1035

Monomethyl phenylphosphonate M-745

[10088-45-6]
Methyl hydrogen phenylphosphonate



(*R*)-*form* of esters

$C_7H_9O_3P$ 172.12
Metab. of Leptophos, L-69 and Leptophos Oxon below.

(*R*)-*form*

Ph ester: Methyl phenyl phenylphosphonate
$C_{13}H_{13}O_3P$ 248.218
Liq. $Bp_{0.02}$ 105-108°. $[\alpha]_D^{20}$ +38.1 (c, 1.45 in $CHCl_3$).

Benzyl ester: Benzyl methyl phenylphosphonate
$C_{14}H_{15}O_3P$ 262.244
Liq. $Bp_{0.02}$ 110-111°. $[\alpha]_D^{20}$ +15.5 (c, 2.15 in $CHCl_3$).

(*S*)-*form*

Ph ester:
Liq. $Bp_{0.02}$ 105-108°. $[\alpha]_D^{20}$ -38.8 (c, 1.24 in $CHCl_3$).

Benzyl ester:
Liq. $Bp_{0.02}$ 110-111°. $[\alpha]_D^{20}$ -17.3 (c, 0.52 in $CHCl_3$).

(±)-*form*
Oil. pK_a 2.97. Heat-sensitive, isol. as Ba or cyclohexylammonium salt.

Mono-cyclohexylammonium salt: [38555-73-6]
Cryst. (Me_2CO). Mp 156-158°.

Mono-dicyclohexylammonium salt: [75620-16-5]
Cryst. (hexane). Mp 132°.

Me ester: See Dimethyl phenylphosphonate in *The Combined Chemical Dictionary.*

(4-Bromo-2,5-dichlorophenyl) ester: [25006-32-0] *(4-Bromo-2,5-dichlorophenyl)methyl phenylphosphonate. Leptophos Oxon*
$C_{13}H_{10}BrCl_2O_3P$ 396.003
►TA0360000

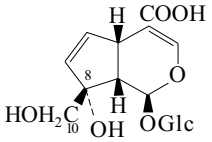
Chloride: See Phenylphosphonochloridic acid in *The Combined Chemical Dictionary.*

[94274-44-9]

Cherbuliez, E. *et al., Helv. Chim. Acta*, 1961, **44**, 1812 (*synth*)
Holmstead, R.L. *et al., Arch. Environ. Contam. Toxicol.*, 1973, **1**, 133; *CA*, **80**, 44526 (*ms*)
Brooks, R.J. *et al., J.O.C.*, 1973, **38**, 1614 (*synth, pmr*)
Lee, P.W. *et al., Arch. Environ. Contam. Toxicol.*, 1976, **4**, 443; *CA*, **86**, 66794 (*deriv*)
Felcht, U. *et al., Chem. Ber.*, 1976, **109**, 3675 (*synth, ir*)
Otsuki, T. *et al., Synthesis*, 1981, 811 (*ester*)
Regitz, M. *et al., Annalen*, 1984, 1641 (*pmr*)
Morgan, B.P. *et al., J.A.C.S.*, 1991, **113**, 297 (*synth, uv, pmr, cmr, P-31 nmr*)
Baker, S.M. *et al., J. Agric. Food Chem.*, 1995, **43**, 503-506 (*Leptophos oxon, cryst struct*)

Monotropein M-746

[5945-50-6]



$C_{16}H_{22}O_{11}$ 390.343
Constit. of *Liquidambar styraciflua* (sweet gum) and *Liquidambar orientalis* (oriental sweet gum). Food flavouring agent. Stabiliser. Cryst. + $1H_2O$ (H_2O). Mp 175° dec. $[\alpha]_D^{18}$ -127.7 (H_2O).

Me ester: [54712-59-3] ***Galioside***
$C_{17}H_{24}O_{11}$ 404.37
Amorph. Poorly sol. hexane. $[\alpha]_D$ -86.2 (MeOH). λ_{max} 189 ; 242 (H_2O) (Berdy).

10-Ac, Me ester: ***Galioside 10-acetate***
$C_{19}H_{26}O_{12}$ 446.407
$[\alpha]_D$ -63.6 (MeOH).

Penta-Ac, Me ester:
Cryst. Mp 150-151° (147-148°). $[\alpha]_D^{18}$ -76.2 (EtOH).

10-Benzoyl, Me ester: Galioside 10-benzoate
$C_{24}H_{28}O_{12}$ 508.478
Amorph. $[\alpha]_D^{23}$ -45 (c, 0.6 in MeOH).

10-O-*(*p-*Hydroxy*-E-*cinnamoyl):* [36138-58-6] ***Vaccinoside***
$C_{25}H_{28}O_{13}$ 536.488
Isol. from flowers of *Vaccinium bracteatum* (sea bilberry). Mp 150-153°. $[\alpha]_D^{17}$ -75.2 (c, 1 in H_2O).

10-O-*(*p-*Hydroxy*-Z-*cinnamoyl):* [75044-72-3] ***Andromedoside***
$C_{25}H_{28}O_{13}$ 536.488
Cryst. Mp 126-128°. $[\alpha]_D$ -26.5 (EtOH).

8-Deoxy, Me ester: [77856-55-4] ***Apodantheroside***
$C_{17}H_{24}O_{10}$ 388.371
Cryst. (Et_2O/hexane) (as penta-Ac). Mp 126° (penta-Ac).

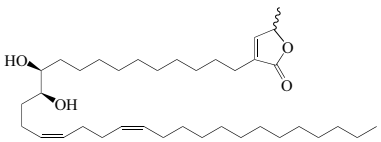
8-Epimer, Me ester: See Gardenosidic acid in *The Combined Chemical Dictionary.*

Bobbitt, J.M. *et al., Chem. Ind. (London)*, 1964, 931 (*pmr*)
Inouye, H. *et al., Chem. Pharm. Bull.*, 1964, **12**, 255; 888 (*isol, uv, ir, pmr, struct*)
Masaki, N. *et al., Tet. Lett.*, 1967, 2367 (*cryst struct*)
Rimpler, H. *et al., Phytochemistry*, 1970, **18**, 1891 (*isol*)
Sakakibara, J. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1979 (*Vaccinoside*)
Bianco, A. *et al., Gazz. Chim. Ital.*, 1978, **108**, 13 (*Galioside*)
Chung, S.G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1980, **313**, 702 (*Andromedoside*)
Bailleul, F. *et al., Phytochemistry*, 1980, **19**, 2763 (*Apodantheroside*)
Damtoft, S. *et al., Phytochemistry*, 1981, **20**, 2717; 1993, **33**, 377 (*isol, pmr, cmr*)
Jensen, S.R. *et al., Phytochemistry*, 1982, **21**, 1623 (*Galioside acetate*)
Karikas, G.A. *et al., Planta Med.*, 1987, **53**, 223 (*Galioside*)
Sakar, M.K. *et al., Fitoterapia*, 1991, **62**, 176 (*Monotropein, pmr*)

Montecristin M-747

[185336-15-6]
3-(11,12-Dihydroxy-15,19-dotriacontadie-

*nyl)-5-methyl-2(5*H*)-furanone, 9CI*



$C_{37}H_{66}O_4$ 574.926
Constit. of *Annona muricata* (soursop). Powder. Mp 62-65°. $[\alpha]_D$ +25 (c, 0.1 in MeOH). λ_{max} 212 (log ϵ 3.8) (MeOH).

Gleye, C. *et al., J.O.C.*, 1997, **62**, 510-513 (*isol, uv, ir, pmr, cmr, ms*)

Montmorillonite M-748

[1318-93-0]

[61029-13-8]

$Na[Al_5MgSi_{12}O_{30}(OH)_6]$

$Al_5H_6MgNaO_{36}Si_{12}$ 1101.254

Struct. has Pyrophyllite double layers with replacement of some octahedral $Al^{3\oplus}$ by $Mg^{2\oplus}$ and interlayer $Na^{\oplus}$ and H_2O.Dull white, grey, yellowish, greenish or pink solid. Vol. increased several fold by adsorption of H_2O. Cation exchange capacity 0.6-1.5 eq kg^{-1}.

Al-poor-*form*

Fuller's earth. Floridin

A natural, porous, absorptive Al silicate comprising a series of amorph., hydrous silicates with a persistent colloidal nature. Used in food processing as a filtration agent and flocculating agent.

Tantalum pillared-*form*

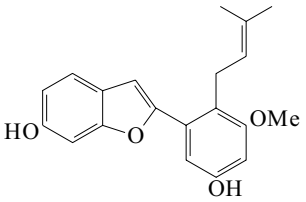
A pillared clay with a basal spacing of 2600 pm at 500°.BET surface are 180 m^2 g^{-1} at 500°. 600 meq of acid sites.

MacEwan, D.M.C. *et al., Trans. Faraday Soc.*, 1948, **44**, 349 (*cryst struct, complexes*)
MacKenzie, R.C. *et al., Trans. Faraday Soc.*, 1948, **44**, 368 (*complexes*)
Barrer, R.M. *et al., J.C.S.*, 1961, 971 (*synth*)
Van Olpen, H. *et al., Introduction to Clay Colloid Chemistry*, 2nd Ed., Wiley, 1977, (*rev, props*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 23; **6**, 197 (*rev, uses*)
Smith, K.A. *et al., Am. Mineral.*, 1983, **68**, 1206 (*Si-29 nmr*)
Kinsey, R.A. *et al., Am. Mineral.*, 1985, **70**, 537 (*Al-27 nmr, Si-29 nmr*)
Tennakoon, D.T.B. *et al., J.C.S. Faraday 1*, 1986, **82**, 545 (*Al-27 nmr, Si-29 nmr*)
Tichit, D. *et al., Clays Clay Miner.*, 1988, **36**, 369 (*pillared form*)
González, F. *et al., Chem. Comm.*, 1991, 587 (*pillared form*)
Guiu, G. *et al., Chem. Comm.*, 1994, 1729 (*Ta pillared form, synth, use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **5**, 3667-3671 (*use*)

Moracin I M-749

[73338-88-2]

6-Hydroxy-2-(5-hydroxy-3-methoxy-2-prenylphenyl)benzofuran



$C_{20}H_{20}O_4$ 324.376
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. Cryst. (EtOAc/toluene). Mp 139-140°.

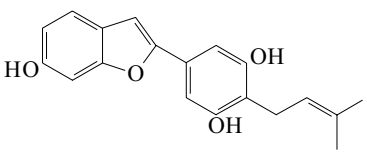
O-*De-Me:* ***De*-O-*methylmoracin I***
$C_{19}H_{18}O_4$ 310.349
Brown powder. Mp 82-83°. λ_{max} 214 (log ϵ 4.47); 310 (log ϵ 4.3) (MeOH).

Deshpande, V.H. *et al., Indian J. Chem.*, 1975, **13**, 453 (*isol*)
Takasugi, M. *et al., CA*, 1980, **92**, 160540 (*isol, struct*)
Mann, I.S. *et al., Tetrahedron*, 1991, **47**, 7991-8000 (*synth, pmr*)
Lee, D. *et al., J. Nat. Prod.*, 2001, **64**, 1286-1293 (*Demethylmoracin I*)

Moracin C M-750

[69120-06-5]

5-(6-Hydroxy-2-benzofuranyl)-2-(3-methyl-2-butenyl)-1,3-benzenediol, 9CI. 2-(3,5-Dihydroxy-4-prenylphenyl)-6-hydroxybenzofuran



$C_{19}H_{18}O_4$ 310.349
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. Plates. Mp 198-199°. λ_{max} 219 (ϵ 31900); 319 (ϵ 40900); 333 (ϵ 34600) (EtOH) (Berdy).

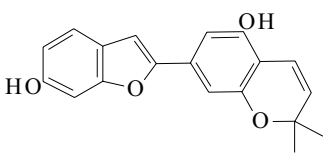
Tri-Ac:
$C_{25}H_{24}O_7$ 436.46
Mp 156-157°.

Deshpande, V.H. *et al., Indian J. Chem.*, 1975, **13**, 453 (*isol*)
Takasugi, M. *et al., CA*, 1980, **92**, 160540 (*isol, struct*)
McAllister, G.D. *et al., J.C.S. Perkin 1*, 1998, 3453-3457 (*synth, pmr*)

Moracin D M-751

[69120-07-6]

*7-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, 9CI*



$C_{19}H_{16}O_4$ 308.333
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. Mp 130-131°. λ_{max} 219 (ϵ 25700); 329 (ϵ 30000); 342 (ϵ 41700); 360 (ϵ 35200) (EtOH) (Berdy).

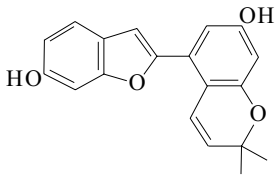
Di-Ac:
Mp 125-126°.

Takasugi, M. *et al., Chem. Lett.*, 1978, 1239 (*isol, struct*)

Moracin E M-752

[73338-84-8]

*5-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-7-ol, 9CI*



$C_{19}H_{16}O_4$ 308.333
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. Mp 184-185°. λ_{max} 218 ; 323 (MeOH) (Berdy).

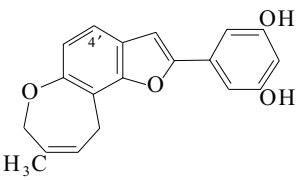
Di-Ac:
Mp 87-88°.

Takasugi, M. *et al., Tet. Lett.*, 1979, 4675 (*isol, struct, props*)

Moracin G M-753

[73338-86-0]

5-(7,10-Dihydro-8-methylfuro[2,3-g][1]benzoxepin-2-yl)-1,3-benzenediol, 9CI



$C_{19}H_{16}O_4$ 308.333
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. Mp 198-199°. λ_{max} 217 ; 314 ; 326 (MeOH) (Berdy).

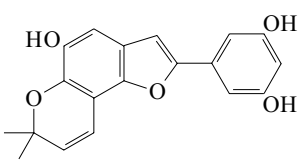
4′-Methoxy: [73338-87-1] ***Moracin H***
$C_{20}H_{18}O_5$ 338.359
From *Morus alba* (white mulberry) infected with *Fusarium solani*. Mp 191-192°. λ_{max} 217 (ϵ 33000); 306 (ϵ 31000); 315 (ϵ 33400); 329 (ϵ 22000) (EtOH) (Berdy).

4′-Methoxy, di-Ac:
$C_{24}H_{23}O_6$ 407.442
Mp 140-141°.

Takasugi, M. *et al., Tet. Lett.*, 1979, 4675 (*isol, struct, props*)

Moracin K M-754

[73338-90-6]

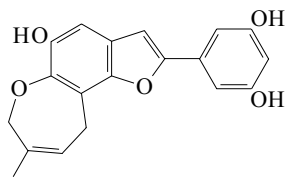


$C_{19}H_{16}O_5$ 324.332
Prod. by *Morus alba* (white mulberry) infected with *Fusarium solani*.

Takasugi, M. *et al., CA*, 1980, **92**, 160540d (*isol*)

Moracin L M-755

[73338-91-7]

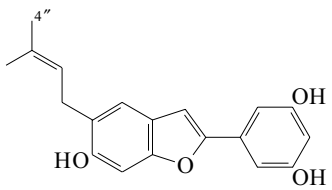


$C_{19}H_{16}O_5$ 324.332
Prod. by *Morus alba* (white mulberry) infected with *Fusarium solani*.

Takasugi, M. *et al., CA*, 1980, **92**, 160540d (*isol*)

Moracin N M-756

[135248-05-4]
2-(3,5-Dihydroxyphenyl)-6-hydroxy-5-prenylbenzofuran



$C_{19}H_{18}O_4$ 310.349
Constit. of the leaves of *Morus alba* (white mulberry) (famine food). Mp 187-188°.

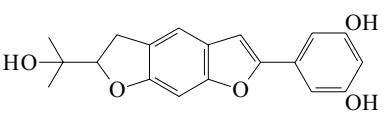
*Δ1″-Isomer(*E-*):* [209264-00-6] *2-(3,5-Dihydroxyphenyl)-6-hydroxy-5-(3-methyl-1-butenyl)benzofuran*. ***Artotonkin***
$C_{19}H_{18}O_4$ 310.349

4″-Hydroxy: [135248-04-3] ***ω-Hydroxymoracin N***
$C_{19}H_{18}O_5$ 326.348
Constit. of the leaves of *Morus alba* (white mulberry) (famine food). Possesses (*E*)-config..

Matsuyama, S. *et al., Agric. Biol. Chem.*, 1991, **55**, 1333; 1409 (*isol, pmr, struct*)
Lien, T.P. *et al., Pharmazie*, 1998, **53**, 353 (*Artotonkin*)

Moracin O M-757

[123702-97-6]
5-[5,6-Dihydro-6-(1-hydroxy-1-methylethyl)benzo[1,2-b:5,4-b′]difuran-2-yl]-1,3-benzenediol, 9CI

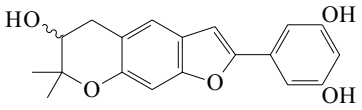


$C_{19}H_{18}O_5$ 326.348
Constit. of *Morus alba* (white mulberry).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 807
Ferrari, F. *et al., Fitoterapia*, 1998, **69**, 554-555 (*pmr*)

Moracin P M-758

[102841-46-3]
5-(6,7-Dihydro-6-hydroxy-7,7-dimethyl-5H-furo[3,2-g][1]benzopyran-2-yl)-1,3-benzenediol, 9CI



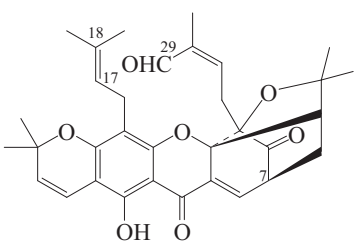
$C_{19}H_{18}O_5$ 326.348
Constit. of *Morus alba* (white mulberry). No phys. props. reported.

3′-O-β-D-Xylopyranoside: [102841-43-0] ***Mulberroside C***
$C_{24}H_{26}O_9$ 458.464
Amorph. powder. $[\alpha]_D^{19}$ -23 (c, 0.1 in MeOH).

Hirakura, K. *et al., J. Nat. Prod.*, 1986, **49**, 218 (*Mulberroside C*)
Hano, Y. *et al., Heterocycles*, 1989, **29**, 807
Ferrari, F. *et al., Fitoterapia*, 1998, **69**, 554-555 (*pmr*)

Morellin M-759

[1183-12-6]



$C_{33}H_{36}O_7$ 544.643
Constit. of seeds of *Garcinia morella* (batuan). Golden needles or rhombic prisms (MeOH or EtOH). Sol. Me_2CO, EtOAc, C_6H_6, Et_2O, $CHCl_3$; fairly sol. MeOH, EtOH, hexane; poorly sol. H_2O. Mp 154°. $[\alpha]_D$ -594 (c, 4.5 in $CHCl_3$). Log P 4.49 (uncertain value) (calc). Isomerises to (*E*)-form on treatment with KOH/Et_2O λ_{max} 234 (ε 30200); 279 (ε 17400); 291 (ε 17400); 361 (ε 14300) (EtOH) (Berdy).

▶ LD_{50} (mus, ipr) 50 mg/kg. PB9268000

*(*E*)-Isomer:* [1064-71-7] ***Isomorellin***
$C_{33}H_{36}O_7$ 544.643
Orange prismatic needles (MeOH). Mp 120-121°. $[\alpha]_D^{28}$ -623 (c, 1.006 in $CHCl_3$).

*(*E*)-Isomer, 29-alcohol:* [149655-53-8] ***Isomorellinol***
$C_{33}H_{38}O_7$ 546.659
$[\alpha]_D^{20}$ -322 (c, 0.125 in $CHCl_3$).

*(*E*)-Isomer, 29-carboxylic acid:* ***Isomorellic acid***
$C_{33}H_{36}O_8$ 560.643
From *Garcinia morella* (batuan). Amorph.

Di-Me acetal: ***Morellin dimethyl acetal***
$C_{35}H_{42}O_8$ 590.712
Yellow gum. $[\alpha]_D^{24}$ -405 (c, 0.1 in $CHCl_3$). λ_{max} 280 (ε 10000); 290 (ε 9332); 361 (ε 4786) (MeOH) (Berdy).

Dihydro: See Dihydroisomorellin in *The Combined Chemical Dictionary.*

Deoxy: ***Deoxymorellin***
$C_{33}H_{36}O_6$ 528.644
Isol. from seeds of *Garcinia morella* (batuan). Orange cryst. (MeOH). Mp 126°. $[\alpha]_D^{28}$ -557 ($CHCl_3$).

29-Alcohol: [55452-65-8] ***Morellinol***
$C_{33}H_{38}O_7$ 546.659
Pigment from *Garcinia morella* (batuan). Yellow needles (MeOH). Mp 149-150°.

29-Carboxylic acid: [5304-71-2] ***Morellic acid***. *α2-Guttiferin*
$C_{33}H_{36}O_8$ 560.643
From *Garcinia morella* (batuan). Amorph. Sol. Et_2O, bases; poorly sol. H_2O. Isomerises on silica λ_{max} 278 ; 360 (EtOH) (Berdy).

▶ LD_{50} (mus, ivn) 100 mg/kg , LD_{50} (mus, ipr) 200 mg/kg , LD_{50} (mus, scu) 400 mg/kg.

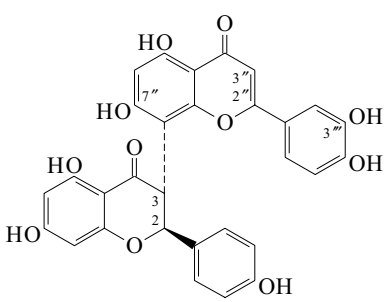
29-Carboxylic acid, Δ18-isomer, 17-hydroxy: ***Gaudichaudiic acid E***
$C_{33}H_{36}O_9$ 576.642
Yellow oil. $[\alpha]_D^{25}$ -160.1 (c, 0.1 in $CHCl_3$). λ_{max} 220 (log ε 4.01); 278 (log ε 3.76); 286 (log ε 3.79); 358 (log ε 3.7) (EtOH).

7-(3-Methyl-2-butenyl), 29-carboxylic acid: ***7-Prenylmorellic***. *7-Isopropylmorellic acid*
$C_{38}H_{44}O_8$ 628.761
Yellow oil. $[\alpha]_D^{30}$ -191.5 (c, 3.4 in $CHCl_3$).

Rao, B.S. *et al., J.C.S.*, 1937, 853 (*isol*)
Kartha, G. *et al., Tet. Lett.*, 1963, 459 (*cryst struct*)
Nair, P.M. *et al., Indian J. Chem.*, 1964, **2**, 402 (*struct*)
Bhat, H.B. *et al., Indian J. Chem.*, 1964, **2**, 405 (*Deoxymorellin*)
Karanjgaonkar, C.G. *et al., Tet. Lett.*, 1966, 687 (*Morellic acid*)
Arnone, A. *et al., Tet. Lett.*, 1967, 4201 (*pmr*)
Yemul, S.S. *et al., Org. Mass Spectrom.*, 1974, **9**, 1063 (*ms*)
Vogeli, U. *et al., Org. Magn. Reson.*, 1975, **7**, 617 (*cmr*)
Adawadkar, P.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 19 (*Morellinol*)
Lin, L.-J. *et al., Magn. Reson. Chem.*, 1993, **31**, 340 (*Isomorellinol*)
Asano, J. *et al., Phytochemistry*, 1996, **41**, 815 (*di-Me acetal*)
Cao, S.-G. *et al., Tetrahedron*, 1998, **54**, 10915-10924 (*Gaudichaudiic acid E*)
Wu, J. *et al., Tet. Lett.*, 2001, **42**, 727-729 (*7-Prenylmorellic acid*)

Morelloflavone M-760

Fukugetin†. Garcinin. BGH II



$C_{30}H_{20}O_{11}$ 556.481

(±)-*form*

Mp 298-299° dec.

2″,3″-Dihydro: ***Dihydromorelloflavone****. GB 2a*

$C_{30}H_{22}O_{11}$ 558.497

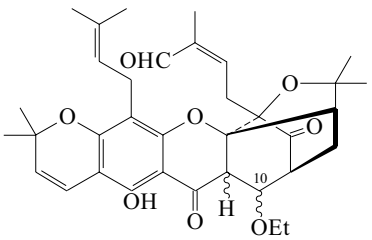
Isol. from *Garcinia morella* (batuan). Pale yellow needles (MeOH). Mp 268-270° (210°) dec. Identity of Dihydromorelloflavone and GB2a not fully establ. No mention of opt. activity.

Adawadkar, P.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 19 (*Dihydromorelloflavone*)

Moreollin M-761

[55221-73-3]

Ethoxydihydromorellin



$C_{35}H_{42}O_8$ 590.712

Identity of Moreollin and the prev. isol. ethoxydihydromorellin (from the same sp.) is probable but not definitely establ.. Constit. of the seed coat of *Garcinia morella* (batuan). Sol. Me_2CO, Et_2O; poorly sol. MeOH, EtOH, H_2O, hexane. Mp 168°. $[\alpha]_D^{26}$ -21.03. λ_{max} 277 ; 328 (MeOH) (Berdy). λ_{max} 235 (ϵ 25120); 266 (ϵ 39400); 275 (ϵ 41600); 305 (ϵ 18200); 316 (ϵ 13800); 365 (ϵ 4070) (EtOH) (Berdy).

(E)-Isomer:Isomoreollin. Ethoxydihydroisomoreollin

$C_{35}H_{42}O_8$ 590.712

Mp 148° (143°). $[\alpha]_D^{26}$ -22.03.

(E)-Isomer, 10-O-de-Et, 10-O-Me: ***Isomoreollin B***

$C_{34}H_{40}O_8$ 576.685

Powder. Mp 58-59°. $[\alpha]_D^{24}$ -37 (c, 0.1 in $CHCl_3$). λ_{max} 269 (ϵ 34700); 278 (ϵ 35500); 319 (ϵ 14450); 362 (ϵ 4600) (EtOH). λ_{max} 269 (ϵ 34673); 278 (ϵ 35481); 362 (ϵ 4571) (MeOH) (Berdy).

Carboxylic acid, O^{10}*-de-Et,* O^{10}*-Me:* ***Moreollic acid***

$C_{34}H_{40}O_9$ 592.685

Powder. Mp 97°. $[\alpha]_D^{27}$ -31 (c, 0.1 in $CHCl_3$). λ_{max} 267 (ϵ 25700); 277 (ϵ 26900); 318 (ϵ 10000); 365 (ϵ 2950) (EtOH). λ_{max} 267 (ϵ 45700); 277 (ϵ 26915); 365 (ϵ 2951) (MeOH) (Berdy).

Bhat, H.B. *et al., Indian J. Chem.*, 1964, **2**, 405 (*isol*)

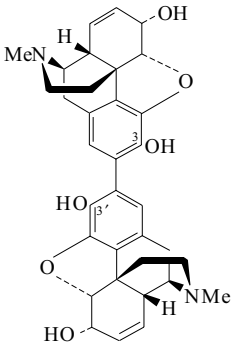
Subba Rao, G.S.R. *et al., Tet. Lett.*, 1974, 1259 (*isol, struct, uv*)

Asano, J. *et al., Phytochemistry*, 1996, **41**, 815 (*Moreollic acid*)

ψ-Morphine M-762

[125-24-6]

7,7′,8,8′-Tetrahydro-4,5:4′,5′-diepoxy-17,17′-dimethyl[2,2′-bimorphinan], 9CI. Pseudomorphine. 2,2′-Bimorphine. Dehydromorphine. Oxydimorphine. Oxymorphine



Absolute configuration

$C_{34}H_{36}N_2O_6$ 568.668

Alkaloid from opium poppies and opium. Rods + $1H_2O$. Insol. MeOH. Mp 330° dec.

Tetra-Ac:

Prisms (MeOH). Mp 294-296°.

3,3′-Di-Me ether:

Mp 155-156°.

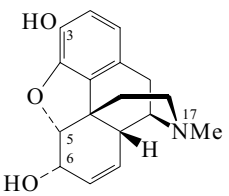
Bentley, K.W. *et al., J.C.S.*, 1959, 2574 (*synth, struct, uv*)

Mushinskaya, S.Kh. *et al., Khim. Prir. Soedin.*, 1971, **7**, 855; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 845 (*isol*)

Morphine, BAN M-763

[57-27-2]

7,8-Didehydro-4,5-epoxy-17-methylmorphinan-3,6-diol, 9CI. Meconium. Morfine



(−)-*form*

$C_{17}H_{19}NO_3$ 285.342Log P 0.24 (uncertain value) (calc).

(-)-*form*

Principal alkaloid of opium (*Papaver somniferum*). Minor constit. of lettuce. Prisms + $1H_2O$ (EtOH aq.), anhyd. prisms (anisole). V. sol. EtOAc, Me_2CO; sol. EtOH; spar. sol. H_2O, Et_2O, $CHCl_3$. Mp 254-256.4° dec. (anhyd.). $[\alpha]_D^{23}$ -130.9 (MeOH). pK_{a1} 8.2; pK_{a2} 9.9 (25°).

▶ Gastrointestinal effects when used therapeutically. Human and exp. reprod. effects. Abuse leads to habituation or addiction. Larger doses produce respiratory depression leading to coma. Can cause death. LD_{50} (rat, orl) 335 mg/kg. QC7875000

N-*Oxide:* [639-46-3] ***Morphine* N-*oxide****. Genomorphine*

$C_{17}H_{19}NO_4$ 301.341

Alkaloid from *Papaver somniferum* (opium poppy). Mp 272-273°.

Di-Me ether: [2859-16-7] ***6-O-Methylcodeine***

$C_{19}H_{23}NO_3$ 313.396

Minor alkaloid of *Papaver somniferum* (opium poppy). Prisms or plates. Mp 140-141°. $[\alpha]_D$ -188.5 (c, 1.09 in 95% EtOH).

[64-31-3]

Bentley, K.W. *et al., Chemistry of the Morphine Alkaloids*, Oxford Univ. Press, 1954, (*isol, bibl, uv*)

Gates, M. *et al., J.A.C.S.*, 1956, **78**, 1380-1393 (*synth*)

Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1965, **54**, 1393 (*di-Me ether, isol, ir, pmr*)

Wheeler, D.M.S. *et al., J.A.C.S.*, 1967, **89**, 4494-4501 (*ms*)

Fridrichsons, J. *et al., Tet. Lett.*, 1968, 2887-2890 (*cryst struct, abs config*)

Fennessy, M.R. *et al., Eur. J. Pharmacol.*, 1969, **8**, 261 (*pharmacol*)

Kametani, T. *et al., J.C.S.(C)*, 1969, 2030-2033 (*synth*)

de Angelis, G.G. *et al., Tetrahedron*, 1969, **25**, 5099-5112 (*ord*)

Heimans, R.L.H. *et al., J. Pharm. Pharmacol.*, 1971, **23**, 831-836 (*metab*)

Bentley, K.W. *et al., The Alkaloids*, (Manske, R.H.F., Ed.), 1971, **13**, 1-163 (*rev, bibl*)

Barber, R.B. *et al., J. Med. Chem.*, 1975, **18**, 1074-1077 (*di-Me ether, Heterocodeine, synth*)

Battersby, A.R. *et al., Tet. Lett.*, 1975, 1873-1876 (*biosynth*)

Bye, E. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 549-554 (*cryst struct*)

Carroll, F.I. *et al., J.O.C.*, 1976, **41**, 996-1001 (*cmr*)

Thenot, J.P.G. *et al., Methods Biochem. Anal.*, 1977, **24**, 1-38 (*rev, glc*)

Factors Affecting Action Narc. [Proc. Meet.], Raven Press, N.Y., 1978, 103; 233; 565; 595 (*rev, pharmacol*)

Hazum, E. *et al., Science (Washington, D.C.)*, 1981, **213**, 1010-1012 (*pharmacol*)

Rice, K.C. *et al., Chem. Biol. Isoquinoline Alkaloids, Int. Symp., Phytochem. Soc. Eur., Abstr. Pap.*, 1985, 191 (*rev, synth*)

Goldstein, A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1985, **82**, 5203-5207 (*isol*)

Toth, J.E. *et al., J.O.C.*, 1987, **52**, 473-475 (*synth*)

Muhtadi, F.J. *et al., Anal. Profiles Drug Subst.*, 1988, **17**, 259 (*rev*)

Toth, J.E. *et al., J.O.C.*, 1988, **53**, 4694-4708 (*synth*)

Parker, K.A. *et al., J.A.C.S.*, 1992, **114**, 9688-9689 (*synth*)

Hong, C.Y. *et al., J.A.C.S.*, 1993, **115**, 11028-11029 (*synth*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1076; 1083

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 5800 (*synonyms*)

Hong, C.Y. *et al., Tet. Lett.*, 1994, **35**, 3453-3456 (*synth*)

Opium Poppy: Botany, Chemistry and Pharmacology, Pharmaceutical Products Press, 1995,

Mulzer, J. *et al., Angew. Chem., Int. Ed.*, 1996, **35**, 2830-2832 (*synth*)

White, J.D. *et al., J.O.C.*, 1997, **62**, 5250-5253 (*synth*)

Mulzer, J. *et al., Chirality*, 1999, **11**, 475-482 (*synth*)

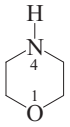
Meuzelaar, G.J. *et al., Eur. J. Org. Chem.*, 1999, 2315-2321 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DVO700; ENK000; MRO500; MRO750

Morpholine, 9CI M-764

[110-91-8]

Tetrahydro-1,4-oxazine. 1-Oxa-4-azacyclohexane. Drewamine



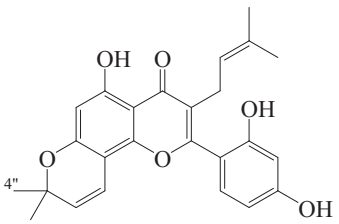
C_4H_9NO 87.121
Permitted (FDA) in edible coatings for fruit and vegetables. Food contaminant arising from its use as a boiler water additive. Hygroscopic oil with ammoniacal odour and caustic props. Misc. H_2O. d_4^{20} 1. Mp -4.9°. Bp 128.9° Bp_6 20°. n_D^{20} 1.4545. pK_a 8.49 (25°). Steam-volatile.

▶ Flammable, fl. p. 37°(oc)/38°(oc), auto-ignition temp. 310°/290°. Corrosive and irritating to skin, eyes and mucous membranes. LD_{50} (rbt, orl) 1050 mg/kg. LD_{50} (rbt, skn) 500 mg/kg. Exp. nephrotoxic. OES: long-term 20 ppm; short-term 30 ppm (Sk). QD6475000

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 1009C
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 382A; 382C; 382D; 383C; 383D; 764D; 765A; 1311A; **2**, 907C; 1129B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 597A; 597C; 598A; 599C; 1250C; 1251A; **2**, 653C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 472A; 472C; 472D; 473D; 785D; 1178B (*ir*)
Jones, L.W. *et al., J.A.C.S.*, 1925, **47**, 2966 (*synth*)
Hampton, B.L. *et al., J.A.C.S.*, 1936, **58**, 2338 (*synth*)
Adv. Chem. Ser., 1955, **15**, 515 (***props***)
Takeuchi, Y. *et al., J.C.S. Perkin 2*, 1974, 1927 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 295 (*rev*)
IARC Monog., 1989, **47**, 199 (*rev, tox*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1912
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2693
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 244
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1555
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 879
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACR750; CHE000; ENL000; NKZ000; MMA250; MRQ500; MRQ600; MRP750; PFS750

Morusin M-765

[62596-29-6]
*2-(2,4-Dihydroxyphenyl)-5-hydroxy-8,8-dimethyl-3-(3-methyl-2-butenyl)-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, 9CI. Mulberrochromene*



$C_{25}H_{24}O_6$ 420.461
Constit. of the root bark of *Morus alba* (mulberry) and other *Morus* spp.. Pale yellow prisms (Et_2O/hexane). Mp 214-216°. λ_{max} 270 (ε 39800); 320 ; 350 (MeOH) (Berdy).

Tri-Ac:
Mp 70-75°.

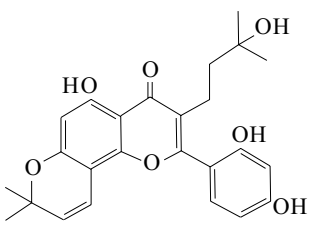
Tri-Me ether:
Mp 140-146°.

4″-Hydroxy: [73343-41-6] ***Albanin B***
$C_{25}H_{24}O_7$ 436.46
Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*.

Nomura, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2898
Chari, V.M. *et al., Z. Naturforsch., B*, 1978, **33**, 1547
Takasugi, M. *et al., CA*, 1980, **92**, 160540d (*Albanin B*)
Hano, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1260 (*cmr*)
Uchida, A. *et al., Acta Cryst. C*, 1996, **52**, 1713 (*cryst struct*)
Maria de Souza, M. *et al., Z. Naturforsch., C*, 2000, **55**, 256 (*activity*)

Morusinol M-766

[62949-93-3]
*2-(2,4-Dihydroxyphenyl)-5-hydroxy-3-(3-hydroxy-3-methylbutyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, 9CI. Oxydihydromorusin*

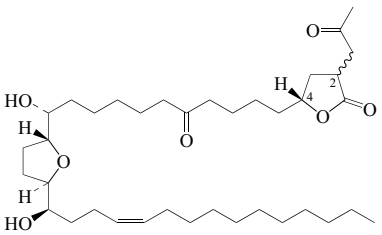


$C_{25}H_{26}O_7$ 438.476
Isol. from root bark of *Morus alba* (white mulberry). Cryst. (MeOH). Mp 215-216°. λ_{max} 206 (ε 22387); 225 (ε 18197); 242 (ε 18200); 269 (ε 27540) (MeOH) (Berdy).

Nomura, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 529; 1978, **26**, 1453 (*isol*)

Mosinone A M-767

[191800-47-2]



$C_{37}H_{64}O_7$ 620.908
Constit. of *Annona squamosa* (sugar apple). Waxy solid. Obt. as a mixture of 2,4-*cis*- and *trans*-isomers λ_{max} 202 (2.96) (MeOH).

Hopp, D.C. *et al., J. Nat. Prod.*, 1997, **60**, 581-586 (*isol, uv*)

Motilin M-768

H-Phe-Val-Pro-Ile-Phe-Thr-A-B-Glu-Leu-Gln-C-D-E-Glu-Lys-Glu-Arg-Asn-Lys-Gly-Gln-OH.

Canine motilin [85490-53-5]
$C_{120}H_{194}N_{36}O_{34}$ 2685.073
Fluffy powder + 5AcOH + 13H_2O. $[\alpha]_D^{25}$ -58 (c, 0.5 in 3% AcOH aq.). Has A = His, B = Ser, C = Lys, D = Ile, E = Arg.

Porcine motilin [9072-41-7]
Human motilin
$C_{120}H_{108}N_{34}O_{35}S$ 2618.446
Fluffy powder + 4AcOH + 8H_2O. $[\alpha]_D^{27}$ -54.5 (c, 0.6 in H_2O). $[\alpha]_D^{26}$ -50 (c, 0.5 in 5% AcOH aq.). Has A = Tyr, B = Gly, C = Arg, D = Met, E = Gln.

13-Leu: [59530-69-7] ***13-Leucinemotilin***. *KW 5139. [Leu^{13}] motilin*

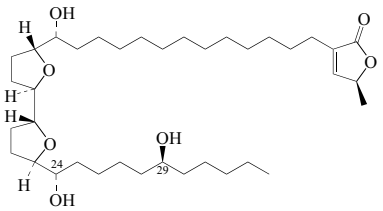
[52906-92-0, 85490-53-5]

Brown, J.C. *et al., Can. J. Biochem.*, 1973, **51**, 533; 1974, **52**, 7 (*isol, struct*)
Wünsch, E. *et al., Z. Naturforsch., C*, 1973, **28**, 235 (*synth*)
Kai, Y. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2346 (*synth*)
Mihara, J. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3589; 3594 (*synth*)
Wuensch, E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1976, **357**, 459-465; 467-476 (*13-Leu*)
Fujino, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 101 (*synth*)
Fox, J.E.T. *et al., Life Sci.*, 1984, **35**, 695 (*rev*)
Kitagawa, K. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3307 (*synth, bibl*)
McIntosh, C.H.S. *et al., Adv. Metab. Disord.*, 1988, **11**, 439 (*rev*)
Khan, N. *et al., Biochemistry*, 1990, **29**, 5743; 1991, **30**, 11271 (*pmr, conformn*)
Nakada, K. *et al., Am. J. Surg.*, 1995, **169**, 294-299 (*13-Leu*)

Motrilin M-769

[138551-27-6]

[157084-75-8]
Annonin III. Squamocin C



$C_{37}H_{66}O_7$ 622.924

Closely related to Narumicin I and Squamostatin A, S-212. Isol. from *Annona cherimolia* (cherimoya), *Annona squamosa* (sugar apple) and *Asimina triloba* (pawpaw). Mp 50-51°. $[\alpha]_D$ +19.5 (c, 0.9 in MeOH). λ_{max} 210 (ϵ 7000) (MeOH). λ_{max} 211 (ϵ 11800) (EtOH) (Berdy).

24-Epimer: [156256-35-8] ***Asiminecin***
$C_{37}H_{66}O_7$ 622.924
Constit. of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D$ +22 ($CHCl_3$). λ_{max} 215 (MeOH).

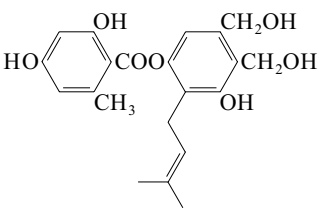
23,24-Diepimer (29ξ-): [201167-32-0] ***Carolin B***
$C_{37}H_{66}O_7$ 622.924
Oil. $[\alpha]_D^{20}$ +5 (c, 0.5 in $CHCl_3$). λ_{max} 208 (log ϵ 3.6) (EtOH). λ_{max} 208 (ϵ 3980) (MeOH) (Berdy).

[141505-62-6]

Cortes, D. *et al., Tetrahedron*, 1991, **47**, 8195-8202 (*isol, pmr, cmr*)
Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*Squamocin C*)
Zhao, G.-X. *et al., J. Med. Chem.*, 1994, **37**, 1971-1976 (*Asiminecin*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)
Queiroz, E.F. *et al., J. Nat. Prod.*, 1998, **61**, 34 (*Carolin B*)

MS 3 M-770

[58265-74-0]
2,4-Dihydroxy-6-methylbenzoic acid 3-hydroxy-4,5-bis(hydroxymethyl)-2-(3-methyl-2-butenyl)phenyl ester, 9CI. 3-Hydroxy-4,5-bis(hydroxymethyl)-2-prenylphenyl 2,4-dihydroxy-6-methylbenzoate



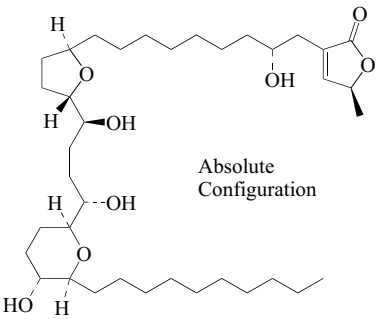
$C_{21}H_{24}O_7$ 388.416
Prod. by the mushroom *Stereum hirsutum*. Needles ($MeOH/CHCl_3$). Sol. MeOH, Et_2O, EtOAc, Py, butanol, dioxan, DMSO; poorly sol. H_2O, hexane, $CHCl_3$, C_6H_6. Mp 92°. λ_{max} (no shifts reported) (Derep). λ_{max} 240 (ϵ 16900); 310 (ϵ 39000) (MeOH/NaOH) (Derep). λ_{max} 270 (ϵ 23300); 305 (ϵ 8630) (MeOH) (Derep). λ_{max} 270 (E1%/1cm 600); 305 (E1%/1cm 224) (MeOH) (Berdy). λ_{max} 270 ; 304 (MeOH-HCl) (Berdy). λ_{max} 240 (E1%/1cm 488); 310 (E1%/1cm 1040) (MeOH-NAOH) (Berdy). λ_{max} 240 ; 270 ; 330 (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 125 - 275 mg/kg. VH3709900

Kurasawa, S. *et al., Agric. Biol. Chem.*, 1975, **39**, 2003; 2009; 1976, **40**, 1781

Mucocin M-771

[170591-47-6]

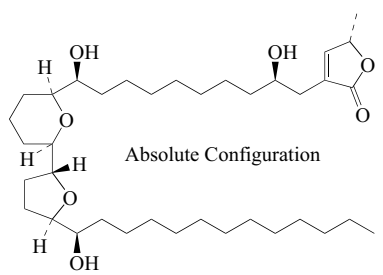


$C_{37}H_{66}O_8$ 638.924
Constit. of the leaves of *Rollinia mucosa* (biriba). Waxy solid. Mp 57-58°. $[\alpha]_D^{23}$ -10.8 (CH_2Cl_2). λ_{max} 207 (log ϵ 3.84) (EtOH). λ_{max} 207 (ϵ 6920) (MeOH).

Shi, G. *et al., J.A.C.S.*, 1995, **117**, 10409-10410 (*isol, uv, ir, pmr, cmr*)
Neogi, P. *et al., J.A.C.S.*, 1998, **120**, 11279-11284 (*synth*)
Takahashi, S. *et al., J.O.C.*, 2002, **67**, 5739-5752 (*synth*)

Muconin M-772

[183195-98-4]

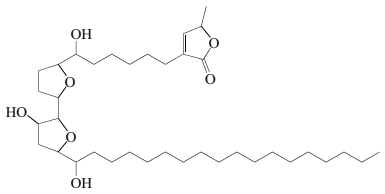


$C_{37}H_{66}O_7$ 622.924
Constit. of *Rollinia mucosa* (biriba). Wax. Mp 75-77° (synthetic). $[\alpha]_D^{27}$ +13.5 (c, 0.28 in $CHCl_3$) (synthetic).

Shi, G. *et al., J.O.C.*, 1996, **61**, 7988 (*isol, struct*)
Schaus, S.E. *et al., J.O.C.*, 1998, **63**, 4876-4877 (*synth*)
Yang, W.-Q. *et al., Tetrahedron*, 2000, **56**, 1451-1461 (*synth*)
Takahashi, S. *et al., Tet. Lett.*, 2002, **43**, 8661-8664 (*synth*)

Mucoxin M-773

[183195-99-5]

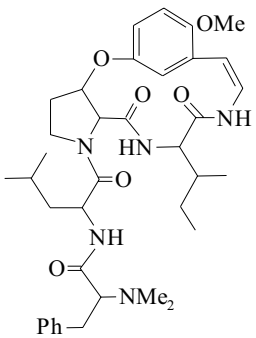


$C_{37}H_{66}O_7$ 622.924
Constit. of *Rollinia mucosa* (biriba). Oil.

Shi, G. *et al., J.O.C.*, 1996, **61**, 7988 (*isol*)

Mucronine D M-774

[38496-00-3]
Daechuine S9



$C_{37}H_{51}N_5O_6$ 661.84
Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date) and *Zizyphus jujuba* var. *inermis*. Amorph. $[\alpha]_D^{20}$ -487 (c, 0.12 in $CHCl_3$).

Dihydro:
Needles (CH_2Cl_2/Et_2O). Mp 250-252° (247°). $[\alpha]_D^{20}$ -225 (c, 0.17 in $CHCl_3$).

N-*De-Me:* [53947-95-8] ***Nummularine A***. N-*Demethylnummularine D*
$C_{36}H_{49}N_5O_6$ 647.813
Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Needles (MeOH). Mp 235-240° dec. $[\alpha]_D^{20}$ -397 (c, 0.2 in $CHCl_3$).

O-*De-Me:* [155656-07-8] **O-*Demethylmucronine D***
$C_{36}H_{49}N_5O_6$ 647.813
$[\alpha]_D^{20}$ -191 (c, 0.3 in $CHCl_3$).

Tschesche, R. *et al., Chem. Ber.*, 1972, **105**, 3106; 1974, **107**, 3180 (*isol, uv, cd, ir, pmr, ms, struct*)
Tschesche, R. *et al., Phytochemistry*, 1976, **15**, 541; 1979, **18**, 702 (*isol*)
Han, B.H. *et al., Pure Appl. Chem.*, 1989, **61**, 443
Barboni, L. *et al., Phytochemistry*, 1994, **35**, 1579 (*O-Demethylmucronine D*)

Mugiline β M-775

[53240-94-1]

H-Pro-[Arg]$_4$-Glu-Thr-Ser-Arg-Pro-Ile-[Arg]$_5$-Ala-Arg-Arg-Ala-Pro-Ile-[Arg]$_5$-Val-Val-[Arg]$_4$-OH

Polypeptide complex consisting of at least 7 components, M1 → M7. Struct. of M6 shown. Isol. from the mature sperm

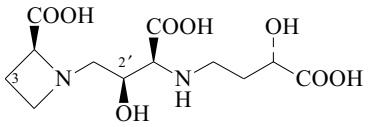
nuclei of the Formosan grey mullet, *Mugil japonicus*.

[110734-13-9, 110734-14-0, 110734-15-1, 110734-16-2]

Okamoto, Y. *et al., J. Biochem. (Tokyo)*, 1987, **101**, 1017 (*struct*)

Mugineic acid M-776

[69199-37-7]
2-Carboxy-α-[(3-carboxy-3-hydroxypropyl)amino]-β-hydroxy-1-azetidinebutanoic acid, 9CI



$C_{12}H_{20}N_2O_8$ 320.299
Excreted from the roots of barley (*Hordeum vulgare*), also in root-washings of oat and rice. Mp 210-212° dec. $[\alpha]_D$ -70.7 (c, 0.97 in H_2O).

2′-Epimer: [74281-81-5] ***Isomugineic acid***
$C_{12}H_{20}N_2O_8$ 320.299
Isol. from roots of barley (*Hordeum vulgare*). $[\alpha]_D$ -97 (c, 1.24 in H_2O).

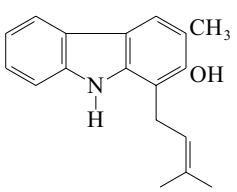
*2′-Deoxy:**2′-Deoxymugineic acid***
$C_{12}H_{20}N_2O_7$ 304.299
Isol. from wheat (*Triticum aestivum*). Cryst. Mp 198.5-200.5°. $[\alpha]_D$ -70.5 (H_2O).

3α-Hydroxy: [74235-23-7] ***3-Hydroxymugineic acid***
$C_{12}H_{20}N_2O_9$ 336.298
Isol. from roots of barley (*Hordeum vulgare*).

Nomoto, K. *et al., Chimia*, 1981, **35**, 249 (*deriv*)
Ohfune, Y. *et al., J.A.C.S.*, 1981, **103**, 2409 (*deriv*)
Sugiura, Y. *et al., Biochemistry*, 1983, **22**, 4842 (*pmr, cmr, cd*)
Procházka, Z. *et al., Experientia*, 1984, **40**, 794 (*rev*)
Sugiura, Y. *et al., J.A.C.S.*, 1985, **107**, 4667 (*pmr, cmr, cd*)
Hamada, Y. *et al., J.O.C.*, 1986, **51**, 5489 (*synth, bibl*)
Kawai, S. *et al., Tet. Lett.*, 1988, **29**, 1053 (*biosynth*)
Hamada, Y. *et al., Tet. Lett.*, 1990, **31**, 5041 (*synth*)
Klair, S.S. *et al., Tet. Lett.*, 1998, **38**, 89-92 (*2′-Deoxymugineic acid, synth*)
Miyakoshi, K. *et al., Tetrahedron*, 2001, **57**, 3355-3360 (*2′-Deoxymugineic acid, synth*)

Mukoenine A M-777

[155519-81-6]
2-Hydroxy-3-methyl-1-prenylcarbazole. 3-Methyl-1-(3-methyl-2-butenyl)-9H-carbazol-2-ol, 9CI. ***Girinimbilol***



$C_{18}H_{19}NO$ 265.354

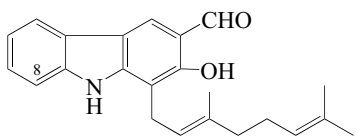
Alkaloid from stem bark and roots of *Murraya koenigii* (curryleaf tree). Needles (hexane/CH_2Cl_2) or prisms. Mp 106° (104-107°). Mukoenine A and Girinimbilol have not been directly compared but they appear to be identical.

O-*Ac:*
Needles (hexane/CH_2Cl_2). Mp 172-174°.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)
Reisch, J. *et al., Phytochemistry*, 1994, **36**, 1073 (*isol, uv, ir, pmr, cmr, ms, struct*)

Mukoenine B M-778

[155519-82-7]
1-(3,7-Dimethyl-2,6-octadienyl)-2-hydroxy-9H-carbazole-3-carboxaldehyde, 9CI. 3-Formyl-1-geranyl-2-hydroxycarbazole. Clausenatine A



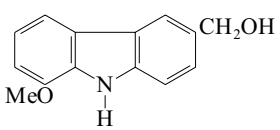
$C_{23}H_{25}NO_2$ 347.456
Alkaloid from *Murraya koenigii* (curryleaf tree). Yellowish powder (Me_2CO). Mp >280°.

8-Hydroxy:3-Formyl-1-geranyl-2,8-dihydroxycarbazole. ***Clauszoline F***
$C_{23}H_{25}NO_3$ 363.455
Yellow powder. λ_{max} 204 ; 216 ; 242 ; 276 ; 291 ; 300 (sh) ; 354 (MeOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096; 1996, **44**, 2231 (*isol, uv, ir, pmr, ms, struct*)
Wu, T.S. *et al., Phytochemistry*, 1999, **52**, 523-527 (*Clausenatine A*)

Mukoline M-779

[87264-41-3]
8-Methoxy-9H-carbazole-3-methanol, 9CI. 6-Hydroxymethyl-1-methoxycarbazole



$C_{14}H_{13}NO_2$ 227.262
Minor alkaloid from roots of *Murraya koenigii* (curryleaf tree). Cryst. (C_6H_6). Mp 118°.

Picrate:
Cryst. (C_6H_6). Mp 230°.

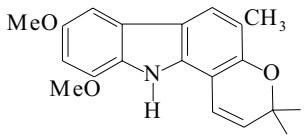
O-*Ac:*
Cryst. (C_6H_6/petrol). Mp 145°.

N-*Me:*
Cryst. (C_6H_6/petrol). Mp 140°.

Roy, S. *et al., J. Indian Chem. Soc.*, 1982, **59**, 1369 (*isol, uv, ir, pmr, ms, struct*)

Mukonicine M-780

[88607-43-6]
3,11-Dihydro-8,10-dimethoxy-3,3,5-trimethylpyrano[3,2-a]carbazole, 9CI

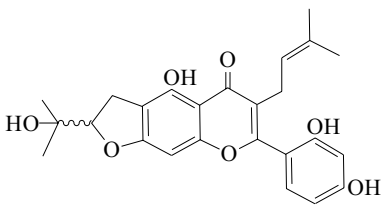


$C_{20}H_{21}NO_3$ 323.391
Alkaloid from the leaves of *Murraya koenigii* (curry leaf tree). Cryst. (C_6H_6/$CHCl_3$). Mp 233-234°.

Mukherjee, M. *et al., Phytochemistry*, 1983, **22**, 2328 (*isol, uv, ir, pmr, ms, struct*)

Mulberranol M-781

[62393-99-1]



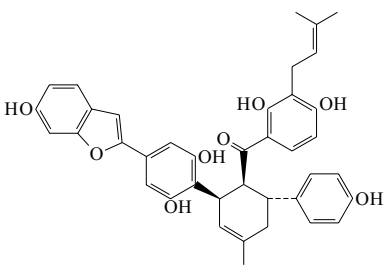
$C_{25}H_{26}O_7$ 438.476
Constit. of the bark of *Morus alba* (white mulberry) (famine food). Yellow amorph. solid.

Tri-Me ether:
Mp 142-145°.

Deshpande, V.H. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 647

Mulberrofuran E M-782

[89803-87-2]

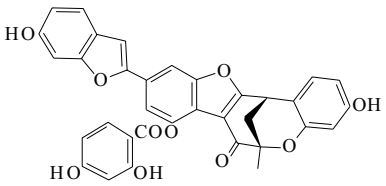


$C_{39}H_{36}O_8$ 632.709
Constit. of callus tissues of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{22}$ +302 (Me_2CO). Similar to Mulberrofuran J λ_{max} 220 (ε 43650); 243 (sh) (ε 16220); 287 (sh) (ε 23440); 297 (sh) (ε 26300); 310 (sh) (ε 32360); 321 (ε 38900); 334 (ε 31620) (EtOH).

Ueda, S. *et al., Chem. Pharm. Bull.*, 1984, **32**, 350 (*isol, uv, ir, pmr, cmr, ms*)

Mulberrofuran M M-783

[101365-03-1]

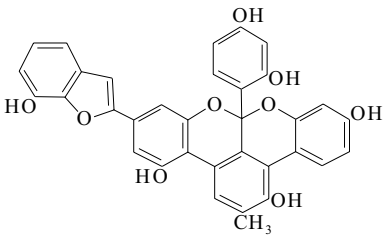


$C_{34}H_{22}O_{10}$ 590.542
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{14}$ +15 (c, 0.02 in MeOH).

Hano, Y. *et al., Heterocycles*, 1986, **24**, 1251

Mulberrofuran P M-784

[101365-02-0]

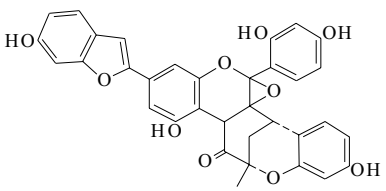


$C_{34}H_{22}O_9$ 574.542
Constit. of *Morus alba* (white mulberry). Blue amorph. powder. $[\alpha]_D^{29}$ +19.5 (c, 0.0113 in EtOH).

Hano, Y. *et al., Heterocycles*, 1986, **24**, 1381

Mulberrofuran Q M-785

[101383-35-1]

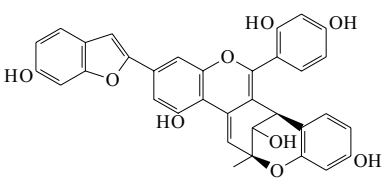


$C_{34}H_{24}O_{10}$ 592.558
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{21}$ +82.4 (c, 0.278 in MeOH).

Hano, Y. *et al., Heterocycles*, 1986, **24**, 1807

Mulberrofuran S M-786

[125090-76-8]

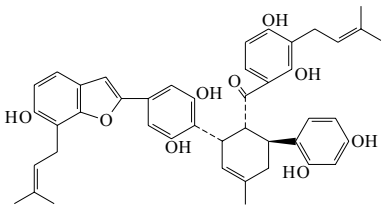


$C_{34}H_{24}O_9$ 576.558
Isolated from the powder on the surface of *Morus alba* bark (white mulberry). Red amorph. powder. $[\alpha]_D^{23}$ +166 (c, 0.13 in EtOH).

Hano, Y. *et al., Heterocycles*, 1989, **28**, 697

Mulberrofuran T M-787

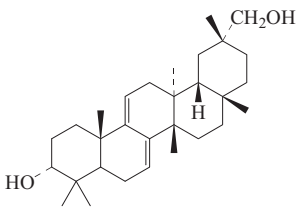
[125882-66-8]



$C_{44}H_{44}O_9$ 716.826
Constit. of *Morus alba* (white mulberry). Powder (Et_2O/hexane). Mp 168-169° dec. $[\alpha]_D^{22}$ +139 (c, 0.1 in EtOH).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 2035 (*isol, pmr, cmr*)

7,9(11)-Multifloradiene-3,29-diol M-788



3α-*form*

$C_{30}H_{48}O_2$ 440.708

3α-*form* [118117-31-0]
Karounidiol
Cryst. Mp 201-203°.

3-O-Benzoyl: [118117-32-1]
$C_{37}H_{52}O_3$ 544.816
Cryst. Mp 119-122°.

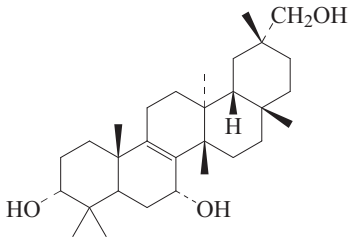
3-O-(4-Aminobenzoyl): [308811-93-0] ***Debenzoylzucchini factor B***
$C_{37}H_{53}NO_3$ 559.831
Constit. of *Cucurbita pepo* seeds. Gum. $[\alpha]_D^{25}$ -111 (c, 0.9 in MeOH). λ_{max} 290 (MeOH).

3-O-(4-Aminobenzoyl), 29-O-benzoyl: [246248-10-2] ***Zucchini factor B***
$C_{44}H_{57}NO_4$ 663.939
Constit. of seeds of pumpkin (*Cucurbita maxima*) and squash (*Cucurbita pepo*). Powder (Et_2O). Mp 204-206°. $[\alpha]_D^{25}$ -130 (c, 0.9 in $CHCl_3$). λ_{max} 240 (sh) ; 290 (log ϵ 4.06) (EtOH).

3β-*form*
3-Epikarounidiol
Cryst. Mp 225-226°. λ_{max} 232 (ϵ 11200); 236 (ϵ 12600); 247 (ϵ 3180) (EtOH) (Derep).

Akihisa, T. *et al., J.C.S. Perkin 1*, 1988, 439 (*isol, pmr, cmr, cryst struct*)
Akihisa, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1101 (*isol, pmr, cmr*)
Appendino, G. *et al., Phytochemistry*, 1999, **51**, 1021-1026 (*Cucurbita ester*)
Appendino, G. *et al., Fitoterapia*, 2000, **71**, 258-263 (*Debenzoylzucchini factor B*)

8-Multiflorene-3,7,29-triol M-789



$C_{30}H_{50}O_3$ 458.723

(3α,7α)-*form*

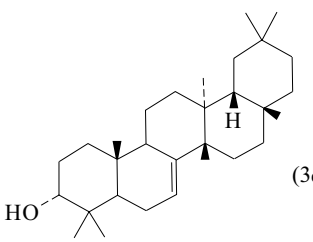
3-O-(4-Aminobenzoyl), 29-benzoyl: [308811-92-9] ***7-Epizucchini factor A***
$C_{44}H_{59}NO_5$ 681.954
Constit. of *Cucurbita pepo* seeds. Gum. $[\alpha]_D^{25}$ -71 (c, 0.8 in MeOH). λ_{max} 289 (MeOH).

(3α,7β)-*form*

3-O-(4-Aminobenzoyl), 29-benzoyl: [246248-09-9] ***Zucchini factor A***
$C_{44}H_{59}NO_5$ 681.954
Constit. of *Cucurbita maxima* and *Cucurbita pepo*. Powder (Et_2O). Mp 158-160°. $[\alpha]_D^{25}$ -52 (c, 0.9 in Py). λ_{max} 289 (log ϵ 4.06) (EtOH).

Appendino, G. *et al., Phytochemistry*, 1999, **51**, 1021-1026 (*Zucchini factor A*)
Appendino, G. *et al., Fitoterapia*, 2000, **71**, 258-263 (*7-Epizucchini factor A*)

7-Multifloren-3-ol M-790



(3α)-*form*

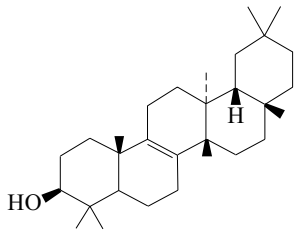
$C_{30}H_{50}O$ 426.724

3β-*form* [2270-62-4]
Multiflorenol
Cryst. (Me_2CO). Mp 188-190°. $[\alpha]_D$ -28 ($CHCl_3$).

Me ether: [14021-27-3] ***3β-Methoxy-7-multiflorene***
$C_{31}H_{52}O$ 440.751
Constit. of the leaf wax of *Saccharum officinarum* (cane sugar). Cryst. (EtOAc). Mp 190-193°. $[\alpha]_D$ -32 (c, 1.9 in $CHCl_3$).

Bryce, T.A. *et al., Tetrahedron*, 1967, **23**, 1283 (*Me ether, isol*)

8-Multifloren-3-ol M-791



$C_{30}H_{50}O$ 426.724

3β-*form* [24462-48-4]

Isomultiflorenol

Constit. of *Cucumis* spp.. Cryst. ($CHCl_3$/MeOH). Mp 182-183°. $[\alpha]_D^{23}$ +27.9 (c, 0.97 in $CHCl_3$).

Ac: ***Isomultiflorenyl acetate***

$C_{32}H_{52}O_2$ 468.762

Constit. of *Benincasa cerifera* (wak gourd). Cryst. (Me_2CO/petrol). Mp 216-217°.

3-Ketone: [22611-26-3] *8-Multifloren-3-one.* ***Isomultiflorenone***

$C_{30}H_{48}O$ 424.709

Cryst. (Me_2CO). Mp 188-195°. $[\alpha]_D^{22}$ +69.1 (c, 1.08 in $CHCl_3$).

Sengupta, P. *et al., Tetrahedron*, 1963, **19**, 123 (*synth*)

Seifert, K. *et al., Pharmazie*, 1976, **31**, 816 (*isol*)

Itoh, T. *et al., Phytochemistry*, 1982, **21**, 2414 (*isol*)

Takai, M. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 185 (*synth*)

Tanaka, R. *et al., Phytochemistry*, 1989, **27**, 3579 (*isol, pmr*)

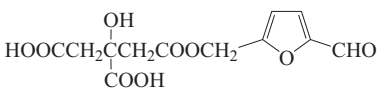
Faure, R. *et al., J. Nat. Prod.*, 1991, **54**, 1564 (*isol, pmr, cmr*)

Cho, H.J. *et al., Phytochemistry*, 1993, **33**, 1407 (*biosynth*)

Mumefural M-792

[222973-44-6]

2-Hydroxy-1,2,3-propanetricarboxylic acid, 1-[(5-formyl-2-furanyl)methyl] ester, 9CI



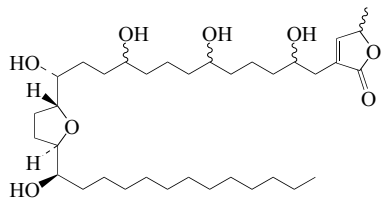
$C_{12}H_{12}O_9$ 300.221

Ester of 5-Hydroxymethyl-2-furancarboxaldehyde, H-587 with Citric acid, C-290. Isol. from fruit juice concentrate of *Prunus mume* (Japanese apricot). Viscous syrup.

Chuda, Y. *et al., J. Agric. Food Chem.*, 1999, **47**, 828-831 (*isol, nmr, uv*)

Muricapentocin M-793

[205304-30-9]



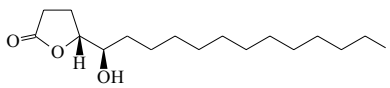
$C_{35}H_{64}O_8$ 612.886

Constit. of *Annona muricata* (soursop). Amorph. solid. $[\alpha]_D$ +8 (c, 0.05 in MeOH). λ_{max} 220 (log ε 3.54) (MeOH).

Kim, G.-S. *et al., J. Nat. Prod.*, 1998, **61**, 432-436 (*isol, pmr, cmr, ms*)

Muricatacin M-794

[134698-86-5]



$C_{17}H_{32}O_3$ 284.438

Constit. of *Annona muricata* (soursop). Cryst. (Et_2O/pentane). Mp 72° (50°). $[\alpha]_D^{20}$ -5.8. $[\alpha]_D^{24}$ -22.9 (c, 1.1 in $CHCl_3$). Nat. prod. is a partial racemate with *ca*. 25% ee of (1′*R*,5*R*) enantiomer illus. Oxidation prod. of Annonacin, A-349.

Reiser, M.J. *et al., Tet. Lett.*, 1991, **32**, 1137 (*isol, pmr, cmr*)

Scholz, G. *et al., Tet. Lett.*, 1991, **32**, 5535 (*synth*)

Tochtermann, W. *et al., Annalen*, 1992, 1069 (*synth*)

Kang, S.K. *et al., J. Carbohydr. Chem.*, 1992, **11**, 807 (*synth*)

Makabe, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1028 (*synth*)

Gravier-Pelletier, C. *et al., Tet. Lett.*, 1994, **35**, 115 (*synth*)

Bonini, C. *et al., J.O.C.*, 1995, **60**, 4803 (*synth, pmr, cmr*)

Quayle, P. *et al., Tet. Lett.*, 1995, **36**, 8087 (*synth*)

Van Aar, M.P.M. *et al., Tetrahedron*, 1995, **51**, 11223 (*synth, ir, pmr, cmr*)

Gypser, A. *et al., J.C.S. Perkin 1*, 1997, 1013 (*synth, pmr, cmr*)

Couladouros, E.A. *et al., Tet. Lett.*, 1999, **40**, 4861-4862 (*synth*)

Baylon, C. *et al., Tet. Lett.*, 2000, **41**, 3833-3835 (*synth*)

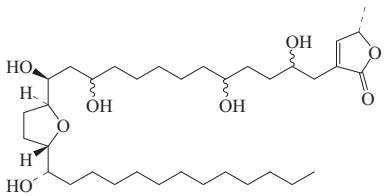
Carda, M. *et al., Eur. J. Org. Chem.*, 2002, 2649-2655 (*synth*)

Konno, H. *et al., Heterocycles*, 2002, **57**, 1793-1797 (*synth*)

Chandrasekhar, M. *et al., Tet. Lett.*, 2002, **43**, 2773-2775 (*synth, bibl*)

Muricatalicin M-795

[179308-46-4]



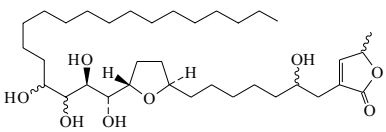
$C_{35}H_{64}O_8$ 612.886

Constit. of *Annona muricata* (soursop). Solid. Mp 105-106°. $[\alpha]_D^{20}$ +17.7 (c, 0.4 in MeOH). λ_{max} 220 (log ε 4.43) (MeCN).

Gui, H.Q. *et al., Chin. Chem. Lett.*, 1996, **7**, 561-564 (*isol, uv, pmr, cmr, ms*)

Muricatalin M-796

[163860-17-1]

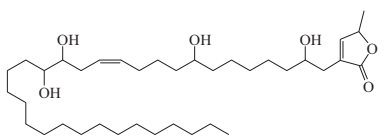


$C_{35}H_{64}O_8$ 612.886

Constit. of *Annona muricata* (soursop). Mp 143-144°. $[\alpha]_D$ +8.8 (c, 0.06 in MeOH). λ_{max} 220 (log ε 3.75) (EtOH).

Gui, H.Q. *et al., Chin. Chem. Lett.*, 1995, **6**, 45-48 (*isol, uv, pmr, cmr*)

Muricatenol M-797



$C_{37}H_{68}O_6$ 608.941

Constit. of the seeds of *Annona muricata* (soursop). Cryst. Mp 50-53°.

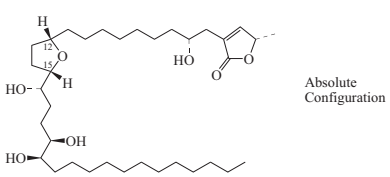
Li, D.Y. *et al., Chin. Chem. Lett.*, 2000, **11**, 239-242

Muricatetrocin A M-798

[153125-14-5]

[163253-84-7]

Howiicin E



$C_{35}H_{64}O_7$ 596.886

Constit. of *Annona muricata* (soursop). Mp 102°. $[\alpha]_D^{25}$ +10.3 (c, 0.15 in $CHCl_3$).

12-Epimer: [153220-48-5] ***Muricatetrocin B***

$C_{35}H_{64}O_7$ 596.886

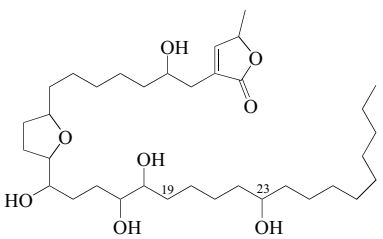
Constit. of *Annona muricata* (soursop) and *Rollinia mucosa* (biriba). Mp 89-

90°. $[\alpha]_D^{25}$ +15 (c, 0.43 in $CHCl_3$).

12,20-Diepimer: [182074-34-6] ***Muricatetrocin C***
$C_{35}H_{64}O_7$ 596.886
Constit. of *Rollinia mucosa* (biriba). Amorph. powder. Mp 65-66°. $[\alpha]_D$ +6.3 (CH_2Cl_2). λ_{max} 224 (log ϵ 3.8) (MeOH).
Rieser, M.J. *et al., Helv. Chim. Acta*, 1993, **76**, 2433-2444; 1994, **77**, 882 (*isol, pmr, cmr, struct, Muricatetrocins*)
Yang, R.-Z. *et al., Zhiwu Xuebao*, 1994, **36**, 561-567; *CA*, **122**, 310664b (*Howiicin E*)
Shi, G.-E. *et al., Bioorg. Med. Chem.*, 1996, **4**, 1281 (*Muricatetrocin C*)
Baeurle, S. *et al., Eur. J. Org. Chem.*, 2000, 2207-2217 (*synth, pmr, cmr, abs config*)
Dixon, D.J. *et al., Chem. Eur. J.*, 2002, **8**, 1621-1636 (*Muricatetrocin C, synth*)

Muricatin A M-799

[160262-48-6]

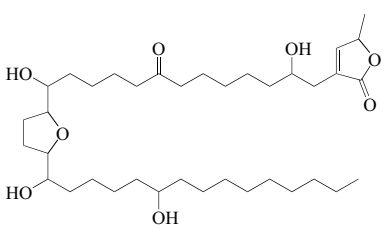


$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Mp 83°. $[\alpha]_D$ +7.1 (c, 0.6 in MeOH).

19-Hydroxy, 23-deoxy: [160262-49-7] ***Muricatin B***†
$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Mp 128°. $[\alpha]_D$ +11.4 (c, 0.2 in MeOH).
Li, C.M. *et al., Chin. Chem. Lett.*, 1994, **5**, 747-750 (*isol, pmr, cmr*)

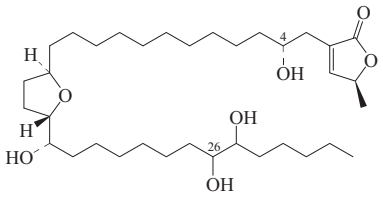
Muricatin C M-800

[160262-50-0]



$C_{37}H_{66}O_8$ 638.924
Constit. of *Annona muricata* (soursop). Mp 61°. $[\alpha]_D$ +15.4 (c, 0.5 in MeOH).
Li, C.M. *et al., Chin. Chem. Lett.*, 1994, **5**, 747-750 (*isol, pmr, cmr*)

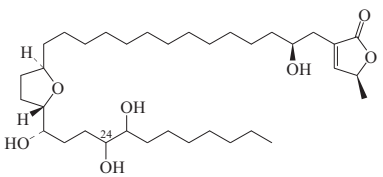
Muricin A M-801



$C_{35}H_{64}O_7$ 596.886
threo-Config. at C-26, C-27. Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +7.2 (c, 0.25 in $CHCl_3$). λ_{max} 210 (log ϵ 3.64) (MeOH).

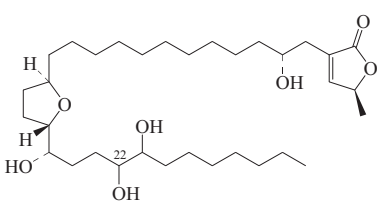
4-Epimer: ***Muricin B***
$C_{35}H_{64}O_7$ 596.886
Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ 0 ($CHCl_3$). λ_{max} 210 (log ϵ 3.65) (MeOH).
Chang, F.-R. *et al., J. Nat. Prod.*, 2001, **64**, 925-931

Muricin C M-802



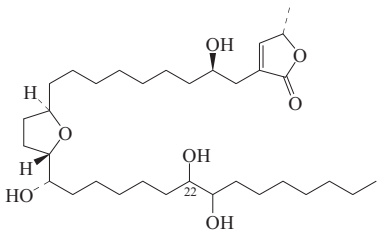
$C_{35}H_{64}O_7$ 596.886
threo-Config. at C-24, C-25. Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +86 (c, 0.15 in $CHCl_3$). λ_{max} 208 (log ϵ 3.73) (MeOH).
Chang, F.-R. *et al., J. Nat. Prod.*, 2001, **64**, 925-931

Muricin D M-803



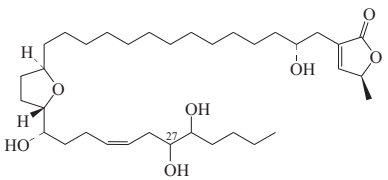
$C_{33}H_{60}O_7$ 568.833
threo-Config. at C-22, C-23. Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +77.6 (c, 0.34 in $CHCl_3$). λ_{max} 208 (log ϵ 3.69) (MeOH).
Chang, F.-R. *et al., J. Nat. Prod.*, 2001, **64**, 925-931

Muricin E M-804



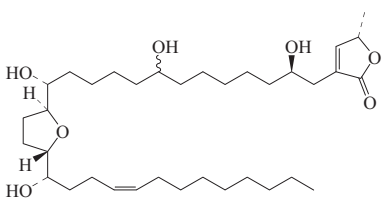
$C_{33}H_{60}O_7$ 568.833
threo-Config. at C-22, C-23. Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +91.4 (c, 0.23 in $CHCl_3$). λ_{max} 208 (log ϵ 3.62) (MeOH).
Chang, F.-R. *et al., J. Nat. Prod.*, 2001, **64**, 925-931

Muricin F M-805



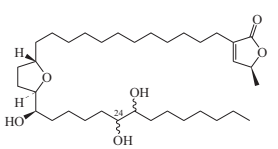
$C_{35}H_{62}O_7$ 594.871
threo-Config. at C-27, C-28. Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +48.2 (c, 0.48 in $CHCl_3$). λ_{max} 208 (log ϵ 3.89) (MeOH).
Chang, F.-R. *et al., J. Nat. Prod.*, 2001, **64**, 925-931

Muricin G M-806



$C_{35}H_{62}O_7$ 594.871
Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +47 (c, 0.63 in $CHCl_3$). λ_{max} 210 (log ϵ 3.52) (MeOH).
Chang, F.-R. *et al., J. Nat. Prod.*, 2001, **64**, 925-931

Muricin H M-807



$C_{35}H_{64}O_6$ 580.887
C-24/C-25 have *threo*-config.. Constit. of the seeds of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D^{25}$ +9.5 (c, 0.76 in $CHCl_3$). λ_{max} 208 (log ϵ 3.64) (MeOH).

Liaw, C.-C. *et al., J. Nat. Prod.*, 2002, **65**, 470-475 (*isol, pmr, cmr, ms*)

Muricine M-808

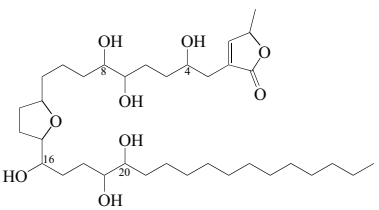
$C_{19}H_{21}NO_4$ 327.379

Struct. unknown. Alkaloid from *Annona muricata* (soursop). Conts. 3OMe groups and no NMe group. Suggested to be identical with De-*N*-methylcorydine.

Hydrobromide:
Mp 242-243°.

Manske, R.H.F. *et al., Alkaloids (N.Y.)*, 1954, **4**, 142

Muricoreacin M-809

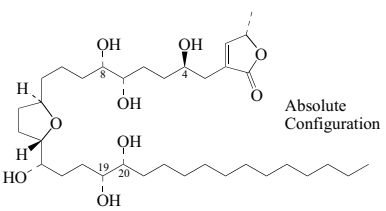


$C_{35}H_{64}O_9$ 628.885
Constit. of the leaves of *Annona muricata* (soursop). Solid. $[\alpha]_D^{23}$ +1.6 (c, 0.06 in MeOH). Relative stereochemistries have been assigned λ_{max} 220 (log ϵ 3.65) (MeOH).

Kim, G.-S. *et al., Phytochemistry*, 1998, **49**, 565-571 (*isol, uv, ir, pmr, cmr, ms*)

Murihexocin A M-810

[167255-47-2]



$C_{35}H_{64}O_9$ 628.885
Acetogenin. Constit. of the leaves of *Annona muricata* (soursop). Wax.

19,20-Diepimer: [166990-05-2] ***Murihexocin B***
$C_{35}H_{64}O_9$ 628.885
Constit. of the leaves of *Annona muricata* (soursop). Powder.

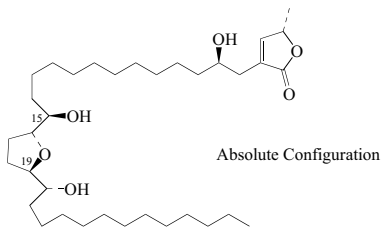
Diastereoisomer: ***Murihexocin C***
$C_{35}H_{64}O_9$ 628.885
Constit. of the leaves of *Annona muricata* (soursop). Solid. $[\alpha]_D^{23}$ +37.5 (c, 0.04 in MeOH). λ_{max} 220 (log ϵ 3.69) (MeOH).

Zeng, L. *et al., Tet. Lett.*, 1995, **36**, 5291-5294 (*isol, pmr, cmr*)
Zeng, L. *et al., Bioorg. Med. Chem.*, 1996, **4**, 1271-1279 (*abs config*)
Kim, G.S. *et al., Phytochemistry*, 1998, **49**, 565-571 (*Murihexocin C*)

Murisolin M-811

[129683-96-1]

[152985-33-6]
Howiicin B



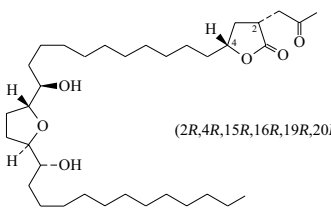
$C_{35}H_{64}O_6$ 580.887
Constit. of *Annona muricata* (soursop) and *Asimina triloba* (paw paw). Amorph. $[\alpha]_D$ +14.8 (c, 0.1 in MeOH). λ_{max} 228 (ϵ 933) (MeOH) (Berdy).

19-Epimer: [170554-60-6] ***16,19-cis-Murisolin***
$C_{35}H_{64}O_6$ 580.887
Constit. of *Asimina triloba* (pawpaw). Amorph. Mp 67-68°. $[\alpha]_D$ +11 (c, 0.1 in CH_2Cl_2). λ_{max} 228 (ϵ 38300) (MeOH) (Berdy).

Diastereoisomer: [170720-10-2] ***Murisolin A***
$C_{35}H_{64}O_6$ 580.887
Constit. of *Asimina triloba* (pawpaw). Powder. Mp 83-84°. $[\alpha]_D$ +17 (c, 0.1 in $CHCl_3$). Has the *erythro*-config. between C-15 and C-16 *or* C-19 and C-20 λ_{max} 226 (ϵ 1050) (MeOH). λ_{max} 226 (ϵ 10800) (MeOH) (Berdy).

Myint, S.H. *et al., Heterocycles*, 1990, **31**, 861 (*isol, pmr, cmr*)
Zhang, L. *et al., Zhiwu Xuebao*, 1993, **35**, 390; *CA*, **120**, 129491 (*Howiicin B*)
Woo, M.H. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 1135 (*isol, pmr, cmr*)

Murisolinone M-812



$C_{35}H_{64}O_6$ 580.887
Struct. given in the lit. lacks a CH_2.

(2*R*,4*R*,15*R*,16*R*,19*R*,20*R*)-*form* [172489-11-1]
cis-*Murisolinone*
Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. Sol. MeOH, $CHCl_3$. Mp 92-93°. $[\alpha]_D$ +13.3 (c, 0.1 in CH_2Cl_2). λ_{max} 220 (log ϵ 3.8) (MeOH).

(2*R*,4*S*,15*R*,16*R*,19*R*,20*R*)-*form* [172489-12-2]
trans-*Murisolinone*
Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. Sol. MeOH, $CHCl_3$. Mp 101-102°. $[\alpha]_D$ +20 (c, 0.1 in CH_2Cl_2). λ_{max} 218 (log ϵ 3.43) (MeOH).

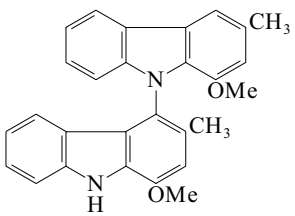
(2ξ,4ξ,15*R*,16*R*,19*R*,20*R*)-*form*

11,12Z-Didehydro: ***Isomurisolenin***
$C_{35}H_{62}O_6$ 578.871
Constit. of *Annona reticulata* (custard apple). Waxy solid. $[\alpha]_D^{24}$ +32.9 (c, 0.3 in $CHCl_3$). Isol. as a mixture of 2,4-*cis*- and *trans*-isomers.

Woo, M.H. *et al., J. Nat. Prod.*, 1995, **58**, 1533 (*isol, pmr, cmr, abs config*)
Chang, F.-R. *et al., Phytochemistry*, 1998, **47**, 1057-1061 (*Isomurisolenin*)

Murrastifoline F M-813

[155519-85-0]
1,1′-Dimethoxy-3,3′-dimethyl-4,9′-bi-9H-carbazole, 9CI

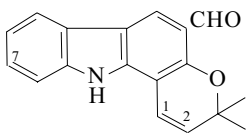


$C_{28}H_{24}N_2O_2$ 420.51
Alkaloid from roots of *Murraya koenigii* (curryleaf tree). Oil. Isol. as a mixture of atropisomers.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)
Bringmann, G. *et al., J.A.C.S.*, 2001, **123**, 2703-2711 (*synth,cd*)

Murrayacine M-814

[27300-29-4]
3,11-Dihydro-3,3-dimethylpyrano[3,2-a]carbazole-5-carboxaldehyde, 9CI



$C_{18}H_{15}NO_2$ 277.322
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Cryst. (EtOAc). Mp 244-245°. $Bp_{0.05}$ 180° subl..

2,4-Dinitrophenylhydrazone:
Mp 280°.

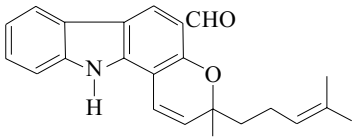
1,2-Dihydro: [17750-37-7] *Cycloheptaphylline. Dihydromurrayacine*
Cryst. (MeOH). Mp 250° (176°).

7-Methoxy: [132160-51-1] ***7-Methoxymurrayacine***
$C_{19}H_{17}NO_3$ 307.348
Mp 211-213°. Numbering systems vary.

Chakraborty, D.P. *et al., J.O.C.*, 1971, **36**, 725; 1973, **38**, 2728 (*isol, uv, ir, pmr, ms, struct, synth*)
Anwer, F. *et al., Indian J. Chem.*, 1973, **11**, 1314 (*synth*)
Oikawa, Y. *et al., Heterocycles*, 1976, **5**, 233 (*synth, ms*)
Roy, S. *et al., Phytochemistry*, 1976, **15**, 356 (*isol, uv, ir*)
Ruangrungsi, N. *et al., J. Nat. Prod.*, 1990, **53**, 946 (*7-Methoxymurrayacine*)
Knölker, H.J. *et al., Tet. Lett.*, 1996, **37**, 7947 (*synth*)

Murrayacinine M-815

[53508-00-2]
3,11-Dihydro-3-methyl-3-(4-methyl-3-pentenyl)pyrano[3,2-a]carbazole-5-carboxaldehyde, 9CI

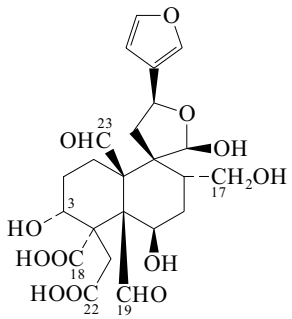


$C_{23}H_{23}NO_2$ 345.44
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Mp 105°. Aldehyde corresponding to Mahanimbine, M-32.

Chakraborty, D.P. *et al., Chem. Ind. (London)*, 1974, 165 (*uv, ir, ms, struct, synth*)
Roy, S. *et al., J. Indian Chem. Soc.*, 1980, **57**, 759 (*synth*)

Musabalbisiane A M-816

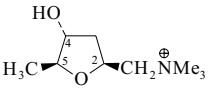
[143183-61-3]



$C_{23}H_{28}O_{12}$ 496.467
Very unusual carbon skeleton. Constit. of *Musa balbisiana*. Cryst. Mp 74-76°. $[\alpha]_D^{18}$ -17.5 (c, 0.1 in $CHCl_3$).
18-Aldehyde, 19-carboxylic acid, 23-alcohol: [143199-58-0] ***Musabalbisiane B***
$C_{23}H_{30}O_{12}$ 498.483
Constit. of *Musa balbisiana*. Amorph. mass. Mp 93-94°. $[\alpha]_D^{18}$ -24.4 (c, 0.06 in $CHCl_3$).
18,19,23-Tris-alcohol, 3-angeloyl: [143183-60-2] ***Musabalbisiane C***
$C_{28}H_{40}O_{12}$ 568.617
Constit. of *Musa balbisiana*. Cryst. Mp 278-280°. $[\alpha]_D^{18}$ -13.3 (c, 0.05 in $CHCl_3$).
Ali, M. *et al., Phytochemistry*, 1992, **31**, 2173 (*isol, pmr, cmr*)

Muscarine M-817

[7619-12-7]
Tetrahydro-4-hydroxy-N,N,N,*5-tetramethyl-2-furanmethanaminium(1+), 9CI*



(2*S*,4*R*,5*S*)-*form*

$C_9H_{20}NO_2^{\oplus}$ 174.262
Sol. EtOH; fairly sol. $CHCl_3$, Et_2O. All 8 stereoisomers have been synthesised.

(2*S*,4*R*,5*S*)-*form* [300-54-9]
Main toxic constit. of the fly fungus *Amanita muscaria* and various *Inocybe* spp.. V. hygroscopic.
► V. toxic if swallowed. Can cause convulsions, coma, death. LD_{50} (mus, ivn) 0.23 mg/kg. Antidote atropine sulfate.
QG3325000

Chloride: [2303-35-7]
$C_9H_{20}ClNO_2$ 209.715
Needles. Mp 181.5-182° , (179-180°). $[\alpha]_D$ +7.4 (c, 3.1 in H_2O).
► QG3500000

(2*R*,4*R*,5*S*)-*form* [6252-44-4]

[35119-38-1]
5-Allomuscarine
Mp 130.8° (as iodide). $[\alpha]_D$ -37.7 (c, 0.8 in H_2O).

(2*R*,4*S*,5*R*)-*form* [92981-62-9]

[35119-35-8]
Mp 179-180° (as chloride). $[\alpha]_D$ -8.4 (EtOH).

(2*S*,4*S*,5*S*)-*form* [6836-08-4]

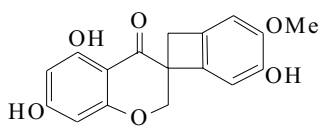
[93226-49-4]
3-Epimuscarine
Cryst. (2-propanol) (as iodide). Mp 170.4° (iodide). $[\alpha]_D$ +43.2 (c, 0.6 in EtOH).

[2936-25-6]

Hardegger, E. *et al., Helv. Chim. Acta*, 1957, **40**, 2383-2389 (*2S,4R,5S-form, synth, abs config*)
Wilkinson, S. *et al., Q. Rev., Chem. Soc.*, 1961, **15**, 153-171 (*rev*)
Eugster, C.H. *et al., Helv. Chim. Acta*, 1969, **52**, 708-715 (*occur, glc*)
Bollinger, H. *et al., Helv. Chim. Acta*, 1971, **54**, 2704-2730 (*synth stereoisomers, abs config, cd*)
Whiting, J. *et al., Can. J. Chem.*, 1972, **50**, 3322-3325 (*synth, pmr*)
Stadelmann, R.J. *et al., Helv. Chim. Acta*, 1976, **59**, 2432-2436 (*occur, stereoisomers*)
Mulzer, J. *et al., Annalen*, 1987, 7-14 (*2S,4R,5S-form, synth, pmr, ir*)
Pirrung, M.C. *et al., Tet. Lett.*, 1988, **29**, 159-162 (*synth, bibl*)
Takano, S. *et al., Chem. Comm.*, 1989, 1371-1372 (*2S,4R,5S-form, synth*)
De Amici, M. *et al., J.O.C.*, 1991, **56**, 67-72 (***synth, stereoisomers, bibl***)
Chan, T.H. *et al., Can. J. Chem.*, 1992, **70**, 2726-2729 (*2S,4R,5S-form, synth*)
Mantell, S.J. *et al., J.C.S. Perkin 1*, 1992, 3023-3027 (*2S,4R,5S-form synth, bibl*)
Norild, J.C. *et al., Synthesis*, 1997, 1128-1130 (*Allomuscarine*)
Popsavin, V. *et al., Carbohydr. Lett.*, 1998, **3**, 1-8 (*synth, Epimuscarine*)

Muscomosin M-818

[99877-68-6]



$C_{17}H_{14}O_6$ 314.294
Constit. of *Muscari comosum* (tassel hyacinth). Cryst. ($CHCl_3$/hexane). Mp 196-198°. $[\alpha]_D$ +68 (c, 0.2 in MeOH). λ_{max} 230 (log ϵ 4.27); 291 (log ϵ 4.38); 336 (log ϵ 3.7) (MeOH).

Adinolfi, M. *et al., Phytochemistry*, 1985, **24**, 2423-2426 (*isol, pmr, cmr*)
Honda, T. *et al., Heterocycles*, 1992, **33**, 291-294 (*synth*)

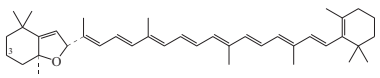
Mutastein M-819

Glycoprotein. Prod. by *Aspergillus terreus* M3328. Comly. used as an ingredient of chewing gum since 1986. Sol. H_2O.

Endo, A. *et al., J. Antibiot.*, 1983, **36**, 203-207 (*isol*)
Hayashida, O. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 588-591 (*isol*)

Mutatochrome M-820

[515-06-0]
5,8-Epoxy-5,8-dihydro-β,β-carotene. Citroxanthin. Flavacin†



(5*S*,8*R*)-*form*

$C_{40}H_{56}O$ 552.882
Constit. of orange peel, *Calendula officinalis* (pot marigold) and *Capsicum annuum* (paprika) and others. Yellow-orange cryst. (C_6H_6/MeOH). Mp 167°.

(5*S*,8*R*)-*form* [90527-81-4]
Cryst. (Et_2O/MeOH). Mp 161°. λ_{max} 250 ; 312 ; 402 ; 425 ; 451 (no solvent reported).

(5*S*,8*S*)-*form* [90527-80-3]
Cryst. (Et_2O/MeOH). Mp 156°. λ_{max} 250 ; 312 ; 402 ; 425 ; 451 (no solvent reported).

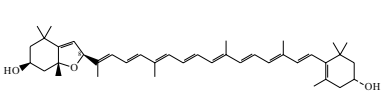
(5ξ,8ξ)-*form*
3-Hydroxy: [30311-63-8] ***Cryptoflavin***. *5,8-Epoxy-5,8-dihydro-β,β-caroten-3-ol. Cryptoxanthin 5,8-epoxide*
$C_{40}H_{56}O_2$ 568.881
Constit. of persimmon (*Diospyros kaki*), star fruit (*Averrhoa carambola*), orange (*Citrus sinensis*) and alfalfa (*Medicago*) spp. Poss. isol. from peach (*Prunus persica*). Leaves (C_6H_6/petrol). Mp 171°. Natural occurrence poorly documented, poss. artifact λ_{max} 459 ; 490 (CS_2). λ_{max} 439 ; 470 (C_6H_6).

[15678-54-3, 31613-49-7]

Karrer, P. *et al., Helv. Chim. Acta*, 1944, **28**, 1695; 1946, **29**, 229; 1947, **30**, 536 (*isol, struct, synth*)
v. Euler, H. *et al., Helv. Chim. Acta*, 1946, **29**, 229; 1947, **30**, 1159 (*synth*)
Bodea, C. *et al., Annalen*, 1963, **666**, 189 (*ir*)
Hertzberg, S. *et al., Phytochemistry*, 1966, **5**, 565; 1971, **10**, 3121
Ignasiak, T. *et al., Biochem. Syst. Ecol.*, 1973, **1**, 97; 1975, **2**, 177 (*isol, Cryptoflavin*)
Eschenmoser, W. *et al., Helv. Chim. Acta*, 1984, **67**, 170
Ebert, G. *et al., Helv. Chim. Acta*, 1985, **24**, 29 (*isol, Cryptoflavin*)

Mutatoxanthin M-821

[31661-06-0]
5,8-Epoxy-5,8-dihydro-β,β-carotene-3,3′-diol. Cryptoxanthin 5,8-epoxide



(8*R*)-*form*

$C_{40}H_{56}O_3$ 584.881
Poss. isol. from *Prunus persica* (peach) and *Diospyros kaki* (persimmon). Leaves (C_6H_6/petrol). Mp 171°. Natural occurrence poorly documented, poss. artifact.

(8*R*)-*form* [85201-99-6]
Constit. of ripe rose hips.

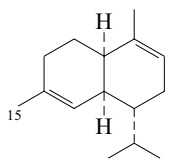
(8*S*)-*form* [85202-00-2]
Constit. of rose hips. Light orange cryst. Mp 213°.

(5ξ,8ξ)-*form*
Red cryst. (MeOH). Mp 177° (sealed tube).

Karrer, P. *et al., Helv. Chim. Acta*, 1946, **29**, 229 (*synth*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 2198; 1983, **66**, 494 (*isol, pmr*)
Bjrnland, T. *et al., Phytochemistry*, 1984, **23**, 1711 (*isol*)
Palermo, J.A. *et al., Phytochemistry*, 1991, **30**, 2983 (*isol, pmr, cmr*)

4,9-Muuroladiene M-822

[31983-22-9]
α*-*Muurolene



(+)-*form*

$C_{15}H_{24}$ 204.355

(+)-*form* [17627-24-6]
Isol. from various plant oils incl. *Pinus mugo* (dwarf mountain pine). $[\alpha]_D$ +17.5 (c, 0.04 in $CHCl_3$).

(-)-*form* [10208-80-7]
Bp_{13} 118°. $[\alpha]_D^{20}$ -52.5. n_D^{22} 1.5051.

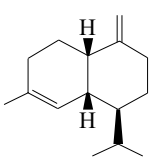
[51260-25-4]

Zabza, A. *et al., Coll. Czech. Chem. Comm.*, 1966, **31**, 3373 (*isol, struct*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)
Dos Santos, M.H. *et al., Rev. Bras. Cienc. Farm.*, 1999, **35**, 297-300 (*activity*)
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr*)

4,10(14)-Muuroladiene M-823

[24268-39-1]

[30021-74-0]
γ*-*Muurolene

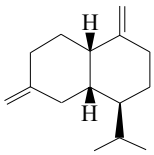


$C_{15}H_{24}$ 204.355
Constit. of *Pinus sylvestris* (Scotch pine). Oil. $[\alpha]_D$ -1.8.

Briggs, L.H. *et al., Aust. J. Chem.*, 1973, **26**, 2229
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*pmr, cmr*)

4(15),10(14)-Muuroladiene M-824

[1136-29-4]
ε*-*Muurolene

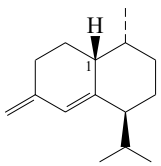


$C_{15}H_{24}$ 204.355
Constit. of ylang-ylang oil. Oil. $[\alpha]_D^{22}$ +50.7 (c, 2.2 in $CHCl_3$).

Burk, L.A. *et al., Tetrahedron*, 1976, **32**, 2083 (*isol*)
Koster, F.-H. *et al., Annalen*, 1986, 78 (*synth, cmr*)

4(15),5,11-Muurolatriene M-825

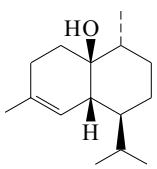
[54324-03-7]
Bicyclosesquiphellandrene



$C_{15}H_{24}$ 204.355
Constit. of *Piper cubeba* (cubeb pepper). Oil.

Terhune, S.J. *et al., Phytochemistry*, 1974, **13**, 1183 (*isol, struct*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1976, **53**, 593 (*synth*)
Melching, S. *et al., Phytochemistry*, 1997, **44**, 1291 (*isol, pmr, ms, gc*)

4-Muurolen-1-ol M-826



(−)-*form*

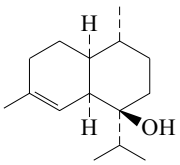
$C_{15}H_{26}O$ 222.37

(+)-*form*
ent-*Epicubenol*
Oil. $[\alpha]_D^{24}$ +111.6 (c, 4.7 in $CHCl_3$).

(-)-*form* [19912-67-5]
Epicubenol. epi-*Cubenol*
Constit. of cubeb pepper (*Piper cubeba*) oil. Oil. $Bp_{2.5}$ 170-180° (bath). $[\alpha]_D^{30}$ -100.6 ($CHCl_3$) (-65).

Ohta, Y. *et al., Tet. Lett.*, 1967, 2073 (*Epicubenol*)
Gerber, N.N. *et al., Phytochemistry*, 1971, **10**, 185 (*isol*)
Adams, D.R. *et al., J.C.S. Perkin 1*, 1975, 1502 (*isol*)
Connolly, J.D. *et al., Phytochemistry*, 1982, **21**, 233 (*isol, struct*)
Cane, D.E. *et al., Tet. Lett.*, 1994, **35**, 5351; 5355 (*synth, biosynth*)
Nabeta, K. *et al., J.C.S. Perkin 1*, 1995, 1935 (*biosynth*)

4-Muurolen-7-ol M-827

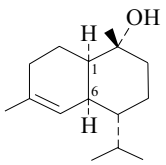


$C_{15}H_{26}O$ 222.37

7β-*form* [86341-93-7]
Chamomillol
Constit. of *Matricaria chamomilla* (German chamomile). Oil.

Reichling, J. *et al., Z. Naturforsch., C*, 1983, **38**, 159 (*isol*)
Brown, G.D. *et al., Phytochemistry*, 1994, **35**, 425 (*isol, pmr, cmr*)

4-Muurolen-10-ol M-828



(1α,6α,7α,10α)-*form*

$C_{15}H_{26}O$ 222.37

(1α,6α,7α,10α)-*form*
ent-T-*Muurolol*
$[\alpha]_D$ +83.4 (c, 2.42 in $CHCl_3$).

(1α,6α,7α,10β)-*form* [5937-11-1]
Cedrelanol. *Brown-algae cadinol. Pilgerol*
Constit. of *Juniperus communis* (juniper). Mp 139-140°. $[\alpha]_D^{20}$ -102 (c, 3.2 in EtOH).

(1β,6β,7β,10β)-*form* [19912-62-0]
T-*Muurolol*
Cryst. Mp 80.5-81.5°. $[\alpha]_D^{23}$ -114 (c, 1 in $CHCl_3$).

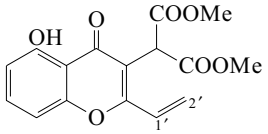
(1β,6β,7β,10α)-*form* [36564-42-8]
Torreyol. *δ-Cadinol. Sesquigoyol. Cedreanol*
Cryst. Mp 139-140°. $[\alpha]_D^{20}$ +102 (c, 3.2 in EtOH). First thought to be a cadinene and therefore appropriately named but since shown to be a muurolane.

[19435-97-3]

Cheng, Y.S. *et al., Chem. Comm.*, 1967, 565 (*isol*)
Nagasampagi, B.A. *et al., Tet. Lett.*, 1968, 1913 (*synth*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 552 (*synth*)
Borg-Karlson, A.-K. *et al., Tetrahedron*, 1981, **37**, 425 (*struct, config*)
Rodriguez-Avial Franke, L.R. *et al., Tetrahedron*, 1984, **40**, 3491 (*synth*)
Tkachev, A.V. *et al., Khim. Prir. Soedin.*, 1990, **26**, 635; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 539 (*pmr, cmr*)
Nagashima, F. *et al., Phytochemistry*, 1994, **37**, 1323 (*ent-T-Muurolol*)

Mycochromone M-829

[71339-45-2]
Dimethyl (2-ethenyl-5-hydroxy-4-oxo-4H-1-benzopyran-3-yl)propanedioate, 9CI



$C_{16}H_{14}O_7$ 318.282
Prod. by *Mycosphaerella rosigena*. Mycotoxin. Yellow needles (EtOAc). Mp 148-149°.

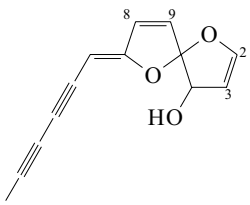
Ac: [71326-01-7]
Mp 151-153°.

1′,2′-Dihydro: [71326-02-8]
Mp 136-137°.

Assante, G. *et al., Phytochemistry*, 1979, **18**, 311 (*isol, struct*)

Mycosinol M-830

[111768-19-5]
7-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.4]nona-2,8-dien-4-ol, 9CI



$C_{13}H_{10}O_3$ 214.22
Variable amts. of information on stereochem. of this compd. and its derivs. Cryst. (Et_2O/petrol). Mp 102°. $[\alpha]_D^{20}$ +44 (c, 0.84 in Et_2O).

Ac (7E-): [17089-08-6]
$C_{15}H_{12}O_4$ 256.257
From *Chrysanthemum coronarium* (chop-suey greens). Cryst. (Et_2O/petrol). Mp 123°. $[\alpha]_D$ +59 (c, 0.57 in Et_2O). Interconverts with the *Z*-form in light.

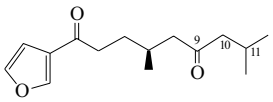
Ac (7Z-):
$C_{15}H_{12}O_4$ 256.257
Isol. *Chrysanthemum coronarium* (chop-suey greens). Mp 123° (91°). $[\alpha]_D$ -868 (c, 0.87 in Et_2O).

[16863-61-9, 17089-43-9, 85317-91-5, 85799-13-9, 85799-15-1]

Bohlmann, F. *et al., Chem. Ber.*, 1961, **94**, 3193; 1963, **96**, 226; 1964, **97**, 1179; 1965, **98**, 2596; 1966, **99**, 990; 2416; 1967, **100**, 3183; 1968, **101**, 1176; 1971, **104**, 11; 1982, **21**, 2543 (*isol, uv, ir, pmr, ord, biosynth, ms*)
Bohlmann, F. *et al., Annalen*, 1963, **668**, 51 (*config*)
Zeisberg, R. *et al., Chem. Ber.*, 1974, **107**, 3800 (*cmr*)
Wrang, P.A. *et al., Phytochemistry*, 1975, **14**, 1027
Marshall, P.S. *et al., Phytochemistry*, 1987, **26**, 2493 (*isol*)
Gao, Y. *et al., Tet. Lett.*, 1996, **37**, 893 (*synth, deriv*)

Myoporone M-831

1-(3-Furanyl)-4,8-dimethyl-1,6-nonanedione, 9CI



(*S*)-*form*

$C_{15}H_{22}O_3$ 250.337
(*S*)-*form* [19479-15-3]
Cryst. (MeOH). Mp 15.5-16.5°. $[\alpha]_D$ -7 (c, 1.39 in MeOH).
▶ RA6500000

(9R)-Alcohol: [72145-16-5] ***Dihydromyoporone***. *6-Myoporol*
$C_{15}H_{24}O_3$ 252.353
Stress metab. of sweet potato (*Ipomoea batatas*). Oil. $[\alpha]_D^{20}$ -3.6 (c, 1.95 in MeOH) (synthetic).
▶ LD_{50} (mus, ipr) 84 mg/kg. RA8254000

10,11-Didehydro: [38462-36-1] ***Dehydromyoporone***
$C_{15}H_{20}O_3$ 248.321
Cryst. (Et_2O/hexane). Mp 32.5-33.5°. $[\alpha]_D$ -15.

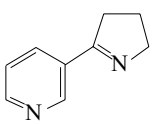
10,11-Epoxy: [68776-17-0] ***Eumorphinone***
$C_{15}H_{20}O_4$ 264.321
Cryst. (Et_2O/petrol). Mp 69.5°. Abs. config. not detd..

10ξ-Hydroxy: [52259-61-7] ***10-Hydroxymyoporone***. *7-Hydroxymyoporone*
Stress metab. of the sweet potato infected with *Ceratocystis fimbriata*. Oil. $[\alpha]_D^{24}$ +12.3 (c, 0.6 in MeOH). Stereochem. undefined.
▶ LD_{50} (mus, ipr) 200 mg/kg. RA6479200

Blackburne, I.D. *et al., Aust. J. Chem.*, 1972, **25**, 1787 (*isol*)
Burka, L. *et al., J.O.C.*, 1974, **39**, 3241 (*7-Hydroxymyoporone*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1155 (*Eumorphinone*)
Burka, L. *et al., Phytochemistry*, 1979, **18**, 873 (*isol*)
Still, W.C. *et al., J.A.C.S.*, 1980, **102**, 7385 (*synth*)
Reich, H. *et al., J.A.C.S.*, 1981, **103**, 3112 (*synth, 7-Hydroxymyoporone*)
Johnson, W.S. *et al., Tet. Lett.*, 1984, **25**, 3951 (*synth, abs config*)
Hess, T. *et al., Tet. Lett.*, 1987, **28**, 5643 (*synth, abs config*)
Anand, R.C. *et al., Tetrahedron*, 1993, **49**, 6515 (*synth, abs config*)
Enders, D. *et al., Synthesis*, 1994, 3127 (*S-form, synth, pmr, cmr*)
Ho, T.-L. *et al., J. Nat. Prod.*, 1997, **60**, 493-494 (*6-Myoporol, synth*)

Myosmine M-832

[532-12-7]
3-(3,4-Dihydro-2H-pyrrol-5-yl)pyridine, 9CI. 3-(1-Pyrrolin-2-yl)pyridine, 8CI. 2-(3-Pyridyl)-1-pyrroline



$C_9H_{10}N_2$ 146.191
Present in hazelnuts and peanuts. Mp 40.5-42°. $Bp_{0.1}$ 55-60°. pK_a 5.26 (24°).

▶ LD_{50} (rat, orl) 1875 mg/kg. UT7660000

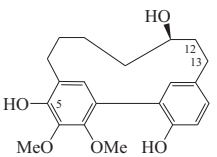
Dipicrate:
Mp 184-185°.

Dipicrolonate:
Mp 213°.

Swain, M.L. *et al., J.A.C.S.*, 1949, **71**, 1341 (*uv*)
Eddy, C.R. *et al., Anal. Chem.*, 1954, **26**, 1428 (*ir*)
Witkop, B. *et al., J.A.C.S.*, 1954, **76**, 5597 (*ir, struct*)
Pople, J.A. *et al., High Resolution Nuclear Magnetic Resonance*, McGraw-Hill, N.Y., 1959, 281 (*pmr*)
Duffield, A.M. *et al., J.A.C.S.*, 1965, **87**, 2926 (*ms*)
Leete, E. *et al., J.O.C.*, 1972, **37**, 4465 (*synth*)
Fejer-Kossey, O. *et al., Phytochemistry*, 1972, **11**, 415 (*isol*)
Brandänge, S. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 93 (*synth*)
Spitzner, D. *et al., Synthesis*, 1977, 242 (*synth*)
Glenn, D.F. *et al., J.O.C.*, 1978, **43**, 2860 (*ms*)
Mahboobi, S. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 175 (*synth, pmr*)
Zwickenflug, W. *et al., J. Agric. Food Chem.*, 1998, **46**, 2703-2706 (*glc, anal*)

Myricanol M-833

[33606-81-4]
16,17-Dimethoxytricyclo[12.3.1.1^{2,6}]nonadeca-1(18),2,4,6(19),14,16-hexaene-3,9,15-triol, 9CI



Absolute Configuration

$C_{21}H_{26}O_5$ 358.433
Needles (Et_2O). Mp 105-125°. $[\alpha]_D^{27.5}$ -65.5 ($CHCl_3$).

11-O-β-D-Xylopyranoside:Myricanol 11-xyloside
$C_{26}H_{34}O_9$ 490.549
Needles (CH_2Cl_2). Mp 229-231°. $[\alpha]_D^{22}$ -46 (c, 0.55 in MeOH). λ_{max} 214 (log ϵ 4.46); 260 (log ϵ 3.97); 298 (log ϵ 3.79) (MeOH).

5-O-β-D-Glucopyranoside: [90052-02-1] *Myricanol 5-glucoside*
$C_{27}H_{36}O_{10}$ 520.575
Constit. of *Myrica rubra* (Chinese bayberry). Mp 220-223°. $[\alpha]_D$ -53.7.

5-O-[(3,4,5-Trihydroxybenzoyl)-(→6)-β-D-glucopyranoside]: [113204-18-5] *Myricanol 5-(6-galloylglucoside)*
$C_{34}H_{40}O_{14}$ 672.682
Constit. of *Myrica rubra* (Chinese bayberry). Cryst. (MeOH aq.). Mp 267-269°. $[\alpha]_D^{24}$ -78.4 (c, 1 in EtOH). λ_{max} 256 (log ϵ 4.2); 285 (log ϵ 4.11) (EtOH).

5-O-[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:
$C_{32}H_{44}O_{14}$ 652.691
Constit. of *Myrica rubra* (Chinese bayberry). Off-white powder. $[\alpha]_D^{21}$ -81.5 (c, 1 in MeOH).

5-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]: [137578-55-3] *Myricanol 5-laminaribioside*
$C_{33}H_{46}O_{15}$ 682.717

Constit. of *Myrica rubra* (Chinese bayberry). Off-white powder. $[\alpha]_D^{21}$ -47.7 (c, 1 in MeOH).

5-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [116107-17-6] *Myricanol 5-β-sophoroside*
$C_{33}H_{46}O_{15}$ 682.717
Constit. of *Myrica rubra* (Chinese bayberry). Off-white powder. $[\alpha]_D^{20}$ -64.6 (c, 1.1 in Py).

Ketone: [32492-74-3] ***Myricanone***
$C_{21}H_{24}O_5$ 356.418
Cryst. (EtOH). Mp 194-196°.

Ketone, 5-deoxy: [110007-10-8] ***5-Deoxymyricanone***
$C_{21}H_{24}O_4$ 340.418
Isol. from bacterial galls of *Myrica rubra* (Chinese bayberry). Amorph.

Ketone, 12-hydroxy: ***Hydroxymyricanone***
$C_{21}H_{24}O_6$ 372.417
Constit. of *Myrica gale* (bog myrtle). Powder. $[\alpha]_D$ -6.1 (c, 0.5 in $CHCl_3$). λ_{max} 213 (ε 35480); 257 (ε 10230); 294 (ε 6920) (MeOH).

Ketone, 12-hydroxy, 5-O-β-D-glucopyranoside: [191999-63-0] ***Myricatomentoside II***
$C_{27}H_{34}O_{11}$ 534.559
Constit. of *Myrica gale* var. *tomentosa*. Needles (MeOH aq.). Mp 148-150°. $[\alpha]_D$ +31.3 (c, 0.5 in MeOH). λ_{max} 213 (log ε 4.48); 249 (log ε 3.99); 295 (log ε 3.67) (MeOH).

Ketone, 12-hydroxy, 5-Me ether: [56222-03-8] ***Porson***
$C_{22}H_{26}O_6$ 386.444
Constit. of *Myrica gale* (bog myrtle). Needles (MeOH). Mp 186-187°. $[\alpha]_D$ -1.8 (c, 2.3 in $CHCl_3$). Gross struct. revised (1995). Abs. config. not certain λ_{max} 213 (ε 38900); 248 (ε 12300); 294 (ε 6025) (EtOH).

Ketone, 12-oxo, 5-Me ether: [171438-25-8] ***12-Dehydroporson***
$C_{22}H_{24}O_6$ 384.428
Constit. of *Myrica gale* (bog myrtle). Pale yellow needles (CH_2Cl_2/MeOH). Mp 191-192°. Exists as α-diketo-tautomer λ_{max} 213 (ε 22910); 249 (ε 6760); 294 (ε 3310) (MeOH).

13-Oxo: [74517-63-8] ***13-Oxomyricanol***
$C_{21}H_{24}O_6$ 372.417
Cryst. (MeOH aq.). Mp 239.5-240°. $[\alpha]_D^{20}$ -36 (c, 0.3 in $CHCl_3$). λ_{max} 224 (log ε 4.23); 262 (log ε 4.24); 281 (sh) (log ε 4.01) (MeOH).

11-Deoxy, 10E,11-didehydro:Myricanene A
$C_{21}H_{24}O_4$ 340.418
Powder.

11-Deoxy, 10E,11-didehydro, 5-O-[α-L-arabinofuranosyl-(1→6)-β-D-glucopyranoside]:
$C_{32}H_{42}O_{13}$ 634.676
Constit. of the bark of *Myrica rubra* (Chinese bayberry). Powder. $[\alpha]_D^{22}$ -0.6 (c, 0.1 in EtOH). λ_{max} 215 (log ε 4.2); 257 (log ε 3.9); 300 (log ε 3.6) (EtOH).

11-Deoxy, 11E,12-didehydro:Myricanene B
$C_{21}H_{24}O_4$ 340.418
Powder.

11-Deoxy, 11E,12-didehydro, 5-O-[α-L-arabinofuranosyl-(1→6)-β-D-glucopyranoside]:
$C_{32}H_{42}O_{13}$ 634.676
Constit. of the stem bark of *Myrica rubra* (Chinese bayberry). Powder. $[\alpha]_D^{22}$ -10.8 (c, 0.1 in EtOH). λ_{max} 214 (log ε 4.5); 253 (log ε 4.1); 297 (log ε 3.7) (EtOH).

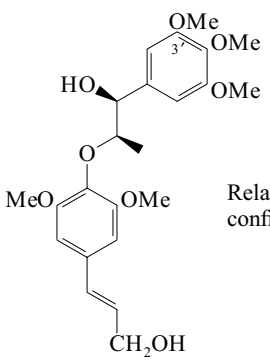
11-Epimer, 5-O-β-D-glucopyranoside: ***Epimyricanol 5-glucoside***
$C_{27}H_{36}O_{10}$ 520.575
Constit. of the bark of *Myrica rubra* (Chinese bayberry). Powder. $[\alpha]_D^{22}$ +81.3 (c, 0.2 in EtOH). λ_{max} 216 (log ε 4.5); 256 (log ε 4.2); 299 (log ε 3.7) (EtOH).

(±)-form
Cubes (EtOAc). Mp 205-206°.

Campbell, R.V.M. *et al., Chem. Comm.*, 1970, 1206 (*isol*)
Begley, M.J. *et al., J.C.S.(C)*, 1971, 3634 (*cryst struct*)
Whiting, D.A. *et al., Tet. Lett.*, 1978, 2335 (*synth*)
Malterud, K.E. *et al., Phytochemistry*, 1980, **19**, 705 (*13-Oxomyricanol*)
Inoue, T. *et al., Yakugaku Zasshi*, 1984, **104**, 37-41 (*5-glucoside*)
Takeda, Y. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2569 (*5-Deoxymyricanone*)
Yaguchi, Y. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1419-1424 (*5-sophoroside, 5-6-galloylglucoside*)
Sun, D. *et al., Phytochemistry*, 1988, **27**, 579 (*cmr*)
Sakurai, N. *et al., Phytochemistry*, 1991, **30**, 3077-3079 (*5-arabinosylglucoside, 5-laminaribioside*)
Nagai, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1674 (*Porson, Dehydroporson*)
Joshi, B.S. *et al., J. Nat. Prod.*, 1996, **59**, 759 (*pmr, cmr, ir, cryst struct*)
Morihara, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 820 (*Myricatomentoside II*)
Tene, M. *et al., Phytochemistry*, 2000, **54**, 975-978 (*11-xyloside*)
Matsuda, H. *et al., Chem. Pharm. Bull.*, 2002, **50**, 208-215 (*Epimyricanol, Myricanenes*)

Myristicanol A M-834

[114892-44-3]
α-[1-[4-(3-Hydroxy-1-propenyl)-2,6-dimethoxyphenoxy]ethyl]-3,4,5-trimethoxybenzenemethanol, 9CI



Relative configuration

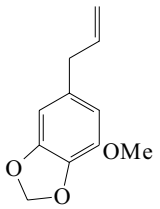
$C_{23}H_{30}O_8$ 434.485
Constit. of the arils of *Myristica fragrans* (mace). Oil. Similar to Polysyphorin.

3′-Demethoxy: [114912-33-3] ***Myristicanol B***
$C_{22}H_{28}O_7$ 404.459
Constit. of the arils of mace *Myristica fragrans*. Oil.

Hattori, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 648 (*isol, ir, pmr, cmr, ms*)

Myristicin M-835

[607-91-0]
4-Methoxy-6-(2-propenyl)-1,3-benzodioxole, 9CI. 1-Methoxy-2,3-methylenedioxy-5-(2-propenyl)benzene. 1-Allyl-3-methoxy-4,5-methylenedioxybenzene



$C_{11}H_{12}O_3$ 192.214
Constit. of dill, nutmeg, parsley and many other essential oils. May be responsible for psychotic effects of nutmeg at large doses. d_{20}^{20} 1.14. Bp_{15} 149-149.5° $Bp_{0.2}$ 95-97°. Log P 2.56 (calc).

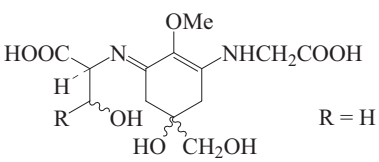
▶ LD_{50} (rat, orl) 4260 mg/kg. CY2625000

Trikojus, W.M. *et al., Nature (London)*, 1939, **144**, 1016 (*synth*)
Surrey, A.R. *et al., J.A.C.S.*, 1948, **70**, 2887 (*synth*)
Redemann, C.E. *et al., J.O.C.*, 1948, **13**, 886 (*synth*)
Lichtenstein, E.P. *et al., J. Agric. Food Chem.*, 1963, **11**, 410 (*use*)
Willhalm, B. *et al., Tetrahedron*, 1964, **20**, 1185 (*ms*)
Cook, W.B. *et al., Can. J. Chem.*, 1966, **44**, 2461 (*isol*)
Shulgin, A.T. *et al., Nature (London)*, 1966, **210**, 380 (*rev*)
Fujita, H. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 3553 (*synth*)
Yakushijin, K. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2879 (*isol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1395
Hallstroem, H. *et al., Nat. Toxins*, 1997, **5**, 186-192 (*tox*)
Benevides, P.J.C. *et al., Phytochemistry*, 1999, **52**, 339-343 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MSA500

Mytilin A M-836

[73112-73-9]

[73522-56-2]
N-[3-[(Carboxymethyl)amino]-5-hydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-ylidene]serine, 9CI. Shinorine. Substance Y. Mycosporin-Gly-Ser



$C_{13}H_{20}N_2O_8$ 332.31
Isol. from the edible mussel *Mytilus*

galloprovincialis (as a 3:1 insep. mixt. with Mytilin B, M-837) and from the red algae *Chondrus endoi* and *Trichocarpus crinitus*. Cryst. Mp 154-156° dec. $[\alpha]_D^{19}$ -3.47. λ_{max} 334 (H_2O).

Chioccara, F. *et al., Tet. Lett.*, 1979, 3181 (*uv, pmr, cmr, ms*)
Tsujino, I. *et al., Bot. Mar.*, 1980, **23**, 65; *CA*, **92**, 124955j (*isol*)
Yabe, K. *et al., CA*, 1981, **95**, 21251j (*isol*)
Grant, P.T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 755
Chioccara, F. *et al., Gazz. Chim. Ital.*, 1985, **115**, 643-647 (*isol, occur*)
Bandaranayake, W.M. *et al., Nat. Prod. Rep.*, 1998, **16**, 159-172 (*rev*)

Mytilin B M-837

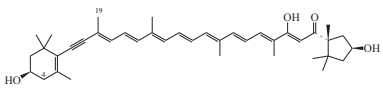
[70579-26-9]
Porphyra 334. Mycosporin-Thr
As Mytilin A, M-836 with
R = CH_3
$C_{14}H_{23}N_2O_8^{\oplus}$ 347.344
Isol. from the edible mussel *Mytilus galloprovincialis* as a 1:3 inseparable mixt. with Mytilin A, M-836. Powder. λ_{max} 334 (ϵ 42300) (H_2O).

[73495-42-8, 79980-53-3]

Takano, S. *et al., Chem. Lett.*, 1979, 419-420 (*isol, uv*)
Chioccara, F. *et al., Tet. Lett.*, 1979, 3181 (*uv, pmr, cmr, ms, struct*)
Kobayashi, J. *et al., Tet. Lett.*, 1981, **22**, 3001-3002 (*isol*)
Grant, P.T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 755 (*isol*)

Mytiloxanthin M-838

[50906-61-1]
7,8-Didehydro-3,3′,8′-trihydroxy-β,κ-carotene-6′-one



$C_{40}H_{54}O_4$ 598.864
Isol. from the mussels *Mytilus edulis*. Reddish needles. Mp 147°.

3′-Ketone: [83746-66-1] ***Mytiloxanthinone.*** *7,8-Didehydro-3,8′-dihydroxy-β,κ-carotene-3′,6′-dione*
$C_{40}H_{52}O_4$ 596.848
Reddish needles. Mp 226-228°.

4-Oxo: [84537-00-8] *7,8-Didehydro-3,3′,8′-trihydroxy-β,κ-carotene-4,6′-dione.* ***4-Oxomytiloxanthin***
$C_{40}H_{52}O_5$ 612.848Struct. assignment is considered tentative by the authors
λ_{max} 447 ; 473 ; 502 (no solvent reported).

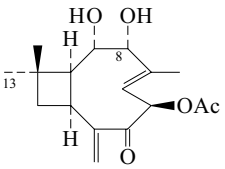
19-Butanoyloxy: [179818-35-0] ***19-Butanoyloxymytiloxanthin***
$C_{44}H_{60}O_6$ 684.954
Red powder. λ_{max} 480 (ϵ 85000) (C_6H_6). λ_{max} 475 (ϵ 94000) (Me_2CO).

19-Hexanoyloxy: [179818-34-9] ***19-Hexanoyloxymytiloxanthin***
$C_{46}H_{64}O_6$ 713.008
Red powder. λ_{max} 480 (ϵ 66900) (C_6H_6). λ_{max} 470 (ϵ 72900) (Me_2CO).

Khare, A. *et al., Tet. Lett.*, 1973, 3921-3924 (*isol*)
Bernhard, K. *et al., Helv. Chim. Acta*, 1982, **65**, 2224-2229 (*4-Oxomytiloxanthin*)
Matsuno, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4309-4315 (*isol, uv, ms, pmr*)
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606-613 (*biosynth*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 419
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495-503 (*isol, pmr, uv, ms*)
Chopra, A.K. *et al., J.C.S. Perkin 1*, 1988, 1383-1388 (*struct, synth*)
Higa, T. *et al., Pure Appl. Chem.*, 1994, **66**, 2227-2230 (*19-acyloxy derivs*)
Kitamura, A. *et al., J. Nat. Toxins*, 1996, **5**, 219-224 (*19-acyloxy derivs*)
Tode, C. *et al., J.C.S. Perkin 1*, 2002, 1581-1587 (*synth*)

Naematolin N-1

[11054-16-3]



Absolute configuration

$C_{17}H_{24}O_5$ 308.374
Cryst. Sol. MeOH, C_6H_6; fairly sol. H_2O; poorly sol. H_2O, hexane. Mp 144-145°. $[\alpha]_D^{22}$ -370 (c, 1.0 in $CHCl_3$). $[\alpha]_D^{22}$ -330. Rare example of *cis*-fused caryophyllane λ_{max} 212 (ϵ 8400); 326 (ϵ 964) (MeOH) (Berdy). λ_{max} 210 (ϵ 8500); 242 ; 326 (ϵ 900) (EtOH) (Berdy).

▶ LD_{50} (mus, ivn) 400 mg/kg. QI1275000

8-Ketone: [92121-62-5] ***Naematolone***
$C_{17}H_{22}O_5$ 306.358
Metab. of *Hypholoma capnoides* (conifer tuft). Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{22}$ +116 (c, 0.46 in $CHCl_3$). λ_{max} 240 (ϵ 2900); 318 (ϵ 340) (MeOH) (Berdy).

13-Hydroxy: [102167-68-0] ***Naematolin B***
$C_{17}H_{24}O_6$ 324.373
Cryst. Mp 122-123°. $[\alpha]_D^{23}$ -352.

Ito, Y. *et al., Chem. Pharm. Bull.*, 1967, **15**, 2009 (*isol*)
Backens, S. *et al., Annalen*, 1984, 1332 (*struct*)
Tsuboyama, S. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1921 (*cryst struct*)

Naled, ANSI, BSI, ISO N-2

[300-76-5]
1,2-Dibromo-2,2-dichloroethyl dimethyl phosphate, 9CI. Dibrom. Bromchlorphos. Bromex†. BRP, JMAF. Flibol Ex. Fosbrom. Alvora

$(MeO)_2P(O)OCHBrCBrCl_2$

$C_4H_7Br_2Cl_2O_4P$ 380.784

▶ TB9450000

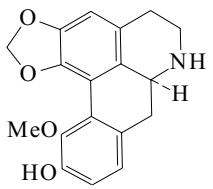
(±)-form
Agricultural insecticide, acaricide, bactericide and fungicide. V. spar. sol. H_2O. d_4^{26} 1.96. Mp 26°. $Bp_{0.5}$ 110°. n_D^{25} 1.5108. Rapidly hydrolysed and degraded in sunlight.

▶ Skin irritant. LD_{50} (rat, orl) 250 mg/kg. LD_{50} (rat, skn) 800 mg/kg. OES: long-term 3 mg m^{-3}; short-term 6 mg m^{-3}.

U.K. Pat., 1957, 855 157; *CA*, **55**, 8748f (*manuf, tox*)
Ger. Pat., 1965, 1 190 246; *CA*, **63**, 4162 (*synth, tox*)
Keith, L.H. *et al., J. Assoc. Off. Anal. Chem.*, 1968, **51**, 1063-1094 (*pmr*)
Getz, M.E. *et al., J. Assoc. Off. Anal. Chem.*, 1968, **51**, 1101-1107 (*tlc*)
Szalontai, G. *et al., J. Chromatogr.*, 1976, **124**, 9-16 (*hplc*)
Stan, H.-J. *et al., Fresenius' Z. Anal. Chem.*, 1977, **287**, 271-285 (*ms*)
Stan, H.-J. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 483-492 (*glc, ms*)
Ripley, B.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 1084-1095 (*glc*)
Dangerous Prop. Ind. Mater. Rep., 1985, **5**, 44-77; 1990, **10**, 62-73 (*rev*)
Betowski, L.D. *et al., CA*, 1988, **109**, 206622 (*hplc-ms*)
Mortimer, R.D. *et al., J. Agric. Food Chem.*, 1991, **39**, 911-916 (*P-31nmr*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A289
Tanner, P.A. *et al., Appl. Spectrosc.*, 1996, **50**, 565-571 (*ir, Raman*)
Pesticide Manual, 11th edn., 1997, no.507
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NAG400

Nandigerine N-3

6,7,7a,8-Tetrahydro-12-methoxy-5H-benzo[g]-1,3-benzodioxolo[6,5,4-de]quinolin-11-ol, 9CI. 10-Hydroxy-11-methoxy-1,2-methylenedioxynoraporphine. Hernangerine



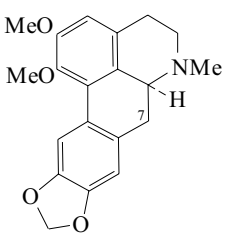
$C_{18}H_{17}NO_4$ 311.337

(S)-form [31520-97-5]
Alkaloid from *Laurus nobilis* (bay laurel). Needles (MeOH). Mp 176-177°. $[\alpha]_D$ +248 (EtOH). Forms MeOH solvate, Mp 99-100°.

Cava, M.P. *et al., Tet. Lett.*, 1966, 1577; 4279 (*Nandigerine, N-Methylnandigerine, uv, pmr, struct*)
Cava, M.P. *et al., Tetrahedron*, 1971, **27**, 2639 (*isol*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80 (*cd*)

Nantenine N-4

[42971-15-3]
5,6,6a,7-Tetrahydro-1,2-dimethoxy-6-methyl-4H-benzo[de][1,3]benzodioxolo[5,6-g]quinoline, 9CI. 1,2-Dimethoxy-9,10-methylenedioxyaporphine. Domestine. Epidicentrine. O-*Methyldomesticine*



(*S*)-*form*

$C_{20}H_{21}NO_4$ 339.39

▶ CE0450000

(S)-form
Mp 139-141°. $[\alpha]_D$ +93 (c, 0.17 in $CHCl_3$). λ_{max} 217 (log ϵ 4.52); 234 (sh) (log ϵ 4.3); 273 (sh) (log ϵ 3.92); 282 (log ϵ 3.96); 309 (log ϵ 4.05); 318 (sh) (log ϵ 4.01) (95% EtOH).

N-*De-Me:* [15401-66-8] *1,2-Dimethoxy-9,10-methylenedioxynoraporphine.* ***Nornantenine***
$C_{19}H_{19}NO_4$ 325.363
Alkaloid from *Laurelia sempervirens* (Peruvian nutmeg). Prisms (Me_2CO/petrol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 163-164°. $[\alpha]_D$ +85 (c, 0.75 in $CHCl_3$). λ_{max} 218 (log ϵ 4.61); 282 (log ϵ 4.06); 308 (log ϵ 4.15) (no solvent reported).

O^2-*De-Me:* [70560-83-7] *2-Hydroxy-1-methoxy-9,10-methylenedioxyaporphine.* ***Isodomesticine***
$C_{19}H_{19}NO_4$ 325.363
Alkaloid from the leaves of *Laurus nobilis* (bay laurel). Amorph. Mp 85°. λ_{max} 216 (log ϵ 4.55); 283 (log ϵ 3.99); 310 (log ϵ 4.07) (EtOH).

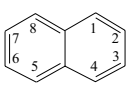
O^2-*De-Me,* N-*de-Me:* [80151-84-4] *2-Hydroxy-1-methoxy-9,10-methylenedioxynoraporphine.* ***Norisodomesticine***
$C_{18}H_{17}NO_4$ 311.337
Alkaloid from the leaves *Laurus nobilis* (bay laurel). Amorph.

*4*R-*Hydroxy,* N-*de-Me:* [69128-21-8] *4-Hydroxynornantenine*
$C_{19}H_{19}NO_5$ 341.363
Alkaloid from the wood of *Laurelia sempervirens* (Peruvian nutmeg). Oil which darkens rapidly on contact with air. Mp 179-181° (as di-Ac).

Johns, S.R. *et al., Aust. J. Chem.*, 1966, **19**, 2331-2338; 1967, **20**, 1457-1462 (*Nordomesticine, Nantenine, Nornantenine, isol, pmr, uv, struct*)
Govindachari, T.R. *et al., Indian J. Chem., Sect. B*, 1969, **7**, 841-843; 1970, **8**, 16-18 (*Domesticine, Isodomesticine, synth*)
Kunitomo, J. *et al., Yakugaku Zasshi*, 1974, **94**, 1149-1153 (*Hydroxynantenine*)
Hoshino, O. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2048-2053; 1978, **26**, 3920 (*Domesticine, Isodomesticine, synth*)
Manikumar, G. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 740-741 (*Nornantenine, synth*)
Urzúa, A. *et al., Tet. Lett.*, 1978, 2649-2652 (*4-Hydroxynornantenine*)
Zabel, V. *et al., Acta Cryst. B*, 1979, **35**, 3126-3129 (*4-Hydroxynornantenine, cryst struct*)
Hoquemiller, R. *et al., J. Nat. Prod.*, 1981, **44**, 551-556 (*Norisodomesticine*)
Pech, B. *et al., J. Nat. Prod.*, 1982, **45**, 560-563 (*Isodomesticine*)

Naphthalene, BSI, ISO N-5

[91-20-3]



$C_{10}H_8$ 128.173
Found in many essential oils. Plates (EtOH) with characteristic odour. Spar. sol. petrol; insol. H_2O. Mp 80.3°. Bp 218°. Steam-volatile. Sublimes readily. Noncarcinogenic.

▶ Fl. p. 77°, autoignition temp. 528°. Eye and skin irritant. Contact with solid can damage eyes. Haemolytic agent (via metabolites) by ingestion. OES: long-term 10 ppm; short-term 15 ppm. QJ0525000

Picrate: [5160-53-2]
Mp 149.5°.

▶ Reacts explosively with N_2O_5.

[1146-65-2, 34509-91-6, 34512-27-1]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 40C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 956A (*ir*)

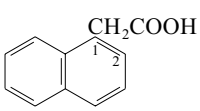
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 877C (*ir*)
Adv. Chem. Ser., 1955, **15**, 203 (***props***)
Almenningene, A. *et al., Acta Cryst.*, 1961, **14**, 1056 (*cryst struct*)
Memory, J.D. *et al., J. Chem. Phys.*, 1966, **45**, 3567 (*pmr*)
Alger, T.D. *et al., J.A.C.S.*, 1966, **88**, 5397 (*cmr*)
Hathaway, C.E. *et al., Spectrochim. Acta A*, 1967, **23**, 881 (*Raman*)
Momicchioli, F. *et al., J.C.S.(B)*, 1970, 1353 (*uv*)
Crecely, R.W. *et al., Org. Magn. Reson.*, 1970, **2**, 613 (*pmr*)
Poponova, R.V. *et al., Zh. Org. Khim.*, 1971, **7**, 2032; *J. Org. Chem. USSR (Engl. Transl.)*, 1971, **7**, 2111 (*ms*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Günther, H. *et al., J. Magn. Reson.*, 1973, **11**, 344 (*cmr*)
Sakurai, H. *et al., J.A.C.S.*, 1973, **95**, 955 (*epr*)
Evans, A.G. *et al., J.C.S. Perkin 2*, 1973, 2091 (*epr*)
Palmer, M.H. *et al., J.C.S. Perkin 2*, 1974, 1893 (*struct*)
Schönfeld, W. *et al., Org. Mass Spectrom.*, 1975, **10**, 321 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **15**, 698 (*rev*)
Wudl, F. *et al., J.O.C.*, 1979, **44**, 2491 (*uv*)
Dowdy, D. *et al., Chem. Ind. (London)*, 1985, 338 (*purifn*)
Boutonnet, J.C. *et al., J. Organomet. Chem.*, 1985, **290**, 153 (*pmr*)
Freeman, H.S. *et al., Dyes Pigm.*, 1988, **9**, 67 (*pmr*)
Pesticide Manual, 9th edn., 1991, No. 8760
Sakamoto, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1981 (*bibl, tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1129
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NAJ500
Franklin, R.B. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 153 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 3041
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 881
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 2504 (*tox*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 419

1-Naphthaleneacetic acid, 9CI, 8CI N-6

[86-87-3]

[26445-01-2]

(1-Naphthyl)acetic acid, BSI, ISO. Planofix. Phyomone. Fruitone N. Rootone. Regenasol. Tre-Hold. NAA



$C_{12}H_{10}O_2$ 186.21

Some trade names apply to the Na salt. Plant growth regulator. Used for control of preharvest fruit drop, flower induction and fruit thinning in various crops such as apples, potatoes, olives and citrus fruits. Needles (H_2O). Mod. sol. alkalis; spar. sol. H_2O; v. sol. Me_2CO, EtOH. Mp 134.5-135.5° (131°). pK_a 4.24 (25°). Log P 2.59 (calc). Dec. on dist..

▶ Skin, mucous membrane and severe eye irritant. LD_{50} (rat, orl) 1000 mg/kg. Exp. reprod. effects. QJ0875000

Me ester: [2876-78-0]
$C_{13}H_{12}O_2$ 200.237
Oil. Bp_{11} 162-165°. $n_D^{25.5}$ 1.5939.

▶ LD_{50} (rat, orl) 1900 mg/kg. QJ1225000

Et ester: [2122-70-5]
$C_{14}H_{14}O_2$ 214.263
Plant growth regulator used to promote root growth. Oil. Bp_{20} 220-225° $Bp_{0.15}$ 100-105° (lit. gives a pressure range).

▶ LD_{50} (rat, orl) 3580 mg/kg. QJ0948000

Chloride: [5121-00-6]
$C_{12}H_9ClO$ 204.655
Yellow oil. Bp_{23} 188° $Bp_{0.05}$ 148-155°.

Amide: [86-86-2] *2-(1-Naphthyl)acetamide, ISO. α-Naphthaleneacetamide. NAD†. Amid-Thin*
$C_{12}H_{11}NO$ 185.225
Plant growth regulator. Needles. Subl. 181-183.

▶ LD_{50} (rat, orl) 1690 mg/kg. QJ0590000

Anilide: [80817-92-1]
$C_{18}H_{15}NO$ 261.323
Needles (C_6H_6/hexane). Mp 156-157°.

Nitrile: [132-75-2] *1-(Cyanomethyl)-naphthalene*
$C_{12}H_9N$ 167.21
Waxy solid. Mp 33-35°. Bp 162-164° Bp_{18} 191-194°. n_D^{20} 1.6192.

▶ AM1240000

Anhydride: [5415-58-7]
$C_{24}H_{18}O_3$ 354.404
Mp 116°.

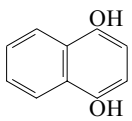
[61-31-4, 15165-79-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 173A; 379C; 463A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1041A; 1216A; 1409A; 1548A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1349A; 1421D (*ir*)
Gardner, F.E. *et al., Science (Washington, D.C.)*, 1939, **90**, 208-209 (*use*)
Ogata, Y. *et al., J.A.C.S.*, 1950, **72**, 4302 (*synth*)
Hitzenberger, G. *et al., Wien. Med. Wochenschr.*, 1958, **108**, 507-509; 1959, **109**, 707 (*pharmacol*)
Gore, R.C. *et al., J. Assoc. Off. Anal. Chem.*, 1971, **54**, 1040-1082 (*uv, ir*)
Pande, C.S. *et al., Fresenius' Z. Anal. Chem.*, 1972, **262**, 365; 1973, **265**, 31 (*detn, Zr, Th*)
Emudianughe, T.S. *et al., Biochem. Soc. Trans.*, 1977, **5**, 1006-1008 (*metab*)
Rajan, S.S. *et al., Acta Cryst. B*, 1978, **34**, 998-1000 (*cryst struct*)
Marshall, J.L. *et al., Org. Magn. Reson.*, 1979, **12**, 163-168 (*cmr*)
Higgins, S.D. *et al., J.C.S. Perkin 1*, 1982, 235-241 (*Me ester, synth, pmr*)
Giordano, C. *et al., J.C.S. Perkin 1*, 1982, 2575-2581 (*synth*)
Engman, L. *et al., J.O.C.*, 1982, **47**, 3946-3949 (*synth*)
Takahashi, K. *et al., J.O.C.*, 1983, **48**, 3566-3568 (*synth*)
Rathore, H.S. *et al., J. Liq. Chromatogr.*, 1987, **10**, 3623-3636 (*tlc*)
Chen, J. *et al., Synthesis*, 1987, 586-587 (*synth*)
Emudianughe, T.S. *et al., Xenobiotica*, 1987, **17**, 815-821 (*metab*)
Org. Synth., Coll. Vol., 6, 1988, 613-615 (*Et ester, synth*)
Husain, S. *et al., J. Chromatogr.*, 1991, **558**, 435-439 (*hplc*)
Org. Synth., 1993, **71**, 146-157 (*Et ester, synth, ir, pmr*)
Synthesis, 1993, **71**, 146-157 (*Et ester, synth, ir, pmr*)
Pesticide Manual, 10th edn., 1994, No. 493; No. 494
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1730
Carretero, A.S. *et al., J. Agric. Food Chem.*, 1998, **46**, 561-565 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NAK000; NAK500; NBD500

1,4-Naphthalenediol, 9CI, 8CI N-7

[571-60-8]

1,4-Dihydroxynaphthalene. Naphthohydroquinone



$C_{10}H_8O_2$ 160.172
Needles (EtOH). Sol. hot H_2O. Mp 176°.

▶ QJ4730000

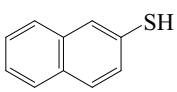
Mono-Me ether: [84-85-5] *4-Methoxy-1-naphthol*
$C_{11}H_{10}O_2$ 174.199
Constit. of the roots of *Asperula odorata* (sweet woodruff). Needles (petrol). Mp 124-126°.

Burnett, A.R. *et al., J.C.S.(C)*, 1968, 854 (*isol, ms, uv, deriv*)

2-Naphthalenethiol N-8

[91-60-1]

2-Naphthyl mercaptan. 2-Mercaptonaphthalene. β-Thionaphthol. FEMA 3314



$C_{10}H_8S$ 160.239
Flavouring ingredient. Cryst. (EtOH) with a disagreeable mercaptan-like odour. Spar. sol. H_2O. Mp 81°. Bp 286° $Bp_{10.3}$ 146.3°. pK_a 6.47 (25°). Spar. steam-volatile.

▶ LD_{50} (mus, orl) 385 mg/kg. QK3930000

S-*Ac:* [831-23-2]
$C_{12}H_{10}OS$ 202.276
Mp 53.5°. Bp_{15} 191°.

S-*Me:* See 2-(Methylthio)naphthalene in *The Combined Chemical Dictionary.*

S-*Et:* [32551-87-4] *2-(Ethylthio)naphthalene. Ethyl 2-naphthyl sulfide*
$C_{12}H_{12}S$ 188.293
Mp 16°. Bp_{15} 170.5°.

S-*Ph:* See 2-(Phenylthio)naphthalene in *The Combined Chemical Dictionary.*

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 430A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1099B (*ir*)
Hannan, R.B. *et al., J.A.C.S.*, 1949, **71**, 3733 (*ir*)
Jacques, J. *et al., Bull. Soc. Chim. Fr.*, 1955, 231 (*synth*)
Schaepma, Y. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1957, **76**, 180 (*synth*)
Dann, O. *et al., Chem. Ber.*, 1958, **91**, 172 (*synth*)
Lawesson, S.O. *et al., Acta Chem. Scand.*, 1966, **20**, 2325 (*ms*)
Org. Synth., 1971, **51**, 139 (*synth*)
Tiecco, M. *et al., Synthesis*, 1983, 751 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 588
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1933-1934
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NAP500

1,4,5-Naphthalenetriol, 9CI N-9

[481-40-3]
1,4,5-Trihydroxynaphthalene. α-Hydrojuglone

$C_{10}H_8O_3$ 176.171
Occurs in green shells of unripe walnuts (*Juglans* sp.). Leaflets or needles (H_2O). Insol. C_6H_6, petrol, $CHCl_3$. Mp 168-170°. Tautomer of β-Hydrojuglone; see under 5-Hydroxy-1,4-naphthoquinone, H-625.

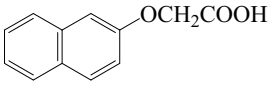
4-O-β-D-Glucopyranoside: [39015-63-9]
$C_{16}H_{18}O_8$ 338.313
Isol. from *Juglans* spp.. Prisms (H_2O). Mp 216° dec. $[\alpha]_D^{21}$ -96.7 (MeOH). λ_{max} 224 (log ϵ 4.6); 306 (log ϵ 4.2); 326 (log ϵ 4.1); 342 (log ϵ 4.1) (EtOH).

5-O-β-D-Glucopyranoside: [22427-33-4]
Hydrojuglone glucoside
$C_{16}H_{18}O_8$ 338.313
Constit. of the leaves of *Carya illinoensis* (pecan). Cryst. (EtOAc). Mp 197° (179-180°).

Willstätter, R. *et al., Ber.*, 1914, **47**, 2796 (*synth*)
Daglish, C. *et al., J.A.C.S.*, 1950, **72**, 4859 (*uv*)
Elsevier's Encycl. Org. Chem., Ser. III, 1953, **12B**, 2155 (*bibl*)
Hayes, N.F. *et al., J.C.S.*, 1955, 904 (*glucoside*)
Cameron, D.W. *et al., J.C.S.(C)*, 1968, 3068 (*5-glucoside*)
Corey, E.J. *et al., Tet. Lett.*, 1975, 2389 (*deriv*)
Mueller, W.U. *et al., Phytochemistry*, 1978, **17**, 1739 (*4-glucoside*)
Hannan, R.L. *et al., J.O.C.*, 1979, **44**, 2153-2158 (*deriv, synth*)
Laatsch, H. *et al., Annalen*, 1980, 140-157 (*deriv, synth, pmr*)
Chorn, T.A. *et al., J.C.S. Perkin 1*, 1984, 1339-1343 (*deriv, synth, ir, pmr*)
Malesani, G. *et al., J. Het. Chem.*, 1987, **24**, 513-517 (*synth, pmr, derivs*)
Jung, M.E. *et al., J.O.C.*, 1987, **52**, 1889-1902 (*deriv, synth, pmr, cmr, ir, ms*)
Gueldner, R.C. *et al., J. Am. Soc. Hortic. Sci.*, 1994, **119**, 498 (*5-glucoside*)
Min, B.-S. *et al., Chem. Pharm. Bull.*, 2000, **48**, 194-200 (*4-glucosides, 4-galloylglucosides*)

(2-Naphthalenyloxy)acetic acid, 9CI N-10

[120-23-0]
(2-Naphthyloxy)acetic acid, 8CI, BSI, ISO. Glycollic acid 2-naphthyl ether. Betapal



$C_{12}H_{10}O_3$ 202.209
Plant growth regulator. Used for control of preharvest fruit drop esp. on grapes, pineapples, strawberries and tomatoes. Prisms (H_2O). Mp 156°.

▶ LD_{50} (rat, orl) 600 mg/kg. AI9659000

Et ester: [6036-14-2]
$C_{14}H_{14}O_3$ 230.263
Plates. Mp 48-49°. Bp_{16} 170-190°. Triboluminescent.

Chloride: [40926-77-0]
$C_{12}H_9ClO_2$ 220.655
Needles (C_6H_6). Mp 54°. Bp_{10} 207°.

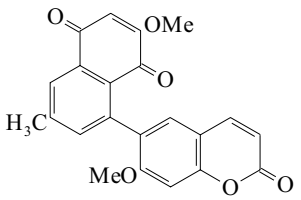
Amide: [35368-77-5]
$C_{12}H_{11}NO_2$ 201.224
Needles or plates. Spar. sol. H_2O. Mp 147°.

[1929-87-9]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1042B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 173D (*ir*)
Ingham, B. *et al., J.C.S.*, 1931, 897 (*synth*)
Pattabhi, V. *et al., Acta Cryst. B*, 1978, **34**, 3118 (*cryst struct*)
Pagani, G. *et al., Farmaco, Ed. Sci.*, 1978, **33**, 332 (*activity*)
Deshmukh, J.G. *et al., Chem. Ind. (London)*, 1986, 179 (*esters*)
Rathore, H.S. *et al., J. Liq. Chromatogr.*, 1987, **10**, 3623 (*tlc*)
Pesticide Manual, 9th edn., 1991, No. 8820
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A290

Naphthoherniarin N-11

[114032-22-3]
2-Methoxy-8-(7-methoxy-2-oxo-2H-1-benzopyran-6-yl)-6-methyl-1,4-naphthalenedione, 9CI

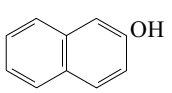


$C_{22}H_{16}O_6$ 376.365
Constit. of *Ruta graveolens* (rue). Cryst. (toluene). Mp 242-244° Mp 285° (278-283°).

Reisch, J. *et al., Annalen*, 1988, 543 (*ir, pmr, uv, synth*)
Rózsa, Z. *et al., Planta Med.*, 1989, **55**, 68 (*isol, uv, pmr, cmr*)

2-Naphthol, 8CI N-12

[135-19-3]
2-Naphthalenol, 9CI. 2-Hydroxynaphthalene. β-Naphthol



$C_{10}H_8O$ 144.173
Trace constit. of essential oils. Plates by subl. Sol. EtOH, Et_2O; v. spar. sol. H_2O. Mp 123°. Bp 285-286°. Reduces Ag-NO_3.NH_3. Volatile in steam, EtOH and Et_2O. Fluoresces strongly in aq. soln (unlike 1-naphthol).

▶ Can cause nephritis by skin absorption. Other adverse systemic effects resulting from overdosage recorded. LD_{50} (rat, orl) 1960 mg/kg. Skin and eye irritant. QL2975000

Na salt: [875-83-2]
Platelets. Mp 120°.

Phosphate: [1136-89-6] *2-Naphthyl dihydrogen phosphate*
$C_{10}H_9O_4P$ 224.153
Cryst. Mp 159-161°.

Ac: [1523-11-1]
$C_{12}H_{10}O_2$ 186.21
Mp 70°.

Benzoyl: [93-44-7] *2-Benzoyloxynaphthalene. Benzonaphthol*
$C_{17}H_{12}O_2$ 248.281
Mp 107°.

3,5-Dinitrobenzoyl:
Mp 210-212°.

Trifluoromethanesulfonyl: [3857-83-8]
$C_{11}H_7F_3O_3S$ 276.236
Cryst. (EtOH aq.). Mp 31-32° (27.5-28°). $Bp_{0.2}$ 86-87°.

Me ether: 2-Methoxynaphthalene, M-266

Et ether: 2-Ethoxynaphthalene, E-256

2-Propenyl ether: [3698-15-5] *2-Allyloxynaphthalene*
$C_{13}H_{12}O$ 184.237
Oil. Bp 108-110°.

2-Methylpropyl ether: [2173-57-1] *2-(2-Methylpropoxy)naphthalene. FEMA 3719*
$C_{14}H_{16}O$ 200.28
Flavouring ingredient. Leaflets (EtOH). Mp 33°. Bp 307°.

1,1,2,2-Tetrafluoroethyl ether: [2796-08-9]
$C_{12}H_8F_4O$ 244.188
Mp 28-30°. $Bp_{0.7}$ 75-76°. n_D^{25} 1.5022.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1109B; **2**, 316D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 307C; 1298C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1042D (*ir*)
Franzen, H. *et al., Ber.*, 1917, **50**, 101-104 (*synth*)
Wang, A.B. *et al., J. Chin. Chem. Soc. (Peking)*, 1933, **1**, 59-63; *CA*, **27**, 573l (*ethers, synth*)
Friedman, O.M. *et al., J.A.C.S.*, 1950, **72**, 624-625 (*phosphate*)
England, D.C. *et al., J.A.C.S.*, 1960, **82**, 5116 (*tetrafluoroethyl ether*)
Klouwen, M.H. *et al., Parfuem. Kosmet.*, 1962, **43**, 195-200; *CA*, **57**, 11325 (*occur*)
Christian, G.D. *et al., Anal. Chim. Acta*, 1968, **41**, 269-274 (*use*)
Occolowitz, J.L. *et al., Aust. J. Chem.*, 1968, **21**, 997-1005 (*ms*)
Christian, G.D. *et al., Talanta*, 1969, **16**, 255-261 (*use*)
Brown, R.F.C. *et al., Aust. J. Chem.*, 1974, **27**, 2385-2391 (*synth*)
Ernst, L. *et al., Chem. Ber.*, 1975, **108**, 2030-2039 (*cmr*)

Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, (*use, ind*)
Rusek, G. *et al., Spectrosc. Lett.*, 1978, **17**, 381-387 (*uv*)
Pant, U.C. *et al., Rev. Roum. Chim.*, 1979, **24**, 471-482 (*synth*)
Abeywickrema, A.N. *et al., J.O.C.*, 1987, **52**, 4072-4078 (*2-propenyl ether, synth, pmr, cmr*)
Crisp, G.T. *et al., Aust. J. Chem.*, 1988, **41**, 1711-1715 (*trifluoromethanesulfonyl, synth, cmr, ms*)
Armstrong, M.M. *et al., J. Coord. Chem.*, 1989, **20**, 81-93 (*phosphate*)
Sund, R.B. *et al., Pharmacol. Toxicol.*, 1993, **72**, 84-89 (*metab*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 588 (*2-methylpropyl ether*)
Thompson, M.J. *et al., J. Chromatogr., B: Biomed. Appl.*, 1996, **677**, 117 (*hplc*)
Bieniek, G. *et al., J. Chromatogr., B: Biomed. Appl.*, 1996, **682**, 167 (*gc*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 111
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1936 (*2-methylpropyl ether*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 885
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NAX000

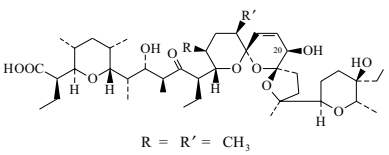
Napin N-13

Storage protein isol. from the seeds of *Brassica napus* (rape).

Byczynska, A. *et al., J. Plant Physiol.*, 1999, **154**, 417-425 (*rev, struct, biosynth*)

Narasin A N-14

[55134-13-9]
4-Methylsalinomycin, 9CI. Monteban. ***Narasin, BAN, INN, USAN****. Narasul. A 28086A. C 18-205. C 7819B. Lilly 79891. Antibiotic A 28086A. Antibiotic C 7819B*



R = R′ = CH_3

$C_{43}H_{72}O_{11}$ 765.035

Polyether antibiotic. Ionophore effective against viruses and particularly against coccidial infections in chickens. Cryst. (Me_2CO aq.). Mp 98-100° Mp 198-200° (double Mp). $[\alpha]_D^{25}$ -54 ($CHCl_3$). Log P 5.54 (uncertain value) (calc).

▶ LD_{50} (mus, ipr) 7 mg/kg. VO8640000

Na salt: [70052-00-5]
Cryst. Mp 158-160°.

▶ QN4590000

Me ester: [63045-44-3]
Mp 160-162°.

20-Ketone: [58439-94-4] ***Narasin B****. A 28086B. Antibiotic A 28086B*
$C_{43}H_{70}O_{11}$ 763.019
Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. Mp 150-153°.

20-Deoxy: [70022-35-4] ***20-Deoxynarasin***
$C_{43}H_{72}O_{10}$ 749.036
Useful feed additive. Sol. MeOH, C_6H_6, DMSO, DMF; fairly sol. hexane; poorly sol. H_2O.

▶ LD_{50} (mus, ipr) 5 mg/kg.

17-Epimer, 20-deoxy: [70051-99-9] ***20-Deoxy-17-epinarasin***
$C_{43}H_{72}O_{10}$ 749.036
Useful feed additive. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O.

▶ LD_{50} (mus, ipr) 201 mg/kg. QN4570000

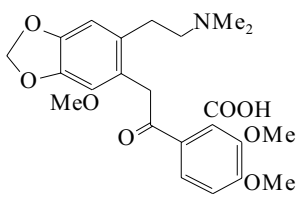
4-Demethyl: See Salinomycin in *The Combined Chemical Dictionary.*

[59979-83-8]

Occolowitz, J.K. *et al., Biomed. Mass Spectrom.*, 1976, **3**, 272 (*struct*)
Dorman, D.E. *et al., Helv. Chim. Acta*, 1976, **59**, 2625 (*biosynth*)
Seto, H. *et al., J. Antibiot.*, 1977, **30**, 530 (*cmr, struct*)
U.S. Pat., 1977, 4 035 481; *CA*, **87**, 116418 (*isol*)
Berg, D.H. *et al., J. Antibiot.*, 1978, **31**, 1 (*isol, struct*)
U.S. Pat., 1979, 4 141 907; *CA*, **91**, 122144 (*isol, props, deriv*)
Caughey, B. *et al., Biochem. Biophys. Res. Commun.*, 1983, **113**, 832 (*pmr, conformn*)
Lewis, M.D. *et al., Diss. Abstr. Int., B*, 1983, **44**, 1829 (*rev, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NBO600
Caughey, B. *et al., Magn. Reson. Chem.*, 1989, **27**, 403 (*pmr*)
Shepherd, M.J. *et al., Food Contaminants: Sources and Surveillance*, Royal Society of Chemistry, 1991, 143 (*anal, rev*)
Riddell, F.G. *et al., Tetrahedron*, 1991, **47**, 10109 (*pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 522
Brimble, M.A. *et al., Tetrahedron*, 1999, **55**, 7661-7706 (*rev, synth*)

Narceine N-15

[131-28-2]
6-[[6-[2-(Dimethylamino)ethyl]-4-methoxy-1,3-benzodioxol-5-yl]acetyl]-2,3-dimethoxybenzoic acid, 9CI



$C_{23}H_{27}NO_8$ 445.468
Alkaloid from *Papaver somniferum* (opium poppy). Cryst. (MeOH/Et_2O or H_2O). Mp 176-178° (trihydrate) Mp 145° (anhyd.). pK_{a1} 3.5; pK_{a2} 9.3 (15°). Log P -1.79 (uncertain value) (calc).

▶ YX5210000

Hydrochloride:
Mp 192-193°.

Picrate:
Mp 195°.

N-*Me:*
Mp 207° (as iodide).

N-*De-Me:* [483-89-6] ***Nornarceine****. Oxynarcotine*
$C_{22}H_{25}NO_8$ 431.441
Alkaloid from *Papaver somniferum* (opium poppy). Cryst. (EtOH). Mp 229° (223-225°). Prob. artifact of demethylation of Narcotine λ_{max} 209 (ε 55700); 230 (sh) (ε 22000); 273 (ε 14500) (EtOH).

1-Oxo: [125187-48-6] ***Narceinone***
$C_{23}H_{25}NO_9$ 459.452
Alkaloid from unlanced dried capsules of *Papaver somniferum* (opium poppy). Cryst. (MeOH). Mp 162°.

8-Demethoxy: [31971-15-0] **N-*Methylhydrasteine***
$C_{22}H_{25}NO_7$ 415.442
Cryst. (EtOH, H_2O or $CHCl_3$/MeOH). Mp 146-147° Mp 150° (hydrate) Mp 223°. Poss. artifact. A uv spectrum has been reported but contains a typographical error. See also Coryrutine.

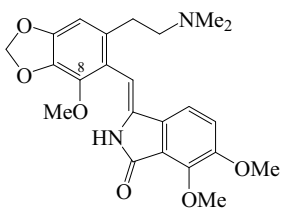
8-Demethoxy, 1-oxo: [41515-85-9] **N-*Methyloxohydrasteine***
$C_{22}H_{23}NO_8$ 429.426
Cryst. ($CHCl_3$/MeOH, H_2O or MeOH). Mp 234-235° Mp 203° (hydrate) Mp 168° (MeOH solvate). See also.

8-Demethoxy, 1-oxo, Et ester: [144525-63-3] ***Papracine***
$C_{24}H_{27}NO_8$ 457.479

Rabe, P. *et al., Annalen*, 1910, **377**, 223-258 (*struct, bibl*)
Addinall, C.R. *et al., J.A.C.S.*, 1933, **55**, 1202-1209; 2153-2163 (*isol, synth*)
Briggs, L.H. *et al., Anal. Chem.*, 1957, **29**, 904-911 (*ir*)
Klötzer, W. *et al., Monatsh. Chem.*, 1972, **103**, 1210-1212 (*Nornarceine, synth, uv, ir, pmr*)
Forgacs, P. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1973, **276**, 105-108; 1974, **279**, 855-857 (*N-Methylhydrasteine, N-Methyloxohydrasteine*)
Blaskó, G. *et al., J.O.C.*, 1982, **47**, 880-885 (*synth, uv, pmr*)
Chaudhuri, P.K. *et al., Phytochemistry*, 1989, **28**, 2002-2003 (*Narceinone*)
Atta-ur-Rahman, *et al., Fitoterapia*, 1992, **63**, 129-135 (*Papracine*)
Rucker, G. *et al., Phytochemistry*, 1994, **36**, 519-523 (*N-Methylhydrasteine methyl ester*)
Baggio, R. *et al., Acta Cryst. C*, 1996, **52**, 703-705 (*cryst struct*)

Narceine imide N-16

[38952-67-9]
*3-[[6-[2-(Dimethylamino)ethyl]-4-methoxy-1,3-benzodioxol-5-yl]methylene]-2,3-dihydro-6,7-dimethoxy-1*H*-isoindol-1-one, 9CI*



(*Z*)-*form*

$C_{23}H_{26}N_2O_6$ 426.468

(*E*)-*form* [75794-87-5]
Cryst. (Me_2CO/cyclohexane). Mp 142-144°.

(*Z*)-*form* [55968-77-9]
Alkaloid from *Papaver somniferum* (opium poppy). Cryst. (Me_2CO). Mp 151-152°. May be an artifact of work-up.

Hydrochloride:
Cryst. (H_2O). Mp 239-240° Mp 249-251°.

Picrate:
Cryst. (EtOH). Mp 249-251°.

N-*Oxide:* [75794-90-0]
Cryst. (Me_2CO aq.). Mp 158-159°.

(ξ)-*form*

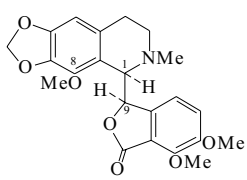
8-Demethoxy: [30341-98-1] ***Fumaridine***. *Hydrastine imide*
$C_{22}H_{24}N_2O_5$ 396.442
Mp 191°. May be an artifact of work-up.

8-Demethoxy, picrate:
Mp 204-205°.

Hodková, J. *et al., J. Nat. Prod.*, 1972, **35**, 61 (*isol, ir, uv, pmr, synth*)
Shamma, M. *et al., Chem. Comm.*, 1975, 89 (*Fumaridine, uv, ir, pmr, struct*)
Trojánek, J. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 681 (*synth, uv, ir*)
Proksa, B. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 2125 (*uv, ir, ms, struct*)
Hussain, S.F. *et al., J. Nat. Prod.*, 1981, **44**, 169 (*Fumaridine, isol, pmr, ms*)

Narcotine N-17

6,7-Dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl)-1(3H)-isobenzofuranone, 9CI. ***Noscapine, BAN, INN***. *Anarkotin. Gnoscopine. Opianine. Tusscapine. NSC 5366. Many other names*



(1*R*,9*R*)-*form*

$C_{22}H_{23}NO_7$ 413.426
pK_a 5.86 (24°).

(1*R*,9*R*)-*form* [3860-46-6]
(-)-β-Narcotine
Mp 181-182° (176°). $[\alpha]_D^{22}$ -100 (c, 1 in dioxan). $[\alpha]_D^{20}$ -87.5 (c, 1 in $CHCl_3$).
► LD_{50} (mus, orl) 840 mg/kg. NP7224500

(1*R*,9*S*)-*form* [128-62-1]
(-)-α-Narcotine. Longatin
Alkaloid from *Papaver somniferum* (opium poppy). Stout needles (EtOH). Mp 176°. $[\alpha]_D$ -200 ($CHCl_3$). Log P 2.74 (uncertain value) (calc). Polymorphic. This is prob. the only nat. occurring stereoisomer but it readily epimerises to (-) β-Narcotine which may be isol. as an artifact. Opt. rotn. highly solv. and concn. dependent λ_{max} 209 (ε 72500); 291 (ε 4000); 309 (ε 4900) (EtOH) (Berdy).
► LD_{50} (mus, ivn) 83 mg/kg. LD_{50} (rat, orl) 1520 mg/kg. Mutagenic props.. RD2625000

Hydrochloride: [912-60-7]
► LD_{50} (mus, orl) 853 mg/kg. Mutagenic props.. NP7225000

Picrate:
Mp 174°.

N-*Oxide:*
Hygroscopic solid. V. sol. H_2O. $[\alpha]_D$ +135 ($CHCl_3$).

O^8-*De-Me:* [521-40-4] ***Narcotoline***
$C_{21}H_{21}NO_7$ 399.399
Alkaloid from straw of *Papaver somniferum* (opium poppy). Rods (MeOH aq.). Mp 202° (189°). $[\alpha]_D$ -189 ($CHCl_3$).

O^8-*De-Me, Ac:*
Mp 208-209°.

(1*S*,9*R*)-*form* [35933-64-3] *(+) α-Narcotine*
Cryst. (EtOH). $[\alpha]_D$ +199.9.

N-*Me:****(+)*-N-*Methyl-α-narcotine***
$C_{23}H_{26}NO_7^{\oplus}$ 428.461

N-*Me, iodide:* [51606-51-0]
$C_{23}H_{26}INO_7$ 555.365
Amorph. $[\alpha]_D$ +42 (c, 0.16 in MeOH).

(1*RS*,9*RS*)-*form* [35933-63-2] *(±)-β-Narcotine. β-Gnoscopine*
Cryst. (EtOH). Mp 184-186° (180°).

Hydrochloride:
Mp 224-226°. Epimerises readily.

(1*RS*,9*SR*)-*form* [6035-40-1] *(±) α-Narcotine. α-Gnoscopine*
Formed in opium, prob. as an artifact. Cryst. (EtOH). V. spar. sol. EtOH. Mp 230-233° (227-230°).
► LD_{50} (rat, ipr) 750 mg/kg. QN5600000

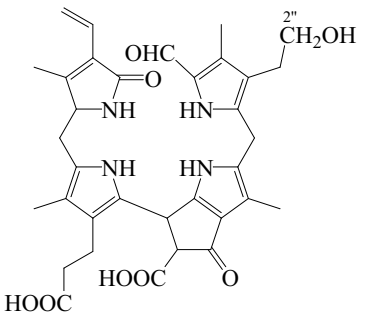
Hydrochloride:
Cryst. + $3H_2O$. Mp 220° Mp 238°.

Picrate:
Mp 188° (185°).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1304B (*nmr*)
Robiquet, M. *et al., Ann. Chim. (Paris)*, 1817, **5**, 275 (*isol*)
Perkin, W.H. *et al., J.C.S.*, 1911, **99**, 775 (*synth, resoln*)
Ohta, M. *et al., Tet. Lett.*, 1963, 859 (*abs config*)
Ohta, M. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1080 (*isol*)
Battersby, A.R. *et al., J.C.S.*, 1965, 1087 (*abs config*)
Snatzke, G. *et al., Tetrahedron*, 1969, **25**, 5059 (*ord*)
Analyst (London), 1972, **97**, 740 (*microanal*)
Kametani, T. *et al., J.C.S. Perkin 1*, 1977, 374 (*synth*)
Al-Yahya, M.A. *et al., Anal. Profiles Drug Subst.*, 1982, **11**, 407 (*rev, synth, props, anal*)
Blaskó, G. *et al., J. Nat. Prod.*, 1982, **45**, 105 (*occur*)
Shono, T. *et al., J.O.C.*, 1983, **48**, 1621 (*synth*)
Moss, D.S. *et al., Acta Cryst. C*, 1984, **40**, 1960 (*cryst struct*)
Johansson, M. *et al., J. Chromatogr.*, 1988, **459**, 301 (*hplc*)
Sariyar, G. *et al., J. Nat. Prod.*, 1990, **53**, 1302 (*N-Methyl-α-narcotine*)
Janssen, R.H.A.M. *et al., Phytochemistry*, 1990, **29**, 3331 (*pmr, cmr, conformn*)
Porter, R. *et al., Mutagenesis*, 1992, **7**, 205
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 750
Tiveron, C. *et al., Mutagenesis*, 1993, **8**, 311
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 8884 (*synonyms*)
Baradarani, M.M. *et al., Tet. Lett.*, 1999, **40**, 7403-7406 (*epimerisation*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NBP275; NOA000; NOA500

Bn-NCC-3 N-18

[173740-48-2]
Brassica napus *Non-fluorescent chlorophyll catabolite 3*



$C_{34}H_{38}N_4O_8$ 630.696
Isol. from rape cotyledons. Solid (as di-K salt).

2″-O-β-D-Glucopyranoside: [173740-47-1]
Bn-*NCC-2*
$C_{40}H_{48}N_4O_{13}$ 792.838
Isol. from rape cotyledons. Solid (as di-K salt).

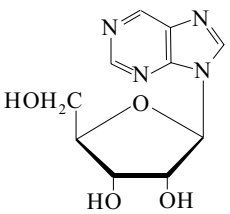
2″-O-Malonyl: [152571-56-7]

[173740-46-0] **Bn-*NCC-1***
$C_{37}H_{40}N_4O_{11}$ 716.743
Isol. from rape cotyledons. Solid (as tri-K salt).

Muehlecker, W. *et al., Helv. Chim. Acta*, 1993, **76**, 2976 (*isol, pmr, cmr, ms*)
Muehlecker, W. *et al., Plant Physiol. Biochem. (Paris)*, 1996, **34**, 61 (*isol*)

Nebularine N-19

[550-33-4]
9-β-D-Ribofuranosyl-9H-purine, 9CI, 8CI. Purinosine



$C_{10}H_{12}N_4O_4$ 252.229
Nucleoside antibiotic. Isol. from the mushroom *Clitocybe nebularis* (clouded agaric). Needles (MeOH). Mp 182-183°. $[\alpha]_D^{35}$ -46.8 (c, 2.0 in H_2O). λ_{max} 262.5 (ε 7 020) (H_2O), 262.8 (5 900) (1*M* HCl), 263 nm (7 110) (pH 9.2).
► LD_{50} (rat, scu) 220 mg/kg. UO9100000

2′,3′,5′-Tri-Ac: [15981-63-2]
$[\alpha]_D^{26}$ -10.8 (c, 1.5 in MeOH).

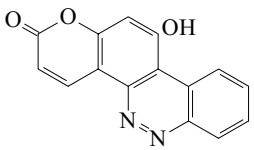
6-Fluoro: See 6-Fluoro-9-ribofuranosyl-9*H*-purine in *The Combined Chemical Dictionary.*

Isono, K. *et al., J. Antibiot., Ser. A*, 1960, **13**, 270-272 (*isol*)
Cory, J.G. *et al., Biochemistry*, 1965, **4**, 1729-1732 (*pharmacol*)
Iwamura, H. *et al., J.O.C.*, 1968, **33**, 1796-1799 (*synth, tri-Ac*)

Takeda, T. *et al., Acta Cryst. B*, 1974, **30**, 825-827 (*cryst struct*)
Ohno, M. *et al., J.A.C.S.*, 1974, **96**, 4326-4327 (*tri-Ac*)
Chenon, M.T. *et al., J.A.C.S.*, 1975, **97**, 4627-4636 (*cmr*)
Westhof, E. *et al., Z. Naturforsch., C*, 1975, **30**, 131-140 (*pmr*)
Gupta, P.K. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 534-537 (*synth*)
Zavgorodnii, S.G. *et al., Bioorg. Khim.*, 1984, **10**, 1496-1507 (*conformn*)
Nair, V. *et al., Synthesis*, 1984, 401-402 (*synth, uv, pmr, cmr, ms*)
Cooper, R. *et al., J. Ind. Microbiol.*, 1986, **1**, 275-276 (*isol*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711-1739 (*rev*)
Nair, V. *et al., Tetrahedron*, 1988, **44**, 7001-7006 (*derivs*)
Worner, K. *et al., Helv. Chim. Acta*, 1999, **82**, 2094-2104 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RJF000

Necatorine N-20

[89915-35-5]
*11-Hydroxy-2*H*-benzo[*c*]pyrano[2,3-*h*]cinnolin-2-one, 9CI*



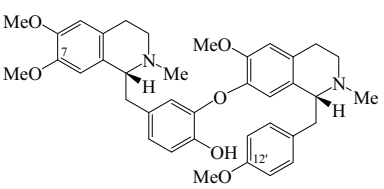
$C_{15}H_8N_2O_3$ 264.24
Alkaloid from the mushroom *Lactarius necator*. Cryst. Mp 220-225°. *L. necator* is considered edible in some countries e.g. Finland, however necatorin is only partially deactivated under cooking conditions.

▶ Highly mutagenic. DJ2622000

Suortti, T. *et al., J. Chromatogr.*, 1983, **255**, 529; 1984, **301**, 303-307 (*isol*)
Suortti, T. *et al., Phytochemistry*, 1983, **22**, 2873 (*pmr, ms, struct*)
Suortti, T. *et al., Food Chem. Toxicol.*, 1984, **22**, 579-581 (*stability*)

Neferine N-21

[2292-16-2]
12′-O-*Methylliensinine*



$C_{38}H_{44}N_2O_6$ 624.775
Alkaloid from the seed embryo of *Nelumbo nucifera* (East Indian lotus). Oil. $[\alpha]_D^{28}$ -37.8 (c, 1.43 in $CHCl_3$). $[\alpha]_D^{27}$ -100 (c, 0.24 in MeOH).

▶ Tumour promotor. SM9495000

Me ether, styphnate:
Mp 139-140° (133-135°). $[\alpha]_D^{29}$ -93.3 (c, 0.6 in Me_2CO) (-81.5).

Methiodide:
Mp 179-181°.

O⁷-De-Me: [6817-41-0] ***Isoliensinine***
$C_{37}H_{42}N_2O_6$ 610.749
Alkaloid from the seed embryo of *Nelumbo nucifera* (East Indian lotus). Oil. $[\alpha]_D^{22}$ +49.3 (Me_2CO). $[\alpha]_D^{29}$ -43.3 ($CHCl_3$).

▶ Tumour promotor.

O⁷-De-Me; hydrochloride (1:2):
Cryst. + $4H_2O$. Mp 185-186°.

O⁷-De-Me; perchlorate (1:2):
Cryst. + $1H_2O$. Mp 200-203°. $[\alpha]_D^{22}$ -70 (Me_2CO).

O¹²′-De-Me: [2586-96-1] ***Liensinine***
$C_{37}H_{42}N_2O_6$ 610.749
Alkaloid from seed embryo of *Nelumbo nucifera* (East Indian lotus). Mp 95-99°. $[\alpha]_D^{31}$ +15.85 (c, 0.883 in Me_2CO).

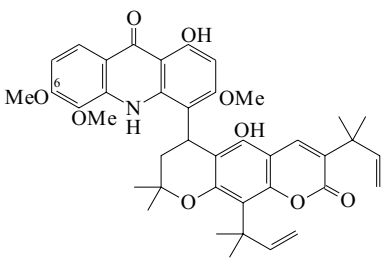
O¹²′-De-Me; perchlorate (1:2):
Mp 212-214°.

O¹²′-De-Me, di-Ac:
Mp 124°.

Chao, Y.C. *et al., Sci. Sin. (Engl. edn.)*, 1962, **11**, 215; *CA*, **57**, 7383i (*isol, Liensinine*)
Hsieh, Y.Y. *et al., Sci. Sin. (Engl. edn.)*, 1964, **12**, 2018; *CA*, **62**, 9183h (*abs config, Liensinine*)
Tomita, M. *et al., Tet. Lett.*, 1964, 2637 (*Isoliensinine*)
Furukawa, H. *et al., Yakugaku Zasshi*, 1965, **85**, 335; 353; *CA*, **63**, 4351ad (*isol, ir, pmr, struct*)
Yang, T.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1970, **17**, 235; *CA*, **74**, 100254g (*isol, uv, ir, pmr*)
Kametani, T. *et al., J. Het. Chem.*, 1970, **7**, 181 (*isol, pmr*)

Neoacrimarine A N-22

[149301-45-1]



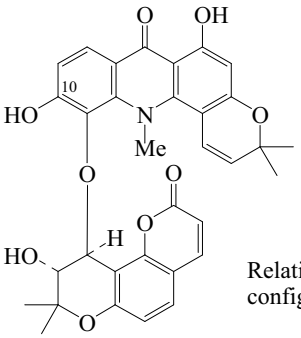
$C_{40}H_{43}NO_9$ 681.781
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisii*) × Dancy tangerine (*Citrus tangerina*)] (Rutaceae). Yellow cubes (Me_2CO). Mp 225-230°. $[\alpha]_D$ 0 ($CHCl_3$).

O⁶-De-Me: [149301-47-3] ***Neoacrimarine B***
$C_{39}H_{41}NO_9$ 667.754
Alkaloid from Yalaha. Yellow cubes (Me_2CO). Mp 240-243°. $[\alpha]_D$ 0 (Py).

Takemura, Y. *et al., Heterocycles*, 1993, **36**, 675 (*isol, uv, ir, pmr, cmr, struct*)

Neoacrimarine C N-23

[155519-79-2]



Relative configuration

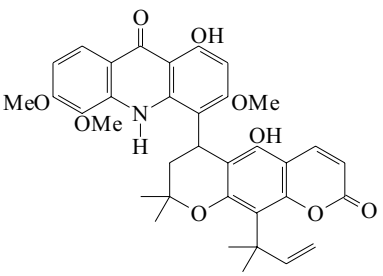
$C_{33}H_{29}NO_9$ 583.593
Yellow cubes. Mp 111-113°. $[\alpha]_D$ +42.3 (c, 0.026 in $CHCl_3$).

10-Deoxy: [217199-06-9] ***Neoacrimarine H***
$C_{33}H_{29}NO_8$ 567.594
Alkaloid from the roots of *Citrus paradisi* (grapefruit). Yellow oil. $[\alpha]_D$ +80.6 (c, 0.07 in $CHCl_3$). λ_{max} 204 ; 265 ; 286 ; 294 (sh) ; 318 ; 343 (sh) ; 410 (MeOH).

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1757-1759; 1998, **46**, 1518-1521 (*isol, uv, ir, pmr, cmr, ms, struct*)

Neoacrimarine E N-24

[158182-13-9]

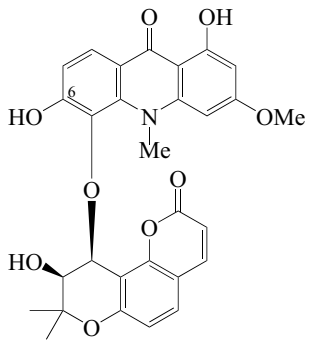


$C_{35}H_{35}NO_9$ 613.663
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisi*) and Dancy tangerine (*Citrus tangerina*)] (Rutaceae). Yellow cubes (Me_2CO). Mp 212-215°. $[\alpha]_D$ -21.6 (c, 0.3 in $CHCl_3$).

Takemura, Y. *et al., Heterocycles*, 1994, **38**, 1937 (*isol, uv, ir, pmr, cmr, ms, struct*)

Neoacrimarine F N-25

[195057-36-4]



$C_{29}H_{25}NO_9$ 531.518

Alkaloid from the roots of *Citrus paradisi* (grapefruit) x *Citrus tangerina* (tangerine). Yellow cubes. Mp 218-220°. $[\alpha]_D$ +130.9 (c, 0.2 in MeOH). λ_{max} 220 (sh) ; 264 ; 295 (sh) ; 330 ; 369 (EtOH).

N-*De-Me:* [217199-08-1] ***Neoacrimarine J***
$C_{28}H_{23}NO_9$ 517.491
Alkaloid from the roots of *Citrus paradisi* (grapefruit). Yellow oil. $[\alpha]_D$ -131.9 (c, 0.05 in $CHCl_3$). λ_{max} 203 ; 218 (sh) ; 263 ; 292 (sh) ; 327 ; 373 (sh) (MeOH).

6-Me ether, N-*de-Me:* [217199-07-0] ***Neoacrimarine I***
$C_{29}H_{25}NO_9$ 531.518
Alkaloid from the roots of *Citrus paradisi* (grapefruit). Yellow oil. $[\alpha]_D$ -157.3 (c, 0.27 in $CHCl_3$). λ_{max} 205 ; 255 (sh) ; 266 ; 292 (sh) ; 326 ; 381 (MeOH).

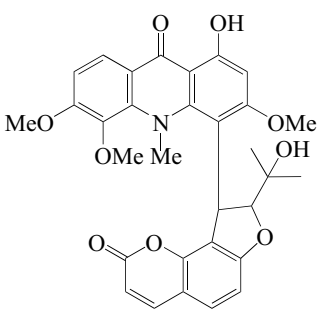
6-Deoxy: [195057-37-5] ***Neoacrimarine G***
$C_{29}H_{25}NO_8$ 515.518
Alkaloid from the roots of *Citrus paradisi* (grapefruit). Yellow oil. $[\alpha]_D$ +130.2 (c, 0.03 in $CHCl_3$). λ_{max} 220 (sh) ; 262 ; 280 (sh) ; 315 ; 324 (MeOH).

Takemura, Y. *et al., Heterocycles*, 1997, **45**, 1411-1414 (*isol, uv, ir, pmr, cmr, ms*)

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1518-1521 (*isol, uv, ir, pmr, cmr, ms*)

Neoacrimarine K N-26

[217199-09-2]



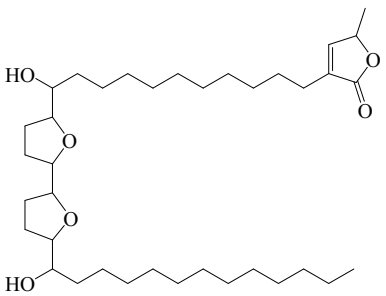
$C_{31}H_{29}NO_9$ 559.571

Alkaloid from the roots of *Citrus paradisi* (grapefruit). Yellow oil. Racemic λ_{max} 204 ; 222 (sh) ; 261 (sh) ; 269 ; 334 ; 393 (MeOH).

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1518-1521 (*isol, uv, ir, pmr, cmr, ms*)

Neoannonin B N-27

[170312-94-4]

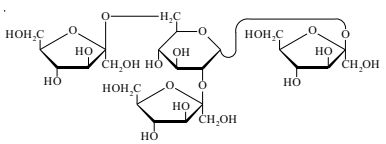


$C_{37}H_{66}O_6$ 606.925

Constit. of the seeds of *Annona squamosa* (sugar apple).

Zheng, X.-C. *et al., Zhiwu Xuebao*, 1995, **37**, 238-243

Neobifurcose N-28



$C_{24}H_{42}O_{21}$ 666.583

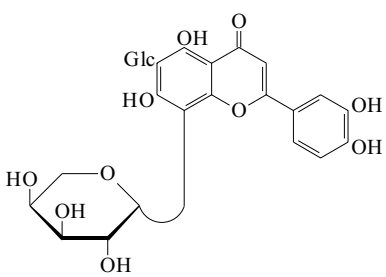
Struct. not confirmed. A trifructosyl glucose with the prob. struct. shown. Isol. from cereals. $[\alpha]_D^{20}$ +14.4 (H_2O).

Schlubach, H.H. *et al., Annalen*, 1958, **614**, 126; 1961, **647**, 41

Neocarlinoside N-29

[83151-89-7]

*8-β-L-Arabinopyranosyl-2-(3,4-dihydroxyphenyl)-6-β-D-glucopyranosyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. 8-β-L-Arabinopyranosyl-6-β-D-glucopyranosyl-3′,4′,5,7-tetrahydroxyflavone. 8-Arabinopyranosyl-6-glucopyranosylluteolin. 8-Arabinosyl-6-glucosylluteolin*



$C_{26}H_{28}O_{15}$ 580.498

Isol. from *Oryza sativa* (rice). Also see Carlinoside.

Linard, A. *et al., Phytochemistry*, 1982, **21**, 797 (*isol*)

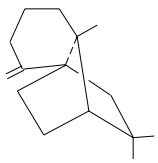
Besson, E. *et al., Phytochemistry*, 1985, **24**, 1061 (*isol*)

Ulubelen, A. *et al., Rev. Latinoam. Quim.*, 1985, **16**, 63 (*isol*)

β-Neoclovene N-30

[56684-96-9]

*Octahydro-2,2,7*a*-trimethyl-4-methylene-1,3*a*-ethano-3*a*H-indene, 9CI*



$C_{15}H_{24}$ 204.355

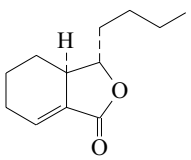
Constit. of ginseng. Flavouring ingredient. $[\alpha]_D^{25}$ -30 (MeOH).

Yoshihara, K. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2078 (*isol, struct*)

Neocnidilide N-31

[4567-33-3]

*3-Butyl-3*a*,4,5,6-tetrahydro-1(3*H*)-isobenzofuranone, 9CI. Sedanolide*



Absolute configuration

$C_{12}H_{18}O_2$ 194.273

Identity with Sedanolide apparently not certain. Constit. of celery oil. Cryst. (hexane). Mp 34.5-35° (24-27°). Bp_4 147-148° $Bp_{0.4}$ 112°. $[\alpha]_D$ -74.7 ($CHCl_3$).

Mitsuhashi, H. *et al., Tetrahedron*, 1964, **20**, 1971 (*struct*)

Nagai, U. *et al., Tetrahedron*, 1965, **21**, 1433

Cocker, W. *et al., J.C.S.(C)*, 1966, 1152 (*synth*)

Yamagishi, T. *et al., Yakugaku Zasshi*, 1977, **97**, 237 (*isol*)

Suzuki, H. *et al., Agric. Biol. Chem.*, 1987, **51**, 3369 (*synth, abs config*)

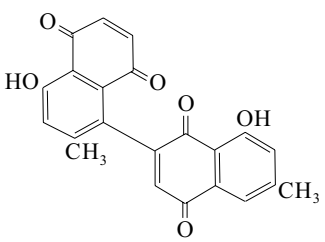
Tanaka, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 2253 (*synth*)

Jiao, X.Z. *et al., Chin. Chem. Lett.*, 2003, **14**, 127-129 (*synth*)

Neodiospyrin N-32

[33916-25-5]

4,8′-Dihydroxy-2,6′-dimethyl[1,2′-binaphthalene]-1′,4′,5,8-tetrone, 9CI



$C_{22}H_{14}O_6$ 374.349

Isol. from roots of *Diospyros kaki* (Japanese persimmon). Orange cryst. Mp 218° (synthetic).

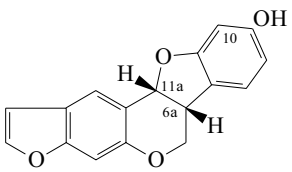
Di-Me ether: [58274-96-7]
Cryst. Mp 245-247°.

Tezuka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2029 (*isol*)

Sankaram, A.V.B. *et al., Tet. Lett.*, 1975, 3627 (*isol*)
Lillie, T.J. *et al., J.C.S. Perkin 1*, 1977, 355 (*struct*)
Kumari, L.K. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 619 (*struct, synth*)
bin Zakaria, M. *et al., Phytochemistry*, 1984, **23**, 1481 (*isol*)

Neodunol N-33

[53766-53-3]
*6a,11a-Dihydro-6*H*-benzofuro[3,2-c]furo[3,2-g][1]benzopyran-9-ol, 9CI*



$C_{17}H_{12}O_4$ 280.279

Pterocarpan numbering shown. Isol. from *Pachyrrhizus erosus* (yam bean). Cryst. (C_6H_6/hexane). Mp 170.5-171.5°. $[\alpha]_D^{22}$ -284.9 (c, 0.8 in $CHCl_3$). λ_{max} 246 (ε 27000) (MeOH) (Berdy). λ_{max} 213 ; 241 ; 248 ; 255 ; 294 (EtOH) (Berdy). λ_{max} 216 ; 248 ; 255 ; 301 (EtOH-NaOH) (Berdy).

Me ether: [53833-80-0] ***9-O-Methylneodunol***
$C_{18}H_{14}O_4$ 294.306
Mp 175°. $[\alpha]_D^{25}$ -217 (c, 0.415 in $CHCl_3$). Rare animal source of a flavonoid.

Me ether, 10-methoxy: [76165-15-6] ***Ambonane***
$C_{19}H_{16}O_5$ 324.332
Light-yellow needles (Et_2O/hexane). Mp 125-127°. $[\alpha]_D$ -214 (c, 0.01 in $CHCl_3$).

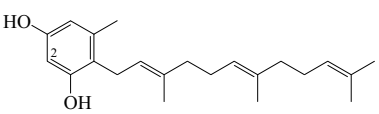
6a,11a-Didehydro: [53766-54-4] ***Neorauteen***. *6*H*-Benzofuro[3,2-c]furo[3,2-g][1]benzopyran-9-ol, 9CI*
$C_{17}H_{10}O_4$ 278.264
Plates (MeOH). Mp 202.5-204°.

6a,11a-Didehydro, Ac:
Needles. Mp 197.5-199°.

Brink, A.J. *et al., Phytochemistry*, 1972, **16**, 273 (*isol*)
Brink, A.J. *et al., Phytochemistry*, 1974, **13**, 1581 (*Neorauteen*)
Chalmers, A.A. *et al., Tetrahedron*, 1977, **33**, 1735-1737 (*cmr*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1979, **34**, 683 (*isol*)
Breytenbach, J.C. *et al., J.C.S. Perkin 1*, 1980, 1804 (*Ambonane*)
Sanduja, R. *et al., J. Het. Chem.*, 1984, **21**, 845 (*isol, deriv, cryst struct, abs config*)

Neogrifolin N-34

[23665-96-5]
5-Methyl-6-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,3-benzenediol



$C_{22}H_{32}O_2$ 328.494

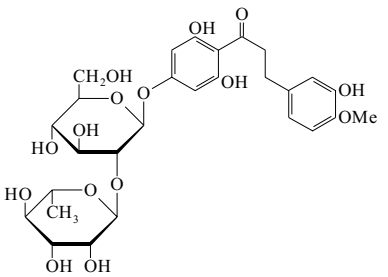
Numbering systems vary. Constit. of *Albatrellus ovinus*. Red-brown oil. λ_{max} 282 (ε 3890) (MeOH) (Derep). λ_{max} 275 ; 281 ; 282 (ε 4080) (MeOH) (Berdy).

2-Hydroxy:5-Methyl-4-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,2,3-benzenetriol. ***3-Hydroxyneogrifolin***
$C_{22}H_{32}O_3$ 344.493
Constit. of *Albatrellus ovinus*. Amorph. powder. λ_{max} 210 (log ε 4.6); 276 (log ε 2.76) (EtOH).

Misasa, H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1660 (*Neogrifolin*)
Nukata, M. *et al., Phytochemistry*, 2002, **59**, 731-737 (*3-Hydroxyneogrifolin*)

Neohesperidin dihydrochalcone N-35

[20702-77-6]
Neohesperidin DHC. E959. FEMA 3811. NHDHC. NHDC



$C_{28}H_{36}O_{15}$ 612.583

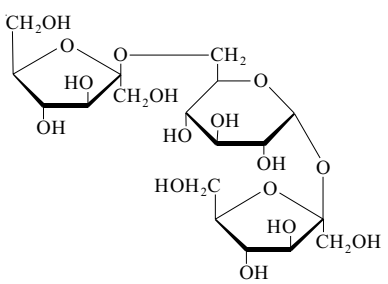
Intensely sweet, 612 times more sweet than sucrose. ADI 5 mg/kg (1987). Permitted in EU at low concs. (=10 ppm) for certain applications, e.g. low-alcohol beer. Generally recognised as safe (GRAS) in the USA. Practical use limited by slow development of taste sensation and peculiar aftertaste. Analogues extensively studied.

▶ LZ5785000

Horowitz, R.M. *et al., J. Agric. Food Chem.*, 1969, **17**, 696 (*rev*)
DuBois, G.E. *et al., J. Med. Chem.*, 1981, **24**, 408
Lina, B.A.R. *et al., Food Chem. Toxicol.*, 1990, **28**, 507 (*tox*)
Bär, A. *et al., Lebensm.-Wiss. Technol.*, 1990, **23**, 371 (*rev, prop*)

Neokestose N-36

[3688-75-3]
O-β-D-Fructofuranosyl-(2→6)-α-D-glucopyranosyl β-D-fructofuranoside. β-D-Fructofuranosyl 6-O-β-D-fructofuranosyl-α-D-glucopyranoside, 8CI. neo-*Kestose. 6^G-Kestotriose*



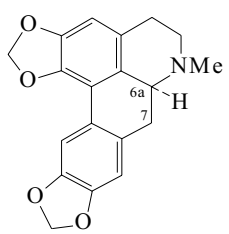
$C_{18}H_{32}O_{16}$ 504.441

A fructan. See Fructans. Isol. from aq. alcoholic extracts of oat stalks. Amorph. $[\alpha]_D^{20}$ +22.2 (c, 2.3 in H_2O).

Gross, D. *et al., J.C.S.*, 1954, 1727 (*synth*)
Schlubach, H.H. *et al., Annalen*, 1961, **647**, 41 (*isol*)
Haq, S. *et al., Can. J. Chem.*, 1961, **39**, 1165 (*isol*)
Gross, D. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 360 (*enzymic synth*)
Kamerling, J.P. *et al., Tetrahedron*, 1972, **28**, 3037 (*pmr*)
Henry, R.J. *et al., Phytochemistry*, 1980, **19**, 1017
De Bruyn, A. *et al., Carbohydr. Res.*, 1991, **211**, 131 (*cmr*)
Liu, J. *et al., Carbohydr. Res.*, 1991, **213**, 43 (*pmr, cmr*)

Neolitsine N-37

1,2:9,10-Bis(methylenedioxy)aporphine



$C_{19}H_{17}NO_4$ 323.348

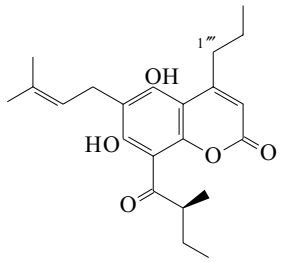
(S)-form [2466-42-4]
Alkaloid from the leaves of *Laurus nobilis* (bay laurel). Needles (Me_2CO). Mp 149-150°. $[\alpha]_D$ +56.5 (c, 1.57 in $CHCl_3$).

N-*De-Me:* [41787-55-7] ***Cryptodorine***. *1,2:9,10-Bismethylenedioxynoraporphine. Norneolitsine*
$C_{18}H_{15}NO_4$ 309.321
Alkaloid from the leaves of *Laurus nobilis* (bay laurel). Unstable cryst.; cryst. + $2H_2O$ (as sulfate). Mp 219-221° (sulfate). $[\alpha]_D^{19}$ +61 ($CHCl_3$).

Hui, W.H. *et al., J.C.S.*, 1965, 2285 (*isol, uv, ir, pmr, ms, struct*)
Cava, M.P. *et al., J.O.C.*, 1968, **33**, 2443 (*isol, uv*)
Bick, I.R.C. *et al., Bull. Soc. Chim. Fr.*, 1972, 4596 (*isol, uv, pmr, ms, struct, Cryptodorine*)
Moltrasio, G.Y. *et al., J.C.S. Perkin 1*, 1973, 349 (*synth, uv*)
Pai, B.R. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 1042 (*synth, uv, pmr, ms, Cryptodorine*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80 (*cd*)
Pech, B. *et al., J. Nat. Prod.*, 1982, **45**, 560 (*isol*)

Neomammein N-38

[37975-64-7]
*5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 9CI. 5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methylbutyryl)-4-propylcoumarin, 8CI. Mammea B/BB*



$C_{22}H_{28}O_5$ 372.46

(*S*)-*form* [5022-20-8]
Constit. of *Mammea americana* (mamey) seeds. Needles (hexane). Mp 122°. $[\alpha]_D^{25}$ -2.93 (c, 4.34 in $CHCl_3$).

1‴-Hydroxy: [188817-90-5] ***Assamene***
$C_{22}H_{28}O_6$ 388.46
Plates ($CHCl_3$/EtOAc). Mp 135°. $[\alpha]_D^{31}$ +38 (c, 0.4 in $CHCl_3$). Abs. config. not determined λ_{max} 203 ; 220 ; 248 ; 330 ; 372 (MeOH). λ_{max} 203 ; 220 ; 248 ; 330 ; 372 (MeOH) (Berdy). λ_{max} 220 ; 295 ; 325 (MeOH-HCl) (Berdy).

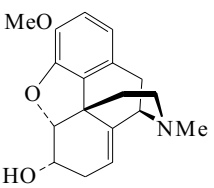
1‴-Acetoxy: [26477-65-6]

[111321-12-1] ***Mammea ElBB***
$C_{24}H_{30}O_7$ 430.497
Isol. from seeds of *Mammea americana* (mamey). Mp 50-53°. $[\alpha]_D^{24}$ -28.5 (EtOH). Abs. config. not detd..

Crombie, L. *et al., J.C.S.(C)*, 1967, 2545 (*isol, ir, uv, pmr, ms*)
Carpenter, I. *et al., J.C.S.(C)*, 1971, 3783; 1972, 2259 (*isol, uv, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317; 345 (*synth*)
Begley, M.J. *et al., J.C.S. Perkin 1*, 1987, 353 (*abs config*)
Bordoloi, M. *et al., Phytochemistry*, 1997, **44**, 939 (*Assamene*)

Neopine N-39

[467-14-1]
8,14-Didehydro-4,5-epoxy-3-methoxy-17-methylmorphinan-6-ol, 9CI. β-Codeine



Absolute configuration

$C_{18}H_{21}NO_3$ 299.369
Minor alkaloid of opium (*Papaver somniferum*). Long needles (cyclohexane). Mp 127.5-127.8°. $[\alpha]_D^{26}$ -28.1 (c, 7.7 in $CHCl_3$).

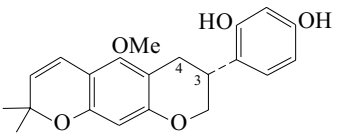
Hydrobromide:
Cryst. (H_2O). Mod. sol. H_2O. Mp 280-285° dec. (darkens at 240°). $[\alpha]_D^{20}$ +17.1 (c. 5.2 in H_2O).

Sulfate:
Cryst. (Me_2CO). Sol. EtOH; v. sol. H_2O. Mp 166-167° dec. $[\alpha]_D^{28}$ +16.4 (c, 3 in H_2O). Slowly dec. in air.

Homeyer, A.H. *et al., J.O.C.*, 1947, **12**, 356 (*isol*)
Small, L. *et al., J.O.C.*, 1947, **12**, 359 (*struct*)
Conroy, H. *et al., J.A.C.S.*, 1955, **77**, 5960 (*synth*)
Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1964, **53**, 1549 (*glc, tlc*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1965, **18**, 1799 (*pmr*)
Weiss, U. *et al., Bull. Soc. Chim. Fr.*, 1965, 3707 (*ord*)
Wheeler, D.M.S. *et al., J.A.C.S.*, 1967, **89**, 4494 (*ms*)
Kuppers, F.J.E.M. *et al., Phytochemistry*, 1976, **15**, 443 (*isol*)

Neorauflavane N-40

[53734-74-0]
4-(3,4-Dihydro-5-methoxy-8,8-dimethyl-2H,8H-benzo[1,2-b:5,4-b′]dipyran-3-yl)-1,3-benzenediol, 9CI



$C_{21}H_{22}O_5$ 354.402

Di-Me ether: [53354-51-1]
Cryst. (C_6H_6/hexane). Mp 132.9°. $[\alpha]_D^{22}$ -7.78 (c, 0.2 in $CHCl_3$).

3,4-Didehydro: [53734-75-1] ***Neorauflavene***
$C_{21}H_{20}O_5$ 352.386
Oil (as di-Me ether).

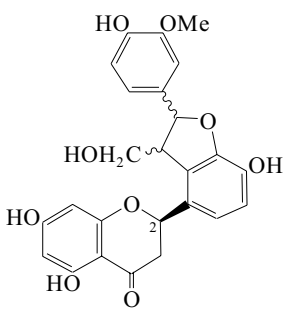
Demethoxy: [406676-62-8] ***Eryvarin C***
$C_{20}H_{20}O_4$ 324.376
Oil. $[\alpha]_D$ +35 (c, 0.1 in MeOH). λ_{max} 204 (log ϵ 4.58); 222 (log ϵ 4.61); 277 (log ϵ 4.06); 311 (log ϵ 3.93) (MeOH).

5-Demethoxy, 4′-Me ether: [160825-65-0] ***Gancaonin X***
$C_{21}H_{22}O_4$ 338.402
Constit. of *Glycyrrhiza uralensis* (Chinese licorice).

Brink, A.J. *et al., Tetrahedron*, 1974, **30**, 311-314 (*isol, di-Me ether*)
Fukai, T. *et al., Nat. Med. (Tokyo)*, 1994, **48**, 203-207 (*Gancaonin X*)
Tanaka, H. *et al., Heterocycles*, 2001, **55**, 2341-2347 (*Eryvarin C*)

Neosilyhermin A N-41

[96291-04-2]



$C_{25}H_{22}O_9$ 466.443
Constit. of *Silybum marianum* (milk thistle). $[\alpha]_D^{26}$ +99 (c, 0.19 in MeOH).

Penta-Ac:
Mp 95-97°. $[\alpha]_D^{26}$ +34.8 (c, 0.315 in $CHCl_3$).

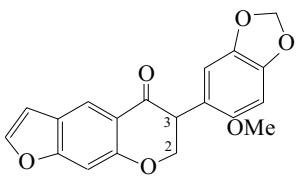
2-Epimer: [96238-87-8] ***Neosilyhermin B***
$C_{25}H_{22}O_9$ 466.443
Constit. of *Silybum marianum* (milk thistle).

2-Epimer, penta-Ac:
Mp 98-100°. $[\alpha]_D^{26}$ +124.8 (c, 0.255 in $CHCl_3$).

Fiebig, M. *et al., Planta Med.*, 1984, **50**, 310

Neotenone N-42

[10091-02-8]
6,7-Dihydro-6-(6-methoxy-1,3-benzodioxol-5-yl)-5H-furo-[3,2-g][1]benzopyran-5-one, 9CI. Neorautenone



$C_{19}H_{14}O_6$ 338.316
Flavonoid numbering shown.

(-)-*form*
Light green-yellow cryst. ($CHCl_3$/MeOH). Mp 152°. $[\alpha]_D^{20}$ -5.5 (c, 0.181 in MeOH).

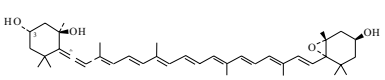
(±)-*form*
Cryst. ($CHCl_3$/MeOH or by subl.). Mp 149° Mp 180° (dimorph.).

2,3-Didehydro: [1242-81-5] ***Dehydroneotenone***
$C_{19}H_{12}O_6$ 336.3
Isol. from *Pachyrrhizus erosus* (yam bean). Cryst. (EtOH). Mp 240-241°.

v. Duuren, B.L. *et al., J.O.C.*, 1961, **26**, 5013 (*isol*)
Crombie, L. *et al., J.C.S.*, 1963, 1569 (*isol*)
Fukui, K. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 2733 (*synth*)
Weber-Schilling, C.A. *et al., Chem. Ber.*, 1971, **104**, 1518 (*synth*)
Oberholzer, M.E. *et al., Tet. Lett.*, 1977, 1165 (*synth*)
van Puyvelde, L. *et al., J. Nat. Prod.*, 1987, **50**, 349 (*isol*)
Phrutivorapongkul, A. *et al., Chem. Pharm. Bull.*, 2002, **50**, 534-537 (*isol, pmr, cmr*)

Neoxanthin N-43

[30743-41-0]
6,7-Didehydro-5′,6′-epoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3,3′,5-triol. Foliaxanthin. Trollixanthin. Trolliflor



$C_{40}H_{56}O_4$ 600.88
Constit. of paprika, lucerne, Valencia orange and other spp.. Light brown-orange cryst. (C_6H_6/Et_2O). Mp 200° (136-139°, 142-145°). $[\alpha]_D^{20}$ +32 ($CHCl_3$). Undergoes thermal isom. into a mixt. of neochromes upon melting. Related to Vaucheriaxanthin λ_{max} 434 ; 464 (MeOH). λ_{max} 437 ; 466 (heptane). λ_{max} 463 ; 493 (CS_2).

3-Ac: [54369-12-9] ***Dinoxanthin***. *Neoxanthin 3-acetate*
$C_{42}H_{58}O_5$ 642.917

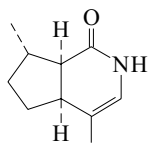
(9′*Z*)-*form* [14660-91-4]
9′-cis-*Neoxanthin*

[52949-72-1, 52949-73-2, 142204-43-1]

Schimmer, B.P. *et al., Biochemistry*, 1966, **5**, 1814; 3649 (*struct*)
de Ville, T.E. *et al., Chem. Comm.*, 1969, 754; 1311 (*struct*)
Cholnoky, L. *et al., J.C.S.(C)*, 1969, 1256 (*isol*)
Nitsche, H. *et al., Z. Naturforsch., C*, 1973, **28**, 641 (*Vaucheriaxanthin*)
Johansen, J.E. *et al., Phytochemistry*, 1974, **13**, 2261; 1980, **19**, 441 (*Dinoxanthin*)
Nitsche, H. *et al., Z. Naturforsch., C*, 1974, **29**, 657 (*synth*)
Buchecker, R. *et al., Phytochemistry*, 1975, **14**, 797 (*struct*)
Swift, I.E. *et al., Phytochemistry*, 1982, **21**, 2859 (*biosynth*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 234 (*bibl*)
Bjoernland, T. *et al., Tet. Lett.*, 1989, **30**, 2577 (*pmr, struct*)
Maerki-Fischer, E. *et al., Helv. Chim. Acta*, 1990, **73**, 1637 (*pmr*)
Baumeler, A. *et al., Helv. Chim. Acta*, 1992, **75**, 773; 1994, **77**, 909 (*synth*)
Strand, A. *et al., J.C.S. Perkin 1*, 2000, 595-598 (*synth*)

Nepetalactam N-44

[115421-73-3]

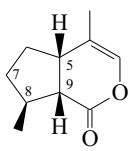


$C_{10}H_{15}NO$ 165.235
Isol. from a commercial sample of catnip oil (*Nepeta cataria*). Cryst. Mp 95-96°. $[\alpha]_D^{25}$ -46.5 (c, 5 in $CHCl_3$). Artifact.

Eisenbraun, E.J. *et al., J.O.C.*, 1988, **53**, 3968-3972 (*isol, uv, ir, pmr, cmr, ms, struct*)

Nepetalactone N-45

*5,6,7,7*a*-Tetrahydro-4,7-dimethylcyclopenta[*c*]pyran-1(4*a*H)-one, 9CI*



(5*S*,8*S*,9*R*)-*form*

$C_{10}H_{14}O_2$ 166.219

(5*S*,8*S*,9*R*)-*form* [21651-62-7]
Constit. of catnip from the catmint plant *Nepeta cataria*. Oil. $[\alpha]_D^{21}$ +37 (c, 27 in $CHCl_3$).

7,8-Didehydro: [66644-99-3] ***Gastrolactone***
$C_{10}H_{12}O_2$ 164.204
Oil. $[\alpha]_D^{24}$ -32.5.

(5*S*,8*S*,9*S*)-*form* [17257-15-7] *Epinepetalactone*
Constit. of *Nepeta cataria* (catnip). Oil. $[\alpha]_D^{21}$ -24.4 (c, 6.2 in $CHCl_3$).

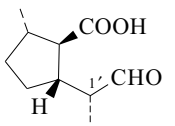
(5*R*,8*S*,9*S*)-*form* [21651-53-6]
Oil. $Bp_{0.1}$ 60°. $[\alpha]_D^{23}$ +81 (c, 0.04 in $CHCl_3$).

(5*R*,8*R*,9*S*)-*form* [105660-81-9]
Oil. $[\alpha]_D^{25}$ -222 (c, 0.84 in $CHCl_3$).

(5*R*,8*S*,9*R*)-*form*
[4581-79-7, 21651-48-9, 108944-20-3]

Achmad, S.A. *et al., Proc. Chem. Soc., London*, 1963, 166 (*synth*)
Eisenbraun, E.J. *et al., J.O.C.*, 1980, **45**, 3811 (*struct, bibl*)
Jones, T.H. *et al., Tet. Lett.*, 1981, **22**, 4373 (*Gastrolactone*)
Bellesia, F. *et al., Phytochemistry*, 1984, **23**, 83 (*biosynth*)
Bottini, A.T. *et al., Phytochemistry*, 1987, **26**, 1200 (*isol*)
De Pooter, H.L. *et al., Phytochemistry*, 1987, **26**, 2311 (*isol*)
Sakurai, K. *et al., Agric. Biol. Chem.*, 1988, **52**, 2369 (*synth*)
Kigawa, M. *et al., Heterocycles*, 1992, **33**, 117 (*synth*)
Unelius, C.R. *et al., Nat. Prod. Lett.*, 1994, **5**, 61 (*Gastrolactone, synth*)
Dawson, G.W. *et al., Bioorg. Med. Chem.*, 1996, **4**, 351 (*synth, biosynth*)
Nangia, A. *et al., Tetrahedron*, 1997, **53**, 14507-14545 (*rev, synth*)

Nepetalic acid N-46



(1′*R*)-*form*

$C_{10}H_{16}O_3$ 184.235

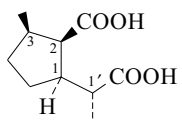
(1′*R*)-*form* [21651-54-7]
Constit. of *Nepeta cataria* (catnip). Cryst. (Et_2O/petrol). Mp 73-75°.

(1′*S*)-*form* [32203-60-4]
Oil.

Taylor, W.I. *et al., Cyclopentanoid Terpene Deriv.*, Marcel Dekker, 1969, 206 (*rev*)
Trave, R. *et al., Gazz. Chim. Ital.*, 1970, **100**, 1061 (*synth, struct*)
Eisenbraun, E.J. *et al., J.O.C.*, 1981, **46**, 3302 (*isol*)

Nepetalinic acid N-47

2-Carboxy-α,3-dimethylcyclopentaneacetic acid, 9CI



$C_{10}H_{16}O_4$ 200.234

(1*R*,2*R*,3*R*,1′*R*)-*form* [50429-20-4]
Cryst. Mp 68°. $[\alpha]_D$ -36 ($CHCl_3$/EtOH).

(1*R*,2*R*,3*R*,1′*S*)-*form* [50429-18-0]
Cryst. Mp 157.5-158°. $[\alpha]_D$ +18.6 ($CHCl_3$/EtOH).

(1*R*,2*R*,3*S*,1′*R*)-*form* [32603-11-5]
Constit. of oil of catnip. Cryst. Mp 85°.

(1*R*,2*R*,3*S*,1′*S*)-*form* [32603-10-4]
Constit. of oil of catnip. Cryst. Mp 117°.

(1*R*,2*S*,3*R*,1′*R*)-*form* [50429-13-5]
Cryst. Mp 121.5-122°. $[\alpha]_D$ -52 ($CHCl_3$/EtOH).

(1*R*,2*S*,3*R*,1′*S*)-*form* [50429-10-2]
Cryst. Mp 123.5°. $[\alpha]_D$ -39 ($CHCl_3$/EtOH).

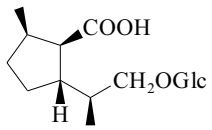
(1*R*,2*S*,3*S*,1′*R*)-*form* [32603-12-6]
Cryst. Mp 115°.

(1*R*,2*S*,3*S*,1′*S*)-*form* [485-06-3]
Cryst. Mp 111°.

Bates, R.B. *et al., J.A.C.S.*, 1958, **80**, 3420
Trave, R. *et al., Gazz. Chim. Ital.*, 1970, **100**, 1061 (*synth, struct*)
Grant, H.G. *et al., Aust. J. Chem.*, 1973, **26**, 2183 (*synth*)
Sakai, T. *et al., J.O.C.*, 1981, **46**, 4774 (*cmr, synth*)

Nepetariaside N-48

[110344-61-1]

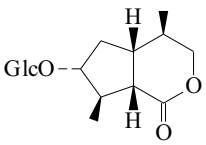


$C_{16}H_{28}O_8$ 348.392
Constit. of *Nepeta cataria* (catnip). Cryst. (EtOAc). Mp 139-141° dec. $[\alpha]_D$ -14 (c, 1.7 in MeOH).

Murai, F. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2533 (*isol, pmr, cmr*)

Nepetaside N-49

[114076-56-1]

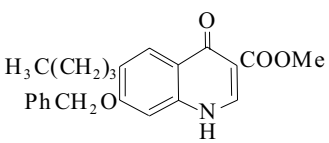


$C_{16}H_{26}O_8$ 346.377
Constit. of *Nepeta cataria* (catnip). Needles (EtOH). Mp 204-205°. $[\alpha]_D^{22}$ -52.5 (c, 0.6 in MeOH).

Xie, S. *et al., Phytochemistry*, 1988, **27**, 469

Nequinate, INN, USAN N-50

[13997-19-8]
Methyl 6-butyl-1,4-dihydro-4-oxo-7-(phenylmethoxy)-3-quinolinecarboxylate, 9CI. Methyl 7-(benzyloxy)-6-butyl-1,4-dihydro-4-oxo-3-quinolinecarboxylate, 8CI. ***Methyl benzoquate, BAN****. Statyl. AY 20385*

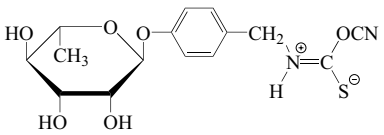


$C_{22}H_{23}NO_4$ 365.428
Antiprotozoan; used as a coccidiostat for poultry and rabbits. Mp 287-288°. Log P 4.55 (uncertain value) (calc).

Bowie, R.A. *et al., Nature (London)*, 1967, **214**, 1349 (*pharmacol*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NCN600
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 584

Niazidin N-51

[198969-42-5]



$C_{15}H_{18}N_2O_6S$ 354.383

Predominant tautomer shown. Constit. of the fresh pods of *Moringa oleifera* (horseradish tree). Amorph. λ_{max} 201 ; 227 ; 242 (MeOH).

Faizi, S. *et al., J. Nat. Prod.*, 1997, **60**, 1317-1321

Nickel N-52

[7440-02-0]

Ni

Ni 58.69

Atomic No. 28. Ground state electron config. $[Ar]3d^8 4s^2$. 9 Isotopes reported of which 5 are stable. Isol. in 1751 by A.F. Cronstedt. Known in alloys in early Chinese history. Biological role uncertain. Abundance: 99 ppm (earth's crust), traces (sea water). Fcc struct.. Catalyst for the hydrogenation of food fats and oils. Lustrous silvery-white, hard, malleable and ductile metal. Mp 1455°. Bp 2920° (2730°). Resistant to Cl_2, F_2, HCl, fused salts. Fairly good resistance to H_2SO_4, organic acids. Passivated by conc. HNO_3. Weakly ferromagnetic.

▶ Hypersensitivity to Ni is common. Ni powders or dry sponges may ignite spontaneousy. QR5950000

[12596-73-5, 12710-90-6, 14701-22-5, 14903-34-5, 18973-71-2, 20508-37-6, 22541-64-6, 37185-69-6, 37353-20-1, 37353-21-2, 37367-12-7]

Mellor Compr. Treat. Inorg. Theor. Chem., 1936, **15**, 1 (*rev, bibl*)

Gmelin Handbook Inorg. Chem., Syst. No. 57, *Suppl. Vol.*, 1965, **B/1**, ; 1967, **A1**, ; **A2/1**, ; 1968, **A2/2**, (*rev, bibl*)

Compr. Inorg. Chem., Pergamon, Oxford, 1973, **3**, 1109 (*rev*)

Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **3**, 1685 (*synth*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **15**, 787 (*rev, bibl*)

Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 1328 (*rev*)

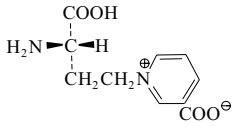
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1955-1956

Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1388 (*haz*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NCW500

Nicotianine N-53

1-(3-Amino-3-carboxypropyl)-3-carboxypyridinium hydroxide inner salt, 9CI



Absolute configuration

$C_{10}H_{12}N_2O_4$ 224.216

(*S*)-*form* [19701-79-2]

L-form

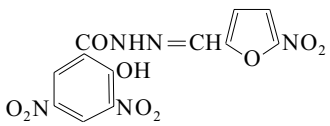
Constit. of *Lentinus edodes* (shiitake). Cryst. (MeOH aq.). Mp 241-243° dec. $[\alpha]_D^{24}$ +24 (c, 2.0 in H_2O).

Noma, M. *et al., Phytochemistry*, 1968, **7**, 1861 (*isol, struct*)

Nifursol, BAN, INN, USAN N-54

[16915-70-1]

2-Hydroxy-3,5-dinitrobenzoic acid [(5-nitro-2-furanyl)methylene]hydrazide, 9CI. 3,5-Dinitrosalicylic acid (5-nitrofurfurylidene)hydrazide, 8CI. Histomon. RT 6912



$C_{12}H_7N_5O_9$ 365.215

Veterinary antiprotozoal, esp. for poultry. Mp 227-229°. Log P 2.3 (calc). Component of Salfuride.

▶ VO2980000

Berndt, E.W. *et al., J. Med. Chem.*, 1969, **12**, 371 (*synth, pharmacol*)

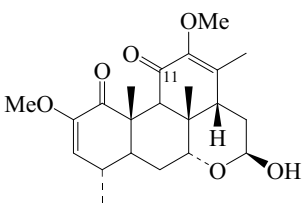
Analyst (London), 1985, **110**, 1013 (*hplc*)

Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 589

Nigakihemiacetal B N-55

[76-77-7]

Neoquassin. Simalikahemiacetal A



$C_{22}H_{30}O_6$ 390.475

Constit. of *Quassia amara* (Surinam quassia). Cryst. (C_6H_6/petrol). Mp 230.5-231°. $[\alpha]_D$ +20 (c, 0.21 in EtOH). $[\alpha]_D^{20}$ +41 ($CHCl_3$). λ_{max} 255 (ε 11650) (MeOH) (Derep).

16-Me ether: [89498-93-1]
$C_{23}H_{32}O_6$ 404.502

16-Et ether: [343943-63-5]
$C_{24}H_{34}O_6$ 418.529

16-Ketone (lactone): Quassin, Q-2

16-Epimer, 16-O-β-D-glucopyranoside: [89200-08-8] ***Picrasinoside B***
$C_{28}H_{40}O_{11}$ 552.617
Cryst. Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 153-153.5°. $[\alpha]_D$ -15.1. λ_{max} 255 (ε 11300) (EtOH) (Berdy).

16-Epimer, 16-Me ether:
$C_{23}H_{32}O_6$ 404.502
Constit. of *Quassia amara* (Surinam quassia). Powder (MeOH). Mp 173-176°.

16-Epimer, 11α-alcohol, 16-Me ether, 11-O-β-D-glucopyranoside:11-α-O-β-D-Glucopyranosyl-16α-O-methylneoquassin
$C_{29}H_{44}O_{11}$ 568.66
Constit. of *Quassia amara* (Surinam quassia). Powder (EtOH). Mp 200° dec.

Carman, R.M. *et al., Aust. J. Chem.*, 1962, **15**, 807 (*pmr*)

Tresca, J.-P. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **273**, 601 (*isol*)

Murae, T. *et al., Tetrahedron*, 1971, **27**, 5147 (*isol*)

Okano, M. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1793 (*deriv*)

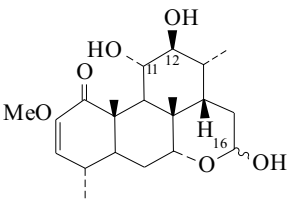
Barbetti, P. *et al., Phytochemistry*, 1993, **32**, 1007-1013 (*Quassia amara constits*)

De Bellis, P. *et al., Fitoterapia*, 1994, **65**, 314 (*pmr, cmr*)

Krebs, H.C. *et al., Z. Naturforsch., B*, 2000, **55**, 100-103 (*Picrasma crenata constits, cryst struct*)

Nigakihemiacetal C N-56

[30760-22-6]



$C_{21}H_{32}O_6$ 380.48

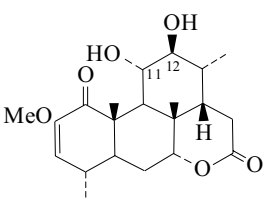
Compds. covered by this entry may not necessarily have the same 16-config..- Cryst. (EtOH). Mp 265-265.5°. $[\alpha]_D$ +49 (c, 0.13 in MeOH).

*12-Ketone:**11-Dihydro-12-norneoquassin***
$C_{21}H_{30}O_6$ 378.464
Isol. from *Quassia amara* (Surinam quassia). Prisms (MeOH). Mp 227-229°. $[\alpha]_D^{20}$ +21 (c, 0.19 in MeOH).

Grandolini, G. *et al., Phytochemistry*, 1987, **26**, 3085 (*11-Dihydro-12-norneoquassin*)

Nigakilactone A N-57

[24148-76-3]



$C_{21}H_{30}O_6$ 378.464

Cryst. (MeOH aq.). Mp 237.5-238°. $[\alpha]_D$ +35 (c, 0.26 in EtOH). λ_{max} 271 (ε 4800) (MeOH) (Derep).

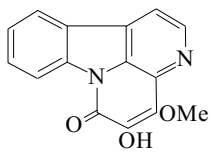
*12-Epimer, 13,18-didehydro:**12α-Hydroxy-13,18-dehyroparain***

$C_{21}H_{28}O_6$ 376.449
Constit. of *Quassia amara* (Surinam quassia). Powder (MeOH). Mp 238-241°.

Barbetti, P. *et al., Phytochemistry*, 1993, **32**, 1007 (*12α-Hydroxy-13,18-dehydroparain*)

Nigakinone N-58

[18110-86-6]
*5-Hydroxy-4-methoxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, 9CI. 5-Hydroxy-4-methoxycanthin-6-one*



$C_{15}H_{10}N_2O_3$ 266.256
Alkaloid from the wood of *Picrasma excelsa* (Jamaican quassiawood). Yellow needles (MeOH). Mp 223-224° dec.

N-*Oxide:* [129722-98-1] ***5-Hydroxy-4-methoxy-6-canthinone 3*-N-*oxide***
$C_{15}H_{10}N_2O_4$ 282.255
Alkaloid from the wood of *Quassia amara* (Surinam quassia). Red-orange powder (EtOH). Mp 300°.

Ac:
Needles (MeOH). Mp 194° dec.

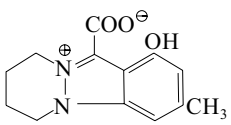
Me ether: [18110-87-7] ***4,5-Dimethoxy-canthin-6-one***. *4,5-Dimethoxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, 9CI. Methylnigakinone*
$C_{16}H_{12}N_2O_3$ 280.282
Pale yellow needles (MeOH). Mp 147.3-147.5°.

Me ether, picrate:
Bright yellow prisms (EtOH). Mp 185-186° dec.

Inamoto, N. *et al., Bull. Chem. Soc. Jpn.*, 1961, **34**, 888 (*isol, uv, ir, struct, deriv*)
Kondo, Y. *et al., Chem. Pharm. Bull.*, 1973, **21**, 837 (*isol, pmr, struct*)
Wagner, H. *et al., Planta Med.*, 1979, **36**, 113 (*isol*)
Yang, J.S. *et al., Yaoxue Xuebao*, 1979, **14**, 167-177 (*activity*)
Forgacs, P. *et al., Planta Med.*, 1982, **46**, 187 (*isol, deriv*)
Barbetti, P. *et al., Planta Med.*, 1990, **56**, 216 (*oxide*)

Nigellicine N-59

[98063-20-8]

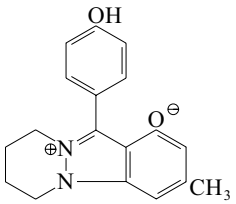


$C_{13}H_{14}N_2O_3$ 246.265
Alkaloid from the seeds of *Nigella sativa* (black cumin). Yellow cryst. (EtOH). Dec. over a wide temp. range λ_{max} 240 (ε 20000); 288 (ε 3310); 296 (ε 3240); 353 (ε 3390) (EtOH) (Derep).

Atta-ur-Rahman, *et al., Tet. Lett.*, 1985, **26**, 2759 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Nigellidine N-60

[120993-86-4]
*6,7,8,9-Tetrahydro-1-hydroxy-11-(4-hydroxyphenyl)-3-methylpyridazino[1,2-*a*]indazol-5-ium inner salt, 9CI*

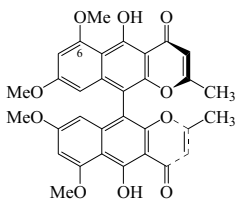


$C_{18}H_{18}N_2O_2$ 294.352
Alkaloid from seeds of *Nigella sativa* (black cumin). Related to Nigellicine, N-59 λ_{max} 230 (ε); 280 (ε); 328 (ε) (MeOH) (Derep).

Atta-ur-Rahman, *et al., Tet. Lett.*, 1995, **36**, 1993 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Nigerone N-61

[76069-41-5]
*5,5′-Dihydroxy-6,6′,8,8′-tetramethoxy-2,2′-dimethyl[10,10′-bi-4*H*-naphtho[2,3-*b*]pyran]-4,4′-dione, 9CI*



Absolute Configuration

$C_{32}H_{26}O_{10}$ 570.551
Prod. by *Aspergillus niger*. Mycotoxin. Orange needles ($CHCl_3$/MeOH). Mp 330°. $[\alpha]_D^{20}$ -287.7 (c, 1 in $CHCl_3$). λ_{max} 226 (ε 51300); 278 (ε 83200); 407 (ε 14100) (MeOH) (Derep).

*6-*O*-De-Me:* [76045-68-6] ***6-O-Demethylnigerone***
$C_{31}H_{24}O_{10}$ 556.525
From *Aspergillus niger*. Mycotoxin. Orange powder. Mp 330°. $[\alpha]_D^{20}$ -235.7 (c, 0.14 in $CHCl_3$). λ_{max} 226 (ε 51300); 278 (ε 83200); 407 (ε 14100) (MeOH) (Derep).

Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1980, 2474 (*isol, uv, ir, pmr, cmr, struct*)
Ehrlich, K.C. *et al., Appl. Environ. Microbiol.*, 1984, **48**, 1 (*isol*)
Koyama, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4049-4055 (*abs config*)

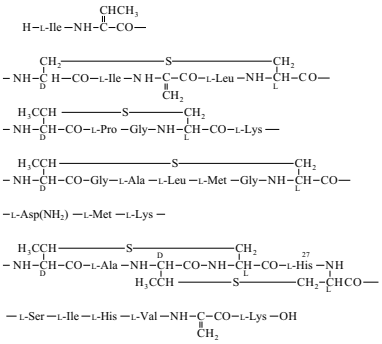
NIP 1 N-62

Protein containing 60 amino acid residues including 10 cysteines. Prod. by the barley pathogen *Rhynchosporium secalis*. Toxic to barley leaves.

Wevelsiep, L. *et al., Physiol. Mol. Plant Pathol.*, 1991, **39**, 471-482 (*isol*)
Rohe, M. *et al., EMBO J.*, 1995, **14**, 4168-4177 (*struct*)

Nisin N-63

[1414-45-5]
E234



$C_{143}H_{230}N_{42}O_{37}S_7$ 3354.111
Lantibiotic. Food preservative, esp. for cheese. Active against Gram-positive bacteria - particularly *Clostridium* and *Bacillus* (the antibacterial action applies to both spores and vegetative cells), but also *Listeria monocytogenes* and lactic acid bacteria. Nisin does not affect Gram-negative bacteria, yeasts and moulds. It has been used for over 50 years commercially as a food preservative without any evidence of bacterial resistance. Cryst. (EtOH). Sol. acids, bases, AcOH; fairly sol. H_2O; poorly sol. Me_2CO, hexane. Stable to boiling in acid soln. λ_{max} 210 (H_2O) (Berdy).
▶ LD_{50} (mus, ivn) 400 - 600 mg/kg.
QU3340000

*27-*L*-Asparagine analogue:* [136850-28-7] ***Nisin Z***
$C_{141}H_{229}N_{41}O_{38}S_7$ 3331.074

*5-(2-Amino-2-butenoic acid), 27-*L*-asparagine analogue:* [144307-02-8] Has lower biol. activity than Nisin Z but increased chemical stability.

*27-*L*-Asparagine, 31-*L*-lysine analogue:* [166188-15-4] Biol. activity similar to that of Nisin Z but has increased solubility.

[137061-46-2]

Mattick, A.T.R. *et al., Nature (London)*, 1944, **154**, 551 (*isol*)
Berridge, N.J. *et al., Biochem. J.*, 1952, **52**, 529-535 (*purifn*)
Gross, E. *et al., J.A.C.S.*, 1971, **93**, 4634-4635 (*struct*)
Fisk, C.L. *et al., Diss. Abstr. Int., B*, 1976, **36**, 4482 (*pmr*)
Wakamiya, T. *et al., Pept. Chem.*, (Publ. 1983), 1982, **20**, 149-154 (*synth*)
Wakamiya, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 2044-2049 (*synth*)
Hurst, A. *et al., Food Sci. (N.Y.)*, 1983, **10**, 327-351 (*rev*)
Chan, W.C. *et al., J.C.S. Perkin 1*, 1989, 2359-2367 (*pmr, conformn*)
Fukase, K. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 1758-1763; 1838-1840; 1992, **65**, 2227-2240 (*synth*)
Jung, G. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 1051-1068 (*rev*)
Mulders, J.W.M. *et al., Eur. J. Biochem.*, 1991, **201**, 581-584 (*Nisin Z*)
Kuipers, O.P. *et al., J. Biol. Chem.*, 1992, **267**, 24340-24346 (*deriv*)

Rollema, H.S. *et al., Appl. Environ. Microbiol.*, 1995, **61**, 2873-2878 (*deriv*)
Lúck, E. *et al., Antimicrobial Food Additives: Characteristics, Uses, Effects*, 2nd edn., Springer-Verlag, 1997, 208-213 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NEB050

[Nitrilotris(methylene)]trisphosphonic acid, 9CI, 8CI N-64

[6419-19-8]
Nitrilotris(methylenephosphonic acid). sym-*Trimethylaminetriphosphonic acid. Dequest 2000. Dequest 2001*

$N[CH_2P(O)(OH)_2]_3$

$C_3H_{12}NO_9P_3$ 299.05

A pentabasic acid with betaine struct. Exists as zwitterion in crystalline state. Corrosion inhibitor, complexing agent, e.g. for scale control, and demetallisation of wines. Permitted for treatment of cooling and retort water for meat and poultry products. Glassy or crystalline solid. Sol. H_2O, insol. org. solvs. Mp 210-215° dec. (201° dec.). pK_{a1} 1.9; pK_{a2} 2; pK_{a3} 4.6; pK_{a4} 5.92; pK_{a5} 7.35; pK_{a6} 10.9 (20°, 0.1*M* Me_4NCl). pK_{a1} 0.3; pK_{a2} 1.5; pK_{a3} 4.64; pK_{a4} 5.86; pK_{a5} 7.3; pK_{a6} 12.1 (25°, H_2O). pK_{a1} 2; pK_{a2} 2; pK_{a3} 4.3; pK_{a4} 5.46; pK_{a5} 6.66; pK_{a6} 12.34 (25°, 1*M* KNO_3). The penta-Na salt marketed as Dequest 2006.

▶ Skin and eye irritant. LD_{50} (rat, orl) 2100 mg/kg. SZ9860000

Hexa-Et ester: [6806-71-9] *Hexaethyl [nitrilotris(methylene)]trisphosphonate*
$C_{15}H_{36}NO_9P_3$ 467.372
Oil. d_4^{20} 1.18. $Bp_{0.8}$ 202-204°. n_D^{20} 1.4534.

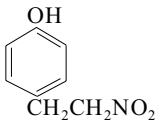
Hexa-Et ester, N-*oxide:* [15834-10-3]
$C_{15}H_{36}NO_{10}P_3$ 483.371
Cryst. Mp 171°.

[2235-43-0, 20592-85-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 920A (*ir*)
Petrov, K.A. *et al., Zh. Obshch. Khim.*, 1959, **29**, 591; *J. Gen. Chem. USSR (Engl. Transl.)*, 1959, **29**, 587 (*hexa-Et*)
Moedritzer, K. *et al., J.O.C.*, 1966, **31**, 1603 (*synth, props, pmr, P-31 nmr*)
Carter, R.P. *et al., Inorg. Chem.*, 1967, **6**, 939; 943 (*pmr, N-oxide*)
Daly, J.J. *et al., J.C.S.(A)*, 1967, 212 (*cryst struct*)
Krüger, F. *et al., Chem.-Ztg.*, 1972, **96**, 691 (*synth*)
U.S. Pat., 1974, 3 832 393; *CA*, **82**, 112160 (*use*)
Grigor'ev, A.I. *et al., Zh. Neorg. Khim.*, 1974, **19**, 1970; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 1079 (*ir, complexes*)
Nikitina, L.V. *et al., Zh. Obshch. Khim.*, 1974, **44**, 1598; 1669; *J. Gen. Chem. USSR (Engl. Transl.)*, 1974, **44**, 1568; 1641; 1975, **45**, 546; 552 (*props, ir, complexes*)
Goeva, L.V. *et al., Radiokhimiya*, 1982, **24**, 591; *Sov. Radiochem. (Engl. Transl.)*, 1982, **24**, 489 (*complexes*)
Popov, K.I. *et al., Zh. Neorg. Khim.*, 1982, **27**, 2756; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1982, **27**, 1562 (*P-31 nmr, pmr, props, struct*)
Rudomino, M.V. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1984, 2768; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1984, 2535 (*synth, pmr*)
Kaslina, N.A. *et al., Zh. Obshch. Khim.*, 1985, **55**, 534; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 472 (*props*)
Appleton, T.G. *et al., Inorg. Chem.*, 1986, **25**, 726 (*cmr, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 129 (*use*)

4-(2-Nitroethyl)phenol, 9CI N-65

[37567-58-1]
1-(4-Hydroxyphenyl)-2-nitroethane



$C_8H_9NO_3$ 167.164
Pale yellow oil.

O-*β-D-Glucopyranoside:* [74213-96-0] ***Thalictoside***
$C_{14}H_{19}NO_8$ 329.306
Cryst. ($MeOH/CHCl_3$). Mp 138-139° (102-103°). $[\alpha]_D^{25}$ -48.8 (c, 1.1 in MeOH).

O-*[3,4-Dihydroxycinnamoyl-(→6)-β-D-glucopyranoside]:* [114217-01-5]
$C_{23}H_{25}NO_{11}$ 491.451
Amorph. yellow powder. $[\alpha]_D^{20}$ -25.3 (c, 0.44 in MeOH).

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [153287-94-6] ***Arabinothalictoside***
$C_{19}H_{27}NO_{12}$ 461.422
Powder. $[\alpha]_D^{20}$ -51.3 (c, 0.8 in MeOH). λ_{max} 220 (ε 9355); 271 (ε 2620) (MeOH).

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:4-(2-Nitroethyl)phenyl primeveroside*
$C_{19}H_{27}NO_{12}$ 461.422
Constit. of *Annona squamosa* (sugar apple). Cryst. (EtOH). Mp 125°. $[\alpha]_D^{20}$ -70 (c,2 in EtOH). λ_{max} 274 (log ε 3.05) (EtOH).

Me ether:1-Methoxy-4-(2-nitroethyl)benzene. 1-(4-Methoxyphenyl)-2-nitroethane. ***Lysichitalexin***
$C_9H_{11}NO_3$ 181.191
Pale yellow oil.

Chirkunov, E.V. *et al., CA*, 1972, **77**, 126172r (*synth*)
Forgacs, P. *et al., Phytochemistry*, 1980, **19**, 1251 (*primeveroside*)
Ina, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 726 (*isol, struct, synth, deriv*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1109 (*deriv*)
Shimomura, H. *et al., Phytochemistry*, 1988, **27**, 644 (*derivs*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 492-499 (*Arabinothalictoside*)
Hanawa, F. *et al., Phytochemistry*, 2000, **53**, 55-58 (*isol, Lysichitalexin*)

Nitrogen, 11CI N-66

[7727-37-9]
Dinitrogen. E941

N≡N

N 14.007

Atomic No. 7. Ground state electron config. $[He]2s^22p^3$. 8 Isotopes known, of which 2 are stable, ^{14}N and ^{15}N. Recognition attributed to Rutherford, Scheele, Cavendish and Priestley in 18th century. Abundant in nature. Forms 78% by vol. of earth's atmosphere. In addition to the α-form (cubic, fcc) and β-form (hexagonal) there is a high pressure tetragonal (γ) form. α → β form at -238°. N≡N 110 pm. Used as a propellant and aerating agent in foods. Colourless, odourless, v. stable, non-flammable gas. Generally unreactive. V. sl. sol. H_2O; sol. liq. NH_3. d 0.8. Mp -210°. Bp -196°. T_{crit} -146°; P_{crit} 35 atm; V_{crit} 5.17 cm^3. Reacts with Li at r.t. to give Li_3N.

▶ QW9700000

[12185-02-3, 12185-04-5, 12596-60-0, 12596-63-3, 13966-04-6, 14158-22-6, 14158-23-7, 14452-70-1, 15721-56-9, 17439-59-7, 17778-87-9, 17778-88-0, 18396-22-0, 20508-99-0, 29817-79-6, 40549-08-4, 55128-57-9]

Mellor Compr. Treat. Inorg. Theor. Chem., 1928, **8**, 360; 1964, **8/I, Part 1**, 1 (*bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 4, 1936, (*bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 147 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **15**, 932 (*rev, bibl*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 466 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1960-1961
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 142; 245
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1345 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NGP500; NGP510

Nitrogen chloride (NCl_3) N-67

[10025-85-1]
Nitrogen trichloride. Trichloramine. Chlorine nitride

NCl_3 (C_{3v})

Cl_3N 120.365

Interatomic distance: N–Cl 175.9 pm; angle: ClNCl 107.1°. Once sold as Agene, a flour bleaching agent. V. unstable yellow liq. with strong odour. Sol. CCl_4, $CHCl_3$. Mp -40°. Bp 70°.

▶ Solns. up to 20% NCl_3 are stable in various solvs. without danger of explosion, otherwise highly dangerous. NCl_3 detonation held responsible for causing major ammonium nitrate explosion at Toulouse in 2001. QW9740000

Inorg. Synth., 1939, **1**, 65 (*synth*)
Ferrari, C.G. *et al., Cereal Chem.*, 1945, **20**, 101-112 (*use*)
Gmelin Handbook Inorg. Chem., Syst No. 6, 1969, **B2**, 483 (*rev*)
Bürgi, H.B. *et al., J. Mol. Struct.*, 1971, **10**, 31 (*struct*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 462 (*synth*)
Jander, J. *et al., Adv. Inorg. Chem. Radiochem.*, 1976, **19**, 2 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 565
Soulard, M. *et al., J.C.S. Dalton*, 1981, 2300 (*anal, equilib*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 5050-5052 (*use*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NGQ500

Nitrogen oxide (N_2O), 11CI N-68

[10024-97-2]

Nitrous oxide, JAN, USAN. Dinitrogen monoxide. Laughing gas. FEMA 2779. E942

N═N═O ($C_{\infty v}$)

N_2O 44.013

Interatomic distances: N–N 112.8, N–O 118.4 pm. Aerosol propellant for foods. Flavouring ingredient. Colourless, non-flammable gas. Sl. sol. H_2O; sol. Et_2O; freely sol. $CHCl_3$, EtOH. Mp -90.6°. Bp -88.5°.

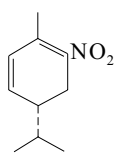
▶ OES: long-term 100 ppm (1995 proposed). Exp. adverse effects on bone marrow function, immune system, CNS, liver and reproductive system. LC_{50} (rat, ihl) 1068 mg1m^3 (4 h exposure). Evidence suggests that N_2O oxidises and inactivates Vitamin B_{12} (as Methyl cobalamin). QX1350000

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1689C (*ir*)
Griggs, J.L. *et al., J. Mol. Spectrosc.*, 1968, **25**, 34 (*struct*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 316 (*rev*)
Watson, J.K.G. *et al., J. Mol. Spectrosc.*, 1973, **48**, 479 (*struct*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 468 (*synth*)
Nitrous Oxide/N_2O, (Ed. Eger E.I.), Edward Arnold, 1985, (*book*)
Brodsky, J.B. *et al., Med. Toxicol.*, 1986, **1**, 362 (*tox*)
Gillman, M.A. *et al., Br. J. Anaesth.*, 1987, **59**, 143 (*rev, pharmacol*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 323-324
Gillman, M.A. *et al., Int. J. Neurosci.*, 1994, **76**, 5 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 594 (*rev*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1260
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1963 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NGU000

2-Nitro-*p*-mentha-1,5-diene N-69

[73041-74-4]

2-Methyl-5-(1-methylethyl)-1-nitro-1,3-cyclohexadiene. 5-Isopropyl-2-methyl-1-nitro-1,3-cyclohexadiene



$C_{10}H_{15}NO_2$ 181.234

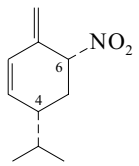
(R)-form

Constit. of *Angelica archangelica* (angelica). Oil. $[\alpha]_D^{20}$ -161 (c, 0.5 in $CHCl_3$).

Escher, S. *et al., Helv. Chim. Acta*, 1979, **62**, 2061

6-Nitro-*p*-mentha-1(7),2-diene N-70

3-Methylene-6-(1-methylethyl)-4-nitrocyclohexene. 6-Isopropyl-3-methylene-4-nitrocyclohexene



(4*R**,6*R**)-*form*

$C_{10}H_{15}NO_2$ 181.234

(4R*,6R*)-form [73069-40-6]

cis-*form*

Constit. of *Angelica archangelica* (angelica). Oil.

(4R*,6S*)-form [73041-75-5]

trans-*form*

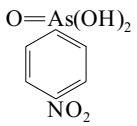
Constit. of *Angelica archangelica* (angelica). Oil.

Escher, S. *et al., Helv. Chim. Acta*, 1979, **62**, 2061

(4-Nitrophenyl)arsonic acid, 9CI N-71

[98-72-6]

p-*Nitrobenzenearsonic acid, 8CI. **Nitarsone, INN, USAN**. Hep-A-Stat. Histostat. NSC 5085*



$C_6H_6AsNO_5$ 247.039

Antiprotozoal, antihistomonad; mainly used for poultry. Pale yellow leaflets (H_2O). Spar. sol. cold MeOH, H_2O, EtOH. Mp 298-300° dec. pK_{a1} 2.9; pK_{a2} 7.8 (22°). Log P -0.2 (calc). Reduced by Fe^{II} → (4-Aminophenyl)arsonic acid. Treatment with SO_2/HCl gives (4-Nitrophenyl)arsonous dichloride and with SO_2/HBr gives (4-nitrophenyl)arsonous dibromide.

▶ CY6125000

[19428-29-6]

Jacobs, W.A. *et al., J.A.C.S.*, 1918, **40**, 1580 (*synth*)
Org. Synth., Coll. Vol., 3, 1955, 665 (*synth*)
McGregor, J.K. *et al., Poultry Sci.*, 1964, **43**, 1026 (*pharmacol*)
Sullivan, T.W. *et al., Poultry Sci.*, 1972, **51**, 1582 (*nitarsone, use, tox*)
Modro, T.A. *et al., Tetrahedron*, 1972, **28**, 3867 (*synth, uv*)
Zakirov, D.U. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1977, 910; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1977, 834 (*nqr*)
Yambushev, F.D. *et al., Zh. Obshch. Khim.*, 1981, **51**, 2232; *J. Gen. Chem. USSR (Engl. Transl.)*, 1981, **51**, 1919 (*synth*)
Cullen, W.R. *et al., Appl. Organomet. Chem.*, 1988, **2**, 1 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NIJ500

3-Nitropropanoic acid, 9CI N-72

[504-88-1]

*3-Nitropropionic acid, 8CI. **Bovinocidin**. Hiptagenic acid*

$O_2NCH_2CH_2COOH$

$C_3H_5NO_4$ 119.077

Isolated from *Aspergillus* sp. and moulds contaminating food. Cryst. ($CHCl_3$). V. sol. H_2O, EtOH, Et_2O; sol. warm $CHCl_3$; insol. petrol. Mp 64-65°. pK_a 9.1.

▶ LD_{50} (rat, ipr) 67 mg/kg. Exp. neoplastic agent.. UF6220000

Et ester: [3590-37-2]
$C_5H_9NO_4$ 147.13
Liq. Bp 161-165°.

Chloride: [51834-15-2]
$C_3H_4ClNO_3$ 137.522
Liq. Bp_{10} 123°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 543D (*ir*)
Carter, C.L. *et al., Nature (London)*, 1949, **164**, 575 (*isol*)
Hass, H.B. *et al., J.A.C.S.*, 1951, **73**, 1858 (*synth*)
Sutor, D.J. *et al., Acta Cryst.*, 1954, **7**, 767 (*cryst struct*)
Anzai, K. *et al., J. Antibiot., Ser. A*, 1960, **13**, 133 (*isol, props*)
Birkinshaw, J.H. *et al., Biochem. J.*, 1964, **93**, 478 (*biosynth*)
Finnegan, R.A. *et al., J. Pharm. Sci.*, 1965, **54**, 1136 (*isol, ester*)
Wasaki, T. *et al., J. Food Sci.*, 1974, **38**, 1162 (*occur*)
Seebach, D. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 321 (*use, deriv*)
Gustine, D.L. *et al., J. Anim. Sci.*, 1977, **44**, 1107 (*metab*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 363
Baxter, R.L. *et al., J.C.S. Perkin 1*, 1992, 2495; 1994, 2297 (*biosynth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 755
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NIY500

N-Nitrosodimethylamine N-73

[62-75-9]

N-*Methyl*-N-*nitrosomethanamine, 9CI. Dimethylnitrosamine*

Me_2NNO

$C_2H_6N_2O$ 74.082

Food contaminant esp. in cured meat products. Yellow liq. d_4^{10} 1.01. Bp_{774} 153°. Forms azeotrope with H_2O, Bp 99.3°.

▶ Probable human carcinogen. Eye and skin irritant.. LD_{50} (rat, orl) 58 mg/kg. LC_{50} (rat, ihl) 78 ppm (4h exposure). Exp. carcinogen and teratogen. Exp. hepatotoxic and reprod. effects. Fl. p. 61°. IQ0525000

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 234E (*ir*)
Looney, C.E. *et al., J.A.C.S.*, 1957, **79**, 6136 (*synth, pmr, ir*)
Karabatsos, G.J. *et al., J.A.C.S.*, 1964, **86**, 4373 (*pmr, uv*)
Levin, I.W. *et al., J. Chem. Phys.*, 1970, **53**, 2505 (*ir*)
Krebs, B. *et al., Chem. Ber.*, 1975, **108**, 1130 (*cryst struct*)
Rainey, W.T. *et al., Biomed. Mass Spectrom.*, 1978, **5**, 395 (*ms*)

IARC Monog., 1978, **17**, 125; *Suppl*. 7, 67 (*rev, tox*)
Gouesnard, J.P. *et al., Org. Magn. Reson.*, 1979, **12**, 263 (*nmr*)
N-Nitroso Compounds, (ed. Scanlan, R.A. *et al*), ACS Symposium Series 174, American Chemical Society, 1981, (*book*)
Tricker, A.R. *et al., Food Chem. Toxicol.*, 1991, **29**, 729-732 (*occur*)
Relevance to Human Cancer of N-Nitroso Compounds, Tobacco and Mycotoxins, (ed. O'Neill, I.K. *et al*), IARC Scientific Publications, No. 105, IARC, Lyon, 1991, (*book*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3766-3768 (*use*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 513
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NKA600
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 663 (*tox, rev*)

Nitrosyl chloride ((NO)Cl), 11CI N-74

[2696-92-6]

ClNO (C_s)

ClNO 65.459

Interatomic distances: Cl-N 197.5, N-O 113.9 pm; angle: ClNO 113.3°. Bleaching agent for flour. Orange-yellow gas condensing to a deep red liq. The dry gas slowly attacks glass. Sol. fuming H_2SO_4. d^{-12} 1.42. Mp -61.5°. Bp -6.4°. Hydrol. to HNO_2, HNO_3, NO and HCl. d (gas) 2.99 gl^{-1}. T_{crit} 167°, P_{crit} 92.4 atm.

▶ QZ7883000

Inorg. Synth., 1939, **1**, 55; 1953, **4**, 48; 1968, **11**, 194 (*synth, vp, ir*)
Millen, D.J. *et al., J.C.S.*, 1961, 1322 (*struct*)
Gmelin Handbook Inorg. Chem., Syst. No. 6, 1969, **B2**, 500 (*bibl*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 474 (*synth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3770-3771 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1962-1963
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMH000

Nitrosylsulfuric acid N-75

[7782-78-7]

Nitrosyl hydrogen sulfate. Sulfuric acid monoanhydride with nitrous acid. Nitrosyl sulfate. Nitrososulfuric acid. Nitrosulfonic acid. Nitroxylsulfuric acid. Nitrose. Lead chamber crystals. Chamber crystals

$HOS(O)_2ONO$

HNO_5S 127.078

Used for bleaching cereal milling products. White cryst., stable in dry air. Readily hydrol. Sol. H_2SO_4. Mp 73.5° dec. Dec. in moist air.

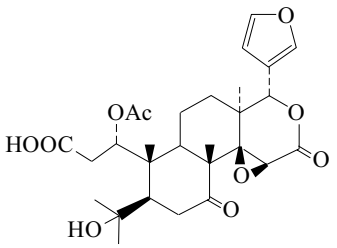
▶ Corrosive, toxic. QZ7886700

Gmelin Handbook Inorg. Chem., Syst. No. 9, 1963, **B3**, 1639 (*rev, bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 755; **2**, 299 (*uses*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 403 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMJ000

Nomilinic acid N-76

[35930-20-2]

1-Acetoxy-1,2-dihydroobacunoic acid



$C_{28}H_{36}O_{10}$ 532.586

Constit. of grapefruit seeds. Noncryst.; cryst. (Et_2O/hexane) (as Me ester). Mp 108-110° (Me ester).

O-*β-D-Glucopyranoside:* [113301-65-8]
$C_{34}H_{46}O_{15}$ 694.728
Isol. from lemons *Citrus limon*. Cryst. Mp 250-252° dec. $[\alpha]_D^{20}$ +35.44 (c, 0.75 in MeOH).

Me ester, O-*β-D-glucopyranoside: Methyl nomilinate 17-glucoside*
$C_{35}H_{48}O_{15}$ 708.755
Isol. from satsuma (*Citrus unshiu*) peel. Amorph. solid. $[\alpha]_D$ +20.32 (c, 0.09 in MeOH). Shows no significant antitumour activity.

O-*De-Ac:* [35930-21-3] ***Deacetylnomilinic acid***
$C_{26}H_{34}O_9$ 490.549
Constit. of the extract of grapefruit seeds. Noncryst.

Lactone: [1063-77-0] ***Nomilin***
$C_{28}H_{34}O_9$ 514.571
Constit. of grapefruit (*Citrus paradisi*).

Lactone, O-*de-Ac:* [3264-90-2] ***Deacetylnomilin***. *Isolimonin*
$C_{26}H_{32}O_8$ 472.534
Isol. from orange (*Citrus sinensis*) and finger lime (*Microcitrus australasica*). Tablets (EtOH). Mp 263-265°.

Dreyer, D.L. *et al., J.O.C.*, 1965, **30**, 749 (*Deacetylnomilin*)
Dreyer, D.L. *et al., Phytochemistry*, 1966, **5**, 367 (*rev*)
Bennett, R.D. *et al., Phytochemistry*, 1971, **10**, 3065
Marcelle, G.B. *et al., Tet. Lett.*, 1981, 505 (*7,11-Diacetoxydihydronomilin*)
Hasegawa, S. *et al., Phytochemistry*, 1986, **25**, 1323; 2523 (*biosynth*)
Herman, Z. *et al., Phytochemistry*, 1987, **26**, 2247 (*biosynth*)
Matsubara, Y. *et al., Agric. Biol. Chem.*, 1990, **54**, 1143 (*glucoside*)
Sawabe, A. *et al., Carbohydr. Res.*, 1999, **315**, 142-147 (*glucoside, Me ester glucoside*)

Nonacosane N-77

[630-03-5]

$H_3C(CH_2)_{27}CH_3$

$C_{29}H_{60}$ 408.793

Constit. of the leaves of *Brassica oleracea* (Brussels sprouts) and other plants. Cryst. (petrol). Mp 64°. Bp_{40} 346-348° $Bp_{0.05}$ 196-198°.

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 8B (*ir*)
Gluud, W. *et al., Ber.*, 1919, **52**, 1039 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 16 (*occur*)
Kami, T. *et al., J. Agric. Food Chem.*, 1975, **23**, 795 (*glc, ms*)
Behari, M. *et al., Curr. Sci.*, 1976, **45**, 481 (*isol*)
Ulubelen, L. *et al., Planta Med.*, 1976, **29**, 258 (*isol*)
Koehlen, L. *et al., Z. Pflanzenphysiol.*, 1976, **77**, 99 (*isol*)

1,10-Nonacosanediol N-78

[180005-29-2]

$H_3C(CH_2)_{18}CH(OH)(CH_2)_8CH_2OH$

$C_{29}H_{60}O_2$ 440.792

Constit. of the leaf wax of *Papaver somniferum* (opium poppy).

Jetter, R. *et al., Phytochemistry*, 1996, **42**, 1617-1620 (*isol, ms*)

1,18-Nonacosanediol N-79

$H_3C(CH_2)_{10}CH(OH)(CH_2)_{16}CH_2OH$

$C_{29}H_{60}O_2$ 440.792

Incorr. descr. in the text of the paper and in the CAS abstract as the 1,8-diol. Correctly indexed by CAS.

(+)-*form* [151454-22-7]
Constit. of *Papaver somniferum* (opium poppy). Mp 107°. $[\alpha]_D$ +4 (c, 1.8 in $CHCl_3$).

Bhakuni, R.S. *et al., J. Indian Chem. Soc.*, 1992, **69**, 889 (*isol*)

6,8-Nonacosanediol N-80

[96850-33-8]

$C_{29}H_{60}O_2$ 440.792

(6*S*,8*R*)-*form*
erythro-*form*
Constit. of the flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 72-74°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105-108 (*isol*)
Ukiya, M. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1187-1189 (*abs config*)

8,10-Nonacosanediol N-81

$C_{29}H_{60}O_2$ 440.792

(8*R,10*S**)-*form*** [193419-77-1]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 52-55°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, pmr, ms*)

6,8-Nonacosanedione N-82

$H_3C(CH_2)_{20}COCH_2CO(CH_2)_4CH_3$

$C_{29}H_{56}O_2$ 436.76

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

8,10-Nonacosanedione, 9CI N-83

[58170-84-6]

$H_3C(CH_2)_{18}COCH_2CO(CH_2)_6CH_3$

$C_{29}H_{56}O_2$ 436.76

Constit. of the pollen of *Helianthus annuus* (sunflower).

Evans, D. *et al., Phytochemistry*, 1975, **14**, 2447 (*isol, chromatog, ms*)
Matsuzaki, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 2341 (*isol, uv, pmr, ms*)
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

10,12-Nonacosanedione N-84

$H_3C(CH_2)_{16}COCH_2CO(CH_2)_8CH_3$

$C_{29}H_{56}O_2$ 436.76

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

12,14-Nonacosanedione, 9CI N-85

[58141-94-9]

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_{10}CH_3$

$C_{29}H_{56}O_2$ 436.76

Constit. of the pollen of *Helianthus annuus* (sunflower).

Horn, D.H.S. *et al., Aust. J. Chem.*, 1964, **17**, 464 (*isol*)
Evans, D. *et al., Phytochemistry*, 1975, **14**, 2447 (*isol, chromatog, ms*)
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

14,16-Nonacosanedione, 9CI N-86

[72089-30-6]

[230955-83-6]
16-Hydroxy-15-nonacosen-14-one, 9CI

$H_3C(CH_2)_{12}COCH_2CO(CH_2)_{12}CH_3$

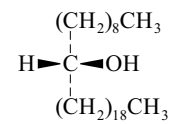
$C_{29}H_{56}O_2$ 436.76

Enolised β-diketone. Constit. of barley wax.

Mikkelsen, J.D. *et al., Carlsberg Res. Commun.*, 1979, **44**, 133-147 (*isol*)
Otsuka, H. *et al., Nat. Med. (Tokyo)*, 1998, **52**, 533-535 (*isol, tautom*)

10-Nonacosanol N-87

[2606-50-0]
Ginnol. Celidoniol



(*S*)-*form*

$C_{29}H_{60}O$ 424.792

(*S*)-*form*

Wax from *Ginkgo biloba* (ginkgo). Cryst. (EtOH, Me_2CO or hexane). Mp 81-81.5°. $[\alpha]_D^{20}$ +2.18 (c, 1.1 in $CHCl_3$).

Ac:
$C_{31}H_{62}O_2$ 466.83
Cryst. (Me_2CO). Mp 44.5-45.5°.

Bentley, H.R. *et al., J.C.S.*, 1955, 596 (*isol*)
Kariyone, T. *et al., Yakugaku Zasshi*, 1959, **79**, 51; 54; 58 (*isol, struct*)
Seone, E. *et al., Chem. Ind. (London)*, 1961, 1080 (*isol, struct*)
Beckmann, S. *et al., Z. Naturforsch., B*, 1968, **23**, 471 (*isol*)
Naruto, S. *et al., Phytochemistry*, 1972, **11**, 2644 (*isol*)
De Pascual, T. *et al., An. Quim.*, 1975, **71**, 110 (*isol*)
Caldicott, A.B. *et al., Phytochemistry*, 1975, **14**, 1799 (*isol*)
Isono, H. *et al., Yakugaku Zasshi*, 1976, **96**, 957 (*glc, ms*)
Fuhrhop, J.H. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 350 (*bibl*)
Kusumi, T. *et al., Chem. Lett.*, 1994, 1093 (*abs config*)
Jetter, R. *et al., Planta*, 1994, **195**, 257 (*occur, cryst struct*)
Langer, F. *et al., J.O.C.*, 1996, **61**, 8229-8243 (*synth, ir, pmr, cmr, ms*)
Berkenbusch, T. *et al., Tetrahedron*, 1998, **54**, 11471-11480 (*synth*)

15-Nonacosanol, 9CI N-88

[2764-81-0]

$H_3C(CH_2)_{13}CH(OH)(CH_2)_{13}CH_3$

$C_{29}H_{60}O$ 424.792

Isol. from wax of the strawberry tree *Arbutus unedo* and Brussels sprouts (*Brassica oleracea* var. *gemmintera*). Mp 83.1-83.8°.

Sahai, P.N. *et al., Biochem. J.*, 1932, **26**, 403 (*isol*)
Soza, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1950, **230**, 995 (*isol*)

10-Nonacosanone N-89

[504-56-3]
Ginnone. Celidonione

$H_3C(CH_2)_{18}CO(CH_2)_8CH_3$

$C_{29}H_{58}O$ 422.777

Isol. from plant wax from *Ginkgo biloba* (ginkgo). Cryst. (EtOH aq.). Mp 74-75°.

Oxime:
$C_{29}H_{59}NO$ 437.791
Cryst. (EtOH). Mp 49-50°.

Semicarbazone:
Cryst. (EtOH aq.). Mp 45-46°.

Piper, H. *et al., Biochem. J.*, 1932, **25**, 2072 (*synth*)
Seoane, E. *et al., Chem. Ind. (London)*, 1961, 1080 (*isol*)
Dodova, A.M. *et al., Phytochemistry*, 1973, **12**, 2239 (*isol, ms, struct*)
Ulubelen, A. *et al., Planta Med.*, 1973, **24**, 290 (*isol*)
Soeder, R.W. *et al., Phytochemistry*, 1975, **14**, 2508 (*isol, glc, ms*)

15-Nonacosanone, 9CI N-90

[2764-73-0]
Ditetradecyl ketone. Dimyristyl ketone

$H_3C(CH_2)_{13}CO(CH_2)_{13}CH_3$

$C_{29}H_{58}O$ 422.777

Isol. from cabbage leaves (*Brassica oleracea*). Platelets (C_6H_6/EtOH). Mp 80.5-81°.

Collison, D.L. *et al., Biochem. J.*, 1931, **25**, 606 (*isol*)
Kolattukudy, P.E. *et al., Phytochemistry*, 1971, **10**, 3047-3051 (*biosynth*)
Matsota, N.P. *et al., Zh. Prikl. Khim. (Leningrad)*, 1971, **44**, 1823; *CA*, **76**, 3358c (*synth*)

20-Nonacosene-2,4-dione N-91

$H_3C(CH_2)_7CH=CH(CH_2)_{15}COCH_2COCH_3$

$C_{29}H_{54}O_2$ 434.744

(*Z*)-*form*

Ximenoylacetone

Constit. of the epicuticular waxes of *Vanilla fragrans* (vanilla) and *Vanilla tahitensis* (Tahitian vanilla).

Ramaroson-Raonizafinimanana, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 4739-4743 (*isol*)

Nonadecane N-92

[629-92-5]

$H_3C(CH_2)_{17}CH_3$

$C_{19}H_{40}$ 268.525

Isol. from apple wax. Mp 32°. Bp 330° Bp_{30} 212°.

▶ Fl. p. >100°, autoignition temp. 230°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 5C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 4D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 5D (*ir*)
Hildebrandt, J.H. *et al., J.A.C.S.*, 1929, **51**, 2487
Cocker, W. *et al., J.C.S.*, 1963, 677 (*isol*)
Carnduff, J. *et al., Phytochemistry*, 1966, **5**, 1029 (*isol*)
Roelofs, W.L. *et al., Science (Washington, D.C.)*, 1971, **171**, 684
Olf, H.G. *et al., J. Chem. Phys.*, 1973, **59**, 534 (*Raman*)
Balinova-Tsvetkova, A. *et al., Dokl. Skh. Akad. (Sofia)*, 1974, **7**, 45; *CA*, **83**, 32911c (*glc*)
Wong, J.W. *et al., J. Chem. Ecol.*, 1984, **10**, 463

4,6-Nonadecanedione N-93

$H_3C(CH_2)_{12}COCH_2COCH_2CH_2CH_3$

$C_{19}H_{36}O_2$ 296.492

Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-nonadecanone
$C_{19}H_{38}O_2$ 298.508
Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-4-nonadecanone
$C_{19}H_{38}O_2$ 298.508
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

1,2,4-Nonadecanetriol N-94

$H_3C(CH_2)_{14}CH(OH)CH_2CH(OH)-CH_2OH$

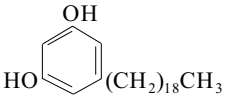
$C_{19}H_{40}O_3$ 316.523

Constit. of the unripe fruit of *Persea americana* (avocado). Cytotoxic agent. Powder. Mp 79-81°. Config. not determined λ_{max} 200 (no solvent reported).

Oberlies, N.H. *et al., J. Nat. Prod.*, 1998, **61**, 781-785 (*isol, pmr, cmr, ms*)

5-Nonadecyl-1,3-benzenediol, 9CI N-95

[35176-46-6]
1,3-Dihydroxy-5-nonadecylbenzene. 5-Nonadecylresorcinol



$C_{25}H_{44}O_2$ 376.621
Constit. of wheat bran. Cryst. (hexane). Mp 96.5-97.5°.

Di-Ac:
$C_{29}H_{48}O_4$ 460.696
Cryst. (EtOH). Mp 67.5-68°.

Di-Me ether:1,3-Dimethoxy-5-nonadecylbenzene
$C_{27}H_{48}O_2$ 404.675
Mp 56.5-57.5°.

10′,11′-Didehydro(Z-):

[52483-22-4] *5-(10-Nonadecenyl)-1,3-benzenediol. 5-(10-Nonadecenyl)resorcinol*
$C_{25}H_{42}O_2$ 374.606
Constit. of wheat and rye flour.

12′,13′-Didehydro(Z-): [189562-06-9] *5-(12-Nonadecenyl)-1,3-benzenediol. 5-(12-Nonadecenyl)resorcinol*
$C_{25}H_{42}O_2$ 374.606
Constit. of wheat and rye flour.

14′,15′-Didehydro(Z-): [187523-39-3] *5-(14-Nonadecenyl)-1,3-benzenediol. 5-(14-Nonadecenyl)resorcinol*
$C_{25}H_{42}O_2$ 374.606
Constit. of wheat and rye flour.
Amorph.

10′,11′,13′,14′-Tetradehydro(Z,Z-):
[189562-02-5] *5-(10,13-Nonadecadienyl)-1,3-benzenediol. 5-(10,13-Nonadecadienyl)resorcinol*
$C_{25}H_{40}O_2$ 372.59
Constit. of wheat and rye flour.

*2′-Oxo:**1-(3,5-Dihydroxyphenyl)-2-nonadecanone**. 5-(2-Oxononadecyl)-1,3-benzenediol*
$C_{25}H_{42}O_3$ 390.605
Cryst. (EtOAc). Mp 90-92°. λ_{max} 282 (ε 1560) (MeOH).

Wenkert, E. *et al., J.O.C.*, 1964, **29**, 435 (*isol, synth, pmr*)
Cirigottis, K.A. *et al., Aust. J. Chem.*, 1974, **27**, 345 (*occur*)
Tyman, J.H.P. *et al., Chem. Soc. Rev.*, 1979, **8**, 499 (*rev*)
Anh, N.H. *et al., Planta Med.*, 1996, **62**, 479 (*Nonadecenylbenzenediol*)
Suzuki, Y. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 480-486 (*isol, ms*)
Filip, P. *et al., Z. Naturforsch., C*, 2002, **57**, 1004-1008 (*2′-oxo*)

2,4-Nonadienal, 9CI N-96

[6750-03-4]
FEMA 3212
$H_3C(CH_2)_3CH{=}CHCH{=}CHCHO$
$C_9H_{14}O$ 138.209

(2*E*,4*E*)-*form* [5910-87-2]
Flavour and fragrance ingredient. Present in American cranberry, raw asparagus, peas, wheat bread, Russian cheeses, caviar, raw fatty fish, roast beef, boiled mutton, cooked chicken, roasted filberts, roasted peanuts, soybean, mushrooms and tomatoes. It may also be formed by lipid oxidation in foodstuffs such as skimmed milk and edible fats and oils. Liq. with strong, fatty, floral odour. d_4^{25} 0.86. Bp_{10} 97-98°. n_D^{27} 1.5184.

2,4-Dinitrophenylhydrazone:
Mp 136-138°.

(2*Z*,4*E*)-*form* [5910-86-1]
V. pale yellow liq. $Bp_{0.5}$ 75°.

2,4-Dinitrophenylhydrazone:
Cryst. Mp 147-148°.

[5910-86-1, 21661-99-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 475C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 743B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 565C (*ir*)
Näf, F. *et al., Helv. Chim. Acta*, 1974, **57**, 1309 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NMV775
Furber, M. *et al., J.C.S. Perkin 1*, 1989, 683 (*synth, uv, ir, pmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1965-1966 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMV775

2,6-Nonadienal, 9CI N-97

[26370-28-5]
$H_3CCH_2CH{=}CHCH_2CH_2CH{=}CHCHO$
$C_9H_{14}O$ 138.209

(2*E*,6*E*)-*form* [17587-33-6]
FEMA 3766
Occurs in beef and mutton tallows and is formed during deep frying of fat. Also present in lingonberry, cowberry, mango, cucumber, cornmint oil, raw lean fish, cooked trassi and cooked shrimp. Flavouring agent. Bp_{11} 88-89°. n_D^{20} 1.4420.

Di-Et acetal: [106950-34-9] *1,1-Diethoxy-2,6-nonadiene. FEMA 3378*
$C_{13}H_{24}O_2$ 212.331
Flavouring ingredient. $Bp_{0.2}$ 67-70°. n_D^{20} 1.4439.

(2*E*,6*Z*)-*form* [557-48-2]
Violet-leaf aldehyde. Cucumber aldehyde. FEMA 3377
Constit. of cherry, melon, peas, cooked potato, wheat bread, other breads, milk, lean and fatty fish, black tea, oyster, clam and other foods. Primary odourant in cucumbers. Present in cucumber juice. Flavouring agent. Liq. with cucumber odour. d 0.87. Bp 187° Bp_{11} 94-98°. n_D^{20} 1.4460.
► Skin irritant. LD_{50} (rat, orl) > 5000 mg/kg. RA5391800

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 743C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 565D (*ir*)
Ruzicka, L. *et al., Helv. Chim. Acta*, 1942, **25**, 760; 1944, **27**, 1561 (*isol, synth*)
Seifert, R.M. *et al., J. Agric. Food Chem.*, 1968, **16**, 880 (*synth*)
Hariel, J. *et al., Soap, Perfum. Cosmet.*, 1969, **42**, 571 (*use*)
Meyers, A.I. *et al., J.O.C.*, 1973, **38**, 36 (*synth*)
Kajiwara, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 1617 (*synth, ir*)
Tadema, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1976, **95**, 66 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 769 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NMV760; NMV775
Shieberle, P. *et al., J. Food Sci.*, 1990, **55**, 193-195 (*isol*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1991, 567 (*synth, ir, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 595-596 (*di-Et acetal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1966-1968 (*di-Et acetal, occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMV760

3,6-Nonadienal, 9CI N-98

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CHO$
$C_9H_{14}O$ 138.209

(3*E*,6*Z*)-*form* [57386-95-5]
Bp_{22} 94-95°.

(3*Z*,6*Z*)-*form* [21944-83-2]
Constit. of cucumber flavour. Bp_{14} 86-91°.

Kajiwara, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 1617; 1977, **41**, 1481 (*synth, nmr*)
Phillips, D.R. *et al., Phytochemistry*, 1978, **17**, 355

2,4-Nonadien-1-ol, 9CI N-99

[62488-56-6]
FEMA 3951
$H_3CCH_2CH_2CH_2CH{=}CHCH{=}CHCH_2OH$
$C_9H_{16}O$ 140.225
Food flavourant (presumably as mixt. of geom. isomers) for a variety of foods. Liq. with fatty/green taste.

(2*E*,4*E*)-*form* [64576-90-5]
Oil. $Bp_{0.3}$ 80°.

Ac: [72648-91-0]
$C_{11}H_{18}O_2$ 182.262
Oil.

(2*E*,4*Z*)-*form* [16195-69-0]
Oil. d_4^{20} 0.88. $Bp_{0.03}$ 50°. n_D^{20} 1.4885.

1-Naphthylcarbamoyl:
Cryst. (heptane). Mp 73-74°.

(2*Z*,4*E*)-*form* [106335-88-0]
Liq. $Bp_{0.1}$ 50° (bulb).

(2*Z*,4*Z*)-*form* [106335-90-4]
Liq. $Bp_{0.1}$ 50° (bulb).

(2ξ,4ξ)-*form*
Isol. from cucumber.

Bergelson, L.D. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1967, 843-850; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1967, 810-815 (*2E,4Z-form, synth, uv*)
Petragnani, N. *et al., Farmaco, Ed. Sci.*, 1977, **32**, 627-634 (*2E,4E-form, synth, pmr*)
Stille, J.K. *et al., J.A.C.S.*, 1987, **109**, 813-817 (*2Z,4E-form, 2Z,4Z-form, synth, pmr, cmr*)
Ishii, Y. *et al., J.O.C.*, 1993, **58**, 6818-6825 (*Ac, synth, pmr, cmr*)
Kazmaier, U. *et al., Tetrahedron*, 1998, **54**, 1491-1496 (*2E,4E-form, synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1298
Li, T.S.C. *et al., Chinese and Related North American Herbs*, CRC Press, 2002, 50 (*occur*)

2,6-Nonadien-1-ol, 9CI N-100

[7786-44-9]
FEMA 2780
$H_3CCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2OH$
$C_9H_{16}O$ 140.225
Flavouring ingredient.

(2*E*,6*E*)-*form* [5820-89-3]
$Bp_{2.5}$ 58° (lit. gives a pressure range).
Benzoyl:
$C_{16}H_{20}O_2$ 244.333
Liq. $Bp_{0.3}$ 137°.

(2*E*,6*Z*)-*form* [28069-72-9] *Violet alcohol. Cucumber alcohol. Violet-leaf alcohol*
Found in *Cucumis sativus* (cucumber), watermelon and prickly pear. Flavouring agent. Liq. with intense violet/green odour. Bp_{11} 98-100°. n_D^{25} 1.4631.
▶ Skin irritant. LD_{50} (mus, orl) > 5000 mg/kg. RA5394000

Ac: [68555-65-7] *FEMA 3952*
$C_{11}H_{18}O_2$ 182.262
Flavouring ingredient. Oil with green apple/melon odour and flavour. Bp_{15} 75°.

(2*Z*,6*Z*)-*form*
Isol. from violet leaves and peppermint oil. Oily liq. Bp_{24} 108-110°.

Ruzicka, L. *et al., Helv. Chim. Acta*, 1944, **27**, 1561 (*struct*)
Zobrist, F. *et al., Helv. Chim. Acta*, 1952, **35**, 2380 (*synth*)
Sondheimer, F. *et al., J.A.C.S.*, 1952, **74**, 4040 (*synth*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1965, **42**, 637 (*synth*)
Ali, M.E. *et al., Sci. Res. (Dacca)*, 1968, **5**, 91 (*isol*)
Kemp, T.R. *et al., J. Agric. Food Chem.*, 1974, **22**, 717
Kemp, T.R. *et al., Phytochemistry*, 1975, **14**, 2637 (*isol*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 771 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NMV780
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1969
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1299-1300; 1302 (*Ac*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

3,6-Nonadien-1-ol N-101

[76649-25-7]
$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2OH$
$C_9H_{16}O$ 140.225

(3*E*,6*Z*)-*form* [56805-23-3]
FEMA 3884
Found in prickly pear. Food flavour. Oil with fatty, cucumber, green pepper odour.
Ac: [211323-05-6] *FEMA 3953*
$C_{11}H_{18}O_2$ 182.262
Food flavour. Oil with fresh green odour. Bp_{15} 75°.

(3*Z*,6*E*)-*form* [53250-56-9]

(3*Z*,6*Z*)-*form* [53046-97-2]
FEMA 3885
Found in melon and cucumber. Food flavour. Bp_{13} 110°.

Kemp, T.R. *et al., J. Agric. Food Chem.*, 1974, **22**, 717-718 (*3Z,6Z-form, isol*)
Kemp, T.R. *et al., Phytochemistry*, 1974, **13**, 1167-1170 (*3Z,6Z-form, isol*)
Kajiwara, T. *et al., Agric. Biol. Chem.*, 1975, **39**, 1617-1621; 1977, **41**, 1481-1484 (*3Z,6Z-form, isol, 3E,6Z-form, synth*)
Nation, J.L. *et al., Environ. Entomol.*, 1975, **4**, 27-30 (*3Z,6Z-form, isol, pharmacol*)
Hatanaka, A. *et al., Phytochemistry*, 1975, **14**, 2589-2592 (*3Z,6Z-form, occur, biosynth*)
Flath, R.A. *et al., J. Agric. Food Chem.*, 1978, **26**, 835-837 (*3E,6Z-form, isol*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1300-1302 (*use*)

Nonanal, 9CI N-102

[124-19-6]
Nonyl aldehyde. Pelargonaldehyde. FEMA 2782
$H_3C(CH_2)_7CHO$
$C_9H_{18}O$ 142.241
Found in various plant sources incl. fresh fruits, citrus peels, cassava (*Manihot esculenta*), rice (*Oryza sativa*). Flavouring ingredient. Liq. with sharp, pleasant odour. d_4^2 0.83. Bp 190-192° Bp_{22} 91-92°. n_D^{20} 1.4240. Polymerises readily with H_2SO_4. Oxidised fairly rapidly in air.
▶ Skin irritant. RA5700000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 732A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 468D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 555B (*ir*)
Aldrich Library of NMR Spectra, **2**, 98A (*pmr*)
Sadtler Standard C-13 NMR Spectra, 8607 (*cmr*)
Scanlan, J.T. *et al., J.A.C.S.*, 1940, **62**, 2305 (*synth*)
Fleet, G.W.J. *et al., Tet. Lett.*, 1972, 3749 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 115 (*rev, tox*)
Botteghi, C. *et al., Chim. Ind. (Milan)*, 1977, **59**, 839 (*synth*)
Johnstone, R.A.W. *et al., Chem. Comm.*, 1978, 354 (*synth*)
Sato, F. *et al., Chem. Lett.*, 1979, 167 (*synth*)
Bowen, R.D. *et al., Org. Mass Spectrom.*, 1983, **18**, 576 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, NMW500
Katritzky, A.R. *et al., J.O.C.*, 1991, **56**, 2143 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMW500

Nonane, 9CI N-103

[111-84-2]
$H_3C(CH_2)_7CH_3$
C_9H_{20} 128.257
Present in numerous plant oils incl. olive oils. Liq. d_4^{20} 0.72. Fp -51. Bp 150.8°.
▶ Narcotic in high concs., flammable, fl. p. 30/31°, autoignition temp. 205°. RA6115000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 2B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 2B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 3B (*ir*)
Mathis, C. *et al., Phytochemistry*, 1964, **3**, 133-141 (*occur*)
Kajdas, C. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1971, **45**, 1771-1775 (*ms*)
Norman, N. *et al., Acta Chem. Scand.*, 1972, **26**, 3913-3916 (*cryst struct*)
Deshayes, H. *et al., Chem. Comm.*, 1975, 439-440 (*synth*)
Baker, A. *et al., Helv. Chim. Acta*, 1977, **60**, 2958-2963 (*synth*)
Boese, R. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 988-992 (*cryst struct*)
Low, L.K. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 318 (*rev, tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 940
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMX000

Nonanedioic acid, 9CI N-104

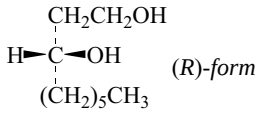
[123-99-9]
*1,7-Heptanedicarboxylic acid. **Azelaic acid, INN, USAN**. Anchoic acid. Lepargylic acid. Emerox 1144. Skinoren. ZK 62498*
$HOOC(CH_2)_7COOH$
$C_9H_{16}O_4$ 188.223
Occurs in rancid fats. Isol. from a few higher plants. Launched 1989Needles or leaflets. Spar. sol. H_2O, Et_2O, C_6H_6; sol. EtOH; Me_2CO. Mp 106.5°. Bp 360° part. dec. Bp_{10} 226°. pK_{a1} 4.56; pK_{a2} 5.53 (25°, 0.1*M* KNO_3). Log P 1.48 (calc). Not steam-volatile.
▶ Skin and eye irritant. CM1980000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 496C; 696D; 842B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 772B; 946B; 1121B; 1357C (*nmr*)
Ger. Pat., 1933, 565 158; *CA*, **27**, 1008 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 53 (*synth*)
Mowry, D.T. *et al., J.A.C.S.*, 1950, **72**, 4439 (*synth*)
Housty, J. *et al., Acta Cryst.*, 1967, **22**, 288 (*cryst struct*)
Mingrone, G. *et al., Drugs Exp. Clin. Res.*, 1983, **9**, 447 (*tox*)
Breathnach, A.S. *et al., Br. J. Dermatol.*, 1984, **111**, 115 (*rev, pharmacol*)
Fukushima, K. *et al., J. Mol. Struct.*, 1986, **146**, 61 (*Raman*)
Řezanka, T. *et al., J. Chromatogr.*, 1987, **408**, 145 (*ms*)
Zakharkin, L.I. *et al., Zh. Org. Khim.*, 1987, **23**, 1328; *J. Org. Chem. USSR (Engl. Transl.)*, 1987, **23**, 1201 (*synth*)
Fitton, A. *et al., Drugs*, 1991, **41**, 780 (*rev, pharmacol*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **8**, 118 (*rev*)
Merwin, L.H. *et al., Magn. Reson. Chem.*, 1992, **30**, 440 (*cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 755
Cotarca, L. *et al., Synthesis*, 1997, 328 (*synth, ir, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ASB750

1,3-Nonanediol, 9CI, 8CI N-105

[23433-07-0]

[121541-59-1]



(*R*)-*form*

$C_9H_{20}O_2$ 160.256

▶RA6475650

(*R*)-*form* [121541-65-9]
Liq. $Bp_{0.1}$ 97-99°. $[\alpha]_D^{22}$ -6 (neat). $[\alpha]_D$ -6.3 (c, 10.0 in EtOH).

(±)-*form* [121651-87-4]
Oil. Bp_{12} 144-146° $Bp_{0.8}$ 90-92°.

N-*Phenylcarbamate:*
Cryst. (2,2,4-trimethylpentane). Mp 83-84.5°.

Bis-N-*phenylcarbamate:*
Cryst. (2,2,4-trimethylpentane). Mp 85-85.5°.

Mono-Ac: [1322-17-4] *FEMA 2783*
$C_{11}H_{22}O_3$ 202.293
Flavouring ingredient. Liq. with an intense floral odour. Mixt. of the 1- and 3-monoacetates.

Di-Ac: [63270-14-4]
$C_{13}H_{24}O_4$ 244.33

Bendz, G. *et al., Acta Chem. Scand.*, 1957, **11**, 903 (*synth*)
Diaper, D.G.M. *et al., Can. J. Chem.*, 1960, **38**, 1976 (*synth*)
Kuleszi, J. *et al., Riechst., Aromen, Koerperpflegem.*, 1969, **19**, 157; *CA*, **71**, 49865r (*synth*)
Akedo, M. *et al., J. Food Sci.*, 1977, **42**, 699; *CA*, **87**, 48469h (*use*)
Kitching, W. *et al., J.O.C.*, 1989, **54**, 3893-3902 (*synth, isol, cmr, pmr, ms*)
Perkins, M.V. *et al., J.C.S. Perkin 1*, 1990, 1111-1117 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 598 (*mono-Ac*)
Kula, J. *et al., Tetrahedron*, 1996, **52**, 11321-11324 (*synth, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1972-1973 (*mono-Ac*)
Kula, J. *et al., Synth. Commun.*, 2001, **31**, 463-467 (*R-form, synth*)

1,4-Nonanediol, 9CI N-106

$C_9H_{20}O_2$ 160.256

(*R*)-*form* [156041-92-8]
$[\alpha]_D^{22}$ +0.6 (c, 0.82 in MeOH) (96% ee).

(±)-*form* [145475-09-8]
d_4^{20} 0.93. Bp_4 133°. n_D^{20} 1.4547.

Di-Ac: [67715-81-5]
$C_{13}H_{24}O_4$ 244.33
Flavouring ingredient.

4-Trimethylsilyl ether: [157870-96-7]
$C_{12}H_{28}O_2Si$ 232.438
$Bp_{0.3}$ 94-95° (bath).

Bukharov, V.G. *et al., Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1961, 135-140; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1961, 119-122 (*synth*)
Nikishin, G.I. *et al., Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1962, 831-834; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1962, 892-897 (*synth*)
Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32(2)**, 60-62; 64-66; 68-70 (*di-Ac, use*)
Ager, D.J. *et al., Chem. Comm.*, 1982, 248-249 (*synth*)
Matsumoto, K. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 1694-1700 (*trimethylsilyl ether*)
Molander, G.A. *et al., J.O.C.*, 1994, **59**, 2676-2678 (*R-form, synth, pmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 599 (*di-Ac, use*)

2,4-Nonanedione, 9CI, 8CI N-107

[6175-23-1]
Caproylacetone
$H_3CCOCH_2CO(CH_2)_4CH_3$
$C_9H_{16}O_2$ 156.224
Light-induced degradn. product of soybean oil. Liq. Fp -18. Bp 211-213° Bp_{20} 105-106° Bp_4 78°. pK_{a1} 9.2 (20°, c 0.01).

Cu complex:
Blue cryst. Sol. org. solvs. Mp 136° (139°).

Swamer, F.W. *et al., J.A.C.S.*, 1950, **72**, 1352 (*synth*)
Bertrand, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 2533 (*synth*)
Org. Synth., Coll. Vol., 5, 1973, 848 (*synth*)
Douglas, D.E. *et al., Lipids*, 1977, **12**, 635 (*synth*)
Guth, H. *et al., Fat Sci. Technol.*, 1989, **91**, 225-230 (*occur, soybean oil*)

1,9-Nonanedithiol, 9CI N-108

[3489-28-9]
1,9-Dimercaptononane. FEMA 3513
$HSCH_2(CH_2)_7CH_2SH$
$C_9H_{20}S_2$ 192.389
Flavouring ingredient. Liq. with heavy odour. Mp -17.5°. Bp 284° Bp_{50} 175-178°. n_D^{20} 1.4999.

Bis-2,4-dinitrophenyl:
Cryst. Mp 131-132°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 261C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 421B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 343C (*ir*)
Hall, W.P. *et al., J.A.C.S.*, 1943, **65**, 1466 (*synth*)
Grogan, C.H. *et al., J.O.C.*, 1955, **20**, 50 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 599
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1973-1974

Nonanoic acid, 9CI N-109

[112-05-0]
Nonoic acid. Pelargonic acid. Octane-1-carboxylic acid. Nonylic acid. FEMA 2784
$H_3C(CH_2)_7COOH$
$C_9H_{18}O_2$ 158.24
Flavouring ingredient. Oily, irritant liq. with characteristic odour and unpleasant taste. d_4^{20} 0.91. Mp 15° Fp 12.24. Bp 255° Bp_1 98.9°. n_D^{20} 1.4309. pK_a 4.95. Spar. steam-volatile.

▶Skin and eye irritant. LD_{50} (mus, orl) 15000 mg/kg. RA6650000

NH_4 salt: [63718-65-0]
Solid (H_2O). Mp 115°.

Me ester: [1731-84-6] *FEMA 2724*
$C_{10}H_{20}O_2$ 172.267
Flavouring ingredient. Isol. from cloves, hops, hyssop oil, vanilla and some wines. Liq. with a wine and coconut-like odour. Insol. H_2O, sol. EtOH, Et_2O. d^{18} 0.88. Mp -35°. Bp 213.5-214° Bp_8 88-91°. n_D^{25} 1.4302.

▶RA6906000

Et ester: [123-29-5] *FEMA 2447*
$C_{11}H_{22}O_2$ 186.294
Flavouring ingredient. Present in pineapple, banana and apple. Liq. with an odour reminiscent of cognac with a rosy-fruity note. Mp -44.5°. Bp 228° Bp_{10} 100-103°.

▶RA6845000

Propyl ester: [6513-03-7] *Propyl nonanoate*
$C_{12}H_{24}O_2$ 200.32
d 0.86. Bp 237°.

Isopropyl ester: [28267-32-5] *Isopropyl nonanoate*
$C_{12}H_{24}O_2$ 200.32
Used in food flavouring. d 0.86. Bp 228°.

2-Methylpropyl ester: [55195-29-4] *2-Methylpropyl nonanoate. Isobutyl pelargonate*
$C_{13}H_{26}O_2$ 214.347
Oil with fruity odour. d 0.86. Bp 260°.

3-Methylbutyl ester: [7779-70-6] *3-Methylbutyl nonanoate. Isoamyl pelargonate*
$C_{14}H_{28}O_2$ 228.374
Present in banana (*Musa sapientum*). Flavouring ingredient. Oil with a fruity cognac-rum flavour.

8-Methylnonyl ester: [109-32-0] *Emolein*
$C_{19}H_{38}O_2$ 298.508

Vinyl ester: [6280-03-1]
$C_{11}H_{20}O_2$ 184.278
Liq. d^{25} 0.87. $Bp_{1.5}$ 65°. n_D^{30} 1.4291. Q/e values for radical polym., Q 0.030, e -0.68.

2-Propenyl ester: [7493-72-3] *FEMA 2036*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. with a characteristic fruity aroma (cognac, pineapple). d_4^{30} 0.87. Bp 230°. n_D^{30} 1.4302.

4-Bromophenacyl ester: [35300-70-0]
Cryst. (EtOH). Mp 68.5°.

Chloride: [764-85-2]
$C_9H_{17}ClO$ 176.685
Liq. Fp -60.5. Bp 215° Bp_{15} 98°.

Amide: [1120-07-6] *Nonanamide, 9CI*
$C_9H_{19}NO$ 157.255
Cryst. Insol. cold H_2O. Mp 92-93° (98.9°).

Nitrile: [2243-27-8] *Nonanenitrile, 9CI. 1-Cyanooctane. Pelargononitrile. Octyl cyanide*
$C_9H_{17}N$ 139.24
Liq. Fp -34.2. Bp 224° Bp_{15} 102-105°. n_D^{20} 1.4260.

▶LD_{50} (mus, orl) 2059 mg/kg. RA6606000

Anhydride: [1680-36-0]
$C_{18}H_{34}O_3$ 298.465
Liq. Fp 5 (16°). Bp_{15} 207°.

[14047-60-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 483B; 607D; 730B; 839D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 754A; 922B; 922C; 1195C; 1354C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 575C; 625D; 626A; 798D (*ir*)
Aldrich Library of NMR Spectra, **2**, 147A (*pmr*)

Deffet, L. *et al., Bull. Soc. Chim. Belg.*, 1931, **40**, 385 (*props*)
Swern, D. *et al., J.A.C.S.*, 1948, **70**, 2334 (*2-propenyl ester*)
Marvel, C.S. *et al., J. Polym. Sci.*, 1958, **27**, 39 (*vinyl ester*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1976, **17**, 1 (*cmr*)
Foglia, T.A. *et al., J. Am. Oil Chem. Soc.*, 1977, **54**, 858A (*ester, synth*)
Krapcho, A.P. *et al., J.O.C.*, 1977, **42**, 3749 (*synth*)
Miyazaki, S. *et al., J. Am. Oil Chem. Soc.*, 1978, **55**, 536 (*synth*)
Evans, D.A. *et al., J.A.C.S.*, 1979, **101**, 371 (*Me ester, synth, ir, pmr*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*vinyl ester, polym*)
Jiricny, J. *et al., J.C.S. Perkin 1*, 1980, 1487 (*nitrile*)
Bowen, R.D. *et al., Org. Mass Spectrom.*, 1983, **18**, 576 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 381; **2**, 29; 257; 531; 600 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 96-97; 1022-1023; 1430; 1807; 1974-1975 (*esters*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Pesticide Manual, 12th edn., 2000, No. 565
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ENW000; NMY000

1-Nonanol, 9CI N-110

[143-08-8]

[28473-21-4]
Nonyl alcohol, 8CI. FEMA 2789

$H_3C(CH_2)_7CH_2OH$

$C_9H_{20}O$ 144.256

Widespread in nature. Occurs in oils of orange, citronella and lemon. Also found in cheese, prickly pears and bread. Flavouring agent. Colourless to yellow liq. with odour of citronella oil. Misc. EtOH, Et_2O, prac. insol. H_2O. d_4^{20} 0.83. Fp -5. Bp 215° $Bp_{7.5}$ 95.6°. n_D^{20} 1.4330. Isononanol (Nonanol N) is a mixt. of nonanol isomers marketed as a solvent.

▶ LD_{50} (mus, orl) 6400 mg/kg. RB1575000

Ac: [143-13-5] *FEMA 2788*
$C_{11}H_{22}O_2$ 186.294
Found in citrus peel oils, kumquat peel oil, wine grapes, apple, melon, milk, beer, gruyere cheese and pepino fruits (*Solanum muricaturm*). Liq. Bp 223.6-224.3° Bp_{10} 101-102°.

2-Methylpropanoyl: [10522-34-6] *Nonyl 2-methylpropanoate, 9CI*
$C_{13}H_{26}O_2$ 214.347
d 0.86. Bp 220°.

Octanoyl: [7786-48-3] *Nonyl octanoate. Nonyl caprylate. FEMA 2790*
$C_{17}H_{34}O_2$ 270.454
Used in food flavouring. Colourless oily liq. with strong bitter orange flavour. d 0.86. Bp 312°.

3,5-Dinitrobenzoyl:
Cryst. Mp 52.2°.

Me ether: [7289-51-2] *1-Methoxynonane, 9CI*
$C_{10}H_{22}O$ 158.283
Liq. Bp_{10} 73-75°.

Et ether: [16979-32-1] *1-Ethoxynonane, 9CI*
$C_{11}H_{24}O$ 172.31
Liq. Bp_{10} 88-91°.

[27458-94-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 111B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 165C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 157C (*ir*)
Aldrich Library of NMR Spectra, **1**, 81A (*pmr*)
Morel, C. *et al., Soap, Perfum. Cosmet.*, 1952, **25**, 512 (*2-methylpropanoyl, octanoyl*)
Sousa, J.A. *et al., J.O.C.*, 1960, **25**, 108 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
McKillop, A. *et al., Tetrahedron*, 1974, **30**, 2467 (*Ac, ethers, synth*)
Seebach, D. *et al., Angew. Chem., Int. Ed.*, 1976, **15**, 438 (*synth*)
Kikugawa, Y. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1939 (*synth*)
Normant, J.F. *et al., Tet. Lett.*, 1977, 3263 (*synth*)
Mikaya, A.I. *et al., Org. Mass Spectrom.*, 1983, **18**, 99 (*ms*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1985, **36**, 253 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1984; 1985 (*occur, props*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 184 (*tox, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NNB400; NNB500

2-Nonanol, 9CI, 8CI N-111

[628-99-9]

[28473-21-4]
FEMA 3315

$C_9H_{20}O$ 144.256

Isol. from various essential oils, orange (*Citrus sinensis*), ginger (*Zingiber officinale*), coconut (*Coces nucifera*). Also present in guava fruit, raw asparagus, various cheeses and wines.

(S)-form [70419-06-6]
Bp_{19} 105°. $[\alpha]_D^{20}$ +11.9 (C_6H_6).

(±)-*form* [74683-66-2]
Fp -35. Bp 193-194° Bp_{10} 84-86°.

Ac: [14936-66-4]
$C_{11}H_{22}O_2$ 186.294
Bp_{30} 108-109°.

3,5-Dinitrobenzoyl:
Mp 43-45°.

Me ether: [54894-33-6] *2-Methoxynonane*
$C_{10}H_{22}O$ 158.283
Bp 186-188°.

[70419-07-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 121B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 182A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 170A (*ir*)
Pickard, R.H. *et al., J.C.S.*, 1911, **99**, 56; 70 (*synth*)
Keil, W. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1942, **274**, 175 (*synth*)
Nair, G.V. *et al., Can. J. Chem.*, 1959, **37**, 1608; 1960, **38**, 177 (*isol*)
McKillop, A. *et al., Tetrahedron*, 1974, **30**, 2467 (*synth*)
Millon, J. *et al., Tet. Lett.*, 1976, 1095 (*synth*)
Normant, J.F. *et al., Bull. Soc. Chim. Fr.*, 1980, 289 (*synth*)
Keinan, E. *et al., J.A.C.S.*, 1986, **108**, 162 (*synth*)
Mori, K. *et al., Annalen*, 1994, 1065 (*S-form*)
Nakamura, K. *et al., J.C.S. Perkin 1*, 2000, 3205-3211 (*S-form, synth, ir, pmr*)

3-Nonanol, 9CI N-112

[624-51-1]

[28473-21-4]
Ethylhexylcarbinol

$C_9H_{20}O$ 144.256

Constit. of Scotch spearmint oil and yarrow oil from *Achillea fragrantissima*.

(R)-form [61925-50-6]
$[\alpha]_D^{24}$ -7.4 (c, 8.1 in $CHCl_3$).

(S)-form [61925-49-3]
$[\alpha]_D^{24}$ +9.6 (c, 8.3 in $CHCl_3$).

(±)-*form* [74742-08-8]
Bp_{20} 94°. n_D^{20} 1.4279.

3,5-Dinitrobenzoyl:
Mp 44-45°.

Shalaby, A.F. *et al., J. Pharm. Sci.*, 1964, **53**, 1502; *CA*, **62**, 3879h (*isol*)
Thewalt, K. *et al., J. Prakt. Chem.*, 1964, **26**, 237 (*synth*)
Mukaiyama, T. *et al., Chem. Lett.*, 1976, 893 (*synth*)
Cammert, M.C. *et al., J. Insect Physiol.*, 1978, **24**, 207; *CA*, **90**, 19298u
Japan. Pat., 1978, 78 25 502; *CA*, **89**, 42412d (*synth*)
Spieler, J. *et al., Eur. J. Org. Chem.*, 2000, 391-399 (*R-form, synth, pmr*)

2-Nonanone, 9CI N-113

[821-55-6]
FEMA 2785

$H_3C(CH_2)_6COCH_3$

$C_9H_{18}O$ 142.241

Present in banana, ginger, Brazil nut, attar of rose, clove oil, coconut oil, passionflower, sorghum, asparagus, tomato, corn, wine, cheese, beer, blackcurrant buds, melon, strawberry jam etc. Flavouring ingredient. Oil with rue-like odour and rose/tea-like flavour. Fp -15. Bp 194-196° Bp_{12} 75-77°. n_D^{20} 1.4175.

▶ LD_{50} (rat, orl) 3200 mg/kg. RA8225000

Oxime: [52435-37-7]
$C_9H_{19}NO$ 157.255
Liq. or cryst. Mp 16°. Bp_{15} 131°.

Semicarbazone: [818-06-4]
Solid. Mp 119-120°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 374C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 410D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 495C (*ir*)
Morgan, G.T. *et al., J. Soc. Chem. Ind., London*, 1925, **44**, 108T (*synth*)
Carpenter, W. *et al., J.A.C.S.*, 1967, **89**, 6167 (*ms*)
Olah, G.A. *et al., Synthesis*, 1977, 419 (*synth*)
Demuth, M. *et al., Helv. Chim. Acta*, 1978, **61**, 3136 (*synth*)
Sonnek, G. *et al., J. Prakt. Chem.*, 1978, **320**, 341 (*synth*)
Sato, F. *et al., Chem. Lett.*, 1979, 167 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 393 (*rev, tox*)

Rasmussen, L.E.L. *et al., J. Chem. Ecol.*, 1990, **16**, 2167
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1976-1977 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NMY500

3-Nonanone N-114

[925-78-0]
FEMA 3440
$H_3C(CH_2)_5COCH_2CH_3$
$C_9H_{18}O$ 142.241
Flavouring ingredient. Present in banana, passion fruit and cooked beef. Liq. with a pungent, leafy/fruity flavour. d^{20} 0.83. Fp -8. Bp 190° Bp_{20} 86°. n_D^{20} 1.4208.

Oxime: [22418-72-0]
$C_9H_{19}NO$ 157.255
Liq. Bp_1 70°.

Phenylhydrazone:
Amber oil. Bp_{15} 190-192°.

Semicarbazone: [1669-37-0]
Cryst. (EtOH aq.). Mp 111-112°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 411A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 639B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 495D (*ir*)
Pickard, R.H. *et al., J.C.S.*, 1913, **103**, 1923 (*synth*)
Kraft, M. *et al., Org. Mass Spectrom.*, 1968, **1**, 617 (*ms*)
Yamamoto, Y. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 3682 (*synth, ir, pmr*)
Masuyama, Y. *et al., Tet. Lett.*, 1976, 2967 (*synth*)
Cammaerts, M.C. *et al., J. Insect Physiol.*, 1978, **24**, 207 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 601
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1977-1978

4-Nonanone, 9CI N-115

[4485-09-0]
Amyl propyl ketone. Pentyl propyl ketone
$H_3C(CH_2)_4CO(CH_2)_2CH_3$
$C_9H_{18}O$ 142.241
Isol. from lemongrass. Liq. Bp 187-188° Bp_{20} 75-76°.

Semicarbazone:
Cryst. (EtOH or petrol). Mp 73-74° (rapid heat) (67°, 145°).

4-Nitrophenylhydrazone:
Unstable yellow cryst. (EtOH) or light yellow plates (petrol). Mp 84-85°.

Bryant, S.A. *et al., J.C.S.*, 1931, 2080 (*synth*)
Brodman, B.W. *et al., Sep. Sci. Technol.*, 1967, **2**, 139 (*cryst struct*)
Soussan, G. *et al., Bull. Soc. Chim. Fr.*, 1972, 4228 (*synth*)
Sheikh, M.Y. *et al., Tet. Lett.*, 1972, 257 (*synth*)
McAdoo, D.J. *et al., Org. Mass Spectrom.*, 1974, **9**, 525 (*ms*)
Kende, A.S. *et al., Synth. Commun.*, 1978, **8**, 59 (*synth*)

2-Nonenal, 9CI N-116

[2463-53-8]
FEMA 3213
$H_3C(CH_2)_5CH{=}CHCHO$
$C_9H_{16}O$ 140.225

(E)-form [18829-56-6]
Widespread in nature, in beer, coffee, watermelon, cucumbers, redcurrants, orris oil, palm oil, potatoes etc. Flavouring ingredient. Liq. $Bp_{11.5}$ 88-90° (lit. gives a pressure range).
▶ RA8509050

Semicarbazone: [16742-24-8]
Small needles (MeOH).

2,4-Dinitrophenylhydrazone: [18287-00-8]
Orange-red needles (EtOH). Mp 126°.

(Z)-form [60784-31-8]
No phys. props. reported.

Semicarbazone:
Cryst. (MeOH). Mp 141°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 473B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 739A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 562A (*ir*)
Gamboni, G. *et al., Helv. Chim. Acta*, 1958, **41**, 1603 (*synth*)
Forss, D.A. *et al., Aust. J. Chem.*, 1962, **15**, 163 (*synth, ir, uv*)
Wada, M. *et al., Chem. Lett.*, 1977, 345 (*synth*)
Bestmann, H.J. *et al., Tet. Lett.*, 1977, 121 (*synth, pmr*)
Ficini, J. *et al., Tet. Lett.*, 1977, 3589 (*synth*)
Goodrich, B.S. *et al., J. Chem. Ecol.*, 1978, **4**, 581 (*isol*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 775 (*rev, tox*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1991, 567 (*synth, ir, pmr*)
Kula, J. *et al., J. Am. Oil Chem. Soc.*, 1993, **70**, 643 (*synth*)
Fortes, C.C. *et al., Synth. Commun.*, 1997, **27**, 3917-3941 (*synth, ir, pmr, cmr, ms*)

6-Nonenal N-117

$H_3CCH_2CH{=}CH(CH_2)_4CHO$
$C_9H_{16}O$ 140.225

(Z)-form [2277-19-2]
FEMA 3580
Flavour component of melon (*Cucumis melo*). Also present in cucumber (*Cucumis sativus*), raw lean fish and pepino fruit (*Solanum muricaturm*). Flavouring agent. Liq. with citrus, melon odour. Bp_{17} 83°.
▶ Skin irritant. LD_{50} (mus, orl) >5000 mg/kg. RA8509200

Meyboom, P.W. *et al., J. Am. Oil Chem. Soc.*, 1971, **48**, 143
Kemp, T.R. *et al., Phytochemistry*, 1972, **11**, 3321 (*isol*)
Kemp, T.R. *et al., J. Agric. Food Chem.*, 1974, **22**, 717 (*isol*)
Yasud, K. *et al., J. Am. Oil Chem. Soc.*, 1975, **52**, 307
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 777 (*rev, tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NNA325

1-Nonene, 9CI N-118

[124-11-8]

[27215-95-8]
$H_3C(CH_2)_6CH{=}CH_2$
C_9H_{18} 126.241
Isol. from peaches and beef. Liq. d^{21} 0.73. Fp -88 (-82.2°). Bp 146° Bp_{15} 50°. n_D^{21} 1.4140.
▶ Flammable, fl. p. 26° (oc).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 19A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 14B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 19B (*ir*)
Tschinkel, W.R. *et al., J. Insect Physiol.*, 1975, **21**, 659; 753 (*isol*)
Westmijze, H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1976, **95**, 299 (*synth*)
Miyaura, N. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 2199 (*synth*)
Roberts, J.L. *et al., Tet. Lett.*, 1977, 1299 (*synth*)
Sato, F. *et al., J. Organomet. Chem.*, 1978, **157**, C30 (*synth*)
Muurisepp, A. *et al., Zh. Org. Khim.*, 1978, **14**, 2017 (*ms*)

7-Nonene-3,5-diyn-1-ol, 9CI N-119

[90535-88-9]
$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH_2CH_2OH$
$C_9H_{10}O$ 134.177
Isol. from a mixed culture of *Lentinus edodes* (shiitake) and the pathogen *Trichoderma*.

Tokimoto, K. *et al., Proc. Jpn. Acad., Ser. B*, 1987, **63**, 277-280 (*isol*)

2-Nonenoic acid, 9CI, 8CI N-120

[3760-11-0]
$H_3C(CH_2)_5CH{=}CHCOOH$
$C_9H_{16}O_2$ 156.224
Occurs in mushrooms.

(E)-form [14812-03-4]
FEMA 3954
Isol. from Scotch spearmint oil (*Mentha gracilis*). Flavouring ingredient. Liq. Spar. sol. H_2O. Mp 1-2° (4°). Bp_{14} 146°. Steam volatile.

Me ester: [111-79-5] *Methyl 2-nonenoate. Neofolione. FEMA 2725*
$C_{10}H_{18}O_2$ 170.251
Flavouring ingredient. Liq. with violet-like odour. Insol. H_2O. d_{25}^{25} 0.9. Bp_5 80°.
▶ RA9470000

Et ester: [38112-59-3]
$C_{11}H_{20}O_2$ 184.278
Food preservative (prob. as isomeric mixt. with *Z*-form). Liq. Sol. Et_2O, THF, hexane. Bp_{20} 114°.

4-Bromophenacyl ester:
Cryst. Mp 77.5-78°.

Chloride: [60784-27-2]
$C_9H_{15}ClO$ 174.67
Liq. $Bp_{0.4}$ 70-72°.

Amide: [14952-05-7]
$C_9H_{17}NO$ 155.239
Cryst. (C_6H_6). Mp 131.5° (118-119°). $Bp_{0.73}$ 120° subl..

(Z)-form [1577-98-6]
Liq. at -15°. Fp 2-3. Bp_{15} 140°.

Et ester: [72284-17-4]
Liq. Bp_{15} 108°.

Amide:
Cryst. (C_6H_6). Mp 74-74.5°.

[764-86-3, 17463-01-3]

Blum, M.S. *et al., J. Insect Physiol.*, 1971, **17**,

349 (*use*)
Org. Synth., 1973, **53**, 123 (*synth*)
Katzenellenbogen, J.A. *et al., J.A.C.S.*, 1974, **96**, 6153 (*synth, ir, ms, pmr, ester*)
Yamada, K. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 3431 (*synth, ms, pmr, ester*)
Lombardo, L. *et al., Synthesis*, 1978, 131 (*synth*)
Lucchetti, J. *et al., Tet. Lett.*, 1978, 2693 (*synth*)
Shen, Y. *et al., Synth. Commun.*, 1997, **27**, 4319-4325 (*Me ester*)
Tsuneya, T. *et al., J. Essent. Oil Res.*, 1998, **10**, 507-516 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MNB750

3-Nonenoic acid, 9CI, 8CI N-121

[4124-88-3]
$H_3C(CH_2)_4CH{=}CHCH_2COOH$
$C_9H_{16}O_2$ 156.224

(*E*)-*form* [28163-88-4]
Liq. Sol. Et_2O, insol. H_2O. Fp -4.4. Bp_1 106°.

Me ester: [36781-67-6]
Liq. $Bp_{0.5}$ 69-71°.

4-Bromophenacyl ester:
Cryst. Mp 68.2-69.3°.

Chloride: [764-87-4]
$C_9H_{15}ClO$ 174.67
Liq. $Bp_{4.5}$ 80-81°. Assignment of these props. to the *E*-isomer is not certain.

Amide:
$C_9H_{17}NO$ 155.239
Cryst. (EtOH). Mp 74.5-75°. Assignment of these props. to the *E*-isomer is not certain.

(*Z*)-*form* [41653-98-9]

Me ester: [41654-16-4]

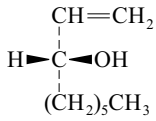
(ξ)-*form*
Isol. from grapes and strawberries.

Me ester: [13481-87-3] *FEMA 3710*
Isol. from guava and hop oil. Flavouring ingredient. Liq. with watermelon-like odour.

Morton, A.A. *et al., J.A.C.S.*, 1950, **72**, 3785 (*synth*)
Groff, T.M. *et al., Ark. Kemi*, 1968, **29**, 179 (*ms, ester*)
Koyama, H. *et al., Agric. Biol. Chem.*, 1972, **36**, 793 (*synth, pmr, ester*)
Kimland, B. *et al., Phytochemistry*, 1973, **12**, 835 (*isol*)
Hattori, R. *et al., Agric. Biol. Chem.*, 1978, **42**, 1351 (*isol*)
Shiota, H. *et al., Koryo*, 1978, **121**, 23 (*isol, ester*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255 (*synth*)
Deng, M.Z. *et al., J.O.C.*, 1992, **57**, 4017-4019 (*E-form Et ester*)
Bulugahapitiya, P. *et al., J.O.C.*, 1997, **62**, 1630-1641 (*E-form Et ester, Z-form Me ester*)
Ragoussis, N. *et al., J.C.S. Perkin 1*, 1998, 3529-3533 (*E-form Me ester, synth, pmr, ir, cmr, ms*)

1-Nonen-3-ol, 9CI N-122

[21964-44-3]
Hexylvinylcarbinol



(*R*)-*form*

$C_9H_{18}O$ 142.241
Isol. from *Petasites japonicus* (sweet coltsfoot).

(*R*)-*form* [79646-41-6]
$[\alpha]_D^{25}$ -17.5 (c, 1.4 in EtOH) (>95% ee).

(±)-*form* [79605-61-1]
Bp 193-194° Bp_{20} 92.5°.

4-Nitrobenzoyl:
Plates (EtOH). Mp 36-37°.

(ξ)-*form*

Ac: [31795-37-6]
$C_{11}H_{20}O_2$ 184.278
Constit. of *Petasites japonicus* (sweet coltsfoot).

[79646-41-6]

Kikuchi, M. *et al., Yakugaku Zasshi*, 1973, **93**, 123-126 (*acetate, isol*)
Dumont, W. *et al., Angew. Chem., Int. Ed.*, 1974, **13**, 804 (*synth*)
Ueno, Y. *et al., Synthesis*, 1980, 1011 (*synth, pmr*)
Martin, V.S. *et al., J.A.C.S.*, 1981, **103**, 6237 (*resoln*)
Halazy, S. *et al., Tet. Lett.*, 1981, 2135 (*synth*)
Boughdady, N.M. *et al., Aust. J. Chem.*, 1987, **40**, 767 (*synth, pmr, ir*)
Gao, Y. *et al., J.A.C.S.*, 1987, **109**, 5765 (*resoln*)
Dittmer, D.C. *et al., J.O.C.*, 1993, **58**, 718 (*synth, pmr, cmr*)

2-Nonen-1-ol N-123

FEMA 3379
$H_3C(CH_2)_5CH{=}CHCH_2OH$
$C_9H_{18}O$ 142.241
Used in food flavouring. Present in melon, cucumber, chicken fat, armagnac, brown algae, nectarine and prickly pear (*Opuntia ficus Indica*).

(*E*)-*form* [31502-14-4]
d_4^{19} 0.85. $Bp_{0.6}$ 68-73°. n_D^{25} 1.4418.

(*Z*)-*form* [41453-56-9]
Bp_{20} 106°.

[22104-79-6]

Zolvist, F. *et al., Helv. Chim. Acta*, 1952, **35**, 2380 (*deriv, E-form*)
Jacobson, M. *et al., J. Med. Chem.*, 1971, **14**, 236 (*synth, E-form*)
Kitching, W. *et al., J.O.C.*, 1989, **54**, 3893 (*pmr, cmr, ms, E-form*)
Daeuble, J.F. *et al., Tet. Lett.*, 1990, **31**, 2397 (*synth, Z-form*)
Subbaraman, A.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 511 (*synth, ir, pmr, Z-form*)
Zhang, Z.-B. *et al., J.C.S. Perkin 1*, 2000, 53-57 (*E-form, synth*)

3-Nonen-1-ol N-124

$H_3C(CH_2)_4CH{=}CHCH_2CH_2OH$
$C_9H_{18}O$ 142.241

(*E*)-*form* [10339-61-4]

(*Z*)-*form* [10340-23-5]
Isol. from cucumber and watermelons. Bp_2 75°.

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 212A (*ir*)
Cavill, G.W.K. *et al., Aust. J. Chem.*, 1966, **19**, 1495 (*isol, synth*)
Jacobson, M. *et al., J. Med. Chem.*, 1971, **14**, 236
Kemp, T.R. *et al., J. Agric. Food Chem.*, 1974, **22**, 717 (*isol*)
Hatanaka, A. *et al., Phytochemistry*, 1975, **14**, 2589 (*isol*)
Kemp, T.R. *et al., Phytochemistry*, 1975, **14**, 2637 (*isol*)
Kocieński, P.J. *et al., J.C.S. Perkin 1*, 1992, 3419 (*synth, ir, pmr*)
Pommier, A. *et al., J.O.C.*, 1995, **60**, 7334 (*synth, pmr, cmr, ir*)

6-Nonen-1-ol N-125

$H_3CCH_2CH{=}CH(CH_2)_4CH_2OH$
$C_9H_{18}O$ 142.241
Liq.

(*E*)-*form* [31502-19-9]
$Bp_{0.1}$ 75-80°.

Ac: [30412-53-4]
$C_{11}H_{20}O_2$ 184.278
Bp_3 89-90°.

(*Z*)-*form* [35854-86-5] *FEMA 3465*
Flavouring ingredient. Present in melon (*Cucumis melo*). Liq.

Jacobson, M. *et al., J. Med. Chem.*, 1971, **14**, 236 (*synth*)
Scholz, D. *et al., Annalen*, 1983, 98 (*synth*)
Buss, A.D. *et al., J.C.S. Perkin 1*, 1987, 2569 (*synth, ir, pmr, ms*)
Brown, H.C. *et al., J.O.C.*, 1988, **53**, 246 (*synth, ir, pmr, cmr*)
Ayrey, P.M. *et al., J.C.S. Perkin 1*, 1992, 3407 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 604
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1981-1982

1-Nonen-4-one, 9CI N-126

[61168-10-3]
$H_3C(CH_2)_4COCH_2CH{=}CH_2$
$C_9H_{16}O$ 140.225
Detected in volatile constituents of *Capsicum annuum grossum*. Bp_{20} 68-71°.

Buttery, R.G. *et al., J. Agric. Food Chem.*, 1969, **17**, 1322 (*ms, glc*)
Sharpless, K.B. *et al., Tet. Lett.*, 1976, 2503 (*synth*)
Fujita, T. *et al., J. Appl. Chem. Biotechnol.*, 1978, **28**, 882 (*synth*)
Watanabe, S. *et al., Yukagaku*, 1979, **28**, 862 (*synth*)
Hegedus, L.S. *et al., Organometallics*, 1982, **1**, 1188 (*synth*)
Arase, A. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 209 (*synth, pmr, ir, ms*)
Wu, C.M. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1172 (*occur*)

2-Nonen-4-one, 9CI N-127

[32064-72-5]
$H_3C(CH_2)_4COCH{=}CHCH_3$
$C_9H_{16}O$ 140.225

(*E*)-*form* [27743-70-0]
Detected in bell pepper and potato volatiles. Liq. Bp_2 100°.

(*Z*)-*form* [71897-99-9]
Liq.

Buttery, R.G. *et al., J. Agric. Food Chem.*, 1969,

17, 1322; 1970, **18**, 538 (*occur, ms*)
Sheikh, Y.M. *et al., Org. Mass Spectrom.*, *Suppl.*, 1970, **4**, 273 (*ms*)
Shetzmiller, S. *et al., Helv. Chim. Acta*, 1973, **56**, 2975 (*synth, pmr, ir, uv, ms*)
Fujita, T. *et al., J. Appl. Chem. Biotechnol.*, 1978, **28**, 882 (*synth*)
Villieras, J. *et al., Synthesis*, 1979, 968 (*synth, pmr*)
Hooz, J. *et al., Synth. Commun.*, 1980, **10**, 667 (*synth, ir, pmr, ms*)
Hegedus, L.S. *et al., Organometallics*, 1982, **1**, 1188 (*synth*)
Ruel, O. *et al., Tet. Lett.*, 1983, **24**, 4829 (*synth*)
Wu, C.M. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1172 (*occur*)

3-Nonen-2-one, 9CI N-128

[14309-57-0]
FEMA 3955
$H_3C(CH_2)_4CH{=}CHCOCH_3$
$C_9H_{16}O$ 140.225

(*E*)-*form* [18402-83-0]
Detected in many food volatiles . Flavouring ingredient. Food flavourant for confectionery etc., (geom. isom. not specified but presumably *E*-form). Oil with agreeable fruity odour. Bp_{32} 106-107° $Bp_{0.5}$ 49-50°. n_D^{28} 1.4452. n_D^{22} 1.4495.

2,4-Dinitrophenylhydrazone:
Orange-red needles (petrol). Mp 83-85°.

(*Z*)-*form* [39103-04-3]
No phys. props. reported.

[98631-60-8]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 646C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 415C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 501C (*ir*)
Maryvonne, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1959, **249**, 884 (*pmr*)
Sturtz, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 2477 (*synth*)
Sheikh, Y.M. *et al., Org. Mass Spectrom.*, *Suppl.*, 1970, **4**, 273 (*ms*)
Klein, E. *et al., Annalen*, 1973, 1004 (*synth*)
Focella, A. *et al., J.O.C.*, 1977, **42**, 3456 (*use*)
Chandrasekharan, V. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 970 (*synth, ir, use*)
Hegedus, L.S. *et al., J.A.C.S.*, 1980, **102**, 4973 (*synth, ir, pmr*)
Jaxa-Chamiec, A.A. *et al., J.C.S. Perkin 1*, 1980, 170 (*synth, use*)

5-Nonen-2-one, 9CI N-129

[27039-84-5]
$H_3CCH_2CH_2CH{=}CHCH_2CH_2COCH_3$
$C_9H_{16}O$ 140.225

(*E*)-*form* [75606-70-1]
Detected in many food volatiles.

(*Z*)-*form* [39924-56-6]
No phys. props. reported.

Dias, J.R. *et al., J.A.C.S.*, 1972, **94**, 473 (*synth, uv, ms*)
Bian, Z. *et al., J. Chem. Ecol.*, 1984, **10**, 451
Fujii, M. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 2423 (*synth, ir*)

8-Nonen-2-one, 9CI N-130

[5009-32-5]
$H_2C{=}CH(CH_2)_5COCH_3$
$C_9H_{16}O$ 140.225
Detected in mold-ripened cheeses. Liq. Bp_{12} 95-97°.

2,4-Dinitrophenylhydrazone:
Cryst. (MeOH or EtOAc). Mp 50°.

Conia, J.M. *et al., Bull. Soc. Chim. Fr.*, 1967, 830 (*synth, ir, Raman*)
Cottier, L. *et al., Bull. Soc. Chim. Fr.*, 1972, 1072 (*synth, ir, Raman*)
Dias, J.R. *et al., J.A.C.S.*, 1972, **94**, 473 (*synth, ms*)
Agosta, W.C. *et al., J.O.C.*, 1976, **41**, 136 (*ms*)

8-Nonen-3-one, 9CI N-131

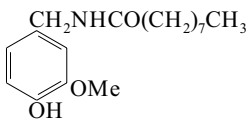
[20013-10-9]
$H_2C{=}CH(CH_2)_4COCH_2CH_3$
$C_9H_{16}O$ 140.225
Detected in mold-ripened cheeses. Liq. d_4^{20} 0.84. Bp_{35} 95-97°. n_D^{20} 1.4411.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 58°.

Portnyagin, Y.M. *et al., Zh. Org. Khim.*, 1968, **4**, 1576; *J. Org. Chem. USSR (Engl. Transl.)*, 1968, **4**, 1515 (*synth*)
Brocard, T. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1976, **282**, 853 (*synth*)

Nonivamide, INN N-132

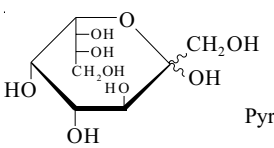
[2444-46-4]
N-*[(4-Hydroxy-3-methoxyphenyl)-methyl]nonanamide, 9CI*. N-*Vanillylnonanamide, 8CI*. *Synthetic capsaicin. Pseudocapsaicin. Pelargonoyl vanillylamide. HH 50. PSVA. FEMA 2787*



$C_{17}H_{27}NO_3$ 293.405
Alkaloid from *Capsicum* spp. Flavouring ingredient. Cryst.; odourless with a pungent burning taste. $Bp_{0.05}$ 200-210°. Log P 3.59 (uncertain value) (calc).

Dirnhuber, P. *et al., J. Physiol. (London)*, 1965, **178**, 41P (*pharmacol*)
Friedrich, H. *et al., Naturwissenschaften*, 1965, **52**, 514
Ger. Pat., 1966, 1 213 855, (*Krewel-Leuffen*); *CA*, **64**, 19504h (*synth*)
Todd, P. *et al., J. Chromatogr. Sci.*, 1975, **13**, 577 (*tlc*)
Jurenitsch, J. *et al., Sci. Pharm.*, 1982, **50**, 64 (*isol*)
Skofitsch, G. *et al., Arzneim.-Forsch.*, 1984, **34**, 154 (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1311
Lo, Y.-C. *et al., Brain Res. Bull.*, 1994, **35**, 15 (*pharmacol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 602
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1979-1980

D-*erythro*-L-*galacto*-Nonulose N-133

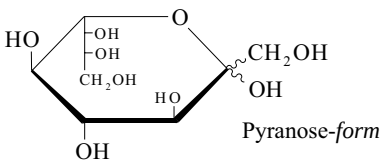


$C_9H_{18}O_9$ 270.236
Present in avocado. $[\alpha]_D^{20}$ -36.2 (c, 5.2 in MeOH aq.).

2,5-Dichlorophenylhydrazone:
Mp 247-249°.

Begbie, R. *et al., Carbohydr. Res.*, 1966, **2**, 272 (*occur*)
Sephton, H.H. *et al., Carbohydr. Res.*, 1966, **2**, 289 (*synth*)

D-*erythro*-L-*gluco*-Nonulose N-134



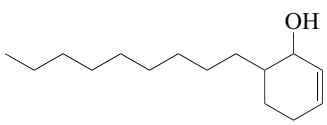
$C_9H_{18}O_9$ 270.236
Isol. from avocado. Syrup. $[\alpha]_D^{20}$ -40 (c, 0.6 in H_2O).

2,5-Dichlorophenylosazone:
Yellow needles. Mp 248-250° dec.

Sephton, H.H. *et al., J.O.C.*, 1963, **28**, 2388 (*isol*)
Begbie, R. *et al., Carbohydr. Res.*, 1966, **2**, 272 (*isol*)
Sephton, H.H. *et al., Carbohydr. Res.*, 1966, **2**, 289 (*synth*)

6-Nonyl-2-cyclohexen-1-ol N-135

Mangalkanol



$C_{15}H_{28}O$ 224.386

(ξ)-*form*

O-*β*-D-*Glucopyranoside:* [259144-63-3]
Mangalkanyl glucoside
$C_{21}H_{38}O_6$ 386.528
Constit. of the root bark of *Mangifera indica* (mango). Pale yellow cryst. ($CHCl_3$/MeOH). Mp 176-178°. λ_{max} 215 (log ε 6.9) (MeOH).

Gupta, J. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1093-1098

2-Nonylheneicosanal N-136

Nonacosane-10-carboxaldehyde. 10-Formylnonacosane
$H_3C(CH_2)_{18}CH(CHO)(CH_2)_8CH_3$
$C_{30}H_{60}O$ 436.803

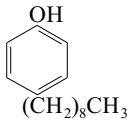
(±)-*form*
Reported from above-ground parts of *Papaver rhoeas* (corn poppy). No phys. props. reported.

Drozdz, B. *et al., Diss. Pharm. Pharmacol.*, 1965, **17**, 527

4-Nonylphenol, 9CI N-137

[104-40-5]

[25154-52-3]



$C_{15}H_{24}O$ 220.354
Environmental pollutant arising from the degradation of nonionic surfactants in sewage. Mp 41-42.5°. Bp_{10} 180-181° $Bp_{1.3}$ 140-142°.

▶ *p*-Alkylphenols have estrogenic props. and have been implicated in feminisation of wildlife. Skin and eye irritant. LD_{50} (rat, orl) 160 mg/kg. SM5600000

Phosphite (3:1): [3050-88-2]
$C_{45}H_{69}O_3P$ 689.012
Light amber oil. d^{25} 0.98. n_D^{20} 1.5262.

Benzoyl: [6316-62-7]
$C_{22}H_{28}O_2$ 324.462
Mp 36.2°.

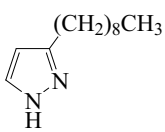
Me ether: [32588-84-4] *1-Methoxy-4-nonylbenzene, 9CI*
$C_{16}H_{26}O$ 234.381
$Bp_{0.5}$ 140°.

[28987-17-9]

Sandulesco, G. *et al., Bull. Soc. Chim. Fr.*, 1930, **47**, 1300-1314 (*synth*)
U.S. Pat., 1956, 2 733 226; *CA*, **50**, 11052a (*phosphite, synth, use*)
Loev, B. *et al., J.O.C.*, 1957, **22**, 988-989 (*synth*)
Lindemann, L.P. *et al., Anal. Chem.*, 1964, **36**, 2414-2417 (*pmr*)
Hedin, P.A. *et al., J. Insect Physiol.*, 1974, **20**, 2135-2142 (*occur*)
Moreno-Manas, M. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 2154-2158 (*Me ether, synth, pmr*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1619-1621 (*synth*)
Dangerous Prop. Ind. Mater. Rep., 1989, **9**, 66 (*rev, haz*)
Krzyzanowska, E. *et al., J. Prakt. Chem.*, 1989, **331**, 617-630 (*synth*)
Rasmussen, L.E.L. *et al., J. Chem. Ecol.*, 1990, **16**, 2167-2181 (*occur*)
Kiedik, M. *et al., Przem. Chem.*, 1991, **70**, 257-259 (*synth*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 6th edn., Van Nostrand Reinhold*, 1984, 2068

3-Nonyl-1*H*-pyrazole, 9CI N-138

[72738-01-3]

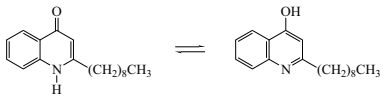


$C_{12}H_{22}N_2$ 194.319
Alkaloid from *Houttuynia cordata* (Yu Xing Cao). Cryst. Sol. Et_2O. Mp 47.5-49.5°. Bp_{22} 195° Bp_9 181°.

Kosuge, T. *et al., Yakugaku Zasshi*, 1952, **72**, 1227-1231; 1954, **74**, 819-820 (*synth*)
Kosuge, T. *et al., J. Biochem. (Tokyo)*, 1954, **41**, 183-186 (*isol*)
U.S. Pat., 1959, 2 883 392; *CA*, **53**, 16155e (*synth*)

2-Nonyl-4(1*H*)-quinolinone N-139

[55396-45-7]
Pyo Ic. *Pseudane IX. 2-Nonyl-4-quinolinol. 4-Hydroxy-2-nonylquinoline*



$C_{18}H_{25}NO$ 271.402
Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O, acids. Mp 138.8-139.2°. λ_{max} 213 (ϵ 23500); 236 (ϵ 26900); 316 (ϵ 10400); 327 (ϵ 10000) (MeOH) (Berdy). λ_{max} 236 (E1%/1cm 1050); 316 (E1%/1cm 431); 328 (E1%/1cm 415) (EtOH) (Berdy).

Oxalate:
Mp 158-159°.

N-*Oxide:* [316-66-5]
$C_{18}H_{25}NO_2$ 287.401
Leaflets (EtOH). Mp 148-149°.

*1′,2′-Didehydro (*E-*):* [60783-01-9]

[1033-24-5] *2-(1-Nonenyl)-4(1*H*)-quinolinone. 4-Hydroxy-2-(1-nonenyl)quinoline. 2-(1-Nonenyl)-4-quinolinol. Δ^1-Pseudene IX. Pyo III*
$C_{18}H_{23}NO$ 269.386
Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 152.8-153.5°. λ_{max} 258 (ϵ 39000); 267 (ϵ 38000); 308 (ϵ 8700); 330 (ϵ 11000) (MeOH) (Berdy). λ_{max} 258 (E1%/1cm 1460); 266 (E1%/1cm 1376); 307 (E1%/1cm 340); 338 (E1%/1cm 434) (EtOH) (Berdy).

3′,4′,6′,7′-Tetradehydro: [29479-51-4] ***2-(3,6-Nonadienyl)-4(1H)-quinolinone***. *4-Hydroxy-2-(3,6-nonadienyl)quinoline. 2-(3,6-Nonadienyl)-4-quinolinol*
$C_{18}H_{21}NO$ 267.37
Mp 103°. Config. of double bonds unknown.

9′-Hydroxy: [29479-52-5] ***2-(9-Hydroxynonyl)-4(1H)-quinolinone***
$C_{18}H_{25}NO_2$ 287.401
Cryst. (Me_2CO). Mp 50°.

*8′-Oxo:2-(8-Oxononyl)-4(1*H*)-quinolinone*
$C_{18}H_{23}NO_2$ 285.385
λ_{max} 216 (log ϵ 4.5); 236 (log ϵ 4.2); 320 (log ϵ 3.8); 332 (log ϵ 3.8) (MeOH).

8′-Oxo, N-*Me:1-Methyl-2-(8-oxononyl)-4(1*H*)-quinolinone*
$C_{19}H_{25}NO_2$ 299.412
λ_{max} 220 (log ϵ 4.2); 235 (log ϵ 4.5); 320 (log ϵ 3.8); 332 (log ϵ 3.8) (MeOH).

NH-form

N-*Me:* [68353-24-2] ***1-Methyl-2-nonyl-4(1H)-quinolinone***
$C_{19}H_{27}NO$ 285.428
Alkaloid from *Ruta graveolens* (rue). Plates (C_6H_6/cyclohexane). Mp 71-75°.

N-*Acetoxymethyl:**1-Acetoxymethyl-2-nonyl-4(1H)-quinolinone***
$C_{21}H_{29}NO_3$ 343.465
Amorph. solid. Mp 79°.

OH-form

*8′-Oxo, Me ether:**4-Methoxy-2-(8-oxononyl)quinoline***. *9-(4-Methoxy-2-quinolinyl)-2-nonanone*
$C_{19}H_{25}NO_2$ 299.412
λ_{max} 228 (log ϵ 4.5); 300 (log ϵ 2.9); 314 (log ϵ 2.8) (MeOH).

Hays, E.E. *et al., J. Biol. Chem.*, 1945, **159**, 725 (*isol, uv*)
Wells, I.C. *et al., J. Biol. Chem.*, 1952, **196**, 331 (*isol, struct, synth*)
Kan-Fan, C. *et al., Phytochemistry*, 1970, **9**, 1283 (*9′-hydroxy, 3′,4′,6′,7′-tetradehydro*)
Ritter, C. *et al., Eur. J. Biochem.*, 1971, **18**, 391 (*biosynth*)
Wratten, S.J. *et al., Antimicrob. Agents Chemother.*, 1977, **11**, 411
Kamikado, T. *et al., Agric. Biol. Chem.*, 1978, **42**, 1515 (*deriv*)
Budzikiewicz, H. *et al., Monatsh. Chem.*, 1979, **110**, 947 (*isol, uv*)
Grundon, M.F. *et al., Phytochemistry*, 1979, **18**, 1768 (*deriv*)
Somanathan, R. *et al., J. Het. Chem.*, 1981, **18**, 1077 (*synth, uv, ir, pmr*)
Ahsan, M. *et al., J. Nat. Prod.*, 1994, **57**, 670 (*1-Acetoxymethyl-2-nonyl-4(1H)-quinolinone*)
Touati, D. *et al., Phytochemistry*, 2000, **53**, 277-279 (*8′-oxo derivs*)
Biavatti, M.W. *et al., J. Braz. Chem. Soc.*, 2002, **13**, 66-70 (*isol, pmr, cmr*)

2-Nonynoic acid, 9CI, 8CI N-140

[1846-70-4]
$H_3C(CH_2)_5C{\equiv}CCOOH$
$C_9H_{14}O_2$ 154.208
Liq. Mp -8°. Bp_{18} 154-156° $Bp_{2.2}$ 122°.

Me ester: [111-80-8] *Methyl octynecarboxylate. FEMA 2726*
$C_{10}H_{16}O_2$ 168.235
Flavouring ingredient. Liq. with violet odour. Insol. H_2O, sol. EtOH. $Bp_{2.3}$ 85° Bp 232°. n_D^{25} 1.4470.

▶ LD_{50} (rat, orl) 2220 mg/kg. RB3450000

Et ester: [10031-92-2] *FEMA 2448*
$C_{11}H_{18}O_2$ 182.262
Flavouring ingredient. Oil. d^{25} 0.9. Bp 227°. n_D^{20} 1.4527.

Amide:
$C_9H_{15}NO$ 153.224
Cryst. (Et_2O/petrol). Mp 94°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 528A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1597A (*ir*)
Wotiz, J.H. *et al., J.O.C.*, 1954, **19**, 1580 (*synth*)
Groff, T.M. *et al., Ark. Kemi*, 1968, **29**, 179 (*ms, ester*)
Silveira, A. Jr. *et al., J. Am. Oil Chem. Soc.*, 1971, **48**, 661 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1975, **13**, 871 (*rev, bibl, ester*)
Org. Synth., 1976, **55**, 73 (*ester*)
Gershon, H. *et al., Can. J. Microbiol.*, 1978, **24**, 593 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 257; 533 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1023; 1810 (*Et ester*)
Fortes, C.C. *et al., Synth. Commun.*, 1997, **27**, 2993-3026 (*synth, Me ester, ir, pmr, cmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MNC000

Nopalinic acid N-141

[63409-16-5]
N-*(4-Amino-1-carboxybutyl)glutamic acid, 9CI.* N^2-*(1,3-Dicarboxypropyl)or-*

nithine. Ornaline

$H_2N(CH_2)_3CH(COOH)NHCH(COOH)CH_2CH_2COOH$

$C_{10}H_{18}N_2O_6$ 262.262

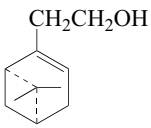
Isol. from *Helianthus annuus* (sunflower).

Firmin, J.L. *et al., Phytochemistry*, 1977, **16**, 761 (*isol, synth*)
Scott, I.M. *et al., Phytochemistry*, 1978, **17**, 1103 (*biosynth*)

Nopol N-142

[128-50-7]

6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-ethanol, 9CI. 6,6-Dimethyl-2-norpinene-2-ethanol, 8CI. Homomyrtenol. FEMA 3938



$C_{11}H_{18}O$ 166.263

(-)-*form* [35836-73-8]

Present in carrots. Flavouring agent for baked goods and candies. Liq. with citrus/pine odour. d 0.973. Bp 230-240° $Bp_{2.8}$ 89°. $[\alpha]_D^{24}$ -37 (neat). n_D^{20} 1.4930.

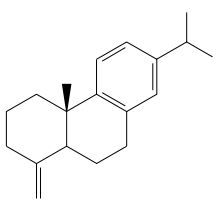
[30982-38-8, 69978-56-9, 107667-90-3, 133098-22-3]

Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 822

18-Nor-4(19),8,11,13-abietatetraene N-143

[22478-62-2]

19-Nordehydro-4(18)-abietene

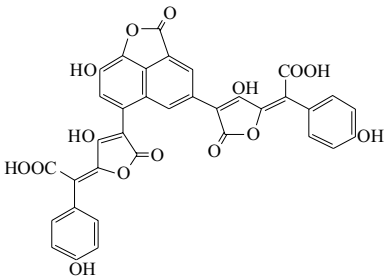


$C_{19}H_{26}$ 254.414

Isol. from oleoresin of *Pinus koraiensis* (Korean pine). Waxy cryst. $[\alpha]_D^{24}$ +147 (c, 0.88 in MeOH). n_D^{22} 1.5340. Prob. an artifact of dehydration of 18-Nor-8,11,13-abietatrien-4-ol.

Bennett, C.R. *et al., Aust. J. Chem.*, 1969, **22**, 1711 (*synth*)
Raldugin, V.A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 595; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 574 (*isol*)

Norbadione A N-144



$C_{35}H_{18}O_{15}$ 678.518

Metabolite of *Xerocomus badius* (kostanjevka). Red needles. Mp 300°.

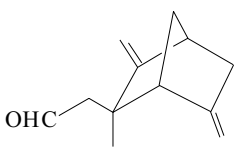
Penta-Me ether, di-Me ester: [90295-69-5] Mp 247-249°.

Steffan, B. *et al., Angew. Chem., Int. Ed.*, 1984, **23**, 445 (*isol, cmr, struct*)
Gill, M. *et al., Phytochemistry*, 1985, **24**, 1351 (*isol*)
Gill, M. *et al., Aust. J. Chem.*, 1994, **47**, 1967 (*cmr*)

Norbicycloekasantalal N-145

[37720-84-6]

10,11,12,13-Tetranor-β-santal-3(15)-en-9-al



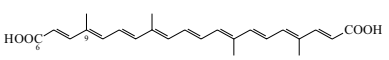
$C_{11}H_{16}O$ 164.247

Flavouring ingredient. Constit. of the famine food *Santalum album* (sandalwood).

Gibson, T. *et al., Tet. Lett.*, 1972, 2207

Norbixin N-146

6,6′-Diapo-6,6′-carotenedioic acid. E160



(9E)-form

$C_{24}H_{28}O_4$ 380.483

Water-soluble food colour. Commercial forms contain mixts. of isomers and their Me esters. Used to colour butter, margarine and other fat-related products.

(9*E*)-*form* [542-40-5]

β-Norbixin. Isonorbixin

Cryst. Mp 250° dec.

►JX3795000

Mono-Me ester: [39937-23-0] ***Bixin***. *β-Bixin. Labile bixin*

$C_{25}H_{30}O_4$ 394.51

Constit. of *Bixa orellana* (annatto). Cryst. (EtOH). Mp 204-206°. λ_{max} 443 ; 475 ; 509 ($CHCl_3$) (Berdy). λ_{max} 475 (ϵ 130000) (C_6H_6) (Berdy).

Di-Me ester: [62697-46-5] trans-*Methylbixin. Isomethylbixin*

$C_{26}H_{32}O_4$ 408.536

Constit. of *Bixa orellana* (annatto). Blue-violet prisms (C_6H_6). Mp 204-205°. λ_{max} 432 ; 456 ; 490 (petrol). λ_{max} 446 ; 473 ; 506 (C_6H_6).

6-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-6′-Me ester: [247030-35-9]

$C_{45}H_{62}O_4$ 666.982

Constit. of *Bixa orellana* (annatto) seeds. λ_{max} 350 ; 432 ; 456 ; 489 (2-methoxy-2-methylpropane).

(9*Z*)-*form*

α-Norbixin

Cryst. (AcOH). Mp 280° dec.

6-Me ester: [6983-79-5] *α-Bixin. Isobixin. Stable bixin*

$C_{25}H_{30}O_4$ 394.51

Principal colouring matter of *Bixa orellana* (annatto) seeds. Cryst. (Me_2CO). Mp 189.5-190.5°.

Di-Me ester: [26585-94-4] cis-*Methylbixin. Natural methylbixin*

$C_{26}H_{32}O_4$ 408.536

Constit. of *Bixa orellana* (annatto). Cryst. Mp 164°.

6-(3,7,11,5-Tetramethyl-2,6,10,14-hexadecatetraenyl)-6′-Me ester: [247030-34-8]

Constit. of *Bixa orellana* (annatto) seeds. λ_{max} 350 ; 426 ; 452 ; 482 (2-methoxy-2-methylpropane).

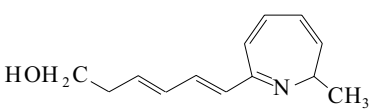
(9*Z*,9′*Z*)-*form*

Di-Me ester: [201996-34-1]

Constit. of *Bixa orellana* (annatto). λ_{max} 350 ; 423 ; 448 ; 476 (2-methoxy-2-methylpropane).

Isler, D. *et al., Helv. Chim. Acta*, 1957, **40**, 1242 (*synth*)
Barber, M.S. *et al., J.C.S.*, 1961, 1625 (*struct*)
Pattenden, G. *et al., J.C.S.(C)*, 1970, 235 (*synth*)
Reith, J.F. *et al., J. Food Sci.*, 1971, **36**, 861 (*isol, struct*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Kelly, D.R. *et al., J. Chem. Res., Synop.*, 1996, 446; *J. Chem. Res., Miniprint*, 1996, 2640 (*isol, pmr, cmr, ms, cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 184 (*rev*)
Mercadante, A.Z. *et al., Phytochemistry*, 1997, **46**, 1379-1383 (*isol, pmr, cmr*)
Häberli, A. *et al., Helv. Chim. Acta*, 1999, **82**, 696 (*synth*)
Mercadente, A.Z. *et al., Phytochemistry*, 1999, **52**, 135-139 (*phytatetraenyl esters*)

Norchalciporol N-147



$C_{13}H_{17}NO$ 203.283

O-*Propanoyl:* [112448-75-6] ***Norchalciporyl propionate***

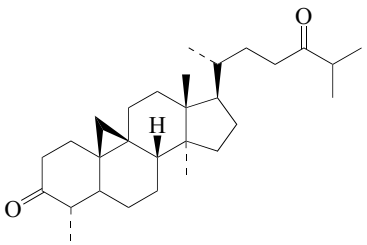
$C_{16}H_{21}NO_2$ 259.347

Pungent principle from fruit-bodies of the edible pfefferröhrling mushroom (*Chalciporus piperatus*). Sl. yellow oil. Sol. MeOH, Et_2O; poorly sol. H_2O. $[\alpha]_D^{22}$ -290 (c, 0.2 in Et_2O). λ_{max} 246 (ϵ 15900) (EtOH) (Berdy).

Sterner, O. *et al., Tetrahedron*, 1987, **43**, 1075 (*isol, uv, ir, pmr, ms, struct*)

29-Norcycloartane-3,24-dione N-148

[207850-22-4]

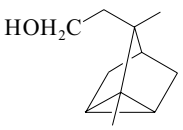


$C_{29}H_{46}O_2$ 426.681
Constit. of fruit peel of *Musa sapientum* (banana).

Akihisa, T. *et al., Phytochemistry*, 1998, **47**, 1107-1110 (*isol, pmr, cmr*)

Norecasantalol N-149

[59460-65-0]
10,11,12,13-Tetranor-α-santalan-9-ol. Nortricycloekasantalol



$C_{11}H_{18}O$ 166.263
Flavouring ingredient. Constit. from oil of the famine food *Santalum album* (sandalwood). Oil. Bp_{10} 114-117°.

Aldehyde: [59300-38-8] ***Norecasantalal***. *10,11,12,13-Tetranor-α-santalan-9-al. Nortricycloekasantalal*
$C_{11}H_{16}O$ 164.247
Flavouring ingredient. Constit. from oil of the famine food *Santalum album* (sandalwood). Oil. Bp 222-224°.

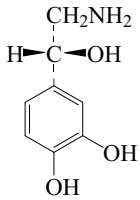
Carboxylic acid: [59300-52-6] ***Norecasantalic acid***. *10,11,12,13-Tetranor-α-santalan-9-oic acid. Nortricycloekasantalic acid*
$C_{11}H_{16}O_2$ 180.246
Flavouring ingredient. Constit. from oil of the famine food *Santalum album* (sandalwood). Cryst. (EtOH). Mp 93°. $[\alpha]_D$ -33.3 (EtOH).

Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737

Ngo, K.-S. *et al., Phytochemistry*, 1999, **50**, 1213-1218 (*pmr, cmr*)

Norepinephrine, INN N-150

4-(2-Amino-1-hydroxyethyl)-1,2-benzenediol, 9CI. α-(Aminomethyl)-3,4-dihydroxybenzyl alcohol, 8CI. 2-Amino-1-(3,4-dihydroxyphenyl)ethanol. 4-(β-Amino-α-hydroxyethyl)catechol. ***Noradrenaline, BAN****. Arterenol*



(*R*)-*form*

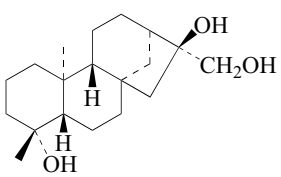
$C_8H_{11}NO_3$ 169.18
Log P -0.99 (calc).

(ξ)-*form*
Present in banana peel and pulp (*Musa paradisiaca*), red plum fruit (*Prunus domestica*), orange pulp (*Citrus sinensis*), potato tubers (*Solanum tuberosum*) and whole purslane (*Portulaca oleracea*). *P. oleracea* is the richest of these sources.

[5794-08-1, 69815-49-2]

Biel, J.H. *et al., J.A.C.S.*, 1954, **76**, 3149-3153 (*synth, pharmacol*)
Waalkes, T.P. *et al., Science (Washington, D.C.)*, 1958, **127**, 648-650 (*isol*)
Udenfriend, S. *et al., Arch. Biochem. Biophys.*, 1959, **85**, 487-490 (*detn, occur*)
Pratesi, P. *et al., J.C.S.*, 1959, 4062-4065 (*abs config*)
Levy, B. *et al., Drill's Pharmacol. Med.*, 4th edn., McGraw-Hill, New York, 1971, 627 (*rev, pharmacol*)
Applewhite, P.B. *et al., Phytochemistry*, 1973, **12**, 191-192 (*occur*)
Donike, M. *et al., Chromatographia*, 1974, **7**, 651-654 (*ms*)
Andersen, A.M. *et al., Acta Chem. Scand., Ser. B*, 1975, **29**, 871-876 (*cryst struct*)
Rajan, K.S. *et al., Bioinorg. Chem.*, 1976, **6**, 93-117 (*uv*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9-18 (*occur, bibl*)
Wilson, T.D. *et al., Anal. Profiles Drug Subst.*, 1982, **11**, 555 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1249
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARL500; NNP050; NNO500; NNO699; ARL750

19-Nor-4,16,17-kauranetriol N-151

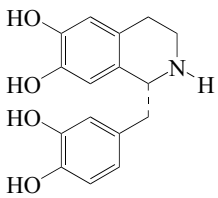


$C_{19}H_{32}O_3$ 308.46
(*ent*-4β,16αOH)-*form* [177742-56-2]
Annosquamosin B
Constit. of *Annona squamosa* (sugar apple). Powder. Mp 263-266°. $[\alpha]_D^{24}$ -47 (c, 0.2 in $CHCl_3$/MeOH).

Wu, Y.C. *et al., J. Nat. Prod.*, 1996, **59**, 635-637 (*isol, pmr, cmr*)

Norlaudanosoline N-152

[4747-99-3]
1-[(3,4-Dihydroxyphenyl)methyl]-1,2,3,4-tetrahydro-6,7-isoquinolinediol, 9CI. Tetrahydropapaveroline. 1-(3,4-Dihydroxybenzyl)-1,2,3,4-tetrahydro-6,7-isoquinolinediol, 8CI



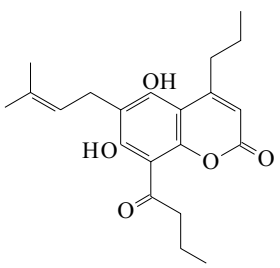
(*R*)-*form*

$C_{16}H_{17}NO_4$ 287.315
Formerly believed to be a biosynthetic precursor of morphine in *Papaver somniferum*, now disproved.

Davies, V.E. *et al., Science (Washington, D.C.)*, 1970, **167**, 1005-1006
Rice, V.C. *et al., J.O.C.*, 1980, **45**, 592-601 (*synth, resoln*)
Hoffman, I.S. *et al., J. Pharmacol. Exp. Ther.*, 1982, **220**, 16-22 (*biochem*)
Brockmann-Hannsen, E. *et al., The Chemistry and Biology of Isoquinoline Alkaloids*, (eds. Phillipson, J.D. *et al*), Springer, 1985, 229-239 (*biosynth*)
Clezy, P.S. *et al., Aust. J. Chem.*, 1988, **41**, 483-491 (*synth, pmr*)
Stadler, R. *et al., Annalen*, 1990, 555-562 (*biosynth*)
Merck Index, 12th edn., 1996, 1575 (*props, bibl*)
Haber, H. *et al., Life Sci.*, 1997, **60**, 77-89 (*formn, detn, ms, glc*)

Normammein N-153

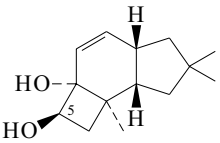
[5085-54-1]
*5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, 9CI. 8-Butyryl-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4-propylcoumarin, 8CI. Mammea B/BC*



$C_{21}H_{26}O_5$ 358.433
Constit. of *Mammea americana* (mamey) seeds. Needles (hexane). Mp 132-133°.

Crombie, L. *et al., J.C.S.(C)*, 1967, 2545 (*isol, ir, uv, pmr, ms*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1987, 317 (*synth*)

14-Nor-7-protoilludene-5,6-diol N-154



$C_{14}H_{22}O_2$ 222.327

(5β,6α)-*form*

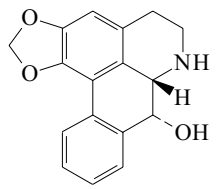
5-(2,4-Dihydroxy-6-methylbenzoyl): [139051-16-4] ***Armillasin***
$C_{22}H_{28}O_5$ 372.46
Metab. of *Armillaria mellea* (honey mushroom). Cryst. Mp 179-181°. $[\alpha]_D^{28}$ +14.3 (c, 0.16 in $CHCl_3$).

5-(2,4-Dihydroxy-6-methylbenzoyl), 6-hexadecanoyl: [139051-17-5] ***Armillatin***
$C_{38}H_{58}O_6$ 610.873
Metab. of *Armillaria mellea* (honey mushroom). Oil.

Yang, J.S. *et al., Planta Med.*, 1991, **57**, 478 (*isol, pmr, cmr*)

Norushinsunine N-155

Michelalbine. Normicheline A



(−)-*form*

$C_{17}H_{15}NO_3$ 281.31

(+)-*form*

N-*Me,* N-*oxide(β-):* ***(+)-Norushinsunine N-oxide***
$C_{18}H_{17}NO_4$ 311.337
Alkaloid from *Cananga odorata* (ylang ylang). Cryst. Mp 177-179°. $[\alpha]_D^{24}$ +50.7 (c, 0.05 in $CHCl_3$). λ_{max} 271 (log ϵ 4.03); 283 (log ϵ 3.98); 320 (log ϵ 3.61) (EtOH).

(-)-*form* [3175-84-6]
Mp 206-207°. $[\alpha]_D^{25}$ -103 (c, 0.60 in $CHCl_3$).

N,O-*Di-Ac:* [3327-33-1]
Mp 243-245°.

N-*Me:* [3175-89-1] ***Ushinsunine****. Micheline A*
$C_{18}H_{17}NO_3$ 295.337
Mp 122-123°. $[\alpha]_D$ -122 (c, 0.37 in MeOH).

▶ CE1055600

N-*Me,* N-*oxide(β-):* ***Ushinsunine β-N-oxide***
$C_{18}H_{17}NO_4$ 311.337
Amorph. $[\alpha]_D$ -52 (c, 0.06 in MeOH).

N,N-*Di-Me:* [61619-44-1] **N-*Methylushinsunine***
$C_{19}H_{20}NO_3^{\oplus}$ 310.372
Cryst. (Me_2CO aq.) (as iodide). Mp 235-237° (iodide). $[\alpha]_D$ -118 (c, 1 in $CHCl_3$).

(±)-*form*

Mp 210-212° (202-203°).

N-*Me:*

Mp 144-145°.

Yang, S.-S. *et al., Hua Hsueh*, 1961, 144; *CA*, **56**, 1489c (*N-Methylushinsunine*)
Yang, T.-H. *et al., Yakugaku Zasshi*, 1962, **82**, 811; 1963, **83**, 216 (*isol*)
Tomita, M. *et al., Yakugaku Zasshi*, 1965, **85**, 77 (*isol, uv, ir, ms, pmr*)
Lu, S.T. *et al., Yakugaku Zasshi*, 1969, **89**, 1313 (*uv, ir, pmr, deriv*)
Kunitomo, J. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1502 (*synth, abs config*)
Cleaver, L. *et al., Aust. J. Chem.*, 1976, **29**, 2003 (*N-Methylushinsunine*)
Kessar, S.V. *et al., Tet. Lett.*, 1980, **21**, 3307 (*synth, Norushinsunine, Ushinsunine*)
Charles, B. *et al., J. Nat. Prod.*, 1987, **50**, 1113 (*Ushinsunine N-oxide*)
Yang, T.H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1988, **35**, 305; *CA*, **110**, 111669j (*Ushinsunine N-oxide*)
Simeon, S. *et al., Pharmazie*, 1989, **44**, 593-597 (*activity*)
Hsieh, T.-J. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 607-612 (*(+)-Ushinsunine N-oxide*)
Wright, C.W. *et al., J. Nat. Prod.*, 2000, **63**, 1638-1640 (*activity*)

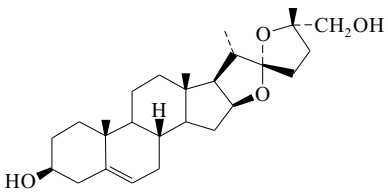
NS LTP N-156

Protein, MW 9 kDa. Inhibits the growth of several fungi *in vitro*. Isol. from seeds of radish *Raphanus sativus*.

Terras, F.R.G. *et al., Plant Physiol.*, 1992, **100**, 1055-1058 (*isol*)

Nuatigenin N-157

[6811-35-4]
22S,25S-Epoxyfurost-5-ene-3β,26-diol



$C_{27}H_{42}O_4$ 430.626
Cryst. Mp 227-228°. $[\alpha]_D^{20}$ -86 (c, 0.1 in $CHCl_3$).

3-O-[α-L-Rhamnosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside], 26-O-β-D-glucopyranoside: [24915-65-9] ***Avenacoside A***
$C_{51}H_{82}O_{23}$ 1063.195
Constit. of *Avena sativa* (oats). $[\alpha]_D^{24}$ +52 (c, 1 in H_2O).

3-O-[α-L-Rhamnosyl-(1→4)-[β-D-glucopyranosyl]-(1→3)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 26-O-β-D-glucopyranoside: [35920-91-3] ***Avenacoside B***
$C_{57}H_{92}O_{28}$ 1225.337
Constit. of *Avena sativa* (oats). $[\alpha]_D^{24}$ +52 (c, 1 in H_2O).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [113561-09-4]
$C_{39}H_{62}O_{13}$ 738.911
Constit. of *Allium vineale* (wild garlic).

3-O-[α-L-Rhamnopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]: [59795-21-0] *26-Desglucoavenacoside A*
$C_{45}H_{72}O_{18}$ 901.053
Constit. of *Avena sativa* (oats).
Amorph. Sol. H_2O, MeOH; poorly sol. hexane.

3-O-[α-L-Rhamnopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]: [59795-22-1] *26-Desglucoavenacoside B*
$C_{51}H_{82}O_{23}$ 1063.195
Constit. of *Avena sativa* (oats).
Amorph. Sol. H_2O, MeOH; poorly sol. hexane.

Tschesche, R. *et al., Chem. Ber.*, 1969, **102**, 2072; 1971, **104**, 3549; 1977, **110**, 2416; 1978, **111**, 3300 (*isol*)
Saijo, R. *et al., Phytochemistry*, 1983, **22**, 733 (*isol*)
Agrawal, P.K. *et al., Phytochemistry*, 1985, **24**, 2479 (*cmr*)
Chen, S. *et al., Tet. Lett.*, 1987, **28**, 5603 (*deriv*)
Mimaki, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3055 (*Lilium braunii saponins*)
Mimaki, Y. *et al., Phytochemistry*, 1990, **29**, 2267; 1995, **38**, 1279 (*isol, pmr, cmr*)

Nukacin ISK-1 N-158

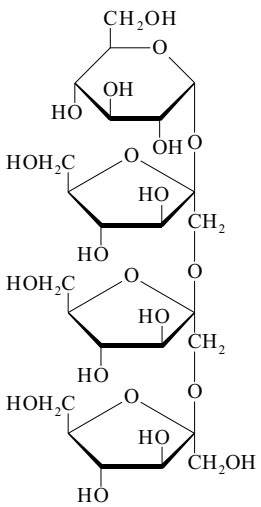
MENSKVMKDIEVANLLEEVQEDEL-NEVLGAKKKSG-VIPTVSHDCHMNSFQFVFTCCS

Lantibiotic containing 57 amino acids. For struct. see ref.. Bacteriocin prod. by *Staphylococcus warneri* ISK-1.

Sashihara, T. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 2420-2428 (*isol, struct*)

Nystose N-159

[13133-07-8]
β-D-Fructofuranosyl-(2→1)-β-D-fructofuranosyl-(2→1)-β-D-fructofuranosyl α-D-glucopyranoside, 9CI. Fungitetraose. 1,1-Kestotetraose



$C_{24}H_{42}O_{21}$ 666.583

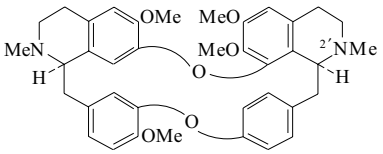
A fructan. Constit. of seeds of onions and roots of Asparagus. Low-calorie sweetening agent for food and chewing gum. Constit. of neosugar which improves the intestinal flora in humans. Cryst. (MeOH/EtOH); cryst. + $1H_2O$; needles + 3MeOH (MeOH aq.). Mp 129-131° (monohydrate) Mp 134° (trihydrate). $[\alpha]_D^{20}$ +10.3 (c, 0.61 in H_2O). Cmr data published prior to 1993 was incorrect.

Tsuchida, H. *et al., Agric. Biol. Chem.*, 1966,

30, 429 (*synth*)
Binkley, W.W. *et al., Carbohydr. Res.*, 1971, **17**, 127; 1972, **23**, 301 (*ms, cmr*)
Kamerling, J.P. *et al., Carbohydr. Res.*, 1972, **25**, 293 (*isol, ms, cryst struct*)
Shiomi, N. *et al., Agric. Biol. Chem.*, 1979, **43**, 2233 (*enzymic synth*)
Uchiyama, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 3315 (*isol*)
Hidaka, H. *et al., Agric. Biol. Chem.*, 1988, **52**, 1181 (*enzymic synth*)
Handbook of Sweetners, (eds. Marie, S. *et al*), Blackie, 1991, 64-65 (*rev*)
Okuyama, K. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 374 (*cryst struct*)
Timmermans, J.W. *et al., Carbohydr. Res.*, 1993, **243**, 379 (*pmr, cmr*)
Jeffery, G.A. *et al., Carbohydr. Res.*, 1993, **247**, 37 (*cryst struct*)
French, A.D. *et al., Carbohydr. Res.*, 1993, **247**, 51 (*struct*)
Buddington, R.K. *et al., Am. J. Clin. Nutr.*, 1996, **63**, 709-716 (*pharmacol*)

Obaberine O-1

[1263-80-5]
6,6′,7,12′-Tetramethoxy-2,2′-dimethyloxyacanthan, 9CI. O-*Methyloxyacanthine*



$C_{38}H_{42}N_2O_6$ 622.76

Alkaloids in this entry have the 1*R*,1′*S*-configuration (Shamma-Moniot numbering convention; older CAS numbering put the primes on the opposite rings). Mp 139-140° Mp 199-200°. $[\alpha]_D^{26}$ +169 (c, 0.147 in MeOH). λ_{max} 280 (MeOH).

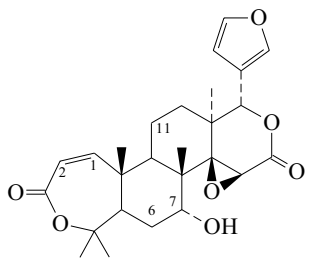
O^{12}-*De-Me:* [548-40-3] ***Oxyacanthine***
$C_{37}H_{40}N_2O_6$ 608.733
Alkaloid from *Berberis vulgaris* (barberry). Cryst. (petrol). Mp 212-214°. $[\alpha]_D^{29}$ +285.6 (c, 0.5 in $CHCl_3$). Log P 7.72 (uncertain value) (calc). Epimer of Repandine λ_{max} 223 ; 283 (log ϵ 3.95) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 50 mg/kg. RR6475000

Fujita, E. *et al., Yakugaku Zasshi*, 1952, **72**, 213-216; *CA*, **47**, 6429a (*Obaberine, Oxyacanthine, struct, synth*)
Battersby, A.R. *et al., J.C.S.*, 1965, 2239-2247 (*Obaberine, Oxyacanthine, ord*)
Baldas, J. *et al., J.C.S. Perkin 1*, 1972, 592-596 (*Obaberine, Oxyacanthine, ms*)

Obacunol O-2

[17182-59-1]
Tricoccin S_{23}



$C_{26}H_{32}O_7$ 456.535
Cryst. (MeOH). Mp 256-260°. $[\alpha]_D$ +73.6.

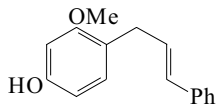
7-Ketone: [751-03-1] ***Obacunone***. *Casimirolide. Tricoccin S_3*
$C_{26}H_{30}O_7$ 454.519
Constit. of *Citrus* spp., *Fortunella margarita* (oval kumquat) and *Casimiroa edulis* (Mexican apple). Cryst. (MeOH). Mp 229-230°. $[\alpha]_D$ -50 ($CHCl_3$). λ_{max} 288 (ϵ 1360) (MeOH) (Derep).

11β-Hydroxy, 7-ketone: [35796-71-5] ***Zapoterin***
$C_{26}H_{30}O_8$ 470.518
Constit. of the seeds of *Casimiroa edulis* (Mexican apple). Mp 257-259°. $[\alpha]_D$ -51 ($CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1961, 255 (*Obacunone, struct*)
Dreyer, D.L. *et al., Tetrahedron*, 1965, **21**, 75 (*Obacunone, pmr*)
Moss, G.P. *et al., J.C.S.(C)*, 1970, 694 (*Zapoterin*)
Taylor, D.A.H. *et al., J. Chem. Res., Synop.*, 1977, 2 (*Obacunone, cmr*)
Jung, H. *et al., Planta Med.*, 2000, **66**, 74 (*Obacunone, activity*)

Obtustyrene O-3

[21148-31-2]
3-Methoxy-4-(3-phenyl-2-propenyl)phenol, 9CI. 4-Cinnamyl-3-methoxyphenol

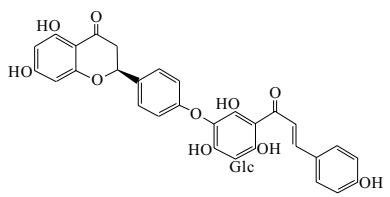


$C_{16}H_{16}O_2$ 240.301
Stress metab. of pea. Oil. $Bp_{0.1}$ 140° (bath).

Gregson, M. *et al., Chem. Comm.*, 1968, 1390 (*occur, struct*)
Gregson, M. *et al., Phytochemistry*, 1978, **17**, 1395 (*isol*)
Carlson, R.E. *et al., Phytochemistry*, 1982, **21**, 1733 (*isol*)

Occidentoside O-4

[77782-91-3]
*2-[4-[3-β-D-Glucopyranosyl-2,4,6-trihydroxy-5-[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]phenoxy]phenyl]-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI*



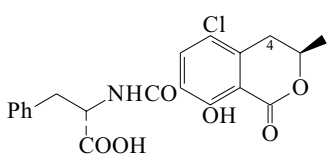
$C_{36}H_{32}O_{15}$ 704.64

Discrepancies in struct. analysis. Isol. from *Anacardium occidentale* (cashew). Pale-yellow microcryst. powder (Me_2CO). Mp 160-161°.

Murthy, S.S.N. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 150 (*isol, struct*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 940 (*struct*)
Murthy, S.S.N. *et al., Planta Med.*, 1982, **45**, 3 (*isol*)
Wannan, B.S. *et al., Biochem. Syst. Ecol.*, 1985, **13**, 105

Ochratoxin A O-5

[303-47-9]
N-*[(5-Chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-7-yl)carbonyl]phenylalanine, 9CI*



$C_{20}H_{18}ClNO_6$ 403.818
Mycotoxin. Prod. by *Aspergillus melleus, Aspergillus sulphureus* and *Penicillium viridicatum*. Potential contaminant of foodstuffs, especially cereals. Found in stored grain products in UK (1997). Cryst. (xylene). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 169°. $[\alpha]_D^{20}$ -118 (c, 1.1 in $CHCl_3$). λ_{max} 213 (ϵ 37600); 332 (ϵ 6500) (MeOH) (Derep). λ_{max} 213 (ϵ 36800); 332 (ϵ 6400) (MeOH) (Berdy). λ_{max} 215 (ϵ 34000); 333 (ϵ 2400) (EtOH) (Berdy).

▶ Possible human carcinogen. Exp. carcinogen and neoplastic agent. Nephrotoxic. Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 20 mg/kg, LD_{50} (pig, orl) 1 mg/kg. V. toxic if swallowed. Implicated in Balkan endemic nephropathy ; LD_{50} (rats, orl) 22 mg/kg. AY4375000

Et ester: [4865-85-4] ***Ochratoxin C***
$C_{22}H_{22}ClNO_6$ 431.872
Metab. of *Aspergillus ochraceus*. Amorph. $[\alpha]_D$ -100 (c, 1.2 in EtOH).

Dechloro: [4825-86-9] ***Ochratoxin B***
$C_{20}H_{19}NO_6$ 369.373
Metab. of *Aspergillus ochraceus*. Cryst. (MeOH). Mp 221°. $[\alpha]_D$ -35 (c, 0.15 in EtOH). λ_{max} 218 (ϵ 33600); 318 (ϵ 6500) (MeOH) (Derep). λ_{max} 218 (ϵ 37200); 318 (ϵ 6900) (EtOH) (Berdy).

▶ Highly toxic orally. AY6825000

4S-*Hydroxy:* [35299-87-7] ***4-Hydroxyochratoxin A***
$C_{20}H_{18}ClNO_7$ 419.817
Cryst. (C_6H_6). Mp 216-218°.

Van der Merwe, K.J. *et al., J.C.S.*, 1965, 7083 (*isol*)
Steyn, P.S. *et al., Tetrahedron*, 1967, **23**, 4449 (*synth*)
Roberts, J.C. *et al., J.C.S.(C)*, 1970, 278 (*synth*)
Yamazaki, M. *et al., Tet. Lett.*, 1971, 2301 (*biosynth*)
Hutchinson, R.D. *et al., Tet. Lett.*, 1971, 4033 (*deriv*)
Maebayashi, Y. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2172 (*biosynth*)
Harwig, J. *et al., Mycotoxins*, 1974, 345 (*rev*)
Kraus, G.A. *et al., J.O.C.*, 1981, **46**, 201 (*synth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220; 1992, **64**, 1029 (*uv, ir, pmr, ms, cd, occur, !rev*)
IARC Monog., 1983, **31**, 191; *Suppl.*, **6**, 434; *Suppl.*, **7**, 271 (*tox, rev*)
Joergensen, K. *et al., Food Addit. Contam.*, 1996, **13**, 95-104 (*occur*)
Stoev, S.D. *et al., Vet. Hum. Toxicol.*, 1998, **40**, 352-360 (*tox, rev*)
Scudamore, K.A. *et al., Food Addit. Contam.*, 1999, **16**, 281-290 (*occur*)
Visconti, A. *et al., J. Chromatogr., A*, 1999, **864**, 89-101 (*hplc*)
Donner, C.D. *et al., Aust. J. Chem.*, 2002, **55**, 213-217 (*synth*)
Harris, J.P. *et al., Phytochemistry*, 2002, **58**, 709-716 (*biosynth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 137; 141; 145; 146
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CHP250

Octacosanal O-6

[22725-64-0]
$H_3C(CH_2)_{26}CHO$
$C_{28}H_{56}O$ 408.75
Isol. from wax of wine grapes (*Vitis vinifera*) and from cabbage leaves (*Brassica oleracea*).

Radler, F. *et al., Aust. J. Chem.*, 1965, **18**, 1059 (*isol*)
Schmid, H.H.O. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1969, **350**, 462 (*isol*)

1,9-Octacosanediol O-7

[180005-28-1]
$H_3C(CH_2)_{18}CH(OH)(CH_2)_7CH_2OH$
$C_{28}H_{58}O_2$ 426.765
Constit. of the leaf wax of *Papaver somniferum* (opium poppy).

(±)-form
Mp 94-95°.
Jetter, R. *et al., Phytochemistry*, 1996, **42**, 1617-1620 (*isol, synth, pmr, cmr, ms*)

1,28-Octacosanediol O-8

[5848-11-3]
$HOCH_2(CH_2)_{26}CH_2OH$
$C_{28}H_{58}O_2$ 426.765
Isol. from apple (*Pyrus malus*) and oat (*Avena sativa*) in esterified form. Cryst. (C_6H_6/Me_2CO). Mp 112.2-112.3°.

Di-Ac:
$C_{32}H_{62}O_4$ 510.839
Mp 80.9-81°. $Bp_{0.5}$ 258°.

Bis(3,4-dihydroxycinnamoyl):1,28-Dicaffeoyloctacosanediol
$C_{46}H_{70}O_8$ 751.054
Occurs in oats (*Avena sativa*).

Bis(3-hydroxy-4-methoxycinnamoyl):1,28-Octacosanediol diferulate
$C_{48}H_{74}O_8$ 779.108
Found in oats (*Avena sativa*).

Murray, K.E. *et al., Aust. J. Chem.*, 1955, **8**, 832
Mazliak, P. *et al., Phytochemistry*, 1962, **1**, 79 (*isol*)
Daniels, D.G.H. *et al., Chem. Ind. (London)*, 1964, 2058; 1965, 1763 (*isol, dicaffeate, diferulate*)
Mukherjee, K.S. *et al., Curr. Sci.*, 1978, **47**, 301 (*isol*)

6,8-Octacosanediol O-9

$C_{28}H_{58}O_2$ 426.765
(6R*,8S*)-form [155800-86-5]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower).
Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

7,9-Octacosanediol O-10

$C_{28}H_{58}O_2$ 426.765
(7R*,9S*)-form [193419-71-5]
erythro-*form*
Constit. of dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 56-58°.
Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

5,7-Octacosanedione O-11

$H_3C(CH_2)_{20}COCH_2CO(CH_2)_3CH_3$
$C_{28}H_{54}O_2$ 422.733
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

6,8-Octacosanedione O-12

$H_3C(CH_2)_{19}COCH_2CO(CH_2)_4CH_3$
$C_{28}H_{54}O_2$ 422.733
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

7,9-Octacosanedione O-13

$H_3C(CH_2)_{18}COCH_2CO(CH_2)_5CH_3$
$C_{28}H_{54}O_2$ 422.733
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

8,10-Octacosanedione O-14

$H_3C(CH_2)_{17}COCH_2CO(CH_2)_6CH_3$
$C_{28}H_{54}O_2$ 422.733
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

10,12-Octacosanedione O-15

$H_3C(CH_2)_{15}COCH_2CO(CH_2)_8CH_3$
$C_{28}H_{54}O_2$ 422.733
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

11,13-Octacosanedione O-16

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_9CH_3$
$C_{28}H_{54}O_2$ 422.733
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

12,14-Octacosanedione O-17

$H_3C(CH_2)_{13}COCH_2CO(CH_2)_{10}CH_3$
$C_{28}H_{54}O_2$ 422.733
Constit. of the pollen of *Helianthus annuus* (sunflower).
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Octacosanol O-18

[557-61-9]
Montanyl alcohol. Cluytyl alcohol
$H_3C(CH_2)_{26}CH_2OH$
$C_{28}H_{58}O$ 410.766
Mp 83.2-83.4°.

Ac: [18206-97-8] *Octacosyl acetate*
$C_{30}H_{60}O_2$ 452.803
Bp_1 245°.

Hexadecanoyl: [78509-52-1] *Octacosyl hexadecanoate*
$C_{44}H_{88}O_2$ 649.178
Cryst. Mp 81-82°.

Octacosanoyl: [66662-27-9] *Octacosyl octacosanoate*
$C_{56}H_{112}O_2$ 817.5

Triacontanoyl: [87538-97-4] *Octacosyl triacontanoate*
$C_{58}H_{116}O_2$ 845.553
Constit. of *Solanum torvum* (pea eggplant). Cryst. (hexane). Mp 70°.

O-*(3-O-Benzoyl-β-D-glucopyranoside):*
[180465-33-2] ***Arundinoside B***
$C_{41}H_{72}O_7$ 677.016
Mp 208-212°. $[\alpha]_D$ -10.2 (Py).

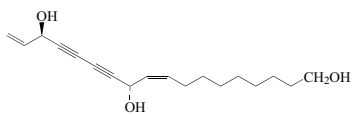
Bleyberg, W. *et al., Ber.*, 1931, **64**, 2504 (*synth*)
Pollard, A. *et al., Biochem. J.*, 1933, **27**, 1889 (*isol*)
Murray, K.E. *et al., Aust. J. Chem.*, 1955, **8**, 424
Mathis, C. *et al., Phytochemistry*, 1964, **3**, 379 (*isol*)
Radler, F. *et al., Aust. J. Chem.*, 1965, **18**, 1059 (*isol*)
Joshi, K.C. *et al., Planta Med.*, 1975, **28**, 190 (*isol*)
Mahmood, U. *et al., Phytochemistry*, 1983, **22**, 167-169 (*Octacosyl triacontanoate*)
Jain, D.C. *et al., Fitoterapia*, 1991, **62**, 93 (*Octacosyl octacosanoate*)
Khetwal, K.S. *et al., Phytochemistry*, 1994, **35**, 1033 (*Octacosanyl hexadecanoate*)
Tandon, M. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 988 (*Arundinoside B*)

10-Octacosene-1,12-diol O-19

[151454-17-0]
$H_3C(CH_2)_{15}CH(OH)CH=CH(CH_2)_8CH_2OH$
$C_{28}H_{56}O_2$ 424.749
Constit. of the tubers of *Colocasia esculenta antiquorum*. Mp 72-73°.
Ali, M. *et al., J. Indian Chem. Soc.*, 1992, **69**, 887 (*isol*)

9,17-Octadecadiene-12,14-diyne-1,11,16-triol, 9CI O-20

[288376-12-5]



(9Z,11S,16R)-form

$C_{18}H_{26}O_3$ 290.402
(9Z,11S,16R)-form
1-Ac: [213905-35-2] *1-Acetoxy-9,17-octadecadiene-12,14-diyne-11,16-diol*
Viscous oil. $[\alpha]_D^{20}$ +318.2 (c, 0.03 in MeCN). λ_{max} 228 ; 245 ; 258 ; 280 ; 320 (no solvent reported).

(9Z,11S,16S)-form [211238-60-7]
$[\alpha]_D^{25}$ +191 (c, 0.3 in $CHCl_3$). λ_{max} 234 (ε 1200); 246 (ε 1000); 260 (ε 700); 284 (ε 400) (MeOH).

1-Ac: [52691-49-3]
$C_{20}H_{28}O_4$ 332.439
Constit. of *Smyrnium olusatrum* (alexanders). Oil. $[\alpha]_D^{25}$ +178.8 (c, 9 in $CHCl_3$).

17,18-Dihydro, 1-Ac: [198490-49-2] *9-Octadecene-12,14-diyne-1,11,16-triol 1-acetate.* ***Oplopantriol acetate***
$C_{20}H_{30}O_4$ 334.455
Oil. $[\alpha]_D^{25}$ +164.5 (c, 5.7 in $CHCl_3$). λ_{max} 206 (ε 14846); 233 (ε 1354); 245 (ε 1277); 259 (ε 808) (EtOH).

Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 3614-3620 (*isol, struct, pmr, ir, ms, uv*)
Kobaisy, M. *et al., J. Nat. Prod.*, 1997, **60**, 1210-1213 (*isol, pmr, cmr*)

Liu, J.-H. *et al., Phytochemistry*, 1998, **49**, 211-213 (*isol, uv, ord, pmr, cmr, ms*)
Papajewski, S. *et al., Planta Med.*, 1998, **64**, 479-481 (*isol, uv, ir, pmr, cmr, ms*)
Choi, Y.E. *et al., Biol. Pharm. Bull.*, 2000, **23**, 884-886 (*isol*)

2,4-Octadecadienoic acid O-21

[76282-17-2]

$H_3C(CH_2)_{12}CH{=}CHCH{=}CHCOOH$

$C_{18}H_{32}O_2$ 280.45

(2*E*,4*E*)-*form* [59404-49-8]

Me ester: [86120-41-4]
$C_{19}H_{34}O_2$ 294.476
Oil.

2-Methylpropylamide: [54794-70-6] **N-*Isobutyl-2,4-octadecadienamide***
$C_{22}H_{41}NO$ 335.572
Mp 92-94° Mp 78-80°.

(2*E*,4*Z*)-*form*

2-Methylpropylamide: ***Pipericine***
$C_{22}H_{41}NO$ 335.572
Constit. of the fruit of *Piper nigrum* (pepper). Oil. λ_{max} 257 (EtOH).

Okogun, J.I. *et al., J.C.S. Perkin 1*, 1974, 2195 (*isol, ms*)
Vig, O.P. *et al., Indian J. Chem.*, 1975, **13**, 1358 (*synth, deriv*)
Akimoto, A. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 90 (*synth*)
Cardillo, G. *et al., Tetrahedron*, 1986, **42**, 917 (*deriv, synth, ir, pmr, cmr, ms*)
Baneriji, A. *et al., Indian J. Chem., Sect. B*, 1988, **27**, 163 (*isol, uv, ir, pmr*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419 (*synth, isobutylamide*)
Siddiqui, B.S. *et al., Phytochemistry*, 1997, **45**, 1617 (*Pipericine*)

9,12-Octadecadienoic acid, 9CI O-22

[2197-37-7]

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_7COOH$

$C_{18}H_{32}O_2$ 280.45
pK_a 4.77 (25°). Log P 7.26 (uncertain value) (calc).

(*E,E*)-*form* [506-21-8]
Linolelaidic acid
Cryst. (MeOH). Sol. Me_2CO, hexane, bases; poorly sol. H_2O. Mp 28-29°. $Bp_{0.8}$ 179-183°.

Me ester: [2566-97-4] *Methyl linolelaidate*
$C_{19}H_{34}O_2$ 294.476
Mp -7.8°. Bp_2 151-152°.

(9*E*,12*Z*)-*form* [2420-55-5]
Mp 1°.

(9*Z*,12*E*)-*form* [2420-42-0]
Mp 1°.

(*Z,Z*)-*form* [60-33-3] *Linoleic acid. Leinolic acid. Telfairic acid. Linolic acid*
Constit. of most vegetable oils and animal fats. The Fe salt is the major component of metallic drier compositions used to line food cans. Liq. Insol. H_2O; sol. EtOH, Et_2O. d_4^{25} 0.9. Mp -5°. Bp_{16} 229-230° $Bp_{0.02}$ 129°. n_D^{20} 1.4697. Undergoes thermal or catalysed dimerisation.

► Skin irritant. Gastrointestinal effects reported by ingestion. Fl. p. >66°.
RF9990000

Na salt: [822-17-3]
Mp 230° dec.

Ca salt: [19704-83-7] *Linocalcium*

Me ester: [112-63-0] *Methyl linoleate*
$C_{19}H_{34}O_2$ 294.476
Mixt. with (FEMA 3411) is used as a flavouring ingredient. Mp -35°. Bp_1 168-170°.

Et ester: [544-35-4]
$C_{20}H_{36}O_2$ 308.503
$Bp_{2.5}$ 175°. n_D^{20} 1.4600.

Isopropyl ester: [22882-95-7] *Isopropyl 9,12-octadecadienoate. Isopropyl linoleate*
$C_{21}H_{38}O_2$ 322.53
Liq. with low viscosity. d 0.87. $Bp_{2.5}$ 179°.

Chloride: [7459-33-8]
$C_{18}H_{31}ClO$ 298.895
$Bp_{0.3}$ 148°. Never marketed

Cyclohexylamide: [25167-65-1] ***Clinolamide, INN.*** *Linolexamide*
$C_{24}H_{43}NO$ 361.61
Mp 34-35°. $Bp_{0.02}$ 180-181°. Log P 8.45 (uncertain value) (calc).

Anhydride: [24909-68-0] *Linoleic anhydride*
$C_{36}H_{62}O_3$ 542.884
$d_4^{23.5}$ 0.9. Mp -4° Fp -18. n_D^{23} 1.4760.

9,10-Epoxide: See 9,10-Epoxy-12-octadecenoic acid, E-174

12,13-Epoxide: See 12,13-Epoxy-9-octadecenoic acid in *The Combined Chemical Dictionary.*

Dimer: [6144-28-1] *Dilinoleic acid*Consists predominantly of monocyclic species together with some bicyclic and tricyclic species.

[3207-50-9, 7779-63-7, 28984-77-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 501C; 643C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 785B; 989B; 989C; 1171B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 686B; 687A (*ir*)
Holde, D. *et al., Ber., B*, 1925, **58**, 1067 (*anhydride*)
Cowan, J.C. *et al., J.A.C.S.*, 1944, **66**, 84 (*synth, dimer*)
Kovac, S. *et al., Chem. Zvesti*, 1962, **16**, 82 (*isopropyl ester*)
Harlow, R.D. *et al., J. Am. Oil Chem. Soc.*, 1963, **40**, 505
Japan. Pat., 1963, 63 625 966; *CA*, **65**, 7066a
Nakatani, H. *et al., Science (Washington, D.C.)*, 1966, **153**, 1267 (*Clinolamide, metab, activity*)
Wheeler, D.H. *et al., J. Am. Oil Chem. Soc.*, 1970, **47**, 242 (*dimer, struct*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1972, **9**, 112 (*synth, pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 754 (*occur*)
Ackman, R.G. *et al., J. Chromatogr. Sci.*, 1974, **12**, 131 (*chromatog*)
Gunstone, F.D. *et al., J. Sci. Food Agric.*, 1976, **27**, 675 (*isol*)
McDaniel, C.A. *et al., J. Chem. Ecol.*, 1987, **13**, 227
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, LGG000; LGF900
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1383
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1791 (*Me ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, LGG000

9,15-Octadecadienoic acid O-23

[13309-77-8]

$H_3CCH_2CH{=}CH(CH_2)_4CH{=}CH(CH_2)_7COOH$

$C_{18}H_{32}O_2$ 280.45All 4 geom. isomers have been synthesised.

(*Z,Z*)-*form* [18402-92-1]
Mangiferic acid
Constit. of mango fruit and human milk.

[17309-05-6, 17600-03-2, 20221-28-7, 20221-29-8, 38700-60-6, 75656-26-7, 84393-26-0]

Butterfield, R.O. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 397 (*synth*)
Stroink, J.B.A. *et al., J. Am. Oil Chem. Soc.*, 1967, **44**, 531 (*synth*)
Murawski, U. *et al., Z. Naturforsch., C*, 1974, **29**, 1 (*isol*)
Snyder, J.M. *et al., J. Am. Oil Chem. Soc.*, 1982, **59**, 469 (*synth*)
Shibahara, A. *et al., Biochim. Biophys. Acta*, 1993, **1170**, 245 (*isol, struct*)
Gruiec, R. *et al., Bull. Soc. Chim. Fr.*, 1994, **131**, 699 (*synth, pmr, cmr*)

11,13-Octadecadien-9-ynoic acid O-24

$H_3C(CH_2)_3CH{=}CHCH{=}CHC{\equiv}C(CH)_7COOH$

$C_{18}H_{28}O_2$ 276.418

(*E,E*)-*form*
Constit. of the root lipids of the famine food *Ximenia americana*. Also from *Santalum acuminatum* (quandong). Cryst. (pentane). Mp 45-46°.

4-Bromophenacyl ester:
Cryst. (EtOH). Mp 62-63°.

Crombie, L.C. *et al., J.C.S.*, 1957, 1632 (*synth*)
Hatt, H.H. *et al., Aust. J. Chem.*, 1960, **13**, 488 (*isol*)
Bu'lock, J.D. *et al., Phytochemistry*, 1963, **2**, 289 (*isol*)
Ketola, M. *et al., Tetrahedron*, 1974, **30**, 2717

Octadecane O-25

[593-45-3]

$H_3C(CH_2)_{16}CH_3$

$C_{18}H_{38}$ 254.498
Found in hop oil and other plant sources. Isol. from *Piper longum* (long pepper). Cryst. (Me_2CO). Mp 28°. Bp 305-307° (317°) Bp_{15} 180-183°.

► Fl. p. >100°, autoignition temp. 227°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 4C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 5B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 5C (*ir*)
Schrauth, W. *et al., Ber.*, 1931, **64**, 1314 (*synth*)
Carey, P.C. *et al., J.C.S.*, 1933, 346 (*synth*)
Nyburg, S.C. *et al., Acta Cryst. B*, 1972, **28**, 2992 (*cryst struct*)
Trenner, N.R. *et al., J. Chromatogr.*, 1972, **71**, 415 (*glc*)

Pacakova, V. *et al., Chromatographia*, 1974, **7**, 171 (*glc*)
Erkelens, J. *et al., J. Catal.*, 1975, **39**, 173 (*ir*)

Octadecanoic acid, 9CI O-26

[57-11-4]
Stearic acid. Bassinic acid. Lactaric acid. Stearophanic acid. Talgic acid. FEMA 3035

$H_3C(CH_2)_{16}COOH$

$C_{18}H_{36}O_2$ 284.481

For salts see Octadecanoic acid salts, O-27. Constit. of most vegetable and animal fats. Food uses include: flavour modifier, adjuvant, defoamer, lubricant, masticatory aid in chewing gum base, component of fruit coatings and clarifying agent in wines. Leaflets. Sol. EtOH, C_6H_6, $CHCl_3$; sl. sol. H_2O. Mp 69.7°. Bp 386° Bp_5 213°. Polymorphic, at least 4 cryst. forms are known.

▶ Skin irritant. Fl. p. 196°, autoignition temp. 395°. WI2800000

Me ester: [112-61-8] *Methyl octadecanoate. Methyl stearate*
$C_{19}H_{38}O_2$ 298.508
Antifoaming agent and fermentation nutrient. Mp 39.1°. Bp_{15} 215°.

▶ Fl. p. 153°. WI4460000

Et ester: [111-61-5] *Ethyl octadecanoate. Ethyl stearate. FEMA 3490*
$C_{20}H_{40}O_2$ 312.535
Flavouring ingredient. Cryst. Mp 33.4° (30.9°). Bp 318° Bp_{10} 199°.

▶ Skin irritant. WI3600000

Butyl ester: [123-95-5] *Butyl octadecanoate. Butyl stearate. FEMA 2214*
$C_{22}H_{44}O_2$ 340.588
Flavouring agent; defoaming agent used in processing beet sugar and yeast. Cryst. (EtOH). Mp 27.5°. Bp_{25} 220-225°.

▶ WI2900000

Amide: [124-26-5] *Octadecanamide. Stearamide. Amide C-18. Kemamide® S*
$C_{18}H_{37}NO$ 283.496
Release agent migrating from food packaging. Cryst. (EtOH). Mp 109°. Bp_{12} 250-251°.

▶ RG0182000

[593-29-3, 4568-28-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 485C; 609C; 609D; 748C; 840B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 757B; 851A; 1169C (*nmr*)
Sadtler Standard Proton NMR Spectra, 9661 (*pmr*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, NY, 1947, **2**, 82 (*use*)
Bricas, E. *et al., Biochemistry*, 1965, **4**, 2254 (*use*)
Malta, V. *et al., J.C.S.(B)*, 1971, 548 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 705 (*occur*)
Schwarz, R.P. *et al., J. Lipid Res.*, 1978, **19**, 12 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 383 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, SLK000
Kaneko, F. *et al., Acta Cryst. C*, 1990, **46**, 1490; 1994, **50**, 245; 247 (*cryst struct*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1993, **65**, 155 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 95; 258 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 355-356; 1023-1024; 2677-2679 (*use, esters, use*)
Dembitsky, V.M. *et al., Phytochemistry*, 2000, **54**, 965-967 (*isol, amide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSL600; MJW000; OAR000; ZMS000; SLK000; CAX350; SJV500; SLL500

Octadecanoic acid salts O-27

Octadecanoates. Stearates
For parent acid see Octadecanoic acid, O-26.

Na salt: [822-16-2]

[19322-83-9] *Sodium octadecanoate. Sodium stearate*
$C_{18}H_{35}NaO_2$ 306.463
Used in foods as a binder, emulsifier and anticaking agent. Soapy-feeling powder with sl. tallow-like odour. A 3:1 salt is also known.

K salt: [593-29-3] *Potassium octadecanoate. Potassium stearate*
$C_{18}H_{35}KO_2$ 322.572
Used in foods as a binder, emulsifier, anticaking agent, defoaming agent and masticatory substance. White powder (EtOH). Commercial product contains palmitate.

Mg salt: [557-04-0]

[114601-81-9] *Magnesium octadecanoate. Magnesium stearate*
$C_{36}H_{70}MgO_4$ 591.252
Used in foods as a binder, emulsifier, anticaking agent, lubricant and release agent, nutrient supplement, defoaming agent and processing aid. Cryst. (EtOH aq.). Mp 132° Mp 183° dec.

Ca salt: [1592-23-0] *Calcium octadecanoate. Calcium stearate*
$C_{36}H_{70}CaO_4$ 607.025
Used in foods as a flavouring adjuvant, lubricant, release agent, stabiliser and thickener, binder, emulsifier and anticaking agent. Cryst. Mp 150-156° (147-149°).

Zn salt: [557-05-1] *Zinc octadecanoate.* ***Zinc stearate, USAN***
$C_{36}H_{70}O_4Zn$ 632.337
Nutrient supplement. Mp 140° (128-130°).

Al salt: [637-12-7] *Aluminium octadecanoate. Aluminium stearate*
$C_{54}H_{105}AlO_6$ 877.401
Used in foods as a buffer, firming agent and neutralising agent. Mp 117-120°.

[3353-05-7, 5136-76-5, 6865-35-6, 10476-84-3]

Koenig, A.E. *et al., J.A.C.S.*, 1914, **36**, 951-961 (*salts*)
Martin, E.P. *et al., J.C.S.*, 1948, 1750-1755 (*Zn salt*)
Lomer, T.R. *et al., Acta Cryst.*, 1952, **5**, 11-17 (*K salt, cryst struct*)
Muller, B.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1977, **310**, 693-704 (*Mg salt*)
Merck Index, 12th edn., 1996, 379; 588; 1750; 5442; 7844; 8827 (*Na salt, K salt, Ca salt, Al salt, Pb salt, NH_4 salt*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 119-120; 425-426; 1633-1635; 2322; 2608-2609; 2991-2992

1-Octadecanol, 9CI O-28

[112-92-5]

[26762-44-7]
Stearyl alcohol. Octadecyl alcohol. Stenol

$H_3C(CH_2)_{16}CH_2OH$

$C_{18}H_{38}O$ 270.498
Solidifying agent for margarine and other foods containing semi-solid fats. Generally recognised as safe (GRAS) status in the USA. Leaves (EtOH), cryst. (petrol). Mp 59.4-59.8°. Bp_{19} 217° Bp_{15} 210°.

▶ LD_{50} (rat, orl) 20000 mg/kg. Autoignition temp. 450°. RG2010000

O-*Phosphate:* [2958-09-0] *Phosphoric acid monooctadecyl ester, 9CI. Monooctadecyl phosphate. Monostearyl phosphate. Octadecyl monophosphate. Octadecyl phosphate. Stearyl monophosphate. Stearyl phosphate*
$C_{18}H_{39}O_4P$ 350.478
Cryst. (petrol). Mp 83°.

O-*Sulfate:*
$C_{18}H_{38}O_4S$ 350.562
Amorph. solid (as Na salt).

Formyl: [5451-75-2] *Octadecyl formate*
$C_{19}H_{38}O_2$ 298.508
Cryst. (petrol). Mp 57.2° (52-53°) Mp 67-68.5°.

Ac: [822-23-1]
$C_{20}H_{40}O_2$ 312.535
Cryst. Mp 33°. Dimorphic.

Me ether: [6838-81-9] *1-Methoxyoctadecane, 9CI*
$C_{19}H_{40}O$ 284.524
Cryst. (Et_2O/EtOH). Mp 30-31°.

Et ether: [62435-06-7] *1-Ethoxyoctadecane, 9CI*
$C_{20}H_{42}O$ 298.551
Mp 35-37°. $Bp_{0.44}$ 166-168°.

Propyl ether: [65018-61-3] *1-Propoxyoctadecane, 9CI*
$C_{21}H_{44}O$ 312.578
Mp 40°. $Bp_{0.4}$ 160-162°.

Butyl ether: [111082-35-0] *1-Butoxyoctadecane, 9CI*
$C_{22}H_{46}O$ 326.605
Cryst. (EtOH). Mp 29°. $Bp_{0.7}$ 152°.

Vinyl ether: [930-02-9] *1-(Ethenyloxy)octadecane, 9CI. Ethenyl octadecyl ether. Octadecyloxyethylene. Stearyloxyethylene. Stearyl vinyl ether. 1-(Vinyloxy)octadecane*
$C_{20}H_{40}O$ 296.535
Mp 29°. Bp_{10} 190°. Undergoes cationic homopolym. Q/e values for radical polym., Q 0.024, e -1.93.

▶ RG0300000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 113C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 168C (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 159D (*ir*)
Aldrich Library of NMR Spectra, **1**, 83A (*pmr*)
Brown, D.A. *et al., J.C.S.*, 1955, 1584-1588 (*phosphate, synth, cryst struct*)
Reppe, W. *et al., Annalen*, 1956, **601**, 84 (*vinyl ether*)
Fishbein, L. *et al., Makromol. Chem.*, 1961, **48**, 221 (*polym, vinyl ether*)
Chatterjee, P.C. *et al., Indian J. Chem.*, 1967, **5**, 160 (*polym, vinyl ether*)
Precht, V.D. *et al., Fette, Seifen, Anstrichm.*, 1976, **78**, 145; 189 (*cryst struct*)
Maya, L. *et al., J. Chromatogr.*, 1980, **190**, 145-149 (*synth*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values, vinyl ether*)
Vetter, W. *et al., Org. Mass Spectrom.*, 1981, **16**, 118 (*ms*)
Yamaoka, R. *et al., Nippon Oyo Dobutsu Konchu Gakkaishi*, 1983, **27**, 77 (*occur*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1985, **36**, 253 (*cmr*)
Rafat Husain, S. *et al., Lipids*, 1987, **22**, 578 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, OAX000
Japan. Pat., 1990, 02 286 690; *CA*, **114**, 185754n (*sepn, purifn*)
Armarego, W.L.F. *et al., Biol. Chem. Hoppe-Seyler*, 1993, **374**, 9 (*ethers*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 498-499
Japan. Pat., 1996, 08 259 576; *CA*, **126**, 31482h (*synth*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1411
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, **3**, 2679-2682
Osvath, R. *et al., Food Chem. News*, 2001, **43**, 7 (*use, status*)
Aiello, A. *et al., J. Nat. Prod.*, 2001, **64**, 219-221 (*sulfate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OAX000

4,8,12,15-Octadecatetraenoic acid, 9CI O-29

[67329-10-6]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2CH{=}CHCH_2CH_2COOH$

$C_{18}H_{28}O_2$ 276.418

Isol. from sardine oil.

[81275-46-9, 106440-10-2]

Toyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1935, **10**, 232 (*isol*)
Hörhammer, L. *et al., Arzneim.-Forsch.*, 1964, **14**, 34 (*isol*)
Mimura, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4562 (*isol*)

6,9,12,15-Octadecatetraenoic acid O-30

[2091-28-3]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$

$C_{18}H_{28}O_2$ 276.418

(6*Z*,9*Z*,12*Z*,15*Z*)-*form* [20290-75-9] ***Stearidonic acid***

Isol. from herring and other fish oils. Pale yellow oil. Mp *ca.* ° -57. n_D^{16} 1.4888.

[73097-00-4, 81275-46-9]

Klenk, E. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1957, **307**, 272 (*isol*)
Craig, B.M. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 209 (*isol*)
De Gomez Dumm, I.N.T. *et al., J. Lipid Res.*, 1975, **16**, 264
De Gomez Dumm, I.N.T. *et al., Lipids*, 1975, **10**, 315
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1991, **59**, 83 (*cmr*)
Griffiths, G. *et al., Phytochemistry*, 1996, **43**, 381 (*isol, biosynth*)

2,4,12-Octadecatrienoic acid O-31

$H_3C(CH_2)_4CH{=}CH(CH_2)_6CH{=}CHCH{=}CHCOOH$

$C_{18}H_{30}O_2$ 278.434

(2*E*,4*E*,12*Z*)-*form*

2-Methylpropylamide: [151391-69-4] *2,4,12-Octadecatrienoic acid isobutylamide.* N-*Isobutyl-2,4,12-octadecatrienamide*

$C_{22}H_{39}NO$ 333.556

Alkaloid from *Piper retrofractum* (Javanese long pepper). Oil. λ_{max} 263 (log ϵ 4.04) (MeOH).

Piperidide: [151391-71-8] *2,4,12-Octadecatrienoic acid piperidide. 1-(2,4,12-Octadecatrienoyl)piperidine*

$C_{23}H_{39}NO$ 345.567

Alkaloid from *Piper retrofractum* (Javanese long pepper).

Kikuzaki, H. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1329-1333 (*isol, amides*)

6,9,12-Octadecatrienoic acid, 9CI O-32

[1686-12-0]

[25448-03-7]

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_4COOH$

$C_{18}H_{30}O_2$ 278.434

(*Z*,*Z*,*Z*)-*form* [506-26-3]

[27213-43-0]

γ-Linolenic acid. ***Gamolenic acid, BAN, INN****. Gammalinolenic acid. Efomase. Epogam. Gammolin. Efemast. Unigam. GLA*

A minor component of many animal lipids. Log P 6.78 (calc).

[122051-95-0]

Bernhard, K. *et al., Helv. Chim. Acta*, 1948, **31**, 977; 981 (*props*)
Riley, J.P. *et al., J.C.S.*, 1949, 2728 (*struct*)
Bus, J. *et al., Chem. Phys. Lipids*, 1976, **17**, 501 (*cmr*)
Lie Ken Jie, M. *et al., Chem. Phys. Lipids*, 1976, **18**, 130 (*cmr*)
Fr. Pat., 1976, 1 603 386, (*Ono*); *CA*, **76**, 84681 (*isol*)
Horrobin, D.F. *et al., Agents Actions*, Suppl., 1992, **37**, 120 (*rev*)
Gunstone, F.D. *et al., Prog. Lipids Res.*, 1992, **31**, 145-161 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1371
Jamal, G.A. *et al., Diabetic Med.*, 1994, **11**, 145 (*rev, pharmacol*)
Guivernau, M. *et al., Prostaglandins, Leukotrienes, Essent. Fatty Acids*, 1994, **51**, 311 (*Evening primrose oil, pharmacol, human*)
Durand, S. *et al., Synthesis*, 1998, 1015-1018 (*synth, pmr, cmr*)

8,10,12-Octadecatrienoic acid O-33

[25448-03-7]

$H_3C(CH_2)_4CH{=}CHCH{=}CHCH{=}CH(CH_2)_6COOH$

$C_{18}H_{30}O_2$ 278.434

(*E*,*E*,*E*)-*form* [822-19-5]

Mp 77-78°.

Maleic anhydride adduct:

Cryst. (petrol). Mp 71°.

(8*E*,10*E*,12*Z*)-*form* [28872-28-8] ***Calendic acid****. Calendulic acid*

Isol. from *Calendula officinalis* (pot marigold) seed oil. Mp 40-40.5°.

Tetracyanoethylene adduct:

Mp 112.5-113.5°.

Maleic anhydride adduct:

Mp 73-74°.

(8*Z*,10*E*,12*Z*)-*form* [18961-59-6] ***Jacaric acid****. Jacaranda acid*

Mp 43.5-44°.

[27213-43-0]

McLean, J. *et al., J.C.S.*, 1956, 777 (*isol*)
Chisholm, M.J. *et al., Can. J. Chem.*, 1960, **38**, 2500 (*isol*)
Chisholm, M.J. *et al., J.O.C.*, 1962, **27**, 3137 (*isol*)
Bergel'son, L.D. *et al., CA*, 1967, **67**, 99692 (*synth*)
Conacher, H.B.S. *et al., Lipids*, 1970, **5**, 434
Crombie, L. *et al., Chem. Comm.*, 1984, 953 (*biosynth*)

9,11,13-Octadecatrienoic acid O-34

[13296-76-9]

[25448-03-7]

$H_3C(CH_2)_3CH{=}CHCH{=}CHCH{=}CH(CH_2)_7COOH$

$C_{18}H_{30}O_2$ 278.434

(9*Z*,11*E*,13*E*)-*form* [506-23-0]

α-Eleostearic acid. Elaeostearinic acid. Margarolic acid. Elaeomargarinic acid

Isol. from seed oil of *Momordica charantia* (bitter melon). Cryst. (MeOH). Mp 49-49.2°. Rapidly polymerises λ_{max} 262 ; 272 ; 293 (cyclohexane) (Berdy).

(9*Z*,11*E*,13*Z*)-*form* [544-72-9]

Punicic acid. Trichosanic acid. Punicinic acid

Found in pomegranate oil (*Punica granatum*). Mp 44-45°. λ_{max} 265 ; 275 ; 287 (cyclohexane).

[27213-43-0]

Farmer, E.H. *et al., J.C.S.*, 1936, 1809-1811 (*punicic acid, isol, struct*)
Alder, H. *et al., Annalen*, 1957, **609**, 24; 36 (*isol*)
Crombie, L. *et al., J.C.S.*, 1957, 1632-1636; 1962, 2449 (*punicic acid, synth*)
Hopkins, C.Y. *et al., Can. J. Chem.*, 1962, **40**, 2078; 1965, **43**, 3160 (*isol, struct*)
Chisholm, M.J. *et al., Can. J. Chem.*, 1964, **42**, 560 (*isol*)
Hopkins, C.Y. *et al., Top. Lipid Chem.*, 1973, **3**, 37 (*rev*)
Tulloch, A.P. *et al., Lipids*, 1979, **14**, 996 (*cmr*)
Tsuboi, S. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 1103 (*synth*)

9,12,15-Octadecatrienoic acid, 9CI O-35

[1955-33-5]

[25448-03-7]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_7COOH$

$C_{18}H_{30}O_2$ 278.434

(*E,E,E*)-*form* [28290-79-1]
Linolenelaidic acid. *Elaidolinolenic acid*
Isol. from seed oil of safflower (*Carthamus tinctorius*). Cryst. (C_6H_6). Mp 29.5-30°. $Bp_{0.8}$ 179-183°. n_D^{27} 1.4655.

(*Z,Z,Z*)-*form* [463-40-1]

[27213-43-0]
α-Linolenic acid
An essential fatty acid. d_4^{20} 0.92. Mp -11.3°. $Bp_{0.07}$ 137° $Bp_{0.05}$ 125°.

*9*R*,10*S*-Epoxide: [36747-82-7] *9,10-Epoxy-12,15-octadecadienoic acid*
$C_{18}H_{30}O_3$ 294.433
Present as a minor component in soybean oil.

12ξ,13ξ-Epoxide: [88159-18-6] *12,13-Epoxy-9,15-octadecadienoic acid*
$C_{18}H_{30}O_3$ 294.433
Isol. from roots of rice plant Fukuyuki. $[\alpha]_D^{20}$ -0.23 (c, 1.71 in $CHCl_3$).

15ξ,16ξ-Epoxide:15,16-Epoxy-9,12-octadecadienoic acid
$C_{18}H_{30}O_3$ 294.433
Isol. from roots of rice plant, also from seed oil of false flax (*Camelina sativa*). $[\alpha]_D^{20}$ +0.27 (c, 1.5 in $CHCl_3$).

[7361-80-0]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **1**, 785C; 990B; 990C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 502B; 643D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 589A; 687C; 687D (*ir*)
Nigam, S.S. *et al., J.C.S.*, 1956, 4049 (*synth*)
Gunstone, F.D. *et al., J.C.S.*, 1959, 2127 (*epoxide*)
Chisholm. M.J., *et al., Can. J. Chem.*, 1963, **41**, 1888; 1965, **43**, 2566 (*isol, uv, ir*)
Strocchi, A. *et al., Rev. Fr. Corps. Gras*, 1969, **13**, 3 (*isom*)
Sen Gupta, A.K. *et al., Chem. Ind. (London)*, 1972, 257 (*epoxide*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 759 (*occur*)
Ackman, R.G. *et al., J. Chromatogr. Sci.*, 1974, **12**, 131 (*cmr*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Rakoff, M. *et al., Chem. Phys. Lipids*, 1982, **31**, 213 (*synth, cmr, glc*)
Kato, T. *et al., Tet. Lett.*, 1983, **24**, 4715 (*epoxides*)
Sandri, J. *et al., Synthesis*, 1995, 271 (*linolenic acid, synth, pmr, cmr, ir*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OAX100

10,14,16-Octadecatrien-12-ynoic acid O-36

$H_3CCH{=}CHCH{=}CHC{\equiv}CCH{=}CH(CH_2)_8COOH$

$C_{18}H_{26}O_2$ 274.402

(10*Z*,14*E*,16*E*)-*form*
Constit. of the roots of *Ximenia americana* (tallow nut). Yellow oil. λ_{max} 229 (log ε 3.84); 240 (log ε 3.52); 253 (log ε 3.44); 267 (log ε 3.87); 283 (log ε 3.29); 367 (log ε 3.29) (MeOH).

Fatope, M.O. *et al., J. Agric. Food Chem.*, 2000, **48**, 1872-1874

9-Octadecenal O-37

[5090-41-5]

$H_3C(CH_2)_7CH{=}CH(CH_2)_7CHO$

$C_{18}H_{34}O$ 266.466

(*Z*)-*form* [2423-10-1]
Oleic aldehyde
Isol. from the oil of hops (*Humulus lupulus*). Also found in the aromas of various cooked meats. Liq. $Bp_{0.001}$ 108-110°.

2,4-Dinitrophenylhydrazone:
Yellow cryst. (EtOH). Mp 67-68°.

[10009-79-7]

Valicenti, A.J. *et al., Chem. Phys. Lipids*, 1976, **17**, 389
Wedmid, Y. *et al., J.O.C.*, 1977, **42**, 3624
Mancuso, A.J. *et al., J.O.C.*, 1978, **43**, 2480
Tatsuki, S. *et al., Appl. Entomol. Zool.*, 1985, **20**, 357
Hedin, P.A. *et al., J. Chem. Ecol.*, 1986, **12**, 2051 (*isol*)
Tsay, S.-C. *et al., J.C.S. Perkin 1*, 1990, 757 (*synth*)

13-Octadecenal, 9CI O-38

[56554-90-6]

$H_3C(CH_2)_3CH{=}CH(CH_2)_{11}CHO$

$C_{18}H_{34}O$ 266.466

(*Z*)-*form* [58594-45-9]
Oil. $Bp_{0.01}$ 110-112°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra , 1992, **1**, 741B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 564A (*ir*)
Ohta, K. *et al., Agric. Biol. Chem.*, 1976, **40**, 1897 (*synth, pmr, ir, ms, glc, activity*)
Kanno, H. *et al., Appl. Entomol. Zool.*, 1978, **13**, 321 (*activity*)
Bestmann, H.J. *et al., Chem. Ber.*, 1979, **112**, 3740 (*synth, pmr, ir, ms, activity*)
McDonough, L.M. *et al., Environ. Entomol.*, 1982, **11**, 711 (*activity*)
Hedin, P.A. *et al., J. Chem. Ecol.*, 1986, **12**, 2051 (*activity*)
Mangold, H.K. *et al., Z. Naturforsch., C*, 1986, **41**, 555 (*synth*)
Lanne, B.S. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1987, **88**, 631 (*isol*)
Robacker, D.C. *et al., J. Chem. Ecol.*, 1989, **15**, 105 (*activity*)
Zagatti, P. *et al., J. Chem. Ecol.*, 1991, **17**, 1399 (*isol, activity*)
Gil, S. *et al., Synth. Commun.*, 1995, **25**, 351; 1996, **26**, 2329 (*synth*)

15-Octadecene-9,11,13-triynoic acid O-39

$H_3CCH_2CH{=}CHC{\equiv}CC{\equiv}CC{\equiv}C(CH_2)_7COOH$

$C_{18}H_{22}O_2$ 270.371
Major component of the lipids of *Santalum acuminatum* (quandong). λ_{max} 212 ; 223 ; 232 ; 244 ; 258 ; 274 ; 291 ; 310 ; 332 (no solvent reported).

Bu'Lock, J.D. *et al., Phytochemistry*, 1963, **2**, 289

2-Octadecenoic acid O-40

[5340-63-6]

$H_3C(CH_2)_{14}CH{=}CHCOOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [2825-79-8]
Cryst. (EtOH or petrol). Mp 58.5°.

Piperidide:1-(1-Oxo-2-octadecenyl)piperidine, 9CI. N-*(2-Octadecenoyl)piperidine.* ***Pipercitine***
$C_{23}H_{43}NO$ 349.599
Alkaloid from the dried seeds of black pepper (*Piper nigrum*). Amorph. powder. λ_{max} 210 (ε 6450) (MeOH).

Siddiqui, B.S. *et al., Heterocycles*, 2002, **57**, 1653-1658 (*Pipercitine*)

6-Octadecenoic acid O-41

$H_3C(CH_2)_{10}CH{=}CH(CH_2)_4COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [593-40-8]
Petroselaidic acid. Tarelaidinic acid
Cryst. ($CHCl_3$ or MeOH). Mp 52.7-53.4° Mp 54-59°.

Me ester: [14620-36-1]
$C_{19}H_{36}O_2$ 296.492
Bp_{10} 208-210° Bp_4 185-186°.

Chloride:
$C_{18}H_{33}ClO$ 300.911
Bp_2 144-146°.

(*Z*)-*form* [593-39-5] *Petroselinic acid*
Found in umbelliferous seed oils e.g. major constit. of oils of parsley, ivy, fennel, celery and others. Cryst. (MeOH or EtOH aq.). Mp 33°. $Bp_{2.5}$ 215-217° (lit. gives a pressure range) $Bp_{0.15}$ 148-152°.

Baker, B.W. *et al., J.C.S.*, 1952, 1804
Lamb, P.B. *et al., J.C.S.*, 1952, 5032 (*synth, config*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539 (*cryst struct*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Batchelor, J.G. *et al., J.O.C.*, 1974, **39**, 1698 (*cmr*)
Parodi, P.W. *et al., J. Dairy Sci.*, 1976, **59**, 1870 (*synth, glc*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224
Conacher, H.B.S. *et al., J. Assoc. Off. Anal. Chem.*, 1978, **61**, 702 (*glc*)
Kaneko, F. *et al., Acta Cryst. C*, 1992, **48**, 1054; 1057 (*cryst struct*)
Cahoon, E.B. *et al., Prog. Lipids Res.*, 1994, **33**, 155 (*rev, biosynth*)

7-Octadecenoic acid O-42

[14122-42-0]

$H_3C(CH_2)_9CH{=}CH(CH_2)_5COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [13126-32-4]
Mp 44.2-44.5°.

(*Z*)-*form* [13126-31-3]
Mp 11.8-12.5° Mp 12.5-13.1°.

Huber, W.F. *et al., J.A.C.S.*, 1951, **73**, 2732 (*cryst struct*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539 (*cryst struct*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Stepaneko, G.A. *et al., Khim. Prir. Soedin.*, 1972, **8**, 709; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 694 (*occur*)
Schwartz, D.P. *et al., Anal. Biochem.*, 1976, **74**, 320

Parodi, P.W. *et al., J. Dairy Sci.*, 1976, **59**, 1870 (*glc*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224

8-Octadecenoic acid O-43

$H_3C(CH_2)_8CH{=}CH(CH_2)_6COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [5684-81-1]
Mp 51.5-52.3° Mp 52-52.6°.

(*Z*)-*form* [5684-71-9]
Mp 22.7-23.8°.

Huber, W.F. *et al., J.A.C.S.*, 1951, **73**, 2730 (*synth*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539 (*cryst struct*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Davies, J.E.D. *et al., J.C.S. Perkin 2*, 1972, 1557 (*ir, Raman*)
Stepanenko, G.A. *et al., Khim. Prir. Soedin.*, 1972, **8**, 709; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 694 (*occur*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224

9-Octadecenoic acid, 9CI O-44

[2027-47-6]

[26764-26-1]

$H_3C(CH_2)_7CH{=}CH(CH_2)_7COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [112-79-8]

[27251-59-8]
Elaidic acid
Minor constit. of plant oils. Cryst. (EtOH). Mp 45-45.5°. Bp_{15} 234° $Bp_{0.8}$ 180-185°. Dimorphic.

►LD_{50} (mus, ivn) 100 mg/kg. JX6125000

(*Z*)-*form* [112-80-1]

[27104-13-8]
Oleic acid. Rapinic acid. Pamolyn 100. MYX 6121. FEMA 2815
Major constit. of plant oils e.g. olive oil (*ca.* 80%), almond oil (*ca.* 80%) and many others, mainly as glyceride. Constit. of tall oil. Also present in apple, melon, raspberry oil, tomato, banana, roasted peanuts, black tea, rice bran, cardamon, plum brandy, peated malt, dairy products and various animal fats. Component of citrus fruit coatings. Emulsifying agent in foods. Oil. Insol. H_2O; sol. EtOH, Et_2O. d_4^{20} 0.9. Mp 12° (labile form) Mp 16° (stable form). Bp_5 203-205°. n_D^{20} 1.4595. Log P 7.75 (uncertain value) (calc). ^{125}I and ^{131}I labelled cpds. are used as radioactive agents (Oleotope). Undergoes BF_3-catalysed dimerisation.

►Skin irritant. LD_{50} (rat, orl) 74000 mg/kg. RG2275000

Na salt: [143-19-1]
Binder, emulsifier, anticaking agent. Mp 232-235°.

►RK1200000

Et ester: [111-62-6] *Ethyl oleate. FEMA 2450*
Flavouring ingredient. Oil with a faint, floral odour. d^{20} 0.87. Bp_{151} 216-217°. n_D^{20} 1.4515.

►RG3715000

Amide: [301-02-0] *Oleamide. Kemamide O*
$C_{18}H_{35}NO$ 281.481
Release agent migrating from food packaging. Scales (EtOH). Sol. MeOH. Mp 75-76°.

[142-17-6, 143-18-0, 544-60-5, 557-07-3, 688-37-9, 1555-53-9, 2462-84-2, 2717-15-9, 3687-46-5, 10402-16-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 501B; 546A; 733B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 782C; 783A; 987A; 987B; 1171A; 1200B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 588A; 588B; 685C; 685D (*ir*)
Gensler, W.J. *et al., J.A.C.S.*, 1951, **73**, 1071 (*synth*)
Org. Synth., 1957, **37**, 66 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 738; 739 (*occur*)
Bonfand, A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1975, **281**, 723 (*synth*)
Bailey, A.W. *et al., J. Am. Oil Chem. Soc.*, 1976, **53**, 89 (*cryst struct, esters*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Ackman, R.G. *et al., J. Chromatogr. Sci.*, 1978, **16**, 204 (*glc*)
Miller, R.A. *et al., J. Liq. Chromatogr.*, 1978, **1**, 291 (*hplc*)
Gross, M.L. *et al., Lipids*, 1986, **21**, 580 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, OHU000
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 182-183; 325-326
Lerner, R. *et al., Science (Washington, D.C.)*, 1995, **268**, 1506 (*isol, amide*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1410; 1704
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1028; 2041-2045; 2580 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAF500; OHU000; OHW000; OIA000

10-Octadecenoic acid O-45

[3386-63-8]
Isooleic acid

$H_3C(CH_2)_6CH{=}CH(CH_2)_8COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [5684-82-2]
Mp 52-52.6°. Bp_3 208-216°.

Amide:
$C_{18}H_{35}NO$ 281.481
Mp 83°.

(*Z*)-*form* [2442-70-8]
Mp 22.2-22.8°.

Huber, F. *et al., J.A.C.S.*, 1951, **73**, 2730 (*synth*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539 (*cryst struct*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224
Venkatachalam, S.R. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 515 (*isol, ms*)

11-Octadecenoic acid O-46

[143-25-9]

$H_3C(CH_2)_5CH{=}CH(CH_2)_9COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [693-72-1]
Vaccenic acid
Occurs in small proportions in ruminant fats (e.g., butter) *via* biohydrogenation of dietary polyene acids. Mp 43.5-44.1°.

Me ester: [6198-58-9]
$C_{19}H_{36}O_2$ 296.492
Bp_3 172-173°.

(*Z*)-*form* [506-17-2] *Asclepic acid*
A minor component of various natural fats. Cryst. (Me_2CO). Mp 14.5-15.5°.

Me ester: [1937-63-9]
$Bp_{0.1}$ 162-164°. n_D^{20} 1.4500.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 987C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 685A (*ir, Asclepic acid*)
Bounds, D.G. *et al., J.C.S.*, 1954, 4219 (*synth*)
Swern, D. *et al., J. Am. Oil Chem. Soc.*, 1955, **32**, 539 (*cryst struct*)
Cohen, M. *et al., Biochemistry*, 1966, **5**, 2385 (*isol*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Noble, R.C. *et al., Br. J. Nutr.*, 1974, **31**, 99
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 213 (*cmr*)
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224 (*isol*)

12-Octadecenoic acid O-47

[7378-88-3]

$H_3C(CH_2)_4CH{=}CH(CH_2)_{10}COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [13126-38-0]
Cryst. (petrol). Mp 39.7-40.1° Mp 52-53°.

(*Z*)-*form* [13126-37-9]
Mp 26.5-27.5° Mp 26.8-27.6°. $Bp_{1.5}$ 196°.

Et ester:
$C_{20}H_{38}O_2$ 310.519
$Bp_{0.4}$ 184°.

Huber, F. *et al., J.A.C.S.*, 1951, **73**, 2730 (*synth*)
Baker, C.D. *et al., J.C.S.*, 1963, 489 (*synth*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Schwartz, D.P. *et al., Anal. Biochem.*, 1976, **74**, 320
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Conacher, H.B.S. *et al., J. Assoc. Off. Anal. Chem.*, 1978, **61**, 702 (*glc*)

13-Octadecenoic acid O-48

[7378-89-4]

$H_3C(CH_2)_3CH{=}CH(CH_2)_{11}COOH$

$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [693-71-0]
Mp 43.5-44.5°.

(*Z*)-*form* [13126-39-1]
Constit. of various lipid fractions from fish and some cooked foods. Mp 26.5-27°.

Me ester: [13058-55-4]
$C_{19}H_{36}O_2$ 296.492
Liq. $Bp_{0.4}$ 145°.

Et ester: [101766-90-9]
$C_{20}H_{38}O_2$ 310.519
Viscous liq.

[42199-38-2, 56338-67-1]

Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1967, **1**, 209; 264; 1977, **18**, 115 (*synth, cmr*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Singh, B. *et al., J. Nat. Prod.*, 1989, **52**, 180 (*isol, ir, pmr, cmr, esters*)
Subbaraman, A.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 865 (*synth, ir*)

15-Octadecenoic acid O-49

[15737-21-0]
$H_3CCH_2CH{=}CH(CH_2)_{13}COOH$
$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [13126-44-8]
Cryst. (EtOH). Mp 59° Mp 61-61.5°.

(*Z*)-*form* [13126-43-7]
Cryst. (Me_2CO). Mp 41-42°.

Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Klok, R. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 222 (*synth*)
Parodi, P.W. *et al., J. Dairy Sci.*, 1976, **59**, 1870 (*isol, synth, glc*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Conacher, H.B.S. *et al., J. Am. Oil Chem. Soc.*, 1978, **61**, 702 (*glc*)
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224

16-Octadecenoic acid O-50

[21739-76-4]
$H_3CCH{=}CH(CH_2)_{14}COOH$
$C_{18}H_{34}O_2$ 282.465

(*E*)-*form* [10440-93-4]
Cryst. (MeOH). Mp 65.6-66.2°.

Me ester: [42199-41-7]
$C_{19}H_{36}O_2$ 296.492
Mp 28.3-28.9°.

(*Z*)-*form* [13126-45-9]
Mp 54°.

Kapp, R. *et al., J.A.C.S.*, 1943, **65**, 2062 (*synth*)
Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311 (*synth*)
Frost, D.J. *et al., Chem. Phys. Lipids*, 1975, **15**, 53 (*pmr*)
Bus, J. *et al., Chem. Phys. Lipids*, 1976, **17**, 501 (*cmr*)
Schwartz, D.P. *et al., Anal. Biochem.*, 1976, **74**, 320
Saito, Y. *et al., Biochim. Biophys. Acta*, 1978, **529**, 224

9-Octadecen-1-ol, 9CI O-51

[593-47-5]
$H_3C(CH_2)_7CH{=}CH(CH_2)_7CH_2OH$
$C_{18}H_{36}O$ 268.482

(*E*)-*form* [506-42-3]
Elaidyl alcohol. Elaidic alcohol
Mp 36-37° (34°). Bp_{18} 216°.

(*Z*)-*form* [143-28-2]
Oleyl alcohol. Oleic alcohol. Francol OA-95
Occurs in fish oils. Emulsion stabiliser, antifoam agent, detergent and release agent for food applications. Pale yellow, oily liq. Insol. H_2O. d_4^{20} 0.85. Bp 360° Bp_{15} 205-210°. n_D^{20} 1.4607. Oligomerises in the presence of BF_3.

▶ Skin and eye irritant. Fl. p. 184/189°, autoignition temp. 363°. RG4120000

Ac: [693-80-1]
$C_{20}H_{38}O_2$ 310.519
Liq. $Bp_{0.04}$ 131-135°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 146A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 220B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 215C (*ir*)
Noller, C.R. *et al., J.A.C.S.*, 1934, **56**, 1563 (*synth*)
Org. Synth., 1935, **15**, 72 (*synth*)
Nyström, R.F. *et al., J.A.C.S.*, 1947, **69**, 1197
Blake, S. *et al., J.C.S.*, 1963, 430 (*isol*)
Ghodssi, M.A. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1966, **262**, 269 (*oligomers*)
Bestman, H.J. *et al., Chem. Ber.*, 1971, **104**, 65 (*Ac, synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OBA000

Octadecylamine O-52

[124-30-1]
1-Octadecanamine, 9CI. 1-Aminooctadecane. Stearylamine
$H_3C(CH_2)_{16}CH_2NH_2$
$C_{18}H_{39}N$ 269.513
Present in food through its use as a boiler water additive. Cryst. Mp 49-52° (46°). Bp_5 183-183.1°.

▶ Skin irritant. LD_{50} (mus, ipr) 250 mg/kg. LD_{50} (mus, orl) 3000 mg/kg. RG4150000

Hydrochloride: [1838-08-0]
Cryst. Mp 160-161°.

▶ RG4375000

N-*Ac:* [3906-22-7]
$C_{20}H_{41}NO$ 311.55
Cryst. ($EtOH/Et_2O$). Mp 84-85°.

N-*Benzoyl:* [19083-52-4] N-*Octadecylbenzamide, 9CI*
$C_{25}H_{43}NO$ 373.621
Mp 85.5-86°.

N-*Me:* [2439-55-6]
$C_{19}H_{41}N$ 283.54
Mp 42-46°.

▶ RG4460000

N,N-*Di-Me:* [124-28-7] N,N-*Dimethyl-1-octadecanamine, 9CI.* ***Dimantine, INN.*** *Dymanthine*
$C_{20}H_{43}N$ 297.566
Fp 22.9. Log P 8.88 (uncertain value) (calc).

▶ Eye and skin irritant. LD_{50} (mus, ipr) 315 mg/kg. RG4200000

N,N-*Di-Me; hydrochloride:* [1613-17-8] ***Dymanthine hydrochloride, USAN.*** *Doda. GS 1339. NSC 5547. Thelmesan*

▶ LD_{50} (rat, orl) 200 mg/kg. RG4210000

N,N-*Di-Me,* N-*oxide:* [2571-88-2]
$C_{20}H_{43}NO$ 313.566Obt. in aq. soln..

[2190-04-7, 19855-61-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 284A; 298C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 455A; 479B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 367D; 383A (*ir*)
Ralston, A.W. *et al., Oil Soap (Chicago)*, 1940, **17**, 89; *CA*, **34**, 3674 (*synth*)
Reck, R.A. *et al., J.O.C.*, 1947, **12**, 517 (*deriv*)
Heck, R.A. *et al., J.O.C.*, 1947, **12**, 517-521 (*N,N-di-Me N-oxide*)
Clemo, G.R. *et al., J.C.S.*, 1952, 4684 (*synth*)
Murr, B.L. *et al., J.A.C.S.*, 1955, **77**, 1684 (*synth*)
Gohlke, R.S. *et al., Anal. Chem.*, 1962, **34**, 1281 (*ms*)
Cavier, R. *et al., Therapie*, 1964, **19**, 265; 947 (*activity, deriv*)
Goto, R. *et al., Nippon Kagaku Zasshi*, 1966, **87**, 1220; *CA*, **66**, 75599 (*synth*)
Kreuger, P.J. *et al., Can. J. Chem.*, 1967, **45**, 1605 (*ir*)
Narayanan, C.R. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 209 (*nmr*)
Douvres, F.W. *et al., Vet. Parasitol.*, 1980, **7**, 195 (*activity*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 776
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1998
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTC400; OBC000; OBE000

5-Octadecynoic acid, 9CI O-53

[676-30-2]
$H_3C(CH_2)_{11}C{\equiv}C(CH_2)_3COOH$
$C_{18}H_{32}O_2$ 280.45
Constit. of the roots of *Ximenia americana* (tallow nut). Cryst. Mp 52°.

[26527-49-1]

Barve, J.A. *et al., Chem. Phys. Lipids*, 1971, **7**, 311-323 (*synth*)
Frost, D.J. *et al., Chem. Phys. Lipids*, 1975, **15**, 53-85 (*pmr*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1976, **17**, 1-13 (*cmr*)
Fatope, M.O. *et al., J. Agric. Food Chem.*, 2000, **48**, 1872-1874 (*isol, pmr, cmr*)

2,4-Octadienal, 9CI O-54

[5577-44-6]
$H_3CCH_2CH_2CH{=}CHCH{=}CHCHO$
$C_8H_{12}O$ 124.182

(*E,E*)-*form* [30361-28-5]
FEMA 3721
Present in roasted beef, bread, cheese, cocoa beans, fresh salted salmon, sturgeon caviar, salmon roe, salmon oil, pickled ham, grapes, cooked mutton, peanuts, rice, roasted sesame seeds and black tea. Flavouring ingredient. Liq. with a fatty, green, sour odour. Bp_{11} 83-85°. n_D^{20} 1.5244.

2,4-Dinitrophenylhydrazone:
Mp 154-156°.

[33819-10-2]

Pippen, E.L. *et al., J.O.C.*, 1958, **23**, 1580 (*synth*)
Yamamoto, K. *et al., Chem. Lett.*, 1979, 713 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 609
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2000

2,6-Octadienal O-55

[149231-57-2]

[76917-23-2]
$H_3CCH{=}CHCH_2CH_2CH{=}CHCHO$
$C_8H_{12}O$ 124.182

d_4^{20} 0.87. Bp_{10} 77-79°. n_D^{20} 1.4665. Phys. props. are for material of unspecified geometry.

(*E,E*)-*form* [56767-18-1]
FEMA 3466
Flavouring ingredient. Component of storage odour development in hydrogenated soybean oil. Characterised spectroscopically.

Goethals, G. *et al., Bull. Soc. Chim. Belg.*, 1937, **46**, 409-422 (*synth*)
Yasuda, K. *et al., J. Am. Oil Chem. Soc.*, 1975, **52**, 307-311 (*E,E-form, isol, ms, ir*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1136 (*E,E-form, use*)

1,3-Octadiene, 9CI O-56

[1002-33-1]

[39491-64-0]

$H_3C(CH_2)_3CH{=}CHCH{=}CH_2$
C_8H_{14} 110.199
Constit. of *Glycine max* (soybean).

(*E*)-*form* [39491-65-1]
Liq. Bp 123-126°. n_D^{21} 1.4483. Obt. mixed with *ca.* 30% *Z* isomer.

Prévost, C. *et al., Bull. Soc. Chim. Fr.*, 1964, 2485 (*synth*)
Beger, J. *et al., J. Prakt. Chem.*, 1984, **326**, 12 (*synth, pmr, ms*)
Engman, L. *et al., J.O.C.*, 1985, **50**, 3170 (*synth, pmr*)
Pellmyr, O. *et al., Biochem. Syst. Ecol.*, 1991, **19**, 623 (*isol*)
Kitahara, T. *et al., Synthesis*, 1994, 692 (*synth, ir, pmr*)

2,3-Octadiene-5,7-diyn-1-ol, 9CI O-57

Lentinamycin
$HC{\equiv}CC{\equiv}CCH{=}C{=}CHCH_2OH$
C_8H_6O 118.135

(-)-*form* [51864-98-3]
$[\alpha]_D^{24}$ -380 (c, 0.09 in CH_2Cl_2).

(±)-*form* [41793-44-6]
Unstable oil.

(ξ)-*form*
Isol. from *Lentinus edodes* (shiitake). λ_{max} 211 ; 235 ; 248 ; 261 ; 276 (no solvent reported).

[64753-26-0]

Bew, R.E. *et al., J.C.S.(C)*, 1966, 129 (*isol, uv, ir*)
Landor, P.D. *et al., J.C.S. Perkin 1*, 1975, 1628 (*synth, uv, ir*)
Kleijn, H. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1982, **101**, 97 (*synth*)
Tokimoto, K. *et al., Proc. Jpn. Acad., Ser. B*, 1987, **63**, 277 (*isol*)
Komemushi, S. *et al., CA*, 1996, **124**, 170149b (*isol, pmr*)

4,7-Octadienoic acid, 9CI O-58

$H_2C{=}CHCH_2CH{=}CHCH_2CH_2COOH$
$C_8H_{12}O_2$ 140.182

(*E*)-*form* [84565-02-6]
Me ester: [189440-77-5] *Anapear*
$C_9H_{14}O_2$ 154.208
Fragrance ingredient with a fruity green pear note.

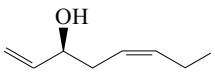
Et ester: [90269-57-1]
Bp_{10} 95-97°.

(*Z*)-*form* [84565-03-7]
Et ester: [69925-33-3]

[72276-09-6]
$C_{10}H_{16}O_2$ 168.235
Aroma component of purple passion fruit (*Passiflora edulis*). Flavouring agent. Liq. with pineapple-like odour. $Bp_{8.5}$ 90-95° (lit. gives a pressure range). n_D^{20} 1.4459.

Furrer, A. *et al., Helv. Chim. Acta*, 1979, **62**, 135-139 (*isol*)
Bhanot, R.K. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 970-971 (*Z-form, Et ester, synth*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 970-971 (*E-form, Et ester, synth, ir, pmr*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255-3264 (*synth, ir, pmr*)
Eur. Pat., 1997, 773 209 (*E-form, Me ester*)

1,5-Octadien-3-ol, 9CI O-59



(*S,Z*)-*form*

$C_8H_{14}O$ 126.198

(3*S*,5*Z*)-*form* [56994-74-2]
$[\alpha]_D$ -8 (c, 0.5 in CH_2Cl_2).

(3ξ,5*E*)-*form* [50306-14-4]

(3ξ,5*Z*)-*form* [50306-18-8]
Off-flavour component of cooked prawns and sand-lobsters.

Woolard, F.X. *et al., Chem. Comm.*, 1975, 486 (*pmr*)
Vanhaelen, M. *et al., J. Chromatogr.*, 1977, **144**, 108
Whitfield, F.B. *et al., Aust. J. Chem.*, 1982, **35**, 373 (*isol*)

2,4-Octadien-1-ol O-60

$H_3CCH_2CH_2CH{=}CHCH{=}CHCH_2OH$
$C_8H_{14}O$ 126.198

(2*E*,4*E*)-*form* [18409-20-6]
FEMA 3956
Flavouring ingredient. Mobile liq. with pleasant fruity odour. Bp_2 70-73°. n_D^{25} 1.4865.

(2*E*,4*Z*)-*form* [56904-85-9]
$Bp_{0.1}$ 48°. n_D^{20} 1.4912.

Ac: [56904-76-8]
$C_{10}H_{16}O_2$ 168.235
$Bp_{0.7}$ 67°.

[119518-99-9, 119519-00-5]

Jacobsen, M. *et al., J.A.C.S.*, 1956, **78**, 5084 (*synth*)
Games, D.E. *et al., Experientia*, 1973, **29**, 532 (*isol*)
Commerçon, A. *et al., Tetrahedron*, 1980, **36**, 1215 (*synth, ir, pmr*)
Tsuboi, S. *et al., J.O.C.*, 1982, **47**, 4478 (*synth, cmr*)
Staddon, B.W. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 235 (*isol, Ac*)
Kuroda, S. *et al., Tet. Lett.*, 1987, **28**, 803 (*synth, pmr*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1990, **67**, 37 (*synth*)
Kaiser, R. *et al., J. Essent. Oil Res.*, 1991, **3**, 129 (*isol*)
Bellina, F. *et al., Synth. Commun.*, 1996, **26**, 3297 (*synth, pmr*)

2,5-Octadien-1-ol O-61

[83861-75-0]

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2OH$
$C_8H_{14}O$ 126.198
Constit. of various fish and other marine animals.

(2*E*,5*Z*)-*form* [67548-36-1]
Bp_{12} 92-93°.

(2*Z*,5*Z*)-*form* [67548-44-1]

[101339-88-2]

Cahiez, C. *et al., Synthesis*, 1978, 528 (*synth, ir, pmr*)
Marner, F.J. *et al., Annalen*, 1982, 579 (*synth*)
Wurzenburger, M. *et al., Lipids*, 1986, **21**, 261
Honda, T. *et al., J.C.S. Perkin 1*, 1999, 23-29 (*synth, ir, pmr, cmr*)

3,5-Octadien-1-ol O-62

$H_3CCH_2CH{=}CHCH{=}CHCH_2CH_2OH$
$C_8H_{14}O$ 126.198

(3*E*,5*E*)-*form* [10573-34-9]
Bp_{12} 94-96°.

α-Naphthylurethane:
Needles (EtOH aq.). Mp 100°.

Ac: [85722-81-2]
$C_{10}H_{16}O_2$ 168.235
Bp_{12} 101-103°.

3,5-Dinitrobenzoyl:
Cryst. (petrol). Mp 54-55°.

(3*E*,5*Z*)-*form* [70664-95-8]
Flavour component of kogyoku apple oil. Bp_5 71-72°.

Ac: [70664-97-0]
Bp_5 74-75°.

(3*Z*,5*E*)-*form* [70664-96-9]
Bp_2 72-74°.

Ac: [85722-82-3]
Bp_5 74-76°.

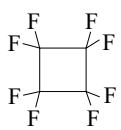
(3*Z*,5*Z*)-*form* [10160-16-4]
Flavour component of kogyoku apple oil. Bp_{12} 95-98°.

Ac: [85722-80-1]
Bp_{12} 101-103°.

Riemschneider, R. *et al., Monatsh. Chem.*, 1965, **96**, 1766 (*synth*)
Iwamoto, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 117; 1984, **48**, 849 (*synth, isol*)

Octafluorocyclobutane, 9CI O-63

[115-25-3]
Perfluorocyclobutane. Fluorocarbon C-318. Freon C318. C318



C_4F_8 200.031
Propellant and aerating agent in foamed or sprayed food products. Gas. Sol. EtOH. Mp -41.4° (-40.7°). Bp -6.04°.

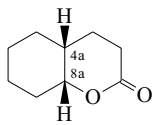
▶ GU1779500

U.S. Pat., 1945, 2 384 821; *CA*, 1877, **40**, 2 384 821 (*synth*)
Lewis, E.E. *et al., J.A.C.S.*, 1947, **69**, 1968 (*synth*)
Atkinson, B. *et al., J.C.S.*, 1953, 2083 (*synth*)
Phillips, W.D. *et al., J. Chem. Phys.*, 1956, **25**, 949 (*nmr*)
Miller, W.T. *et al., J.A.C.S.*, 1957, **79**, 3084 (*synth*)

Manuel, T.A. *et al., J.A.C.S.*, 1961, **83**, 249 (*synth*)
Chang, C.-H. *et al., J. Mol. Struct.*, 1971, **7**, 89 (*struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **1**, 588 (*props*)
Kammermaier, J. *et al., Adv. Low-Temp. Plasma Chem., Technol., Appl.*, 1984, **1**, 326 (*polym*)
Claude, R. *et al., Polym. Mater. Sci. Eng.*, 1987, **56**, 134 (*polym*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CPS000

Octahydro-2*H*-1-benzopyran-2-one O-64

[4430-31-3]
Octahydrocoumarin, 8CI. 2-Hydroxycyclohexanepropanoic acid lactone



(4a*RS*,8a*RS*)-*form*

$C_9H_{14}O_2$ 154.208
Flavouring ingredient.
► Skin irritant. LD_{50} (rat, orl) 3900 mg/kg. GN8261500

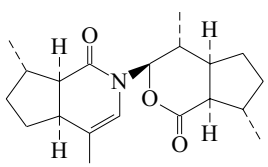
(4a*RS*,8a*RS*)-*form* [23201-43-6]
(±)-cis-*form*
Liq. $Bp_{0.1}$ 88°.

(4a*RS*,8a*SR*)-*form* [14072-79-8]
(±)-trans-*form*
$Bp_{0.4}$ 94-96° $Bp_{0.1}$ 86°. n_D^{25} 1.4882.

Frank, R.L. *et al., J.A.C.S.*, 1951, **73**, 724
House, H.O. *et al., J.O.C.*, 1962, **27**, 4145
Duřěý, P. *et al., Bull. Soc. Chim. Fr.*, 1968, 4653; 5030 (*synth, pmr*)
Dean, C.S. *et al., J.C.S.(C)*, 1968, 1491 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 781 (*rev, tox*)
Griffiths, D.V. *et al., J.C.S. Perkin 2*, 1988, 431 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OBV200

2-[Octahydro-4,7-dimethyl-1-oxocyclopenta[*c*]pyran-3-yl]nepetalactam O-65

[115421-74-4]



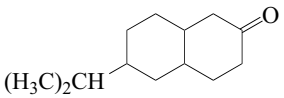
$C_{20}H_{29}NO_3$ 331.454
A mixed dimer of nepetalactam and nepetalic acid, analgous to nepetalic ψ-anhydride. Isol. from a commercial sample of catnip oil (*Nepeta cataria*). Cryst. (2-methylpentane). Mp 116-117°. $[\alpha]_D^{25}$ +3.8 (c, 5 in $CHCl_3$). Artifact.

Eisenbraun, E.J. *et al., J.O.C.*, 1988, **53**, 3968-3972 (*isol, uv, ir, pmr, cmr, ms, struct*)

Octahydro-6-isopropyl-2(1*H*)-naphthalenone, 8CI O-66

[34131-98-1]

[115305-83-4, 115305-93-6]
Octahydro-6-(1-methylethyl)-2(1H)-naphthalenone, 9CI. 6-Isopropyl-2-decalone. Decatone

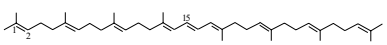


$C_{13}H_{22}O$ 194.316
Fragrance ingredient with a grapefruit-like aroma. Two stereoisomers have been characterised.

Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 371 (*rev*)
Huffman, J.W. *et al., J.O.C.*, 1988, **53**, 3828-3831 (*synth, ir, pmr*)

7,7′,8,8′,11,11′,12,12′-Octahydrolycopene O-67

[540-04-5]
*7,7′,8,8′,11,11′,12,12′-Octahydro-ψ,ψ-carotene. **Phytoene***



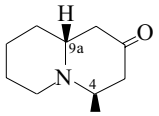
$C_{40}H_{64}$ 544.946
Viscous oil with strong uv fluorescence.

1,2-Epoxide: [26107-96-0] ***Phytoene 1,2-epoxide**. 1,2-Epoxy-1,2,7,7′,8,8′,11,11′,12,12′-decahydro-ψ,ψ-carotene*
$C_{40}H_{64}O$ 560.945
Isol. from ripe tomatoes. λ_{max} 275 ; 285 ; 296 (no solvent reported).

(15Z)-Isomer: [13920-14-4] ***15*-cis-*Phytoene**. 15Z-Phytoene isomer*
Isol. from tomato (*Lycopersicon esculentum* var. 'Tangella'). Pale orange oil. λ_{max} 286 ; 296 (hexane).

Britton, G. *et al., Phytochemistry*, 1969, **8**, 2257 (*epoxide*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1817a (*occur*)
Gregonis, D.E. *et al., Biochemistry*, 1974, **13**, 1538 (*biosynth*)
Khan, N. *et al., J.C.S. Perkin 1*, 1975, 1457 (*struct, synth*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97 (*cmr*)
Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*15Z-Phytoene, ir, pmr, cmr*)
Frecknell, E.A. *et al., Phytochemistry*, 1984, **23**, 1707 (*isol, occur*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 44 (*bibl*)
Ebenezer, W.J. *et al., J.C.S. Perkin 1*, 1993, 1869 (*15Z-Phytoene, ir, pmr, cmr*)

Octahydro-4-methyl-2*H*-quinolizin-2-one, 9CI O-68



(4*R*,9a*R*)-*form*

$C_{10}H_{17}NO$ 167.25

(4*R*,9a*R*)-*form* [66835-10-7]
Myrtine
Alkaloid from *Vaccinium myrtillus* (bilberry) aerial parts. Oil. $[\alpha]_D^{20}$ +3.1 (c, 2.1 in $CHCl_3$) (natural). $[\alpha]_D^{23}$ +11.3 (c, 2.7 in $CHCl_3$) (synthetic). Isol. sample has only 25% opt. purity. This is not due to isom. during isol..

(4*R*,9a*S*)-*form* [82111-02-2]
Epimyrtine
Alkaloid from *Vaccinium myrtillus* (bilberry). Oil. $[\alpha]_D^{20}$ -2.5 (c, 1.2 in $CHCl_3$) (natural). $[\alpha]_D^{23}$ -18 (c, 5.2 in $CHCl_3$) (synthetic). Low opt. purity.

Hydrochloride:
Mp 211-213° dec. $[\alpha]_D^{23}$ -31.7.

(4*RS*,9a*RS*)-*form* [66900-13-8]

[82083-37-2]
Mp 196-198° dec. (as hydrochloride).

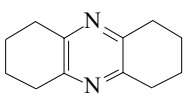
(4*RS*,9a*SR*)-*form* [66900-14-9]

[82083-36-1]
Mp 200-201° dec. (as hydrochloride).

Slosse, P. *et al., Tetrahedron*, 1981, **37**, 4287 (*isol, ir, ms, pmr, cmr, synth, resoln*)
Comins, D.L. *et al., J.O.C.*, 1992, **57**, 5807 (*synth*)
Gelas-Miakhe, Y. *et al., Tet. Lett.*, 1992, **33**, 73 (*synth*)
Pilli, R.A. *et al., J.O.C.*, 1995, **60**, 717 (*synth*)

1,2,3,4,6,7,8,9-Octahydrophenazine O-69

[4006-50-2]
Polycartine B



$C_{12}H_{16}N_2$ 188.272
Flavour enhancer. Mp 112-113° (106-108°). Bp_{11} 135-170°. λ_{max} 260 (ϵ); 323 (ϵ) (MeOH) (Derep).

Hydrochloride: [42383-40-4]
Mp 160-162°.

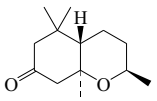
N,N′-Dioxide: [24716-05-0]
$C_{12}H_{16}N_2O_2$ 220.271
Cryst. Mp 230°.

Schäffler, A. *et al., Chem. Ber.*, 1955, **88**, 767 (*synth, uv*)
Fellman, J.H. *et al., J.O.C.*, 1956, **21**, 713 (*synth*)
Wilen, S.H. *et al., Chem. Ind. (London)*, 1969, 237 (*synth*)
Smith, H.E. *et al., Chem. Comm.*, 1970, 1112 (*uv*)
Scheinbaum, M.L. *et al., J.O.C.*, 1970, **35**, 2790 (*oxide*)
Maurer, B. *et al., Helv. Chim. Acta*, 1976, **59**, 1169 (*isol*)

Moritake, M. *et al., Tet. Lett.*, 1987, **28**, 1425 (*isol*)

Octahydro-2,5,5,8*a*-tetramethyl-7*H*-1-benzopyran-7-one, 9CI — O-70

[5835-18-7]
*Tetrahydro-3-oxoedulan. Hexahydro-2,5,5,8*a*-tetramethyl-7-chromanone. 1,3,7,7-Tetramethyl-2-oxabicyclo[4.4.0]decan-9-one*

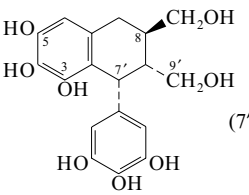


(2*RS*,4*aSR*,8*aSR*)-*form*

$C_{13}H_{22}O_2$ 210.316
Constit. of dried kukoshi berries (*Lycium chinense*) and tobacco oil.

(2*RS*,4*aSR*,8*aSR*)-*form* [183506-08-3]
Mp 53-59°.
U.S. Pat., 1965, 3 217 716; *CA*, **64**, 5466 (*synth, use*)
Sannai, A. *et al., Agric. Biol. Chem.*, 1983, **47**, 2397-2399 (*occur*)
Enzell, C.R. *et al., Mass Spectrom. Rev.*, 1986, **5**, 39-72 (*ms*)
Ito, N. *et al., J.C.S. Perkin 1*, 1996, 2397-2405 (*synth, ir, pmr, ms*)

3,3′,4,4′,5,5′,9,9′-Octahydroxy-2,7′-cyclolignan — O-71



(7′*R*,8*R*,8′*R*)-*form*

$C_{18}H_{20}O_8$ 364.351
Lignan numbering shown.

(7′*R*,8*R*,8′*R*)-*form*

3,3′,5,5′-Tetra-Me ether:
Amorph. solid. $[\alpha]_D^{27}$ -140.8 (c, 0.23 in $CHCl_3$).

3,3′,5,5′-Tetra-Me ether, 9′-O-α-L-arabinopyranoside: [233686-33-4] ***Gaultheroside A***
$C_{27}H_{36}O_{12}$ 552.574
Mp 154-155°. λ_{max} 209 ; 278 (MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-β-D-glucopyranoside:
$C_{28}H_{38}O_{13}$ 582.6
Constit. of the bark of *Aegle marmelos* (bael fruit). Amorph. solid. $[\alpha]_D^{26}$ -144.8 (c, 0.42 in MeOH).

(7′*R*,8*S*,8′*S*)-*form*

3,3′,5,5′-Tetra-Me ether: [31768-94-2] ***(-)-Lyoniresinol***. *Pygeoresinol*
$C_{22}H_{28}O_8$ 420.458
Cryst. (H_2O or MeOH). Mp 171-172° (202-204°). $[\alpha]_D^{31}$ -53.2 (c, 2.01 in Me_2CO). $[\alpha]_D$ -5.24 (MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-sulfate: ***Lyoniresinol 9′-sulfate***
$C_{22}H_{28}O_{11}S$ 500.523
Constit. of the roots of *Polygonum cuspidatum* (Japanese knotweed).
Amorph. powder (as Na salt). $[\alpha]_D^{25}$ -17 (c, 0.13 in MeOH). λ_{max} 205 ; 238 (sh) ; 282 (MeOH).

3,3′,5,5′-Tetra-Me ether, 9-O-xyloside: [75587-29-0] ***Pygeoside***
$C_{27}H_{36}O_{12}$ 552.574
Needles (MeOH aq.). Mp 152-156°. $[\alpha]_D$ +40.2 (c, 1.42 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-β-D-xylopyranoside: [62058-46-2] ***Nudiposide***
$C_{27}H_{36}O_{12}$ 552.574
Mp 175-178° (157-160°). $[\alpha]_D^{29}$ -67 (c, 1.4 in EtOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-α-L-rhamnopyranoside:(-)-Lyoniresinol 9′-rhamnoside
$C_{28}H_{38}O_{12}$ 566.601
Viscous oil (as hexa-Ac). $[\alpha]_D^{20}$ -11.7 (c, 0.03 in $CHCl_3$) (hexa-Ac). λ_{max} 203 (ϵ 52990); 275 (ϵ 1040) (MeOH) (hexa-Ac).

3,3′,5,5′-Tetra-Me ether, 9-O-β-D-glucopyranoside:
$C_{28}H_{38}O_{13}$ 582.6
Oil. $[\alpha]_D$ -23 (c, 0.3 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-β-D-glucopyranoside:
$C_{28}H_{38}O_{13}$ 582.6
$[\alpha]_D$ -110.

Hexa-Me ether: [23212-70-6]
Cryst. (MeOH aq.). Mp 158-160°. $[\alpha]_D^{28}$ -20.7 (c, 0.58 in EtOH).

(7′*S*,8*R*,8′*R*)-*form*

3,3′,5,5′-Tetra-Me ether: [14464-90-5] *4,4′,9,9′-Tetrahydroxy-3,3′,5,5′-tetramethoxy-2,7′-cyclolignan*. ***Lyoniresinol***. *Dimethoxyisolariciresinol*
$C_{22}H_{28}O_8$ 420.458
Mp 115-116° Mp 165-167° (dimorph.). $[\alpha]_D$ +52 (EtOH). $[\alpha]_D$ +13.3 (c, 0.32 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-β-D-xylopyranoside: [34425-25-7] ***Lyoniside***. *Lyonoside*
$C_{27}H_{36}O_{12}$ 552.574
Mp 124-125° Mp 165-165° (dimorph.). $[\alpha]_D$ +43 (MeOH).

3,3′,5,5′-Tetra-Me ether, 9-O-α-L-rhamnopyranoside:
$C_{28}H_{38}O_{12}$ 566.601
Amorph.

3,3′,5,5′-Tetra-Me ether, 4-O-β-D-glucopyranoside:
$C_{28}H_{38}O_{13}$ 582.6
Constit. of *Antidesma membranaceum*. λ_{max} 205 (log ϵ 4.84); 275 (log ϵ 3.5) (MeOH).

3,3′,5,5′-Tetra-Me ether, 9-O-β-D-glucopyranoside:
$C_{28}H_{38}O_{13}$ 582.6
Constit. of the bark of *Aegle marmelos* (bael fruit). Amorph. solid. $[\alpha]_D^{27}$ -51.7 (c, 0.41 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-β-D-glucopyranoside: [87585-32-8]
$C_{28}H_{38}O_{13}$ 582.6
Isol. from bark of *Cinnamomum cassia* (Chinese cinnamon). Amorph. powder. Mp 178-180°. $[\alpha]_D$ +22.4 (c, 1.01 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-[4-hydroxy-3-methoxybenzoyl-(→6)-β-D-glucopyranoside]: ***Fernandoside***
$C_{36}H_{44}O_{16}$ 732.734
Amorph. powder. $[\alpha]_D^{26}$ +25 (c, 1.24 in MeOH). λ_{max} 250 ; 362 (MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-[4-hydroxy-3,5-dimethoxybenzoyl-(→2)-β-D-glucopyranoside]: ***Acanfolioside***
$C_{37}H_{46}O_{17}$ 762.76
Amorph. powder. $[\alpha]_D^{22}$ +28.3 (c, 2.7 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-[4-hydroxy-3,5-dimethoxy-E-cinnamoyl-(→6)-β-D-glucopyranoside]: [147742-23-2] ***Hazaleanin B***
$C_{39}H_{48}O_{17}$ 788.798
Amorph. solid. $[\alpha]_D^{26}$ +7.5 (c, 1.1 in MeOH).

3,3′,5,5′-Tetra-Me ether, 4,9′-di-O-β-D-glucopyranoside:
$C_{34}H_{48}O_{18}$ 744.742
Powder. $[\alpha]_D^{25}$ -21.2 (c, 0.12 in MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: ***Alangilignoside A***
$C_{33}H_{46}O_{17}$ 714.716
Amorph. powder. $[\alpha]_D$ +23.4 (c, 0.9 in MeOH). λ_{max} 209 (log ϵ 4.75); 238 (log ϵ 4.08); 276 (log ϵ 3.55) (MeOH).

3,3′,5,5′-Tetra-Me ether, 9-O-[β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside]:
$C_{34}H_{48}O_{18}$ 744.742
Powder. $[\alpha]_D^{25}$ +0.4 (c, 0.47 in MeOH).

3,3′,5,5′-Tetra-Me ether, di-Ac: ***Gaultherin B***
$C_{26}H_{32}O_{10}$ 504.533
Powder (Me_2CO aq.). Mp 120-121° (99-100°,88-89°). $[\alpha]_D^{23}$ +40 (c, 0.05 in MeOH). λ_{max} 218 (log ϵ 2.34); 274 (log ϵ 0.45) (MeOH).

3,3′,4′,5,5′-Penta-Me ether, 4-O-β-D-glucopyranoside:
$C_{29}H_{40}O_{13}$ 596.627
λ_{max} 205 (log ϵ 4.63); 273 (log ϵ 3.18) (MeOH).

Hexa-Me ether: [7333-11-1]
Cryst. Mp 163-164°. $[\alpha]_D$ +45 ($CHCl_3$).

(7′*S*,8*S*,8′*R*)-*form*

3,3′,5,5′-Tetra-Me ether: [73745-49-0] ***Epilyoniresinol***
Pinkish prisms ($EtOAc/C_6H_6$). Mp 198-200°. $[\alpha]_D$ -28.9 (MeOH).

3,3′,5,5′-Tetra-Me ether, 9′-O-β-D-glucopyranoside: [73706-67-9]
$C_{28}H_{38}O_{13}$ 582.6

3′,4′,5,5′-Tetra-Me ether: [129502-58-5] *3,4,9,9′-Tetrahydroxy-3′,4′,5,5′-tetramethoxy-2,7′-cyclolignan*. ***Lingueresinol***
$C_{22}H_{28}O_8$ 420.458
Cryst. (MeOH). Mp 179-183°. $[\alpha]_D$ +35.9 (c, 1.255 in MeOH). Tentative struct..

(7′*RS*,8*SR*,8′*SR*)-*form*

3,3′,5,5′-Tetra-Me ether: [23212-64-8] ***(±)-Lyoniresinol***
$C_{22}H_{28}O_8$ 420.458
Cryst. ($CHCl_3$). Mp 193-194°.

3,3′,5,5′-Tetra-Me ether, di-Ac:
Cryst. Mp 103°.

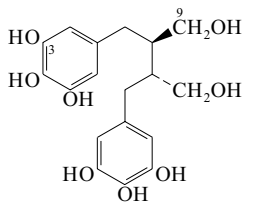
Hexa-Me ether: [23212-66-0]
Cryst. (Et_2O). Mp 162-164°.

[3737-93-7]

Freudenberg, K. *et al., Tet. Lett.*, 1959, **No. 17**, 19 (*isol*)
Weinges, K. *et al., Chem. Ber.*, 1961, **94**, 2522 (*isol*)
Arya, V.P. *et al., Acta Chem. Scand.*, 1962, **16**, 518 (*isol*)
Narnsimbachari, N. *et al., Can. J. Chem.*, 1962, **40**, 1118 (*isol*)
Kato, Y. *et al., Chem. Pharm. Bull.*, 1966, **14**, 1438 (*isol*)
Klyne, W. *et al., J.C.S.(C)*, 1966, 893 (*ord*)
Hostettler, F.D. *et al., Tetrahedron*, 1969, **25**, 2325 (*isol*)
Rowe, J.W. *et al., Phytochemistry*, 1972, **11**, 2513 (*isol*)
Wallis, A.F.A. *et al., Aust. J. Chem.*, 1973, **26**, 1571 (*synth*)
Sakakibura, J. *et al., Yakugaku Zasshi*, 1974, **94**, 1377; *CA*, **82**, 73392g
Ogawa, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2102 (*Nudiposide*)
Mehta, M. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 127 (*synth*)
Vecchietti, V. *et al., Phytochemistry*, 1979, **18**, 1847 (*cmr*)
Chandel, R.S. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 279 (*Pygeoside*)
Varma, M. *et al., Z. Naturforsch., C*, 1980, **35**, 344 (*Epilyoniresinol*)
Hulbert, P.B. *et al., J. Chem. Res., Synop.*, 1981, 27 (*cd, uv*)
Miyamura, M. *et al., Phytochemistry*, 1983, **22**, 215 (*(+)-Lyoniresinol glucoside*)
Dada, G. *et al., J. Nat. Prod.*, 1989, **52**, 1327 (*isol, glycosides*)
Yoshinari, K. *et al., Phytochemistry*, 1990, **29**, 1675 (*isol, (±)-form*)
Sepulveda-Boza, S. *et al., Phytochemistry*, 1990, **29**, 2357 (*Lingueresinol*)
Higuchi, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 534 (*glucosides*)
Shibuya, H. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2639 (*Hazaleanin B*)
Achenbach, R.S. *et al., Planta Med.*, 1992, **58**, 270 (*glucoside*)
Ohashi, K. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1924 (*(-)-Lyoniresinol 9-glucoside*)
Achenbach, H. *et al., Phytochemistry*, 1997, **45**, 325 (*isol, derivs*)
Yuasa, K. *et al., Phytochemistry*, 1997, **45**, 611 (*Alangilignoside A*)
Cortez, D.A.G. *et al., Nat. Prod. Lett.*, 1998, **11**, 255-262 (*(-)-Lyoniresinol rhamnoside*)
Zhang, Z. *et al., Phytochemistry*, 1999, **51**, 469-472 (*Gaultherin B*)
Zhang, Z. *et al., Yaoxue Xuebao*, 1999, **34**, 128-131 (*Gaultheroside A*)
Buske, A. *et al., Eur. J. Org. Chem.*, 2001, 3537-3543 (*Antidesma 4-glucosides*)
Kanchanapoom, T. *et al., Phytochemistry*, 2001, **56**, 369-372; **57**, 1245-1248 (*Acanfolioside, Fernandoside*)
Xiao, K. *et al., Chem. Pharm. Bull.*, 2002, **50**, 605-608 (*Lyoniresinol 9′-sulfate*)

3,3′,4,4′,5,5′,9,9′-Octahydroxylignan O-72

2,3-Bis(3,4,5-trihydroxybenzyl)-1,4-butanediol



(8*R*,8′*R*)-*form*

$C_{18}H_{22}O_8$ 366.367

(8*S*,8′*S*)-*form*

3,3′,5,5′-Tetra-Me ether, 9-O-xylopyranoside: [126882-53-9] ***Ssioriside***
$C_{27}H_{38}O_{12}$ 554.59
Isol. from *Prunus padus* (bird cherry). Powder. $[\alpha]_D^{24}$ +0.7 (c, 1.0 in MeOH).

Yoshinari, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3301 (*Ssioriside*)

Octanal, 9CI O-73

[124-13-0]
Caprylaldehyde. Caprylic aldehyde. Octyl aldehyde. FEMA 2797
$H_3C(CH_2)_6CHO$
$C_8H_{16}O$ 128.214
Isol. from various plant oils esp. *Citrus* spp.. Also present in kumquat peel oil, cardamom, coriander, caraway and other herbs. Flavouring agent, used in artificial citrus formulations. Liq. d_4^{20} 0.82. Bp 163.4° Bp_{20} 72°. n_D^{26} 1.4167.

▶ Flammable. Skin and eye irritant. LD_{50} (rat, orl) 5630 mg/kg. RG7780000

Oxime: [929-55-5]
$C_8H_{17}NO$ 143.228
Cryst. (petrol or EtOH aq.). Mp 60°. Bp_9 112°.

2,4-Dinitrophenylhydrazone: [1726-77-8]
Yellow cryst. (EtOH). Mp 106°.

Semicarbazone:
Cryst. (EtOH). Mp 101°.

Di-Me acetal: [10022-28-3] *1,1-Dimethoxyoctane, 9CI. FEMA 2798*
$C_{10}H_{22}O_2$ 174.283
Flavouring ingredient. Liq. with a woody aroma reminiscent of cognac. Bp 185° Bp_{20} 88-89°. n_D^{22} 1.4153.

Di-Et acetal: [54889-48-4] *1,1-Diethoxyoctane, 9CI*
$C_{12}H_{26}O_2$ 202.336
Liq. Bp 221-223° Bp_{20} 115-117°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 468C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 731C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 555A (*ir*)
Aldrich Library of NMR Spectra, **2**, 97D (*pmr*)
Sadtler Standard C-13 NMR Spectra, 12221 (*cmr*)
Org. Synth., 1967, **47**, 96; 1971, **51**, 39 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 113 (*rev, tox*)
Watanabe, Y. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2490 (*synth*)
Narasaka, K. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 2773 (*synth*)
Akita, Y. *et al., Synthesis*, 1977, 792 (*synth*)
Maccoll, A. *et al., Org. Mass Spectrom.*, 1986, **21**, 251 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, OCO000
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 611-612
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2004-2005 (*use, occur*)
Fields, J.D. *et al., J.O.C.*, 2000, **65**, 5937-5941 (*oxime*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Octane, 9CI O-74

[111-65-9]
$H_3C(CH_2)_6CH_3$
C_8H_{18} 114.23
Found in hop oil. Liq. d_4^{20} 0.7. Fp -56.8. Bp 125.67°. n_D^{20} 1.3974.

▶ Eye, skin and respiratory tract irritant. High vapour conc. narcotic. Highly flammable, fl. p. 13°, autoignition temp. 206/210/220°. OES: long-term 300 ppm; short-term 375 ppm. RG8400000

[17252-77-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 2A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 2A (*nmr*)
Shepard, A.F. *et al., J.A.C.S.*, 1931, **53**, 1949-1958 (*synth*)
Forziati, A.F. *et al., J. Res. Natl. Bur. Stand. (U.S.)*, 1946, **36**, 129-136 (*props*)
Whitesides, G.M. *et al., J.A.C.S.*, 1967, **89**, 5302-5303 (*synth*)
Weil, T.A. *et al., J. Organomet. Chem.*, 1973, **49**, 227-232 (*synth*)
Kabalka, G.W. *et al., J.O.C.*, 1975, **40**, 1834-1835 (*synth*)
Habeeb, J.J. *et al., Chem. Comm.*, 1976, 696 (*synth*)
Boese, R. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 988-992 (*cryst struct*)
Low, L.K. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 307 (*rev, tox*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 942
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OCU000

Octanedioic acid, 9CI O-75

[505-48-6]
Suberic acid, 8CI. 1,6-Hexanedicarboxylic acid
$HOOC(CH_2)_6COOH$
$C_8H_{14}O_4$ 174.196
Isol. from the roots of *Phaseolus vulgaris* (kidney bean). Cryst. (H_2O or C_6H_6/EtOH). Insol. H_2O; sol. Et_2O, C_6H_6. Mp 144°. Bp_{100} 279°. pK_{a1} 4.53; pK_{a2} 5.52 (25°, 0.1*M* KNO_3). Subl. >300°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 496B; 619A; 619B; 696B; 741D; 842A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 772A; 944C; 945A; 1121A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 582C; 644B; 644C; 747A; 801B (*ir*)
Sadtler Standard C-13 NMR Spectra, 10074 (*cmr*)
Green, T.G. *et al., J.C.S.*, 1937, 764 (*synth*)
Cason, J. *et al., J.O.C.*, 1949, **14**, 37 (*synth*)
Hopff, H. *et al., Annalen*, 1966, **691**, 61 (*synth*)
Angelo, B. *et al., C. R. Hebd. Seances Acad. Sci.*, 1971, **273**, 1767 (*synth*)
Takasugi, M. *et al., Chem. Lett.*, 1973, 445 (*isol*)
Chern, C.-I. *et al., J.O.C.*, 1976, **41**, 1077 (*synth*)
Marco, J.A. *et al., Phytochemistry*, 1978, **17**, 1438 (*isol*)
Ansell, M.F. *et al., J.C.S. Perkin 1*, 1984, 1061 (*synth, pmr*)
Fukushima, K. *et al., J. Mol. Struct.*, 1986, **146**, 61 (*Raman*)
Řezanka, T. *et al., J. Chromatogr.*, 1987, **408**, 145 (*ms*)

1,3-Octanediol, 9CI, 8CI O-76

[23433-05-8]

[26762-67-4]

$H_3C(CH_2)_4CH(OH)CH_2CH_2OH$

$C_8H_{18}O_2$ 146.229

▶ RG9604000

(R)-form [120727-18-6]
Constit. of apples. $[\alpha]_D^{25}$ +7.1.

1-O-β-D-Glucopyranoside: [120727-21-1]
$C_{14}H_{28}O_7$ 308.371
Constit. of apples.

1-O-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:
$C_{19}H_{36}O_{11}$ 440.487
Constit. of calabash tree (*Crescentia cujete*) fruits. Oil. $[\alpha]_D$ -40 (c, 0.5 in MeOH).

1-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{20}H_{38}O_{12}$ 470.513
Constit. of calabash tree (*Crescentia cujete*) fruits. Oil. $[\alpha]_D$ -21 (c, 0.3 in MeOH).

Di-Ac: [93222-26-5]
$C_{12}H_{22}O_4$ 230.303
$[\alpha]_D^{25}$ -12.7.

(S)-form

Di-Ac: [93222-25-4]
$[\alpha]_D$ +15.2 (c, 1.7 in CH_2Cl_2).

(±)-form
Preservative for foods and cosmetics. Oil. $Bp_{4.5}$ 81-82°.

[120727-22-2, 124150-19-2]

Cope, A.C. *et al., J.A.C.S.*, 1963, **85**, 3752 (*synth*)
Kulesza, J. *et al., CA*, 1969, **71**, 44865 (*synth*)
Hamming, M. *et al., Arch. Mass Spectral Data*, 1971, **2**, 182 (*ms*)
Medlik-Balan, A. *et al., Tetrahedron*, 1980, **36**, 299 (*synth*)
Barchi, J.J. *et al., J.A.C.S.*, 1984, **106**, 8193 (*synth, di-Ac*)
Schwab, W. *et al., Phytochemistry*, 1989, **28**, 157 (*isol, synth, pmr, cmr, ms, abs config*)
Beuerle, T. *et al., Phytochemistry*, 1996, **43**, 145; 1997, **45**, 1153 (*isol, synth, biosynth*)
Kaneko, T. *et al., Phytochemistry*, 1998, **47**, 259-263 (*isol, glycosides*)

2,3-Octanedione, 9CI O-77

[585-25-1]
2,3-Dioxooctane. Methyl pentyl diketone

$H_3CCOCOCH_2(CH_2)_3CH_3$

$C_8H_{14}O_2$ 142.197
Flavouring material for coffee. Liq. Bp_{17} 65-67°.

Dioxime: [1844-13-9]
$C_8H_{16}N_2O_2$ 172.227
Needles (EtOH aq.). Mp 173°.

Bis-2,4-dinitrophenylhydrazone:
Cryst. (EtOH aq.). Mp 221-224°.

Jones, L.A. *et al., J.O.C.*, 1961, **26**, 228 (*synth*)
Reusch, W. *et al., Tetrahedron*, 1967, **23**, 2893 (*ms*)
Meister, H. *et al., Annalen*, 1969, **724**, 128 (*synth*)
Venien, F. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1973, **277**, 247 (*nmr*)
Bowlus, S.B. *et al., J.O.C.*, 1974, **39**, 3309 (*synth, spectra*)

1,8-Octanedithiol, 9CI O-78

[1191-62-4]
1,8-Dimercaptooctane. FEMA 3514

$HSCH_2(CH_2)_6CH_2SH$

$C_8H_{18}S_2$ 178.362
Flavouring material for soups and meat products. Liq. with sulphurous meaty odour. d_4^{25} 0.96. Mp 0.9°. Bp 269.3°. n_D^{20} 1.5050.

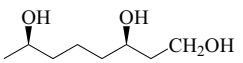
▶ RG9610000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 421A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 343B
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 153F (*ir*)
Hall, W.P. *et al., J.A.C.S.*, 1943, **65**, 1466
Ger. Pat., 1974, 2 417 385, (*IFF*); *CA*, **82**, 123593w (*use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 612 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2005 (*rev*)

1,3,7-Octanetriol O-79

[217650-23-2]

[217650-21-0, 217650-25-4]



(3*R*,7*R*)-*form*

$C_8H_{18}O_3$ 162.228

(3R,7R)-form [217650-11-8]
Constit. of apples. Viscous liq. $[\alpha]_D^{25}$ -14.4 (c, 5.8 in $CHCl_3$).

(3R,7S)-form [182803-48-1]
Constit. of apples. Oil. $[\alpha]_D^{18}$ +2.3 (c, 1 in MeOH).

Fujioka, H. *et al., J.O.C.*, 1996, **61**, 7309-7315 (*synth, pmr*)
Beuerle, T. *et al., J. Nat. Prod.*, 1999, **62**, 35-40 (*isol, synth, ir, pmr, cmr, abs config*)

Octanoic acid, 9CI, INN, USAN O-80

[124-07-2]
Heptane-1-carboxylic acid. Caprylic acid. Octoic acid. n-*Octylic acid. FEMA 2799*

$H_3C(CH_2)_6COOH$

$C_8H_{16}O_2$ 144.213

For salts see Octanoic acid salts, O-81. Widespread in plant oils, free and as glycerides. Also present in apple, banana, orange juice and peel, pineapple, cognac, calamus, blue cheeses, cheddar cheese, Swiss cheese, feta cheese and other cheeses. Flavouring agent, defoamer, lubricant, binder and antimicrobial preservative in cheese wraps. Liq. or cryst. with burning, rancid taste. Sol. alkalis, EtOH, $CHCl_3$; spar. sol. hot H_2O. d_4^{20} 0.91. Mp 16°. Bp 239.7° Bp_{10} 124°. n_D^{20} 1.4335. pK_a 4.89 (25°). Log P 2.94 (calc).

▶ Skin irritant. LD_{50} (rat, orl) approx. 10000 mg/kg. Fl. p. >107°. RH0175000

Me ester: [111-11-5] *Methyl octanoate. Methyl caprylate. FEMA 2728*
$C_9H_{18}O_2$ 158.24
Flavouring agent. Present in many fruits, e.g. apple, apricot, grape, blackberry, cherimoya etc.. Oil with oily, somewhat orange-like taste. d_4^{20} 0.88. Bp 193-194° Bp_{15} 83°. n_D^{20} 1.4180.

▶ RH0778000

Et ester: [106-32-1] *Ethyl octanoate. Ethyl caprylate. FEMA 2449*
$C_{10}H_{20}O_2$ 172.267
Used in many fruit flavourings. Constit. of plant oils. Also present in Swiss cheese, Camembert cheese, wheat bread, port wine, plum brandy, sparkling wine, apple, apricot, banana, cherry, orange, grapefruit, plum and other fruits. Liq. with fruity/flowery odour. Bp 207°. n_D^{20} 1.4178.

▶ RH0680000

Pentyl ester: [638-25-5] *Pentyl octanoate. Amyl caprylate. FEMA 2079*
$C_{13}H_{26}O_2$ 214.347
Flavouring agent. Liq. d^{25} 0.86. Mp -34–35°. Bp 260°. n_D^{25} 1.4262.

3-Methylbutyl ester: [2035-99-6] *3-Methylbutyl octanoate. Isoamyl caprylate. FEMA 2080*
$C_{13}H_{26}O_2$ 214.347
Used in food flavouring. Liq. d 0.86.

Hexyl ester: [1117-55-1] *Hexyl octanoate. Caproyl caprylate. FEMA 2575*
$C_{14}H_{28}O_2$ 228.374
Flavouring ingredient. Liq. with sweet, fruity taste. Mp -31°. Bp 227°.

Heptyl ester: [4265-97-8] *Heptyl octanoate. Heptyl caprylate. FEMA 2553*
$C_{15}H_{30}O_2$ 242.401
Flavouring ingredient. Oil. d^{30} 0.85. Mp -10°. Bp 290° Bp_{14} 160°. n_D^{20} 1.4340.

Octyl ester: [2306-88-9] *Octyl octanoate. Capryl caprylate. FEMA 2811*
$C_{16}H_{32}O_2$ 256.428
Flavouring agent. Liq. with oily, fruity, sweet mildly green taste. d_4^{25} 0.86. Mp -18.1°. Bp 306° Bp_{30} 192.5°. n_D^{20} 1.4352.

2-Propenyl ester: [4230-97-1] *2-Propenyl octanoate. Allyl caprylate. FEMA 2037*
$C_{11}H_{20}O_2$ 184.278
Imitation pineapple flavour. Liq. with fruit-like aroma. d_4^{30} 0.87. Bp 222° $Bp_{5.5}$ 87-88°. n_D^{30} 1.4271.

[557-09-5, 5461-06-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 483A; 607B; 607C; 730A; 838D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 753C; 921C; 922A; 1354B (*nmr*)
Ruhoff, J.R. *et al., J.A.C.S.*, 1933, **55**, 3825-3828 (*synth*)
Langenbeck, W. *et al., Chem. Ber.*, 1956, **89**, 202 (*synth*)
Markley, K.S. *et al., Fatty Acids*, Part 1, Interscience, N.Y., 2nd Ed., 1960, (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 694 (*occur*)
U.S. Pat., 1973, 3 770 782; *CA*, **80**, 14572 (*synth*)
Cahiez, G. *et al., J. Organomet. Chem.*, 1975, **94**, 463 (*synth*)
Baer, T.A. *et al., Tet. Lett.*, 1976, 4697 (*synth*)
Dinizo, S.E. *et al., J.A.C.S.*, 1977, **99**, 182 (*synth*)

Paukstelis, J.V. *et al., J.O.C.*, 1977, **42**, 3941 (*cmr*)
Belova, V.V. *et al., CA*, 1979, **90**, 128252j (*detn, Rh*)
Muehl, P. *et al., Talanta*, 1979, **26**, 227 (*detn, Fe*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1981, **19**, 237 (*rev, tox*)
Kopacz, S. *et al., Zh. Neorg. Khim.*, 1981, **26**, 1625; *CA*, **95**, 50325s (*detn, Co*)
Sokhan, V.F. *et al., Zh. Prikl. Khim. (Leningrad)*, 1981, **54**, 1023; *CA*, **95**, 100983c (*detn, Ti*)
Maccoll, A. *et al., Int. J. Mass Spectrom. Ion Processes*, 1988, **86**, 227 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, OCY000
Lloyd, H.A. *et al., J. Chem. Ecol.*, 1989, **15**, 2589-2599 (*biol, detn*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 319
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 43; 325; 355 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 97; 163-164; 1025; 1283-1284; 1335-1336; 1811; 2006; 2037 (*esters, occur, props*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ENY000; OCY000; ODE200

Octanoic acid salts O-81

Octanoates. Caprylates

For parent acid see Octanoic acid, O-80.

Na salt: [1984-06-1] *Sodium octanoate. Sodium caprylate*
$C_8H_{15}NaO_2$ 166.195
Used in foods as a binder, emulsifier and anticaking agent. d^{27} 1.21. Mp 119-120°.

K salt: [764-71-6] *Potassium octanoate. Potassium caprylate*
$C_8H_{15}KO_2$ 182.304
Used in foods as a binder, emulsifier and anticaking agent. Cryst. (H_2O). Mp 200-210° Mp 353°.

Mg salt: [3386-57-0] *Magnesium octanoate. Magnesium caprylate*
$C_{16}H_{30}MgO_4$ 310.716
Used in foods as a binder, emulsifier and anticaking agent.

Ca salt: [6107-56-8] *Calcium octanoate. Calcium caprylate*
$C_{16}H_{30}CaO_4$ 326.489
Used in foods as a binder, emulsifier and anticaking agent.

Al salt: [6028-57-5] *Aluminium octanoate. Aluminium caprylate*
$C_{24}H_{45}AlO_6$ 456.597
Used in foods as a binder, emulsifier and anticaking agent. Cryst. Mp 82-82.8° Mp 120°.

Fe salt: [6535-20-2] *Iron octanoate. Iron caprylate*
Metallic drier which hastens the drying of oleoresinous coating materials used to line the inner surfaces of food-containing cans. Oxidation state not known; Fe 2-ethylhexanoates are also used.

[74-81-7, 1912-83-0, 4288-15-7, 4696-54-2, 4995-91-9, 6107-56-8, 6535-19-9, 6535-20-2, 18312-04-4]

McBain, J.W. *et al., J.A.C.S.*, 1920, **42**, 426-460 (*synth*)
Soderlund, G. *et al., Z. Phys. Chem.*, 1970, **70**, 39-46 (*Na salt, ir, pmr*)
Kumar, N. *et al., Can. J. Chem.*, 1987, **65**, 740-743 (*synth, props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 110; 372-373; 1616; 2287; 2535

1-Octanol, 9CI O-82

[111-87-5]

[29063-28-3]
n-*Octyl alcohol. Caprylic alcohol. FEMA 2800*

$H_3C(CH_2)_6CH_2OH$
$C_8H_{18}O$ 130.23
Occurs in the form of esters in some essential oils. Flavouring agent. Liq. with penetrating aromatic odour. d_4^{20} 0.83. Mp -16.7°. Bp 194.45° Bp_{19} 98°. n_D^{20} 1.4295.
▶ Skin irritant. LD_{50} (mus, orl) 1790 mg/kg. RH6550000

Sulfate, Na salt: [142-31-4] *Sodium octyl sulfate*
Used in washing/lye peeling of fruits and vegetables, poultry scald agent. Mp 195° dec.
▶ WT1175000

Formyl: [112-32-3] *Octyl formate. FEMA 2809*
$C_9H_{18}O_2$ 158.24
Fragrance and flavouring ingredient. Present in Scotch spearmint oil and grilled or roast beef. Liq. with fruity odour. d 0.87. Bp_{740} 197-199°.
▶ Skin irritant. LQ9290000

Ac: [112-14-1] *Octyl acetate. FEMA 2806*
$C_{10}H_{20}O_2$ 172.267
Present in citrus peel oils, wheat bread, cheddar cheese, wines, banana, sour cherry and other foodstuffs. Flavour ingredient. Liq. Bp 211.5° Bp_{30} 112-113°.
▶ Skin irritant. LD_{50} (rat, orl) 3000 mg/kg. AJ1400000

Propanoyl: [142-60-9] *Octyl propanoate. FEMA 2813*
$C_{11}H_{22}O_2$ 186.294
Flavouring ingredient. Isol. from *Pastinaca satica* (parsnip). d 0.87. Bp 226°. n_D 1.4225.

Butanoyl: [110-39-4] *Octyl butanoate. FEMA 2807*
$C_{12}H_{24}O_2$ 200.32
Used in fruit food flavouring. d 0.86. Bp 244°.

2-Methylpropanoyl: [109-15-9] *Octyl 2-methylpropanoate. FEMA 2808*
$C_{12}H_{24}O_2$ 200.32
Used in food flavouring. d 0.87. Bp 237°.

2-Methylbutanoyl: [29811-50-5] *Octyl 2-methylbutyrate. FEMA 3604*
$C_{13}H_{26}O_2$ 214.347
Flavouring ingredient. Liq. $Bp_{1.4}$ 125-126°. n_D^{20} 1.4254.

3-Methylbutanoyl: [7786-58-5] *Octyl 3-methylbutanoate. Octyl isovalerate. FEMA 2814*
$C_{13}H_{26}O_2$ 214.347
Flavouring agent. Liq. with intense fatty, fruity odour. d 0.86. Bp 245°.

Heptanoyl: [5132-75-2] *Octyl heptanoate. FEMA 2810*
$C_{15}H_{30}O_2$ 242.401
Flavouring ingredient. Liq. d^{20} 0.85. Mp -21.5°. Bp 291°. n_D^{20} 1.4349.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 111A; 603B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 165B; 903B; 1456B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 157B; 610C (*ir*)
Sadtler Standard Proton NMR Spectra, 6392 (*pmr*)
Gartenmeister, R. *et al., Annalen*, 1886, **233**, 226; 272; 281 (*propanoyl, butanoyl, hexanoyl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 109
Fruwert, J. *et al., Z. Phys. Chem. (Leipzig)*, 1968, **238**, 262 (*ir*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 76 (*occur*)
Org. Synth., 1973, **53**, 77 (*synth*)
Akabori, S. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2991 (*Ac*)
Kozhin, S.A. *et al., CA*, 1976, **84**, 155497a (*isol*)
Japan. Pat., 1977, 77 00 006; *CA*, **86**, 189198k (*synth*)
Bowen, R.D. *et al., Org. Mass Spectrom.*, 1983, **18**, 576 (*ms*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1985, **36**, 253 (*cmr*)
Zahalka, H.A. *et al., Synthesis*, 1986, 763 (*formyl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, OEG000; OEI000; OEY100
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 623-630 (*heptanoyl, 2-methylbutanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2009; 2026; 2031; 2039 (*occur, use, esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OEG000; OEI000; OEY100

2-Octanol, 9CI O-83

[123-96-6]

[29063-28-3]
Capryl alcohol. FEMA 2801

$C_8H_{18}O$ 130.23
The use of the name capryl alcohol for this isomer is misleading and should be discouraged. It would be expected to apply to 1-octanol.
▶ Fl. p. 71/88°. RH0795000

(R)-form [5978-70-1]
Bp_{20} 86°. $[\alpha]_D^{17}$ -9.9.

Hydrogen phthalate:
Needles (petrol). Mp 75°. $[\alpha]_D^{24}$ -48.4.

Benzoyl: [78687-05-5]
$C_{15}H_{22}O_2$ 234.338
$Bp_{0.6}$ 90°. $[\alpha]_D$ -34.3 (c, 1.5 in CH_2Cl_2).

(S)-form [6169-06-8]
Bp_{20} 86°. $[\alpha]_D^{17}$ +9.9.

Benzoyl: [34881-29-3]
$Bp_{0.6}$ 90°. $[\alpha]_D^{18}$ +33.5 (MeCl).

(±)-form [4128-31-8]
Flavouring ingredient. Oily refractive liq. with aromatic yet unpleasant odour. d_4^{25} 0.82. Mp -38.6°. Bp 180°. n_D^{20} 1.4203.

Ac: [2051-50-5]
$C_{10}H_{20}O_2$ 172.267
Bp_{744} 194.5° Bp_{15} 84°.

Me ether: [1541-09-9] *2-Methoxyoctane*
$C_9H_{20}O$ 144.256
Bp_{44} 76-77°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 120B; 120C; 120D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 180C; 181A; 181B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 168D; 169A; 169B (*ir*)
Kenyon, J. *et al., J.C.S.*, 1923, **123**, 18
Org. Synth., 1926, **6**, 68 (*synth*)
Bohnsack, H. *et al., Ber.*, 1942, **75**, 502 (*isol*)
Doering von E., W. *et al., J.A.C.S.*, 1952, **74**, 2997 (*abs config*)
Cristol, S.J. *et al., J.A.C.S.*, 1955, **77**, 2512
Goering, H.L. *et al., J.A.C.S.*, 1956, **78**, 2270
Gil-Av, E. *et al., J. Chromatogr.*, 1965, **17**, 408 (*use*)
Fruwert, J. *et al., Z. Phys. Chem. (Leipzig)*, 1968, **238**, 262 (*ir*)
Whitney, T.A. *et al., Polym. Prepr. (Am. Chem. Soc., Div. Polym. Chem.)*, 1971, **13**, 688 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Keinan, E. *et al., J.A.C.S.*, 1986, **108**, 162 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 614
Reyes, A. *et al., Synth. Commun.*, 1995, **25**, 1053 (*resoln*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2010-2012
Nakamura, K. *et al., J.C.S. Perkin 1*, 2000, 3205-3211 (*S-form, synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ODE000

3-Octanol, 9CI O-84

[589-98-0]

[29063-28-3]
FEMA 3581

$C_8H_{18}O$ 130.23
Present in *Mentha* spp. oils, sage, soybeans, porcini (*Boletus edulis*), wines and other foodstuffs. Flavouring agent.
► RH0855000
(*R*)-*form* [70492-66-9]
Bp_{24} 82°. $[\alpha]_D$ -12.5 (1 in $CHCl_3$).
(*S*)-*form* [22658-92-0]
Present in Japanese peppermint oil and many other essential oils. Bp 178.5-179.5° Bp_{16} 76°. $[\alpha]_D$ +10.1 (c, 0.82 in $CHCl_3$).
O-*β*-D-*Glucopyranoside:* [129742-31-0]
$C_{14}H_{28}O_6$ 292.372
Constit. of spearmint (*Mentha spicata* var. *crispa*). $[\alpha]_D^{21}$ -29 (c, 0.2 in MeOH).
(±)-*form* [20296-29-1]
Flavouring agent, used in mushroom flavours and lavender compositions. d_{15}^{15} 0.83. Bp 176-177.5°. n_D^{20} 1.4279.
► Skin and eye irritant.
Ac: [50373-56-3] *FEMA 3583*
$C_{10}H_{20}O_2$ 172.267
Flavouring ingredient. Liq. with a sweet peach-like flavour. Bp 191-191.5°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 121A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 181C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 169C (*ir*)
Pickard, R.H. *et al., J.C.S.*, 1913, **103**, 1944 (*synth*)
Woods, G.F. *et al., J.A.C.S.*, 1956, **78**, 4380 (*synth*)
Cason, J. *et al., J.O.C.*, 1961, **26**, 3645 (*synth*)
Spiteller, G. *et al., Angew. Chem.*, 1965, **77**, 393 (*ms*)
Fruwert, J. *et al., Z. Phys. Chem. (Leipzig)*, 1968, **238**, 262 (*ir*)
Fried, J. *et al., J.A.C.S.*, 1972, **94**, 4342 (*abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 78 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 881 (*rev, tox*)
Tang, K.-C. *et al., J. Med. Chem.*, 1981, **24**, 1277 (*synth, pmr*)
Brand, J.M. *et al., J. Chem. Ecol.*, 1987, **13**, 357 (*isol*)
Shimizu, S. *et al., J. Essent. Oil Res.*, 1990, **2**, 81 (*glucoside*)
Kamezawa, M. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 598 (*synth*)
Paolucci, C. *et al., J.O.C.*, 1995, **60**, 169 (*synth, pmr, cmr*)
Bonini, C. *et al., J.O.C.*, 1995, **60**, 4803 (*synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2011-2012; 2027-2028 (*occur, props*)
Yamamura, S. *et al., Phytochemistry*, 1998, **48**, 131-136 (*glucoside, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OCY100

2-Octanone, 9CI O-85

[111-13-7]
FEMA 2802

$H_3CCH_2(CH_2)_4COCH_3$

$C_8H_{16}O$ 128.214
Trace constit. of plant oils. Also present in apple, apricot, banana, papaya, wheat bread, other breads, cheddar cheese, Swiss cheese, coffee, black tea, roasted filbert, plum brandy and cooked shrimp. Flavouring ingredient. Liq. d_4^{20} 0.82. Fp -16. Bp 172.92° Bp_{11} 59-60°. n_D^{20} 1.4151.
► Skin irritant. LD_{50} (rat, ipr) 800 mg/kg. RH1484000
Oxime: [7207-49-0]
$C_8H_{17}NO$ 143.228
Oil. Bp_{725} 213-214° Bp_{15} 116.5°.
2,4-Dinitrophenylhydrazone:
Orange cryst. (EtOH). Mp 58°.
Semicarbazone:
Cryst. (EtOH aq.). Mp 123°.
Di-Et acetal: [101924-52-1] *2,2-Diethoxyoctane*
$C_{12}H_{26}O_2$ 202.336
Bp_{16} 101-103°.
Δ^1-Enol-*form* *1-Octen-2-ol*
Ac: [26735-84-2]
$C_{10}H_{18}O_2$ 170.251
Bp_{42} 108°.
Me ether: [42367-31-7] *2-Methoxy-1-octene*
$C_9H_{18}O$ 142.241
Bp 166-168°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 410B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 638C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 494C (*ir*)
Moureu, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1904, **138**, 287; 1920, **171**, 652 (*synth*)
Verhulst, G. *et al., Bull. Soc. Chim. Belg.*, 1932, **41**, 501 (*synth*)
Fruwert, J. *et al., Z. Phys. Chem. (Leipzig)*, 1968, **238**, 262; 401 (*ir*)
Hudrlik, P.F. *et al., J.O.C.*, 1973, **38**, 4254 (*synth, spectra*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ODG000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2012-2013 (*occur, props*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

3-Octanone, 9CI O-86

[106-68-3]
Ethyl pentyl ketone. Amyl ethyl ketone.
FEMA 2803

$H_3C(CH_2)_4COCH_2CH_3$

$C_8H_{16}O$ 128.214
Flavouring ingredient. Liq. with a strong, penetrating, fruity odour reminiscent of lavender. d^{15} 0.83. Bp 165-166° (170°). n_D^{23} 1.4156.
► Skin, eye and mucous membrane irritant. LD_{50} (mus, ipr) 406 mg/kg. RH1485000
Semicarbazone:
Cryst. (EtOH aq.). Mp 117-117.5° (112°).
2,4-Dinitrophenylhydrazone:
Mp 67°.
Di-Me ketal:3,3-Dimethoxyoctane
$C_{10}H_{22}O_2$ 174.283
Bp_{26} 90-92°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 410C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 639A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 494D (*ir*)
Pickard, R.H. *et al., J.C.S.*, 1913, **103**, 1936 (*derivs*)
Asinger, F. *et al., Chem. Ber.*, 1957, **90**, 485 (*synth, bibl*)
Shuikin, N.I. *et al., Zh. Obshch. Khim.*, 1957, **27**, 402; *CA*, **51**, 15489i (*synth*)
Shimizu, S. *et al., Agric. Biol. Chem.*, 1961, **25**, 263 (*isol*)
Fruwert, J. *et al., Z. Phys. Chem. (Leipzig)*, 1968, **238**, 262 (*ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 615
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2013-2014
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ODI000

2,4,6-Octatriynoic acid O-87

[51193-80-7]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCOOH$

$C_8H_4O_2$ 132.118
Constit. of *Kuehneromyces mutabilis* (two-toned wood tuft) and *Russula vesca* (bare-toothed russule).

Me ester: [62796-54-7]
$C_9H_6O_2$ 146.145

Cryst. (petrol). Mp 56-58°.

Bohlmann, F. *et al., Chem. Ber.*, 1956, **89**, 2268 (*synth*)
Jones, E.R.H. *et al., J.C.S.*, 1957, 2012 (*synth*)
Hearn, M.T.W. *et al., J.C.S. Perkin 1*, 1973, 2785 (*isol*)

2,4,6-Octatriyn-1-ol O-88

[13033-21-1]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH_2OH$

C_8H_6O 118.135

Constit. of *Kuehneromyces mutabilis* (two-toned wood tuft) and *Russula vesca* (bare-toothed russule). Plates (CCl_4); pale-cream needles (pentane). Mp 93°.

Curtis, R.F. *et al., J.C.S.(C)*, 1971, 186 (*synth, uv, ir, pmr*)
Hearn, M.T.W. *et al., J.C.S. Perkin 1*, 1973, 2785

3,5,7-Octatriyn-1-ol, 9CI O-89

[6071-20-1]

$HC{\equiv}CC{\equiv}CC{\equiv}CCH_2CH_2OH$

C_8H_6O 118.135

Isol. from *Lentinus edodes* (shiitake). λ_{max} 209 (no solvent reported).

Bew, R.E. *et al., J.C.S.(C)*, 1966, 129 (*synth, ir, uv*)
Tokimoto, K. *et al., Proc. Jpn. Acad., Ser. B*, 1987, **63**, 277 (*isol*)

2-Octenal, 9CI O-90

[2363-89-5]
FEMA 3215

$H_3C(CH_2)_4CH{=}CHCHO$

$C_8H_{14}O$ 126.198

Flavouring ingredient.

►RH2130000

(*E*)-*form* [2548-87-0]
Liq. Bp_{19} 84-86°. n_D^{20} 1.4500.
2,4-Dinitrophenylhydrazone:
Mp 125-126°.

(*Z*)-*form*
Bp_{15} 81-82°. 92% pure.
Di-Et acetal:1,1-Diethoxy-2-octene
$C_{12}H_{24}O_2$ 200.32
Bp_{14} 104-106°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 738A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 561C (*ir*)
v. Romburgh, P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1938, **57**, 494 (*isol*)
Baker, J.T. *et al., Aust. J. Chem.*, 1969, **22**, 1793
Riehl, J.J. *et al., Tet. Lett.*, 1969, 3139 (*synth*)
Corey, E.J. *et al., J.A.C.S.*, 1971, **93**, 1724 (*ir, pmr*)
Makin, S.M. *et al., Zh. Org. Khim.*, 1974, **10**, 2044 (*synth*)
Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 617
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2015-2016
Fortes, C.C. *et al., Synth. Commun.*, 1997, **27**, 3917-3941 (*synth, pmr, cmr, ir, ms*)

5-Octenal, 9CI O-91

$H_3CCH_2CH{=}CHCH_2CH_2CH_2CHO$

$C_8H_{14}O$ 126.198

(*E*)-*form* [41547-29-9]
Liq. Bp_{12} 57-59°.

(*Z*)-*form* [41547-22-2]
FEMA 3749
Flavouring ingredient. Liq. Bp_{12} 57-62°. n_D^{20} 1.4360.

Waechli, P. *et al., Helv. Chim. Acta*, 1978, **61**, 885 (*synth, ir, pmr*)
Mikami, K. *et al., Tetrahedron*, 1986, **42**, 2911 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 623
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2017

6-Octenal, 9CI O-92

[63826-25-5]

$H_3CCH{=}CHCH_2CH_2CH_2CH_2CHO$

$C_8H_{14}O$ 126.198

Listed in the EAFUS Food Additive Database (Jan. 2001).

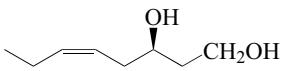
(*E*)-*form* [63196-63-4]
Liq. Bp_{50} 86-88°. $n_D^{24.5}$ 1.4362.
2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 100-101°.

(*Z*)-*form* [63196-64-5] No phys. data reported.

LeBel, N.A. *et al., J.A.C.S.*, 1964, **86**, 3759 (*synth*)
Marvell, E.N. *et al., J.O.C.*, 1977, **42**, 3336 (*synth, ir, pmr*)
Denmark, S.E. *et al., J.A.C.S.*, 1986, **108**, 1306 (*synth*)

5-Octene-1,3-diol O-93

[71677-23-1, 71677-24-2]



(3*R*,5*Z*)-*form*

$C_8H_{16}O_2$ 144.213

(3*R*,5*Z*)-*form* [130272-38-7]
Constit. of apple juice. $[\alpha]_D^{25}$ -14.1.

(3*RS*,5*Z*)-*form*
Bp_2 106-107°.

(3ξ,5*Z*)-*form*
1-Ac:
$C_{10}H_{18}O_3$ 186.25
Constit. of apples. C-3 stereochem not known for isolate.

[71677-25-3, 71677-26-4]

Yajima, I. *et al., Agric. Biol. Chem.*, 1984, **48**, 849 (*isol, synth, ir, pmr, ms*)
Beuerle, T. *et al., Phytochemistry*, 1996, **43**, 145 (*isol, synth*)

6-Octene-2,4-diynedioic acid O-94

HOOCCH=CHC≡CC≡CCOOH

$C_8H_4O_4$ 164.117

(*E*)-*form*
*1-Monoamide:**Diatretin 1**. Diatretyne I*
$C_8H_5NO_3$ 163.132
Cryst. (MeOH). Sol. MeOH, Et_2O, bases; poorly sol. H_2O, acids. Mp 198° (explodes). (*E*)-form assumed λ_{max} 223 (ϵ 37200); 260 (ϵ 11000); 275 (ϵ 16600); 291 (ϵ 23300); 310 (ϵ 18800) (EtOH) (Berdy).

►Explodes on melting; LD_{50} (mus, ivn) 50 mg/kg.

1-Mononitrile: [463-15-0] *7-Cyano-2-heptene-4,6-diynoic acid. **Diatretin 2**. Diatretyne II. Nudic acid B*
$C_8H_3NO_2$ 145.117
Prod. by *Camarophyllus virgineus* (snowy wax cap). Cryst. (Et_2O/petrol). Sol. MeOH, bases, Et_2O, Py; poorly sol. hexane, H_2O, acids. Mp 179-180° dec. λ_{max} 231 (ϵ 46200); 239 (ϵ 58000); 268 (ϵ 7500); 285 (ϵ 14200); 304 (ϵ 20000); 322 (ϵ 14300) (MeOH) (Berdy).

►LD_{50} (mus, ivn) 13 mg/kg. MJ8977000

[3625-68-1]

Anchel, M. *et al., J.A.C.S.*, 1952, **74**, 1588; 1953, **75**, 4621 (*isol, struct*)
Anchel, M. *et al., Arch. Biochem. Biophys.*, 1958, **78**, 100 (*isol*)
Ashworth, P.J. *et al., J.C.S.*, 1958, 950 (*synth*)
Anchel, M. *et al., Mycologia*, 1962, **54**, 249
Thaller, V. *et al., J.C.S. Perkin 1*, 1972, 2032 (*isol, ms, nmr*)
Hearn, M.T.W. *et al., J.C.S. Perkin 2*, 1976, 1027 (*cmr*)
Jones, E.R.H. *et al., J. Chem. Res., Synop.*, 1981, 157 (*biosynth*)
Magalhaes, A.F. *et al., J. Braz. Chem. Soc.*, 1995, **6**, 361-364 (*synth*)

7-Octene-3,5-diyn-1-ol, 9CI O-95

[114020-45-0]
Lentialexin

$H_2C{=}CHC{\equiv}CC{\equiv}CCH_2CH_2OH$

C_8H_8O 120.151

Prod. by a mixed culture of *Lentinus edodes* (shiitake) and *Trichoderma polysporum*. Sol. H_2O, Et_2O. λ_{max} 238 ; 251 ; 264 ; 282 (MeOH) (Berdy).

Tokimoto, K. *et al., Proc. Jpn. Acad., Ser. B*, 1987, **63**, 277-280 (*isol*)
Japan. Pat., 1988, 88 44542; *CA*, **109**, 127328n (*isol*)

2-Octenoic acid, 9CI O-96

[1470-50-4]
1-Heptene-1-carboxylic acid

$H_3C(CH_2)_4CH{=}CHCOOH$

$C_8H_{14}O_2$ 142.197

(*E*)-*form* [1871-67-6]
FEMA 3957
Food flavourant for baked goods and candies. Mp 2°. Bp_{12} 135-136°.

Me ester: [7367-81-9] *FEMA 3712*
$C_9H_{16}O_2$ 156.224
Flavouring ingredient. Liq. Bp_{12} 80°. n_D 1.4399.

Et ester: [7367-82-0] *FEMA 3344*
$C_{10}H_{18}O_2$ 170.251
Flavouring agent. Liq. Bp_{10} 93-96°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 500D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 780B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 586C (*ir*)
Colonge, J. *et al., Annalen*, 1965, **684**, 10-14 (*ir*)
Cainelli, G. *et al., Chem. Comm.*, 1973, 94-95 (*E-form, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 260; 536 (*esters*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1027; 1815-1816 (*esters*)

4-Octenoic acid, 9CI O-97

[18294-89-8]
3-Heptene-1-carboxylic acid
$H_3CCH_2CH_2CH{=}CHCH_2CH_2COOH$
$C_8H_{14}O_2$ 142.197

(*E*)-*form* [18776-92-6]
Liq. d_{20} 0.93. Mp -4°. Bp_{15} 132° $Bp_{1.5}$ 93°. n_D^{20} 1.4441.

(*Z*)-*form* [18654-81-4]
Liq. d_{20} 0.93. Mp -35°. $Bp_{0.8}$ 96°. n_D^{20} 1.4417.

Me ester: [21063-71-8] *FEMA 3367*
$C_9H_{16}O_2$ 156.224
Constit. of pineapple and other fruit aromas. Flavouring ingredient. Bp_{11} 90°.

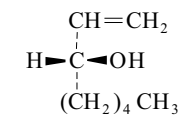
Et ester: [34495-71-1] *FEMA 3344*
$C_{10}H_{18}O_2$ 170.251
Constit. of pineapple and other fruit aromas. Flavouring ingredient. Bp_{11} 105°.

[1732-00-9, 78989-37-4, 81586-83-6]

Knight, J.A. *et al., J.O.C.*, 1959, **24**, 400 (*synth*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1967, **1**, 209 (*synth*)
Firmenich, R. *et al., Helv. Chim. Acta*, 1971, **54**, 1880 (*isol, ms, esters*)
Naf, F. *et al., Helv. Chim. Acta*, 1971, **54**, 1939 (*synth, pmr, ester*)
Bestmann, H.J. *et al., Annalen*, 1981, 1705 (*ester*)
Huhtasaari, M. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 537 (*synth, pmr*)
Thompson, C.M. *et al., J.O.C.*, 1989, **54**, 890 (*ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1026; 1814 (*esters, occur, use*)

1-Octen-3-ol, 9CI O-98

[3391-86-4]
Amyl vinyl carbinol. Matsutake alcohol. Matsutakeol. FEMA 2805



(R)-form

$C_8H_{16}O$ 128.214
► LD_{50} (rat, orl) 340 mg/kg. RH3300000

(*R*)-*form*
Isol. from a number of essential oils, e.g. lavender, leek, mint and mushrooms. Food odorant responsible for typical mushroom odour. Flavouring ingredient. Mp 175°. $[\alpha]_D^{20}$ -18.4 (neat) (c, 7.3 in EtOH).

O-*β*-D-*Glucopyranoside:* [209863-00-3]

[74356-49-3]
$C_{14}H_{26}O_6$ 290.356
Constit. of spearmint (*Mentha spicata* var. *crispa*). $[\alpha]_D^{21}$ +10 (c, 0.5 in MeOH).

O-[*β*-D-*Xylopyranosyl*-(1→6)-*β*-D-*glucopyranoside*]: [209863-01-4]
$C_{19}H_{34}O_{10}$ 422.472
Constit. of spearmint (*Mentha spicata* var. *crispa*). $[\alpha]_D^{21}$ -60 (c, 0.1 in MeOH).

O-[*β*-D-*Glucopyranosyl*-(1→6)-*β*-D-*glucopyranoside*]: [209465-69-0] ***Calaliukiuenoside***
$C_{20}H_{36}O_{11}$ 452.498
Powder. $[\alpha]_D^{28}$ -45.4 (MeOH).

O-[*β*-D-*Glucopyranosyl*-(1→2)-[*β*-D-*xylopyranosyl*-(1→6)]-*β*-D-*glucopyranoside*]: ***Ebracteatoside B***
$C_{25}H_{44}O_{15}$ 584.614
Amorph. powder. $[\alpha]_D^{22}$ -45 (c, 2.1 in MeOH).

Ac:

[2442-10-6] *FEMA 3582*
$C_{10}H_{18}O_2$ 170.251
Present in *Mentha* spp. oils, lavender oil, anise hyssop, various mushrooms and melon. Flavouring agent. Liq. with lavender odour. Bp 190°. $[\alpha]_D^{20}$ +5.4 (neat).

Hydrogen phthalate:
Mp 57°.

(*S*)-*form* [62247-46-5]

[22658-80-6]
$[\alpha]_D^{17}$ +10.7 (EtOH).

(±)-*form* [74072-82-5]
Liq. with intense earthy odour. Bp 173.5°. n_D^{20} 1.4378.

Butanoyl: [16491-54-6] *1-Ethenylhexyl butanoate. 1-Octen-3-yl butyrate. FEMA 3612*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Liq. $Bp_{3.5}$ 80-81°. n_D^{20} 1.4285.

Hydrogen phthalate:
Mp 79°.

(ξ)-*form*
O-[*β*-L-*Arabinopyranosyl*-(1→6)-*β*-D-*glucopyranoside*]: [205178-45-6]
$C_{19}H_{34}O_{10}$ 422.472
Solid. $[\alpha]_D^{25}$ -27 (c, 0.3 in MeOH). Stereochem. not determined.

[2442-10-6, 3687-48-7, 24587-53-9, 50999-79-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 143C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 215C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 210C (*ir*)
Honkanen, E. *et al., Acta Chem. Scand.*, 1963, **17**, 858 (*isol*)
Tsuji, J. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1701 (*synth, spectra*)
Roumestant, M.L. *et al., Synthesis*, 1976, 755 (*synth*)
McGahren, W.J. *et al., J.O.C.*, 1977, **42**, 1659 (*abs config*)
Nakai, T. *et al., Tet. Lett.*, 1977, 2425 (*synth*)
Takabe, K. *et al., Synth. Commun.*, 1980, **10**, 89 (*synth*)
Whitfield, F.B. *et al., Aust. J. Chem.*, 1982, **35**, 373 (*isol*)
Shimazaki, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 3073 (*synth*)
Dittmer, D.C. *et al., J.O.C.*, 1993, **58**, 718 (*synth, pmr, cmr, bibl*)
Toyota, M. *et al., Phytochemistry*, 1993, **32**, 1235 (*Ac, isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 622; **2**, 617; 620 (*butanoyl, Ac, props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2018-2019; 2023-2024; 2025-2026 (*Ac, butanoyl, occur, props*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 886-888 (*Calaliukiuenoside*)
Wang, S. *et al., J. Nat. Prod.*, 1998, **61**, 508-510 (*arabinosylglucoside*)
Yamamura, S. *et al., Phytochemistry*, 1998, **48**, 131-136 (*glycosides*)
Kanchanapoom, T. *et al., Phytochemistry*, 2001, **58**, 811-817 (*Ebracteatoside B*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ODW000

2-Octen-1-ol, 9CI O-99

[22104-78-5]
Isomatsutakeol
$H_3C(CH_2)_4CH{=}CHCH_2OH$
$C_8H_{16}O$ 128.214

(*E*)-*form* [18409-17-1]
FEMA 3887
Found in grapes, ripe bananas, mushroom volatiles and various other vegetable sources. Food flavour/aroma component. Bp_{11} 87-89°.

Ac: [3913-80-2] *2-Octenyl acetate. FEMA 3516*
$C_{10}H_{18}O_2$ 170.251
Present in banana. Flavouring agent. Bp_{13} 82-84°. n_D^{20} 1.4333.

Butanoyl: [84642-60-4] *FEMA 3517*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient. Bp_8 112-113°. n_D^{20} 1.4365.

(*Z*)-*form* [26001-58-1]
Bp_{10} 85-87°.

3,5-Dinitrobenzoyl:
Mp 60°.

[26806-12-2]

Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1955, 953 (*synth*)
Osbond, J. *et al., J.C.S.*, 1961, 5270 (*synth*)
Schlosser, M. *et al., Synthesis*, 1972, 575 (*synth*)
Sood, R. *et al., Tet. Lett.*, 1974, 423 (*synth*)
Pyysalo, H. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 235 (*isol*)
Tsuji, J. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1701
Tsuji, J. *et al., Tet. Lett.*, 1979, 39 (*synth, spectra*)
Porter, N.A. *et al., J.O.C.*, 1985, **50**, 2252 (*synth, pmr, cmr*)
Nicolaou, K.C. *et al., Synthesis*, 1986, 453 (*synth, ir, pmr*)
Binns, M.R. *et al., Aust. J. Chem.*, 1987, **40**, 281 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 621-622 (*rev, esters*)
Richardson, T.I. *et al., J.O.C.*, 1996, **61**, 4219 (*Z-form, synth, ir, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2023-2025 (*rev, esters*)
Mau, J.-L. *et al., J. Agric. Food Chem.*, 1998, **46**, 4587-4591 (*isol*)
Capon, R.J. *et al., J.O.C.*, 1998, **63**, 75-83 (*synth, ir, pmr, cmr*)

2-Octen-4-ol, 9CI O-100

[4798-61-2]

$C_8H_{16}O$ 128.214

(*R*,*E*)-*form*
Oil. $[\alpha]_D$ -6.1 (c, 3.31 in EtOH) (94% ee).

(±)-(*E*)-*form* [20125-81-9]
FEMA 3888
Food flavourant for baked goods and

candies. Bp 175° Bp_{20} 83°.

3,5-Dinitrobenzoyl:
Plates (EtOH aq.). Mp 54°.

(±)-(*Z*)-*form* [22287-00-9]

Ac:
$C_{10}H_{18}O_2$ 170.251
Bp_{45} 105-107°.

Hargreaves, G.H. *et al., J.C.S.*, 1947, 756 (*synth*)
Dauben, W.G. *et al., J.O.C.*, 1970, **35**, 374 (*synth*)
Gocmen, M. *et al., Bull. Soc. Chim. Fr.*, 1973, 1310 (*synth*)
Umbreit, M.A. *et al., J.A.C.S.*, 1977, **99**, 5526 (*synth*)
Ishida, A. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 2077 (*synth*)
Belelie, J.L. *et al., J.O.C.*, 2001, **66**, 5552-5555 (*R,E-form*)

3-Octen-1-ol, 9CI O-101

[18185-81-4]

$H_3C(CH_2)_3CH{=}CHCH_2CH_2OH$

$C_8H_{16}O$ 128.214

(*E*)-*form* [20125-85-3]
Found in ripe bananas. Bp_{12} 86°.

(*Z*)-*form* [20125-84-2]
FEMA 3467
Flavouring ingredient present in banana, passionfruit and green peas. Liq. Insol. H_2O, sol. EtOH. d^{20} 0.85. Bp_{15} 95-96°. n_D^{20} 1.4457.

Normant, H. *et al., C. R. Hebd. Seances Acad. Sci.*, 1948, **226**, 733
Rossi, R. *et al., Gazz. Chim. Ital.*, 1978, **108**, 709
Alexakis, A. *et al., Tetrahedron*, 1980, **36**, 1961 (*synth, ir, pmr*)
Mitra, R.B. *et al., Synthesis*, 1989, 694 (*synth, ir, pmr*)
Ducoux, J.P. *et al., J.O.C.*, 1993, **58**, 1290 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 618
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2017-2018

3-Octen-2-ol O-102

[76649-14-4]

[57648-55-2, 69668-89-9, 105087-04-5, 105087-06-7, 133646-97-6]
FEMA 3602

$C_8H_{16}O$ 128.214
Flavouring ingredient. Produced from mold (*Penicillium cyclopium, Aspergilus amstelodami*) affected wheat grains. Also present in fish oil and krill products.

(*R*,*E*)-*form* [81801-15-2]
Bp_{18} 105-115° (bulb). $[\alpha]_D^{24}$ +1.5 (c, 1.8 in MeOH) (79% op).

(±)-(*E*)-*form* [122211-24-9]
Bp_{20} 80-81°. n_D^{20} 1.4258.

Noyori, R. *et al., J.A.C.S.*, 1984, **106**, 6717-6725 (*R-form, synth*)
Corey, L.D. *et al., Can. J. Chem.*, 1987, **65**, 1821-1827 (*synth, pmr, ms*)
Boerjesson, T. *et al., Cereal Chem.*, 1989, **66**, 300-304 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 618 (*use*)

5-Octen-1-ol, 9CI O-103

$H_3CCH_2CH{=}CH(CH_2)_3CH_2OH$

$C_8H_{16}O$ 128.214

(*E*)-*form* [64275-74-7]
Bp_{14} 91.5°.

Ac: [71978-07-9]
$C_{10}H_{18}O_2$ 170.251
Oil.

(*Z*)-*form* [64275-73-6]
FEMA 3722
Constit. of apples, banana and passionfruit. Flavouring ingredient. Liq. with green, fatty odour. d_4^{20} 0.85. Bp_{12} 96-98°. n_D^{20} 1.4472.

Sulfate:
$C_8H_{16}O_4S$ 208.278
Amorph. solid. Stated as *E*-isomer in parts of text.

Ac: [71978-00-2]
Constit. of bananas. Oil.

Propanoyl: [196109-18-9] *5-Octenyl propanoate. FEMA 3890*
$C_{11}H_{20}O_2$ 184.278
Used in food flavouring. Liq. with melon, green, fatty odour. $Bp_{0.5}$ 70°.

Ficini, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 119 (*synth*)
Waelchli, P.C. *et al., Helv. Chim. Acta*, 1978, **61**, 885 (*synth, tetrahydropyranyl ethers*)
Brown, D.C. *et al., J.O.C.*, 1979, **44**, 3457 (*E-form, synth*)
Yajima, I. *et al., Agric. Biol. Chem.*, 1984, **48**, 849 (*Z-form, isol, synth, ir, pmr, ms*)
Kaiser, R. *et al., J. Essent. Oil Res.*, 1991, **3**, 129 (*Z-form, isol*)
Aiello, A. *et al., J. Nat. Prod.*, 2000, **63**, 1590-1592 (*isol, sulfate*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1359 (*use*)

7-Octen-2-ol, 9CI O-104

[39546-75-3]

[211695-55-5]

$C_8H_{16}O$ 128.214

(*S*)-*form* [129234-94-2]
Liq. $[\alpha]_D^{20}$ +11.2 (c, 4.3 in Me_2CO).

(±)-*form*
Oil. Bp_{64} 83-85°. n_D^{21} 1.4380.

(ξ)-*form*
Present in goat's cheese.

Sumitani, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 1511-1515 (*synth, pmr*)
Mori, K. *et al., Annalen*, 1992, 1011-1017 (*synth, pmr*)
Buchin, S. *et al., Lait*, 1998, **78**, 673-687 (*detn, cheese*)
Fuerstner, A. *et al., Tetrahedron*, 1999, **55**, 8215-8230 (*S-form, synth, pmr, cmr, ms*)

1-Octen-3-one, 9CI O-105

[4312-99-6]
FEMA 3515

$H_3C(CH_2)_4COCH{=}CH_2$

$C_8H_{14}O$ 126.198
Mushroom flavour component (shiitake, matsutake). Also present in cranberry, melon, cape gooseberry, peas, potato, mustards, wheat bread, other breads, coriander seed, dill basil varieties and soybean. Contributes to aroma of cooked artichokes (*Cynara scolymus*) and many other foods. Bp_{14} 63-65°.

2,4-Dinitrophenylhydrazone: [92325-46-7]
Mp 124°.

Sasson, Y. *et al., Can. J. Chem.*, 1974, **52**, 3825 (*synth*)
Grieco, P.A. *et al., Chem. Comm.*, 1974, 497 (*synth*)
Pyysalo, H. *et al., Acta Chem. Scand., Ser. B*, 1976, **30**, 235 (*isol*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1978, **26**, 791-793 (*isol*)
Marczak, S. *et al., Synth. Commun.*, 1990, **20**, 1511 (*synth*)
Venturello, C. *et al., J.O.C.*, 1991, **56**, 5924 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 619 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2021 (*rev*)
Cha, Y.-J. *et al., CA*, 1998, **130**, 310820q (*isol*)
Mau, J.-L. *et al., J. Agric. Food Chem.*, 1998, **46**, 4587-4591 (*isol*)

2-Octen-4-one, 9CI O-106

[4643-27-0]
FEMA 3603

$H_3C(CH_2)_3COCH{=}CHCH_3$

$C_8H_{14}O$ 126.198
Flavouring ingredient. Present in roasted hazelnut and white bread.

(*E*)-*form* [22286-99-3]
Bp_{740} 178°.

2,4-Dinitrophenylhydrazone:
Orange needles (EtOH). Mp 108-109°.

Stutsman, P.S. *et al., J.A.C.S.*, 1939, **61**, 3303 (*synth*)
Dauben, W.G. *et al., J.O.C.*, 1970, **35**, 374 (*synth, spectra*)
Engel, P.S. *et al., J.A.C.S.*, 1976, **98**, 2683 (*synth*)
Claude, L.R. *et al., Tet. Lett.*, 1978, 1137 (*synth*)
Nakai, T. *et al., Tet. Lett.*, 1978, 2895 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 620
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2021-2022

3-Octen-2-one O-107

[1669-44-9]
FEMA 3416

$H_3C(CH_2)_3CH{=}CHCOCH_3$

$C_8H_{14}O$ 126.198
Vanilla volatile, mushroom flavour component of *Boletus edulis* (porcini). Also present in asparagus, baked or French fried potato, raw lean fish, chicken fat, white wine, roasted filbert, coriander seed and rice. Flavouring ingredient.

(*E*)-*form* [18402-82-9]
Oil. Bp_{50} 100°.

2,4-Dinitrophenylhydrazone:
Mp 93°.

(*Z*)-*form* [51193-77-2]
Oil. Bp_{50} 68-69°.

2,4-Dinitrophenylhydrazone:
Mp 93°.

Heilman, R. *et al., Bull. Soc. Chim. Fr.*, 1957, 119 (*synth, uv, ir*)
Clinet, J.C. *et al., Tet. Lett.*, 1978, 1137 (*synth*)
Beak, P. *et al., J.A.C.S.*, 1980, **102**, 3848 (*synth*)

Grayson, D.H. *et al., J.C.S. Perkin 1*, 1986, 2137 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 619 (*rev*)
Barbero, A. *et al., J.C.S. Perkin 1*, 1995, 1525 (*synth, ir, pmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, (*rev*)

5-Octen-2-one O-108

[36359-70-3]

$H_3CCH_2CH{=}CHCH_2CH_2COCH_3$

$C_8H_{14}O$ 126.198

Isol. from bergamot orange (*Citrus bergamia*) and black tea.

(*E*)-*form* [19093-20-0]

Bp 169-173° Bp_{11} 59-61.5°.

Semicarbazone:

Cryst. (petrol). Mp 62.5-63.5°.

2,4-Dinitrophenylhydrazone:

Mp 65.5-66°.

(*Z*)-*form* [22610-86-2]

Bp_{20} 68-70° Bp_{10} 54-57°.

Semicarbazone:

Leaflets (EtOH aq.). Mp 114-114.5°.

2,4-Dinitrophenylhydrazone:

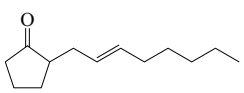
Plates (EtOH aq.). Mp 67.5°.

Crombie, L. *et al., J.C.S.*, 1952, 869 (*synth*)
Harper, S.H. *et al., J.C.S.*, 1955, 1512 (*synth*)
Sundt, E. *et al., Helv. Chim. Acta*, 1964, **47**, 408 (*isol, pmr, ms*)
Crombie, L. *et al., J.C.S.(C)*, 1969, 1016 (*synth, ir, pmr*)
Ballini, R. *et al., Synthesis*, 1986, 849 (*synth, ir, pmr*)
McKenzie, T.C. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 435 (*synth*)

2-(2-Octenyl)cyclopentanone O-109

[65737-52-2]

[98314-99-9]



(*E*)-*form*

$C_{13}H_{22}O$ 194.316

(*E*)-*form* [98314-98-8]

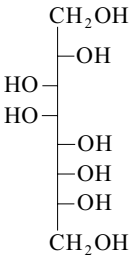
FEMA 3889

Flavouring ingredient. Liq. with peach-like odour and a hint of jasmine. d^{20} 0.9. Bp_2 85°.

Luo, F.-T. *et al., Tet. Lett.*, 1985, **26**, 2177-2180 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1358-1359 (*use*)

D-*erythro*-D-*galacto*-Octitol, 8CI O-110

[27655-86-3]



$C_8H_{18}O_8$ 242.225

Isol. from avocado. Cryst. (EtOH aq.). Mp 170-171°. $[\alpha]_D^{20}$ -12 (c, 0.4 in 5% ammonium molybdate) (monohydrate).

Octa-Ac:

$C_{24}H_{34}O_{16}$ 578.523

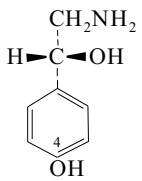
Mp 99-100°. $[\alpha]_D^{20}$ +1 (c, 1.0 in $CHCl_3$).

Charlson, A.J. *et al., J.A.C.S.*, 1960, **82**, 3428 (*isol, synth, octa-Ac*)
Brimacombe, J.S. *et al., J.C.S. Perkin 1*, 1986, 815 (*synth*)

Octopamine, INN O-111

[104-14-3]

*α-(Aminomethyl)-4-hydroxybenzenemethanol, 9CI. α-(Aminomethyl)-*p*-hydroxybenzyl alcohol, 8CI. 2-Amino-1-(4-hydroxyphenyl)ethanol.* p-*(β-Amino-α-hydroxyethyl)phenol. Norsympathol. Norsynephrine. Noroxedrine. Many other names*



(*R*)-*form*

$C_8H_{11}NO_2$ 153.18

► LD_{50} (rat, orl) 1240 mg/kg. LD_{50} (mus, ipr) 600 mg/kg. DN7350000

(*R*)-*form* [876-04-0]

Alkaloid from leaves of tabasco pepper (*Capsicum frutescens*), nutgrass (*Cyperus rotundus*) and leaves or fruit of *Citrus* spp. Occurs in many animal tissues; found in high concs. in octopus. Cryst. (H_2O). Mp 160° approx. $[\alpha]_D^{25}$ -37.4 (c, 1 in H_2O). $[\alpha]_D$ -56 (c, 1 in 1*M* HCl).

(ξ)-*form*

N-*(*E*-Cinnamoyl):* [87596-52-9] N-*[2-Hydroxy-2-(4-hydroxyphenyl)ethyl]-3-phenyl-2-propenamide.* **N-*[2-Hydroxy-2-(4-hydroxyphenyl)ethyl]cinnamide.*** N-*Cinnamoyl-2,4′-dihydroxyphenethylamine.* N-*Cinnamoyloctopamine*

$C_{17}H_{17}NO_3$ 283.326

Alkaloid from the leaves of *Aegle marmelos* (bael). Needles (MeOH). Mp 158° (solidifies and remelts at 228-231°).

N-*(4-Hydroxy-*E*-cinnamoyl):* [66648-45-1]

[88700-34-9, 152433-78-8] **N-trans-p-*Coumaroyloctopamine***

$C_{17}H_{17}NO_4$ 299.326

Alkaloid from roots of bell pepper (*Capsicum annuum* var. *grossum*). Cryst. Mp 214-215°.

N-*(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* [66648-44-0] **N-trans-*Feruloyloctopamine***

$C_{18}H_{19}NO_5$ 329.352

Constit. of roots of bell pepper (*Capsicum annuum* var. *grossum*). Powder. Mp 164-165° (as tri-Ac).

4-O-*(3-Methyl-2-butenyl),* N-*cinnamoyl:* [81532-00-5] N-*[2-Hydroxy-2-[4-[(3-methyl-2-butenyl)oxy]phenyl]ethyl]-3-phenyl-2-propenamide.* N-*2-Hydroxy-2-[4-(3,3-dimethylallyloxy)phenyl]ethylcinnamide.* ***Marmeline.*** N-*Cinnamoyl*-O-*prenyloctopamine*

$C_{22}H_{25}NO_3$ 351.444

Alkaloid from the leaves and unripe fruits of *Aegle marmelos* (bael). Needles (MeOH or $CHCl_3$/hexane). Mp 159-161° (156-157°).

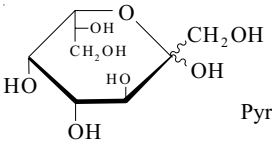
4-O-*(3-Methyl-2-butenyl), β-Me ether,* N-*(*E*-cinnamoyl):* [70546-92-8] Aegle marmelos *Alkaloid C*

$C_{23}H_{27}NO_3$ 365.471

Alkaloid from leaves of *Aegle marmelos* (bael). Cryst. (C_6H_6/hexane). Mp 110°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1290D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 613B (*nmr*)
Bretschneider, H. *et al., Monatsh. Chem.*, 1949, **80**, 530 (*resoln*)
Corrigan, J.R. *et al., J.A.C.S.*, 1953, **75**, 6258 (*synth*)
Ascher, M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **84**, 1021 (*synth*)
Kappe, T. *et al., J. Med. Chem.*, 1964, **7**, 569 (*resoln*)
Hardwick, B.C. *et al., Plant Physiol.*, 1969, **44**, 1745 (*ir, uv*)
Wheaton, T.A. *et al., Lloydia*, 1970, **33**, 244-254 (*occur*)
Hengstmann, J.H. *et al., Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1974, **283**, 93 (*metab*)
Paxton, K. *et al., Acta Cryst. B*, 1977, **33**, 2143 (*cryst struct*)
Axelrod, J. *et al., Nature (London)*, 1977, **265**, 501 (*rev*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*occur*)
Manandhar, M.D. *et al., Phytochemistry*, 1978, **17**, 1814 (*Aegle marmelos Alkaloid C*)
Yoshihara, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 2593-2598 (*cinnamoyl derivs*)
Sharma, B.R. *et al., Phytochemistry*, 1981, **20**, 2606 (*Marmeline*)
Govindachari, T.R. *et al., Phytochemistry*, 1983, **22**, 755 (*N-cinnamoyl*)
Redouane, K. *et al., Agressologie*, 1984, **25**, 3 (*rev*)
Midgley, J.M. *et al., J.C.S. Perkin 2*, 1989, 963-964 (*cryst struct, abs config, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1250
Matsuda, F. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 625-627 (*N-Coumaroyloctopamine*)
Lee, C. *et al., J. Nat. Prod.*, 2001, **64**, 659-660 (*N-Feruloyl-O-methyloctopamine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKT250

D-*glycero*-L-*galacto*-Octulose O-112



Pyranose-*form*

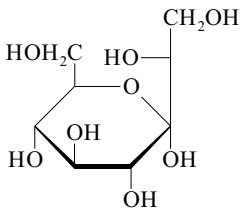
$C_8H_{16}O_8$ 240.21
Present in ripe avocados. $[\alpha]_D^{20}$ -57 (c, 2 in H_2O).

2,5-Dichlorophenylhydrazone:
Mp 178-180°.

Sephton, H.H. *et al., J.O.C.*, 1963, **28**, 1691 (*occur, synth*)
Sephton, H.H. *et al., Carbohydr. Res.*, 1966, **2**, 289 (*occur, synth*)
Schaffer, R. *et al., The Carbohydrates*, Academic Press, 1972, 69 (*rev*)

D-*glycero*-D-*ido*-3-Octulose O-113

[78174-72-8]
D-gluco-L-glycero-*3-Octulose*



$C_8H_{16}O_8$ 240.21
First reported naturally occurring 3-octulose. Main constit. in aq. extracts of *Laurus nobilis* leaves (bay laurel) and buds.

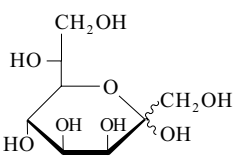
α-form
Cryst. (MeOH). Mp 173-176°. $[\alpha]_D$ +66 (c, 1.0 in H_2O) (+55.7).

Hepta-Ac:
$C_{22}H_{30}O_{15}$ 534.47
Mp 128-131°. $[\alpha]_D$ +69 (c, 0.41 in $CHCl_3$).

Schaffer, R. *et al., J.O.C.*, 1963, **28**, 1929
Westelund, E. *et al., Carbohydr. Res.*, 1981, **91**, 21 (*synth, ms, cmr*)
Sakata, K. *et al., Agric. Biol. Chem.*, 1989, **53**, 2539 (*isol, cmr, ms*)

D-*glycero*-D-*manno*-Octulose, 8CI O-114

[13111-79-0]



Pyranose-*form*

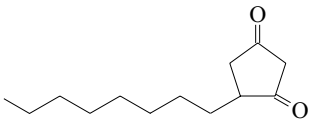
$C_8H_{16}O_8$ 240.21
Present in avocado (*Persea gratissima*), alfalfa (*Medicago sativa*), roots of opium poppy (*Papaver somniferum*). $[\alpha]_D^{20}$ +20 (c, 1.1 in MeOH).

2,5-Dichlorophenylhydrazone:
Mp 169-170°.

Charlson, A.J. *et al., J.A.C.S.*, 1960, **82**, 3428 (*occur*)
Haustveit, G. *et al., Acta Chem. Scand.*, 1970, **24**, 3059 (*occur*)

4-Octyl-1,3-cyclopentanedione, 9CI O-115

[126624-26-8]
Tsibulin 1



$C_{13}H_{22}O_2$ 210.316
Phytoalexin from onion (*Allium cepa*) bulbs. Pale-yellow oil. λ_{max} 207 ; 220 ; 246 (EtOH) (Berdy).

Tverskoy, L. *et al., Phytochemistry*, 1991, **30**, 799 (*isol*)

2-Octynoic acid, 9CI O-116

[5663-96-7]
1-Heptyne-1-carboxylic acid
$H_3C(CH_2)_4C{\equiv}CCOOH$
$C_8H_{12}O_2$ 140.182
Liq. d_4^{13} 0.96. Fp 2-5. Bp 180-220° dec. Bp_{19} 148-149°. n_D^{20} 1.4595.
▶ RI2725000

Me ester: [111-12-6] *Methyl 2-octynoate. Methyl heptyne carbonate. FEMA 2729*
$C_9H_{14}O_2$ 154.208
Flavouring ingredient. Liq. with violet odour. Bp_{20} 107° Bp_{10} 94°. n_D^{20} 1.4464.
▶ RI2735000

Et ester: [10519-20-7]
$C_{10}H_{16}O_2$ 168.235
$Bp_{0.2}$ 51-52°.

Chloride:
$C_8H_{11}ClO$ 158.627
Bp_{17} 88-90°.

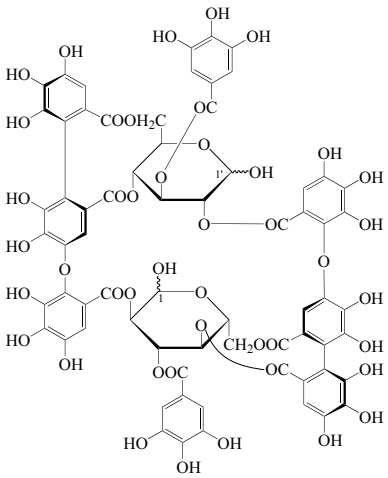
Amide:
$C_8H_{13}NO$ 139.197
Plates (EtOH). Mp 91°.

Nitrile:1-Cyanoheptyne
$C_8H_{11}N$ 121.182
Bp 194-196° Bp_{13} 80-81°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 943B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 525B; 527C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1596D (*ir*)
Zoss, A.O. *et al., J.A.C.S.*, 1941, **63**, 1152 (*synth*)
Nametkin, I.S.S. *et al., CA*, 1942, **36**, 3783 (*synth*)
Newman, M.S. *et al., J.A.C.S.*, 1949, **71**, 1292 (*synth*)
Wotiz, J.H. *et al., J.A.C.S.*, 1949, **71**, 3441 (*ir*)
Bohlmann, F. *et al., Chem. Ber.*, 1967, **100**, 3706 (*ms*)
Gershon, H. *et al., Can. J. Microbiol.*, 1978, **24**, 593 (*use*)
Sprecher, H. *et al., Prog. Chem. Fats Other Lipids*, 1978, **15**, 219 (*rev*)
Wuts, P.G.M. *et al., J.O.C.*, 1989, **53**, 5989 (*Me ester, synth, pmr, cmr, ir*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1992, 1929 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 536
Hutzinger, M.W. *et al., J.O.C.*, 1995, **60**, 4595 (*Me ester, synth, ir, pmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1816
Fortes, C.C. *et al., Synth. Commun.*, 1997, **27**, 2993-3026 (*synth, Me ester, ir, pmr, cmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MND275

Oenothein B O-117

[104987-36-2]



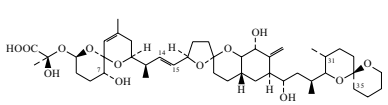
$C_{68}H_{48}O_{44}$ 1569.101
Exists as an equilibrated mixt. of α- and β-anomers.Amorph. powder. $[\alpha]_D$ +179 (c, 1 in MeOH). λ_{max} 208 (ϵ 59000); 218 (ϵ 120000) (MeOH) (Berdy).

1-O-(3,4,5-Trihydroxybenzoyl)(1β-):
[189302-95-2] ***Eugeniflorin D_1***
$C_{75}H_{52}O_{48}$ 1721.207
Constit. of *Eugenia uniflora* (Surinam cherry). Light-brown powder + $6H_2O$. $[\alpha]_D$ +28 (c, 1 in MeOH). λ_{max} 218 (log ϵ 5.16); 268 (log ϵ 4.8) (MeOH).

Miyamoto, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 814 (*pharmacol*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2269 (*struct, pmr*)
Hatano, T. *et al., J.C.S. Perkin 1*, 1990, 2735 (*isol, pmr, cmr*)
Miyamoto, K. *et al., Jpn. J. Cancer Res.*, 1993, **84**, 99 (*pharmacol*)
Lee, M.-H. *et al., Phytochemistry*, 1997, **44**, 1343-1349 (*Eugeniflorin D_1*)
Santos, S.C. *et al., Fitoterapia*, 2001, **72**, 95-97 (*isol, pmr, cmr*)

Okadaic acid O-118

[78111-17-8]
9,10-Deepithio-9,10-didehydroacanthifolicin. PL toxin II



$C_{44}H_{68}O_{13}$ 805.013
Found in the marine sponges *Halichondria okadai* and *Halichondria melanodocia* and shellfish. Metab. of *Prorocentrum lima*. Diarrhetic shellfish toxin. Cryst. (C_6H_6/$CHCl_3$). Sol. MeOH, hexane; poorly sol.

H_2O, hexane. Mp 164-166°. $[\alpha]_D^{20}$ +53.3 (c, 0.182 in $CHCl_3$).

► LD_{50} (mus, ivn) .192 mg/kg. AA8227800

Me ester:
Cryst. (hexane/C_6H_6). Mp 127-133°. $[\alpha]_D^{25}$ +28 (c, 0.38 in $CHCl_3$).

p-*Bromophenacyl ester:*
Mp 134-135°.

(4-Formyl-2-methylene-4-pentenyl) ester: ***DTX6***
$C_{51}H_{76}O_{14}$ 913.153
Amorph. powder. $[\alpha]_D^{25}$ +3.3 (c, 0.1 in $CHCl_3$). λ_{max} 242 ; 270 (EtOH).

*6-Hydroxy-2-methyl-2*E,*4*E*-hexadienyl ester:* [145781-81-3]
$C_{51}H_{78}O_{14}$ 915.169

*7-Hydroxy-2-methyl-2*E,*4*E*-heptadienyl ester:* [145814-30-8]
$C_{52}H_{80}O_{14}$ 929.196

*7-Hydroxy-2,4-dimethyl-2*E,*4*E*-heptadienyl ester:* [157376-74-4]
$C_{53}H_{82}O_{14}$ 943.222
Amorph. powder. $[\alpha]_D$ +21.4 (c, 0.5 in $CHCl_3$). λ_{max} 264 (ϵ 14822) (EtOH) (Berdy).

*7-Hydroxy-4-methyl-2-methylene-4*E*-heptenyl ester:* [145814-31-9]
$C_{53}H_{82}O_{14}$ 943.222
Amorph. powder. $[\alpha]_D$ +17.3 (c, 0.1 in $CHCl_3$). λ_{max} 263 (EtOH) (Berdy).

Glycine amide: [123764-98-7] ***Glycookadaic acid***
$C_{46}H_{71}NO_{14}$ 862.065

Tetra-Ac:
$[\alpha]_D^{20}$ +153 (c, 1.4 in $CHCl_3$).

7-Deoxy: [136993-62-9] ***7-Deoxyokadaic acid***
$C_{44}H_{68}O_{12}$ 789.014
Cryst.

*35*R-*Methyl:* [81720-10-7] ***Dinophysistoxin 1***. *DTX1*
$C_{45}H_{70}O_{13}$ 819.04
Metab. of *Dinophysis fortii*. Found in scallops and mussels. Component toxin in diarrhetic shellfish poisoning. Solid. Sol. MeOH, C_6H_6; poorly sol. hexane. Mp 134°. $[\alpha]_D^{20}$ +28.

► LD_{99} 100 µg/kg (i.p. mice).

*35*R-*Methyl, 14,15-dihydro:* ***14,15-Dihydrodinophysistoxin 1***
$C_{45}H_{72}O_{13}$ 821.056
Amorph. solid. $[\alpha]_D^{25}$ +19 (c, 0.4 in $CHCl_3$).

*35*S-*Methyl, 7*-O-*acyl:* ***Dinophysistoxin 3***. *DTX3*
Metab. of *Dinophysis acuminata*. Found in scallops and mussels. Component toxin of diarrhetic shellfish poisoning. Solid. Contains 13% C_{14}, 29% C_{16}, 12% C_{18}, 23% C_{20} and 23% C_{22} fatty acids.

► LD_{50} (mus, ipr) 800 mg/kg.

*35*S-*Methyl, 7*-O-*hexadecanoyl:*
$C_{61}H_{100}O_{14}$ 1057.453
Formed from Dinophysistotoxin 3 on standing. Solid. Mp 78°. $[\alpha]_D^{20}$ +5.9 (c, 0.041 in $CHCl_3$).

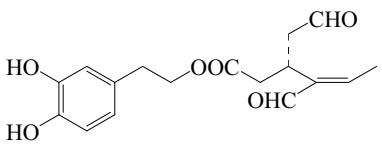
*35*R-*Methyl, 31-methyl:* ***Dinophysistoxin 2***. *DTX2*
$C_{44}H_{68}O_{13}$ 805.013
Metab. of *Dinophysis* spp.. Amorph. solid. Mp 128-130°. $[\alpha]_D$ +15.49 (c, 0.213 in $CHCl_3$).

Tachibana, K. *et al., J.A.C.S.*, 1981, **103**, 2469 (*isol, cryst struct, spectra*)
Japan. Pat., 1982, 82 11 986; *CA*, **96**, 217820
Murakami, W. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 69; *CA*, **96**, 139; 380 (*isol*)
Muraka, W. *et al., Nippon Suisan Gakkaishi*, 1982, **48**, 549; *CA*, **97**, 52852 (*deriv*)
Yasumoto, T. *et al., Tetrahedron*, 1985, **41**, 1019 (*deriv*)
Ichikawa, Y. *et al., Tetrahedron*, 1987, **43**, 4737; 4742; 4749; 4759 (*synth*)
Nagai, H. *et al., J. Appl. Phycol.*, 1990, **2**, 305-308 (*7-Deoxyokadaic acid*)
Norte, M. *et al., Tetrahedron*, 1991, **47**, 7437; 1994, **50**, 9175 (*pmr, cmr, esters*)
Hu, T. *et al., Chem. Comm.*, 1992, 39 (*Dinophysistoxin 2*)
Hu, T. *et al., J. Nat. Prod.*, 1992, **55**, 1631 (*esters*)
Norte, M. *et al., Tet. Lett.*, 1994, **35**, 1441 (*Dinophysistoxin 1*)
Sakai, R. *et al., J. Nat. Prod.*, 1995, **58**, 773 (*Dihydrodinophysistoxin 1*)
Matsumori, N. *et al., Tetrahedron*, 1995, **51**, 12229 (*nmr, conformn*)
Forsyth, C.J. *et al., J.A.C.S.*, 1997, **119**, 8381-8382 (*synth*)
Urbanek, R.A. *et al., J.A.C.S.*, 1998, **120**, 2523-2533; 2534-2542 (*synth*)
Ley, S.V. *et al., J.C.S. Perkin 1*, 1998, 3907-3911 (*synth*)
Perry, N.B. *et al., Nat. Prod. Lett.*, 1998, **11**, 305-312 (*Glycookadaic acid*)
Leftley, J.W. *et al., Natural Toxicants in Food*, (ed. Watson, D.H.), CRC Press, 1998, 182-224 (*rev*)
Suarez-Gomez, B. *et al., J. Nat. Prod.*, 2001, **64**, 1363-1364 (*DTX6*)

Oleacein O-119

[149183-75-5]

[151194-90-0]
2-(3,4-Dihydroxyphenyl)ethyl 4-formyl-3-formylmethyl-4-hexenoate. 3,4-DHPEA-EDA



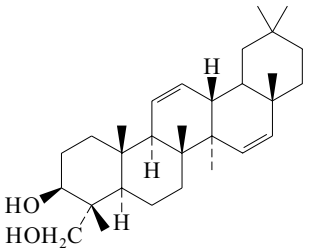
$C_{17}H_{20}O_6$ 320.341
Secoiridoid. Constit. of *Olea europaea* (olive). Also from *Jasminum grandiflorum* (Royal jasmine). Amorph. powder. $[\alpha]_D^{25}$ +6.5.

3′-Deoxy: [289030-99-5]

[151194-92-2] ***3′-Deoxyoleacein***. *4-HPEA-EDA*
$C_{17}H_{20}O_5$ 304.342
Constit. of *Olea europaea* (olive).

Montedoro, G. *et al., J. Agric. Food Chem.*, 1993, **41**, 2228-2234 (*isol*)
Lo Scalzo, R. *et al., J. Nat. Prod.*, 1993, **56**, 621-623 (*isol, pmr*)
Hansen, K. *et al., Phytomedicine*, 1996, **2**, 319-325 (*isol, activity*)
Somanaldhan, B. *et al., Planta Med.*, 1998, **64**, 246-250 (*isol*)
Paiva-Martins, F. *et al., J. Agric. Food Chem.*, 2001, **49**, 4214-4219 (*isol*)

12,15-Oleanadiene-3,23-diol O-120



$C_{30}H_{48}O_2$ 440.708

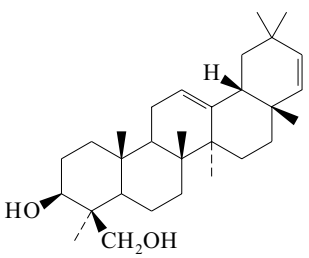
3β-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→6)[α-D-galactopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-α-D-galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-β-D-glucuronoside]:* [30937-16-7] ***Phaseoloside D***
$C_{65}H_{104}O_{31}$ 1381.518
Isol. from *Phaseolus vulgaris* (kidney bean).

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-α-D-galactopyranosyl-(1→2)[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranosyl-(1→4)-α-D-galactopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-β-D-glucuronoside]:* [30915-09-4] ***Phaseoloside E***
$C_{77}H_{124}O_{41}$ 1705.802
Isol. from *Phaseolus vulgaris* (kidney bean).

Chirva, V.Y. *et al., Khim. Prir. Soedin.*, 1970, **6**, 377; 559; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 386; 575 (*isol, struct*)
Lazur'evskii, G.V. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1971, **199**, 226; *CA*, **75**, 115903 (*struct*)

12,21-Oleanadiene-3,24-diol O-121

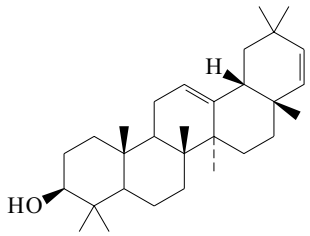


$C_{30}H_{48}O_2$ 440.708

3β-*form* [595-14-2]
Soyasapogenol C. *Soyasapogenol M_1. Sapogenol C*
Constit. of soya bean saponin, green gram (*Phaseolus radiatus*), *Trifolium repens* (white clover) and other plants.. Cryst. (MeOH). Mp 238-239°. $[\alpha]_D^{21}$ +70.7 ($CHCl_3$).

Cainelli, G. *et al., Helv. Chim. Acta*, 1958, **41**, 2053 (*struct*)
Smith, H.M. *et al., Tetrahedron*, 1958, **4**, 111 (*struct*)
McLean, J. *et al., Phytochemistry*, 1963, **2**, 179 (*isol*)
Nes, W.D. *et al., Phytochemistry*, 1981, **20**, 2299 (*cmr*)

12,21-Oleanadien-3-ol O-122

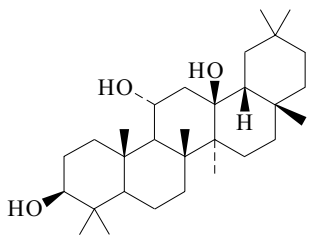


$C_{30}H_{48}O$ 424.709

3β-*form* [86425-22-1]
Anhydrosophoradiol
Isol. from azuki bean (*Vigna angularis*) seeds. Needles ($CHCl_3$/MeOH). Mp 180-181°. $[\alpha]_D^{13}$ +54.8 (c, 0.7 in $CHCl_3$). Artifact.

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 664 (*isol*)

3,11,13-Oleananetriol O-123



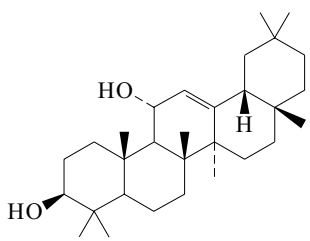
$C_{30}H_{52}O_3$ 460.739

(3β,11α,13β)-*form* [85643-69-2]
Constit. of *Pistacia vera* (pistachio). Cryst. (hexane). Mp 208-210°. $[\alpha]_D$ +5.5 (c, 1.1 in $CHCl_3$).

[85643-70-5, 85643-71-6, 85643-72-7]

Monaco, P. *et al., Phytochemistry*, 1982, **21**, 2408

12-Oleanene-3,11-diol O-124



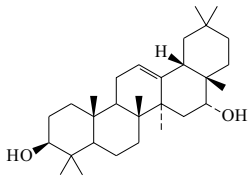
$C_{30}H_{50}O_2$ 442.724

(3β,11α)-*form* [5282-14-4]
Cryst. (MeOH). Mp 227-230°.

11-Me ether: [268541-26-0] *11-Methoxy-12-oleanen-3-ol.* ***Triptohypol F***
$C_{31}H_{52}O_2$ 456.751
Constit. of *Myroxylon balsamum* (Tolu balsam). Cryst. ($CHCl_3$). Mp 172-173°. $[\alpha]_D$ +12.4 (c, 0.73 in CH_2Cl_2).

Mathias, L. *et al., J. Braz. Chem. Soc.*, 2000, **11**, 195-198; *CA*, **133**, 102002 (*11-Me ether*)
Fujita, R. *et al., Phytochemistry*, 2000, **53**, 715-722 (*Triptohypol F*)

12-Oleanene-3,16-diol O-125



(3β,16α)-*form*

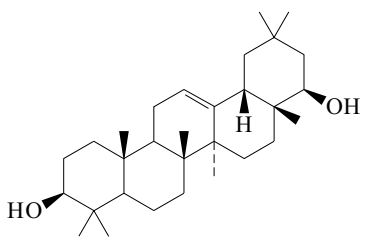
$C_{30}H_{50}O_2$ 442.724

(3β,16β)-*form* [595-17-5]
Maniladiol
Constit. of *Calendula officinalis* (pot marigold). Cryst. (MeOH aq.). Poorly sol. hexane. Mp 220-221°. $[\alpha]_D^{19}$ +68 ($CHCl_3$).

(3α,16β)-*form* [122564-89-0]
Constit. of *Canarium album* (Chinese white olive). Cryst. Mp 290-292°. $[\alpha]_D^{23}$ +51 (c, 1 in $CHCl_3$).

Djerassi, C. *et al., J.A.C.S.*, 1953, **75**, 5940-5942; 1956, **78**, 2312-2315; 1957, **79**, 3525 (*Maniladiol, struct, isol*)
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 2465-2490 (*Maniladiol*)
Arriaga-Giner, F.J. *et al., Phytochemistry*, 1986, **25**, 719-721 (*Maniladiol, isol*)
Guang-Yi, L. *et al., Phytochemistry*, 1988, **27**, 2283-2286 (*Maniladiol, cmr*)
Tamai, M. *et al., Planta Med.*, 1989, **55**, 44-47 (*3α,16β-form*)
Nkengfack, A.E. *et al., J. Nat. Prod.*, 1990, **53**, 1552-1556 (*Maniladiol, cmr*)
Quijano, L. *et al., Phytochemistry*, 1998, **49**, 2065-2068 (*Maniladiol, cryst struct*)

12-Oleanene-3,22-diol O-126



$C_{30}H_{50}O_2$ 442.724

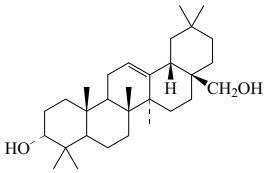
(3β,22β)-*form* [6822-47-5]
Sophoradiol
Needles. Poorly sol. hexane. Mp 219-220°. $[\alpha]_D$ +113.

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucuronopyranoside]: [82793-02-0] ***Azukisaponin I***
$C_{42}H_{68}O_{13}$ 780.991
Isol. from seeds of *Vigna angularis* (azuki bean). Cryst. (EtOH). Mp 215-217°. $[\alpha]_D^{28}$ +16 (c, 0.3 in MeOH).

[86500-79-0, 86500-80-3]

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2294; 1983, **31**, 674 (*Azukisaponin I, isol, struct*)

12-Oleanene-3,28-diol O-127



3α-*form*

$C_{30}H_{50}O_2$ 442.724

3β-*form* [545-48-2]
Erythrodiol. *Homoolestranol*
Found in grapes, olives, pot marigold (*Calendula officinalis*) and other plants. Needles (Me_2CO). Mp 235-237°. $[\alpha]_D$ +77.

3-Decanoyl: [36286-67-6] *Erythrodiol 3-decanoate*
$C_{40}H_{68}O_3$ 596.975
Isol. from leaves of the famine food *Madhuca longifolia*. Mp 152°.

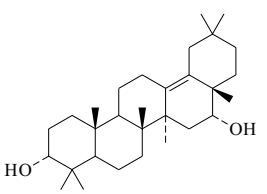
3-Hexadecanoyl: [19833-13-7] *Erythrodiol 3-palmitate*
$C_{46}H_{80}O_3$ 681.136
Isol. from the famine food *Madhuca longifolia*. Cryst. (Me_2CO). Mp 121-123°.

28-Aldehyde: [17020-22-3] *3β-Hydroxy-12-oleanen-28-al.* ***Oleanolic aldehyde***
$C_{30}H_{48}O_2$ 440.708
Found in grapes and olives. Cryst. Mp 168-172°. $[\alpha]_D$ +72.

[52801-09-9, 55869-95-9]

Shamma, M. *et al., J.O.C.*, 1959, **24**, 726; 1962, **27**, 4512 (*isol, pmr*)
Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688 (*ms*)
Eyton, W.B. *et al., Tetrahedron*, 1965, **21**, 2697 (*pmr*)
Savoir, R. *et al., Bull. Soc. Chim. Belg.*, 1967, **76**, 335 (*pmr*)
Kasprzyk, Z. *et al., Phytochemistry*, 1969, **8**, 1921 (*biosynth*)
Ito, S. *et al., Tet. Lett.*, 1969, 2905 (*pmr*)
Yosioka, I. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1186 (*deriv*)
Bhatnagar, S.C. *et al., Phytochemistry*, 1972, **11**, 465; 1533 (*decanoate, hexadecanoate*)
Monaco, P. *et al., Phytochemistry*, 1974, **13**, 1992 (*Oleanolic aldehyde*)
Doddrell, D.M. *et al., Tet. Lett.*, 1974, 2381 (*cmr*)
Nakano, T. *et al., Planta Med.*, 1975, **27**, 89 (*hexadecanoate*)
Nes, W.D. *et al., Phytochemistry*, 1981, **20**, 2299 (*cmr, abs config*)
Corey, E.J. *et al., J.A.C.S.*, 1993, **115**, 8871 (*synth*)
Kamiya, K. *et al., Phytochemistry*, 1997, **44**, 141 (*Oleanolic aldehyde, pmr, cmr*)

13(18)-Oleanene-3,16-diol O-128



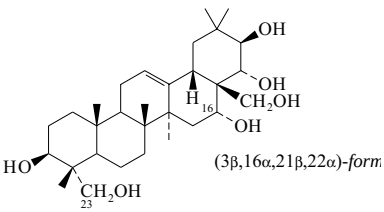
(3α,16α)-*form*

$C_{30}H_{50}O_2$ 442.724

(3α,16α)-*form*
Constit. of *Canarium album* (Chinese white olive). Cryst. Mp 290-292°. $[\alpha]_D^{23}$ +51 (c, 1 in $CHCl_3$).

(3β,16β)-*form* [37384-13-7]
Coflodiol. *Ursadiol (obsol.)*†
Isol. from *Calendula officinalis* (pot marigold). Cryst. Mp 240-242°. $[\alpha]_D^{25}$ -48 (c, 0.2 in $CHCl_3$). Formerly thought to be an ursane.
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1977, **51**, 2493
Tamai, M. *et al., Planta Med.*, 1989, **55**, 44 (*isol*)

12-Oleanene-3,16,21,22,23,28-hexol O-129



(3β,16α,21β,22α)-*form*

$C_{30}H_{50}O_6$ 506.721

(3β,16α,21β,22α)-*form* [13844-22-9]
Theasapogenol A
Sapogenol isol. from seeds of china tea and other plants. May or may not be present in the leaves. Found together with various acylated derivs. and their glucosides for which refs. are given. Mp 301-303°. $[\alpha]_D$ +14 (c, 0.51 in Py).

*21-Angeloyl, 22-Ac, 3-*O*-[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]:* [259748-69-1] ***Assamsaponin D***
$C_{59}H_{92}O_{27}$ 1233.36
Constit. of Assam tea (*Camellia sinensis* var. *assamica*) seeds. Cryst. ($CHCl_3$/MeOH). Mp 190.6-191.2°. $[\alpha]_D^{26}$ +15.6 (c, 0.1 in MeOH).

22-Angeloyl: [200492-44-0]
$C_{35}H_{56}O_7$ 588.823
Constit. of Assam tea (*Camellia sinensis* var. *assamica*) seeds. Cryst. Mp 202-204°.

23-Aldehyde: [15399-41-4]
3β,16α,21β,22α,28-Pentahydroxy-12-oleanen-23-al. ***Theasapogenol E***. *Camelliagenin E*
$C_{30}H_{48}O_6$ 504.706
Sapogenin from seeds of China tea (*Thea sinensis*) and *Camellia sasanqua*. Cryst. Mp 270-273°. $[\alpha]_D$ +640 (Py).

23-Aldehyde, 22-angeloyl: [200492-42-8]
$C_{35}H_{54}O_7$ 586.807
Constit. of Assam tea (*Camellia sinensis* var. *assamica*). Cryst. Mp 186-189°.

*23-Aldehyde, 21-angeloyl, 22-Ac, 3-*O*-[β-D-galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]:* [220114-28-3] ***Theasaponin E1***
$C_{59}H_{90}O_{27}$ 1231.344
Constit. of Japanese tea (*Camellia sinensis*) seeds. Cryst. ($CHCl_3$/MeOH aq.). Mp 246-248°. $[\alpha]_D^{25}$ +8.9 (c, 1.1 in MeOH).

*23-Aldehyde, 21-angeloyl, 22-Ac, 3-*O*-[β-D-galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]:* [316157-16-1] ***Assamsaponin G***
$C_{60}H_{92}O_{28}$ 1261.37
Constit. of Assam tea (*Camellia sinensis* var. *assamica*) seeds. Cryst. ($CHCl_3$/MeOH). Mp 187.7-188.5°. $[\alpha]_D^{26}$ +14.9 (c, 0.1 in MeOH).

*23-Aldehyde, 21-angeloyl, 28-Ac, 3-*O*-[β-D-galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]:* [220114-30-7] ***Theasaponin E2***
$C_{59}H_{90}O_{27}$ 1231.344
Constit. of Japanese tea (*Camellia sinensis*) seeds. Cryst. ($CHCl_3$/MeOH aq.). Mp 240-242°. $[\alpha]_D^{25}$ +22.2 (c, 1.2 in MeOH).

*23-Aldehyde, 21-angeloyl, 28-Ac, 3-*O*-[β-D-galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]:* [316157-17-2] ***Assamsaponin H***
$C_{60}H_{92}O_{28}$ 1261.37
Constit. of Assam tea (*Camellia sinensis* var. *assamica*) seeds. Cryst. ($CHCl_3$/MeOH). Mp 206.3-207.6°. $[\alpha]_D^{26}$ +41 (c, 0.1 in MeOH).

*23-Aldehyde, 21-angeloyl, 16,22-di-Ac, 3-*O*-[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]:* [259748-07-7] ***Assamsaponin B***
$C_{61}H_{92}O_{28}$ 1273.381
Constit. of Assam tea (*Camellia sinensis* var. *assamica*). Cryst. ($CHCl_3$/MeOH). Mp 199-200°. $[\alpha]_D^{26}$ +21.6 (c, 0.1 in MeOH).

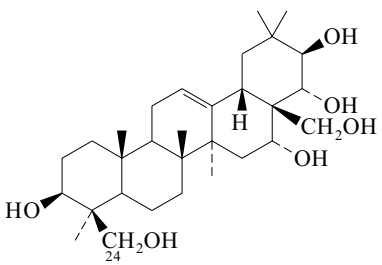
*23-Aldehyde, 21-angeloyl, 16,22-di-Ac, 3-*O*-[β-D-galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]:* [316157-15-0] ***Assamsaponin F***
$C_{62}H_{94}O_{29}$ 1303.407
Constit. of Assam tea (*Camellia sinensis* var. *assamica*) seeds. Cryst. ($CHCl_3$/MeOH). Mp 209.8-210.3°. $[\alpha]_D^{26}$ +8.8 (c, 0.1 in MeOH).

*23-Aldehyde, 21-tigloyl, 28-Ac, 3-*O*-[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]:* [259748-14-6] ***Assamsaponin C***
$C_{59}H_{90}O_{27}$ 1231.344
Constit. of Assam tea (*Camellia sinensis* var. *assamica*) seeds. Cryst. ($CHCl_3$/MeOH). Mp 201-202°. $[\alpha]_D^{28}$ +21 (c, 0.1 in MeOH).

*23-Aldehyde, 21-tigloyl, 28-Ac, 3-*O*-[β-D-galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]:* [316157-18-3] ***Assamsaponin I***
$C_{60}H_{92}O_{28}$ 1261.37
Constit. of Assam tea (*Camella sinensis* var. *assamica*) seeds. Cryst. ($CHCl_3$/MeOH). Mp 208.2-209.5°. $[\alpha]_D^{26}$ +35.6 (c, 0.1 in MeOH).

Yoshioka, I. *et al., Tet. Lett.*, 1966, 5979 (*Theasapogenol A*)
Ito, S. *et al., Tet. Lett.*, 1967, 1127 (*isol, struct, deriv*)
Subba Rao, G. *et al., Chem. Comm.*, 1968, 1681 (*struct*)
Yosioka, I. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1186 (*Theasapogenol E*)
Aurada, E. *et al., Sci. Pharm.*, 1982, **50**, 331 (*isol, deriv*)
Yoshikawa, K. *et al., Tet. Lett.*, 1989, **30**, 1103 (*isol*)
Maeda, M. *et al., Tet. Lett.*, 1989, **30**, 1547 (*isol*)
Wei, J. *et al., Zhongguo Zhongyao Zazhi*, 1997, **22**, 228-230; *CA*, **128**, 72912h (*Camellia sinensis esters*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1901-1906 (*Theasaponins E_1 and E_2*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1759-1764 (*Assamsaponins*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1720-1725 (*Assamsaponins F-I, Theasaponin E_1, activity*)

12-Oleanene-3,16,21,22,24,28-hexol O-130

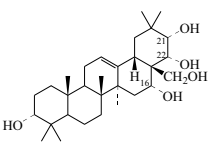


$C_{30}H_{50}O_6$ 506.721

(3β,16α,21β,22α)-*form* [20853-07-0]
Protoescigenin. *Protoaescigenin*
Mp 310°. $[\alpha]_D^{20}$ +30.5 (c, 0.7 in EtOH).

24-Aldehyde: [25122-87-6] *3,16,21,22,28-Pentahydroxy-12-oleanen-24-al*. ***Camelliagenin D***
Isol. from seeds of *Camellia sinensis* (Japanese tea) and *Camellia sasanqua*. Cryst. Mp 250-258°. $[\alpha]_D$ +39.2.
Ito, S. *et al., Tet. Lett.*, 1967, 1127 (*Camelliagenin D*)

12-Oleanene-3,16,21,22,28-pentol O-131



(3α,16α,21α,22α)-*form*

$C_{30}H_{50}O_5$ 490.722

(3β,16α,21β,22α)-*form* [13844-01-4]
Barringtogenol C. *Barrigenol R_2. Theasapogenol B. Jegosapogenol. Giganteumgenin M. Jegosapogenol A. Proschiwalligenin PB_1. Saniculagenin D. Escinidin. Aescinidin. Acutangenol B. Careyagenol A*
Sapogenin from *Thea sinensis* (tea). Cryst. ($CHCl_3$). Mp 302-308°. $[\alpha]_D^{20}$ +32.6 (c, 0.7 in dioxan).

*21-Angeloyl, 28-Ac, 3-*O*-[[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1*

→3)]-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [259748-74-8] ***Assamsaponin E***
$C_{59}H_{92}O_{26}$ 1217.36
Constit. of *Camellia sinensis* var. *assamica* (Assam tea). Cryst. ($CHCl_3$/MeOH). Mp 189.4-190.4°. $[\alpha]_D^{27}$ +23.8 (c, 0.1 in MeOH).

22-Angeloyl: [200492-43-9]
$C_{35}H_{56}O_6$ 572.824
Constit. of *Camellia sinensis* var. *assamica* (Assam tea). Cryst. Mp 230-234°.

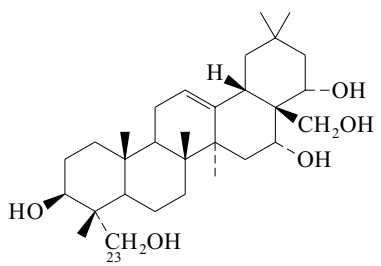
21-Cinnamoyl, 16,22-di-Ac, 3-O-[β-D-galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [160539-68-4]
$C_{65}H_{94}O_{27}$ 1307.441
Constit. of *Camellia sinensis* var. *sinensis* (tea).

22-Cinnamoyl, 16,21-di-Ac, 3-O-[β-D-galactopyranosyl-(1→2)-[α-D-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [316157-19-4] ***Assamsaponin J***
$C_{66}H_{96}O_{27}$ 1321.468
Constit. of *Camellia sinensis* var. *assamica* (Assam tea). Cryst. ($CHCl_3$/MeOH). Mp 200.2-201°. $[\alpha]_D^{26}$ +36 (c, 0.1 in MeOH).

[56144-10-6]

Hiller, K. *et al., Pharmazie*, 1975, **30**, 105 (*Giganteumgenins*)
Barua, A.K. *et al., J. Indian Chem. Soc.*, 1976, **53**, 209 (*isol*)
Kapunda, M. *et al., Bull. Soc. Chim. Belg.*, 1984, **93**, 497
Jiménez, E. *et al., Can. J. Chem.*, 1989, **67**, 2071 (*isol, pmr, cmr, cryst struct*)
Massiot, G. *et al., Phytochemistry*, 1992, **31**, 3571 (*cmr*)
Sagesaka, Y.M. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 2036 (*Barringtogenol C, cmr, Camellia sinensis saponin*)
Wei, J. *et al., Zhongguo Zhongyao Zazhi*, 1997, **22**, 228-230; *CA*, **128**, 72912h (*Camellia sinensis ester*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1759-1764 (*Assamsaponin E*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1720-1725 (*Assamsaponin J*)

12-Oleanene-3,16,22,23,28-pentol O-132



$C_{30}H_{50}O_5$ 490.722

(3β,16α,22α)-*form* [14440-27-8]
Camelliagenin C. *Theasapogenol C*
Sapogenin from the seeds of *Camellia japonica*. Cryst. Mp 280-283°. $[\alpha]_D$ +25.3 (EtOH).

22-Angeloyl, 3-O-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [156250-58-7] ***Camelliasaponin C1***
$C_{58}H_{92}O_{26}$ 1205.349
Constit. of *Camellia japonica*. Cryst. Mp 165.8-167.2°. $[\alpha]_D$ +4.3 (MeOH).

22-Tigloyl, 3-O-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [156317-51-0] ***Camelliasaponin C2***
$C_{58}H_{92}O_{26}$ 1205.349
Constit. of *Camellia japonica*. Cryst. Mp 177.6-178.9°. $[\alpha]_D$ +8.8 (MeOH).

23-Aldehyde: [14511-74-1] *3β,16α,22α,28-Tetrahydroxy-12-oleanen-23-al.* ***Camelliagenin B.*** *Camelliasapogenol II*
Sapogenin from seeds of *Camellia japonica* and from *Camellia sasanqua*. Cryst. Mp 200-205°. $[\alpha]_D$ +48.

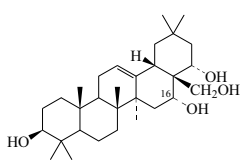
23-Aldehyde, 22-angeloyl, 3-O-[β-D-xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [259747-95-0] ***Assamsaponin A***
$C_{57}H_{88}O_{25}$ 1173.307
Constit. of *Camellia sinensis* var. *assamica* (Assam tea). Cryst. ($CHCl_3$/MeOH). Mp 211.7-212.2°. $[\alpha]_D^{26}$ +19.6 (c, 0.1 in MeOH).

23-Aldehyde, 22-angeloyl, 3-O-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [156250-57-6] ***Camelliasaponin B1***
$C_{58}H_{90}O_{26}$ 1203.333
Constit. of *Camellia japonica*. Mp 209.6-211.1°. $[\alpha]_D$ +23.7 (MeOH).

23-Aldehyde, 22-tigloyl, 3-O-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [156317-50-9] ***Camelliasaponin B2***
$C_{58}H_{90}O_{26}$ 1203.333
Constit. of *Camellia japonica*. Cryst. Mp 233.5-235.6°. $[\alpha]_D$ +20.7 (MeOH).

Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 743; 1996, **44**, 1899 (*Camelliasaponins*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1759-1764 (*Assamsaponin A*)

12-Oleanene-3,16,22,28-tetrol O-133



(3β,16α,22α)-*form*

$C_{30}H_{50}O_4$ 474.723

(3β,16α,22α)-*form* [53227-91-1]
Camelliagenin A. *Barrigenol A_2. Theasapogenol D. Camelliasapogenol I. Dihydropriverogenin A. Proschiwalligenin PA_2. Theasapogenin I*
Sapogenin from the seeds of *Camellia japonica*. Cryst. Mp 290-293°. $[\alpha]_D$ +20 (EtOH).

22-Angeloyl, 3-O-[β-D-galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [183020-18-0] ***Camelliasaponin A1***
$C_{58}H_{92}O_{25}$ 1189.35
Constit. of *Camellia japonica*. Cryst. (MeOH aq.). Mp 185.8-187°. $[\alpha]_D^{25}$ +22.9 (c, 0.2 in MeOH).

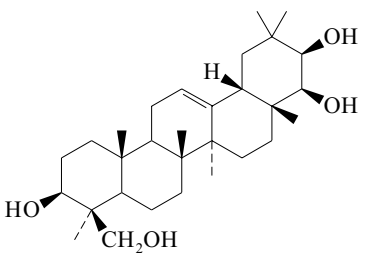
22-Tigloyl, 3-O-[β-D-galactopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [183183-15-5] ***Camelliasaponin A2***
$C_{58}H_{92}O_{25}$ 1189.35
Constit. of *Camellia japonica*. Cryst. (MeOH aq.). Mp 215.3-217.2°. $[\alpha]_D^{25}$ +8 (c, 1 in MeOH).

28-Aldehyde: [18443-26-0] *3,16,22-Trihydroxy-12-oleanen-28-al.* ***Priverogenin A***
$C_{30}H_{48}O_4$ 472.707
Sapogenin from *Primula veris* (cowslip). Cryst. (Et_2O). Mp 198-202°. $[\alpha]_D^{20}$ -4.2 (c, 0.53 in $CHCl_3$).

28-Aldehyde, 16-Ac: [26339-85-5]
$C_{32}H_{50}O_5$ 514.744
Sapogenin from *Primula veris* (cowslip). Cryst. (C_6H_6). Mp 200-204°. $[\alpha]_D^{20}$ -18.7 (c, 0.52 in $CHCl_3$).

Sandoval, A. *et al., J.A.C.S.*, 1957, **79**, 4468
Tschesche, R. *et al., Annalen*, 1966, **696**, 160 (*Priverogenin A*)
Tschesche, R. *et al., Tet. Lett.*, 1968, 183
Khong, P.W. *et al., Aust. J. Chem.*, 1975, **28**, 165; 1976, **29**, 1351
Dimbi, M.Z. *et al., Bull. Soc. Chim. Belg.*, 1983, **92**, 473 (*derivs*)
Chakravarty, A.K. *et al., Phytochemistry*, 1987, **26**, 2345 (*deriv, pmr, cmr*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1899; 1998, **46**, 1102-1107 (*Camelliasaponins, Alternosides*)

12-Oleanene-3,21,22,24-tetrol O-134



$C_{30}H_{50}O_4$ 474.723

(3β,21β,22β)-*form* [508-01-0]
Soyasapogenol A. *Soyasapogenol M_4*
Constit. of soya bean saponin. Cryst. (MeOH). Mp 308-312°. $[\alpha]_D^{21}$ +102.3 ($CHCl_3$).

22-O-α-L-Arabinopyranoside: ***Antibiotic MK 800-62F1***. *MK 800-62F1*
$C_{35}H_{58}O_8$ 606.838
Powder. $[\alpha]_D^{22}$ +65 (c, 1 in Py). Mp >200°.

3-O-[α-L-Arabinopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[2,3,4-tri-O-acetyl-β-D-xylopyranosyl-(1→3)-α-L-arabinopyranoside]: [117230-35-0] ***Acetylsoyasaponin A6***
$C_{57}H_{88}O_{25}$ 1173.307
Constit. of soybean *Glycine max*. Fine

cryst. + $3H_2O$ (EtOH). Mp 240-244°. $[\alpha]_D^{16}$ +14.2 (c, 0.2 in MeOH).

3-O-[α-L-Arabinopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]: [117210-16-9] ***Acetylsoyasaponin A_3***
$C_{60}H_{92}O_{27}$ 1245.371
Constit. of soybean (*Glycine max*). Fine cryst. + $5H_2O$ (EtOH). Mp 257-260°. $[\alpha]_D^{20}$ +23.6 (c, 0.5 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside]: [168288-04-8] ***Kudzusaponin SA_1***
$C_{42}H_{68}O_{15}$ 812.99
Constit. of kudzu (*Pueraria lobata*). Amorph. powder. $[\alpha]_D^{25}$ +12.1 (c, 0.38 in Py aq.).

3-O-[β-D-Galactopyranoside-(1→2)-β-D-glucuronopyranoside], 21-O-β-D-xylopyranoside: [162558-96-5] ***Lupinoside PA_2***
$C_{47}H_{76}O_{19}$ 945.106
Amorph. powder. $[\alpha]_D^{25}$ -1.6 (c, 0.45 in Py).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-α-L-arabinopyranoside: [168288-05-9] ***Kudzusaponin SA_2***
$C_{47}H_{76}O_{19}$ 945.106
Constit. of kudzu (*Pueraria lobata*). Amorph. powder. $[\alpha]_D$ +1.6 (c, 0.11 in DMSO).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[2,3,4-tri-O-acetyl-β-D-xylopyranosyl-(1→3)-α-L-arabinopyranoside]: [117230-34-9] ***Acetylsoyasaponin A_5***
$C_{58}H_{90}O_{26}$ 1203.333
Constit. of soybean (*Glycine max*). Fine cryst. + $4H_2O$ (EtOH). Mp 260-264°. $[\alpha]_D^{16}$ +9.7 (c, 0.7 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]: [78693-93-3] ***Soyasaponin A_2***
$C_{53}H_{86}O_{24}$ 1107.248
Isol. from soybean. Fine cryst. + $3H_2O$ (MeOH aq.). Sol. MeOH, EtOH, H_2O; poorly sol. $CHCl_3$, Et_2O, hexane. Mp 231-232°. $[\alpha]_D^{26}$ +25.3 (c, 1 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]: [117230-32-7] ***Acetylsoyasaponin A_2***
$C_{61}H_{94}O_{28}$ 1275.397
Constit. of soybean (*Glycine max*). Fine cryst. + $3H_2O$ (EtOH). Mp 276-278°. $[\alpha]_D^{18}$ +18.8 (c, 0.3 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]: [114077-04-2] ***Soyasaponin A_3***
$C_{48}H_{78}O_{19}$ 959.133
Isol. from soybean (*Glycine max*). Amorph. powder. $[\alpha]_D^{27}$ -14.2 (c, 0.55 in Py).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 21-O-β-D-xylopyranoside: [162558-95-4] ***Lupinoside PA_1***
$C_{53}H_{86}O_{23}$ 1091.249
Amorph. powder. $[\alpha]_D^{25}$ -15.3 (c, 0.52 in MeOH).

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-α-L-arabinopyranoside: [179910-78-2] ***Kudzusaponin SA_4***
$C_{47}H_{74}O_{20}$ 959.09
Constit. of kudzu (*Pueraria lobata*). Amorph. powder. $[\alpha]_D^{25}$ +5.2 (c, 0.6 in Py aq.).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[2,3,4-tri-O-acetyl-β-D-xylopyranosyl-(1→3)-α-L-arabinopyranoside]: [117230-33-8] ***Acetylsoyasaponin A_4***
$C_{64}H_{100}O_{31}$ 1365.475
Constit. of soybean (*Glycine max*). Fine cryst. + $2H_2O$ (EtOH). Mp 255-258°. $[\alpha]_D^{16}$ +13.5 (c, 0.1 in MeOH).

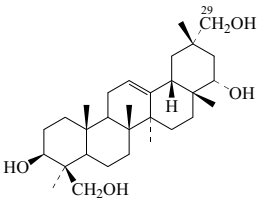
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]: [78693-94-4] ***Soyasaponin A_1***
$C_{59}H_{96}O_{29}$ 1269.39
Isol. from soybean (*Glycine max*). Fine cryst. + $4H_2O$ (MeOH aq.). Sol. MeOH, H_2O, EtOH; poorly sol. $CHCl_3$, hexane, Et_2O. Mp 240-242°. $[\alpha]_D^{26}$ +23.2 (c, 0.91 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-[2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl-(1→3)-α-L-arabinopyranoside]: [118194-13-1] ***Acetylsoyasaponin A_1***
$C_{67}H_{104}O_{33}$ 1437.539
Constit. of soybean (*Glycine max*). Fine cryst. + $4H_2O$ (EtOH). Mp 263-265°. $[\alpha]_D^{16}$ +17 (c, 0.6 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22-O-α-L-arabinopyranoside: [168288-06-0] ***Kudzusaponin SA_3***
$C_{53}H_{86}O_{23}$ 1091.249
Constit. of kudzu (*Pueraria lobata*). Amorph. powder. $[\alpha]_D^{25}$ -2.8 (c, 0.74 in DMSO).

Smith, H.M. *et al., Tetrahedron*, 1958, **4**, 111 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2294 (*struct*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1985, **33**, 589; 1069; 1988, **36**, 2819; 2829 (*Soyasaponins*)
Kinjo, J. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1293 (*cmr*)
Curl, C.L. *et al., J. Nat. Prod.*, 1988, **51**, 122 (*Soyasaponin A_3*)
Kinjo, J. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1874 (*Lupinosides*)
Arao, T. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1176; 1997, **45**, 362 (*Kudzusaponins*)
Miyao, H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1222 (*Soyasaponin A_3*)
Yoshimoto, Y. *et al., J. Antibiot.*, 2000, **53**, 569-574; 575-578 (*MK 800-62F1*)

12-Oleanene-3,22,24,29-tetrol O-135



(3β,22α)-*form*

$C_{30}H_{50}O_4$ 474.723

(3β,22α)-*form*

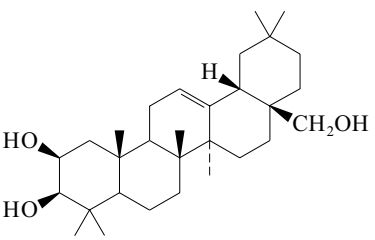
3-O-[β-D-Arabinopyranosyl-(1→3)-β-D-arabinopyranoside]: [211944-26-2]
$C_{40}H_{66}O_{12}$ 738.954
Constit. of *Acorus calamus* (sweet flag). Cryst. ($CHCl_3$). Mp 270°.

(3β,22β)-*form* [121994-06-7] ***Abrisapogenol B***
Needles. Mp 278-280°. $[\alpha]_D$ +26.1 (Py).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]: [149691-29-2] ***Robinioside E***
$C_{48}H_{78}O_{19}$ 959.133
Powder+$3H_2O$ (as Me ester). $[\alpha]_D^{26}$ -12.2 (c, 0.92 in MeOH) (Me ester).

Takeshita, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 846 (*isol, pmr*)
Sun, R.Q. *et al., Phytochemistry*, 1990, **29**, 2032 (*cmr*)
Miyao, H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1222 (*Robinioside E*)
Rai, R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 473-476 (*arabinosylarabinoside*)

12-Oleanene-2,3,28-triol O-136



$C_{30}H_{50}O_3$ 458.723

(2β,3β)-*form* [83991-75-7]
2β-Hydroxyerythrodiol
Cryst. ($CHCl_3$/MeOH). Mp 248° Mp 110-112°. $[\alpha]_D$ +69.8 ($CHCl_3$).

2,3-Bis[L-rhamnopyranosyl(1→4)-β-D-glucopyranoside]: [86264-32-6] ***Melilotin***†
$C_{54}H_{90}O_{21}$ 1075.292
Isol. from flowers of *Melilotus alba* (white melilot). No phys. props. reported.

3-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]: [155767-96-7] ***Castaraleside G***
$C_{48}H_{78}O_{18}$ 943.133
Gum (as Me ester). $[\alpha]_D^{20}$ +32.2 (c, 0.9 in MeOH) (Me ester).

3-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-xylopyranosyl-(1→2)-β-D-glucuronopyranoside]: [155767-97-8] ***Castaraleside***

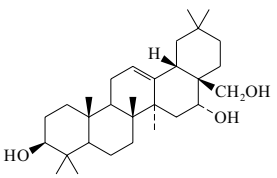
H
$C_{47}H_{76}O_{17}$ 913.107
Gum (as Me ester). $[\alpha]_D^{20}$ +43.3 (c, 0.15 in MeOH).

28-Carboxylic acid: 2,3-Dihydroxy-12-oleanen-28-oic acid, D-574

[86190-18-3, 86190-19-4, 86190-20-7, 86190-21-8]

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1806 (*isol*)
Nicollier, G. *et al., J. Nat. Prod.*, 1983, **46**, 183 (*Melilotin*)
Ahmed, W. *et al., Chem. Pharm. Bull.*, 1994, **42**, 314 (*Castaralesides*)
Shiojima, K. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1640 (*isol, pmr, cmr*)

12-Oleanene-3,16,28-triol O-137



(3β,16α)-*form*

$C_{30}H_{50}O_3$ 458.723

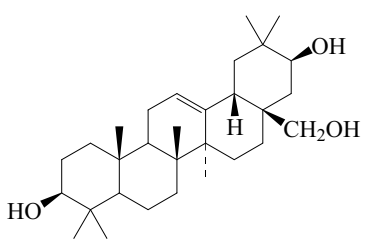
(3β,16α)-*form* [465-95-2]
Primulagenin A. *Armillarisgenin C. Schiwalligenin B_1*
Cryst. ($CHCl_3$/MeOH). Mp 249.5-250°. $[\alpha]_D$ +58 (c, 0.7 in $CHCl_3$). Identity of Primulagenin A and Armillarisgenin C not definitely confirmed.

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→2)]-β-D-glucuronopyranoside]:* [380303-70-8] ***Camellioside D***
$C_{54}H_{88}O_{24}$ 1121.275
Constit. of *Camellia japonica*. Cryst. (MeOH aq.). Mp 222-225°. $[\alpha]_D^{26}$ -3.2 (c, 0.1 in MeOH).

(3β,16β)-*form* [465-94-1]
Longispinogenin
Constit. of *Calendula officinalis* (pot marigold). Cryst. (Me_2CO). Mp 247-249°. $[\alpha]_D^{25}$ +51 ($CHCl_3$).

Djerassi, C. *et al., J.A.C.S.*, 1954, **76**, 4089-4091 (*Longispinogenin, struct*)
Tori, K. *et al., Tet. Lett.*, 1976, 4163-4166; 4167-4170 (*Longispinogenin, cmr*)
Yoshikawa, M. *et al., Heterocycles*, 2001, **55**, 1653-1657 (*Camellioside D*)

12-Oleanene-3,21,28-triol O-138



$C_{30}H_{50}O_3$ 458.723

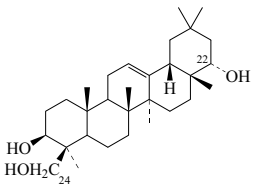
(3β,21β)-*form*
Cryst. ($CHCl_3$). Mp 108°.

28-O-*[β-D-Arabinopyranosyl-(1→3)-β-D-arabinopyranosyl-(1→3)-β-D-arabinopyranoside]:* [243468-98-6]
$C_{45}H_{74}O_{15}$ 855.071
Constit. of the seeds of *Dendrocalamus strictus* (male bamboo). Cryst. ($CHCl_3$). Mp 118°.

28-Carboxylic acid: 3,21-Dihydroxy-12-oleanen-28-oic acid, D-581

Rai, R. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 518-520

12-Oleanene-3,22,24-triol O-139



(3β,22α)-*form*

$C_{30}H_{50}O_3$ 458.723

(3β,22β)-*form* [595-15-3]
Soyasapogenol B. *Soyasapogenol M_2*
Constit. of soya bean saponin, *Medicago, Astragalus, Trifolium* spp.. Cryst. (MeOH). Mp 258-259°. $[\alpha]_D^{30.5}$ +92.4 ($CHCl_3$). Originally assigned 3,21,24-trihydroxy struct..

3-O-*α-L-Arabinopyranoside:* [170663-67-9]
Melilotoside A
$C_{35}H_{58}O_7$ 590.839
Constit. of *Melilotus albus* (white melilot).

24-O-*β-D-Glucopyranoside:* [115334-08-2]
$C_{36}H_{60}O_8$ 620.865
Constit. of French bean seeds (*Phaseolus vulgaris*). Cryst. (MeOH). Mp 278-280° dec. $[\alpha]_D$ +57 ($CHCl_3$).

3-O-*β-D-Glucuronopyranoside:* [99541-89-6]
$C_{36}H_{58}O_9$ 634.849
Constit. of the seeds of *Trifolium incarnatum* (crimson clover).

3-O-*[α-L-Arabinopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [108906-97-4]
Soyasaponin IV
$C_{41}H_{66}O_{13}$ 766.965
Constit. of soya bean *Glycine max*.

3-O-*[β-D-Galactopyranosyl-(1→2)-α-L-arabinopyranoside]:* [170663-68-0] ***Melilotoside B***
$C_{41}H_{68}O_{12}$ 752.981
Constit. of *Melilotus albus* (white melilot).

3-O-*[β-D-Galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [55304-02-4]
Soyasaponin III
$C_{42}H_{68}O_{14}$ 796.991
Constit. of soya bean *Glycine max*. Cryst. (MeOH). Sol. MeOH, EtOH, H_2O; poorly sol. $CHCl_3$, hexane, Et_2O. Mp 215-216°. $[\alpha]_D^{29}$ +15 (c, 0.5 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [82793-03-1] ***Azukisaponin II***
$C_{42}H_{68}O_{14}$ 796.991
Isol. from seeds of azuki bean (*Vigna angularis*) and alfalfa (*Medicago sativa*). Needles + $2H_2O$ (MeOH). Mp 216-217°. $[\alpha]_D^{25}$ +27.5 (c, 0.2 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [55319-36-3] ***Soyasaponin II***
$C_{47}H_{76}O_{17}$ 913.107
Constit. of soya bean *Glycine max*. Cryst. (MeOH). Sol. MeOH, H_2O, EtOH; poorly sol. $CHCl_3$, Et_2O, hexane. Mp 212-215°. $[\alpha]_D^{29}$ -9.6 (c, 0.5 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-α-L-arabinopyranoside]:* [170678-03-2] ***Melilotoside C***
$C_{47}H_{78}O_{16}$ 899.124
Constit. of *Melilotus albus* (white melilot).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [51330-27-9] ***Soyasaponin I***
$C_{48}H_{78}O_{18}$ 943.133
Constit. of soya bean *Glycine max*. Cryst. (MeOH). Sol. MeOH, EtOH, H_2O; poorly sol. $CHCl_3$, hexane, Et_2O. Mp 238-240°. $[\alpha]_D^{14}$ -8.5 (c, 1.0 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22*-O-*[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [130444-08-5] ***Bersimoside I***
$C_{60}H_{98}O_{28}$ 1267.417
Constit. of the seeds of *Trifolium incarnatum* (crimson clover).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-galactopyranosyl-(1→4)-β-D-glucuronopyranoside]:*
$C_{48}H_{78}O_{18}$ 943.133
Constit. of cowpea seeds (*Vigna unguiculata* ssp. *unguiculata*). Cryst. Mp 268-270° dec. $[\alpha]_D^{28}$ -29.6 (c, 0.05 in DMSO).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [82793-05-3] ***Azukisaponin V. Hispidacin***
$C_{48}H_{78}O_{18}$ 943.133
Isol. from seeds of azuki bean (*Vigna angularis*). Cryst. + $2H_2O$ (MeOH). Mp 245-297° (228-229°). $[\alpha]_D$ -22.5 (c, 0.42 in MeOH). $[\alpha]_D^{28}$ +0.4 (c, 1.1 in MeOH). High opt. rotn. value refers to Hispidacin.

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [114590-20-4] ***Soyasaponin V***
$C_{48}H_{78}O_{19}$ 959.133
Constit. of seeds of soybean (*Glycine max*) and French bean (*Phaseolus vulgaris*).

3-O-*[β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside]:* [137231-80-2] ***Phaseoluside A***
$C_{48}H_{80}O_{18}$ 945.149
Isol. from the seeds of French bean (*Phaseolus vulgaris*). Mp 245-248° dec. $[\alpha]_D^{25}$ +25.1 (c, 1 in Py).

3-O-*[α-L-Arabinopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-β-D-galactopyranosyl-(1→2)-α-L-arabinopyrano-*

side]: [172659-13-1] ***Melilotoside D***
$C_{52}H_{86}O_{20}$ 1031.239
Constit. of *Melilotus albus* (white melilot).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→3)]-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* ***Melilotussaponin O_1***
$C_{53}H_{86}O_{22}$ 1075.249
Constit. of *Melilotus officinalis* (sweet clover). Amorph. powder. $[\alpha]_D^{25}$ +5.7 (c, 0.5 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [170034-93-2] ***Medinoside E***
$C_{54}H_{88}O_{23}$ 1105.275
Constit. of alfalfa *Medicago sativa*. Cryst. (MeOH). Mp 218-221°.

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 22*-O-*[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranoside]:* [234761-05-8]
$C_{65}H_{106}O_{32}$ 1399.533
Constit. of soybean molasses (*Glycine max*). Amorph. powder. $[\alpha]_D^{25}$ -16.4 (c, 0.51 in MeOH).

22-Malonyl, 3-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [333334-36-4] ***Pisumsaponin I***
$C_{51}H_{80}O_{21}$ 1029.18
Constit. of garden pea *Pisum sativum*. Powder. $[\alpha]_D^{24}$ +5.8 (c, 0.9 in MeOH).

22-(2,3-Dihydro-5-hydroxy-6-methyl-4-oxo-2-pyranyl) ether, 3-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [143519-54-4] ***Chromosaponin I***. *Soyasaponin βg*
$C_{54}H_{84}O_{21}$ 1069.245
Constit. of garden pea (*Pisum sativum*) and scarlet runner bean (*Phaseolus coccineus*) seeds. Powder. Mp 210-212° dec. $[\alpha]_D^{17}$ -82.6 (c, 0.5 in MeOH aq.).

*22-(2,3-Dihydro-5-hydroxy-6-methyl-4-oxo-4*H*-pyran-2-yl) ether, 3*-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [244776-46-3] ***AzIII***
$C_{54}H_{82}O_{22}$ 1083.229
Constit. of azuki bean *Vigna angularis*. $[\alpha]_D^{23}$ -68.3 (c, 0.4 in MeOH aq.). λ_{max} 292 (MeCN).

*22-(2,3-Dihydro-5-hydroxy-6-methyl-4-oxo-4*H*-pyran-2-yl) ether, 3*-O-*[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [244776-47-4] ***AzIV***
$C_{54}H_{84}O_{22}$ 1085.244
Constit. of azuki bean *Vigna angularis*. $[\alpha]_D^{23}$ -80.8 (c, 0.4 in MeOH aq.). λ_{max} 292 (MeCN).

*22-(2,3-Dihydro-5-hydroxy-6-methyl-4-oxo-4*H*-pyran-2-yl) ether, 3*-O-*[β-D-glucopyranosyl-(1→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [244776-45-2] ***AzII***
$C_{54}H_{82}O_{23}$ 1099.228
Constit. of azuki bean *Vigna angularis*. $[\alpha]_D^{23}$ -37.4 (c, 0.43 in MeOH). λ_{max} 292 (MeCN).

22-O-(5,6-Dihydro-3-hydroxy-2-methyl-4-oxo-6-pyranyl) ether, 3-O-*[β-D-glucopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [157263-01-9] ***Soyasaponin αa***
$C_{53}H_{82}O_{21}$ 1055.218
Constit. of scarlet runner bean (*Phaseolus coccineus*) seeds.

22-O-(5,6-Dihydro-3-hydroxy-2-methyl-4-oxo-6-pyranyl) ether, 3-O-*[β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [149636-84-0] ***Soyasaponin αg***
$C_{54}H_{84}O_{22}$ 1085.244
Constit. of scarlet runner bean (*Phaseolus coccineus*) seeds.

24-Aldehyde:3,22-Dihydroxy-12-oleanen-24-al. ***Sandosapogenol***
$C_{30}H_{48}O_3$ 456.707
Sapogenin from French bean (*Phaseolus vulgaris*) seed. Powder. $[\alpha]_D^{24}$ +61.2 (c, 1.38 in $CHCl_3$).

24-Aldehyde, 3-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [333334-37-5] ***Pisumsaponin II***
$C_{48}H_{76}O_{18}$ 941.118
Constit. of garden pea *Pisum sativum*. Powder. $[\alpha]_D^{24}$ -2.2 (c, 0.9 in MeOH).

24-Aldehyde, 3-O-*[β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* ***Sandosaponin B***
$C_{48}H_{76}O_{19}$ 957.117
Constit. of French bean (*Phaseolus vulgaris*) seed. Cryst. (MeOH aq.). Mp 212-213°. $[\alpha]_D^{28}$ +34.8 (c, 0.3 in MeOH).

22-Ketone: [6750-59-0] *3,24-Dihydroxy-12-oleanen-22-one.* ***Soyasapogenol E***
$C_{30}H_{48}O_3$ 456.707
Constit. of soya bean (*Glycine max*). Noncryst.

22-Ketone, 3-O-*β-D-glucuronopyranoside:* [143519-22-6] ***Cloversaponin I***
$C_{36}H_{56}O_9$ 632.833
Constit. of *Trifolium repens* (white clover). Amorph. powder (as Me ester). $[\alpha]_D$ +21.1 (c, 0.1 in MeOH) (Me ester).

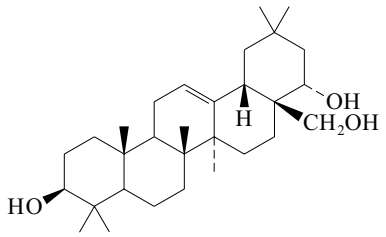
22-Ketone, 3-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [117210-14-7] ***Dehydrosoyasaponin I***. *DHS-1*
$C_{48}H_{76}O_{18}$ 941.118
Constit. of soya bean (*Glycine max*) and alfalfa (*Medicago sativa*). Cryst. powder. Mp 272-280°. $[\alpha]_D^{24}$ -43.2 (c, 0.5 in Py).

22-Ketone, 3-O-*[β-D-glucopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [135272-91-2] ***Sandosaponin A***
$C_{48}H_{76}O_{19}$ 957.117
Constit. of French bean (*Phaseolus vulgaris*) seed. Cryst. (MeOH aq.). Mp 200-201°. $[\alpha]_D^{23}$ -5.8 (c, 0.8 in MeOH).

[86500-81-4, 86511-98-0, 86764-24-1]

Willner, D. *et al., J.C.S.*, 1964, 5885 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1976, **24**, 121; 1982, **30**, 2294; 1983, **31**, 674; 683; 698; 716 (*isol, cryst struct, glycosides*)
Kaneda, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1287 (*isol*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4267 (*isol*)
Burrows, J.C. *et al., Phytochemistry*, 1987, **26**, 1214 (*Soyasaponin IV*)
Kang, S.S. *et al., J. Nat. Prod.*, 1988, **51**, 335 (*Soyasapogenol E, cmr*)
Curl, C.L. *et al., J. Sci. Food Agric.*, 1988, **43**, 101 (*Soyasaponin V*)
Jain, D.C. *et al., Phytochemistry*, 1988, **27**, 1216 (*24-glucoside*)
Kubo, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2229 (*Dehydrosoyasaponin I*)
Everett, J.R. *et al., Anal. Proc. (London)*, 1990, **27**, 184 (*pmr, cmr, ms, ir*)
Baxter, R.L. *et al., J. Nat. Prod.*, 1990, **53**, 298 (*pmr, cmr*)
Sun, R. *et al., Phytochemistry*, 1990, **29**, 2032; 1991, **30**, 2707 (*derivs*)
Ding, Y. *et al., Chem. Pharm. Bull.*, 1991, **39**, 496
Mahato, S.B. *et al., Phytochemistry*, 1991, **30**, 3389 (*Hispidacin, cmr*)
Jain, D.C. *et al., Planta Med.*, 1991, **57**, 94 (*Phaseoluside A*)
Sakamoto, S. *et al., Phytochemistry*, 1992, **31**, 1773-1777 (*Cloversaponins*)
Tsurumi, S. *et al., Phytochemistry*, 1992, **31**, 2435 (*Chromosaponin I*)
McManus, O.B. *et al., Biochemistry*, 1993, **32**, 6128-6133 (*Dehydrosoyasaponin 1, pharmacol*)
Timbekova, A.E. *et al., Khim. Prir. Soedin.*, 1993, **29**, 705; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 626 (*Medinoside E*)
Tsujino, Y. *et al., Chem. Lett.*, 1994, 711 (*Chromosaponin I*)
Khodakov, G.V. *et al., Khim. Prir. Soedin.*, 1994, **30**, 756; 762; *Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 704; 709 (*Melilotosides*)
Yoshiki, Y. *et al., Phytochemistry*, 1994, **36**, 1009 (*Soyasaponins αa, αg, βg*)
Noorwala, M. *et al., J. Nat. Prod.*, 1995, **58**, 1070 (*Vigna unguiculata glycoside*)
Grishkovets, V.I. *et al., Khim. Prir. Soedin.*, 1995, **31**, 709; *Chem. Nat. Compd. (Engl. Transl.)*, 1995, **31**, 596 (*3-glucoside*)
Mohamed, K.M. *et al., Phytochemistry*, 1995, **40**, 1237 (*Bersimosides*)
Miyao, H. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1222 (*Soyasaponin I, Dehydrosoyasaponin I, Abrisaponin SB, pmr, cmr*)
Pelizzoni, F. *et al., Gazz. Chim. Ital.*, 1996, **126**, 275 (*Azukisaponin V, pmr, cmr*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 877-882 (*Sandosapogenol, Sandosaponins*)
Mbafor, J.T. *et al., Phytochemistry*, 1997, **44**, 1151 (*Sigmosides*)
Udayama, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 526-527 (*Melilotussaponin O_1*)
Giangiacomo, K.M. *et al., J. Gen. Physiol.*, 1998, **112**, 485-501 (*Dehydrosoyasaponin 1, pharmacol*)
Hosny, M. *et al., J. Nat. Prod.*, 1999, **62**, 853-858 (*Glycine max saponin*)
Iida, T. *et al., Phytochemistry*, 1999, **51**, 1055-1058 (*AzII, AzIII, AzIV*)
Oh, S.-R. *et al., Planta Med.*, 2000, **66**, 506-510 (*activity*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 73-77 (*Pisumsaponins*)

12-Oleanene-3,22,28-triol O-140



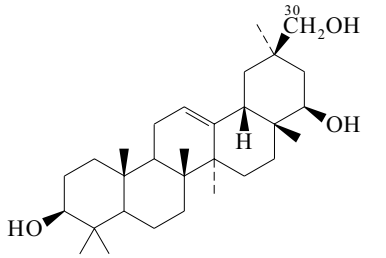
$C_{30}H_{50}O_3$ 458.723

(3β,22α)-*form* [20475-26-7]
22α-Hydroxyerythrodiol
Constit. of *Camellia sasanqua*. Cryst. (MeOH). Mp 279-282°. $[\alpha]_D^{20}$ +37 (c, 1 in Py).

3-O[β-D-Galactofuranosyl(1→2)-O-[β-D-galactofuranosyl(1→4)]-β-D-mannopyranoside]: [76556-16-6] ***Derrissaponin***
$C_{48}H_{80}O_{18}$ 945.149
Amorph. Mp 230° dec. $[\alpha]_D^{20}$ -27 (c, 1.7 in MeOH).

Yosioka, I. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1237 (*struct*)
Tori, K. *et al., Tet. Lett.*, 1974, 4227 (*cmr*)
Cherry, R.F. *et al., Aust. J. Chem.*, 1977, **30**, 1397 (*isol*)
Parente, J.F. *et al., Ann. Acad. Bras. Ci&eenc.*, 1980, **52**, 503; *CA*, **94**, 99764c (*Derrissaponin*)

12-Oleanene-3,22,30-triol O-141



$C_{30}H_{50}O_3$ 458.723

(3β,22β)-*form* [10379-65-4]
Abrisapogenol D
Needles. Mp 290-291°. $[\alpha]_D$ +76.9 (Py).

30-Carboxylic acid, 22-Ac, 3-O-[α-L-rhamnopyranosyl(1→2)-β-D-glucuronopyranosyl(1→2)-glucuronate]: [118536-87-1] ***Licoricesaponin D3***
$C_{50}H_{76}O_{21}$ 1013.138
Isol. from roots of *Glycyrrhiza uralensis* (Chinese licorice). Powder. $[\alpha]_D^{20}$ -5 (MeOH).

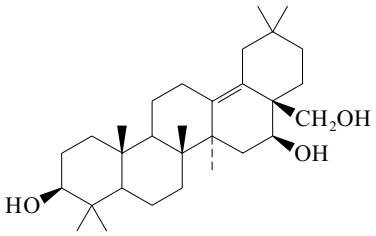
30-Carboxylic acid, 30→22 lactone: [10379-62-1] *3β-Hydroxy-12-oleanen-30,22β-olide.* ***Desoxoglabrolide***
$C_{30}H_{46}O_3$ 454.692
Saponin from *Glycyrrhiza glabra* (licorice). Cryst. (2-propanol). Mp 274-278°. $[\alpha]_D^{25}$ +59.6 (c, 0.52 in $CHCl_3$).

30-Carboxylic acid, 30→22 lactone, 3-O-[α-L-rhamnopyranosyl-(1→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Licoricesaponin F3***
$C_{48}H_{72}O_{19}$ 953.085
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Mp 215-217°. $[\alpha]_D$ -20 (MeOH).

[118525-50-1]

Russo, G. *et al., Corsi. Semin. Chim.*, 1968, **11**, 20 (*Desoxoglabrolide*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3710; 1991, **39**, 244 (*Licoricesaponin D3, Licoricesaponin F3*)

13(18)-Oleanene-3,16,28-triol O-142



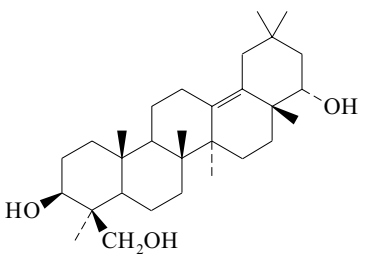
$C_{30}H_{50}O_3$ 458.723

(3β,16β)-*form* [26540-64-7]
Heliantriol A₁. *Coflotriol*
Isol. from flowers of *Helianthus annuus* (sunflower) and *Calendula officinalis* (pot marigold). Needles (EtOAc). Mp 279-281°. $[\alpha]_D$ -36.7 (c, 1 in $CHCl_3$).

Tri-Ac:
Cryst. (MeOH). Mp 229°.

Kubota, T. *et al., Tetrahedron*, 1967, **23**, 3333 (*synth*)
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 2465 (*isol*)

13(18)-Oleanene-3,22,24-triol O-143



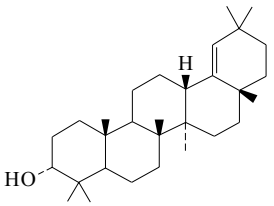
$C_{30}H_{50}O_3$ 458.723

(3β,22α)-*form*

22-Me ether: [65892-76-4] *22-Methoxy-13(18)-oleanene-3,24-diol.* ***Soyasapogenol D***. *Soyasapogenol M_3*
$C_{31}H_{52}O_3$ 472.75
Soybean saponin (from *Glycine max*).. Cryst. (Me_2CO/MeOH). Mp 298-299°. $[\alpha]_D^{31}$ -60.8 ($CHCl_3$). Shown to be 21- or 22-methoxy by Cainelli *et al*. CA uses the 21-methoxy struct. but the most recent assignment seems to be that of Ružička. Prob. artifact.

Meyer, A. *et al., Helv. Chim. Acta*, 1950, **33**, 687 (*isol*)
Cainelli, G. *et al., Helv. Chim. Acta*, 1958, **41**, 2053 (*struct*)
Ružička, L. *et al., Pure Appl. Chem.*, 1963, **6**, 505 (*struct, biosynth*)
Jurzysta, M. *et al., J. Chromatogr.*, 1978, **148**, 517 (*isol*)

18-Oleanen-3-ol O-144



3α-*form*

$C_{30}H_{50}O$ 426.724

3β-*form* [465-02-1]
Germanicol. *Isolupeol*. *Morol*
Cryst. Mp 220-223°. $[\alpha]_D^{17}$ +5.8 (c, 2 in $CHCl_3$).

O-*Cinnamoyl:* [65883-48-9]
$C_{39}H_{56}O_2$ 556.87
Isol. from shea butter.

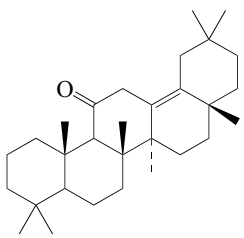
Me ether: [5945-45-9] *3β-Methoxy-18-oleanene.* ***Miliacin***. *Prosol*. *Panicol*
$C_{31}H_{52}O$ 440.751
Obt. from *Panicum miliaceum* (proso millet),. Cryst. (Me_2CO/C_6H_6). Mp 283°. $[\alpha]_D$ +22 (+8) ($CHCl_3$).

[30300-37-9]

Sugiyama, N. *et al., Nippon Kagaku Zasshi*, 1961, **82**, 1051; 1054; 1057; *CA*, **57**, 13810n (*Miliacin*)
Peers, K.E. *et al., J. Sci. Food Agric.*, 1977, **28**, 1000-1009 (*O-cinnamoyl*)
Smetanina, O.F. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 2463-2465 (*Miliacin, cryst struct*)

13(18)-Oleanen-11-one O-145

[18674-26-5]
Mangiferoleanone



$C_{30}H_{48}O$ 424.709
Constit. of the root bark of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 223-225° (186-188°). $[\alpha]_D$ -48.

Barton, D.H.R. *et al., J.C.S.(C)*, 1968, 1031-1040 (*synth*)
Gupta, J. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1093-1098 (*isol, ir, pmr, ms*)

Oleanolic acid bisdesmosides O-146

Saponins of 3-Hydroxy-12-oleanen-28-oic acid, H-663 with glycosides at 3 and glycosyl esters at 28.

Diglycosides

3-O-α-L-Arabinopyranoside, 28-O-β-D-glucopyranosyl ester: [93091-75-9]
$C_{41}H_{66}O_{12}$ 750.965
Isol. from ginseng (*Panax* sp.). Cryst. Mp 220°. $[\alpha]_D^{25}$ +10.3 (c, 0.0033 in MeOH).

Triglycosides

3-O-α-L-*Arabinopyranoside, 28*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [120481-38-1]
$C_{47}H_{76}O_{17}$ 913.107
Constit. of *Aralia elata* (Japanese angelica tree) and *Decaisnea fargesii* (blue sausagefruit). Powder + $2^{1}/_{2}$ H_2O. Mp 227-230°. $[\alpha]_D$ +9.7 (c, 0.2 in MeOH).

3-O-*[[1S-(Carboxymethoxy)carboxymethyl]-(→3)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [182322-57-2] ***Spinacoside C***
$C_{46}H_{70}O_{19}$ 927.048
Present in spinach (*Spinacia oleracea*) and Malabar spinach (*Basella rubra*). Cryst. (MeOH aq.). Mp 220-222°. $[\alpha]_D^{24}$ +10.2 (MeOH). $[\alpha]_D$ +6.8 (c, 0.3 in CD_3OD).

3-O-*[[2-Carboxy-1-(carboxymethoxy)-2-hydroxyethyl]-(→3)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [168111-48-6] ***Achyranthoside C***. *Betavulgaroside III*
$C_{47}H_{72}O_{20}$ 957.074
Constit. of roots and leaves of sugar beet (*Beta vulgaris*). Cryst. Mp 212-214°. $[\alpha]_D$ +10.8 (MeOH).

3-O-*[α-L-Arabinofuranosyl-(1→4)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [7518-22-1] ***Araloside A***. *Oleanoside E*
$C_{47}H_{74}O_{18}$ 927.091
From *Aralia elata* (Japanese angelica tree). Needles (MeOH). Mp 213-215°. $[\alpha]_D^{20}$ -26.7 (c, 1.9 in MeOH).

► FM3374500

3-O-*[α-L-Arabinopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [114006-82-5] ***Cynarasaponin H***
$C_{47}H_{74}O_{18}$ 927.091
Constit. of *Cynara cardunculus* (cardoon).

3-O-*[α-L-Arabinopyranosyl-(1→2)-6*-O-*methyl-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [117804-22-5]
$C_{48}H_{76}O_{18}$ 941.118
Constit. of *Cynara cardunculus* (cardoon).

3-O-*[α-L-Arabinopyranosyl-(1→3)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [95851-41-5] ***Hemsloside Ma 1***. *Momordin II*
$C_{47}H_{74}O_{18}$ 927.091
Constit. of Chinese cucumber (*Momordica cochinchinensis*). Powder. $[\alpha]_D^{24}$ +16.3 (c, 0.93 in MeOH).

3-O-*[α-L-Arabinopyranosyl-(1→3)-6*-O-*methyl-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [95851-50-6] ***Momordin IIa***
$C_{48}H_{76}O_{18}$ 941.118
Constit. of Chinese cucumber (*Momordica cochinchinensis*). Needles (MeOH). Mp 247-249°. $[\alpha]_D^{21}$ +14.1 (c, 1.24 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→3)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [96990-19-1] *Momordin IIc*. ***Quinoside D***
$C_{47}H_{74}O_{18}$ 927.091
Constit. of quinoa grains (*Chenopodium quinoa*), and root of Chinese cucumber (*Momordica cochinchinensis*). Powder + $2H_2O$. Mp 270-275° dec. $[\alpha]_D^{21}$ +5.7 (c, 1 in MeOH).

3-O-*[β-D-Galactopyranosyl-(1→3)-β-D-glucopyranoside], 28*-O-*β-D-glucuronopyranosyl ester:*
$C_{48}H_{76}O_{19}$ 957.117
Constit. of *Aralia elata* (Japanese angelica tree). Powder (as Me ester). $[\alpha]_D$ +7.1 (c, 1 in MeOH) (Me ester).

3-O-*[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranoside], 28*-O-*α-D-glucopyranosyl ester:* [34381-98-1] ***Calenduloside B***
$C_{48}H_{78}O_{18}$ 943.133
Constit. of the roots of *Calendula officinalis* (pot marigold). Cryst. (MeOH). Mp 232-234°. $[\alpha]_D^{20}$ +57.2 (c, 0.5 in MeOH).

3-O-*[β-D-Galactopyranosyl-(1→3)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [26020-29-1]

[29893-98-9] ***Calenduloside H***. *Calendulaglycoside C*
$C_{48}H_{76}O_{19}$ 957.117
Isol. from marigold leaves (*Calendula officinalis*). Mp 198-203°. $[\alpha]_D^{20}$ +22.1 (MeOH). Tentative struct. for Calendulaglycoside C.

3-O-*[β-D-Galactopyranosyl-(1→3)-6*-O-*methyl-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [155740-14-0] ***Calenduloside H methyl ester***
$C_{49}H_{78}O_{19}$ 971.144
Constit. of marigold (*Calendula officinalis*). Powder. $[\alpha]_D^{30}$ +12.4 (c, 0.5 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [34367-04-9] ***Ginsenoside Ro***. *Chikusetsusaponin V. Polysciasaponin* P_3
$C_{48}H_{76}O_{19}$ 957.117
Constit. of *Panax ginseng* (ginseng). Cryst. (MeOH). Mp 239-241°. $[\alpha]_D^{22}$ +15.3 (c, 1 in MeOH).

► LD_{50} (mus, ipr) 656 mg/kg. FM3375000

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [107241-05-4]

[178894-82-1] ***Tuberoside A***
$C_{48}H_{76}O_{19}$ 957.117
Isol. from ulluco tubers *Ullucus tuberosus*. Mp 200-208°.

Tetraglycosides

3-O-*[α-L-Arabinofuranosyl-(1→3)*-O-*[α-L-arabinofuranosyl-(1→4)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [7518-23-2] ***Araloside B***. *Oleanoside C*
$C_{52}H_{82}O_{22}$ 1059.207
From *Aralia elata* (Japanese angelica tree). Amorph.

3-O-*[α-L-Arabinopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [96158-12-2] ***Hemsloside Ma 2***. *Momordin IIe*
$C_{52}H_{82}O_{22}$ 1059.207
Constit. of Chinese cucumber (*Momordica cochinchinensis*). Powder. $[\alpha]_D^{23}$ +11.8 (c, 1.1 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [119617-28-6] ***Momordin IId***
$C_{52}H_{82}O_{22}$ 1059.207
Constit. of Chinese cucumber (*Momordica cochinchinensis*). Powder. $[\alpha]_D^{23}$ +1.98 (c, 1.06 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [156856-39-2] ***Tarasaponin VI***†. *Elatoside C*
$C_{53}H_{84}O_{23}$ 1089.233
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. Mp 208.5-209.5°. $[\alpha]_D$ -1.6 (MeOH). Tarasaponin VI and Elatoside C not compared. Different groups of workers have allocated Tarasaponin names to closely related compds..

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)*-6-O-*octyl-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [256531-73-4] ***Araloside* S_1**
$C_{61}H_{100}O_{23}$ 1201.447
Constit. of *Aralia elata* (Japanese angelica tree).

3-O-*[β-D-Xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-α-L-arabinopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [144118-18-3] ***Caraganoside A***. *Tarasaponin VII. Elatoside F*
$C_{52}H_{84}O_{21}$ 1045.223
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. Mp 212.5-214°. $[\alpha]_D$ +24.3 (MeOH). Caraganoside A and Tarasaponin VII not compared.

3-O-*[β-D-Xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [91204-06-7] ***Tarasaponin V. Elatoside K***
$C_{53}H_{84}O_{23}$ 1089.233
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. (MeOH aq.). Amorph. powder (MeOH) (as Me ester). Mp 219-222°. $[\alpha]_D^{26}$ +2 (c, 0.1 in MeOH).

3-O-*[β-D-Xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [178894-83-2] ***Tuberoside B***
$C_{53}H_{84}O_{23}$ 1089.233
Constit. of ulluco tubers (*Ullucus tuberosus*). Powder. Mp 203-206°.

3-O-*[β-D-Xylopyranosyl-(1→2)-[(2-carboxy-1-carboxymethoxy-2-hydroxyethyl)-(→3)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [184288-94-6] ***Betavulgaroside IX***
$C_{52}H_{80}O_{24}$ 1089.19
Constit. of sugarbeet. Cryst. ($CHCl_3$/MeOH). Mp 213-214°. $[\alpha]_D^{26}$ +17 (c, 0.1 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [209802-26-6] ***Lablaboside A***
$C_{54}H_{86}O_{23}$ 1103.26
Constit. of hyacinth bean seeds (*Doli-*

chos lablab). Cryst. (MeOH aq.). Mp 184-185.5°. $[\alpha]_D^{26}$ -9.3 (c, 1.2 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→3)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:*
$C_{54}H_{86}O_{23}$ 1103.26
Constit. of the famine food *Ximenia americana* (tallow nut).

3-O-*[β-D-Galactopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [55446-15-6] ***Araloside C***. *Oleanoside A*
$C_{53}H_{84}O_{23}$ 1089.233
Constit. of *Aralia elata* (Japanese angelica tree). Amorph.

3-O-*[β-D-Galactopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-6*-O-*butyl-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [329969-14-4] ***Congmunoside XIV***
$C_{57}H_{92}O_{23}$ 1145.34
Constit. of root bark of *Aralia elata* (Japanese angelica tree).

3-O-*[β-D-Galactopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [156856-40-5] ***Elatoside D***
$C_{54}H_{86}O_{24}$ 1119.259
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. Mp 188.5-189.5°. $[\alpha]_D$ +6.9 (MeOH).

3-O-*[β-D-Galactopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [58231-98-4] ***Calenduloside D***
$C_{54}H_{88}O_{23}$ 1105.275
Constit. of the roots of *Calendula officinalis* (pot marigold). Cryst. + 1½ H_2O. Mp 245-247°. $[\alpha]_D^{27}$ +16 (c, 0.5 in MeOH).

3-O-*[β-D-Galactopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→4)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [29660-94-4] ***Calendulaglycoside A***
$C_{54}H_{86}O_{24}$ 1119.259
Isol. from marigold (*Calendula officinalis*).

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-arabinofuranosyl-(1→4)]-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* ***Tarasaponin IV***
$C_{53}H_{86}O_{22}$ 1075.249
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder (MeOH) (Me ester). Mp 196-206° dec. (Me ester). $[\alpha]_D$ -22.6 (c, 1.1 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→3)-[α-L-arabinofuranosyl-(1→4)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [96627-72-4] ***Stipuleanoside R₂***
$C_{53}H_{84}O_{23}$ 1089.233
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder (MeOH) (Me ester). Mp 210-215° dec. (Me ester). $[\alpha]_D$ -15.5 (c, 1.2 in MeOH) (Me ester).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [340963-86-2] ***Araliasaponin V***. *Congmunoside V*
$C_{54}H_{88}O_{23}$ 1105.275
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder. $[\alpha]_D$ -11.3 (c, 0.2 in Py).

3-O-*[β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [144077-05-4] ***Araloside G***
$C_{54}H_{88}O_{23}$ 1105.275
Constit. of *Aralia elata* (Japanese angelica tree).

3-O-*[β-D-Glucopyranosyl-(1→2)-[[2-carboxy-1-(carboxymethoxy)-2-hydroxyethyl]-(→3)]-β-D-glucuronopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [168009-91-4]

[168111-49-7] ***Achyranthoside D***. ***Betavulgaroside V***
$C_{53}H_{82}O_{25}$ 1119.216
Constit. of leaves and root of sugarbeet. Cryst.; amorph. powder (as tri-Me ester). Mp 205-206°. $[\alpha]_D$ +12.5 (MeOH). Identity of Betavulgaroside V with Achyranthoside D is not yet fully established.

Pentaglycosides

3-O-*[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranoside], 28*-O-*[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [36284-77-2] ***Eleutheroside M***. *Hederacoside B. Hederasaponin B. Hederacolchiside C. Tauroside G_2. Glycoside L-G_2*
$C_{59}H_{96}O_{25}$ 1205.392
Isol. from *Eleutherococcus (Acanthopanax) senticosus* (Siberian ginseng). $[\alpha]_D^{20}$ -28.8 (c, 4.9 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-arabinopyranoside], 28*-O-*[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [35790-96-6] ***Eleutheroside L***
$C_{59}H_{96}O_{25}$ 1205.392
Isol. from *Eleutherococcus (Acanthopanax) senticosus* (Siberian ginseng).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [135545-77-6] ***Acutoside B***
$C_{58}H_{94}O_{25}$ 1191.366
Constit. of Chinese okra (*Luffa acutangula*). Amorph. powder. Mp 225-250° dec. $[\alpha]_D^{24}$ -18.3 (c, 1 in MeOH aq.).

3-O-*[β-D-Glucopyranosyl-(1→3)-[α-L-arabinopyranosyl-(1→4)]-β-D-glucuronopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [344911-91-7]
$C_{59}H_{94}O_{28}$ 1251.375
Constit. of root bark of *Aralia elata* (Japanese angelica tree).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside], 28*-O-*β-D-glucopyranosyl ester:* [344911-90-6] ***Congmunoside X***
$C_{60}H_{98}O_{28}$ 1267.417
Constit. of root bark of *Aralia elata* (Japanese angelica tree).

Hexaglycosides

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28*-O-*[α-L-arabinopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [135575-17-6] ***Acutoside E***
$C_{63}H_{102}O_{29}$ 1323.481
Constit. of Chinese okra (*Luffa acutangula*). Needles. Mp 246-251°. $[\alpha]_D^{24}$ -14.2 (c, 1 in MeOH aq.).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [135575-16-5] ***Acutoside D***
$C_{63}H_{102}O_{29}$ 1323.481
Constit. of Chinese okra (*Luffa acutangula*). Amorph. powder. Mp 260-265° dec. $[\alpha]_D^{24}$ -21.4 (c, 1 in MeOH aq.).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28*-O-*[β-D-xylopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [135545-78-7] ***Acutoside F***
$C_{63}H_{102}O_{29}$ 1323.481
Constit. of Chinese okra (*Luffa acutangula*). Amorph. powder. Mp 215-223° dec. $[\alpha]_D^{24}$ -25.3 (c, 1 in MeOH aq.).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside], 28*-O-*[α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranosyl] ester:* [208390-15-2] ***Lablaboside F***
$C_{66}H_{106}O_{31}$ 1395.545
Constit. of hyacinth bean seeds (*Dolichos lablab*). Cryst. (MeOH aq.). Mp 200.6-202°. $[\alpha]_D^{24}$ -46.1 (c, 1.3 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [329969-11-1] ***Congmunoside XII***
$C_{65}H_{106}O_{32}$ 1399.533
Constit. of root bark of *Aralia elata* (Japanese angelica tree).

Heptaglycosides

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 28*-O-*[α-L-arabinopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[β-D-xylopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester:* [135545-79-8] ***Acutoside G***
$C_{68}H_{110}O_{33}$ 1455.597
Constit. of Chinese okra (*Luffa acutangula*). Amorph. powder. Mp 250-252° dec. $[\alpha]_D^{24}$ -22.5 (c, 1 in H_2O).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→2)]-α-L-arabinopyranoside], 28*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [329969-12-2] ***Congmunoside XIII***
$C_{71}H_{116}O_{37}$ 1561.675
Constit. of root bark of *Aralia elata* (Japanese angelica tree).

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Oleanolic acid 3-glycosides O-147

Saponins of 3-Hydroxy-12-oleanen-28-oic acid, H-663 that have glycosides at 3 but no 28-glycosyl esters.

Monoglycosides

3-O-β-D-Glucuronopyranoside: [26020-14-4] ***Calenduloside E***. *Calendulaglycoside F. Momordin Ib. Polysciasaponin P_7. Silphioside F*
$C_{36}H_{56}O_9$ 632.833
Constit. of *Calendula officinalis* (pot marigold), *Beta vulgaris* (sugar beet) and *Momordica cochinchinensis* (Chinese cucumber). Needles (MeOH). Mp 264-267° dec. $[\alpha]_D$ +20.4 (c, 0.8 in MeOH).

Diglycosides

3-O-[[1S-(Carboxymethoxy)carboxymethyl]-(→3)-β-D-glucuronopyranoside]: [182322-58-3] ***Spinacoside D***
$C_{40}H_{60}O_{14}$ 764.906
Constit. of *Spinacia oleracea* (spinach) and *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 183-185°. $[\alpha]_D^{25}$ +11.4 (MeOH). $[\alpha]_D$ +10.7 (c, 0.2 in CD_3OD).

3-O-[[2-Carboxy-1-(carboxymethoxy)-2-hydroxyethyl]-(→3)-β-D-glucuronopyranoside]: [168010-06-8] ***Betavulgaroside IV***
$C_{41}H_{62}O_{15}$ 794.932
Constit. of *Beta vulgaris* (sugar beet). Cryst. Mp 186-187°. $[\alpha]_D$ +43.1 (MeOH).

3-O-[α-L-Arabinopyranosyl-(1→3)-β-D-glucuronopyranoside]: [95851-40-4] ***Momordin I***. *Hemsloside Am1*
$C_{41}H_{64}O_{13}$ 764.949
Constit. of *Momordica cochinchinensis* (Chinese cucumber). Powder (MeOH). Mp 235-240° dec. $[\alpha]_D^{16}$ +28 (c, 0.4 in $CHCl_3$/MeOH aq.).

3-O-[α-L-Arabinopyranosyl-(1→3)-6-O-methyl-β-D-glucuronopyranoside]: [95851-46-0] ***Momordin Ia***
$C_{42}H_{66}O_{13}$ 778.976
Constit. of *Momordica cochinchinensis* (Chinese cucumber). Powder (Me_2CO). $[\alpha]_D^{22}$ +28.2 (c, 0.99 in MeOH).

3-O-[β-D-Xylopyranosyl-(1→3)-β-D-glucuronopyranoside]: [96990-18-0] ***Momordin Ic***
Constit. of *Momordica cochinchinensis* (Chinese cucumber). Powder (MeOH). Mp 240° dec. $[\alpha]_D^{21}$ +15.4 (c, 1.03 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→4)-α-L-arabinopyranoside]: [35790-94-4] ***Mubenin B***. *Eleutheroside I. Raddeanin B*
$C_{41}H_{66}O_{11}$ 734.966
Isol. from *Eleutherococcus (Acanthopanax) senticosus* (Siberian ginseng). Cryst. Mp 234-235°. $[\alpha]_D^{30}$ +9.6 (c, 1.15 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranoside]: [32725-74-9]
[98819-24-0] ***Calenduloside A***
$C_{42}H_{68}O_{13}$ 780.991
Isol. from roots of *Calendula officinalis* (pot marigold). Monohydrate. Mp 260-262°. $[\alpha]_D^{20}$ +41.4 (c, 0.5 in MeOH).

3-O-[β-D-Galactopyranosyl-(1→3)-β-D-glucuronopyranoside]: [26020-15-5] ***Calenduloside G***. *Calendulaglycoside G*
$C_{42}H_{66}O_{14}$ 794.975
Constit. of *Calendula officinalis* (pot marigold). Mp 117-119° dec Mp 205-210° (dihydrate). $[\alpha]_D^{20}$ +24.1 (MeOH).

3-O-[β-D-Galactopyranosyl-(1→3)-β-D-glucuronopyranoside], 6′-Me ester: [155740-15-1] ***Calenduloside G methyl ester***
$C_{43}H_{68}O_{14}$ 809.002
Constit. of *Calendula officinalis* (pot marigold). Powder. Mp 228-230°. $[\alpha]_D^{28.4}$ +22.2 (c, 0.47 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-xylopyranoside]: [215171-28-1]
$C_{41}H_{66}O_{12}$ 750.965
Constit. of the stems of *Pisum sativum* (pea).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [58231-99-5] ***Acutoside A***
$C_{42}H_{68}O_{13}$ 780.991
Constit. of *Luffa acutangula* (Chinese okra). Amorph. powder. Mp 265-270° dec. $[\alpha]_D^{24}$ +36.5 (c, 1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucuronopyranoside]: [25406-56-8] ***Spinasaponin A***
$C_{42}H_{66}O_{14}$ 794.975
Constit. of *Spinacia oleracea* (spinach).

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-glucuronopyranoside]: [38424-95-2] ***Calendulaglycoside E***. *Ladyginoside A*
$C_{42}H_{66}O_{14}$ 794.975
Isol. from *Calendula officinalis* (pot marigold). Cryst. (EtOH). Mp 240-242°. $[\alpha]_D^{20}$ +17.5 (c, 0.8 in MeOH).

Triglycosides

3-O-[α-L-Arabinopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→6)-β-D-glucopyranoside]: [189161-61-3] ***Pitheduloside B***
$C_{46}H_{74}O_{16}$ 883.081
Constit. of *Pithecellobium dulce* (Manila tamarind). Needles. Mp 220-222°. $[\alpha]_D$ +10.5 (c, 5.7 in Py).

3-O-[α-L-Arabinopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-β-D-glucuronopyranoside]: [96158-13-3] ***Momordin Ie***
$C_{46}H_{72}O_{17}$ 897.065
Constit. of *Momordica cochinchinensis* (Chinese cucumber). Powder (MeOH). $[\alpha]_D^{21}$ +20.5 (c, 1.03 in MeOH).

3-O-[α-L-Arabinopyranosyl-(1→2)-[β-D-glucopyransoyl-(1→3)]-β-D-glucuronopyranoside]: [121521-92-4] ***Durupcoside B***
$C_{47}H_{74}O_{18}$ 927.091
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. (MeOH) (as di-Me ester). Mp 227-230° (di-Me ester). $[\alpha]_D^{22}$ +8.5 (c, 0.4 in Py) (di-Me ester).

3-O-[β-D-Xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→6)-β-D-glucopyranoside]: [189161-62-4] ***Pitheduloside C***
$C_{46}H_{74}O_{16}$ 883.081
Constit. of *Pithecellobium dulce* (Manila tamarind). Needles. Mp 182-184°. $[\alpha]_D$ +3.6 (c, 3.7 in Py).

3-O-[β-D-Xylopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [119617-27-5] ***Momordin Id***

Constit. of *Momordica cochinchinensis* (Chinese cucumber). Needles (MeOH). Mp 233-235°. $[\alpha]_D^{21}$ +12.7 (c, 1.2 in MeOH).

3-O-[β-D-Xylopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [155836-04-7] ***Tarasaponin II. Elatoside A***
$C_{47}H_{74}O_{18}$ 927.091
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. Mp 198.5-200.5°. $[\alpha]_D$ +14.1 (MeOH). Tarasaponin II and Elatoside A not compared.

3-O-[β-D-Xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-3-O-acetyl-β-D-glucuronopyranoside]: [333333-27-0] ***Goyasaponin III***
$C_{49}H_{76}O_{19}$ 969.128
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{24}$ -1.9 (c, 0.5 in Py).

3-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [160845-07-8]
$C_{48}H_{78}O_{17}$ 927.134
Constit. of *Ruta graveolens* (rue). Cryst. Mp 223-224°. $[\alpha]_D^{25}$ +16.5 (MeOH).

3-O-[β-D-Galactopyranosyl-(1→2)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [156856-38-1] ***Elatoside B***
$C_{48}H_{76}O_{19}$ 957.117
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. Mp 186-187°. $[\alpha]_D$ +15.3 (MeOH).

3-O-[β-D-Galactopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]: [58231-97-3] ***Arvensoside D. Calenduloside C***
$C_{48}H_{78}O_{18}$ 943.133
Constit. of *Calendula officinalis* (pot marigold). Cryst. (MeOH). Mp 226-228°. $[\alpha]_D^{27}$ +32 (c, 0.5 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[α-L-arabinofuranosyl-(1→4)]-β-D-glucuronopyranoside]: [107656-74-6] ***Durupcoside A***
$C_{47}H_{74}O_{18}$ 927.091
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. (MeOH) (as di-Me ester). Mp 225-228° (di-Me ester). $[\alpha]_D^{22}$ -27.2 (c, 0.3 in Py) (di-Me ester).

3-O-[β-D-Glucopyranosyl-(1→3)-[α-L-arabinopyranosyl-(1→4)]-β-D-glucuronopyranoside]: [96627-79-1] ***Tarasaponin I. Stipuleanoside R_1***
$C_{47}H_{74}O_{18}$ 927.091
Constit. of *Aralia elata* (Japanese angelica tree). Needles (MeOH aq.) (as di-Me ester). Mp 196-202° dec. (di-Me ester). $[\alpha]_D$ -10.5 (c, 1.03 in MeOH) (di-Me ester).

3-O-[β-D-Glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-α-L-arabinopyranoside]: [156980-30-2] ***Elatoside E. Tarasaponin III***
$C_{46}H_{74}O_{16}$ 883.081
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. Mp 192.5-194°. $[\alpha]_D$ +43.6 (MeOH). $[\alpha]_D^{25}$ +21.2 (c, 2.1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-[β-D-galactopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [29660-93-3] ***Calendulaglycoside B***
$C_{48}H_{76}O_{19}$ 957.117
Isol. from *Calendula officinalis* (pot marigold).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucuronopyranoside]: [52657-00-8] ***Elatoside I***
$C_{48}H_{76}O_{19}$ 957.117
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. (MeOH aq.). Mp 263-265°. $[\alpha]_D^{29}$ +17.4 (c, 0.1 in MeOH).

Tetraglycosides

3-O-[α-L-Arabinopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]: [189161-87-3] ***Pitheduloside F***
$C_{52}H_{84}O_{21}$ 1045.223
Constit. of *Pithecellobium dulce* (Manila tamarind). Needles. Mp 226-228°. $[\alpha]_D$ +6.1 (c, 3.6 in Py).

3-O-[β-D-Xylopyranosyl-(1→2)-α-L-arabinopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]: [189161-92-0] ***Pitheduloside G***
$C_{52}H_{84}O_{21}$ 1045.223
Constit. of *Pithecellobium dulce* (Manila tamarind). Needles. Mp 193-195°. $[\alpha]_D$ +7.5 (c, 1.4 in Py).

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Nagao, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 599 (*Acutoside A*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2069-2071; 1994, **42**, 1354-1356 (*Elatosides*)
Ahmad, V.U. *et al., Pak. J. Sci. Ind. Res.*, 1993, **36**, 54; *CA*, **120**, 102005u (*Guaianin N*)
Srivastava, S.K. *et al., Fitoterapia*, 1994, **65**, 301 (*Ruta graveolens saponin*)
Sakai, S. *et al., Phytochemistry*, 1994, **35**, 1319-1324 (*Tarasaponins I and II*)
Satoh, Y. *et al., Phytochemistry*, 1994, **36**, 147-152 (*Tarasaponin III*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1878-1882 (*Elatoside I*)
Yoshikawa, M *et al., Heterocycles*, 1995, **41**, 1621-1626 (*Betavulgarosides*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1212-1217 (*Betavulgaroside IV*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1915; 1923 (*Elatosides A and B*)
Kang, S.S. *et al., Int. J. Pharmacogn.*, 1996, **34**, 119-123; *CA*, **125**, 110261t (*Durupcosides A and B*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 561 (*Betavulgarosides, abs config*)
Nigam, S.K. *et al., Phytochemistry*, 1997, **44**, 1329 (*Pithedulosides*)
Yadava, R.N. *et al., CA*, 1998, **129**, 335563a (*3-glucosylxyloside*)
Yoshikawa, M. *et al., Heterocycles*, 1998, **49**, 93-96 (*Spinacoside D*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1717-1724 (*Betavulgaroside IV, abs config*)
Lavaud, C. *et al., Fitoterapia*, 2000, **71**, 338-340 (*Calenduloside E, pmr, cmr*)
Gao, C. *et al., Yunnan Zhiwu Yanjiu*, 2000, **22**, 103-108; *CA*, **133**, 161775m (*Hemsloside AM1*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 54-63 (*Goyasaponin III*)

Oleanolic acid glycosyl esters O-148

Saponins of 3-Hydroxy-12-oleanen-28-oic acid, H-663 that have glycosyl esters at 28 but no glycosides at 3.

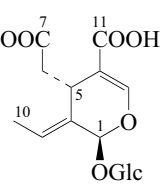
Monoglycosides

Me ether, β-D-glucopyranosyl ester: [51996-63-5]
$C_{37}H_{60}O_8$ 632.876
Isol. from *Calendula officinalis* (pot marigold).

Takabe, S. *et al., Carbohydr. Res.*, 1979, **76**, 101-108 (*Cussonoside B, synth*)
Kikuchi, M. *et al., Yakugaku Zasshi*, 1982, **102**, 533 (*Ligustrin A*)
Akai, E. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3715-3723 (*Rotundiosides B and C*)
Dubois, M.A. *et al., Planta Med.*, 1986, **52**, 80-83 (*Cussonoside B*)
Shao, Y. *et al., Planta Med.*, 1995, **61**, 446-449 (*Asteryunnanoside F*)
Koichi, M. *et al., Phytochemistry*, 1997, **46**, 977-979 (*Ligustrins*)
Grishkovets, V.I. *et al., Khim. Prir. Soedin.*, 1999, **35**, 87-90; *Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 70-72 (*Helicoside L-8a*)

Oleoside O-149

[178600-68-5]



$C_{16}H_{22}O_{11}$ 390.343

There is considerable confusion regarding the struct. of Oleoside. Both the 11-methyl ester and the 7,11-dimethyl ester have erroneously been described as Oleoside in some papers.

11-Me ester: [60539-23-3] ***Oleoside 11-methyl ester***
$C_{17}H_{24}O_{11}$ 404.37
Constit. of *Jasminum sambac* (Arabian jasmine). Amorph. solid. $[\alpha]_D^{24}$ -176 (c, 0.3 in MeOH).

Di-Me ester: [30164-95-5] ***Oleoside dimethyl ester.*** *Secologanoside 7-methyl ester*
$C_{18}H_{26}O_{11}$ 418.397
Constit. of *Olea europaea* (olive).

Amorph. powder. $[\alpha]_D$ -115 (MeOH). The name Secologanoside 7-methyl ester ($\Delta^{8(9)}$) is not consistent with the struct. of Secologanin ($\Delta^{8(10)}$).

7-β-D-Glucopyranosyl ester, 11-Me ester: [115623-36-4] ***Methyl glucooleoside***
$C_{23}H_{34}O_{16}$ 566.512
Powder. $[\alpha]_D^{16}$ -164.7 (c, 0.51 in MeOH).

1,5-Diepimer, 11-Me ester: [180063-39-2] ***Jaspolyside***
$C_{17}H_{24}O_{11}$ 404.37
Amorph. solid. $[\alpha]_D^{24}$ -53 (c, 0.075 in MeOH).

10-Hydroxy: See 10-Hydroxyoleoside in *The Combined Chemical Dictionary.*

Inouye, H. *et al., Tetrahedron*, 1974, **30**, 201 (*Oleoside, struct*)
Gariboldi, P. *et al., Phytochemistry*, 1986, **25**, 865 (*di-Me ester*)
Tanahashi, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 5032 (*11-Me ester*)
Kuwajima, H. *et al., Phytochemistry*, 1989, **28**, 1409 (*derivs*)
Damtoft, S. *et al., Phytochemistry*, 1992, **31**, 4197; 1993, **34**, 1291 (*biosynth, pmr, cmr*)
Sugiyama, M. *et al., Phytochemistry*, 1993, **34**, 1169 (*di-Me ester*)
Damtoft, S. *et al., Phytochemistry*, 1995, **40**, 773 (*biosynth*)
Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Peking)*, 1996, **43**, 171 (*isol, pmr, cmr*)
Shen, Y.-C. *et al., Phytochemistry*, 1996, **42**, 1629 (*Jaspolyside*)
Kuwajima, H. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1634-1637 (*biosynth*)

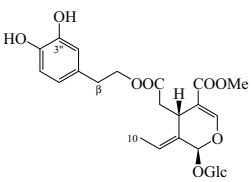
Oleracins O-150

Structs. unknown. Betacyanin pigments from *Portulaca oleracea* (purslane) stems. Oleracins I and II recognised.

Piattelli, M. *et al., Phytochemistry*, 1964, **3**, 547

Oleuropein O-151

[32619-42-4]



Absolute Configuration

$C_{25}H_{32}O_{13}$ 540.52
Bitter principle of olives. Nutriceutical with antioxidant props.. Cryst. (EtOAc). Mp 89-91°. $[\alpha]_D^{26}$ -168 (c, 0.67 in MeOH). Log P -1.75 (uncertain value) (calc). Artifact λ_{max} 228 (ϵ 17900); 233 (ϵ 15850); 280 (ϵ 5250); 284 (ϵ 3020) (MeOH) (Berdy). λ_{max} 230 (E1%/1cm 277); 232 (ϵ 14135); 282 (ϵ 2973); 326 (E1%/1cm 49) (EtOH) (Berdy).

► LD_{50} (mus, ipr) 1300 mg/kg , LD_{50} (mus, orl) 3000 mg/kg.

Parent acid: [52077-55-1] ***Demethyloleuropein***
$C_{24}H_{30}O_{13}$ 526.493
Present in olive fruits and the bark of *Syringa vulgaris*. Indicator of maturity in olives which increases as the fruit ripens. Cryst. (EtOH). Mp 145-147°. $[\alpha]_D^{20}$ -157 (c, 0.4 in EtOH).

3″-Deoxy: [35897-92-8] ***Ligustroside.*** *Ligstroside*
$C_{25}H_{32}O_{12}$ 524.521
Found in olives (*Olea europaea*). Noncryst. $[\alpha]_D$ -110.7 (c, 1 in EtOH). $[\alpha]_D^{20}$ -181.1 (c, 0.6 in MeOH).

10-Acetoxy: ***10-Acetoxyoleuropein***
$C_{27}H_{34}O_{15}$ 598.557
Constit. of osmanthus leaves (*Osmanthus fragrans*). Powder. $[\alpha]_D^{21}$ -191 (c, 1.1 in MeOH).

10-Acetoxy, 3″-deoxy: [57799-95-8] ***10-Acetoxyligustroside***
$C_{27}H_{34}O_{14}$ 582.557
Constit. of osmanthus leaves (*Osmanthus fragrans*). Powder. $[\alpha]_D^{18}$ -143.9 (c, 1 in MeOH).

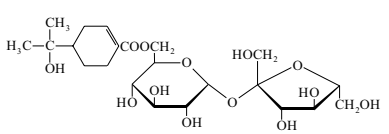
*β-Methoxy(*R-*):* [256498-10-9] *β-Methoxyoleuropein.* ***2″-Methoxyoleuropein***
$C_{26}H_{34}O_{14}$ 570.546
Constit. of *Jasminum officinale* var. *grandiflorum* (royal jasmine). Amorph. powder. $[\alpha]_D^{24}$ -172 (c, 1 in MeOH). λ_{max} 233 (log ϵ 4.22); 281 (log ϵ 3.5) (MeOH).

*β-Methoxy(*S-*):* [256498-11-0]
$C_{26}H_{34}O_{14}$ 570.546
Constit. of *Jasminum officinale* var. *grandiflorum* (royal jasmine). Amorph. powder. $[\alpha]_D^{25}$ -121 (c, 0.98 in MeOH). λ_{max} 232 (log ϵ 4.15); 281 (log ϵ 3.4) (MeOH).

Shasha, B. *et al., J.O.C.*, 1961, **26**, 1948 (*isol*)
Panizzi, L. *et al., Gazz. Chim. Ital.*, 1965, **95**, 1279 (*isol*)
Asaka, Y. *et al., Chem. Lett.*, 1972, 141 (*isol, struct*)
Inouye, H. *et al., Chem. Pharm. Bull.*, 1974, **22**, 676 (*biosynth*)
Inouye, H. *et al., Tetrahedron*, 1974, **30**, 201 (*abs config*)
Inouye, H. *et al., Phytochemistry*, 1975, **14**, 304; 2029; 1982, **21**, 2305 (*10-Acetoxyoleuropein, 10-Acetoxyligustroside*)
Inouye, H. *et al., J. Chromatogr.*, 1976, **118**, 201 (*ms*)
Kikuchi, M. *et al., CA*, 1985, **103**, 147026 (*isol, pmr, cmr*)
Kurkin, V.A. *et al., Khim. Prir. Soedin.*, 1990, **26**, 695-697; *Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 592-593 (*Demethyloleuropein*)
Bianco, A. *et al., J. Nat. Prod.*, 1992, **55**, 760 (*synth*)
Shen, Y.-C. *et al., J. Chin. Chem. Soc. (Peking)*, 1996, **43**, 171 (*pmr, cmr*)
Esti, M. *et al., J. Agric. Food Chem.*, 1998, **46**, 32-35 (*occur*)
Tanahashi, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1582-1586 (*β-methoxy derivs*)

6-*O*-Oleuropeoylsucrose O-152

[17651-05-7]
6-[4-(1-Hydroxy-1-methylethyl)-1-cyclohexene-1-carboxylate] sucrose, 8CI

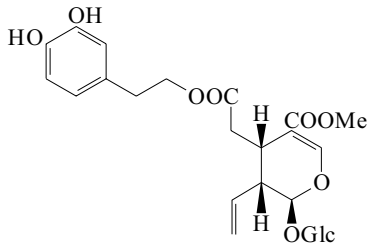


$C_{22}H_{36}O_{13}$ 508.519
Constit. of the root bark of the olive (*Olea europaea*). Cryst. (EtOH). Mp 199-200°. $[\alpha]_D^{28}$ -3.9 (c, 1.1 in H_2O).

Scarpati, M.L. *et al., Tet. Lett.*, 1966, 5673 (*isol*)

Oleuroside O-153

[116383-31-4]



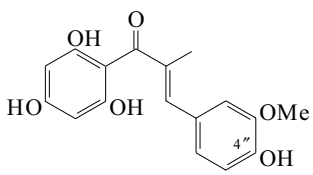
$C_{25}H_{32}O_{13}$ 540.52
Constit. of *Olea europaea* (olive). Powder. $[\alpha]_D^{17}$ -83.7 (c, 1.03 in MeOH).

Hexa-Ac:
Needles (EtOH). Mp 122-123°. $[\alpha]_D^{17}$ -82.8 (c, 1 in $CHCl_3$).

Kuwajima, H. *et al., Phytochemistry*, 1988, **27**, 1757

Olivin O-154

3-(4-Hydroxy-3-methoxyphenyl)-2-methyl-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one. 2′,4,4′,6-Tetrahydroxy-3-methoxy-α-methylchalcone



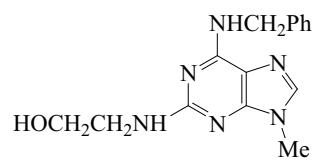
$C_{17}H_{16}O_6$ 316.31
Claimed to be isol. from olive leaves *Olea europaea*, along with a glucoside, but this could not be substantiated. Cryst. (EtOH/EtOAc). Mp 300°.

4″-O-(Glucosylglucoside): ***Olivin 4-diglucoside***
$C_{29}H_{36}O_{16}$ 640.594
Isol. from *Olea europaea* (olive). Cryst. (MeOH aq.). Mp 220-225°. $[\alpha]_D^{20}$ -61.7 (Py).

Bočková, H. *et al., Coll. Czech. Chem. Comm.*, 1964, **29**, 1484 (*isol, uv, ir, struct*)
Hänsel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1970, **303**, 860

Olomoucine O-155

[101622-51-9]
2-[[9-Methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]ethanol, 9CI. 6-(Benzylamino)-2-(2-hydroxyethylamino)-9-methylpurine



$C_{15}H_{18}N_6O$ 298.347

Constit. of the cotyledons of radish. Cryst. (MeOH/EtOAc/petrol). Mp 126°. λ_{max} 232 (ϵ 23260); 290 (ϵ 12880) (EtOH aq.).

Parker, C.W. *et al., Phytochemistry*, 1986, **25**, 303-310 (*synth*)
Tao, G.Q. *et al., J. Plant Growth Regul.*, 1991, **10**, 179-185 (*isol*)
Schulze-Gahmen, U. *et al., Proteins*, 1995, **22**, 378-391 (*cryst struct with ATP*)
Havlicek, L. *et al., J. Med. Chem.*, 1997, **40**, 408-412 (*synth, activity*)
Nugiel, D.A. *et al., J.O.C.*, 1997, **62**, 201-203 (*synth*)

Omega-3 Marine Triglycerides, BAN — O-156

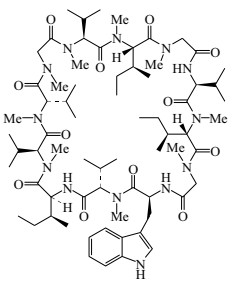
Maxepa

Mixt. of fatty acid triglycerides (from marine fish) containing 18% 5,8,11,14,17-Eicosapentaenoic acid, E-16 and 12% 4,7,10,13,16,19-Docosahexaenoic acid, D-998. Mixt. of fatty acid triglycerides (from marine fish) containing 18% 5,8,11,14,17-Eicosapentaenoic acid, E-16 and 12% 4,7,10,13,16,19-Docosahexaenoic acid, D-998. Reduces plasma triglycerides; dietary supplement. Component of numerous preparations.

Glomset, J.A. *et al., N. Engl. J. Med.*, 1985, **312**, 1253 (*rev*)
Ballard-Barbash, R. *et al., Lancet*, 1988, **1**, 1081 (*rev*)
Lees, R.S. *et al., Omega-3 Fatty Acids Health Dis., 1990*, M. Dekker, New York (see *Food Sci. Technol.* (N.Y.), v37 1990), 1990, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 991

Omphalotin A — O-157

[186511-50-2]



Absolute Configuration

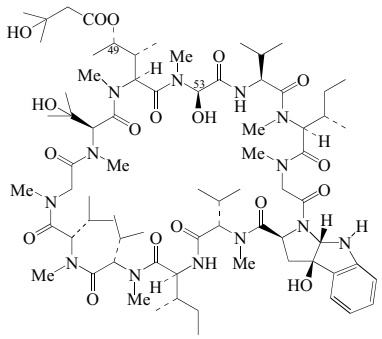
$C_{69}H_{115}N_{13}O_{12}$ 1318.747

Cyclic peptide. Prod. by *Omphalotus olearius* (common chanterelle). Oil. Sol. MeOH, Me_2CO, 2-propanol; fairly sol. EtOAc; poorly sol. cyclohexane.

Mayer, A. *et al., Nat. Prod. Lett.*, 1997, **10**, 25-32; 33-38 (*isol, ir, pmr, cmr*)
Buechel, E. *et al., Tetrahedron*, 1998, **54**, 5345-5352 (*abs config*)
Sewald, N. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 4661-4663 (*synth*)
Thern, B. *et al., Angew. Chem., Int. Ed.*, 2002, **114**, 2401-2403 (*synth*)

Omphalotin B — O-158

[208394-46-1]



$C_{74}H_{123}N_{13}O_{18}$ 1482.862

Cyclic peptide. Prod. by *Omphalotus olearius* (common chanterelle). Cryst. Sol. MeOH, $CHCl_3$, Me_2CO; poorly sol. H_2O. Mp 180-183°. $[\alpha]_D^{22}$ -246 (c, 1 in MeOH).

*53-Ac:**Omphalotin C***
$C_{76}H_{125}N_{13}O_{19}$ 1524.899
Prod. by *Omphalotus olearius* (common chanterelle). Cryst. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. Mp 173-178°. $[\alpha]_D^{22}$ -242 (c, 1 in MeOH).

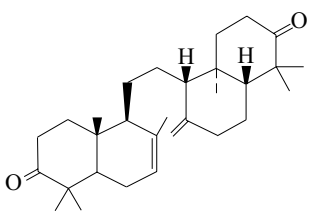
*49-Deacyl, 49,53-di-Ac:**Omphalotin D***
$C_{73}H_{119}N_{13}O_{18}$ 1466.819
Prod. by *Omphalotus olearius* (common chanterelle). Cryst. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. H_2O. Mp 165-170°. $[\alpha]_D^{22}$ -254 (c, 1 in MeOH).

Buechel, E. *et al., Tetrahedron*, 1998, **54**, 5345-5352 (*isol, pmr, cmr*)

7,14(27)-Onoceradiene-3,21-dione — O-159

[19940-78-4]

α,γ-Onoceradienedione

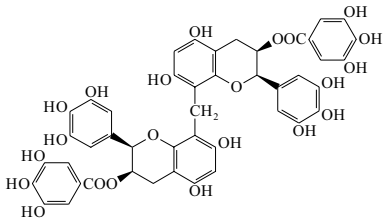


$C_{30}H_{46}O_2$ 438.692
Constit. of *Lansium domesticum* (langsat). Cryst. Mp 127-128°.

Habaguchi, K. *et al., Tet. Lett.*, 1968, 3731

Oolonghomobisflavan A — O-160

[126737-60-8]

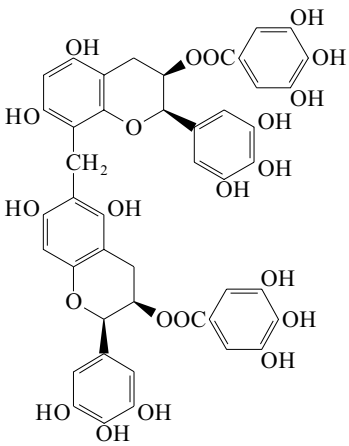


$C_{45}H_{36}O_{22}$ 928.766
Constit. of oolong tea. Tan powder + $4H_2O$. $[\alpha]_D^{26}$ -271 (c, 1 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3255 (*isol, struct*)

Oolonghomobisflavan B — O-161

[126715-88-6]

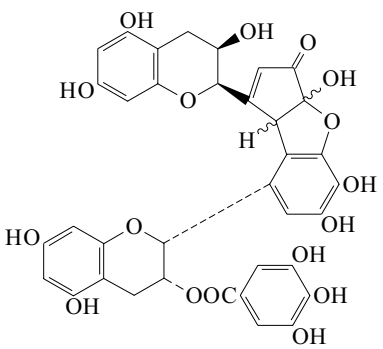


$C_{45}H_{36}O_{22}$ 928.766
Isol. from oolong tea. Tan powder + $3H_2O$. $[\alpha]_D^{26}$ -205 (c, 1 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3255 (*isol, struct*)

Oolongtheanin — O-162

[116310-05-5]



$C_{36}H_{28}O_{17}$ 732.607
Isol. from *Camellia sinensis* var. *viridis* (oolong tea). Off-white powder + $2H_2O$. $[\alpha]_D^{21}$ -112.9 (c, 0.9 in Me_2CO).

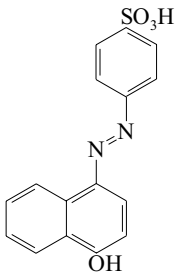
Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1676 (*isol, pmr, cmr, struct*)

Orange I O-163

[523-44-4]

[574-69-6]

4-[(4-Hydroxy-1-naphthalenyl)azo]benzenesulfonic acid, 9CI. 4-(4-Sulfophenylazo)-1-naphthol. C.I. Acid Orange 20. α-Naphthol orange. Tropaeolin 000. C.I. 14600



$C_{16}H_{12}N_2O_4S$ 328.348

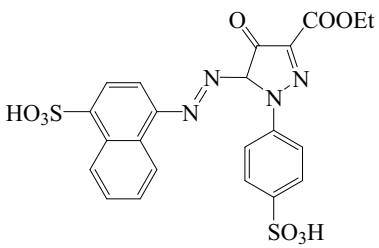
Strictly, the name Orange I and other synonyms apply to the sodium salt. CAS no. refers to Na salt. Formerly used as a food colouring; now banned by the FDA. Reddish-brown powder giving orange soln. (Na salt). Na salt sol. H_2O; sl. sol. EtOH; insol. common org. solvs. Banned by the FDA for food use.

Whitmore, W.F. *et al., J.A.C.S.*, 1937, **59**, 1501
Fierz-David, H.E. *et al., Helv. Chim. Acta*, 1946, **29**, 1718
Colour Index, 3rd Ed., 1971, **4**, 4065 (*rev*)
IARC Monog., 1975, **8**, 173; *Suppl.* 7, 69 (*rev, tox*)
Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, (*use, ind*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG010

Orange B O-164

[15139-76-1]

*Ethyl 4,5-dihydro-5-oxo-4-[(4-sulfo-1-naphthalenyl)azo]-1-(4-sulfophenyl)-1H-pyrazole-3-carboxylate, 9CI. Ethyl 5-oxo-4-[(4-sulfo-1-naphthyl)azo]-1-(*p*-sulfophenyl)-2-pyrazoline-3-carboxylate, 8CI. C.I. 19235. C.I. Acid Orange 137*



$C_{22}H_{18}N_4O_9S_2$ 546.538

Oxo-hydrazone ArNHN=C-CO- and azoenol ArN=NC=C(OH)- tautomers also possible and are likely to predominate. Colourant for frankfurter and sausage casings. Dull orange cryst. Trade names and CAS no. refer to the di-Na salt.

U.S. Pat., 1966, 3 285 906; *CA*, **66**, 30016q (*synth, use, uv*)
Collins, T.F.X. *et al., Toxicol. Ind. Health*, 1995, **11**, 387-397; 1996, **12**, 45-57 (*tox*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2054-2055 (*use*)

Orcein O-165

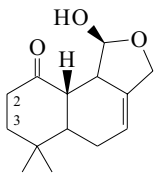
[1400-62-0]

C.I. Natural Red 28

Reddish-brown dye; a mixt. of 14 compds. with a phenoxazone struct.. Once used as a food colouring but now banned throughout the EC. Dark brown cryst.

Musso, H. *et al., Chem. Ber.*, 1956, **89**, 1659-1673; 1957, **90**, 1808-1814 (*isol, struct*)
Musso, H. *et al., Planta Med.*, 1960, **8**, 431-446 (*struct*)
Beecken, H. *et al., Angew. Chem.*, 1961, **73**, 665-688 (*rev, struct*)

Oreadone O-166



$C_{14}H_{20}O_3$ 236.31

Formyl: **O-*Formyloreadone***
$C_{15}H_{20}O_4$ 264.321
Metab. of *Marasmius oreades* (fairy ring mushroom). Glass. $[\alpha]_D^{24}$ +278 (c, 0.07 in MeOH).

3α-Hydroxy: [124869-06-3] ***3α-Hydroxyoreadone***
$C_{14}H_{20}O_4$ 252.31
Metab. of *Marasmius oreades* (fairy ring mushroom). Prisms (CH_2Cl_2/hexane). Mp 103-108°. $[\alpha]_D^{24}$ +130.2 (c, 1 in MeOH).

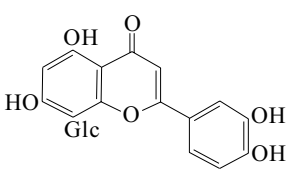
2,3-Didehydro: [124869-07-4] ***Dehydrooreadone***
$C_{14}H_{18}O_3$ 234.294
Metab. of *Marasmius oreades* (fairy ring mushroom). Solid.

Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371 (*isol, pmr, cmr, struct*)

Orientin O-167

[28608-75-5]

8-β-D-Glucopyranosyl-3′,4′,5,7-tetrahydroxyflavone. 8-β-D-Glucopyranosylluteolin. 8-Glucosylluteolin. Lutexin



$C_{21}H_{20}O_{11}$ 448.382

Isol. from *Hordeum vulgare* (barley) and *Passiflora incarnata* (maypops). Pale yellow cryst. (EtOH aq.). Mp 265-267° dec. $[\alpha]_D^{20}$ +18.4 (c, 1.4 in Py).

▶ DJ3009300

7-O-Sulfate:
$C_{21}H_{20}O_{14}S$ 528.447

7-O-β-D-Glucopyranoside: [61361-16-8]
$C_{27}H_{30}O_{16}$ 610.524

7-O-(O-Sulfatoglucoside):
$C_{27}H_{30}O_{19}S$ 690.589

3′-O-β-D-Glucopyranoside: [85708-47-0]
$C_{27}H_{30}O_{16}$ 610.524

4′-O-β-D-Glucopyranoside: [38950-95-7]
$C_{27}H_{30}O_{16}$ 610.524

7-O-α-L-Rhamnopyranoside: [29432-29-9]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Linum usitatissimum*.

2″-Ac: [71880-89-2] ***2″-O-Acetylorientin***
$C_{23}H_{22}O_{12}$ 490.42
Light yellow cryst. (EtOH aq.). Mp 236-237°.

6″-Ac: [112160-04-0] ***6″-O-Acetylorientin***
$C_{23}H_{22}O_{12}$ 490.42
Mp 190-193°. $[\alpha]_D^{24}$ -58.7 (c, 0.13 in Py).

2″,6″-Di-Ac: [131507-99-8] ***2″,6″-Diacetylorientin***
$C_{25}H_{24}O_{13}$ 532.457
Isol. from *Rumex acetosa* (sorrel). Yellow prisms (MeCN aq.). Mp 175-176°. $[\alpha]_D^{21}$ +36 (c, 0.69 in MeOH).

2″-O-(3,4,5-Trihydroxybenzoyl): ***2″-O-Galloylorientin***
$C_{28}H_{24}O_{15}$ 600.489
Yellow amorph. powder. $[\alpha]_D^{20}$ -228.7 (c, 0.15 in MeOH).

2″-O-(3,4-Dihydroxycinnamoyl): ***2″-O-Caffeoylorientin***
$C_{30}H_{26}O_{14}$ 610.527
λ_{max} 249 ; 272 (sh) ; 295 (sh) ; 336 (MeOH).

5-Me ether: [6980-21-8] ***Parkinsonin A***
$C_{22}H_{22}O_{11}$ 462.409
Yellow cryst. + $1H_2O$ (EtOH aq.). Mp 224° dec. $[\alpha]_D^{28}$ -32 (c, 0.52 in Py).

7-Me ether: [6980-41-2] ***Isoswertiajaponin***
$C_{22}H_{22}O_{11}$ 462.409
Isol. from *Gnetum gnemon* (bago). Yellow cryst. (Me_2CO/MeOH). Mp 258-261° dec. (252°).

3′-Me ether: 8-Glucosyl-4′,5,7-trihydroxy-3′-methoxyflavone, G-205

4′-Me ether: [15822-81-8] *8-Glucopyranosyldiosmetin*
$C_{22}H_{22}O_{11}$ 462.409
Cryst. (MeOH). Mp 267-268°.

3′,7-Di-Me ether: [89915-55-9]
$C_{23}H_{24}O_{11}$ 476.436
Isol. from a hybrid sugarcane (*Saccharum*) mill syrup.

2″-O-β-L-Arabinofuranosyl:
$C_{26}H_{28}O_{15}$ 580.498

2″-O-β-Arabinopyranosyl:Orientin 2″-arabinopyranoside
$C_{26}H_{28}O_{15}$ 580.498

2″-O-β-Arabinopyranosyl, 7-Me ether:Isoswertiajaponin 2″-arabinoside
$C_{27}H_{30}O_{15}$ 594.525

2″-O-β-D-Xylopyranosyl: [11003-05-7] ***Adonivernitol***. *Adonivernith*
$C_{26}H_{28}O_{15}$ 580.498
Yellow needles (EtOH). Mp 204°. $[\alpha]_D^{22}$ -67.3 (c, 0.74 in Py).

6″-O-β-D-Xylopyranosyl:
$C_{26}H_{28}O_{15}$ 580.498
Mp 202-205° dec. $[\alpha]_D^{20}$ -22 (c, 1.0 in EtOH).

2″-O-β-D-Glucopyranosyl: [64661-76-3]
Flavocannabiside
$C_{27}H_{30}O_{16}$ 610.524
Pale yellow cryst. Mp 213.5-214° dec.

2″-O-α-L-Rhamnopyranosyl: [81398-30-3]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Fortunella japonica* (round kumquat). Yellow needles. Mp 225-227° (218-220°).

2″-O-α-L-Rhamnopyranosyl, 4′-O-β-D-glucopyranoside: [87454-41-9]
$C_{33}H_{40}O_{20}$ 756.667

2″-O-α-L-Rhamnopyranosyl, 4′-Me ether: [98891-92-0]
$C_{28}H_{32}O_{15}$ 608.552
Isol. from *Fortunella japonica* (round kumquat). Yellow needles. Mp 214-216°.

4″-O-α-L-Rhamnopyranosyl, 4′-Me ether: [229471-74-3]
$C_{28}H_{32}O_{15}$ 608.552
Yellowish-brown solid. Mp 211-213°. $[\alpha]_D^{24}$ -18 (c, 0.3 in MeOH). λ_{max} 211 ; 240 ; 271 ; 342 (MeOH).

2″-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranosyl]:
$C_{33}H_{40}O_{20}$ 756.667

1″-Epimer: [7480-94-6] ***Epiorientin***. *8-C-α-D-Glucopyranosylluteolin*
$C_{21}H_{20}O_{11}$ 448.382
Light yellow cryst. (EtOH). Mp 300°.

1″-Epimer, 5,7-di-Me ether: [6980-22-9]
Parkinsonin B
$C_{23}H_{24}O_{11}$ 476.436
Yellow prisms + $1H_2O$ (MeOH). Mp 300°.

Siekel, W. *et al., J.O.C.*, 1959, **24**, 1995 (*isol*)
Koeppen, H. *et al., Biochem. J.*, 1962, **83**, 507; 1965, **97**, 444 (*isol, synth*)
Horowitz, S. *et al., Chem. Ind. (London)*, 1964, 499 (*isol*)
Koeppen, B.H. *et al., Z. Naturforsch., B*, 1964, **19**, 173 (*pmr*)
Chopin, J. *et al., Tet. Lett.*, 1966, 3657 (*synth*)
Bhatia, V.K. *et al., Tetrahedron*, 1966, **22**, 1147 (*Parkinsonin*)
Komatsu, M. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1567 (*Isoswertiajaponin*)
Bhatia, V.K. *et al., Phytochemistry*, 1967, **6**, 1033 (*Epiorientin, Parkinsonin B*)
Gentili, B. *et al., J.O.C.*, 1968, **33**, 1571 (*4′-Me ether*)
Chernobai, V.T. *et al., Khim. Prir. Soedin.*, 1968, **4**, 51; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 43 (*6″-xylosyl*)
Williams, C.A. *et al., Phytochemistry*, 1972, **11**, 2507; 1973, **12**, 2417; 1974, **13**, 1557 (*4′-glucoside, sulfates*)
Seshadri, R. *et al., Indian J. Chem.*, 1974, **12**, 783 (*isol*)
Zemtsova, G.N. *et al., Khim. Prir. Soedin.*, 1975, **11**, 516; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 538 (*isol*)
Wagner, H. *et al., Phytochemistry*, 1975, **14**, 1089 (*Adonivernith*)
Paris, R.R. *et al., Plant. Med. Phytother.*, 1976, **10**, 144 (*7-glucoside*)
Yoshizaki, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 3408 (*isol*)
Komissarenko, N.F. *et al., Khim. Prir. Soedin.*, 1977, **13**, 287; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 252 (*isol*)
Segelman, A.B. *et al., Phytochemistry*, 1978, **17**, 824 (*Flavocannabiside*)
Kitanov, G. *et al., Khim. Prir. Soedin.*, 1979, **15**, 154; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 129 (*2″-Ac*)
Nichols, K.W. *et al., Phytochemistry*, 1979, **18**, 1078 (*4′-Me ether*)
Markham, K.R. *et al., Phytochemistry*, 1980, **19**, 415 (*2″-arabinofuranoside*)
Smith, D.M. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 37 (*rutinoside*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2342 (*Isoswertiajaponin*)
Nikolov, N. *et al., Planta Med.*, 1982, **44**, 50 (*2″-rhamnoside*)
Escobar, L.K. *et al., Phytochemistry*, 1983, **22**, 796 (*derivs*)
Mabry, T.J. *et al., J. Nat. Prod.*, 1984, **47**, 127 (*3′,7-di-Me ether*)
Kumamoto, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 2613 (*2″-rhamnoside*)
Wilson, A. *et al., Phytochemistry*, 1985, **24**, 1685 (*7-glucoside*)
Congora, C. *et al., Helv. Chim. Acta*, 1986, **69**, 251 (*isol*)
Hori, K. *et al., Yakugaku Zasshi*, 1987, **107**, 774 (*6″-Ac*)
Kato, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2277 (*2″,6″-Diacetylorientin*)
Webby, R.F. *et al., Phytochemistry*, 1994, **36**, 1323 (*2″-arabinopyranosides*)
Greca, M.D. *et al., Phytochemistry*, 1998, **49**, 1299-1304 (*Isoswertiajaponin*)
Leitao, S.G. *et al., Phytochemistry*, 1998, **49**, 2167-2169 (*2″-Caffeoylorientin*)
Ali, Z. *et al., Nat. Prod. Lett.*, 1999, **13**, 121-129 (*4′-Me 4″-rhamnosyl*)
Kumazawa, T. *et al., Carbohydr. Res.*, 2001, **334**, 183-193 (*synth*)
Latté, K.P. *et al., Phytochemistry*, 2002, **59**, 419-424 (*2″-Galloylorientin*)

Ornithinoalanine O-168

N^5-*(2-Amino-2-carboxyethyl)ornithine, 9CI*
$HOOCCH(NH_2)CH_2NH(CH_2)_3CH(NH_2)COOH$
$C_8H_{17}N_3O_4$ 219.24

DL-L-*form* [25693-39-4]
Amino acid formed by alkaline hydrol. of silk, wool and other proteins, esp. lactalbumin and caseins. Present in Mozzarella cheese. Mp 190°.

Hydrochloride:
Hygroscopic cryst. + $1H_2O$ (EtOH aq.).

Picrate:
Mp 185-188°.

DL-DL-*form* [27686-06-2]
Mp 200° dec.

Ziegler, K. *et al., Nature (London)*, 1967, **214**, 404 (*isol, synth*)
Pedro, M. *et al., CA*, 1969, **71**, 50494a; 1970, **72**, 67263t (*synth*)
Boschin, G. *et al., J. Agric. Food Chem.*, 1999, **47**, 939-944 (***synth, pmr, hplc***)

Ornithokinin O-169

[14042-92-3]
6-L-Threonine-8-L-leucinebradykinin
H-Arg-Pro-Pro-Gly-Phe-Thr-Pro-Leu-Arg-OH
$C_{48}H_{77}N_{15}O_{11}$ 1040.23
Analogue of Bradykinin. Isol. from chicken blood. No phys. props. reported.

Kimura, M. *et al., Eur. J. Biochem.*, 1987, **168**, 493; 1988, **172**, 784 (*isol, struct*)

N-Ornithyltaurine O-170

2-[(2,5-Diamino-1-oxopentyl)amino]ethanesulfonic acid, 9CI
$H_2N(CH_2)_3CH(NH_2)CONHCH_2CH_2SO_3H$
$C_7H_{17}N_3O_4S$ 239.295

(*S*)-*form* [98349-67-8]
L-form
Proposed salt substitute esp. for soy sauce. The originally-claimed saltiness at this compound was disputed, but has subsequently been confirmed. Hygroscopic solid. $[\alpha]_D^{25}$ -0.1 (c, 1 in H_2O).

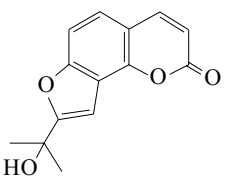
Hydrochloride: [90970-64-2]
Equal to NaCl in saltiness. Cryst. + $1H_2O$. Mp 125-130°. $[\alpha]_D^{25}$ +8.5 (c, 1 in H_2O).

N^{α},N^{δ}-*Bis(benzyloxycarbonyl):* [90990-60-6]
Cryst. + $2.5H_2O$. Mp 85-88°. $[\alpha]_D^{25}$ -13.5 (c, 1 in H_2O).

Huynh-ba, T. *et al., J. Agric. Food Chem.*, 1987, **35**, 165-168; 1990, **38**, 1993 (*synth, props*)
Nakamura, K. *et al., J. Agric. Food Chem.*, 1990, **38**, 1994; 1996, **44**, 2481-2485 (*synth, props*)

Oroselol O-171

[1891-25-4]
8-(1-Hydroxy-1-methylethyl)-2H-furo[2,3-h]-1-benzopyran-2-one, 9CI, 8CI



$C_{14}H_{12}O_4$ 244.246
Cryst. Mp 156-157°.

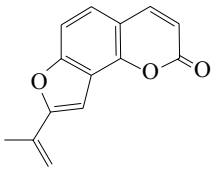
Me ether: ***Archangin***
$C_{15}H_{14}O_4$ 258.273
From *Angelica archangelica* (angelica). Cryst. (Et_2O/petrol). Mp 116-118°. Artifact.

O-*β-D-Glucopyranoside:* [161842-80-4]
Edulisin VI
$C_{20}H_{22}O_9$ 406.388
Constit. of the fruit of *Angelica edulis*.

Halpern, O. *et al., Helv. Chim. Acta*, 1957, **40**, 758 (*isol*)
Nielsen, B.E. *et al., Acta Chem. Scand.*, 1964, **18**, 932 (*struct*)
Grenz, M. *et al., Chem. Ber.*, 1969, **102**, 1673 (*isol*)
Lemmich, E. *et al., Acta Chem. Scand.*, 1970, **24**, 2893 (*isol*)
Gonzáles, A.G. *et al., An. Quim.*, 1976, **72**, 568 (*isol*)
Duffley, R.P. *et al., Synth. Commun.*, 1977, **8**, 175 (*synth*)
Bose, A.K. *et al., Tetrahedron*, 1979, **35**, 13 (*cmr*)
Zubia, E. *et al., Tetrahedron*, 1992, **48**, 4239 (*synth*)
Mizuno, A. *et al., Chin. J. Phys. (Taipei)*, 1994, **46**, 249; *CA*, **122**, 209702n (*Edulisin VI*)
Lee, Y.R. *et al., Tetrahedron*, 1995, **51**, 3087 (*synth, pmr*)

Oroselone O-172

[1760-27-6]
*8-(1-Methylethenyl)-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9CI. Kvannin*



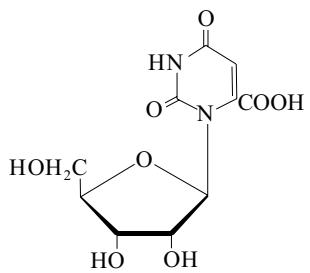
$C_{14}H_{10}O_3$ 226.231
Constit. of *Angelica archangelica* (angelica). Cryst. Mp 188-189° (170-174°).

1′,2′-Dihydro, 1′-hydroxy: Oroselol, O-171

Halpern, O. *et al., Helv. Chim. Acta*, 1957, **40**, 758
Steck, W. *et al., Can. J. Chem.*, 1969, **47**, 2425
Zakharov, P.I. *et al., Khim. Prir. Soedin.*, 1974, **10**, 560; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 575 (*ms*)
Schreiber, F.G. *et al., J. Chem. Res., Synop.*, 1978, 92 (*synth*)
Zubia, E. *et al., Tetrahedron*, 1992, **48**, 4239 (*synth*)
Lee, Y.R. *et al., Tetrahedron*, 1995, **51**, 3087 (*synth, pmr*)

Orotidine O-173

[314-50-1]
1,2,3,6-Tetrahydro-2,6-dioxo-3-β-D-ribofuranosyl-4-pyrimidinecarboxylic acid, 9CI. 3-β-D-Ribofuranosylorotic acid, 8CI. 6-Carboxyuridine, 8CI



$C_{10}H_{12}N_2O_8$ 288.213
Isol. from *Phaseolus vulgaris* (kidney bean). Mp 200° (turns brown near). λ_{max} 267 (ϵ 9570) (0.1*N* HCl) (Derep). λ_{max} 265 (ϵ 8960) (0.1*N* NaOH) (Derep). λ_{max} 268 (ϵ 8900) (MeOH) (Derep).

Cyclohexylammonium salt:
Mp 182-183.5° dec. λ_{max} 265 (ϵ 9700) (0.1*M* HCl). λ_{max} 265 (ϵ 7750) (0.1*M* NaOH).

5′-Phosphate: [2149-82-8] *Orotidine 5′-(dihydrogen phosphate), 8CI. Orotidylic acid. OMP*
$C_{10}H_{13}N_2O_{11}P$ 368.193
Formed in the biosynthetic pathway in yeast. Trihydrate (as Na salt).

Moffatt, J.G. *et al., J.A.C.S.*, 1963, **85**, 1118 (*synth*)
Curran, W.V. *et al., J.O.C.*, 1966, **31**, 201 (*synth*)
Hruska, F.E. *et al., J.A.C.S.*, 1971, **93**, 1795 (*conformn, pmr*)
Holy, A. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 738 (*synth*)

Orthoperiodic acid O-174

[10450-60-9]
Periodic acid. Paraperiodic acid
$(HO)_5I{=}O$
H_5IO_6 227.94
Sterilizing agent for containers and devices used in milk production. White hygroscopic cryst., dec. to $I_2O_5 + O_2 + H_2O$ at Mp. Sol. H_2O; sl. sol. Et_2O. Mp 122° Mp 130° (128.5° dec.). pK_{a1} 1.64; pK_{a2} 8.36; pK_{a3} 14.98 (25°). Forms a wide range of salts. Involved in various equilibria in aq. soln..

▶ Corrosive. Powerful oxidising agent especially in acid soln..

Na, di-K salt, tetrahydrate: [135014-68-5] *Potassium sodium orthoperiodate(VII) tetrahydrate*
Cryst. Formulated as *cis*-$[IO_4(OH)_2]^{3\ominus}.K_2Na.4H_2O$; bond lengths I–O 183-185, I–OH 197-198 pm.

Penta-Na salt: [18122-72-0] *Sodium paraperiodate. Sodium iodate*
INa_5O_6 337.85
White solid. Mp 800° (dec.). Dec. H_2O.

Inorg. Synth., 1939, **1**, 172 (*synth*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 1453 (*rev*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 334 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 238 (*use*)
Merck Index, 11th edn., 1989, No. 7123 (*props*)
Kellersohn, T. *et al., Acta Cryst. C*, 1991, **47**, 1133 (*synth, cryst struct*)
Ger. Pat., 1994, 4 301 277; *CA*, **121**, 178338w (*use*)

Oryzacystatin O-175

Two proteins with no disulfide bonds. Isol. from mature rice grains *Oryza sativa*.

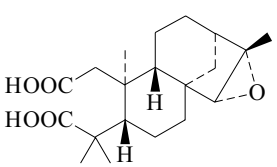
Oryzacystatin I
Sol. H_2O. Contains 107 aminoacid residues.

Oryzacystatin II
Sol. H_2O. Contains 102 amino acid residues.

Abe, K. *et al., Agric. Biol. Chem.*, 1985, **49**, 3349-3350; 1987, **51**, 2763-2768 (*Oryzacystatin I, isol*)
Abe, K. *et al., J. Biol. Chem.*, 1987, **262**, 16793-16797 (*Oryzacystatin I, struct*)
Kondo, H. *et al., J. Biol. Chem.*, 1990, **265**, 15832-15837 (*Oryzacystatin II, isol, struct*)
Kudo, N. *et al., J. Biochem. (Tokyo)*, 1998, **123**, 568-570 (*Oryzacystatin I, cryst struct*)
Nagata, K. *et al., Biochemistry*, 2000, **39**, 14753-14760 (*Oryzacystatin I, pmr, N-15 nmr, struct*)

Oryzalic acid A O-176

[134859-97-5]

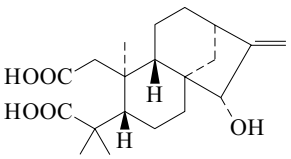


$C_{20}H_{30}O_5$ 350.454
Isol. from rice leaves. Needles. Mp 203-204°. $[\alpha]_D^{22}$ +1.9 (c, 0.26 in MeOH).

Kono, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 803 (*isol, pmr, cmr*)

Oryzalic acid B O-177

15-Hydroxy-2,3-seco-16-kaurene-2,3-dioic acid

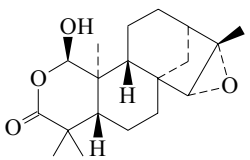


$C_{20}H_{30}O_5$ 350.454
Isol. from leaves of a blight-resistant rice cultivar. Needles (EtOH/Me_2CO/hexane). Mp 237-238°. $[\alpha]_D^{22}$ -49 (c, 0.63 in MeOH). λ_{max} (MeOH) (Berdy).

Watanabe, M. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 113 (*isol, pmr, cmr*)

Oryzalide A O-178

[128500-67-4]

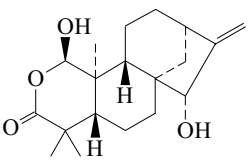


$C_{19}H_{28}O_4$ 320.428
Isol. from rice leaves. Needles. Mp 204-205°. $[\alpha]_D^{22}$ +3.6 (c, 0.33 in MeOH).

Watanabe, M. *et al., Agric. Biol. Chem.*, 1990, **54**, 1103 (*isol, pmr, cmr, cryst struct*)
Kono, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 803 (*isol, pmr, cmr, cryst struct*)

Oryzalide B O-179

[134885-94-2]

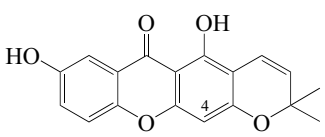


$C_{19}H_{28}O_4$ 320.428
Isol. from rice leaves. Needles. Mp 196-197°. $[\alpha]_D^{20}$ -58 (c, 1.65 in MeOH). λ_{max} 212 (ϵ 720) (MeOH) (Berdy).

Kono, Y. *et al., Agric. Biol. Chem.*, 1991, **55**, 803 (*isol, pmr, cmr*)

Osajaxanthone O-180

[1043-08-9]
*5,8-Dihydroxy-2,2-dimethyl-2*H*,6*H*-pyrano[3,2-*b*]xanthen-6-one, 9CI, 8CI*



$C_{18}H_{14}O_5$ 310.306
Yellow prisms (EtOAc). Mp 265°.

Di-Ac:
Cryst. (EtOH aq.). Mp 203-204°.

4-Hydroxy: ***Atroviridin***
$C_{18}H_{14}O_6$ 326.305
Constit. of *Garcinia atroviridis* (gelugor). Amorph. yellow powder. Mp 257-259°. λ_{max} 205 (log ϵ 4.48); 235 (log ϵ 4.46); 262 (log ϵ 4.41); 288 (log ϵ 4.71); 298 (log ϵ 4.75); 356 (log ϵ 3.8); 404 (log ϵ 3.83) (MeOH).

Jackson, B. *et al., J.C.S.(C)*, 1967, 2500 (*isol*)
Carpenter, I. *et al., J.C.S.(C)*, 1969, 486 (*isol*)
Gottlieb, O.R. *et al., Phytochemistry*, 1969, **8**, 665 (*isol*)
Jain, A.C. *et al., Tetrahedron*, 1969, **25**, 2787 (*synth*)
Lewis, J.R. *et al., J.C.S.(C)*, 1970, 1662 (*synth*)
Deshpande, V.H. *et al., Indian J. Chem.*, 1973, **11**, 518 (*isol*)
Anand, S.M. *et al., Indian J. Chem.*, 1973, **11**, 1233
Gunasekera, S.P. *et al., J.C.S. Perkin 1*, 1977, 11 (*isol*)
Lopez, J.L.C. *et al., Phytochemistry*, 1977, **16**, 1101 (*isol*)
Lopes, V. *et al., Phytochemistry*, 1997, **44**, 191 (*rev, occur*)
Kosin, J. *et al., Phytochemistry*, 1998, **47**, 1167-1168 (*Atroviridin*)
Tisdale, E.J. *et al., Tet. Lett.*, 2003, **44**, 3281-3284 (*Atroviridin, synth*)

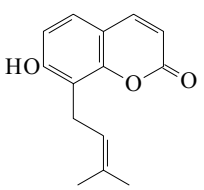
Osmotin-like protein O-181

Acidic protein. Isol. from overripe persimmon (*Diospyros texana*). Shows antifungal activity.

Pat. Coop. Treaty (WIPO), 1994, 94 08 010; *CA*, **121**, 76153q (*isol*)

Osthenol O-182

[484-14-0]
*7-Hydroxy-8-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, 9CI. 7-Hydroxy-8-prenylcoumarin*



$C_{14}H_{14}O_3$ 230.263
Isol. from seeds of *Apium graveolens*. Cryst. (C_6H_6 or H_2O). Mp 124-125°. $Bp_{0.1}$ 160-169°.

O-*β-D-Glucopyranoside:* ***Vellein***
$C_{20}H_{24}O_8$ 392.405
Cryst. + ½ H_2O. Mp 187.5-189°.

O-*β-D-Galactopyranoside:* [192938-65-1]
$C_{20}H_{24}O_8$ 392.405
Mp 106-108°. λ_{max} 210 ; 250 ; 260 ; 320 (no solvent reported).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:β-Gentiobiosylosthenol*
$C_{26}H_{34}O_{13}$ 554.547
Needles (H_2O). $[\alpha]_D^{26}$ 0 (c, 0.337 in MeOH). Ill-defined Mp.

Me ether: [484-12-8] *7-Methoxy-8-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one. 7-Methoxy-8-prenylcoumarin.* ***Osthol***
$C_{15}H_{16}O_3$ 244.29
Cryst. (EtOH aq.). Sol. MeOH, $CHCl_3$. Mp 85°. λ_{max} 258 (ϵ 4300); 322 (ϵ 8000) (MeOH) (Berdy). λ_{max} 247 (ϵ 6431); 258 (ϵ 7074); 322 (ϵ 18221) (EtOH) (Berdy).
▶ LD_{50} (rat, orl) 2905 mg/kg. GN7700000

Me ether, 2′,3′-epoxide: Meranzin, M-195

O-*(3-Methyl-2-butenyl):* [36149-95-8] *8-Prenyl-7-prenyloxycoumarin.* ***Ramosin***†
$C_{19}H_{22}O_3$ 298.381
Mp 66.5-68°.

O-*(2,3-Epoxy-3-methylbutyl):* [63187-29-1] ***Myrselline***
$C_{19}H_{22}O_4$ 314.38
Cryst. (Et_2O/hexane). Mp 99°.

O-*(2,3-Dihydroxy-3-methylbutyl):* [63187-30-4] ***Myrsellinol***
$C_{19}H_{24}O_5$ 332.396
$[\alpha]_D$ +44 (c, 1 in $CHCl_3$).

O-*(3,7-Dimethyl-2*E*,6*E*-octadienyl):* ***O-Geranylosthenol***
$C_{24}H_{30}O_3$ 366.499
Cryst. (Et_2O/heptane). Mp 44-45°.

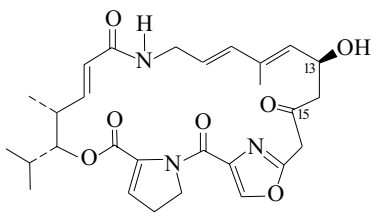
2′,3′-Dihydro, 3′-chloro, Me ether: ***Osthol hydrochloride***
$C_{15}H_{17}ClO_3$ 280.75
Platelets (petrol). Mp 98-99°. Prob. artifact.

2′,3′-Dihydro, 3′-hydroxy, O^7*-Me:8-(3-Hydroxy-3-methylbutyl)-7-methoxy-2*H*-1-benzopyran-2-one. 8-(3-Hydroxy-3-methylbutyl)-7-methoxycoumarin.* ***Osthol hydrate***. *2′-Deoxymeranzin hydrate*
$C_{15}H_{18}O_4$ 262.305
Yellowish cryst. Mp 60-62°. λ_{max} 207 (log ϵ 4.02); 322 (log ϵ 2.72) ($CHCl_3$).

Hollis, A.F. *et al., Aust. J. Chem.*, 1961, **14**, 101 (*Osthol hydrochloride*)
Kapoor, S.K. *et al., Phytochemistry*, 1968, **7**, 147 (*Osthol*)
Murray, R.D.H. *et al., Tetrahedron*, 1971, **27**, 1247 (*synth*)
Dreyer, D.L. *et al., Phytochemistry*, 1972, **11**, 705 (*Ramosin*)
Bandopadhyay, M. *et al., Indian J. Chem.*, 1974, **12**, 23 (*synth*)
Raj, K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 332 (*synth*)
Danchul, T.Y. *et al., Khim. Prir. Soedin.*, 1977, **13**, 575; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 479 (*Osthol*)
Hifnawy, M.S. *et al., Phytochemistry*, 1977, **16**, 1035 (*Myrselline, Myrsellinol*)
Kumar, R. *et al., Phytochemistry*, 1978, **17**, 2111 (*Osthol*)
Gashimov, N.F. *et al., Khim. Prir. Soedin.*, 1979, **15**, 15; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 11 (*Ramosin*)
Sasaki, H. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1847 (*β-Gentiobiosylosthenol*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, (*occur*)
Meyer, B.N. *et al., J. Nat. Prod.*, 1985, **48**, 952 (*O-Geranylosthenol*)
Srivastava, S.D. *et al., J. Indian Chem. Soc.*, 1996, **73**, 666-668 (*7-galactoside*)
Fujioka, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 96-100 (*Osthol, pmr, cmr*)
Cai, J.-N. *et al., J. Nat. Prod.*, 2000, **63**, 485-488 (*Osthol hydrate*)
Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, 2002, **83**, 1-619 (*rev*)

Ostreogrycin A O-183

[21411-53-0]
Mikamycin A. Pristinamycin II$_A$. Staphylomycin M$_1$. Streptogramin A. Syncothrecin A. Synergistin A$_1$. Virginiamycin M$_1$. Vernamycin A. E129A. PA 114A. 1745Z$_3$A. 547C. Antibiotic 14752-2. Antibiotic E129A. Antibiotic PA 114A. Antibiotic 1745Z$_3$A. Antibiotic 547C. Factor M



$C_{28}H_{35}N_3O_7$ 525.6
Depsipeptide-type antibiotic.Cryst. (EtOAc). Mp 200° dec. $[\alpha]_D^{23}$ -209 (c, 1 in EtOH). Log P 0.39 (uncertain value) (calc). λ_{max} 303 (ϵ 15800) (EtOH/HCl) (Derep). λ_{max} 293 (ϵ 21900) (EtOH/NaOH) (Derep). λ_{max} 228 (ϵ 32400); 272 (sh) (ϵ 10000) (95% EtOH) (Derep). Discontinued

Mixture with ca. *25% other Virginamycins:* [11006-76-1] ***Virginiamycin, BAN, INN, USAN***. *Cebin V. Eskalin V. Eskamicin. Stafac. Stephylomycin. Mikamycin. Ostreogrycin. Patricin. Pristinamycin. Streptogramin. Vernamycin*
Antibacterial food additive. Discontinued. Powder. $[\alpha]_D$ -124 (c, 0.05 in EtOH). Dec. at 138-140°.
▶ LD_{50} (mus, orl) 2100 mg/kg. ZA4850000

13-Deoxy: [118693-65-5] ***Antibiotic L 156588***. *L 156588*
$C_{28}H_{35}N_3O_6$ 509.601
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. λ_{max} 212 (ϵ 28400); 275 (ϵ 38900) (MeOH) (Derep). λ_{max} 213 (E1%/1cm 542) (MeOH) (Berdy).

13-Deoxy, 13,14-epoxy: [119465-45-1] ***Antibiotic L 156587***. *L 156587*
$C_{28}H_{33}N_3O_7$ 523.585
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. λ_{max} 212 (ϵ 27700); 325 (ϵ 21100) (MeOH) (Derep).

13-Deoxy, 13,14-epoxy, 15-alcohol: ***Antibiotic L 156586***. *L 156586*
$C_{28}H_{35}N_3O_7$ 525.6
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. The C-15 epimer is Antibiotic L 156906 and is semisynthetic λ_{max} 212 (ϵ 28400); 275 (ϵ 38900) (MeOH) (Derep).

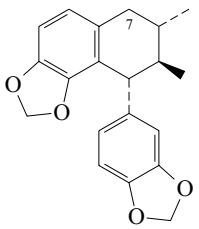
[118693-64-4, 118759-89-0]

Ball, S. *et al., Biochem. J.*, 1958, **68**, 24P (*isol*)
Kingston, D.G.I. *et al., J.C.S.(C)*, 1966, 1669 (*nmr, ir, ms*)
Delpierre, G.R. *et al., Tet. Lett.*, 1966, 369 (*struct*)
Preud'Homme, J. *et al., Bull. Soc. Chim. Fr.*, 1968, 585 (*isol, ms, struct*)
Crooy, P. *et al., J. Antibiot.*, 1972, **25**, 371
Bycroft, B.W. *et al., J.C.S. Perkin 1*, 1977, 2464 (*cmr, pmr, conformn*)
Ogata, K. *et al., J. Antibiot.*, 1978, **31**, 1313 (*isol, ir, nmr*)

Kingston, D.G.I. *et al., J.A.C.S.*, 1983, **105**, 5106 (*biosynth*)
Biot, A.M. *et al., Drugs Pharm. Sci.*, 1984, **22**, 695 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, VRF000
Paris, J.M. *et al., Recent Prog. Chem. Synth. Antibiot.*, 1990, 183 (*rev*)
Shepherd, M.J. *et al., Food Contaminants: Sources and Surveillance*, Royal Society of Chemistry, 1991, 175 (*anal*)
Lam, Y.K.T. *et al., J. Antibiot.*, 1991, **44**, 613 (*derivs*)
Kingston, D.G.I. *et al., Environ. Sci. Res.*, 1992, **44**, 105 (*rev, biosynth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 224
Pechere, J.-C. *et al., Drugs*, (Suppl. 1), 1996, **51**, 13 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VRF000

Otobain O-184

3,4:3′,4′-Bis(methylenedioxy)-2,7′-cyclolignan. Otobite



(−)-*form*

$C_{20}H_{20}O_4$ 324.376

Lignan numbering shown.

(-)-*form* [3738-01-0]
Cryst. (petrol). Mp 136-137°. $[\alpha]_D$ -43 (c, 0.8 in $CHCl_3$).

7-Oxo: [34426-79-4] ***Otobanone***. *7-Oxootobain*
$C_{20}H_{18}O_5$ 338.359
Isol. from nutmeg (*Myristica fragrans*). Mp 175-176°. $[\alpha]_D$ -27.1 (c, 0.7 in $CHCl_3$).

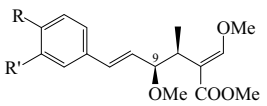
8-Epimer, 7-oxo: ***Isootobanone***
$C_{20}H_{18}O_5$ 338.359
Amorph. $[\alpha]_D^{26}$ -55.9 (c, 0.72 in $CHCl_3$). λ_{max} 235 (log ϵ 4.19); 285 (log ϵ 3.85); 312 (log ϵ 3.67) (MeOH).

(+)-*form*
*5-Methoxy, 7′,8′*R-*didehydro:* [98767-35-2] *5-Methoxy-3,4:3′,4′-bis(methylenedioxy)-2,7′-cyclolign-7′-ene*
$C_{21}H_{20}O_5$ 352.386
Cryst. (MeOH). Mp 152°. $[\alpha]_D^{20}$ +51.7 (c, 0.8 in $CHCl_3$). λ_{max} 279 (ϵ 1200); 292 (ϵ 1050); 332 (ϵ 300) (MeOH).

(±)-*form*
Cryst. (petrol). Mp 171-173°.

Gilchrist, T. *et al., J.C.S.*, 1962, 1780 (*isol*)
Wallis, R. *et al., J.C.S.*, 1963, 1445 (*pmr*)
Klyne, W. *et al., J.C.S.(C)*, 1966, 893 (*abs config*)
Maclean, I. *et al., J.C.S.(C)*, 1966, 1717 (*synth*)
McMurry, T.B.H. *et al., Tet. Lett.*, 1966, 975 (*synth*)
Kuo, Y.H. *et al., Experientia*, 1976, **32**, 828 (*isol*)
Martinez, V.J.C. *et al., Phytochemistry*, 1985, **24**, 1867-1868 (*5-methoxydidehydro deriv*)
Kuo, Y.H. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2310 (*isol, pmr*)
Li, T.M. *et al., Chin. Chem. Lett.*, 1997, **8**, 43-46 (*Artabotryside A*)
Kuo, Y.-H. *et al., Tet. Lett.*, 2001, **42**, 6731-6735 (*Isootobanone*)

Oudemansin O-185



Absolute Configuration

R, R' = H Oudemansin A
R = Cl, R' = OMe Oudemansin B
R = OMe, R' = H Oudemansin X

Oudemansin A [73341-71-6]
Methyl 4-methoxy-2-(methoxymethylene)-3-methyl-6-phenyl-5-hexenoate, 9CI
$C_{17}H_{22}O_4$ 290.358
Metab. of *Oudemansiella mucida* (porcelain fungus). Cryst. (petrol). Sol. MeOH, $CHCl_3$; fairly sol. hexane; poorly sol. H_2O. Mp 44°. $[\alpha]_D^{22}$ -17 (c, 1 in EtOH). λ_{max} 208 (ϵ 24500); 216 (ϵ 17000); 245 (ϵ 30200); 254 (sh) (ϵ 27500); 283 (ϵ 2290); 292 (ϵ 1700) (MeOH) (Derep).

*9-*O*-De-Me:* [225937-85-9] ***9-Hydroxyoudemansin A***. *9-De-*O*-methyloudemansin A. Noroudemansin A*
$C_{16}H_{20}O_4$ 276.332
Oil. $[\alpha]_D^{20}$ -29.2 (c, 0.5 in $CHCl_3$). $[\alpha]_D^{25}$ -64.3 (c, 0.24 in MeOH). λ_{max} 205 (log ϵ 5.36); 248 (log ϵ 5.36); 282 (sh) (log ϵ 4.64); 291 (sh) (log ϵ 4.64) (MeOH).

Oudemansin B [87081-56-9] *Methyl 6-(4-chloro-3-methoxyphenyl)-4-methoxy-2-(methoxymethylene)-3-methyl-5-hexenoate, 9CI*
$C_{18}H_{23}ClO_5$ 354.829
Yellowish oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D^{22}$ -8.3 (c, 1.52 in $CHCl_3$). λ_{max} 219 (ϵ 21900); 248 (ϵ 17800); 261 (ϵ 16600); 270 (sh) (ϵ 12900); 299 (ϵ 4680); 312 (ϵ 3090) (dioxan) (Derep).

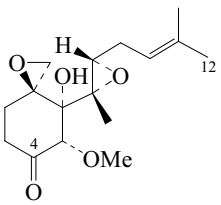
Oudemansin X [130640-32-3] *Methyl 4-methoxy-2-(methoxymethylene)-6-(4-methoxyphenyl)-3-methyl-5-hexenoate, 9CI*
$C_{18}H_{24}O_5$ 320.385
Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ -20.35 (c, 0.14 in EtOH). Similar to Strobilurin A, S-253 λ_{max} 206 (ϵ 24000); 260 (ϵ 26300); 292 (sh) (ϵ 7080) (MeOH) (Derep).

Anke, T. *et al., J. Antibiot.*, 1979, **32**, 1112; 1983, **36**, 661; 1990, **43**, 1010 (*isol, cryst struct*)
Meyer, H.H. *et al., Annalen*, 1984, 791 (*synth, abs config*)
Akita, H. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1242; 1992, **40**, 2847 (*synth*)
Kowalski, C.J. *et al., J.A.C.S.*, 1985, **107**, 1429 (*synth*)
Kellmerton, J. *et al., Tet. Lett.*, 1986, **27**, 2443 (*synth, bibl*)
Akita, H. *et al., Tet. Lett.*, 1986, **27**, 5397 (*Oudemansin B*)
Wittman, M.D. *et al., J.O.C.*, 1987, **52**, 4303 (*synth*)
Honda, T. *et al., Chem. Comm.*, 1992, 1218 (*synth*)
Chida, N. *et al., J.C.S. Perkin 1*, 1993, 1957 (*synth, abs config*)
Umezawa, I. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1111-1118 (*synth, Oudemansin X*)
Akita, H. *et al., J.C.S. Perkin 1*, 1995, 2159 (*synth*)
Kleinwaechter, P. *et al., J. Antibiot.*, 1999, **52**, 332-334 (*9-Hydroxyoudemansin A*)
Engler-Lohr, M. *et al., Z. Naturforsch., C*, 1999, **54**, 163-168 (*9-Hydroxyoudemansin A*)

Ovalicin O-186

[19683-98-8]

[137490-44-9]
Graphinone. FR 125756. Antibiotic FR 125756. SL 1846. Antibiotic SL 1846



$C_{16}H_{24}O_5$ 296.363

Sesquiterpene antibiotic. Found in lettuce seeds. Cryst. (C_6H_6/hexane). Mp 93-94°. $[\alpha]_D^{22}$ -75 (c, 1 in MeOH). Structurally related to Fumagillin λ_{max} 285 (ϵ 43) (MeOH) (Derep).

▶ RP3680500

O-*De-Me:* ***O-Demethylovalicin***. *Antibiotic USF 3506A. USF 3506A*
$C_{15}H_{22}O_5$ 282.336
Oil. $[\alpha]_D^{26}$ -32.9 (c, 0.1 in EtOH).

4α-Alcohol: [28400-07-9] ***Antibiotic FR 125035***. *FR 125035*
$C_{16}H_{26}O_5$ 298.378
Powder. Sol. MeOH, $CHCl_3$. $[\alpha]_D$ -73 ($CHCl_3$). λ_{max} 200 (EtOH). λ_{max} (EtOH) (Berdy).

12-Hydroxy: ***12-Hydroxyovalicin***. *Mer-F3. Antibiotic Mer-F3*
$C_{16}H_{24}O_6$ 312.362
Oil. $[\alpha]_D^{29}$ -46 (c, 0.5 in MeOH).

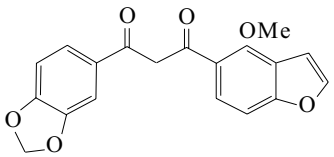
Stereoisomer: [220509-38-6] ***Antibiotic AM 6105***. *AM 6105*
$C_{16}H_{24}O_5$ 296.363

Sassa, T. *et al., Agric. Biol. Chem.*, 1970, **34**, 649 (*struct*)
Bollinger, P. *et al., Helv. Chim. Acta*, 1973, **56**, 819 (*cryst struct*)
Cane, D.E. *et al., J.A.C.S.*, 1977, **99**, 6132 (*biosynth*)
Hartman, G.L. *et al., Planta Med.*, 1978, **34**, 231 (*rev*)
Corey, E.J. *et al., J.A.C.S.*, 1985, **107**, 256 (*synth, bibl*)
Cane, D.E. *et al., Tet. Lett.*, 1987, **28**, 6545 (*biosynth*)
Japan. Pat., 1991, 91 47 120; *CA*, **115**, 278158g (*FR 125035, FR 125756*)
Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1995, 1551 (*synth*)
Ito, C. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1993-1996 (*O-Demethylovalicin*)
Kuboki, H. *et al., J. Antibiot.*, 1999, **52**, 590-593 (*12-Hydroxyovalicin*)
Japan. Pat., 1999, 99 29 561; *CA*, **130**, 181559k (*AM 6105*)

Ovalitenone O-187

[64280-22-4]

1-(1,3-Benzodioxol-5-yl)-3-(4-methoxy-5-benzofuranyl)-1,3-propanedione, 9CI. Glabra I



$C_{19}H_{14}O_6$ 338.316

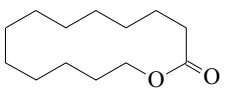
Isol. from *Rhus chinensis* (Chinese gall). Yellow cubes (C_6H_6). Mp 123-126°.

Sharma, P. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 866 (*isol*)
Gupta, R.K. *et al., Phytochemistry*, 1977, **16**, 1104 (*isol*)
Garg, G.P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 658 (*isol*)
Garg, G.P. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 646 (*synth*)
Islam, A. *et al., Tet. Lett.*, 1979, 4879 (*synth*)
Ahmad, J. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 420 (*isol*)
Lee, Y.R. *et al., Tetrahedron*, 1995, **51**, 4909 (*synth, pmr, cmr*)

Oxacyclotetradecan-2-one, 9CI, 8CI O-188

[1725-04-8]

Tridecanolide. Tridecanolactone



$C_{13}H_{24}O_2$ 212.331

Constit. of blackberries (*Rubus* sp.) and *Angelica archangelica* (angelica). Cryst. (MeOH at -50° or subl.). Mp 27.5° (25°). $Bp_{3.8}$ 122°.

Hunsdiecker, H. *et al., Chem. Ber.*, 1947, **80**, 129
Taskinen, J. *et al., Acta Chem. Scand., Ser. B*, 1975, **29**, 757 (*isol*)
Trost, B.M. *et al., J.A.C.S.*, 1980, **102**, 4743 (*synth*)
Regen, S.L. *et al., J.A.C.S.*, 1982, **104**, 2064 (*synth*)
Boden, E.P. *et al., J.O.C.*, 1985, **50**, 2394 (*synth*)
Ishii, Y. *et al., J.O.C.*, 1988, **53**, 5549 (*synth*)
Matsuyama, H. *et al., J.O.C.*, 1989, **54**, 5218 (*synth*)
Torra, N. *et al., Tetrahedron*, 1989, **45**, 863 (*synth*)
Wiberg, K.B. *et al., J.A.C.S.*, 1991, **113**, 971 (*cryst struct, synth*)
White, J.D. *et al., Tet. Lett.*, 1993, **34**, 3515 (*synth*)

Oxalic acid, 8CI O-189

[144-62-7]

[6153-56-6]

Ethanedioic acid, 9CI. Clover acid

HOOCCOOH

$C_2H_2O_4$ 90.035

Present in many plants and vegetables. Toxin from rhubarb, esp. the leaves but also present in the stems. Cryst. + $2H_2O$ (H_2O). V. sol. H_2O; mod. sol. EtOH; spar. sol. Et_2O. $d_4^{18.5}$ 1.65. Mp 189.5° (anhyd. α-form) Mp 101.5° (dihydrate). pK_{a1} 1.23; pK_{a2} 3.85 (25°,H_2O). Hydrate dehydrates on heating and sublimes at 150-60°. Anhydrous acid exists as orthorhombic α-form and metastable monoclinic β-form.

▶ Hg and Ag salts are explosive. Skin and severe eye irritant. Aq. solns. corrosive, and toxic by ingestion causing muscular tremors and convulsions. Acute poisoning can be fatal or result in acute renal failure. Salts are similarly toxic. OES: long-term 1 mg m^{-3}; short-term 2 mg m^{-3}. RO2450000

Mono-K salt: [127-95-7] *Potassium binoxalate*
Cryst. + $1H_2O$.

Ce(III) salt: [139-42-4] ***Cerium oxalate***

Mono-NH_4 salt: [5972-72-5]
Cryst. + $1H_2O$.

Di-NH_4 salt: [1113-38-8]

[6009-70-7, 14258-49-2]
Mp 133° dec. (monohydrate).

▶ Toxic.

Mono-Me ester: [600-23-7]
$C_3H_4O_4$ 104.062
Liq. Bp 108-109°.

Di-Me ester: [553-90-2] *Dimethyl oxalate*
$C_4H_6O_4$ 118.089
Monoclinic prisms. Mp 54°. Bp 163.5°.

▶ RO2850000

Et-Me ester: [615-52-1]
$C_5H_8O_4$ 132.116
Liq. $Bp_{0.1}$ 58°.

Di-Et ester: See Diethyl oxalate in *The Combined Chemical Dictionary.*

Dipropyl ester: [615-98-5]
$C_8H_{14}O_4$ 174.196
Liq. Bp 214-215°.

Diisopropyl ester: [615-81-6]
$C_8H_{14}O_4$ 174.196
Liq. Bp 193-194° Bp_3 41-42°.

Dibutyl ester: [2050-60-4]
$C_{10}H_{18}O_4$ 202.25
Constit. of *Juglans regia* (walnut) and *Panax ginseng* (ginseng). Liq. Mp -29°. Bp 239-240°.

Bis(2-methylpropyl) ester: [2050-61-5]
$C_{10}H_{18}O_4$ 202.25
Liq. Bp 229-231°.

Di-tert-*butyl ester:* [691-64-5]
$C_{10}H_{18}O_4$ 202.25
Cryst. (hexane). Mp 70-72° (69-70°).

Vinyl-Et ester: [52032-00-5]
$C_6H_8O_4$ 144.127
d_4^{20} 1.06. Bp_5 60°. n_D^{20} 1.4282. Undergoes radical polym. Q/e values for copolym., Q 0.018, e -1.80.

Di-2-propenyl ester: [615-99-6] *Diallyl oxalate*
$C_8H_{10}O_4$ 170.165
d^{20} 1.16. Bp 217-219°. n_D^{20} 1.4481.

Dibenzyl ester: [7579-36-4]
$C_{16}H_{14}O_4$ 270.284
Cryst. Mp 80°.

Bis(4-methylbenzyl) ester: [18241-31-1]
$C_{18}H_{18}O_4$ 298.338
Cryst. Mp 99-100° (EtOH).

Di-Ph ester: [3155-16-6]
$C_{14}H_{10}O_4$ 242.231
Cryst. (EtOH or hexane). Mp 135-137°.

▶ RO2880000

Difluoride: See Oxalyl fluoride in *The Combined Chemical Dictionary.*

Monochloride: [4732-69-8] *Chlorooxoacetic acid, 9CI. Chloroglyoxylic acid, 8CI. (Chlorocarbonyl)formic acid. Oxalic monochloride*
C_2HClO_3 108.481Obt. as Me ester.

Chloride-Me ester: [5781-53-3] *Methyl chlorooxoacetate. Methoxalyl chloride*
$C_3H_3ClO_3$ 122.508
Fuming liq. Bp 118-120° (125°).

Chloride-Et ester: [4755-77-5] *Ethyl chlorooxoacetate. Ethoxalyl chloride*
$C_4H_5ClO_3$ 136.534
Liq. d_4^{20} 1.22. Bp 135°.

▶ Lachrymator.

Chloride-Et ester, oxime: See Chloro(hydroxyimino)acetic acid in *The Combined Chemical Dictionary.*

Dichloride: See Oxalyl chloride in *The Combined Chemical Dictionary.*

Dibromide: [15219-34-8] *Oxalyl bromide*
$C_2Br_2O_2$ 215.829
Green liq. Mp -19.3°. Bp_{720} 102-103° Bp_{10} 16-17°.

▶ Mixtures with K or Na/K alloy are explosive. Eye, skin and respiratory tract irritant.

Monoamide: [471-47-6] *Aminooxoacetic acid, 9CI. Oxamic acid. Oxaminic acid. Oxalamic acid. Aminocarbonylformic acid. Oxoglycine*
$C_2H_3NO_3$ 89.051
Cryst. (H_2O). Spar. sol. H_2O; insol. EtOH, Et_2O. Mp 210° dec.

Amide-Et ester: [617-36-7] *Ethyl oxamate. Oxamethane. Ethoxalamide*
$C_4H_7NO_3$ 117.104
Cryst. Mp 115-116°.

Methylamide: [29262-58-6] *Methyloxamic acid*
$C_3H_5NO_3$ 103.077
Cryst. (H_2O or EtOH). Mp 145-146°. Steam-volatile. Sublimes.

Dimethylamide: [32833-96-8] *(Dimethylamino)oxoacetic acid, 9CI. Dimethyloxamic acid*
$C_4H_7NO_3$ 117.104
Prisms (MeOH). Sol. H_2O, EtOH; spar. sol. Et_2O, C_6H_6. Mp 130° dec.

Dimethylamide-Et ester: [16703-52-9] *Ethyl* N,N-*dimethyloxamate*
$C_6H_{11}NO_3$ 145.158
Bp_{15} 119°.

Diamide: [471-46-5] *Oxamide. Ethanediamide, 9CI. Oxalamide*
$C_2H_4N_2O_2$ 88.066
Triclinic needles. Spar. sol. EtOH, hot H_2O. Dec. >320°.

▶ Eye irritant. LD_{50} (rat, orl) 447 mg/kg. RO4900000

Diamide, N,N-*di-Me:* [600-39-5] N,N-*Dimethylethanediamide, 9CI.* N,N-*Dimethyloxamide*
$C_4H_8N_2O_2$ 116.119
Cryst. (EtOH/Me_2CO). Mp 138°.

Bis(methylamide): [615-35-0] sym-*Dimethyloxamide*

$C_4H_8N_2O_2$ 116.119
Leaflets or needles (H_2O). Sol. hot H_2O; mod. sol. EtOH. Mp 217°.

Bis(dimethylamide): [1608-14-6] *Tetramethyloxamide. Tetramethylethanediamide, 9CI*
$C_6H_{12}N_2O_2$ 144.173
Needles (Et_2O). Mp 78-79°.

Bis(cyclohexylamide): [3299-64-7] N,N′-*Dicyclohexylethanediamide, 9CI.* N,N′-*Dicyclohexyloxamide*
$C_{14}H_{24}N_2O_2$ 252.356
Prisms ($CHCl_3$/MeOH). Mp 243-248°.

Amide-hydrazide: [515-96-8] *Semioxamazide, 8CI. Aminooxamide*
$C_2H_5N_3O_2$ 103.08
Leaflets (H_2O). Mp 220-221° dec.

►AF2620000

Monoanilide: [500-72-1] *Oxanilic acid. Oxo(phenylamino)acetic acid, 9CI*
$C_8H_7NO_3$ 165.148
Needles (C_6H_6). Sol. EtOH, Et_2O, $CHCl_3$; mod. sol. hot H_2O; spar. sol. C_6H_6. Mp 149-150°.

►RP3150000

Monoanilide-Et ester: [1457-85-8] *Ethyl oxanilate*
$C_{10}H_{11}NO_3$ 193.202
Cryst. (EtOH). Mp 66-67°.

Dianilide: [620-81-5] *Oxanilide.* sym-*Diphenyloxamide. Oxalanilide*
$C_{14}H_{12}N_2O_2$ 240.261
Leaflets (C_6H_6 or $PhNO_2$). Sol. C_6H_6; spar. sol. hot EtOH; insol. H_2O, Et_2O. Mp 252-254°.

Monohydrazide: [6292-65-5]
$C_2H_4N_2O_3$ 104.065
Mp 300°.

Dihydrazide: [996-98-5]
$C_2H_6N_4O_2$ 118.095
Cryst. Sol. common org. solvs. Mp 241° dec.

►RO2840000

Mononitrile: See Cyanoformic acid in *The Combined Chemical Dictionary.*

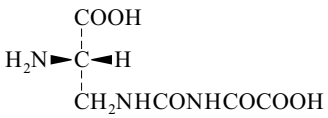
Dinitrile: See Cyanogen in *The Combined Chemical Dictionary.*

[127-96-8, 338-70-5, 6100-20-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 490A; 613B; 613D; 737D; 739D; 766B; 766C; 767A; 770A; **2**, 388C; 1287C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 764B; 933C; 934B; 934C; 1208A; 1252B; **2**, 1422A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 635D; 636B; 636C; 772C (*ir*)
Fischer, E. *et al., Ber.*, 1889, **22**, 1930 (*synth, niccolox*)
Kerp, W. *et al., Ber.*, 1897, **30**, 586 (*synth, aminooxoacetic acid hydrazide*)
Johnson, E.I. *et al., J.C.S.*, 1930, 1510 (*synth*)
Rakusin, M.A. *et al., Chem.-Ztg.*, 1931, **55**, 128 (*hydrate*)
Sah, P.P.T. *et al., J.A.C.S.*, 1931, **53**, 3901 (*esters, props*)
Org. Synth., Coll. Vol., 1, 1932, 259 (*ester*)
U.S. Pat., 1934, 1 948 441; *CA*, **28**, 2728 (*synth*)
Kuras, M. *et al., Coll. Czech. Chem. Comm.*, 1947, **12**, 198 (*detn, Ni*)
Voter, R.C. *et al., Anal. Chem.*, 1949, **21**, 1320 (*detn, Ni*)
Leonard, N.J. *et al., J.O.C.*, 1950, **15**, 42 (*use, aminooxoacetic acid hydrazide*)
Pierce, J.S. *et al., J.A.C.S.*, 1951, **73**, 2595 (*synth, ethyl oxanilate*)
Richardson, A.G. *et al., J.A.C.S.*, 1952, **74**, 4011 (*use, ethyl oxanilate*)
Overberger, C.G. *et al., J.A.C.S.*, 1958, **80**, 4556 (*chloride-Et ester*)
Welcher, R.P. *et al., J.A.C.S.*, 1959, **81**, 2541 (*Ethyl oxamate*)
Pearse, G.A. *et al., Anal. Chem.*, 1960, **32**, 213 (*synth, detn, Ni*)
Lespagnoll, C. *et al., Bull. Soc. Chim. Fr.*, 1960, 110 (*esters*)
Kawabata, N. *et al., Kogyo Kagaku Zasshi*, 1962, **65**, 70; *CA*, **47**, 4850c (*synth, polym, vinyl ethyl ester*)
Nivière, P. *et al., Anal. Abstr.*, 1967, **14**, 668 (*detn, Cu*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 767; 1975, **5**, 487
Jankovic, S. *et al., Anal. Abstr.*, 1968, **15**, 3626 (*detn, Cu*)
Trahanovsky, W.S. *et al., J.A.C.S.*, 1968, **90**, 2839-2842 (*bis-4-methylbenzyl ester*)
Kolthoff, I.M. *et al., Quant. Chem. Anal.*, 4th Edn., MacMillan, New York, 1971, (*use*)
Shingaki, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3567 (*Ethyl oxamate*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 835 (*occur*)
Hagen, K. *et al., J.A.C.S.*, 1973, **95**, 4796 (*bromide*)
Ito, A. *et al., Org. Mass Spectrom.*, 1973, **7**, 1279 (*ms*)
Derissen, J.L. *et al., Acta Cryst. B*, 1974, **30**, 2240 (*cryst struct*)
Kuse, S. *et al., Anal. Chim. Acta*, 1974, **70**, 65 (*use*)
Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, (*use*)
Clark, G.R. *et al., J.C.S. Dalton*, 1976, 1528 (*detn, Cu*)
Aja, D. *et al., J. Mol. Struct.*, 1977, **37**, 160 (*conformn*)
Desseyn, H.O. *et al., Spectrochim. Acta A*, 1977, **33**, 633 (*oxamides, ir*)
Williamson, K.L. *et al., J. Magn. Reson.*, 1978, **30**, 367 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **16**, 618 (*rev*)
de Villepin, J. *et al., Spectrochim. Acta A*, 1978, **34**, 1009; 1019 (*ir, Raman*)
Tripathi, G.N.R. *et al., J. Mol. Struct.*, 1979, **54**, 19 (*ir, Raman, struct, aminooxoacetic acid hydrazide*)
Fritz, E. *et al., Annalen*, 1981, 1015 (*bisdimethylamide*)
Berkovitch-Yellin, Z. *et al., J.A.C.S.*, 1982, **104**, 4052 (*cryst struct*)
Back, R.A. *et al., Can. J. Chem.*, 1984, **62**, 1414 (*uv*)
Baer, A. *et al., Int. J. Vitam. Nutr. Res., Suppl.* 28, 1985, (*rev, metab*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A18**, 247 (*rev*)
Marczenko, Z. *et al., Separation and Spectrophotometric Determination of Elements*, Horwood, Chichester, 1986, (*use*)
Dangerous Prop. Ind. Mater. Rep., 1989, **9**, 13 (*rev, haz*)
Hashimoto, M. *et al., Inorg. Chim. Acta*, 1989, **166**, 17 (*ir, cmr, Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1397
Albrecht, S. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 1780 (*occur*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **5**, 3459-3460 (*chloride-Me ester, use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3812-3814 (*use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3814 (*dibromide, use*)
Tsai, I.-L. *et al., Phytochemistry*, 1997, **44**, 1383 (*N,N′-dicyclohexyloxamide*)
Strazzoli, P. *et al., J.C.S. Perkin 1*, 1998, 2553-2557 (*mono-Me ester, synth, ir, pmr, cmr, ms*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4935 (*tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0682
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 948; 949; 1118
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OKY000; OLA000; OLO000

Oxalylalbizziine O-190

*3-[[[(Carboxycarbonyl)amino]carbonyl]amino]alanine, 9CI. 2-Amino-6*N*-oxalylureidopropionic acid*



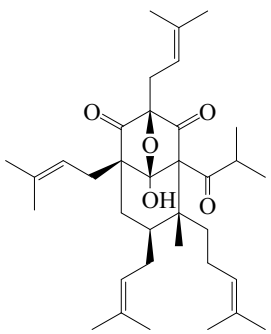
$C_6H_9N_3O_6$ 219.154

(*S*)-*form* [99694-81-2]
L-form
Isol. from seeds of *Acacia catechu* (black catechu).

Evans, C.S. *et al., Phytochemistry*, 1985, **24**, 2273; 1990, **29**, 2159 (*isol, cryst struct*)

Oxepahyperforin O-191

[59014-02-7]



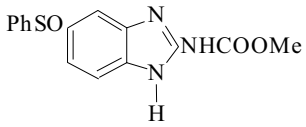
$C_{35}H_{52}O_5$ 552.793

Oxygenated deriv. of Hyperforin, H-835. Constit. of *Hypericum perforatum* (St. John's Wort). Viscous oil. $[\alpha]_D^{20}$ -73.7 (c, 0.8 in $CHCl_3$). λ_{max} 272 (log ϵ 3.83) ($CHCl_3$).

Verotta, L. *et al., J. Nat. Prod.*, 2000, **63**, 412-415

Oxfendazole, BAN, INN, USAN O-192

[53716-50-0]
*Methyl [5-(phenylsulfinyl)-1*H*-benzimidazol-2-yl]carbamate, 9CI. Benzelmin. Nanthic. Synanthic. Systamex. RS 8858*



$C_{15}H_{13}N_3O_3S$ 315.352
Anthelmintic, used in cattle, sheep and horses. Cryst. (MeOH/$CHCl_3$). Mp 253° dec. Log P 2.31 (calc).

▶ Exp. reprod. and teratogenic effects. FD0808000

Averkin, E.A. *et al., J. Med. Chem.*, 1975, **18**, 1164 (*synth, pharmacol*)
Bogan, J.A. *et al., Drugs of Today (Barcelona)*, 1979, **15**, 98 (*rev*)
Prichard, R.K. *et al., Vet. Parasitol.*, 1993, **46**, 113 (*rev*)
Blanchflower, W.J. *et al., Analyst (London)*, 1994, **119**, 1325 (*hplc-ms*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 122
Rose, M.D. *et al., Food Addit. Contam.*, 1997, **14**, 15-26 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OMY500

Oxirane, 9CI O-193

[75-21-8]
Ethylene oxide, 8CI. Epoxyethane. Oxacyclopropane. Oxidoethane. Dihydrooxirene. FEMA 2433



C_2H_4O 44.053
Flavouring ingredient. Used in food processing as a solubiliser, stabiliser, processing aid, wetting agent, surfactant, defoaming agent and dough conditioner. Gas or liq. with pleasant ethereal odour. Sol. H_2O, EtOH, Et_2O, Me_2CO. d_{10}^{10} 0.88. Mp -111.7°. Bp 10.8°. n_D^7 1.3597.

▶ Extremely flammable, fl. p. -20°, autoignition temp. 429/440°. Probable human carcinogen. Eye, skin and respiratory irritant. High conc. can cause pulmonary oedema. LD_{50} (rat, orl) 72 mg/kg. LC_{50} (rat, ihl) 800 ppm (4h exposure). Exp. carcinogen and teratogen. Exp. reprod. effects. MEL: long-term 5 ppm. KX2450000

[9002-90-8]

U.S. Pat., 1960, 2 960 511; *CA*, **55**, 9427
Rodd's Chem. Carbon Compd. (3rd edn.), 1965, **1D**, 19; Vol. IVA, 1973, 3 (*rev, bibl*)
Basch, H. *et al., J. Chem. Phys.*, 1969, **51**, 52 (*uv*)
Fay, C.K. *et al., J.O.C.*, 1973, **38**, 3122 (*pmr*)
Harrison, A.G. *et al., Org. Mass Spectrom.*, 1974, **9**, 221 (*ms*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 297
Whitham, G.H. *et al., J.C.S. Perkin 2*, 1975, 861 (*cmr*)
Bertie, J.E. *et al., J. Chem. Phys.*, 1978, **68**, 97 (*cryst struct*)
Cataliotti, R. *et al., Chem. Phys.*, 1982, **72**, 293 (*ir, Raman*)
IARC Monog., 1985, **36**, 189; *Suppl.* 7, 205; *Suppl.* 6, 300 (*rev, tox*)
Luger, P. *et al., Angew. Chem., Int. Ed.*, 1986, **25**, 276 (*cryst struct*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1986, **6**, 225 (*rev, polymers*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH, Weinheim, 1987, **A10**, 117 (*rev*)
Alkylene Oxides and Their Polymers; Surfactant Science Series, Vol. 35, (Eds. Bailey, F.E. *et al*), Dekker, New York, 1991,
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **9**, 915 (*rev, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 230
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 974-975
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0777
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 600
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EJN500
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 338 (*tox, rev*)

3-Oxoalkanoic acid glycerides O-194

Comly. available mixtures of mono- and diglycerides of $RCOCH_2COOH$. Present in butter and milk fat. Additives for baked goods and imitation dairy products.

3-Oxohexanoic acid glycerides [128331-47-5]

[91052-72-1]
FEMA 3770
Fatty flakes.

3-Oxooctanoic acid glycerides [128331-48-6]

[91052-68-5]
FEMA 3771
Fatty flakes.

3-Oxodecanoic acid glycerides [128331-45-3]
FEMA 3767
Fatty flakes.

3-Oxododecanoic acid glycerides [128362-26-5]

[91052-70-9]
FEMA 3768
Fatty flakes.

3-Oxotetradecanoic acid glycerides [128331-49-7]

[91052-73-2]
FEMA 3772
Fatty flakes.

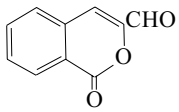
3-Oxohexadecanoic acid glycerides [128331-46-4]

[91052-71-0]
FEMA 3769
Fatty flakes.

Burdock, G.A. *et al., Food Technol. (Chicago)*, 1990, **44(2)**, 78; 80; 82; 84; 86 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1390-1395 (*occur, use*)

1-Oxo-1*H*-2-benzopyran-3-carboxaldehyde, 9CI O-195

[34328-51-3]
3-Formylisocoumarin. Isocoumarin-3-carboxaldehyde. Artemidinal

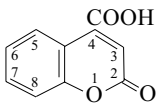


$C_{10}H_6O_3$ 174.156
Isol. from tarragon (*Artemisia dracunculus*). Pale-yellow needles (C_6H_6). Mp 178-179°.

Mallabaev, A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 257; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 248 (*isol*)
Nadkarni, D.R. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 185 (*synth*)
Chatterjea, J.N. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 359 (*synth*)

2-Oxo-2*H*-1-benzopyran-4-carboxylic acid, 9CI O-196

[27393-46-0]
Coumarin-4-carboxylic acid



$C_{10}H_6O_4$ 190.155
Occurs in *Salvia triloba* (Greek sage). Needles (Me_2CO/petrol). Subl. 198-200. Yellow soln. in alkali.

Et ester: [4825-95-0]
$C_{12}H_{10}O_4$ 218.209
Needles (EtOH aq.). Mp 77-78°.

Nitrile: [359842-85-6] *4-Cyano-2H-1-benzopyran. 4-Cyanocoumarin*
$C_{10}H_5NO_2$ 171.155
Mp 185°.

v. Pechmann, H. *et al., Ber.*, 1901, **34**, 421 (*synth, deriv*)
Dey, B.B. *et al., J.C.S.*, 1915, 1644 (*synth*)
Kawai, M. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 1590 (*synth*)
v. Strandtmann, M. *et al., J. Het. Chem.*, 1972, **9**, 175 (*synth*)
Doganis, B. *et al., CA*, 1973, **78**, 33856x (*isol*)
Joshi, S.D. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 399 (*synth*)
Schwebel, D. *et al., Synthesis*, 2001, 1111-1113 (*nitrile*)

3-Oxobutanal, 9CI O-197

[625-34-3]
Acetoacetaldehyde. Formylacetone
$H_3CCOCH_2CHO \Leftrightarrow H_3CCOCH{=}CHOH$
$C_4H_6O_2$ 86.09
Very unstable. Isol. as Na deriv..Sol. H_2O.

1-Ac: [13945-19-2]
$C_6H_8O_3$ 128.127
Liq. $Bp_{0.5}$ 40°.

Di-Me acetal: [5436-21-5] *4,4-Dimethoxy-2-butanone, 9CI. FEMA 3381*
$C_6H_{12}O_3$ 132.159
Flavouring ingredient. Bp_2 38°.

Ethylene ketal: [18871-63-1] *2-Methyl-1,3-dioxolane-2-acetaldehyde, 9CI. 3,3-(Ethylenedioxy)butanal*
$C_6H_{10}O_3$ 130.143
Oil. Bp_{13} 80-85°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985,

1, 423B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 657B (*nmr*)
U.S. Pat., 1942, 2 262 817; *CA*, **36**, 1331 (*synth*)
George, W.O. *et al., J.C.S.(B)*, 1968, 132 (*pmr*)
Franke, W.K. *et al., Fette, Seifen, Anstrichm.*, 1980, **82**, 370 (*rev, deriv*)
Lipinski, C.A. *et al., J.O.C.*, 1984, **49**, 566 (*synth*)
Potman, R.P. *et al., J.O.C.*, 1985, **50**, 1955 (*deriv, synth, pmr, ms*)
Yamashita, A. *et al., J.O.C.*, 1989, **54**, 3625 (*ketal*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 630 (*di-Me acetal*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2073-2074 (*di-Me acetal*)

2-Oxobutanoic acid, 9CI O-198

[600-18-0]
3-Methylpyruvic acid. 2-Ketobutyric acid. FEMA 3723
$H_3CCH_2COCOOH$
$C_4H_6O_3$ 102.09
Flavour ingredient. Plates. Sol. H_2O, EtOH. Mp 31-32°. Bp_{12} 66°. pK_{a1} 2.5 (25°).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 466C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 531A; 556A (*ir*)
Anatol, J. *et al., Bull. Soc. Chim. Fr.*, 1972, 189 (*synth, bibl*)
Cooper, A.J.L. *et al., J. Biol. Chem.*, 1975, **250**, 527 (*pmr*)
Kozlowski, R. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 75 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 631
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1522-1523

3-Oxobutanoic acid, 9CI O-199

[541-50-4]
Acetoacetic acid. Acetonecarboxylic acid. Acetylacetic acid. Diacetic acid
$H_3CCOCH_2COOH \Leftrightarrow H_3CC(OH)=CHCOOH$
$C_4H_6O_3$ 102.09
Syrup or cryst. Misc. H_2O. Mp 36-37°. Bp 100° dec.. pK_{a1} 3.6 (25°). Strong but unstable acid. On warming loses $CO_2 \rightarrow Me_2CO$.

Et ester: Ethyl acetoacetate, E-260

Butyl ester: [591-60-6] *Butyl acetoacetate. FEMA 2176*
$C_8H_{14}O_3$ 158.197
Flavouring agent. Oil. d^{25} 0.98. Bp_6 83-85° Bp_{16} 100-103°. n_D^{25} 1.4245.
▶AK5100000

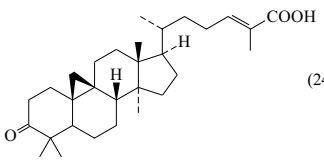
2-Methylpropyl ester: [7779-75-1] *2-Methylpropyl 3-oxobutanoate. Isobutyl acetoacetate. FEMA 2177*
$C_8H_{14}O_3$ 158.197
Flavouring ingredient. Liq. d^{25} 0.97. Bp_{11} 84.5°. n_D^{25} 1.4219.

3-Methylbutyl ester: [2308-18-1] *3-Methylbutyl 3-oxobutanoate. Isoamyl acetoacetate. FEMA 3551*
$C_9H_{16}O_3$ 172.224
Flavouring ingredient. Bp 222-224°.

Benzyl ester: [5396-89-4] *Benzyl acetoacetate. FEMA 2136*
$C_{11}H_{12}O_3$ 192.214
Flavouring ingredient. Oil with a floral odour and fruity taste. Bp_{10} 156-159°. n_D^{20} 1.5120.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 552D; 687A; 688C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1097B; 1227B; **2**, 1238B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 743A (*ir*)
Krampitz, L.O. *et al., Arch. Biochem.*, 1948, **17**, 82 (*synth*)
Biochem. Prep., 1963, **10**, 1 (*synth*)
Kurgane, B.V. *et al., Zh. Org. Khim.*, 1974, **10**, 2306; *J. Org. Chem. USSR (Engl. Transl.)*, 1974, **10**, 2321 (*esters*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 56; 77; 375; 387 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 261; 318-319; 1418; 1442-1443 (*esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BPV250; MFX250; DHI600

3-Oxocycloart-24-en-26-oic acid O-200



(24E)-form

$C_{30}H_{46}O_3$ 454.692
24*Z*-form illus..
(24*E*)-*form* [13878-90-5]
Mangiferonic acid
Isol. from *Mangifera indica* (mango). Cryst. Mp 187-189°.
(24*Z*)-*form* [55511-14-3]
Schizandronic acid. *Schisandronic acid. Ganwuweizic acid*
Cryst. (MeOH). Mp 167-168.5°.

Takahashi, K. *et al., Chem. Pharm. Bull.*, 1975, **23**, 538; 1976, **24**, 2000 (*isol, struct, cmr*)
Sy, L.-K. *et al., Phytochemistry*, 1997, **44**, 1099 (*cmr*)

10-Oxo-8-decenoic acid O-201

[79868-90-9]
9-Formyl-8-nonenoic acid
$OHCCH=CH(CH_2)_6COOH$
$C_{10}H_{16}O_3$ 184.235
(*E*)-*form* [69152-89-2]
Constit. of the mushroom *Agaricus bisporus* (button mushroom). Cryst. (EtOAc). Mp 49-51°.

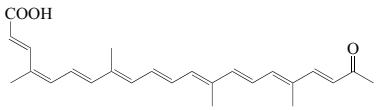
Me ester: [67803-48-9]
$C_{11}H_{18}O_3$ 198.261
Liq. $Bp_{0.1}$ 108-113°.
(*Z*)-*form* [69152-91-6]
Mp 36-40° (impure).

[65114-83-2]

Smith, J.R.L. *et al., Tetrahedron*, 1978, **34**, 1381 (*synth*)
Ranganathan, D. *et al., Tetrahedron*, 1980, **36**, 1869 (*synth, ester*)
Dasaradhi, L. *et al., Synth. Commun.*, 1991, **21**, 183 (*synth, ester*)
Mau, J.L. *et al., Diss. Abstr. Int., B*, 1992, **53**, 2115 (*isol*)
Mau, J.L. *et al., Phytochemistry*, 1992, **31**, 4059 (*isol*)
Pang, Z. *et al., Acta Chem. Scand.*, 1994, **48**, 408 (*isol*)

6′-Oxo-6,5′-diapo-6-carotenoic acid O-202

20-Oxo-4,8,13,17-tetramethyl-2,4,6,8,10,12,14,16,18-heneicosanonaenoic acid

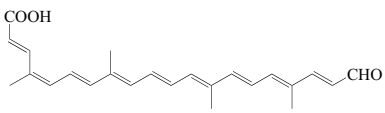


$C_{25}H_{30}O_3$ 378.51
(9*Z*)-*form*
Me ester: [201996-49-8]
$C_{26}H_{32}O_3$ 392.537
Constit. of *Bixa orellana* (annatto).
λ_{max} 430 ; 455 ; 486 (2-methoxy-2-methylpropane).

Mercadante, A.Z. *et al., Phytochemistry*, 1997, **46**, 1379-1383 (*isol, pmr, cmr*)

6′-Oxo-6,6′-diapo-6-carotenoic acid O-203

20-Oxo-4,8,13,17-tetramethyl-2,4,6,8,10,12,14,16,18-eicosanonaenoic acid

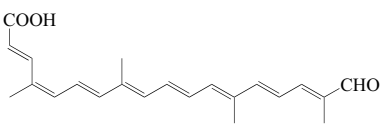


$C_{24}H_{28}O_3$ 364.483
(9*Z*)-*form*
Me ester: [201996-46-5]
$C_{25}H_{30}O_3$ 378.51
Constit. of *Bixa orellana* (annatto).
λ_{max} 434 ; 459 ; 490 (2-methoxy-2-methylpropane).

Mercadante, A.Z. *et al., Phytochemistry*, 1997, **46**, 1379-1383 (*isol, pmr, cmr*)

8′-Oxo-6,8′-diapo-6-carotenoic acid O-204

18-Oxo-4,8,13,17-tetramethyl-2,4,6,8,10,12,14,16-octadecaoctaenoic acid



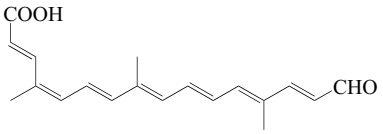
$C_{22}H_{26}O_3$ 338.446
(9*Z*)-*form*
Me ester: [101034-51-9]
$C_{23}H_{28}O_3$ 352.472
Constit. of *Bixa orellana* (annatto).
λ_{max} 337 ; 415 ; 441 ; 470 (2-methoxy-2-methylpropane).

Mercadante, A.Z. *et al., Phytochemistry*, 1997,

46, 1379-1383 (*isol, pmr, cmr*)

10′-Oxo-6,10′-diapo-6-carotenoic acid O-205

16-Oxo-4,8,13-trimethyl-2,4,6,8,10,12,14-hexadecaheptaenoic acid



$C_{19}H_{22}O_3$ 298.381

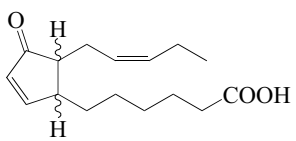
(9*Z*)-*form*

Me ester: [201996-43-2]
$C_{20}H_{24}O_3$ 312.408
Constit. of *Bixa orellana* (annatto). λ_{max} 398 ; 420 ; 445 (2-methoxy-2-methylpropane).

Mercadante, A.Z. *et al., Phytochemistry*, 1997, **46**, 1379-1383 (*isol, pmr, cmr*)

9-Oxo-1,2-dinor-5,10-prostadienoic acid O-206

[197247-23-7]
4-Oxo-5-(2-pentenyl)-2-cyclopentene-1-hexanoic acid. 12-Oxo-2,3-dinor-10,15-phytodienoic acid



$C_{16}H_{24}O_3$ 264.364
Isol. from potato (*Solanum tuberosum*).

Weber, H. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1997, **94**, 10473-10478 (*isol, struct*)

3-Oxododecanal, 9CI O-207

[56505-80-7]
Houttuynin
$H_3C(CH_2)_8COCH_2CHO$
$C_{12}H_{22}O_2$ 198.305
Isol. from *Houttuynia cordata* (Yu Xing Cao). Yellow oil. Mp 6-8°. Polymerises readily. Forms an enol benzoate, Mp 54°.

Takuo, K. *et al., Yakugaku Zasshi*, 1952, **72**, 1227-1231 (*isol*)
Noguchi, T. *et al., Yakugaku Zasshi*, 1956, **76**, 386-389 (*synth*)

12-Oxo-10-dodecenoic acid O-208

11-Formyl-10-undecenoic acid
$OHCCH{=}CH(CH_2)_8COOH$
$C_{12}H_{20}O_3$ 212.288

(*E*)-*form* [65410-38-0]
Traumatin. Traumatic half aldehyde
Found in *Thea sinensis* chloroplasts. Solid (cyclohexane/Et_2O). Mp 65-66°.

Me ester: [63024-87-3]
Amber liq. Mp 0.7°. $Bp_{0.05}$ 109-111°.

(*Z*)-*form*

Me ester:
$C_{13}H_{22}O_3$ 226.315
$Bp_{0.23}$ 126-131°.

Kajiwara, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 8 (*synth, bibl*)
Hatanaka, A. *et al., Phytochemistry*, 1977, **16**, 1828 (*isol*)
Bestmann, H.J. *et al., Tet. Lett.*, 1977, 121 (*synth, pmr*)
Rakoff, H. *et al., Synth. Commun.*, 1979, **9**, 185 (*synth, pmr, ir*)
Bestmann, H.J. *et al., Annalen*, 1981, 1705 (*synth, ir, pmr*)
Gaede, B.J. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 461 (*synth, pmr, cmr, bibl*)
Dasaradhi, L. *et al., Synth. Commun.*, 1991, **21**, 183 (*synth*)

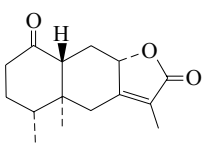
15-Oxo-11-eicosenoic acid O-209

$H_3C(CH_2)_4COCH_2CH_2CH{=}CH(CH_2)_9COOH$
$C_{20}H_{36}O_3$ 324.503

(*Z*)-*form* [182145-55-7]
Isol. from wheat flour infested with the beetle *Oryzaephilus surinamensis*.

Nakajima, S. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1546; 1997, **61**, 551 (*isol, synth, pmr*)

1-Oxo-7(11)-eremophilen-12,8-olide O-210



(4α,5α,8α,10β)-*form*

$C_{15}H_{20}O_3$ 248.321

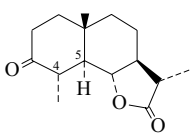
(4α,5α,8α,10β)-*form* [12656-97-2]
Istanbulin B
Constit. of *Smyrnium olusatrum* (alexanders). Cryst. Mp 167°. $[\alpha]_D^{20}$ +120.6 (MeOH).

(4β,5β,8β,10β)-*form*
Oil. $[\alpha]_D^{24}$ -73 (c, 0.43 in $CHCl_3$).

Cox, P.J. *et al., Tetrahedron*, 1980, **36**, 3437 (*cryst struct*)
Buděšínský, M. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1311 (*abs config*)
Bohlmann, F. *et al., Bull. Soc. Chim. Belg.*, 1986, **95**, 707 (*isol, pmr*)

3-Oxo-12,6-eudesmanolide O-211

Santonan



(4α,5α,6α,11α)-*form*

$C_{15}H_{22}O_3$ 250.337

(4α,5α,6α,11α)-*form* [13902-54-0]
Artepaulin. *α-Tetrahydrosantonin*
Cryst. (EtOH). Mp 158°. $[\alpha]_D^{18}$ +17.8 (MeOH).

(4β,5β,6α,11α)-*form* [17956-11-5]
β-Tetrahydrosantonin
Cryst. (Et_2O). Mp 105°. $[\alpha]_D^{18}$ +9.3 (MeOH).

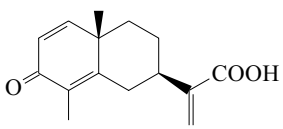
(4β,5α,6α,11α)-*form* [14804-46-7]
γ-Tetrahydrosantonin
Cryst. (EtOH). Mp 96-97°. $[\alpha]_D^{20}$ +7.3.

(4β,5α,6α,11β)-*form* [14804-47-8]
Cadabicilone
Constit. of the famine food *Cadaba farinosa* (luqata sigmama). Cryst. ($CHCl_3$/Et_2O). Mp 118-120°.

Banerji, J.C. *et al., J.C.S.*, 1957, 5041 (*synth*)
Hendrickson, J.B. *et al., J.C.S.*, 1962, 1678 (*synth*)
Narayanan, C.R. *et al., J.O.C.*, 1968, **33**, 3156 (*struct*)
Adekenov, S.M. *et al., Khim. Prir. Soedin.*, 1983, **19**, 238; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 234 (*isol*)
Ahmad, V.U. *et al., Z. Naturforsch., B*, 1990, **45**, 1100 (*Cadabicilone*)

3-Oxo-1,4,11(13)-eudesmatrien-12-oic acid O-212

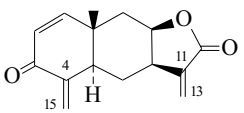
[135594-80-8]



$C_{15}H_{18}O_3$ 246.305
Constit. of *Artemisia vulgaris* (mugwort). Gum. $[\alpha]_D$ -80 (c, 0.36 in $CHCl_3$).

Marco, J.A. *et al., Phytochemistry*, 1991, **30**, 2403 (*isol, pmr, cmr*)
Marco, J.A. *et al., Magn. Reson. Chem.*, 1992, **30**, 678 (*cmr*)

3-Oxo-1,4(15),11(13)-eudesmatrien-12,8-olide O-213



8β-*form*

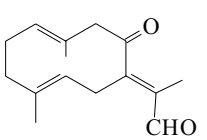
$C_{15}H_{16}O_3$ 244.29

8β-*form* [15569-50-3]
Encelin. *Dehydrofarinosin*
Constit. of *Inula helenium* (elecampane). Cryst. (EtOAc/hexane). Mp 195-196°. $[\alpha]_D^{26}$ -16.5 (c, 3.67 in $CHCl_3$). λ_{max} 213 (ϵ 15200); 239 (ϵ 10600) (MeOH) (Berdy). λ_{max} 210 (ϵ 15140); 239 (ϵ 10570) (EtOH) (Berdy).

Geissman, T.A. *et al., J.O.C.*, 1968, **33**, 656 (*Encelin*)
Bohlmann, F. *et al., Annalen*, 1986, 799 (*isol, pmr*)
Milman, I.A. *et al., Khim. Prir. Soedin.*, 1990, **26**, 307; *Chem. Nat. Compd. (Engl. Transl.)*, 251 (*rev*)
Cantrell, C.L. *et al., Planta Med.*, 1999, **65**, 351-355 (*activity*)

8-Oxo-1(10),4,7(11)-germacratrien-13-al O-214

[129673-85-4]
Germacrone-13-al



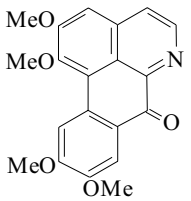
$C_{15}H_{20}O_2$ 232.322
Constit. of *Curcuma longa* (turmeric).

Viscous oil.

Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201 (*isol, pmr, cmr*)

Oxoglaucine O-215

[5574-24-3]
*1,2,9,10-Tetramethoxy-7*H*-dibenzo[*de,g*]-quinolin-7-one, 9CI. Liriodendron base.* O-*Methylatheroline*



$C_{20}H_{17}NO_5$ 351.358
Alkaloid from *Annona purpurea* (soncoya). Mp 227-229° (195-197°).

O^1*-De-Me,* N^1*-Me, inner salt:* [34421-18-6]
Corunnine*. Glauvine*
$C_{20}H_{17}NO_5$ 351.358
Violet needles (EtOH) (also descr. as green). Mp 255-257°.

O^1*-De-Me,* N^1*-Me, perchlorate:*
Purple needles. Mp 293-295°.

O^9*-De-Me:* [5140-35-2] ***Atheroline***
$C_{19}H_{15}NO_5$ 337.331
Mp 250-260° dec. λ_{max} 252 (ϵ 50100); 299 (ϵ 39800); 323 (ϵ 39800); 400 (ϵ 15800) (EtOH/KOH) (Derep). λ_{max} 242 (ϵ 39800); 272 (ϵ 39800); 292 (ϵ 25100); 352 (ϵ 12600); 380 (ϵ 10000); 433 (ϵ 5010) (EtOH) (Derep).

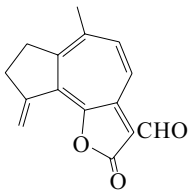
► RB6035000

O^9*-De-Me, Ac:*
Yellow needles (Py). Mp 190-195°.

Buchanan, M.A. *et al., J.O.C.*, 1960, **25**, 1389 (*isol, uv*)
Cohen, J. *et al., J.O.C.*, 1961, **26**, 4143 (*isol, uv, synth*)
Bick, I.R.C. *et al., Tet. Lett.*, 1965, 2399 (*Atheroline, isol, ir, pmr, uv*)
Bick, I.R.C. *et al., Aust. J. Chem.*, 1967, **20**, 1403 (*ms*)
Tomita, M. *et al., Yakugaku Zasshi*, 1968, **88**, 1143 (*isol, pmr*)
Ribas, I. *et al., Tet. Lett.*, 1971, 3093; 1973, 3617 (*Corunnine, uv, ir, pmr, struct, synth*)
Cava, M.P. *et al., J.O.C.*, 1972, **37**, 2936 (*Atheroline, synth, ir, pmr, uv*)
Yakhontova, L.D. *et al., Khim. Prir. Soedin.*, 1972, **8**, 214; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 212 (*Corunnine, uv, pmr*)
Kupchan, S.M. *et al., Chem. Comm.*, 1973, 915 (*Corunnine, synth*)
Castedo, L. *et al., Heterocycles*, 1975, **3**, 449; 1980, **14**, 1131 (*Corunnine, synth, struct*)
Chen, C.-L. *et al., Phytochemistry*, 1976, **15**, 1161 (*Corunnine, isol, uv, pmr*)
Kametani, T. *et al., Tetrahedron*, 1977, **33**, 1069 (*Atheroline, synth*)
Hufford, C.D. *et al., J. Pharm. Sci.*, 1980, **69**, 1180-1182 (*activity*)
Marsaioli, A.J. *et al., Phytochemistry*, 1980, **19**, 995 (*cmr*)
Saá, C. *et al., Tet. Lett.*, 1985, **26**, 4559 (*synth*)
Martínez, E. *et al., Planta Med.*, 1988, **54**, 361 (*isol, uv, ir, pmr, ms*)
Atanes, N. *et al., J.O.C.*, 1991, **56**, 2984 (*synth*)

13-Oxo-1(10),4(15),5,7(11),8-guaiapentaen-12,6-olide O-216

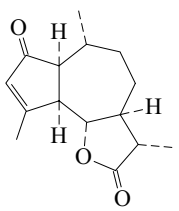
[97915-46-3]
Lettucenin A



$C_{15}H_{12}O_3$ 240.258
Phytoalexin from *Lactuca sativa* var. *capitata* (head lettuce). Unstable yellow cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 175-176°. λ_{max} 233 (ϵ 25600); 255 (ϵ 15600); 329 (ϵ 25000); 446 (ϵ 32000) (MeOH) (Derep). λ_{max} 234 ; 332 ; 446 (EtOH) (Berdy). λ_{max} 238 ; 431 (MeOH-NaOH) (Berdy).

Takasugi, M. *et al., Chem. Comm.*, 1985, 621
Monde, K. *et al., Chem. Lett.*, 1990, 1283 (*synth*)
Bennett, M.H. *et al., Phytochemistry*, 2002, **60**, 255-261 (*biosynth*)

2-Oxo-3-guaien-12,6-olide O-217



$C_{15}H_{20}O_3$ 248.321

(1α,5α,6α,10α,11α)-*form* [82460-83-1]
Carpesialactone
Viscous liq. with bitter taste. Bp_5 200-202°. The identity of Bohlmann's sample with an earlier sample of undetd. 10 and 11 stereochem. is not certain.

► Powerful irritant.

(1β,5α,6α,10β,11α)-*form* [132296-37-8]
Cichoralexin
Constit. of *Cichorium intybus* (chicory) inoculated with *Pseudomonas cichorii*. Cryst. (hexane). Mp 145-146°. λ_{max} 225 (ϵ 12900) (MeOH) (Berdy).

(1α,5α,6α,10β,11β)-*form* [112001-11-3]
Cladantholide
Cryst. Mp 160-161°. $[\alpha]_D^{20}$ +309 (c, 0.5 in $CHCl_3$).

Kariyone, T. *et al., Yakugaku Zasshi*, 1955, **75**, 39; *CA*, **50**, 890 (*struct*)
Naito, S. *et al., Yakugaku Zasshi*, 1955, **75**, 93; 325; *CA*, **50**, 891; 1680 (*struct, synth*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 460 (*isol, struct*)
Monde, K. *et al., Phytochemistry*, 1990, **29**, 3449 (*Cichoralexin*)
Daniewski, W.M. *et al., Phytochemistry*, 1993, **34**, 1639 (*Cladantholide*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)
Lee, E. *et al., J.A.C.S.*, 1997, **119**, 8391-8392 (*synth*)

5-Oxohexadecanoic acid, 9CI O-218

[70444-63-2]
5-Oxopalmitic acid. 5-Ketopalmitic acid
$H_3C(CH_2)_{10}CO(CH_2)_3COOH$
$C_{16}H_{30}O_3$ 270.411
Cryst. (MeOH, C_6H_6 or petrol). Mp 88°.

Me ester: [54527-00-3]
$C_{17}H_{32}O_3$ 284.438
Mp 47.5-48.5°.

Robinson, G.M. *et al., J.C.S.*, 1930, 745-751 (*synth*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883-890 (*isol*)
Naoshima, Y. *et al., Agric. Biol. Chem.*, 1983, **47**, 1431-1434 (*Me ester, synth, ir, pmr, ms*)
Lhommet, G. *et al., Synth. Commun.*, 1996, **26**, 3897-3901 (*synth, ir, cmr*)

7-Oxohexadecanoic acid, 9CI O-219

[54527-29-6]
7-Oxopalmitic acid. 7-Ketopalmitic acid
$H_3C(CH_2)_8CO(CH_2)_5COOH$
$C_{16}H_{30}O_3$ 270.411
Cryst. (MeOH or petrol). Mp 78°.

[54527-09-2, 120622-69-7]

Robinson, G.M. *et al., J.C.S.*, 1930, 745-751 (*synth*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883-890 (*isol*)
Cross, B.E. *et al., J.C.S. Perkin 1*, 1975, 2523-2526 (*synth*)

8-Oxohexadecanoic acid, 9CI O-220

[2777-52-8]
8-Oxopalmitic acid. 8-Ketopalmitic acid
$H_3C(CH_2)_7CO(CH_2)_6COOH$
$C_{16}H_{30}O_3$ 270.411
Trace constit. of milk fat. Cryst. (MeOH). Mp 77-78°.

Amide:
$C_{16}H_{31}NO_2$ 269.426
Mp 58°.

[54527-10-5]

Bodenstein, M. *et al., Ber.*, 1894, **27**, 3397-3405 (*synth*)
Robinson, G.M. *et al., J.C.S.*, 1930, 745-751 (*synth*)
Tulloch, A.P. *et al., Can. J. Chem.*, 1965, **43**, 415-420 (*isol*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883-890 (*isol*)

9-Oxohexadecanoic acid, 9CI O-221

[54527-30-9]
9-Oxopalmitic acid. 9-Ketopalmitic acid
$H_3C(CH_2)_6CO(CH_2)_7COOH$
$C_{16}H_{30}O_3$ 270.411
Trace constit. of milk fat. Cryst. (EtOAc). Mp 73.5-74.5°.

Me ester: [54527-11-6]
$C_{17}H_{32}O_3$ 284.438
Cryst. (petrol). Mp 37-38°.

Davies, L.A. *et al., J.A.C.S.*, 1928, **50**, 1749-1755 (*synth*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883-890 (*isol, glc, ms*)
Radhakrishnan, R. *et al., J.A.C.S.*, 1982, **104**, 3990-3997 (*Me ester, ester, synth, ir*)
Misharin, A.Yu. *et al., Synthesis*, 1985, 656-659 (*Me ester, synth, ir, pmr*)

11-Oxohexadecanoic acid, 9CI O-222

[2388-81-0]
11-Oxopalmitic acid. 11-Ketopalmitic acid
$H_3C(CH_2)_4CO(CH_2)_9COOH$
$C_{16}H_{30}O_3$ 270.411
Trace constit. of milk fat. Cryst. (EtOAc). Mp 74-75°.

Semicarbazone:
Mp 118°.

Me ester: [54527-12-7]
$C_{17}H_{32}O_3$ 284.438
Needles (petrol). Mp 38-39°.

Davies, L.A. *et al., J.A.C.S.*, 1928, **50**, 1749-1755 (*synth*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883-890 (*isol, glc, ms*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1023-1026 (*Me ester*)

5-Oxohexanal O-223

[505-03-3]
γ-Acetylbutyraldehyde. Soyanal
$H_3CCOCH_2CH_2CH_2CHO$
$C_6H_{10}O_2$ 114.144
Poss. obt. from soya. d^{18} 1.02. Bp_{18} 94-95°. n_D^{28} 1.4615.

Mono-2,4-dinitrophenylhydrazone:
Yellow leaflets. Mp 110-111° (107-108° dec.).

Bis-2,4-dinitrophenylhydrazone:
Orange needles. Mp 142-143° dec Mp 184°.

Nakajima, M. *et al., Nippon Kagaku Kaishi*, 1949, **70**, 49; *CA*, **45**, 7015c
Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 370 (*synth*)
Garnick, R.L. *et al., J.A.C.S.*, 1978, **100**, 4213 (*synth, pmr*)

2-Oxohexanedioic acid, 9CI O-224

[3184-35-8]
2-Oxoadipic acid
$HOOC(CH_2)_3COCOOH$
$C_6H_8O_5$ 160.126
Present in pea seedlings. Cryst. (Et_2O). Mp 127°.

Di-Et ester: [99683-30-4]
$C_{10}H_{16}O_5$ 216.233
Bp_{16} 157°.

Di-Et ester, oxime:
$C_{10}H_{17}NO_5$ 231.248
Mp 52-53°.

Di-Et ester, semicarbazone:
Mp 118°.

Oxime:
$C_6H_9NO_5$ 175.141
Cryst. Mp 151-152° dec.

Phenylhydrazone:
Mp 243°.

Semicarbazone:
Mp 210-215°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 824C (*nmr*)
Dieckmann, W. *et al., Ber.*, 1900, **33**, 586 (*synth*)
Virtanen, A.I. *et al., Acta Chem. Scand.*, 1954, **8**, 1720 (*isol*)
U.S. Pat., 1960, 2 883 420; *CA*, **54**, 2180 (*synth*)
U.S. Pat., 1961, 2 990 410; *CA*, **55**, 25764 (*synth*)
Nelson, R.B. *et al., Org. Prep. Proced. Int.*, 1973, **5**, 55 (*synth*)

3-Oxohexanoic acid, 9CI O-225

[4380-91-0]
3-Oxocaproic acid. Butyrylacetic acid
$H_3CCH_2CH_2COCH_2COOH$
$C_6H_{10}O_3$ 130.143

Me ester: [30414-54-1]
$C_7H_{12}O_3$ 144.17
Bp_{14} 85°.

Et ester: [3249-68-1] *FEMA 3683*
$C_8H_{14}O_3$ 158.197
Flavouring agent. Liq. with a slightly fatty odour. Bp_{20} 102-103° $Bp_{0.5}$ 57-60°. n_D^{20} 1.4362.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 690A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1104C (*nmr*)
Kagan, H.B. *et al., Bull. Soc. Chim. Fr.*, 1966, 1819 (*synth*)
Kaneda, A. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 228 (*synth*)
Roth, M. *et al., Helv. Chim. Acta*, 1971, **54**, 710 (*synth*)
Rathke, M.W. *et al., Tet. Lett.*, 1971, 2953 (*synth*)
Couffignal, R. *et al., J. Organomet. Chem.*, 1977, **127**, C65 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 261 (*Et ester*)
Cadman, M.L.F. *et al., J.C.S. Perkin 1*, 1995, 1397 (*Me ester, synth, ir, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1029 (*Et ester*)

4-Oxo-2-hexen-1-al O-226

$H_3CCH_2COCH{=}CHCHO$
$C_6H_8O_2$ 112.128

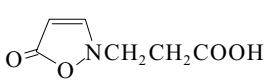
(E)-form [2492-43-5]
Constit. of soy sauce. Yellow oil with pungent pleasant odour. Bp_{19} 91-92°.

Bis(dinitrophenylhydrazone):
Dark red cryst. Mp 247-248° dec.

Gilby, A.R. *et al., Aust. J. Chem.*, 1964, **17**, 1311 (*pmr*)
Pinder, A.R. *et al., J.C.S.*, 1965, 2955 (*isol, uv, synth*)
Ward, J.P. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 989 (*synth*)

5-Oxo-2(5*H*)-isoxazolepropanoic acid, 9CI O-227

[92279-63-5]
2-(2-Carboxyethyl)-3-isoxazolin-5-one



$C_6H_7NO_4$ 157.126
Needles (Me_2CO aq.). Mp not recorded.

Nitrile: [51580-99-5] ***5-Oxo-2(5H)-isoxazolepropanenitrile, 9CI.*** *2-(2-Cyanoethyl)-3-isoxazolin-5-one*
$C_6H_6N_2O_2$ 138.126
Constit. of *Pisum sativum* (peas).

v. Rompuy, L. *et al., J.C.S. Perkin 1*, 1973, 2503 (*synth*)
Ikegami, F. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2450 (*isol, uv, ir, pmr, ms, struct*)

2-Oxo-4-methylenepentanedioic acid O-228

[55601-65-5]
α-Keto-γ-methyleneglutamic acid
$H_2C{=}C(COOH)CH_2COCOOH$
$C_6H_6O_5$ 158.11
Found in peanut (*Arachis hypogaea*).

2,4-Dinitrophenylhydrazone:
Mp 228° dec.

5-Amide:
$C_6H_7NO_4$ 157.126

Towers, G.H.N. *et al., J.A.C.S.*, 1954, **76**, 1959
Fowden, L. *et al., Biochem. J.*, 1955, **59**, 228

4-Oxononanal, 9CI O-229

[74327-29-0]
$H_3C(CH_2)_4COCH_2CH_2CHO$
$C_9H_{16}O_2$ 156.224
Present in used frying oils and water melon aroma. Tentatively identified in roast chicken fat. Liq. Bp_{15} 92-94° Bp_3 81-82°.

Kulinkovich, O.G. *et al., Synthesis*, 1984, 886 (*synth*)
Geraghty, N.W.A. *et al., Synthesis*, 1989, 603 (*synth*)
Takeoka, G.R. *et al., J. Agric. Food Chem.*, 1995, **43**, 22-26 (*occur, anal*)

5-Oxooctadecanoic acid O-230

[16694-31-8]
5-Oxostearic acid. 5-Ketostearic acid
$H_3C(CH_2)_{12}CO(CH_2)_3COOH$
$C_{18}H_{34}O_3$ 298.465
Trace constit. of milk fat.

Semicarbazone:
Mp 197°.

Me ester: [2380-20-3]
$C_{19}H_{36}O_3$ 312.492
Mp 49.5°.

Dodecyl ester:Dodecyl 5-oxooctadecanoate. Actinomycin B1†. Actinomycin J2
$C_{30}H_{58}O_3$ 466.786
Cryst. Mp 59-61° Mp 81.5°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1105A (*nmr*)
Brown, W.B. *et al., Biochem. J.*, 1935, **29**, 631
Hirata, Y. *et al., Bull. Chem. Soc. Jpn.*, 1949, **22**, 121 (*dodecyl ester*)
Tulloch, A.P. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 833 (*glc*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883 (*isol, glc, ms*)
Tulloch, A.P. *et al., Can. J. Chem.*, 1977, **55**, 1135 (*cmr*)

9-Oxooctadecanoic acid O-231

[4114-74-3]
9-Oxostearic acid. 9-Ketostearic acid
$H_3C(CH_2)_8CO(CH_2)_7COOH$
$C_{18}H_{34}O_3$ 298.465
Trace constit. of milk fat. Cryst. (EtOH). Mp 83°.

Amide:
$C_{18}H_{35}NO_2$ 297.48
Mp 79°.

Behrend, O. *et al., Ber.*, 1896, **29**, 806 (*synth*)
Robinson, G.M. *et al., J.C.S.*, 1926, 2204 (*synth*)

Tulloch, A.P. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 833 (*glc*)
Kenney, H.E. *et al., J. Am. Oil Chem. Soc.*, 1971, **48**, 765 (*synth*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883 (*isol, glc, ms*)
Tulloch, A.P. *et al., Can. J. Chem.*, 1977, **55**, 1135 (*cmr*)

10-Oxooctadecanoic acid O-232

[4158-12-7]
10-Oxostearic acid. 10-Ketostearic acid
$H_3C(CH_2)_7CO(CH_2)_8COOH$
$C_{18}H_{34}O_3$ 298.465
Trace constit. of milk fat. Cryst. Mp 76°.

Me ester: [1842-70-2]
$C_{19}H_{36}O_3$ 312.492
Mp 47-51°.

Amide:
$C_{18}H_{35}NO_2$ 297.48
Cryst. (C_6H_6/petrol). Mp 80°.

Baruch, J. *et al., Ber.*, 1894, **27**, 1742 (*synth*)
Robinson, G.M. *et al., J.C.S.*, 1926, 2204 (*synth*)
Tulloch, A.P. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 833 (*glc*)
Kenney, H.E. *et al., J. Am. Oil Chem. Soc.*, 1971, **48**, 765 (*synth*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883 (*isol, glc, ms*)
Zhdanov, R.I. *et al., Bioorg. Khim.*, 1976, **2**, 395
Tulloch, A.P. *et al., Can. J. Chem.*, 1977, **55**, 1135 (*cmr*)

11-Oxooctadecanoic acid O-233

[2388-83-2]
11-Oxostearic acid. 11-Ketostearic acid
$H_3C(CH_2)_6CO(CH_2)_9COOH$
$C_{18}H_{34}O_3$ 298.465
Trace constit. of milk fat. Cryst. (EtOH/AcOH). Mp 65°.

Tulloch, A.P. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 833 (*glc*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883 (*isol, glc, ms*)
Tulloch, A.P. *et al., Can. J. Chem.*, 1977, **55**, 1135 (*cmr*)

4-Oxo-9,11,13,15-octadecatetraenoic acid O-234

$H_3CCH_2(CH=CH)_4(CH_2)_4COCH_2CH_2COOH$
$C_{18}H_{26}O_3$ 290.402

(9Z,11E,13E,15Z)-form [17699-21-7]
Obt. from *Chrysobalanus icaco* seed oil.

Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1967, **1**, 349

13-Oxo-9-octadecenoic acid O-235

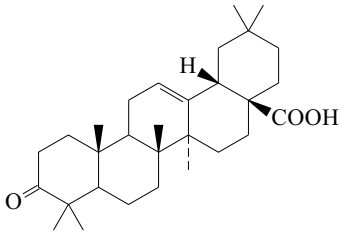
$H_3C(CH_2)_4COCH_2CH_2CH=CH(CH_2)_7COOH$
$C_{18}H_{32}O_3$ 296.449

(Z)-form [38205-11-7]
Isol. from wheat flour infested with the beetle *Oryzaephilus surinamensis*.

Nakajima, S. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1546; 1997, **61**, 551 (*isol, synth, pmr*)

3-Oxo-12-oleanen-28-oic acid O-236

[17990-42-0]
Oleanonic acid



$C_{30}H_{46}O_3$ 454.692
Cryst. (MeOH). Mp 226-229°. $[\alpha]_D$ +101 (c, 1.63 in $CHCl_3$).

Me ester: [1721-58-0]
$C_{31}H_{48}O_3$ 468.718
Isol. from *Pistacia vera* (pistachio) and *Zizyphus jujuba* (Chinese date). Cryst. (MeOH). Mp 184-185°. $[\alpha]_D$ +94 (c, 1.26 in $CHCl_3$).

Oxime:
Cryst. (EtOH). Mp 294° dec.

Me ester, oxime:
Cryst. (EtOH/C_6H_6). Mp 245-248°.

18α-form [73522-35-7]
No phys. props. reported.

[6785-78-0]

Drefahl, G. *et al., Chem. Ber.*, 1960, **93**, 1967 (*synth*)
Savoir, R. *et al., Bull. Soc. Chim. Belg.*, 1967, **76**, 335 (*synth, pmr*)
Renwick, J.D. *et al., J.C.S.(C)*, 1969, 2544 (*cd, ord*)
Seo, S. *et al., Tet. Lett.*, 1975, 7 (*cmr*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1489 (*18α-form*)
Gzella, A. *et al., Acta Cryst. C*, 1999, **55**, 2153-2156 (*cryst struct*)

2-Oxopentanedioic acid, 9CI O-237

[328-50-7]
2-Oxoglutaric acid. α-Ketoglutaric acid. FEMA 3891
$HOOCCH_2CH_2COCOOH$
$C_5H_6O_5$ 146.099
Flavouring ingredient. Cryst. (Me_2CO/C_6H_6). Mp 115°.

Imidazole salt: [67708-20-7] *Imidazole ketoglutarate. Retencal*

Oxime: [2211-15-6]
$C_5H_7NO_5$ 161.114
Prisms (H_2O). Mp 152° dec.

Semicarbazone: [2704-31-6]
Cryst. (H_2O). Mp 220°.

2,4-Dinitrophenylhydrazone: [1237-47-4]
Mp 213° dec.

Di-Me ester: [13192-04-6]
$C_7H_{10}O_5$ 174.153
Mp 129-131° (as 2,4-dinitrophenylhydrazone). $Bp_{0.4}$ 90-95°.

Di-Et ester: [5965-53-7]
$C_9H_{14}O_5$ 202.207
Bp_{13} 144°.

Di-Et ester, semicarbazone:
Cryst. (EtOH aq.). Mp 114°.

[305-72-6, 997-43-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 532B; 686A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 824B; 1108B (*nmr*)

Metzler, D.E. *et al., J.A.C.S.*, 1954, **76**, 644 (*synth*)
Org. Synth., Coll. Vol., 3, 1955, 510 (*synth*)
Weygand, F. *et al., Annalen*, 1962, **658**, 128 (*synth*)
Kretovich, V.L. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 471; *CA*, **61**, 16438 (*occur*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 531 (*use*)
Tsugawa, R. *et al., Agric. Biol. Chem.*, 1969, **33**, 158 (*biosynth*)
Fr. Pat., 1969, 2 005 402; *CA*, **73**, 34808 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 870 (*occur*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 3906
Pat. Coop. Treaty (WIPO), 1996, 96 10 927; *CA*, **125**, 56856a (*use*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1393 (*use*)

2-Oxopentanoic acid, 9CI O-238

[1821-02-9]
2-Oxovaleric acid. α-Ketovaleric acid
$H_3CCH_2CH_2COCOOH$
$C_5H_8O_3$ 116.116
Isol. from *Trigonella caerulea* (sweet trefoil). Liq. Mod. sol. H_2O. d_4^{14} 1.1. Mp 6-7°. Bp 179° Bp_{12} 78°. n_D^{20} 1.4283.

Schreiber, J. *et al., Bull. Soc. Chim. Fr.*, 1956, 1361 (*synth*)
Japan. Pat., 1961, 61 16 628; *CA*, **57**, 3460 (*synth*)
Anatol, J. *et al., Bull. Soc. Chim. Fr.*, 1972, 189 (*synth*)
Ney, K.H. *et al., Gordian*, 1986, **86**, 9; *CA*, **105**, 5347q (*isol*)
Singh, J. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 501 (*synth*)
Simchen, G. *et al., Annalen*, 1992, 607 (*synth, pmr*)

4-Oxopentanoic acid, 9CI O-239

[123-76-2]
Levulinic acid, 8CI. 3-Acetylpropionic acid. FEMA 2627
$H_3CCOCH_2CH_2COOH$
$C_5H_8O_3$ 116.116
Found in beet, caramel etc. Also reported in papaya (*Carica papaya*), wheat bread, rice bran, sake and Chinese quince fruit (*Chaenomeles legenaria*). Also prod. by lychee (*Litchi chinensis*), Malabar spinach (*Basella rubra*) and *Phyllophora* spp. Flavour ingredient. Plates or leaflets with tart, whisky taste. V. sol. H_2O, EtOH, Et_2O; insol. hydrocarbons. Mp 33.5°. Bp 245° Bp_{14} 143-147°. pK_a 4.62.

▶ Skin irritant. LD_{50} (rat, orl) 1850 mg/kg. OI1575000

Et ester: [539-88-8] *Ethyl levulinate. FEMA 2442*
$C_7H_{12}O_3$ 144.17
Flavouring ingredient. Liq. d^{20} 1.01. Bp 199-201° $Bp_{0.1}$ 38°. n_D^{20} 1.4220.

▶ OI1700000

Butyl ester: [2052-15-5] *Butyl levulinate. FEMA 2207*
$C_9H_{16}O_3$ 172.224
Flavouring agent. Liq. with a bitter burning taste. d^{20} 0.97. Bp 229-231°

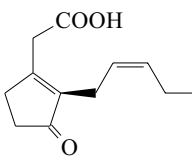
$Bp_{5.5}$ 106-108° $Bp_{0.1}$ 61°. n_D^{20} 1.4283.
▶OI1695000

[591-64-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 531B; 685B; 685C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 823A; 1102B; 1102C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 741D (*ir*)
Sadtler Standard C-13 NMR Spectra, 2217 (*cmr*)
Sah, P.P.T. *et al., J.A.C.S.*, 1930, **52**, 4881 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 335 (*synth*)
Cowley, M.A. *et al., J.A.C.S.*, 1933, **55**, 3463 (*bibl*)
Mattox, V.R. *et al., J.A.C.S.*, 1948, **70**, 882 (*use*)
Leonard, R.H. *et al., Ind. Eng. Chem.*, 1956, **48**, 1331 (*rev*)
Cooper, A.J.L. *et al., J. Biol. Chem.*, 1975, **250**, 527 (*pmr*)
Brown, D.W. *et al., J. Chem. Technol. Biotechnol.*, 1982, **32**, 920 (*esters*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 308
Srzić, D. *et al., Org. Mass Spectrom.*, 1988, **23**, 829 (*ms*)
Merck Index, 11th edn., 1989, 3775 (*Et ester*)
Sizov, A.Y. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1990, 474; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1990, 412 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 854
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 92; 244; 429
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 349-350; 1004-1005; 1570-1571
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EFS600; LFH000

3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid O-240

3,7-Didehydrojasmonic acid

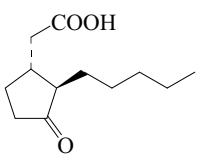


$C_{12}H_{16}O_3$ 208.257

(Z)-*form* [120282-76-0]
Constit. of *Vicia faba*. Oil. λ_{max} 236 (log ϵ 3.81) (MeOH).
Miersch, O. *et al., Phytochemistry*, 1989, **28**, 339

3-Oxo-2-pentylcyclopentaneacetic acid, 9CI O-241

[3572-64-3]



(1*R*,2*R*)-*form*

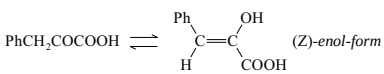
$C_{12}H_{20}O_3$ 212.288

(1*R*,2*R*)-*form* [98674-52-3]
Dihydrojasmonic acid
Isol. from *Vicia faba* and *Secale cereale* (rye). Oil. $[\alpha]_D^{22}$ -28.3 (c, 0.1 in MeOH).
Me ester: [24851-98-7] *Methyl dihydrojasmonate. Hedione. FEMA 3408*
$C_{13}H_{22}O_3$ 226.315
Flavouring ingredient. Liq. Bp_3 102-108° (Bp_4 118-119°).
▶GY2453800

(1*R*,2*S*)-*form* [96844-45-0]
Dihydroisojasmonic acid
$[\alpha]_D^{25}$ +10.5 (c, 0.1 in MeOH).
Renold, W. *et al., Helv. Chim. Acta*, 1974, **57**, 1301 (*ms*)
Roman, K. *et al., Tet. Lett.*, 1974, 3413
Shono, T. *et al., J.A.C.S.*, 1975, **97**, 6144 (*synth*)
Torii, S. *et al., J.O.C.*, 1975, **40**, 2221 (*synth, ir, pmr, ms*)
Matsuda, I. *et al., J.O.C.*, 1980, **45**, 237 (*ir, pmr*)
Tsuji, J. *et al., Tet. Lett.*, 1980, **21**, 1475 (*synth*)
Miersch, O. *et al., Phytochemistry*, 1987, **26**, 1037-1039; 1989, **28**, 339-340 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 496 (*Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1753-1754 (*Me ester*)

2-Oxo-3-phenylpropanoic acid O-242

[156-06-9]
α-Oxobenzenepropanoic acid, 9CI. Phenylpyruvic acid. 2-Hydroxy-3-phenyl-2-propenoic acid, 9CI. α-Hydroxycinnamic acid. FEMA 3892



$C_9H_8O_3$ 164.16
Exists as (*Z*)-enol-form in solid state; enol predominates in organic solvents; equilibrium in aq. soln.. Flavouring ingredient. Plates ($CHCl_3$). Spar. sol. hot H_2O. Mp 157° dec. Oxidises in air. Reduces boiling Fehling's soln..

[52178-60-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 273A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 998B (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 519 (*synth*)
Weygand, F. *et al., Annalen*, 1962, **658**, 128 (*synth*)
Igarashi, M. *et al., J.O.C.*, 1967, **32**, 3399 (*synth*)
Anatol, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **272**, 1159 (*synth*)
Kulkarni, B.D. *et al., Indian J. Chem.*, 1975, **13**, 1097 (*synth*)
Sciacovelli, O. *et al., Z. Naturforsch., C*, 1976, **31**, 5 (*ms, cmr, pmr*)
Ramage, R. *et al., J.C.S. Perkin 1*, 1984, 1531 (*synth, ir*)
Fujita, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 242 (*anal*)
Hanai, K. *et al., J. Phys. Chem.*, 1989, **93**, 6013 (*ir, Raman*)
Hanai, K. *et al., J. Mol. Struct.*, 1991, **245**, 21 (*ir, pmr, uv*)
Kuwae, A. *et al., Spectrochim. Acta A*, 1993, **49**, 125 (*cmr*)
Marais, C. *et al., J.C.S. Perkin 1*, 1996, **2915**, (*isol, biosynth, synth*)
Okabe, N. *et al., Acta Cryst. C*, 1997, **53**, 1449-1450 (*cryst struct*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1394 (*use*)

3-Oxo-3-phenylpropanoic acid O-243

[614-20-0]
β-Oxobenzenepropanoic acid, 9CI. Benzoylacetic acid
$PhCOCH_2COOH$
$C_9H_8O_3$ 164.16
Spar. sol. H_2O, petrol. Mp 103-104° dec.

Me ester: [614-27-7]
$C_{10}H_{10}O_3$ 178.187
Oil. Bp_{15} 152°.

Et ester: [94-02-0] *FEMA 2423*
$C_{11}H_{12}O_3$ 192.214
Flavouring ingredient. Oil with a brandy-like odour and bitter whisky-like taste. Insol. H_2O, misc. EtOH, Et_2O. Bp 265-270°. n_D^{20} 1.5338.
▶AF4878000

Amide: [3446-58-0]
$C_9H_9NO_2$ 163.176
Mp 113°.

Anilide: [959-66-0] *2-Benzoylacetanilide. β-Oxo-N-phenylbenzenepropanamide*
$C_{15}H_{13}NO_2$ 239.273
Cryst. (C_6H_6, toluene). Sol. EtOH, Me_2CO, C_6H_6. Mp 107-108°.

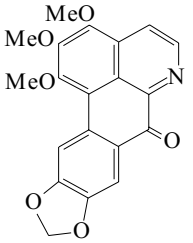
Nitrile: [614-16-4] *Benzoylacetonitrile. β-Oxohydrocinnamonitrile*
C_9H_7NO 145.16
Mp 82-83°. Bp_{10} 160°.

Di-Et acetal:3,3-Diethoxy-3-phenylpropanoic acid
$C_{13}H_{18}O_4$ 238.283
Mp 68° dec.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1506C (*nmr*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1026E (*ir*)
Dorsch, J.B. *et al., J.A.C.S.*, 1932, **54**, 2960 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 80; 415 (*deriv*)
Sarkar, A.K. *et al., Anal. Chem.*, 1967, **39**, 1608 (*detn, Be, Ti*)
Sarkar, A.K. *et al., Anal. Lett.*, 1968, **1**, 323 (*detn, Hg, V*)
Mandal, S.K. *et al., J. Indian Chem. Soc.*, 1973, **50**, 424 (*detn, U*)
Das, J. *et al., J. Indian Chem. Soc.*, 1977, **54**, 278 (*detn, Re*)
Merck Index, 11th edn., 1989, No. 3726
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 219 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 952-953 (*Et ester*)
Giardina, G.A.M. *et al., J. Med. Chem.*, 1997, **40**, 1794-1807 (*amide*)

Oxophoebine O-244

[109175-37-3]
1,2,3-Trimethoxy-7H-benzo[de][1,3]benzodioxolo[5,6-g]quinolin-7-one, 9CI. 1,2,3-Trimethoxy-9,10-methylenedioxyoxoaporphine



$C_{20}H_{15}NO_6$ 365.342
Amorph. red solid. λ_{max} 211 ; 240 ; 274 ; 379 ; 477 (MeOH) (Berdy).

3-Demethoxy: [15358-38-0] *1,2-Dimethoxy-9,10-methylenedioxyoxoaporphine.* ***Oxonantenine***
$C_{19}H_{13}NO_5$ 335.315
Alkaloid from *Laurelia sempervirens* (Peruvian nutmeg). Glistening yellow needles (EtOH). Mp 215-218° dec Mp 225-227° dec Mp 297-299°. λ_{max} 228 ; 242 ; 270 ; 285 ; 318 ; 360 (MeOH) (Berdy).

1,3-Bis(demethoxy): [172924-21-9] ***Hernanymphine***
$C_{18}H_{11}NO_4$ 305.289
Yellowish prisms ($CHCl_3$/MeOH). Mp 263-265°. Rare substitution pattern (no oxygenation at C-1).

Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 1457 (*Oxonantenine, isol, uv, ir, pmr, ms, struct*)
Chiu, S.Y.C. *et al., J. Nat. Prod.*, 1982, **45**, 229 (*Oxonantenine, isol, uv, ir, pmr, ms*)
Castro, O. *et al., J. Nat. Prod.*, 1986, **49**, 1036 (*Oxophoebine, isol, uv, pmr, ms, struct*)
Harrigan, G.G. *et al., J. Nat. Prod.*, 1994, **57**, 68-73 (*Oxophoebine, isol*)
Chen, J.J. *et al., J. Nat. Prod.*, 1996, **59**, 156 (*Hernanymphine*)

2-Oxopropanal, 9CI O-245

[78-98-8]
Pyruvaldehyde, 8CI. Pyruvic aldehyde. Methylglyoxal. Pyroracemic aldehyde. Propanalone. NSC 79019. FEMA 2969
$H_3CCOCHO$
$C_3H_4O_2$ 72.063
Flavouring ingredient. Yellow liq. with pungent odour and a pungent sweet caramel flavour, giving yellowish-green vapour. Sol. EtOH, C_6H_6. d_{20}^{20} 1.06. Bp 72°. $n_D^{17.5}$ 1.4002. pK_{a1} 11 (30°,hydrate). Liq. is bimolecular at r.t. rapidly polymerising to amorph. glassy mass.
► Eye irritant. LD_{50} (rat, orl) 1165 mg/kg.
UZ0700000

[31915-82-9, 51640-14-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 422D; 480B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 656C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 508C (*ir*)
Fischer, O.L. *et al., Ber.*, 1924, **57**, 1506 (*synth*)
Weygand, F. *et al., Chem. Ber.*, 1957, **90**, 1230 (*synth*)
Steinbauer, E. *et al., Monatsh. Chem.*, 1962, **93**, 303 (*synth*)
Tetsuzo, K. *et al., CA*, 1964, **61**, 638 (*synth*)
Bestman, H.-J. *et al., Chem. Ber.*, 1969, **102**, 2259 (*synth*)
Freedberg, W.B. *et al., J. Bacteriol.*, 1971, **108**, 137-144 (*isol*)
Asuero, A.G. *et al., Microchem. J.*, 1980, **25**, 14 (*synth*)
Yamaguchi, T. *et al., Agric. Biol. Chem.*, 1982, **46**, 849 (*tox*)
Baltes, H. *et al., Angew. Chem., Int. Ed.*, 1982, **21**, 540 (*synth*)
IARC Monog., 1991, **51**, 443 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 711
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2397-2398; 2399-2400
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PQC000

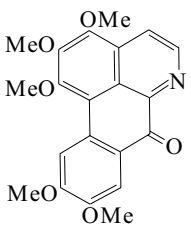
Oxopropanedioic acid, 9CI O-246

[473-90-5]
Mesoxalic acid, 8CI. Oxomalonic acid. Ketomalonic acid
HOOCCOCOOH
$C_3H_2O_5$ 118.046
Free acid exists as the covalent hydrate. Occurs in *Medicago sativa* (alfalfa). Tentatively identified in rhizosphere of sterile white mustard plants (*Sinapis alba*).
► OX7480000

Scheffer, F. *et al., Naturwissenschaften*, 1967, **54**, 118-119 (*occur*)

Oxopurpureine O-247

[32845-27-5]
*1,2,3,9,10-Pentamethoxy-7*H*-dibenzo[de,g]quinolin-7-one, 9CI. 1,2,3,9,10-Pentamethoxyoxoaporphine*

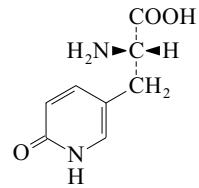


$C_{21}H_{19}NO_6$ 381.384
Alkaloid from the stems and leaves of *Annona purpurea* (soncoya). Cryst. + ½ toluene; yellow needles (EtOH). Mp 198-202° dec. (192-194°). Log P 2.34 (calc). λ_{max} 251 ; 282 ; 354 ; 394 ; 456 (MeOH) (Berdy). λ_{max} 215 (ϵ 3200); 248 (ϵ 2180); 278 (ϵ 3320); 389 (ϵ 640) (EtOH) (Berdy).

Sonnet, P.E. *et al., J. Pharm. Sci.*, 1971, **60**, 1254 (*isol, uv, ir, pmr, struct*)
Martinez, E. *et al., Planta Med.*, 1988, **54**, 361 (*isol, uv, ir, pmr, ms*)

3-(2-Oxo-5-pyridinyl)alanine O-248

*5-(2-Amino-2-carboxyethyl)-2(1*H*)-pyridinone. 2-Amino-3-(2-oxo-5-pyridinyl)propanoic acid*

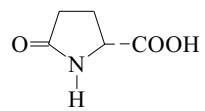


$C_8H_{10}N_2O_3$ 182.179
(S)-form [140681-92-1]
L-form

Yamano, K. *et al., Tetrahedron*, 1992, **48**, 1457 (*isol, synth, struct*)

5-Oxo-2-pyrrolidinecarboxylic acid O-249

5-Oxoproline, 9CI. ***Pidolic acid, INN****. α-Aminoglutaric acid lactam. Glutimic acid lactam. Glutimic acid. Glutiminic acid. Pyroglutamic acid. 2-Pyrrolidone-5-carboxylic acid*



(*R*)-*form*

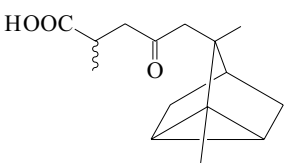
$C_5H_7NO_3$ 129.115Log P -1.27 (calc).
(S)-form [98-79-3]
L-form
Found in vegetables, fruits and molasses. Cryst. (H_2O). Mp 156-157°. $[\alpha]_D^{20}$ -11.45 (c, 4.44 in H_2O).

[28874-51-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 791A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1289C; 1290A; 1291A; 1291B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 789C; 789D (*ir*)
Gibian, H. *et al., Annalen*, 1961, **640**, 145 (*synth, bibl*)
Japan. Pat., 1970, 70 11 144; *CA*, **73**, 35763 (*synth*)
Pattabhi, V. *et al., J.C.S. Perkin 2*, 1974, 1085 (*cryst struct*)
Taira, Z. *et al., Acta Cryst. B*, 1977, **33**, 3823 (*cryst struct*)
Hardy, P.M. *et al., Synthesis*, 1978, 290 (*synth*)
Schmidt, U. *et al., Synthesis*, 1978, 752 (*synth*)
Abraham, G.N. *et al., Mol. Cell. Biochem.*, 1981, **38**, 181 (*rev*)
Rigo, B. *et al., J. Het. Chem.*, 1995, **32**, 1489 (*occur*)

9-Oxo-α-santalan-12-oic acid O-250

Ketosantalic acid



$C_{15}H_{22}O_3$ 250.337

Flavouring ingredient. Constit. of Indian sandalwood oil. Oil. $Bp_{0.3}$ 180°. $[\alpha]_D^{29}$ -30 (c, 1.4 in $CHCl_3$).

Me ester, semicarbazone:
Cryst. (EtOH). Mp 183-185°.

Ranibai, P. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 1006

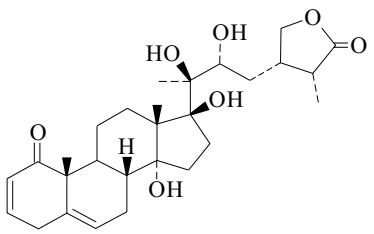
6-Oxotetradecanoic acid O-251

[1619-89-2]
6-Ketomyristic acid
$H_3C(CH_2)_7CO(CH_2)_4COOH$
$C_{14}H_{26}O_3$ 242.358
Trace constit. of milk fat. Cryst. (petrol). Mp 70-71°.

Semicarbazone:
Mp 129-131°.

Keskin, H. *et al., CA*, 1954, **48**, 10618 (*synth*)
Christie, W.W. *et al., J.C.S.*, 1963, 5768; 1964, 5833 (*isol*)
Wadia, M.S. *et al., Tetrahedron*, 1969, **25**, 3841 (*ms*)
Weihrauch, J.L. *et al., Lipids*, 1974, **9**, 883 (*ms*)

1-Oxo-14,17,20,22-tetrahydroxy-2,5-ergostadien-26,28-olide O-252



$C_{28}H_{40}O_7$ 488.62
(14α,17β,20*R*,22*R*,24*S*,25*R*)-*form* [85643-90-9]
Perulactone B
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. (EtOAc). Mp 217-218°. $[\alpha]_D$ +56.5 (c, 0.1 in MeCN).

Sahai, M. *et al., J. Chem. Res., Synop.*, 1982, 346

13-Oxo-9,11-tridecadienoic acid, 9CI O-253

[125407-60-5]
OHCCH=CHCH=CH$(CH_2)_7$COOH
$C_{13}H_{20}O_3$ 224.299
Stress metabolite of the pseudocereal *Chenopodium album* (lambsquarters).

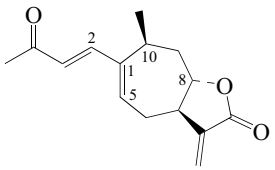
Me ester: [86153-27-7]

[120728-18-9, 129422-78-2, 129422-79-3]
$C_{14}H_{22}O_3$ 238.326
Oil.

[33812-31-6, 33812-63-4]

Kann, N. *et al., J.O.C.*, 1990, **55**, 5312-5323 (*Me ester, synth, ir, pmr, cmr*)
Tahara, S. *et al., Experientia*, 1994, **50**, 137-141 (*isol*)
Yondo, Y. *et al., Biochim. Biophys. Acta*, 1995, **1255**, 9-15

4-Oxo-1(5),2,11(13)-xanthatrien-12,8-olide O-254



(8α,10β)-*form*

$C_{15}H_{18}O_3$ 246.305
(8β,10β)-*form*
8-Epixanthatin
Constit. of *Helianthus annuus* (sunflower).

Deuel, P.G. *et al., J.A.C.S.*, 1957, **79**, 3778 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1441 (*isol*)
Omar, A.A. *et al., Phytochemistry*, 1984, **23**, 915 (*isol*)
Ahmed, A.A. *et al., Phytochemistry*, 1990, **29**, 2211 (*isol, pmr*)
Lanzetta, R. *et al., Phytochemistry*, 1991, **30**, 1121 (*isol, pmr, cmr*)
Yokotani-Tomita, K. *et al., Phytochemistry*, 1997, **46**, 503-506 (*8-Epixanthatin, pmr*)

2,2′-Oxybisethanol, 9CI O-255

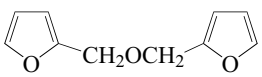
[111-46-6]
Diethylene glycol, 8CI. Bis(2-hydroxyethyl) ether. Diglycol. Digol. 2,2′-Dihydroxydiethyl ether. Ethylene diglycol. 3-Oxa-1,5-pentanediol
$HOCH_2CH_2OCH_2CH_2OH$
$C_4H_{10}O_3$ 106.121
Extremely hygroscopic syrupy liq. Sol. H_2O, EtOH, Me_2CO, Et_2O; insol. C_6H_6, toluene, CCl_4. d_4^{15} 1.12. Mp -6.5°. Bp 244° Bp_{14} 133° Bp_7 119-120°. n_D^{20} 1.4472. Vp 0.01 mmHg (30°).
▶ Fl. p. 124°, autoignition temp. 224/229°. Eye and human skin irritant. Exp. reprod. and teratogenic effects. OES: long-term 23 ppm. ID5950000
Dioctadecanoyl: [109-30-8] *Diethylene glycol distearate*
$C_{40}H_{78}O_5$ 639.053
Diluent in colour additive mixtures for colouring eggshells.

[3088-31-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1922, **1**, 206C; 223B; 225B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 324A; 341B; 342C; 343C; 344A; **2**, 1242B; 1610B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 270C; 270D; 293C; 296A (*ir*)
Sadtler Standard Proton NMR Spectra, 179 (*pmr*)
Cretcher, L.H. *et al., J.A.C.S.*, 1925, **47**, 164 (*synth*)
Liston, L. *et al., J.A.C.S.*, 1938, **60**, 1264 (*synth*)
Jen, T.-K. *et al., CA*, 1960, **54**, 19468; 1961, **55**, 22116 (*synth*)
Austin, G.T. *et al., Chem. Eng. (N.Y.)*, 1974, **81**, 143 (*rev*)
Large, R. *et al., Org. Mass Spectrom.*, 1976, **11**, 582 (*ms*)
Dennis, E.A. *et al., J. Phys. Chem.*, 1977, **81**, 957 (*cmr*)
Kawashima, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3255 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **12**, 695 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 814 (*dioctadecanoyl*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3832
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1601; 2395
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 142; 455
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BKN750; CBR000; DJE000; HFN000; DJD600; CBQ750

2,2′-[Oxybis(methylene)bisfuran], 9CI O-256

[4437-22-3]
Bis(2-furylmethyl) ether. Di-α-furfuryl ether. FEMA 3337



$C_{10}H_{10}O_3$ 178.187
Flavouring ingredient. Oil. d^{20} 1.14. Bp_2 101-102°. n_D^{20} 1.5088.

Zanetti, J.E. *et al., J.A.C.S.*, 1927, **49**, 1065-1067 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 162
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 825-826
Lautens, M. *et al., J.O.C.*, 1997, **62**, 4418-4427 (*synth, pmr, cmr, ir*)

Oxygen, 11CI O-257

[7782-44-7]
E948
O_2
O 15.999
Atomic No. 8. Ground state electron config. $[He]2s^22p^4$. Discovered in 1770's by J.P. Priestley and C.W. Scheele. There are 8 isotopes of which 3 are stable; ^{17}O is useful in nmr spectroscopy. Abundant in atmosphere: forms 20.946% of air. Most abundant element on earth's surface.
▶ RS2060000
Dioxygen:
O_2 31.999
Colourless, odourless, tasteless neutral gas. Condenses to paramagnetic blue liq. and blue solid. Reacts with all elements except He, Ne, Ar. V. sl. sol. H_2O (5.54 g per 100 cm^3 at 0°, 1.93 g per 100 cm^3 at 100°); more sol. org. solvs. d^{-183} 1.13. Mp -218.4°. Bp -183°. Paramagnetic with $2e^{\ominus}$ in antibonding π orbitals. T_{crit} -118.8°; P_{crit} 49.7 atm. Solid O_2 exists in α- (rhombic), β- (rhombohedral), and γ- (cubic) forms. O=O 120.8 pm.
Trioxygen: [10028-15-6] ***Ozone, 11CI***
O_3 47.998
Antimicrobial agent used in the production of bottled water. Also used in the treatment of meat, poultry and

other foodstuffs. Colourless gas; deep blue liq. with characteristic odour at low concn.; blue- or violet-black solid. Sl. sol. H_2O. d^{-183} 1.78. Mp -192.5° Mp -251°. Bp -112.3°. Struct. established in 1872. Interatomic distance: O–O 127.8 pm; angle: OOO 116.8°.

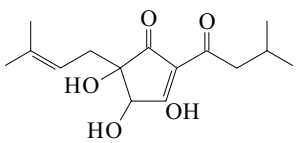
► Explosive. V. toxic. Detect. limit by smell *ca*. 0.01ppm. RS8225000

[8063-77-2, 11062-77-4, 12596-83-7, 14127-63-0, 14127-64-1, 14127-65-2, 14127-66-3, 14274-89-6, 14337-01-0, 14581-93-2, 14915-07-2, 17410-58-1, 17778-80-2, 21450-98-6, 32767-18-3]

Mellor Compr. Treat. Inorg. Theor. Chem., 1922, **1**, 344; 877 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 3, 1951, **2**, 1; 1960, **4**, 1 (*rev, bibl*)
Org. Synth., Coll. Vol., 3, 1955, **3**, 673 (*synth, O_3*)
Tanaka, T. *et al., J. Mol. Spectrosc.*, 1970, **33**, 538 (*struct, O_3*)
Compr. Inorg. Chem., Pergamon, 1973, **2**, 685; 785 (*rev O_2, O_3*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 347; 350 (*synth O_2, O_3*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **16**, 653; 683 (*rev, O_2, O_3*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2078 (*O_3*)
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 148; 246
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1394; 1418 (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OQW000; ORW000

Oxyhumulinic acid O-258

[469-30-7]
3,4,5-Trihydroxy-5-(3-methyl-2-butenyl)-2-(3-methyl-1-oxobutyl)-2-cyclopenten-1-one, 9CI



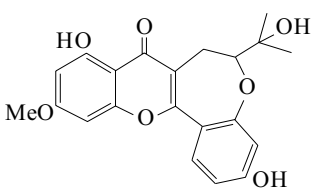
$C_{15}H_{22}O_5$ 282.336
Secondary prod. present in beer derived from Humulone, H-317. *cis*- and *trans*-isomers recognised.

[26110-48-5, 26146-34-9]

Verzele, M. *et al., Bull. Soc. Chim. Belg.*, 1957, **66**, 391; 1964, **73**, 268
Cant, E. *et al., Org. Mass Spectrom.*, 1972, **6**, 977 (*ms, bibl*)

Oxyisocyclointegrin O-259

[60791-47-1]

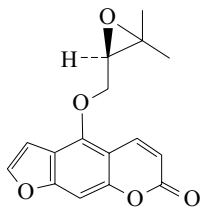


$C_{21}H_{20}O_7$ 384.385
Constit. of heartwood of *Artocarpus integer* (champedak). Pale-yellow cryst. (Me_2CO/C_6H_6). Mp 251-252°.

Pendse, A.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 69 (*isol*)

Oxypeucedanin O-260

[737-52-0]
Prangolarin



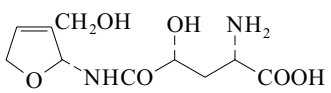
(*R*)-*form*

$C_{16}H_{14}O_5$ 286.284
(***R*)-*form*** [3173-02-2]
Isol. from *Angelica glauca*. Cryst. ($CHCl_3/Et_2O$). Mp 104-105°. $[\alpha]_D^{30}$ +20.1 ($CHCl_3$).
(***S*)-*form*** [26091-73-6]
Cryst. ($Et_2O/CHCl_3$). Mp 103-104°. $[\alpha]_D^{20}$ -14 (c, 0.9 in $CHCl_3$).
► LV1054000
(±)-***form*** [28919-33-7]
Cryst. ($CHCl_3/Et_2O$). Mp 140.5-142°.

Späth, E. *et al., Ber.*, 1933, **66**, 914; 1939, **72**, 52 (*struct, synth*)
Ghosal, C.R. *et al., Chem. Ind. (London)*, 1963, 1430 (*isol, struct*)
Vulfson, N.S. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **155**, 1104 (*ms*)
Lemmich, J. *et al., Phytochemistry*, 1971, **10**, 3333 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1372 (*occur*)
Gonzáles, A.G. *et al., An. Quim.*, 1973, **69**, 1141 (*isol*)
Atkinson, E. *et al., Phytochemistry*, 1974, **13**, 853 (*isol*)
Reisch, J. *et al., Phytochemistry*, 1975, **14**, 1889 (*isol*)
Serkerov, S.V. *et al., Khim. Prir. Soedin.*, 1976, 94 (*isol*)
Yost, G.S. *et al., Phytochemistry*, 1977, **16**, 1097 (*isol, pharmacol*)

Oxypinnatanine O-261

[52329-55-2]
N-*[2,5-Dihydro-3-(hydroxymethyl)-2-furanyl]-4-hydroxyglutamine, 9CI*



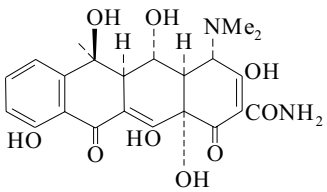
$C_{10}H_{16}N_2O_6$ 260.246
Constit. of *Hemerocallis fulva* (day lily). Cryst. (EtOH aq.). Mp 182-185° dec. $[\alpha]_D^{24}$ +5.5 (c, 0.8 in H_2O).

Grove, M.D. *et al., Tetrahedron*, 1973, **29**, 2715 (*synth*)
Kruger, G.J. *et al., J. S. Afr. Chem. Inst.*, 1976, **29**, 24 (*struct*)
Wagner, I. *et al., Angew. Chem., Int. Ed.*, 1983, **22**, 816 (*struct*)

Oxytetracycline, BAN, BSI, INN, JMAF O-262

[79-57-2]

[6153-64-6]
Abbocin. Berkmycen. Clinimycin†. Galsenomycin. Geomycin†. Oxydon. Stecsolin. Terramycin. Geotilin. Teravit. Tetran. Oxypam. Oxyterracine. NSC 9169. OTC



$C_{22}H_{24}N_2O_9$ 460.44
Tetracycline antibiotic. Clinically used broad-spectrum antibacterial antibiotic. Approved by FDA for use in fish and animal feeds. Light-yellow cryst. + $0.8Me_2CO$ or needles + $2H_2O$ (MeOH aq.). Sol. acids, Me_2CO, bases, MeOH; fairly sol. EtOAc, $CHCl_3$; poorly sol. C_6H_6, hexane, H_2O, Et_2O. Mp 181-182° dec. (hydrate) Mp 200° dec. (Me_2CO solvate). $[\alpha]_D^{25}$ -196.6 (0.1*M* HCl). $[\alpha]_D^{25}$ -2.1 (0.1*M* NaOH). $[\alpha]_D^{25}$ +26.5 (MeOH). pK_{a1} 3.27; pK_{a2} 7.32; pK_{a3} 9.11 (25°). Log P -3.95 (calc). Not the same as Geomycin from *S. xanthophaeus*. Also used as Ca salt (Oxytetracycline calcium, USAN) λ_{max} 220 (ϵ 13000); 268 (ϵ 18000); 355 (ϵ 13300) (0.1*N* HCl) (Derep). λ_{max} 247 (ϵ 18600); 265 (ϵ 17800); 375 (ϵ 16800) (MeOH/NaOH) (Derep). λ_{max} 270 (ϵ 18600); 370 (ϵ 15800) (MeOH) (Derep). λ_{max} 270 (E1%/1cm 361); 370 (E1%/1cm 343) (MeOH) (Berdy). λ_{max} 269 (E1%/1cm 766); 353 (E1%/1cm 560) (H_2SO_4) (Berdy). λ_{max} 249 ; 276 ; 353 (pH 4.5 buffer) (Berdy). λ_{max} 245 ; 264 ; 375 (MeOH-NaOH) (Berdy). λ_{max} 270 ; 359 (MeOH-HCl) (Berdy).
► Gastrointestinal, reprod. and other adverse effects reported when used therapeutically. LD_{50} (rat,orl) 4800 mg/kg. Exp. reprod. and teratogenic effects ; LD_{50} (mus, ivn) 178 mg/kg , LD_{50} (mus, scu) 700 mg/kg , LD_{50} (mus, orl) 7000 mg/kg. QI7875000

Hydrochloride: [2058-46-0] *Oxytetracycline hydrochloride, USAN. Oxytetrin*
Needles (MeOH), yellow platelets (H_2O).
► LD_{50} (mus, orl) 6696 mg/kg. Exp. reprod. and teratogenic effects. QI8225000

Na salt:
Lemon-yellow cryst. (MeOH) + $2H_2O$.

Di-Ac:
Cryst. (MeOH). Mp 208-213° dec. $[\alpha]_D^{25}$ +214 (MeOH).

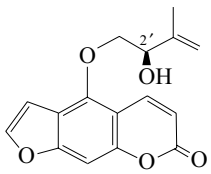
[15251-48-6]

Hochstein, F.A. *et al., J.A.C.S.*, 1951, **73**, 5008; 1952, **74**, 3707; 1953, **75**, 5455 (*struct*)
Hoffman, D.R. *et al., J.O.C.*, 1966, **31**, 792 (*ms*)
Muxfeldt, M. *et al., J.A.C.S.*, 1968, **90**, 6534 (*synth*)

Hughes, R.E. *et al., J.A.C.S.*, 1971, **93**, 1037 (*cryst struct*)
Asleson, G.L. *et al., J.A.C.S.*, 1975, **97**, 6246 (*nmr*)
Prewo, R. *et al., J.A.C.S.*, 1977, **99**, 1117 (*cryst struct*)
Thomas, R. *et al., Chem. Comm.*, 1983, 128; 1984, 442; 1985, 802 (*biosynth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 6512 (*synonyms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HOH500; HOI000
Curtis, R.D. *et al., Can. J. Chem.*, 1991, **69**, 834 (*N-15 nmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **3**, 331 (*rev*)
Pesticide Manual, 9th edn., 1991, No. 9290
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 190
Huang, T.S. *et al., J. Agric. Food Chem.*, 1997, **45**, 2602-2605 (*detn in fish*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HOH500; HOI000

Pabulenol P-1

[37551-62-5]
Pangeline. Gosferol



$C_{16}H_{14}O_5$ 286.284

The name Pangeline has historical precedence but Pabulenol is more common in the lit. Opt. rotns. vary and the use of the different synonyms for isolates having different opt. rotns. does not seem well-defined.

(*R*)-*form* [33783-80-1]
Constit. of *Ruta graveolens* (rue). Cryst. Mp 136.5-138.5° Mp 123-125°. $[\alpha]_D^{18}$ +8.6 (c, 0.46 in EtOH).

2′-O-*Angeloyl:* [33884-53-6] ***Angeloylpangeline***
$C_{21}H_{20}O_6$ 368.385
Cryst. Mp 87-88°. $[\alpha]_D$ -27.

3′,4′-Dihydro: [14685-06-4] ***Pranferol***. *Pranpherol*
$C_{16}H_{16}O_5$ 288.299
Cryst. (EtOH). Mp 108.5-111°. $[\alpha]_D^{19}$ -19.38 (c, 4.5 in $CHCl_3$).

3′,4′-Dihydro, 2′-ketone: [5058-15-1] ***Pabulenone***. *Isooxypeucedanin*
$C_{16}H_{14}O_5$ 286.284
Cryst. (Et_2O). Mp 146-148° (131-132°).

(*S*)-*form* [33889-70-2]
Mp 134-135°. $[\alpha]_D^{25}$ -3.8 (EtOH).

(±)-*form*
Cryst. (EtOH). Mp 136.5-138.5°.

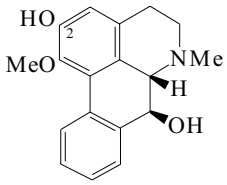
3′,4′-Dihydro:(±)-Pranferol
$C_{16}H_{16}O_5$ 288.299
Cryst. (EtOH). Mp 133°.

[14685-06-4]

Neilsen, B.E. *et al., Acta Chem. Scand.*, 1965, **19**, 1810 (*isol*)
Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1965, **5**, 3; 1971, **7**, 522; 1972, **8**, 49; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **5**, 3; 1971, **7**, 498; 1972, **8**, 43 (*isol, synth*)
Kuznetsova, G.A. *et al., Khim. Prir. Soedin.*, 1966, **2**, 310; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 252 (*Pranferol*)
Ognyanov, I. *et al., Dokl. Bolg. Akad. Nauk*, 1971, **24**, 315 (*isol*)
Basa, S.C. *et al., Tet. Lett.*, 1971, 1977 (*isol*)
Chatterjea, A. *et al., Tetrahedron*, 1972, **28**, 5175 (*isol*)
Reisch, J. *et al., Phytochemistry*, 1975, **14**, 1889-1890 (*Pabulenone*)
Babu, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2565 (*isol*)
Méndez, J. *et al., Phytochemistry*, 1983, **22**, 2599 (*isol*)
Grande, M. *et al., Phytochemistry*, 1986, **25**, 505 (*isol*)
Adebajo, A.C. *et al., Fitoterapia*, 2000, **71**, 334-337 (*pmr*)
Zhou, P. *et al., Phytochemistry*, 2000, **53**, 689 (*R-form, Pranferol, activity*)

Pachyconfine P-2

[62951-75-1]
*5,6,6*a*,7-Tetrahydro-1-methoxy-6-methyl-4*H*-dibenzo[*de,g*]quinoline-2,7-diol, 9CI. 2,7-Dihydroxy-1-methoxyaporphine. 6-Hydroxyasimilobine*



$C_{18}H_{19}NO_3$ 297.353
Mp 198° (as hydrochloride). $[\alpha]_D$ -150 (c, 0.7 in $CHCl_3$).

N-*Oxide:* [112494-70-9] ***Pachyconfine* N-*oxide***
$C_{18}H_{19}NO_4$ 313.352
Cryst. (MeOH). Mp 176-180°. $[\alpha]_D$ -164 (c, 0.41 in $CHCl_3$).

N-*De-Me:* [112571-90-1] *2,7-Dihydroxy-1-methoxynoraporphine.* ***Norpachyconfine***
$C_{17}H_{17}NO_3$ 283.326
Amorph. $[\alpha]_D$ -281 (c, 0.07 in $CHCl_3$).

O^2-*Me:* [107882-18-8] *7-Hydroxy-1,2-dimethoxyaporphine.* ***Nuciferidine***
$C_{19}H_{21}NO_3$ 311.38Obt. impure. Negative opt. rotn..

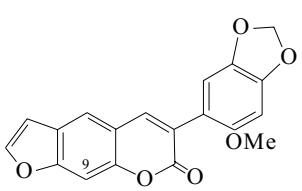
O^2-*Me,* N-*de-Me:* [112494-69-6] ***Nornuciferidine***
$C_{18}H_{19}NO_3$ 297.353
$[\alpha]_D$ -80 (c, 0.16 in EtOH).

6-Epimer, N-*de-Me:* [77410-38-9] ***Anaxagoreine***
$C_{17}H_{17}NO_3$ 283.326
Alkaloid from *Cananga odorata* (ylang ylang). Amorph. Mp 198-200°. $[\alpha]_D$ -174 (c, 0.5 in EtOH).

Bévalot, F. *et al., Ann. Pharm. Fr.*, 1977, **35**, 65; *CA*, **86**, 185953e (*isol, uv, pmr, ms, struct*)
Hocquemiller, R. *et al., Planta Med.*, 1981, **41**, 48 (*Anaxagoreine*)
Rasamizafy, S. *et al., J. Nat. Prod.*, 1986, **49**, 1078; 1987, **50**, 674 (*Nuciferidine, Nornuciferidine*)
Debourges, D. *et al., J. Nat. Prod.*, 1987, **50**, 664 (*Norpachyconfine, Pachyconfine N-oxide*)
Kessar, S.V. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 818 (*synth, Nuciferidine*)
Hsieh, T.J. *et al., J. Chin. Chem. Soc. (Taipei)*, 1999, **46**, 607-612 (*Anaxagoreine*)

Pachyrrhizin P-3

[10091-01-7]
*6-(6-Methoxy-1,3-benzodioxol-5-yl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. 6-(2-Methoxy-4,5-methylenedioxyphenyl)-furocoumarin. Neorautone*



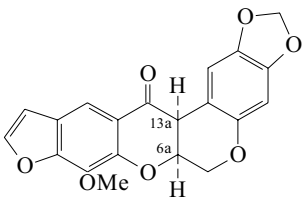
$C_{19}H_{12}O_6$ 336.3
Constit. of *Pachyrrhizus erosus* (yam bean). Yellow-green needles. Mp 207-209°.

9-Methoxy: ***Neofolin***
$C_{20}H_{14}O_7$ 366.326
Greenish-yellow needles (Me_2CO, EtOAc or C_6H_6), white amorph. solid (MeOH), brownish cubes (1,2-dichloroethylene) (trimorph.). Mp 155.5-157.5° (amorph.) Mp 167-168.5° (cubes) Mp 189.5-190.5° (needles).

Norton, L.B. *et al., J.A.C.S.*, 1945, **67**, 1609 (*isol*)
Simanitsch, E. *et al., Monatsh. Chem.*, 1957, **88**, 541 (*struct*)
Rajagopalan, P. *et al., Tet. Lett.*, 1959, **No. 21**, 5 (*synth*)
Abrams, C. *et al., CA*, 1963, **59**, 2917 (*isol, struct*)
Crombie, L. *et al., J.C.S.*, 1963, 1569 (*pmr*)
Brink, C.M. *et al., J. S. Afr. Chem. Inst.*, 1966, **19**, 24 (*Neofolin*)
Van Puyvelde, L. *et al., J. Nat. Prod.*, 1987, **50**, 349 (*isol, pmr, cmr, ms*)
Phrutivorapongkul, A. *et al., Chem. Pharm. Bull.*, 2002, **50**, 534-537 (*isol, pmr, cmr*)

Pachyrrhizone P-4

*6*a*,13*a*-Dihydro-8-methoxy-1,3-dioxolo[6,7][1]benzopyrano[3,4-*b*]furo[3,2-*g*]benzopyran-13(16*H*)-one, 9CI*



$C_{20}H_{14}O_7$ 366.326
CA numbering illus..

(+)-*form* [42485-00-7]
Needles. Mp 232-240° dec Mp 250-251° (sealed tube) Mp 272° (block). $[\alpha]_D^{20}$ +100 (c, 0.39 in $CHCl_3$).

Ac:
Mp 147°.

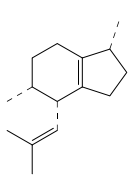
Oxime:
Cryst. Mp 267-268° dec. (279° block).

*6*a*,13*a*-Didehydro:* [28607-94-5] ***Dehydropachyrrhizone***
$C_{20}H_{12}O_7$ 364.311
Pale-yellow needles ($CHCl_3$/MeOH). Mp 260-262° dec.

(±)-*form*
Mp 250° dec. (265° block).

Meijer, T.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1946, **65**, 835 (*struct*)
Bickel, H. *et al., Helv. Chim. Acta*, 1953, **36**, 664 (*uv, ir*)
Reed, R.I. *et al., J.C.S.*, 1963, 5949 (*ms*)
Krishnamurti, M. *et al., Curr. Sci.*, 1966, **35**, 167 (*biosynth*)
Krishnamurti, M. *et al., Tetrahedron*, 1970, **26**, 3023 (*Dehydropachyrrhizone*)
Uchiyama, M. *et al., Agric. Biol. Chem.*, 1973, **37**, 1227 (*synth*)

1(6),10-Pacifigorgiadiene P-5



Absolute Configuration

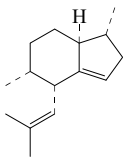
$C_{15}H_{24}$ 204.355

(+)-*form* [351222-70-3]
Oil.

(-)-*form*
Constit. of *Valeriana officinalis* (valerian). Oil.

Paul, C. *et al., Phytochemistry*, 2001, **57**, 307-313 (*isol, pmr, cmr*)

1(9),10-Pacifigorgiadiene P-6



Absolute Configuration

$C_{15}H_{24}$ 204.355

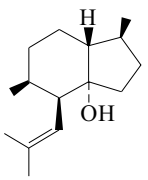
(+)-*form* [351222-62-3]
Constit. of *Valeriana officinalis* (valerian). Oil.

(-)-*form* [351222-69-0]
Oil.

Paul, C. *et al., Phytochemistry*, 2001, **57**, 307-313 (*isol, pmr, cmr*)

Pacifigorgiol P-7

*Octahydro-1,5-dimethyl-4-(2-methyl-1-propenyl)-3*a*H-inden-3*a*-ol, 9CI*



(+)-*form*

$C_{15}H_{26}O$ 222.37

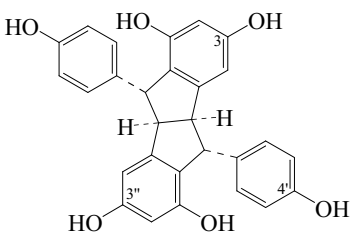
(+)-*form* [84014-68-6]
Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O. $[\alpha]_D$ +41 (c, 1.02 in $CHCl_3$).

(-)-*form* [90988-77-5]
Constit. of *Valeriana officinalis* (valerian). Oil. $[\alpha]_D$ -45.3 (c, 0.724 in $CHCl_3$).

Martin, M. *et al., Pure Appl. Chem.*, 1982, **54**, 1915 (*synth*)
Izac, R.R. *et al., Tet. Lett.*, 1982, **23**, 3743 (*isol, cryst struct*)
Bos, R. *et al., Phytochemistry*, 1986, **25**, 1234 (*isol*)

Pallidol P-8

[105037-88-5]



$C_{28}H_{22}O_6$ 454.478
Amorph. powder. Mp 300° dec.

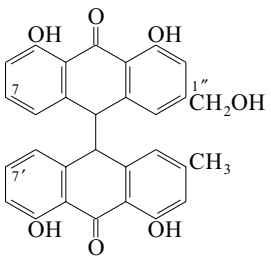
3-O-β-D-Glucopyranoside:
$C_{34}H_{32}O_{11}$ 616.62
Isol. from Riesling wine.

3,3″-Di-O-β-D-glucopyranoside:
$C_{40}H_{42}O_{16}$ 778.762
Isol. from Riesling wine.

Khan, M.A. *et al., Phytochemistry*, 1986, **25**, 1945
Ohyama, M. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3057-3060 (*activity*)
Baderschneider, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 2681-2686 (*glucosides*)

Palmidin B P-9

[17062-56-5]
*4,4′,5,5′-Tetrahydroxy-2-(hydroxymethyl)-2′-methyl-[9,9′-bianthracene]-10,10′(9*H*,9′*H*)-dione, 9CI. Aloeemodin-chrysophanol bianthrone*



$C_{30}H_{22}O_7$ 494.5
Isol. from roots of *Rheum palmatum* (Turkey rhubarb) also cascara (*Rhamnus purshiana*).

7′-Hydroxy: [17062-55-4] ***Palmidin A***. *Aloeemodin-emodin bianthrone*
$C_{30}H_{22}O_8$ 510.499
From roots of *Rheum palmatum* (Turkey rhubarb) and from cascara.

7-Hydroxy, 1″-deoxy: [17177-86-5] ***Palmidin C***. *Emodin-chrysophanol bianthrone*
$C_{30}H_{22}O_7$ 494.5
From roots of *Rheum palmatum* (Turkey rhubarb), also cascara. λ_{max} 220 ; 272 ; 362 (no solvent reported).

Lemli, J. *et al., Planta Med.*, 1964, **12**, 107
Lemli, J. *et al., J. Nat. Prod.*, 1965, **28**, 63 (*isol, uv*)
Kinget, R. *et al., Planta Med.*, 1967, **15**, 233 (*isol, uv*)

Palmidin D P-10

Struct. unknown. Possible Chrysophanol-Physcion dianthrone. Contit. of the roots of *Rheum palmatum* (Turkey rhubarb).

Lemli, J. *et al., Planta Med.*, 1964, **12**, 107 (*isol*)
Friedrich, H. *et al., Phytochemistry*, 1973, **12**, 1459 (*isol*)

Palmidrol, INN P-11

[544-31-0]
N-*(2-Hydroxyethyl)hexadecanamide, 9CI*. N-*(2-Hydroxyethyl)palmitamide. Impulsin. Palmitan. PEA*

$H_3C(CH_2)_{14}CONHCH_2CH_2OH$

$C_{18}H_{37}NO_2$ 299.496
Isol. from soybean lecithin, egg yolk and peanut meal. Cryst. (EtOH aq.). Mp 98-99°. Log P 6 (calc).

Roe, E.T. *et al., J.A.C.S.*, 1952, **74**, 3442 (*synth*)
Kuehl, F.A. *et al., J.A.C.S.*, 1957, **79**, 5577 (*isol*)
Benvenuti, F. *et al., Boll. Soc. Ital. Biol. Sper.*, 1968, **44**, 809; *CA*, **69**, 85237e (*pharmacol*)
Perlik, F. *et al., Acta Phytopathol. Acad. Sci. Hung.*, 1971, **39**, 395 (*pharmacol*)
Miyasaka, T. *et al., Chem. Lett.*, 1985, **6**, 701 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1397

Palygorskite, 9CI P-12

[12174-11-7]

[1337-76-4]
Attapulgite

$Mg_5[Si_2O_5]_4(OH)_2.8H_2O$

$H_{18}Mg_5O_{34}Si_8$ 908.331

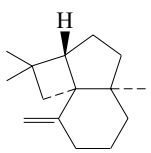
Mineral. The name palygorskite is used both for the group of fibrous clay minerals in the attapulgite-sepiolite series, and for the specific mineral specimens that are similar to sepiolite except for some replacement of Mg by Al. A layer silicate. Also formulated as $(Mg,Al)_2Si_4O_{10}(OH).4H_2O$. Used in foods as a clarifying and flocculating agent. White or grey monoclinic or orthorhombic cryst.

▶ RT6400000

Christ, C.L. *et al., Am. Mineral.*, 1969, **54**, 198 (*cryst struct*)
Jones, B.F. *et al., Rev. Mineral.*, 1988, **19**, 631 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 636
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAE750

3(15)-Panasinsanene P-13

[56684-97-0]
*Decahydro-2,2,4*a*-trimethyl-8-methylenecyclobut[*c*]indene, 9CI. **β-Panasinsene***

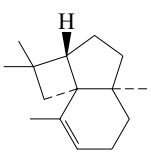


$C_{15}H_{24}$ 204.355
Isol. from ginseng oil. Oil. d_4^{20} 0.89. $[\alpha]_D^{20}$ -25 (c, 1 in MeOH).

Yoshihara, K. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2078 (*isol, struct*)
McMurry, J.E. *et al., Tet. Lett.*, 1980, 2477 (*synth*)
Iwabuchi, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1975 (*isol*)

10-Panasinsanene P-14

[56633-28-4]
*1,2,2*a*,3,4,4*a*,5,6-Octahydro-2,2,4*a*,8-tetramethylcyclobut[*c*]indene, 9CI. **α-Panasinsene***

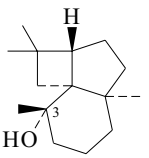


$C_{15}H_{24}$ 204.355

Constit. of ginseng oil. Oil. $[\alpha]_D^{25}$ -17 (c, 1.17 in $CHCl_3$).

Yoshihara, K. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2078 (*isol, struct*)
McMurry, J.E. *et al., Tet. Lett.*, 1980, 2477 (*synth*)
Iwabuchi, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1975 (*isol*)

3-Panasinsanol P-15



3α*OH-form*

$C_{15}H_{26}O$ 222.37

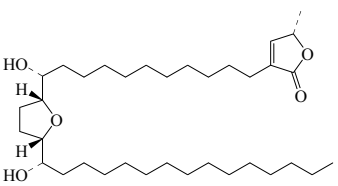
3α*OH-form* [109785-99-1]
Panasinsanol B
Constit. of *Panax ginseng* (ginseng). Oil. $[\alpha]_D^{25}$ -44.3 (c, 0.70 in $CHCl_3$).

3β*OH-form* [80374-27-2]
Panasinsanol A
Constit. of *Panax ginseng* (ginseng). Oil. $[\alpha]_D^{25}$ -51.9 (c, 0.54 in $CHCl_3$).

Iwabuchi, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1975

Panatellin P-16

[205439-32-3]



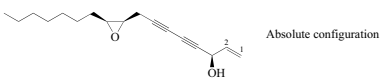
Relative Configuration

$C_{35}H_{64}O_5$ 564.888
Constit. of the roots of *Annona muricata* (soursop). Powder. Mp 62-64°. $[\alpha]_D$ +20 (c, 0.6 in MeOH). λ_{max} 220 (log ϵ 3.65) (MeOH).

Gleye, C. *et al., J. Nat. Prod.*, 1998, **61**, 576-579 (*isol, uv, ir, pmr, cmr, ms*)

Panaxydol P-17

[72800-72-7]
8-(3-Heptyloxiranyl)-1-octene-4,6-diyn-3-ol, 9CI. 9,10-Epoxy-1-heptadecene-4,6-diyn-3-ol



Absolute configuration

$C_{17}H_{24}O_2$ 260.375
Isol. from *Panax ginseng* (ginseng). Also from *Panax quinquefolium* (American ginseng). $[\alpha]_D$ -19.5 (c, 0.6 in MeOH).

Ac: [121820-32-4] ***Acetylpanaxydol***
$C_{19}H_{26}O_3$ 302.413
Constit. of *Panax quinquefolium* (American ginseng). λ_{max} 201 (ϵ 6260); 209 ; 221 (ϵ 620); 228 ; 231 (ϵ 745); 244 (ϵ 700); 254 ; 257 (ϵ 425) (EtOH) (Berdy).

9,12-Octadecadienoyl(Z,Z-): [155551-19-2] ***Panaxydol linoleate***
$C_{35}H_{54}O_3$ 522.81
Constit. of *Panax ginseng* (ginseng). Oil. $[\alpha]_D$ -14.3 (c, 11 in $CHCl_3$).

O-*Succinoyl:* [146368-20-9]
$C_{21}H_{28}O_5$ 360.449
λ_{max} 231 (ϵ 990); 243 (ϵ 810); 257 (ϵ 480) (EtOH) (Berdy).

3-Ketone: [126146-63-2] *8-(3-Heptyloxiranyl)-1-octene-4,6-diyn-3-one, 9CI. 9,10-Epoxy-1-heptadecene-4,6-diyn-3-one.* ***Ginsenoyne E. 3-Oxopanaxydol. PQ 3. Panaquinquecol 3***
$C_{17}H_{22}O_2$ 258.36
Isol. from *Panax quinquefolium* (American ginseng) and *Panax ginseng* (ginseng). Pale yellow oil. $[\alpha]_D$ -36.9 (c, 0.68 in MeOH). $[\alpha]_D$ -82.9 (c, 0.8 in $CHCl_3$).

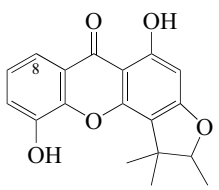
1,2-Dihydro, 1-chloro, 2-hydroxy: [114687-51-3] *1-Chloro-9,10-epoxy-4,6-heptadecadiyne-2,3-diol.* ***Chloropanaxydiol***
$C_{17}H_{25}ClO_3$ 312.835
Isol. from the dried callus of *Panax ginseng* (ginseng). $[\alpha]_D$ -37.2 (c, 0.2 in MeOH).

[134731-68-3, 139035-31-7, 139757-60-1, 155475-72-2]

Poplawski, J. *et al., Phytochemistry*, 1980, **19**, 1539 (*isol, struct, synth*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4206; 1991, **39**, 521 (*isol, pmr, cmr, struct*)
Ahn, B.-Z. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1989, **322**, 223 (*Acetylpanaxydol*)
Chung, C.B. *et al., Bull. Korean Chem. Soc.*, 1991, **12**, 122 (*abs config*)
Hirakura, K. *et al., Phytochemistry*, 1991, **30**, 3327; 1994, **35**, 963 (*isol, ir, cmr, uv, ms, pmr, Panaxydol linoleate*)
Kobayashi, M. *et al., Tetrahedron*, 1997, **53**, 15691-15700 (*abs config*)
Lu, W. *et al., Tet. Lett.*, 1998, **39**, 9521-9522 (*synth*)
Yadav, J.S. *et al., Tetrahedron*, 2002, **58**, 4955-4961 (*synth*)

Pancixanthone B P-18

[174232-29-2]
*1,2-Dihydro-5,10-dihydroxy-1,1,2-trimethyl-6*H*-furo[2,3-*c*]xanthen-6-one, 9CI*



$C_{18}H_{16}O_5$ 312.321
Yellow powder. $[\alpha]_D$ +3 (c, 0.1 in $CHCl_3$). λ_{max} 215 ; 238 (sh) ; 246 ; 256 (sh) ; 320 ; 362 (MeOH).

8-Hydroxy: ***Garbogiol***
$C_{18}H_{16}O_6$ 328.321
Constit. of *Garcinia cambogia*.
Amorph. pale yellow solid. Racemic
λ_{max} 206 ; 225 ; 257 ; 281 ; 346 (MeOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 1996, **44**, 441-443 (*isol, uv, ir, pmr, cmr, ms*)
Iinuma, M. *et al., Phytochemistry*, 1998, **47**, 1169-1170 (*Garbogiol*)

Pancreatin, BAN, JAN, USAN P-19

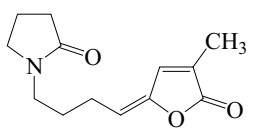
[8049-47-6]
Cotazym†. *Diastase vera*. *Pancrease*†. *Pancrex*. *Panteric*. *Pankrotanon*. *Zypanar*
Isol. from pancreas of pig and cow. Digestive enzyme. Used in replacement therapy. Used to prepare protein hydrolysates for pre- and post-operative diets. Yellow amorph. powder. Component of Donnazyme, Entozyme and Stamyl.

▶ LD_{50} (rat, orl) >10000 mg/kg. LD_{50} (rat, ipr) 2550 mg/kg. RT9033000

U.S. Pat., 1965, 3 223 594, (*North American Philips*); *CA*, **64**, 8578g (*synth*)
Lang, H. *et al., Gastroenterologia*, 1967, **107**, 203 (*pharmacol*)
Bar, D. *et al., Bull. Soc. Pharm. Lille*, 1970, 135 (*rev*)
Groezinger, K.H. *et al., Arzneim.-Forsch.*, 1972, **22**, 1152 (*activity*)
Lalasidis, G. *et al., J. Agric. Food Chem.*, 1978, **26**, 751-758 (*use*)
Zentler-Munro, P.L. *et al., Aliment. Pharmacol. Ther.*, 1987, **1**, 575 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1397
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2083 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAF600

Pandamarilactam 3x P-20

[189179-33-7]
*1-[4-(4-Methyl-5-oxo-2(5*H*)-furanylidene)butyl]-2-pyrrolidinone, 9CI*



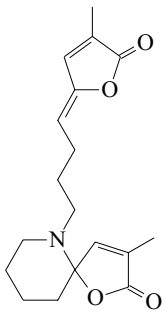
$C_{13}H_{17}NO_3$ 235.282
Food flavouring. Alkaloid from *Pandanus amaryllifolius*.

*(*Z*)-Isomer:* [189179-35-9] ***Pandamarilactam 3y***
$C_{13}H_{17}NO_3$ 235.282
Alkaloid from *Pandanus amaryllifolius*. Food flavouring.

Sjaifullah, A. *et al., CA*, 1997, **126**, 297535w (*isol*)
Takayama, H. *et al., Heterocycles*, 1999, **50**, 75-78 (*synth*)

Pandamarilactone 1 P-21

[152606-63-8]



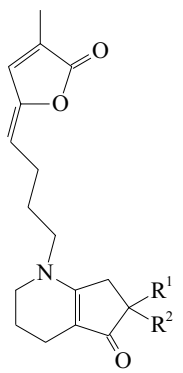
$C_{18}H_{23}NO_4$ 317.384

Alkaloid from leaves of *Pandanus amaryllifolius*. Food flavouring. Yellow amorph. solid. $[\alpha]_D$ -33 (c, 0.1 in MeOH).

Nonato, M.G. *et al., Phytochemistry*, 1993, **34**, 1159 (*isol, uv, ir, pmr, cmr, struct*)

Pandamarilactone 31 P-22

[152606-64-9]



R^1 = OMe, R^2 = CH_3

$C_{19}H_{25}NO_4$ 331.411

Food flavouring. Alkaloid from leaves of *Pandanus amaryllifolius*. Amorph. solid. $[\alpha]_D$ -2 (c, 0.1 in MeOH).

Nonato, M.G. *et al., Phytochemistry*, 1993, **34**, 1159 (*isol, uv, ir, pmr, cmr, struct*)

Pandamarilactone 32 P-23

[152606-65-0]

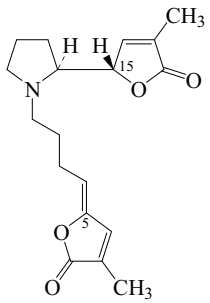
As Pandamarilactone 31, P-22 with $R^1R^2 = CH_2$

$C_{18}H_{21}NO_3$ 299.369

Food flavouring. Major alkaloid from leaves of *Pandanus amaryllifolius*. Amorph. solid.

Nonato, M.G. *et al., Phytochemistry*, 1993, **34**, 1159 (*isol, uv, ir, pmr, cmr, struct*)

Pandamarilactonine A P-24



Relative Configuration

$C_{18}H_{23}NO_4$ 317.384

Relative config. revised in 2002. Alkaloid from *Pandanus amaryllifolius*. Food flavouring. Amorph. powder. $[\alpha]_D^{23}$ +35 (c, 4.4 in $CHCl_3$). Partial racemate λ_{max} 207 (log ε 1.82); 232 (sh) ; 275 (log ε 2.43) (MeOH).

N-*Dealkyl:3-Methyl-5-(2-pyrrolidinyl)-2(5*H*)-furanone.* ***Norpandamarilactonine A***

$C_9H_{13}NO_2$ 167.207

Alkaloid from *Pandanus amaryllifolius*. Food flavouring. Amorph. powder. Racemic λ_{max} 207 (log ε 2.29); 252 (log ε 0.35); 274 (log ε 0.44) (MeOH).

*5*E-*Isomer:* ***Pandamarilactonine C***

$C_{18}H_{23}NO_4$ 317.384

Alkaloid from *Pandanus amaryllifolius*. Food flavouring. Amorph. powder. $[\alpha]_D^{23}$ +26.2 (c, 1 in $CHCl_3$). λ_{max} 201 (log ε 3.67); 220 (sh) ; 275 (log ε 4.23) (MeOH).

15-Epimer: ***Pandamarilactonine B***

$C_{18}H_{23}NO_4$ 317.384

Alkaloid from *Pandanus amaryllifolius*. Food flavouring. Amorph. powder. Racemic λ_{max} 207 (log ε 1.72); 232 (sh) ; 275 (log ε 2.49) (MeOH).

15-Epimer, N-*dealkyl:* ***Norpandamarilactonine B***

$C_9H_{13}NO_2$ 167.207

Alkaloid from *Pandanus amaryllifolius*. Food flavouring. Amorph. powder. Racemic λ_{max} 207 (log ε 2.58); 253 (log ε 0.29); 274 (log ε 0.36) (MeOH).

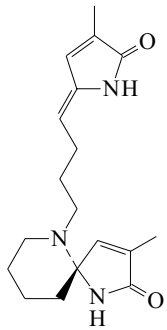
*15-Epimer, 5*E-*isomer:* ***Pandamarilactonine D***

$C_{18}H_{23}NO_4$ 317.384

Alkaloid from *Pandanus amaryllifolius*. Food flavouring. Amorph. powder. Racemic λ_{max} 203 (log ε 4.3); 234 (sh) ; 276 (log ε 4.38) (MeOH).

Takayama, H. *et al., J.A.C.S.*, 2000, **122**, 8635-8639 (*isol*)
Takayama, H. *et al., J. Nat. Prod.*, 2001, **64**, 1224-1225 (*Norpandamarilactonines*)
Takayama, H. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1303-1304 (*isol, synth, pmr, cmr*)
Busqueé, F. *et al., Tet. Lett.*, 2002, **43**, 5583-5585 (*synth*)

Pandamarine P-25



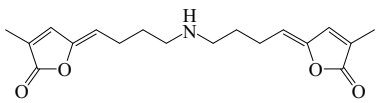
$C_{18}H_{25}N_3O_2$ 315.414

(±)-*form* [145940-69-8]

Major alkaloid from leaves of *Pandanus amaryllifolius*. Plates (MeOH/EtOAc/Et_2O). Mp 210-211°.

Byrne, L.T. *et al., Aust. J. Chem.*, 1992, **45**, 1903 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)

Pandanamine P-26



$C_{18}H_{23}NO_4$ 317.384

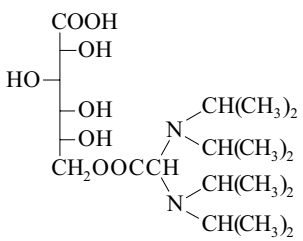
Food flavouring. Alkaloid from *Pandanus amaryllifolius*. Amorph. powder. λ_{max} 203 (log ε 1.86); 242 (sh) ; 273 (log ε 1.15) (MeOH).

Takayama, H. *et al., J.A.C.S.*, 2000, **122**, 8635-8639 (*synth*)
Takayama, H. *et al., Tet. Lett.*, 2001, **42**, 2995-2996 (*isol*)

Pangamic acid, 8CI P-27

[11006-56-7]

Vitamin B_{15}, 8CI. D-*Gluconic acid 6-bis[bis(1-methylethyl)amino]acetate, 9CI.* D-*Gluconic acid 6-bis(diisopropylamino)acetate*



$C_{20}H_{40}N_2O_8$ 436.545

Struct. dubious, not properly characterised. Isol. from apricot kernel, also said to be present in cereals etc. Said to be a vitamin of significance in, *inter alia*, hypertension control.

[13149-69-4]

Krebs, E.T. *et al., CA*, 1952, **46**, 4622 (*isol*)
Janicki, J. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Biol.*, 1968, **16**, 273; *CA*, **69**, 97040y
Siong, T.E. *et al., CA*, 1980, **93**, 192084v
Merck Index, 10th edn., 1983, No. 6871

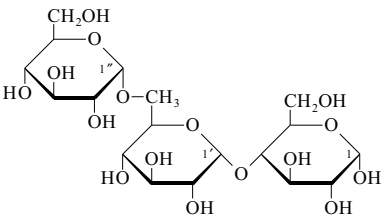
Riemschneider, R. *et al., CA*, 1984, **100**, 33504d (*rev*)

Panose, 9CI P-28

[33401-87-5]

[25193-53-7]

O-α-D-*Glucopyranosyl-(1→6)*-O-α-D-*glucopyranosyl-(1→4)*-D-*glucose, 9CI. 4-α-Isomaltosylglucose*



α-Pyranose-*form*

$C_{18}H_{32}O_{16}$ 504.441

Metab. of *Aspergillus niger*. Isol. from wort and beer. Mp 223° dec. (195-198°). $[\alpha]_D^{25}$ +163 → +155.5 (c, 4.0 in H_2O). $[\alpha]_D$ +147 (H_2O).

α-Pyranose-*form*

Benzyl glycoside, decabenzyl: [85011-47-8]
$C_{95}H_{98}O_{16}$ 1495.81
Syrup. $[\alpha]_D^{20}$ +75 (c, 1.0 in $CHCl_3$).

β-Pyranose-*form*

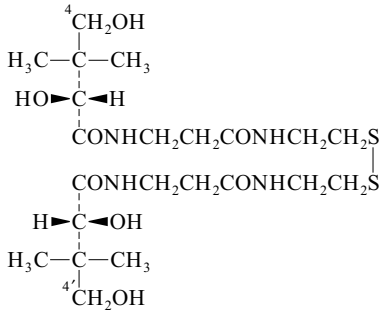
2″,3″,4″,6″-Tetrabenzyl, 1,2,2′,3,3′,6-hexa-Ac: [93417-47-1]
$C_{58}H_{68}O_{22}$ 1117.162
Cryst. (EtOH/2-propanol). Mp 152-153°. $[\alpha]_D^{20}$ +51.3 (c, 2.0 in $CHCl_3$).

Pan, S.C. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 341 (*enzymic synth*)
Wolfrom, M.L. *et al., Chem. Comm.*, 1966, 2 (*synth, struct*)
Bathgate, G.N. *et al., Chem. Ind. (London)*, 1969, 520 (*isol*)
Helferich, B. *et al., Chem. Ber.*, 1973, **106**, 2508 (*synth*)
Colson, P. *et al., J.A.C.S.*, 1974, **96**, 8081 (*conformn, cmr*)
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 188 (*synth, α-benzyl gly synth, cmr*)
Takeo, K. *et al., Carbohydr. Res.*, 1984, **133**, 135 (*synth, β-pyr deriv synth, cmr*)
Imberty, S. *et al., Carbohydr. Res.*, 1988, **181**, 4 (*cryst struct*)
Jeffery, G.A. *et al., Carbohydr. Res.*, 1991, **222**, 47 (*cryst struct*)

Pantethine, JAN P-29

[303-05-9]

N,N′-*[Dithiobis[2,1-ethanediylimino(3-oxo-3,1-propanediyl)]]bis[2,4-dihydroxy-3,3-dimethylbutanamide], 9CI.* N,N′-*[Dithiobis(ethyleneiminocarbonylethylene)]bis[2,4-dihydroxy-3,3-dimethylbutyramide], 8CI. Bis(pantothenyl-2-aminoethyl)disulfide*



$C_{22}H_{42}N_4O_8S_2$ 554.728

(*R*,*R*)-*form* [16816-67-4]
D-*form. Lipodel. Pantetina. Panthecin. Pantomin. Pantosin*
Cryst. (MeOH/Me_2CO), glass (H_2O). $[\alpha]_D^{22}$ +17.9 (c, 3.2 in H_2O). Hydrol. by acids.

▶ LD_{50} (mus, ipr) 4800 mg/kg. Exp. reprod. and teratogenic effects. ES4392700

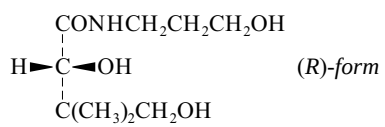
4,4′-Diphosphate: [17451-69-3]
$C_{22}H_{44}N_4O_{14}P_2S_2$ 714.687
Powder (MeOH) (as Ba salt). $[\alpha]_D^{20}$ +12.2 (c, 1 in H_2O).

Brown, G.M. *et al., J.A.C.S.*, 1953, **75**, 1691 (*occur, purifn*)
Viscontini, M. *et al., Helv. Chim. Acta*, 1954, **37**, 375 (*synth, tlc, deriv*)
Bowman, R.E. *et al., J.C.S.*, 1954, 1171 (*anal, rev, bibl*)
Moffatt, J.G. *et al., J.A.C.S.*, 1961, **83**, 663 (*chromatog*)
Shimizu, M. *et al., Chem. Pharm. Bull.*, 1965, **13**, 180 (*synth, chromatog, ir, uv*)
Nagase, O. *et al., Chem. Pharm. Bull.*, 1967, **15**, 648 (*phosphate, synth*)
Zhdanovich, E.S. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 337 (*synth, ir*)
Hashimoto, M. *et al., Chem. Lett.*, 1972, 595 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAG150

Panthenol, BAN, INN, USAN P-30

[62507-76-0]

2,4-Dihydroxy-N-*(3-hydroxypropyl)-3,3-dimethylbutanamide, 9CI. Panthoderm. Pantothenyl alcohol. Pantothenol*



(*R*)-*form*

$C_9H_{19}NO_4$ 205.253
Log P -2.52 (calc).

(*R*)-*form* [81-13-0]
Dexpanthenol, BAN, INN, USAN. *Pantol. Bepanthon*
Dietary supplement. Viscous oil. V. sol. H_2O; spar. sol. Et_2O. d_{20}^{20} 1.2. $Bp_{0.2}$ 118-120°. $[\alpha]_D^{20}$ +29.7 (c, 0.03 in H_2O). n_D^{20} 1.4970.

▶ ES4316000

4′-Phosphate: [25531-31-1]
$C_9H_{20}NO_7P$ 285.233
$[\alpha]_D^{28}$ +13.5 (c, 1.0 in H_2O) (Ba salt).

3″-Phosphate: [25531-30-0]
$C_9H_{20}NO_7P$ 285.233
$[\alpha]_D^{22}$ +22.6 (c, 1.0 in H_2O) (di-Li salt).

Tri-Ac:
$C_{15}H_{25}NO_7$ 331.365
$Bp_{0.000005}$ 130°. $[\alpha]_D^{20}$ -4.65 (EtOH).

(*S*)-*form* [74561-18-5]
$[\alpha]_D^{20}$ -28.4 (c, 0.03 in H_2O).

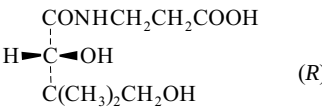
(±)-*form* [16485-10-2]
Cryst. (EtOAc). Sol. H_2O. Mp 60-61°. $Bp_{0.02}$ 118-120°.

[17307-32-3, 74561-18-5]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1233B (*nmr*)
Schnider, O. *et al., CA*, 1947, **41**, 6199a (*synth*)
Bonati, F. *et al., Farmaco, Ed. Sci.*, 1959, **14**, 43 (*synth*)
Ger. Pat., 1960, 1 067 443; *CA*, **56**, 11450i (*synth*)
Gavein, T.W. *et al., Seifen, Oele, Fette, Wachse*, 1963, **89**, 203 (*synth, rev*)
Hosokawa, Y. *et al., Chem. Pharm. Bull.*, 1969, **17**, 202 (*synth, pmr*)
Shimizu, S. *et al., Agric. Biol. Chem.*, 1974, **38**, 1989 (*pharmacol*)
Kozlova, G.S. *et al., Khim.-Farm. Zh.*, 1977, **11**, 69 (*synth*)
J. Am. Coll. Toxicol., 1987, **6**, 139 (*tox, rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1374
Arai, T. *et al., J. Chromatogr.*, 1989, **474**, 405 (*hplc, resoln*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1361
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2085-2087
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAG200

Pantothenic acid, BAN P-31

N-*(2,4-Dihydroxy-3,3-dimethyl-1-oxobutyl)-β-alanine, 9CI. Vitamin B_5*



(*R*)-*form*

$C_9H_{17}NO_5$ 219.237
Log P -1.52 (calc).

(*R*)-*form* [79-83-4]
Present in liver tissue and widespreat in plants in small amts.. Extremely hygroscopic, viscous oil. $[\alpha]_D^{25}$ +37.5 (H_2O). Low acute toxicity.

▶ RU4729000

Na salt: [867-81-2] *Pancal*
Dietary supplement. Mp 171-178°. $[\alpha]_D^{21}$ +27.7 (c, 5 in H_2O).

Ca salt: [137-08-6] ***Calcium pantothenate, INN, USAN.*** *Calpanate. Pantholin. Many other names*
Nutrient supplement, may be used in infant formulas. Enzyme cofactor vitamin. Cryst. (MeOH). Mp 195-196°. $[\alpha]_D^{26}$ +28.2 (c, 2 in Me_2CO). Anisotropic. Component of Stuartinic.

▶ RU4375000

4′-O-β-D-Glucopyranoside: [29493-59-2]
$C_{15}H_{27}NO_{10}$ 381.379
Isol. from tomato juice. Hygroscopic powder. $[\alpha]_D$ -11.2 (c, 1 in H_2O).

Amide: [7757-97-3] *Pantothenamide*
Dietary supplement as a source of

pantothenic acid. Cryst. Sl. sol. H_2O, butanol; insol. C_6H_6, Et_2O. Mp 114-116° (99-101°).

(±)-*form* [599-54-2]
Viscous oil.

Ca salt: [63409-48-3]
Dietary supplement. Mp 138° dec. (monohydrate).

[6363-38-8, 6381-63-1]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1237A (*nmr*)
Woolley, D.W. *et al., J. Biol. Chem.*, 1939, **129**, 673 (*synth*)
Reichstein, T. *et al., Helv. Chim. Acta*, 1940, **23**, 650; 1276; 1941, **24**, 185 (*synth, cryst struct*)
Stiller, E.T. *et al., J.A.C.S.*, 1940, **62**, 1776; 1779; 1784; 1941, **63**, 1237; 2846 (*synth*)
Woolley, D.W. *et al., J.A.C.S.*, 1940, **62**, 2251 (*synth*)
Harris, S.A. *et al., J.A.C.S.*, 1941, **63**, 2662 (*synth*)
Hill, R.K. *et al., Biochem. Biophys. Res. Commun.*, 1970, **38**, 181 (*abs config*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1001 (*cryst struct*)
Imamoto, S. *et al., Methods Enzymol.*, 1979, **62**, 227 (*glucosides*)
Fox, H.M. *et al., Handbook of Vitamins*, (ed., Machlin, L.J.), Marcel Dekker, N.Y., 1984, 437 (*rev*)
Fischer, G.C. *et al., J.O.C.*, 1985, **50**, 2011 (*amide*)
Morrow, C.J. *et al., J.O.C.*, 1986, **51**, 1955 (*synth, cmr, pmr*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1356
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CAU750
Pei, F.K. *et al., Chin. J. Chem.*, 1991, **9**, 212 (*cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1046
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 401-405; 2084-2085; 2582-2583 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CAU750

Paolins P-32

Three fractions isol. with MWs 9000-10000, 1400-1700, and 700. Structs. unknown. Isol. from the common clam *Mercenaria mercenaria*. Sol. H_2O.

Li, C.P. *et al., Ann. N.Y. Acad. Sci.*, 1965, **130**, 374-382 (*isol*)

Papain, USAN P-33

[9001-73-4]
Caroid. Papayotin. Vegetable pepsin. Arbuz. Nematolyt. Summetrin. Tromasin. Velardon. Vermizym. E.C. 3.4.22.2

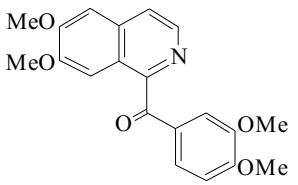
A peptidase enzyme. Purified proteolytic substance derived from papaya *Carica papaya*. Meat tenderiser. Also used to reduce chillhaze in beer. Used in the prepn. of precooked cereals and prodn. of protein hydrolysates. Component of Panafil.

▶ RU4950000

Zoch, E. *et al., Arzneim.-Forsch.*, 1969, **19**, 1593 (*rev, isol, uses*)
Arnon, R. *et al., Methods Enzymol.*, 1970, **19**, 226 (*rev*)
Liener, I.E. *et al., Adv. Chem. Ser.*, 1974, **136**, 202 (*rev, props, uses*)
Kamphius, I.G. *et al., J. Mol. Biol.*, 1984, **179**, 233 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1398
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2087-2089 (*rev, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAG500

Papaveraldine P-34

[522-57-6]
6,7-Dimethoxy-1-(3,4-dimethoxybenzoyl)isoquinoline. Xanthaline†



$C_{20}H_{19}NO_5$ 353.374
Isol. from *Papaver somniferum* preparations (opium). Mp 210°. Probably an artifact.

Hydrochloride:
Mp 198-199°.

Picrate:
Mp 208-209°.

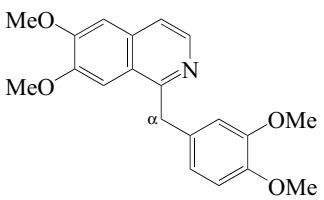
N-*Me:* [7668-80-6] **N-*Methylpapaveraldinium***. N-*Methylxanthalinium*
$C_{21}H_{22}NO_5^{\oplus}$ 368.408
Mp 159.5-161° (as chloride). CAS no. refers to chloride.

3′-O-*De-Me,* N-*Me:* [219915-63-6] ***Thalprzewalskiinone***
$C_{20}H_{20}NO_5^{\oplus}$ 354.382
Yellow cryst. (as iodide). Mp 196-197° (iodide). Revised struct. (2001) λ_{max} 256 (log ϵ 4.38); 302 (log ϵ 3.89); 326 (log ϵ 3.94) (MeOH).

Noller, C.R. *et al., J.A.C.S.*, 1950, **72**, 17 (*uv*)
Guthrie, D.A. *et al., Can. J. Chem.*, 1955, **33**, 729 (*synth*)
Kunitomo, J. *et al., Yakugaku Zasshi*, 1966, **86**, 456; *CA*, **65**, 10633g (N-*Methylpapaveraldinium*)
Wu, W.-N. *et al., J. Nat. Prod.*, 1980, **43**, 143 (*ir, pmr, ms*)
Wasserman, H.H. *et al., Tet. Lett.*, 1989, **30**, 869 (*synth*)
Al-Howiriny, T.A. *et al., J. Nat. Prod.*, 2001, **64**, 823-826 (*Thalprzewalskiinone*)

Papaverine, BAN P-35

[58-74-2]
6,7-Dimethoxy-1-(3,4-dimethoxybenzyl)isoquinoline. Papaveroline tetramethyl ether. NSC 35443



$C_{20}H_{21}NO_4$ 339.39
Alkaloid from *Papaver somniferum* (opium poppy). Prisms (EtOH/Et_2O). Mp 147-148°. pK_a 6.4 (25°). Log P 3.37 (calc). λ_{max} 239 (ϵ 67500); 279 (ϵ 7380); 314 (ϵ 4000); 327 (ϵ 4660) (EtOH) (Berdy).

▶ Gastrointestinal and other adverse effects reported when used therapeutically, can cause drowsiness and dizziness by ingestion. LD_{50} (rat, orl) 325mg/kg. NW8450000

Hydrochloride: [61-25-6] *Papaverine hydrochloride, USAN. Cerespan. Pavabid. Brovon*
Rods (H_2O). Mp 221-222° dec. Component of Copavin.

▶ Adverse therapeutic effects similar to papaverine. LD_{50} (rat, orl) 360 mg/kg. Exp. teratogen. NW8575000

N-*Me:* [19716-71-3] ***Densiberine***. N-*Methylpapaverine*
$C_{21}H_{24}NO_4^{\oplus}$ 354.425
Cryst. (EtOH) (as chloride). Mp 156-157° (chloride). CAS no. refers to chloride λ_{max} 222 ; 256 ; 317 (EtOH).

α-*Oxo:* See Papaveraldine, P-34

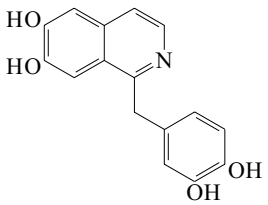
α-*Methoxy:* [180386-76-9] ***Setigerine***. α-*Methoxypapaverine*
$C_{21}H_{23}NO_5$ 369.416Racemic.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 878B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 457C (*nmr*)
Hofmann, A. *et al., Helv. Chim. Acta*, 1954, **37**, 849 (*uv*)
Guthrie, D.A. *et al., Can. J. Chem.*, 1955, **33**, 729 (*synth*)
Popp, F.D. *et al., J.A.C.S.*, 1957, **79**, 3773 (*synth*)
Saferstein, R. *et al., CA*, 1974, **80**, 44458m (*ms*)
Brochmann-Hanssen, E. *et al., J.C.S. Perkin 1*, 1975, 1531 (*biosynth*)
Manske, R.H.F. *et al., The Alkaloids*, Ed., Academic Press, N.Y., 1975, 209 (*pharmacol, tox*)
Neuman, M. *et al., Drugs of Today (Barcelona)*, 1976, **12**, 278 (*rev*)
Shtokalo, M.I. *et al., Zh. Anal. Khim.*, 1976, **31**, 2366 (*detn, Zr*)
Whipple, G.H. *et al., Angiology*, 1977, **28**, 737 (*rev*)
Tomimatsu, T. *et al., CA*, 1977, **87**, 23573z (*pmr*)
Marsaioli, A.J. *et al., Phytochemistry*, 1978, **17**, 1655 (*cmr*)
Wilen, G. *et al., J. Pharm. Pharmacol.*, 1982, **34**, 264 (*metab*)
Skripchuk, V.G. *et al., Zh. Anal. Khim.*, 1983, **38**, 2198 (*detn, Te*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 5642 (*synonyms*)
Hifnawy, M.S. *et al., Anal. Profiles Drug Subst.*, 1988, **17**, 367 (*rev*)
Turano, A. *et al., AIDS Res. Hum. Retroviruses*, 1989, **5**, 183 (*anti-HIV activity*)
Janssen, R.H.A.M. *et al., Phytochemistry*, 1989, **28**, 2833 (*pmr, cmr*)
Hirsenkorn, R. *et al., Tet. Lett.*, 1991, **32**, 1775 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1399
Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1996, **61**, 1047-1052 (*Setigerine*)
Marek, J. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1996, **211**, 649; 651-652 (*cryst struct, Papaverine, Setigerine*)

Khamidov, I.I. *et al., Khim. Prir. Soedin.*, 1997, **33**, 420-423; *Chem. Nat. Compd. (Engl. Transl.)*, 1997, **33**, 323-325 (*Densiberine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAH000; PAH250

Papaveroline, BAN, INN P-36

[574-77-6]
1-[(3,4-Dihydroxyphenyl)methyl]-6,7-isoquinolinediol, 9CI. 1-(3,4-Dihydroxybenzyl)-6,7-dihydroxyisoquinoline. Modus†. Udieci active substance



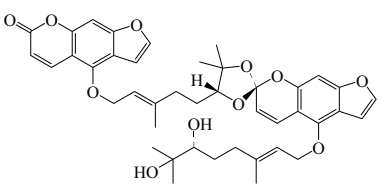
$C_{16}H_{13}NO_4$ 283.283
Cryst. powder + $2H_2O$, becoming anhyd. at *ca*. 100°. Mp 150° dec. Log P 2.79 (calc).

4′,6,7-Tri-Me ether: [18694-10-5] *1-(3-Hydroxy-4-methoxybenzyl)-6,7-dimethoxyisoquinoline.* ***Palaudine***
$C_{19}H_{19}NO_4$ 325.363
Minor alkaloid from opium (*Papaver somniferum*). Prisms (EtOH). Mp 175-176°.

[23740-72-9]

Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1968, **57**, 940 (*Palaudine*)

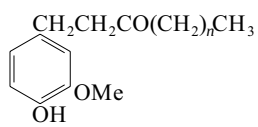
Paradisin C P-37



$C_{42}H_{46}O_{11}$ 726.819
Constit. of grapefruit juice (*Citrus paradisi*). Solid. $[\alpha]_D^{25}$ -17 (c, 0.12 in $CHCl_3$). λ_{max} 225 (log ϵ 4.3); 245 (log ϵ 5.7); 267 (log ϵ 3.2); 311 (log ϵ 2) (MeOH).

Ohta, T. *et al., Tetrahedron*, 2002, **58**, 6631-6635 (*isol, pmr, cmr*)

Paradol P-38



A series of homologues. The Paradol no. is indicated by *n* in the diag..

[7]Paradol [53172-04-6]
1-(4-Hydroxy-3-methoxyphenyl)-3-undecanone
$C_{18}H_{28}O_3$ 292.417
Constit. of *Amomum melegueta* (grains of paradise). Cryst. Mp 35.5-36.5°.

[8]Paradol [27113-23-1]
1-(4-Hydroxy-3-methoxyphenyl)-3-dodecanone
$C_{19}H_{30}O_3$ 306.444
Constit. of *Amomum melegueta* (grains of paradise). Cryst. Mp 42-43°.

Ac: [36700-49-9]
$C_{21}H_{32}O_4$ 348.481
Constit. of *Amomum melegueta* (grains of paradise).

1,2,4,5-Tetradehydro:1-(4-Hydroxy-3-methoxyphenyl)-1,4-dodecadien-3-one. ***[8]Dehydroshogaol***
$C_{19}H_{26}O_3$ 302.413
Constit. of *Zingiber officinale* (ginger). Yellow syrup. Possesses (*E*,*E*)-config. λ_{max} 258 (log ϵ 3.96); 357 (log ϵ 4.1) (MeOH).

[10]Paradol [36700-48-8]
1-(4-Hydroxy-3-methoxyphenyl)-3-tetradecanone
$C_{21}H_{34}O_3$ 334.498
Constit. of *Amomum melegueta* (grains of paradise). Cryst. Mp 50-51°.

*1,2,4,5-Tetradehydro (*E,E-*):1-(4-Hydroxy-3-methoxyphenyl)-1,4-tetradecadien-3-one.* ***[10]Dehydroshogaol***
$C_{21}H_{30}O_3$ 330.466
Constit. of *Zingiber officinale* (ginger). Yellow syrup. λ_{max} 257 (log ϵ 4.04); 355 (log ϵ 4.18) (MeOH).

Connell, D.W. *et al., Aust. J. Chem.*, 1970, **23**, 369 (*isol*)
Ger. Pat., 1974, 2 349 537; *CA*, **81**, 13256 (*synth*)
Tackie, A.N. *et al., Phytochemistry*, 1975, **14**, 853 (*isol*)
Wu, T.-S. *et al., Phytochemistry*, 1998, **48**, 889-891 (*Dehydroshogaols*)

Paraffin wax P-39

[8002-74-2]
Crystalline petroleum wax. Synthetic wax. Fischer-Tropsch paraffin. FEMA 3216

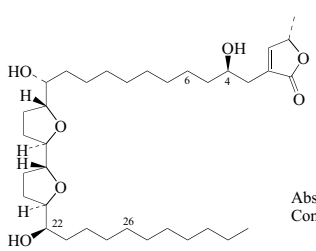
Solid mixture of saturated hydrocarbons derived from the Fischer-Tropsch process. Masticatory substance in chewing gum base, adhesive component, coatings, glazing agent (Japan). Mp 50-57°.

Ash, M. *et al., Handbook of Food Additives*, Gower, 1995, 632 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2093-2094

Parviflorin P-40

[152378-19-3]

[166735-11-1]
Atemoyacin A. Squamocin E. 22-Epimolvizarin



Absolute Configuration

$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona squamosa* (sugar apple) and *Annona atemoya* (custard apple). Wax. $[\alpha]_D$ +20.9 (c, 0.2 in MeOH). λ_{max} 223 (ϵ 8405) (EtOH) (Berdy).

22-Epimer, 4-deoxy: [125205-43-8] ***Neoannonin***. *Squamocin J*
$C_{35}H_{62}O_6$ 578.871
Constit. of *Annona squamosa* (sugar apple). Wax. Sol. MeOH, hexane; poorly sol. H_2O. Mp 85-86.5° (62-64°). $[\alpha]_D^{22}$ +18.8 (c, 1.35 in MeOH). λ_{max} 215 (ϵ 12000) (MeOH) (Berdy).

*4-Deoxy, 6*S*-hydroxy:* [152340-16-4] ***Bullacin***
$C_{35}H_{62}O_7$ 594.871
Wax. $[\alpha]_D$ +15.6 (c, 0.3 in $CHCl_3$). λ_{max} 213 (ϵ 5623) (MeOH) (Berdy).

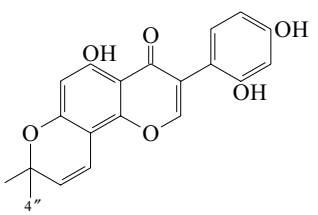
*22-Epimer, 4-deoxy, 26*S*-hydroxy:* [159934-23-3] ***Squamocin B***
$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona squamosa* (sugar apple). Wax. $[\alpha]_D^{25}$ +27.6 (c, 0.2 in MeOH).

8-Hydroxy: [194413-43-9] ***Annonisin***
$C_{35}H_{62}O_8$ 610.87
Constit. of *Annona atemoya* (custard apple). Amorph. solid. $[\alpha]_D^{20}$ +30 (c, 0.2 in $CHCl_3$). λ_{max} 209 (log ϵ 3.9) (MeOH).

Kawaza, K. *et al., Agric. Biol. Chem.*, 1989, **53**, 2719 (*Neoannonin*)
Gu, Z.-M. *et al., Heterocycles*, 1993, **36**, 2221-2228 (*Bullacin*)
Ratnayake, S. *et al., Can. J. Chem.*, 1994, **72**, 287 (*isol*)
Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*Squamocins*)
Chen, W,-S, *et al., Chin. J. Chem.*, 1995, **13**, 263-266 (*Atemoyacin A*)
Hoye, T.R. *et al., J.A.C.S.*, 1996, **118**, 1801-1802 (*synth*)
Duret, P. *et al., Phytochemistry*, 1997, **45**, 1423-1426 (*Annonisin*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)

Parvisoflavone A P-41

[50277-01-5]
*3-(2,4-Dihydroxyphenyl)-5-hydroxy-8,8-dimethyl-4*H,*8*H-*benzo[1,2-*b:*3,4-*b′]dipyran-4-one, 9CI*



$C_{20}H_{16}O_6$ 352.343
Obt. only as a mixt. with Parvisoflavone B. Isol. from *Phaseolus aureus* (mung bean). Yellow cryst. ($Me_2CO/CHCl_3$) (mixt.). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 235-239°. λ_{max} 214 (ϵ 38200); 263 (ϵ 29600) (MeOH) (Berdy).

Tri-Me ether:
Mp 166-168°. Pure.

4′′-Hydroxy: [104691-88-5] ***Hydroxyparvisoflavone A***

$C_{20}H_{16}O_7$ 368.342
Yellow plates. Mp 172-174°.

Assumpção, R.M.V. *et al., Phytochemistry*, 1973, **12**, 1188 (*isol, uv, ir, pmr, ms, struct*)
O'Neill, M.J. *et al., Z. Naturforsch., C*, 1983, **38**, 693 (*isol*)
Hashidoko, Y. *et al., Agric. Biol. Chem.*, 1986, **50**, 1797 (*isol, pmr, deriv*)

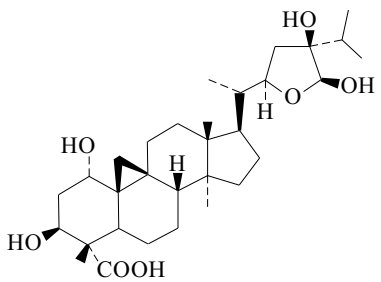
PAS I P-42

Glycoprotein, MW 20-50 Da. Isol. from whey. Shows antiviral activity.

Japan. Pat., 1996, 96 99 896; *CA*, **125**, 41755t (*isol*)

Passifloric acid P-43

[64147-49-5]



$C_{31}H_{50}O_7$ 534.732
Prisms (MeOH).

β-D-Glucopyranosyl ester: [1392-82-1] ***Passiflorine***†
$C_{37}H_{60}O_{12}$ 696.874
Constit. of *Passiflora edulis* (passion fruit). Cryst. (MeOH). Mp 183°. $[\alpha]_D$ +47.1 (Py).

Bombardelli, E. *et al., Phytochemistry*, 1975, **14**, 2661 (*isol*)
Andreeti, G.D. *et al., J.C.S. Perkin 2*, 1977, 605 (*struct*)

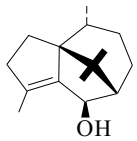
Patatin P-44

A family of closely related glycoproteins with apparent molecular weight of 40 kD. The major storage protein in potato tubers comprising 40% of total soluble protein. Not present in leaves, roots or stems. Possesses lipid acylesterase activity which may be implicated in host defense mechanism. A number of genetic variants are listed in the CAS Index guide, the CAS nos. of which are listed here. The full struct. of at least one genetic variant is known.

[94490-28-5, 94490-29-6, 104299-04-9, 104299-06-1, 120669-71-8, 120669-72-9]

Racusen, D. *et al., J. Food Biochem.*, 1980, **4**, 43-52 (*isol*)
Mignery, G.A. *et al., Nucleic Acids Res.*, 1984, **12**, 7987-8000 (*amino acid sequence*)
Stonnewald, U. *et al., Planta*, 1989, **179**, 171-180 (*struct*)
Pots, A.M. *et al., Eur. J. Biochem.*, 1998, **252**, 66-72 (*conformn, cd, uv*)

4-Patchoulen-6-ol P-45



$C_{15}H_{24}O$ 220.354

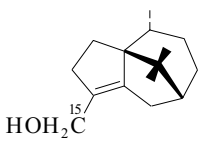
6β-*form* [17806-54-1]
Patchoulenol
Cryst. Mp 74°. $[\alpha]_D^{30}$ -54.23 (c, 3.8 in $CHCl_3$).

Ketone: [5986-54-9] *4-Patchoulen-6-one.* ***Patchoulenone***. *Narucinone*
$C_{15}H_{22}O$ 218.338
Constit. of *Cyperus rotundus* (nutgrass). Cryst. (MeOH). Mp 52.5°. $[\alpha]_D$ -97.1 (c, 8 in $CHCl_3$). Struct. of Narucinone revised in 1992 λ_{max} (MeOH) (Berdy).

Trivedi, B. *et al., Coll. Czech. Chem. Comm.*, 1964, **24**, 1675 (*isol*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1965, **13**, 629 (*struct*)
Nerali, S.B. *et al., Tet. Lett.*, 1967, 2447 (*isol*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 43 (*synth*)
Hisham, A. *et al., Magn. Reson. Chem.*, 1992, **30**, 295-297 (*Narucinone*)
Achenbach, H. *et al., Phytochemistry*, 1995, **38**, 1037 (*Patchoulenone, pmr, cmr*)
Thebtaranorth, C. *et al., Phytochemistry*, 1995, **40**, 125 (*isol, pmr, cmr*)
Banwell, M. *et al., Chem. Comm.*, 1998, 1851-1852 (*synth*)

4-Patchoulen-15-ol P-46

[16981-80-9]
Cyperenol



$C_{15}H_{24}O$ 220.354
Cryst. Mp 94°. $[\alpha]_D^{30}$ -12.1 (c, 4.3 in $CHCl_3$).

Ac: [115334-13-9] ***Cyperenyl acetate***
$C_{17}H_{26}O_2$ 262.391
Oil. $[\alpha]_D$ -5.1 (c, 0.8 in $CHCl_3$).

15-Aldehyde: [115334-16-2] *4-Patchoulen-15-al*. ***Cyperenal***
$C_{15}H_{22}O$ 218.338
Oil. $[\alpha]_D$ +9.6 (c, 0.4 in $CHCl_3$).

15-Carboxylic acid: [112667-88-6] *4-Patchoulen-15-oic acid*. ***Cyperenoic acid***
$C_{15}H_{22}O_2$ 234.338
Cryst. (Me_2CO/hexane). Mp 162-164°. $[\alpha]_D^{25}$ -18.8 (c, 0.08 in $CHCl_3$).

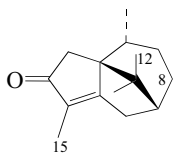
15-Carboxylic acid, Me ester: [190393-31-8] ***Methyl cyperenoate***
$C_{16}H_{24}O_2$ 248.364
Oil. $[\alpha]_D^{21}$ -8 (c, 1.1 in $CHCl_3$). λ_{max} 241 (log ϵ 3.96) (MeOH).

Deoxy: [2387-78-2] *4-Patchoulene.* ***Cyperene***. *Cyperene I. 4-Isopatchoulene. α-Cyperene*
$C_{15}H_{24}$ 204.355
Isol. from *Cyperus rotundus* (nutgrass) and other plants. Bp_5 104°. $[\alpha]_D^{20}$ -20 (neat). n^{20} 1.5058.

Trivedi, B. *et al., Tet. Lett.*, 1964, 1197 (*Cyperene*)
Nerali, S.B. *et al., Tet. Lett.*, 1967, 2447 (*Cyperenol*)
Dreyfus, H. *et al., Tet. Lett.*, 1969, 3757 (*abs config*)
Jacobs, H. *et al., J. Nat. Prod.*, 1987, **50**, 835 (*Cyperenoic acid*)
Boonyaratavej, S. *et al., J. Nat. Prod.*, 1988, **51**, 769 (*Cyperenoic acid, cryst struct*)
Takano, S. *et al., Phytochemistry*, 1988, **27**, 1197 (*Cyperenyl acetate, Cyperenal*)
Achenbach, H. *et al., Eur. J. Pharm. Sci.*, 1994, **2**, 128 (*isol, activity*)
Achenbach, H. *et al., Phytochemistry*, 1997, **45**, 149-157 (*Methyl cyperenoate*)

4-Patchoulen-3-one P-47

[3466-15-7]
Cyperotundone. *Cyperenone. Articulone. Isopatchoulenone*



$C_{15}H_{22}O$ 218.338
Constit. of *Cyperus rotundus* (nutgrass). Cryst. (petrol). Mp 46-47.5°. $Bp_{0.5}$ 136-138°. $[\alpha]_D$ +40.4 (c, 3.2 in $CHCl_3$). λ_{max} 244 (EtOH) (Berdy).

2,4-Dinitrophenylhydrazone:
Red cryst. (EtOH). Mp 231-232°.

8α-Hydroxy:8-Hydroxy-4-patchoulen-3-one. ***8-Hydroxycyperotundone***
$C_{15}H_{22}O_2$ 234.338
Gum.

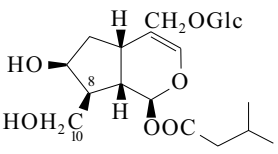
12,15-Diacetoxy: [98211-44-0] *12,15-Diacetoxycyperenone*
$C_{19}H_{26}O_5$ 334.411
Oil.

15-(3-Hydroxy-3-methylbutanoyloxy):
[98211-43-9]
$C_{20}H_{30}O_4$ 334.455
Oil.

Hikino, H. *et al., Tetrahedron*, 1967, **23**, 2169 (*struct*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **66**, 43 (*synth*)
Neville, G.A. *et al., Tetrahedron*, 1968, **24**, 3891 (*pmr, ms, bibl*)
Singh, P. *et al., Phytochemistry*, 1985, **24**, 1525-1529 (*deriv*)
Ybarra, M.I. *et al., Phytochemistry*, 1992, **31**, 3627 (*8-Hydroxycyperotundone*)

Patrinoside P-48

[53962-20-2]



$C_{21}H_{34}O_{11}$ 462.493
Amorph.

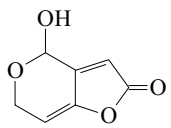
▶ LZ5901000

8-Epimer, 6′-O-*β-D-glucopyranosyl:* [64703-88-4] ***Kanokoside D***
$C_{27}H_{44}O_{16}$ 624.635
Constit. of *Valeriana officinalis* (valerian) root. Amorph., cryst. (as nona-Ac). Mp 179-181° (nona-Ac). $[\alpha]_D$ -30 (MeOH) (nona-Ac). A gentiobioside.

Endo, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2140 (*Kanokoside D*)

Patulin P-49

[149-29-1]
*4-Hydroxy-4*H-*furo[3,2-c]pyran-2(6*H*)-one, 9CI, 8CI. Clavacin. Clavatin. Claviformin. Expansin. Flavicin. Gigantic acid*†. *Mycoin C_3. Penicidin. Terinin. YS 1649. Antibiotic YS 1649. Sch 351633. Antibiotic Sch 351633*



$C_7H_6O_4$ 154.122
Mycotoxin, found as a contaminant of foods, e.g. apple juice. Sometimes detd. in apple juice. Prisms or plates (Et_2O or $CHCl_3$). Mp 111°. $[\alpha]_D^{21}$ -6.2 ($CHCl_3$). Log P -2.4 (uncertain value) (calc). λ_{max} (no shifts reported) (Derep). λ_{max} 292 (ϵ 13400) (0.1*N* NaOH) (Derep). λ_{max} 276 (ϵ 14800) (H_2O or MeOH) (Derep).

▶ Exp. neoplastic agent and teratogen. LD_{50} (rat, orl) 27.8 mg/kg. Exp. kidney and gastrointestinal effects. LV2625000

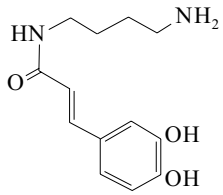
Phenylhydrazone:
Mp 149-150°.

Ac: [6192-26-3]
Prisms (EtOH aq.). Mp 118-120°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1151C (*nmr*)
Birkinshaw, J.H. *et al., Lancet*, 1943, **245**, 625 (*isol, struct*)
Bergel, F. *et al., J.C.S.*, 1944, 415 (*isol, struct*)
Woodward, R.B. *et al., J.A.C.S.*, 1950, **72**, 1428 (*synth*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)
Lalau-Kéraly, F. *et al., C. R. Hebd. Seances Acad. Sci.*, 1965, **261**, 4028 (*ir*)
Ciegler, A. *et al., Microb. Toxins*, (eds. Ciegler, A. *et al*), Academic Press, 1971, **V1**, 409 (*rev*)
Scott, P.M. *et al., Mycotoxins*, (ed. Purchase, I.F.H.), Elsevier, 1974, 383 (*rev*)
Wilson, D.M. *et al., Adv. Chem. Ser.*, 1976, **149**, 90 (*rev*)
Hubbard, C.R. *et al., Acta Cryst. B*, 1977, **33**, 928 (*cryst struct*)
Sekiguchi, J. *et al., Tet. Lett.*, 1979, 41 (*biosynth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2219 (*uv, ir, pmr, ms*)
Iijima, H. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3534 (*biosynth*)
IARC Monog., 1986, **40**, 83; *Suppl.* 7, 69 (*rev, tox*)
Gill, G.B. *et al., Tet. Lett.*, 1988, **29**, 2875 (*synth*)
Sejas, J.A. *et al., Heterocycles*, 1989, **29**, 181 (*synth*)
Tarter, E.J. *et al., J. Chromatogr.*, 1991, **538**, 441 (*glc*)
Bennett, M. *et al., J.C.S. Perkin 1*, 1991, 929 (*synth*)
Tada, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2167 (*synth*)
Yoo, S.-J. *et al., J. Microb. Biotechnol.*, 1995, **5**, 31 (*YS 1649*)
Boukouvalas, J. *et al., Tet. Lett.*, 1995, **36**, 7175 (*synth, bibl*)
Chu, M. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 1949-1952 (*Sch 351633*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 511
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMV000

Paucine P-50

[29554-26-5]
N-*(4-Aminobutyl)-3-(3,4-dihydroxyphenyl)-2-propanamide, 9CI.* N-*(3,4-Dihydroxycinnamoyl)-1,4-butanediamine. Caffeoylputrescine*



$C_{13}H_{18}N_2O_3$ 250.297
Alkaloid from the famine food *Pentaclethra macrophylla and from Persea gratissima* (avocado).

Hydrochloride: [59862-95-2]
Cryst. + $2H_2O$. Mp 247-250° dec.

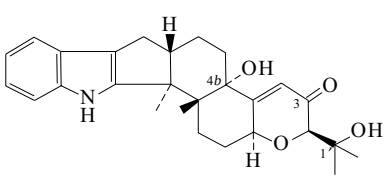
O$^{3'}$-Me: Subaphylline, S-256

[26148-06-1]

Hollerbach, A. *et al., Monatsh. Chem.*, 1970, **101**, 141 (*uv, ir, pmr, ms, struct*)
Mizusaki, S. *et al., Phytochemistry*, 1971, **10**, 1347 (*isol, uv, ir, pmr, synth*)
Buta, J.G. *et al., Phytochemistry*, 1972, **11**, 1188 (*isol, uv, ir, pmr*)
Mbadiwe, E.I. *et al., Phytochemistry*, 1973, **12**, 2546 (*isol*)
Cabanne, F. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1976, **282**, 1959 (*uv*)
Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*occur*)
Keller, H. *et al., Phytochemistry*, 1996, **42**, 389-396 (*isol, pmr, cmr*)

Paxilline P-51

[57186-25-1]



$C_{27}H_{33}NO_4$ 435.562
Tremorgenic agent from *Penicillium paxilli, Acremonium lorii, Emericella foveolata, Emericella desertorum* and *Emericella striata*. Plates (Me_2CO). Mp 252°. λ_{max} 231 (ϵ 41700); 280 (ϵ 9330); 290 (sh) (ϵ 8320) (EtOH) (Derep). λ_{max} 230 ; 280 (MeOH) (Berdy).

▶ LD_{50} (mus, orl) >227 mg/kg; produces tremors. DJ2830000

1′-O-*Ac:* [121998-08-1] ***1′*-O-*Acetylpaxilline***
$C_{29}H_{35}NO_5$ 477.599
Mycotoxin from the mycelium of *Emericella striata*. Needles (EtOAc). Subl. 262-265. λ_{max} 231 (ϵ 41700); 280 (ϵ 9330); 290 (sh) (ϵ 8320) (EtOH) (Derep). λ_{max} 231 (ϵ 42000); 280 (ϵ 9300); 290 (ϵ 8100) (EtOH) (Berdy).

3β-Alcohol, 3-Ac: [133613-75-9] ***PC-M5′***
$C_{29}H_{37}NO_5$ 479.615
Tremorgenic mycotoxin from *Penicillium crustosum*. Cryst. powder. Mp 162-164°.

*4*b-*Deoxy:* [112900-05-7] ***Dehydroxypaxilline***
$C_{27}H_{33}NO_3$ 419.563
Metab. of *Emericella striata*. Leaflets (MeOH). Mp 232-234°.

*4*b-*Deoxy, 3β-alcohol:* [133613-76-0] ***PC-M6***. *10-Hydroxy-13-deoxypaxilline. 3-Hydroxy-4-deoxypaxilline*
$C_{27}H_{35}NO_3$ 421.578
Tremorgenic mycotoxin from *Penicillium crustosum*, *Penicillium paxilli* and *Acremonium lolii*. Cryst. powder. Mp 260-263° dec. Numbering systems vary.

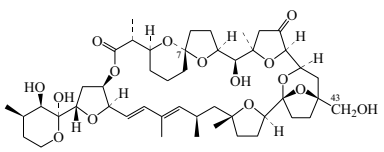
14aα-Hydroxy: [157530-30-8] ***14a-Hydroxypaxilline***. *7-Hydroxypaxilline*
$C_{27}H_{33}NO_5$ 451.561
Metab. from *Penicillium paxilli*. Also identified chromatographically in *Acremonium lolii*. Apparently not tremorgenic. Numbering systems vary.

*14aα-Hydroxy, 4*b-*deoxy:* [157530-29-5] ***14a-Hydroxy-4b-deoxypaxilline***. *7-Hydroxy-13-deoxypaxilline*
$C_{27}H_{33}NO_4$ 435.562
Metab. of *Penicillium paxilli* and *Acremonium lolii*. Numbering systems vary.

Cole, R.J. *et al., Can. J. Microbiol.*, 1974, **20**, 1159 (*isol, uv, ir, pmr, ms*)
Springer, J.P. *et al., Tet. Lett.*, 1975, 2531; 1980, 231 (*pmr, cd, cryst struct, abs config*)
Weedon, C.M. *et al., Phytochemistry*, 1987, **26**, 969
Nozawa, K. *et al., J.C.S. Perkin 1*, 1988, 2607 (*Dehydroxypaxilline*)
Nozawa, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1387 (*1′-O-Acetylpaxilline*)
Betina, V. *et al., Mycotoxins, Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 365 (*rev*)
Hosoe, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3473 (*PC-M5′, PC-M6*)
Antkowiak, R. *et al., Alkaloids (N.Y.)*, 1991, **40**, 249 (*isol, derivs*)
Mantle, P.G. *et al., Phytochemistry*, 1994, **36**, 1209 (*7-Hydroxypaxilline, 7-Hydroxy-13-deoxypaxilline, 10-Hydroxy-13-deoxypaxilline*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 386

Pectenotoxin 1 P-52

[97564-90-4]



Absolute configuration

$C_{47}H_{70}O_{15}$ 875.061

Polyether antibiotic. Found in scallops. Metab. of *Dinophysis acuminata*. Component toxin of shellfish poisoning. Cryst. (MeCN aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 208-209°. $[\alpha]_D^{20}$ +17.1 (c, 0.41 in MeOH). Pectenotoxin 8 and Pectenotoxin 9 have been isol. and identified as artifacts λ_{max} 235 (ϵ 12400) (MeOH) (Berdy).

43-Aldehyde: [97560-25-3] ***Pectenotoxin 3***
$C_{47}H_{68}O_{15}$ 873.045
Metab. of *Dinophysis acuminata*. Shellfish toxin. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 159-160°. $[\alpha]_D^{20}$ +2.22 (c, 0.135 in MeOH). λ_{max} 235 (ϵ 11000) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.35 mg/kg.

43-Carboxylic acid: [124843-18-1] ***Pectenotoxin 6***
$C_{47}H_{68}O_{16}$ 889.045
Constit. of *Dinophysis* sp. Shellfish toxin. λ_{max} 237 (ϵ 37000) (MeOH) (Berdy).

Dihydro (?): [97560-27-5] ***Pectenotoxin 5***
$C_{47}H_{72}O_{15}$ 877.077
Metab. of *Dinophysis acuminata*. Shellfish toxin. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 235 (MeOH) (Berdy).

43-Deoxy: [97564-91-5] ***Pectenotoxin 2***
$C_{47}H_{70}O_{14}$ 859.062
From *Dinophysis acuminata*. Shellfish toxin. Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +16.2 (c, 0.105 in MeOH). λ_{max} 235 (ϵ 16000) (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 0.2 mg/kg.

43-Deoxy, parent hydroxyacid: [212502-87-9] ***Pectenotoxin 2 secoacid***
$C_{47}H_{72}O_{15}$ 877.077
From *Perna canaliculus* (New Zealand green mussel). Ring-opened parent hydroxyacid of the lactone.

7-Epimer: [97560-26-4] ***Pectenotoxin 4***
$C_{47}H_{70}O_{15}$ 875.061
From *Dinophysis acuminata*. Shellfish toxin. Solid. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D^{20}$ +2.07 (c, 0.193 in MeOH).

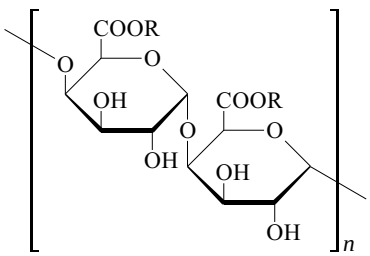
7-Epimer, 43-carboxylic acid: ***Pectenotoxin 7***
$C_{47}H_{68}O_{16}$ 889.045
From *Dinophysis* sp.. λ_{max} 237 (ϵ 37000) (MeOH) (Berdy).

7-Epimer, 43-deoxy, parent hydroxyacid: [212502-88-0] ***7-Epipectenotoxin 2 secoacid***
$C_{47}H_{72}O_{15}$ 877.077
From *Perna canaliculus* (New Zealand green mussel).

Yasumoto, T. *et al., Tetrahedron*, 1985, **41**, 1019 (*isol, cryst struct, spectra*)
Murata, M. *et al., Agric. Biol. Chem.*, 1986, **50**, 2693 (*deriv*)
Lee, J.S. *et al., Bioact. Mol.*, 1989, **10**, 327 (*Pectenotoxin 6*)
Jung, J.H. *et al., J. Nat. Prod.*, 1995, **58**, 1722 (*Pectenotoxin 2, pmr, cmr, activity*)
Sasaki, K. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1783-1785 (*pmr, abs config*)
Daiguji, M. *et al., Chem. Lett.*, 1998, 653-654 (*isol, secoacids*)
Sasaki, K. *et al., J.O.C.*, 1998, **63**, 2475-2480 (*isol, struct*)

Pectic acid P-53

[9046-40-6]
Pectinic acid. Pectin



Colloidal polygalacturonic acids which are essentially completely deesterified and with varying degrees of neutralisation are referred to as pectic acids. Pectinic acids are colloidal polygalacturonic acids with more than a negligible content of Me ester groups with varying degrees of neutralisation. The term pectins refers to those water-soluble pectinic acids of varying Me ester content and degree of neutralisation that are capable of forming gels with sugar and acid under suitable conditions. In pectins, the α-(1→4)-linked D-polygalacturonate sequences are interrupted with (1→2)-L-rhamnose residues, neutral sugars, e.g. D-galactose and L-arabinose, form side chains on the pectin molecules. The mol. wt. of pectins is 20,000 - 400,000. Present in cell walls of all plant tissues. Up to 30% w/w of this polysaccharide can be isol. from orange and lemon rind. Used in food processing as a gelling agent, stabiliser, thickener and emusifier.

[9000-69-5]

Norris, F.W. *et al., Biochem. J.*, 1937, **31**, 1945 (*rev*)
Markovic, O. *et al., Coll. Czech. Chem. Comm.*, 1981, **46**, 266 (*isol*)
Walkinshaw, M.D. *et al., J. Mol. Biol.*, 1981, **153**, 1055 (*cryst struct*)
Japan. Pat., 1988, 63 89 501; *CA*, **109**, 75610b (*manuf*)
Jarvis, M.C. *et al., Carbohydr. Res.*, 1995, **275**, 131-145 (*cmr*)
Renard, M.G.C.C. *et al., Carbohydr. Res.*, 1995, **275**, 155-165 (*pmr, cmr*)
Merck Index, 12th edn., 1996, 7194
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2104-2108

Pediocins P-54

[133108-87-9]

Bacteriocins. Food biopreservatives. Bacteriocins.

Pediocin A [100215-40-5]
Isol. from *Pediococcus pentosaceus* 43200.

Pediocin ACM [194369-20-5]
Isol. from *Pediococcus acidilactici* M.

Pediocin ISK 1 [221191-15-7]
Prod. by *Pediococcus* sp. ISK-1 on aged fermented rice bran.

Pediocin F [219562-11-5]
Isol. from *Pediococcus acidilactici* F from fermented sausage.

Pediocin JD [145018-66-2]
Isol. from *Pediococcus acidilactici* JD1-23.

Pediocin L50 [165659-79-0]
Isol. from *Pediococcus acidilactici* L50.

Pediocin N5p [157856-98-9]
Prod. by *Pediococcus pentosaceus* isol. from wine.

Pediocin PA1 [111745-56-3]

[120367-03-5]
Pediocin AcH
Isol. from *Pediococcus acidilacici* PAC-10 and 43200. A 4629 Da polypeptide with 44 amino acid residues and 2 disulfide bonds.

Pediocin PO2 [149779-78-2]
Isol. from *Pediococcus acidilactici* PO2.

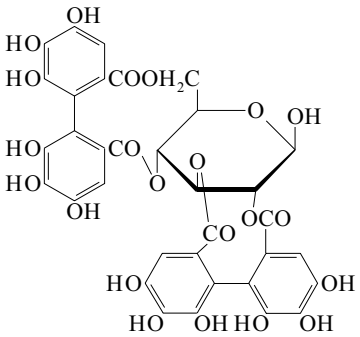
Pediocin SJ-1 [147444-83-5]

Pediocin 5 [158193-12-5]
Isol. from *Pediococcus acidilactici* UL5.

Bhunia, A.K. *et al., J. Appl. Bacteriol.*, 1988, **65**, 261-268 (*Pediocin AcH, isol*)
Henderson, J.T. *et al., Arch. Biochem. Biophys.*, 1992, **295**, 5-12 (*Pediocin PA1, struct*)
Schved, F. *et al., J. Appl. Bacteriol.*, 1993, **74**, 67-77 (*Pediocin SJ-1*)
Huang, J. *et al., Int. Dairy J.*, 1994, **4**, 429-443 (*Pediocin 5*)
Piva, A. *et al., Microbiology (Reading, U.K.)*, 1994, **140**, 697-702 (*Pediocin A*)
Cintas, L.M *et al., Appl. Environ. Microbiol.*, 1995, **61**, 2643-2648 (*Pediocin L50*)
Christensen, D.P. *et al., Appl. Environ. Microbiol.*, 1995, **63**, 2643-2648 (*Pediocin JD*)
Strasser de Saad, A.M. *et al., J. Appl. Bacteriol.*, 1995, **78**, 423-426 (*Pediocin N5p*)
Wan, J. *et al., J. Appl. Bacteriol.*, 1995, **79**, 671-676 (*Pediocin PO2*)
Ray, B. *et al., NATO ASI Ser., Ser. H*, 1996, **98**, 155-203 (*rev*)
Elegado, F.B. *et al., Int. J. Food Microbiol.*, 1997, **37**, 1-11 (*Pediocin ACM*)
Kimura, H. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2341-2345 (*Pediocin ISK 1*)
Osmanagaoglu, O. *et al., Turk. J. Biol.*, 1998, **22**, 217-228; *CA*, **130**, 107322m (*Pediocin F*)

Pedunculagin P-55

[7045-42-3]
2,3;4,6-Bis-(S)-hexahydroxydiphenoyl-D-glucopyranose. Juglanin†



$C_{34}H_{24}O_{22}$ 784.55

Exists as an equilibrated mixt. of α- and β-anomers.Amorph. sandy solid. $[\alpha]_D^{25}$ +106 (c, 2 in MeOH).

1-O-*(3,4,5-Trihydroxybenzoyl) (1β-)*:***1-O-*Galloylpedunculagin***

$C_{41}H_{28}O_{26}$ 936.657

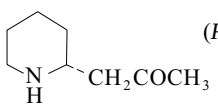
Tannin from *Rubus fruticosus* (blackberry) and *Rubus idaeus* (raspberry). Light brown amorph. powder + $1H_2O$. $[\alpha]_D^{20}$ +34.9 (c, 0.6 in MeOH).

Schmidt, O.T. *et al., Annalen*, 1965, **690**, 150
Gupta, R.K. *et al., J.C.S. Perkin 1*, 1982, 2525 (*1*-O-*Galloylpedunculagin*)
Okuda, T. *et al., J.C.S. Perkin 1*, 1983, 1765 (*ir, uv, cd, pmr, cmr*)
Ishimatea, M. *et al., Phytochemistry*, 1989, **28**, 3179 (*isol, pmr*)
Feldman, K.S. *et al., J.O.C.*, 1996, **61**, 2606 (*synth, pmr, cmr*)
Lee, S.-H. *et al., Yakhak Hoeji*, 1997, **41**, 524-529 (*activity*)

Pelletierine P-56

[4396-01-4]

1-(2-Piperidinyl)-2-propanone, 9CI. 2-Acetonylpiperidine. Isopelletierine. 8-Methylnorlobelone



(R)-form

$C_8H_{15}NO$ 141.213

Pelletierine was originally given the erroneous struct. of 3-(2-piperidinyl)propanal. The early use of the names Pelletierine and Isopelletierine is confusing.Log P 0.56 (calc).

(*R*)-*form* [2858-66-4]

Alkaloid from pomegranate. Liq. $[\alpha]_D^{23}$ -18.1 (c, 8.18 in EtOH). The isoln. of the (*R*)-form is doubtful in view of its ready racemisation and of the fact that the opt. rotn. recorded for the isolate exceeded that of the resolved base.

► RX9625000

Picrate:

Mp 131-132°.

N-*Me:*

$[\alpha]_D^{14}$ -51.5 (c, 4.8 in EtOH).

(*S*)-*form* [2858-67-5]

Liq. $[\alpha]_D^{23}$ +17.9 (c, 9.41 in EtOH aq.).

(±)-*form* [539-00-4]

Alkaloid from pomegranate. Bp_{14} 91-92°. pK_a 9.45 (15°). Readily oxid. in air.

► RX9635000

Hydrochloride: [5984-61-2]

Needles. Mp 143°.

Picrate:

Mp 150-151° (147-149°).

N-*Benzoyl:*

$C_{15}H_{19}NO_2$ 245.321

Prisms or plates. Mp 75°.

N-*Me:****Methylisopelletierine***. α-N-*Methylpelletierin-β-one. Methylpelletierine*

$C_9H_{17}NO$ 155.239

Alkaloid from pomegranate. Misc. H_2O. Bp_{26} 114-117°. Strong base. The isoln. of this alkaloid in opt. active form was reported by Tanret (1880), but this has not been repeated.

N-*Me; hydrochloride:*

Mp 158°.

N-*Me; hydrobromide:*

Mp 151-153°.

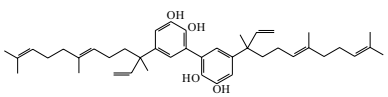
N-*Me, picrate:*

Mp 158°.

Hess, K. *et al., Ber.*, 1917, **50**, 1192 (*isol*)
Galinowsky, F. *et al., Monatsh. Chem.*, 1951, **82**, 551; 1953, **84**, 1221; 1954, **85**, 1012 (*struct*)
Mortimer, P.I. *et al., J.C.S.*, 1957, 3967 (*isol*)
Franck, B. *et al., Chem. Ber.*, 1958, **91**, 2803 (*isol*)
Kuwata, S. *et al., Bull. Chem. Soc. Jpn.*, 1960, **33**, 1668; 1672 (*isol, struct, bibl*)
Gilman, R.E. *et al., Bull. Soc. Chim. Fr.*, 1961, 1993 (*struct*)
Khanna, K.L. *et al., J. Pharm. Sci.*, 1962, **51**, 1194 (*isol*)
Drillien, G. *et al., Bull. Soc. Chim. Fr.*, 1963, 2393 (*rev*)
Beyerman, H.C. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 80 (*abs config*)
Fitch, W.L. *et al., J.O.C.*, 1974, **39**, 2974 (*isol, deriv*)
Hanaoka, M. *et al., Yakugaku Zasshi*, 1974, **94**, 531; *CA*, **81**, 13670r (*synth*)
Krasnov, E.A. *et al., Khim. Prir. Soedin.*, 1977, 585; *Chem. Nat. Compd. (Engl. Transl.)*, 492 (*isol, deriv*)
Cymerman Craig, J. *et al., J.O.C.*, 1978, **43**, 347 (*cd*)
Quick, J. *et al., J.O.C.*, 1979, **44**, 573 (*synth*)
Nagasaka, T. *et al., Heterocycles*, 1989, **29**, 155 (*synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAO500

Peltatol A P-57

[140872-94-2]



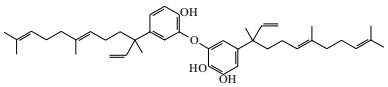
$C_{42}H_{58}O_4$ 626.918

Constit. of *Pothomorphe peltata*. Pale yellow oil. $[\alpha]_D$ +14.2 (c, 2.3 in CH_2Cl_2). Log P 13.37 (uncertain value) (calc). λ_{max} 218 (ϵ 22700); 232 (ϵ 23800); 264 (sh) (ϵ); 310 (ϵ 5560) (MeOH/NaOH) (Derep). λ_{max} 224 (ϵ 24300); 253 (ϵ 9950); 291 (ϵ 4400) (MeOH) (Derep).

Gustafson, K.R. *et al., J.O.C.*, 1992, **57**, 2809 (*isol, pmr, cmr*)

Peltatol B P-58

[140872-95-3]



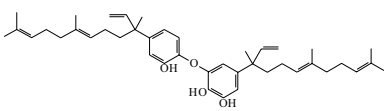
$C_{42}H_{58}O_4$ 626.918

Constit. of *Pothomorphe peltata*. Oil. $[\alpha]_D$ -8.8 (c, 0.7 in $CHCl_3$). Log P 13.93 (uncertain value) (calc). λ_{max} 281 (ϵ 4500) (MeOH) (Derep).

Gustafson, K.R. *et al., J.O.C.*, 1992, **57**, 2809 (*isol, pmr, cmr*)

Peltatol C P-59

[140872-96-4]



$C_{42}H_{58}O_4$ 626.918

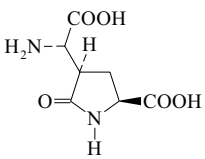
Constit. of *Pothomorphe peltata* (Piperaceae). Oil. $[\alpha]_D$ +6 (c, 0.5 in $CHCl_3$). λ_{max} (solvent not reported) (Derep). λ_{max} 281 (ϵ 4500) (MeOH) (Derep).

Gustafson, K.R. *et al., J.O.C.*, 1992, **57**, 2809 (*isol, pmr, cmr*)

Penmacric acid P-60

[55297-13-7]

α-Amino-5-carboxy-2-oxo-3-pyrrolidineacetic acid, 9CI. 3-(1-Aminocarboxymethyl)-2-pyrrolidone-5-carboxylic acid



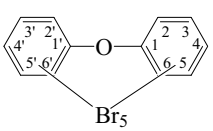
Absolute configuration

$C_7H_{10}N_2O_5$ 202.166

Constit. of the seeds of the famine food *Pentaclethra macrophylla*. Cryst. (H_2O). $[\alpha]_D^{20}$ +6 (c, 0.034 in H_2O). $[\alpha]_D$ +35 (c, 0.070 in 0.1*N* HCl).

Dupont, L. *et al., Acta Cryst. B*, 1975, **31**, 1018 (*cryst struct*)
Welter, A. *et al., Phytochemistry*, 1975, **14**, 1347 (*isol, struct*)
Mbadiwe, E.I. *et al., Phytochemistry*, 1975, **14**, 1351 (*isol, struct*)

Pentabromodiphenyl ethers P-61



$C_{12}H_5Br_5O$ 564.691

Persistent environmental pollutant, detected in fish and human breast milk. Present in land-applied sewage sludge.

2,2′,4,4′,5-Pentabromodiphenyl ether [60348-60-9]

1,2,4-Tribromo-5-(2,4-dibromophenoxy)benzene, 9CI. PBDE 99. BDE 99

$C_{12}H_5Br_5O$ 564.691
Mp 92.3°.

►Developmental neurotoxin in mice.

2,2′,4,4′,6-Pentabromodiphenyl ether
[189084-64-8]
1,3,5-Tribromo-2-(2,4-dibromophenoxy)benzene. PBDE 100. BDE 100

$C_{12}H_5Br_5O$ 564.691
Mp 97-98°.

[32534-81-9]

Environ. Health Criter., *No. 162, Polybrominated Diphenyl Ethers*, WHO, 1994, (*rev, tox, occur*)
Oern, U. *et al., Acta Chem. Scand.*, 1996, **50**, 802-807 (*synth, ms, pmr, uv*)
Marsh, G. *et al., Environ. Sci. Technol.*, 1999, **33**, 3033-3037 (*synth, uv, pmr, ms*)
Hu, J. *et al., Magn. Reson. Chem.*, 2000, **38**, 375-378 (*pmr, cmr*)
Ryan, J.J. *et al., Organohalogen Compd.*, 2000, **47**, 57-60 (*detn in breast milk*)
Strandman, T. *et al., Organohalogen Compd.*, 2000, **47**, 61-64 (*detn*)
Eriksson, P. *et al., Environ. Health Perspect.*, 2001, **109**, 903-908 (*tox*)
Hale, R.C. *et al., Nature (London)*, 2001, **412**, 140-141 (*detn, occur*)

2,3,4,5,6-Pentachlorobenzyl alcohol P-62

[16022-69-8]
2,3,4,5,6-Pentachlorobenzenemethanol, 9CI. Blastin

$(C_6Cl_5)CH_2OH$

$C_7H_3Cl_5O$ 280.364
Fungicide. Effective against foliar-blast disease of rice caused by *Pyricularia oryzae, Drechslera oryzae* and *Rhizoctonia solani*. Needles. Mp 193°. Not used commercially.

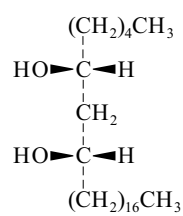
Ac:
$C_9H_5Cl_5O_2$ 322.401
Cryst. (EtOH). Mp 87-90°.

Me ether:1,2,3,4,5-Pentachloro-6-(methoxymethyl)benzene
$C_8H_5Cl_5O$ 294.39
Mp 100-102°.

Et ether:1,2,3,4,5-Pentachloro-6-(ethoxymethyl)benzene
$C_9H_7Cl_5O$ 308.417
Mp 65-66°.

Beilstein, F. *et al., Annalen*, 1869, **152**, 224 (*synth*)
Ross, S.D. *et al., J.A.C.S.*, 1949, **71**, 2756 (*deriv*)
Row, K.V.S.R. *et al., Pesticides*, 1979, **13**, 27 (*use*)
Eur. Pat., 1989, 305 196; *CA*, **111**, 40668r (*synth*)

6,8-Pentacosanediol P-63



$C_{25}H_{52}O_2$ 384.685

(6*R,8*S**)-*form*** [155800-84-3]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 59-62°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

4,6-Pentacosanedione P-64

$H_3C(CH_2)_{18}COCH_2COCH_2CH_2CH_3$

$C_{25}H_{48}O_2$ 380.653
Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-pentacosanone
$C_{25}H_{50}O_2$ 382.669
Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-4-pentacosanone
$C_{25}H_{50}O_2$ 382.669
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

6,8-Pentacosanedione P-65

$H_3C(CH_2)_{16}COCH_2CO(CH_2)_4CH_3$

$C_{25}H_{48}O_2$ 380.653
Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-8-pentacosanone
$C_{25}H_{50}O_2$ 382.669
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

7,9-Pentacosanedione P-66

$H_3C(CH_2)_{15}COCH_2CO(CH_2)_5CH_3$

$C_{25}H_{48}O_2$ 380.653
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

10,12-Pentacosanedione P-67

$H_3C(CH_2)_{12}COCH_2CO(CH_2)_8CH_3$

$C_{25}H_{48}O_2$ 380.653
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

Pentacosanoic acid P-68

[506-38-7]
Hyenic acid

$H_3C(CH_2)_{23}COOH$

$C_{25}H_{50}O_2$ 382.669
Isol. from *Citrus bergamia* (bergamot orange). Cryst. (Me_2CO). Mp 84-85°.

Me ester:
$C_{26}H_{52}O_2$ 396.696
Cryst. (Me_2CO). Mp 61-62°.

Et ester:
$C_{27}H_{54}O_2$ 410.722
Cryst. (Me_2CO). Mp 58-59°. $Bp_{0.5}$ 216-217°.

Nitrile:
$C_{25}H_{49}N$ 363.669
Cryst. (Me_2CO). Mp 58-59°.

Razafindrazaka, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 1633 (*isol*)
Schildknecht, H. *et al., Fette, Seifen, Anstrichm.*, 1964, **66**, 176 (*synth*)
Sundt, E. *et al., Helv. Chim. Acta*, 1964, **47**, 408 (*isol*)
Tember, G.A. *et al., CA*, 1974, **80**, 47410 (*synth*)

7-Pentacosanone P-69

[31469-35-9]

$H_3C(CH_2)_{17}CO(CH_2)_5CH_3$

$C_{25}H_{50}O$ 366.669
Constit. of *Papaver somniferum* (opium poppy). Mp 69°.

Baser, I.A. *et al., CA*, 1971, **74**, 99408 (*synth*)
Bhakuni, R.S. *et al., J. Indian Chem. Soc.*, 1992, **69**, 889 (*isol*)

16-Pentacosene-2,4-dione P-70

$H_3C(CH_2)_7CH=CH(CH_2)_{11}COCH_2COCH_3$

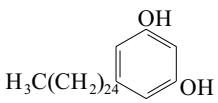
$C_{25}H_{46}O_2$ 378.637

(*Z*)-*form*
Erucoylacetone
Constit. of the epicuticular waxes of *Vanilla fragrans* (vanilla) and *Vanilla tahitensis* (Tahitian vanilla).

Ramaroson-Raonizafinimanana, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 4739-4743 (*isol*)

5-Pentacosyl-1,3-benzenediol, 9CI P-71

[70110-61-1]
5-Pentacosylresorcinol



$C_{31}H_{56}O_2$ 460.782
Constit. of cereal grains.

Kozubek, A. *et al., J. Chromatogr.*, 1984, **295**, 304 (*isol*)
Gohil, S. *et al., J. Sci. Food Agric.*, 1988, **45**, 43 (*isol*)
Suzuki, Y. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 480-486 (*isol, ms*)

2,4-Pentadecadienal P-72

$H_3C(CH_2)_9CH=CHCH=CHCHO$

$C_{15}H_{26}O$ 222.37

(2*E*,4*Z*)-*form* [85769-29-5]
β*-*Triticene
Antifungal constit. of *Triticum aestivum* (wheat). Oil. Poorly sol. hexane. λ_{max} 276 (ε 10000) (EtOH) (Derep). λ_{max} 278 (EtOH) (Berdy).

Spendley, P.J. *et al., Phytochemistry*, 1982, **21**, 2403

5,10-Pentadecadien-1-ol P-73

$H_3C(CH_2)_3CH=CH(CH_2)_3CH=CH(CH_2)_3CH_2OH$

$C_{15}H_{28}O$ 224.386
Flavouring ingredient. Constit. of the flowers of sweet violet (*Viola odorata*). All four stereoisomers have been prepared.

Ohloff, G. *et al., Helv. Chim. Acta*, 1977, **60**, 1161

Cu, J.Q. *et al., Phytochemistry*, 1992, **31**, 571 (*occur*)

6,9-Pentadecadien-2-one P-74

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_3COCH_3$

$C_{15}H_{26}O$ 222.37

(6*Z*,9*Z*)-*form* [78405-86-4]
Constit. of *Lindera benzoin* (spicebush). Oil.

Ueyama, Y. *et al., Flavour Fragrance J.*, 1990, **5**, 85 (*occur*)
Anderson, J.E. *et al., J. Nat. Prod.*, 1992, **55**, 71 (*isol, pmr, cmr*)

Pentadecanal P-75

[2765-11-9]

$H_3C(CH_2)_{13}CHO$

$C_{15}H_{30}O$ 226.401
Isol. from essential oil of *Cinnamomum micranthum* and from lemon oil (*Citrus limon*). Mp 24-25°. Bp_{25} 185° $Bp_{0.2}$ 103-106°. Readily forms a polymer Mp 69-70°.

Oxime:
$C_{15}H_{31}NO$ 241.416
Cryst. (EtOH aq.). Mp 86°.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 107-108°.

Semicarbazone:
Mp 108-109°.

Lauer, W.M. *et al., J.A.C.S.*, 1941, **63**, 1153 (*synth*)
Fujita, Y. *et al., CA*, 1944, **41**, 3509; 1963, **58**, 10506 (*isol*)
Ikeda, R.M. *et al., J. Agric. Food Chem.*, 1962, **10**, 98 (*isol*)
Org. Synth., 1971, **51**, 39 (*synth*)
Enders, D. *et al., Chem. Eur. J.*, 1995, **1**, 382 (*synth, pmr, cmr*)

Pentadecane P-76

[629-62-9]

$H_3C(CH_2)_{13}CH_3$

$C_{15}H_{32}$ 212.418
Mp 10°. Bp 270° Bp_{10} 136°.
► LD_{50} (mus, ivn) 3494 mg/kg. RZ1800000
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 4B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 3D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 4D (*ir*)
Vogel, A.I. *et al., J.C.S.*, 1946, 137 (*synth*)
Bergmann, G. *et al., Angew. Chem., Int. Ed.*, 1972, **11**, 1032 (*cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAY750

2-Pentadecanone, 9CI P-77

[2345-28-0]
FEMA 3724

$H_3C(CH_2)_{12}COCH_3$

$C_{15}H_{30}O$ 226.401
Isol. from hop (*Humulus lupulus*), coconut (*Cocos nucifera*) and other oils. Also found in American cranberry, feijoa fruit, quince, asparagus, ginger, wheat bread, soybean, cooked rice and cheeses. Flavouring ingredient. Mp 39°. Bp 294° $Bp_{0.7}$ 104-106°.

Oxime:
$C_{15}H_{31}NO$ 241.416
Mp 63-65°.

Semicarbazone:
Mp 124-125°.

Krafft, F. *et al., Ber.*, 1879, **12**, 1668
Baumgarten, P. *et al., Ber.*, 1943, **76**, 213
Weichet, J. *et al., Chem. Listy*, 1957, **51**, 127
Rieche, A. *et al., Z. Chem.*, 1964, **4**, 177
Czech. Pat., 1969, 131 766; *CA*, **72**, 132025
McDaniel, C.A. *et al., J. Chem. Ecol.*, 1987, **13**, 227

6,9,12-Pentadecatrien-2-one P-78

$H_3CCH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_3COCH_3$

$C_{15}H_{24}O$ 220.354

(6*Z*,9*Z*,12*Z*)-*form* [139328-79-3]
Constit. of the ripe berries of *Lindera benzoin* (spicebush). Oil.

Anderson, J.E. *et al., J. Nat. Prod.*, 1992, **55**, 71 (*isol, pmr*)

3-Pentadecenal P-79

[140899-08-7]

$H_3C(CH_2)_{10}CH{=}CHCH_2CHO$

$C_{15}H_{28}O$ 224.386
Constit. of the leaves of *Viola odorata* (sweet violet).

Cu, J.Q. *et al., Phytochemistry*, 1992, **31**, 571 (*occur*)

1-Pentadecene, 9CI P-80

[13360-61-7]

[27251-68-9]

$H_3C(CH_2)_{12}CH{=}CH_2$

$C_{15}H_{30}$ 210.402
Occurs in beef and oakmoss oleoresin. Mp -2.8°. Bp 268.2° Bp_{10} 133-137°. Log P 8.14 (uncertain value) (calc).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 21A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 15D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 20D (*ir*)
Schmidt, A.W. *et al., Ber.*, 1941, **74**, 1313
Vinnits'kii, O.M. *et al., Neftekhimiya*, 1969, **9**, 767 (*synth*)
Keville, R. *et al., J. Insect Physiol.*, 1975, **21**, 81

7-Pentadecene, 9CI P-81

[15430-98-5]

[27251-68-9]

$H_3C(CH_2)_6CH{=}CH(CH_2)_5CH_3$

$C_{15}H_{30}$ 210.402

(*E*)-*form* [16416-37-8]
Occurs in corn oil. Bp_7 121.5-122° Bp_{20} 140°.

Asinger, F. *et al., Ber.*, 1943, **76**, 585 (*synth*)
Villieras, J. *et al., Bull. Soc. Chim. Fr.*, 1967, 1511 (*synth, ir*)
Kocienski, P.J. *et al., J.C.S. Perkin 1*, 1978, 829 (*ir, ms, pmr, synth*)

9-Pentadecene-12,14-diyne-1,11-diol, 9CI P-82

[108112-83-0]

[114020-68-7]

$HC{\equiv}CC{\equiv}CCH(OH)CH{=}CH(CH_2)_7CH_2OH$

$C_{15}H_{22}O_2$ 234.338
Isol. from *Solanum melongena* (aubergine) calluses.

Japan. Pat., 1986, 86 221 140; *CA*, **106**, 194797r (*isol*)

9-Pentadecenoic acid P-83

[15451-50-0]

[26444-04-2]

$H_3C(CH_2)_4CH{=}CH(CH_2)_7COOH$

$C_{15}H_{28}O_2$ 240.385
Occurs in animal fat.

(*Z*)-*form*

[29255-62-7]
$Bp_{0.5}$ 152-153°.

Me ester: [14101-90-7]
$C_{16}H_{30}O_2$ 254.412
Bp_2 134-138°.

Et ester: [56219-09-1]
$C_{17}H_{32}O_2$ 268.439
$Bp_{0.01}$ 109°.

Vaver, V.A. *et al., Izv. Akad. Nauk Kaz. SSR, Ser. Khim.*, 1966, 2241; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1966, 2178 (*synth*)
Sen Gupta, A.K. *et al., Chem. Phys. Lipids*, 1969, **3**, 371 (*Me ester*)

Pentadecylbenzene, 9CI P-84

[2131-18-2]
1-Phenylpentadecane

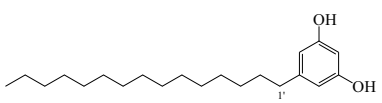
$Ph(CH_2)_{14}CH_3$

$C_{21}H_{36}$ 288.515
Rather poorly documented. Constit. of the mussel (*Mytilus galloprovincialis*).

U.K. Pat., 1961, 884 700; *CA*, **57**, 4591b (*synth*)
Mironov, O.G. *et al., CA*, 1991, **114**, 161123 (*isol*)

5-Pentadecyl-1,3-benzenediol, 9CI P-85

[3158-56-3]
5-Pentadecylresorcinol. ***Adipostatin A***. *Cardol*



$C_{21}H_{36}O_2$ 320.514
Isol. from cereals and other plants. Cryst. (petrol or C_6H_6). Mp 95.5-96° (91-92°). λ_{max} 221 (sh) (ε 7000); 272 (ε 1590); 278 (ε 1570) (MeOH) (Derep).

8′,9′Z-Didehydro: [22910-86-7] *5-(8-Pentadecenyl)-1,3-benzenediol*. ***Bilobol***. *Trifurcatol A_2*. *Cardolmonoene*
$C_{21}H_{34}O_2$ 318.498
Isol. from *Ginkgo biloba* (ginkgo) fruits. Cryst. (pentane). Mp 36-37°.

8′,9′Z,11′,12′Z-Tetradehydro: [79473-25-9] *5-(8,11-Pentadecadienyl)-1,3-benzenediol*. ***Cardol***. *Cardoldiene*
$C_{21}H_{32}O_2$ 316.483
Isol. from *Anacardium occidentale*

(cashew). Mp 55-55.5° as di-Ac. The name Cardol is also used for the mixt. of phenols differing in hydrogenation level in the side chain.

▶ Irritant, sensitiser.

8′,9′Z,11′,12′Z,14,15-Hexadehydro: [79473-24-8]

[111047-32-6] *5-(8,11,14-Pentadecatrienyl)-1,3-benzenediol.* ***Cardoltriene***
$C_{21}H_{30}O_2$ 314.467
Constit. of *Anacardium occidentale* (cashew). Liq.

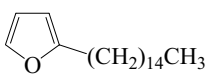
▶ Irritant, sensitiser.

2′-Oxo: [209901-15-5] *1-(3,5-Dihydroxyphenyl)-2-pentadecanone. 5-(2-Oxopentadecyl)-1,3-benzenediol*
$C_{21}H_{34}O_3$ 334.498
Isol. from etiolated rice seedlings.

Ridley, D.D. *et al., Aust. J. Chem.*, 1968, **21**, 2979 (*synth*)
Cirigottis, K.A. *et al., Aust. J. Chem.*, 1974, **27**, 345 (*Bilobol*)
Tyman, J.H.P. *et al., Chem. Soc. Rev.*, 1979, **8**, 499 (*rev*)
Baylis, C.J. *et al., J.C.S. Perkin 1*, 1981, 132 (*isol, pmr, synth, Cardol, Cardoltriene*)
Tsuge, N. *et al., J. Antibiot.*, 1992, **45**, 886 (*isol, pmr, cmr, props*)
Lytollis, W. *et al., J.A.C.S.*, 1995, **117**, 12683 (*isol, synth, Bilobol*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995, (*bibl*)
Fuerstner, A. *et al., J.O.C.*, 1997, **62**, 2332 (*synth*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 889

2-Pentadecylfuran P-86

[59958-20-2]

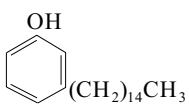


$C_{19}H_{34}O$ 278.477
Constit. of *Persea americana* (avocado).

Rodriguez-Saona, C.R. *et al., J. Chem. Ecol.*, 1998, **24**, 867-889 (*isol*)
Rodriguez-Saona, C.R. *et al., J. Nat. Prod.*, 1999, **62**, 191-193 (*synth, activity*)

3-Pentadecylphenol P-87

[501-24-6]
1-Hydroxy-3-pentadecylbenzene. Cyclogallipharol. Hydroginkgol. Hydrocardanol. Anacardol. Cardanol $C_{15:0}$



$C_{21}H_{36}O$ 304.515
Minor constit. of lipids of *Anacardium occidentale* (cashew nut). Cryst. (petrol). Mp 54.5°. $Bp_{1.5}$ 197°.

Ac: [52122-74-4]
$C_{23}H_{38}O_2$ 346.552
Mp 42°.

Benzoyl:
$C_{28}H_{40}O_2$ 408.623
Mp 54°.

Me ether:1-Methoxy-3-pentadecylbenzene
$C_{22}H_{38}O$ 318.542
Mp 29-30°. Bp_{15} 240-244° $Bp_{1.5}$ 175-177°.

8′,9′-Didehydro(Z-): [501-26-8] *3-(8-Pentadecenyl)phenol. Cardanol$_{15:1}$. Anacardol. Ginkgol. Cardanolmonoene*
Major constit. of lipids of *Anacardium occidentale* (cashew nut). Isol. from fruit of *Ginkgo biloba* (ginkgo). Oil. Bp_4 221-223°. Log P 8.9 uncertain value (calc).

10,11ξ-Didehydro:3-(10-Pentadecenyl)-phenol
$C_{21}H_{34}O$ 302.499

8′,9′,11′,12′-Tetradehydro (Z,Z-): [51546-63-5] *3-(8,11-Pentadecadienyl)phenol.* ***Cardanoldiene***
$C_{21}H_{32}O$ 300.483
Minor component of lipids of *Anacardium occidentale* (cashew nut). Oil.

8′,9′,11′,12′,14′,15′-Hexadehydro (Z,Z,Z-): [79353-39-2] *3-(8,11,14-Pentadecatrienyl)phenol*
$C_{21}H_{30}O$ 298.467
Constit. of lipids of *Anacardium occidentale* (cashew nut).

▶ Irritant.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 871D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1074B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1006B (*ir*)
Prelog, V. *et al., Helv. Chim. Acta*, 1947, **30**, 675 (*synth*)
Kaufmann, H.P. *et al., Fette, Seifen, Anstrichm.*, 1967, **69**, 437 (*isol*)
Tyman, J.H.P. *et al., Chem. Soc. Rev.*, 1979, **8**, 499 (*rev*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995, (*bibl*)
Franke, K. *et al., Planta Med.*, 2001, **67**, 477-479 (*10,11-didehydro*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 889

2,4-Pentadienal, 9CI P-88

[764-40-9]
FEMA 3217
$H_2C{=}CHCH{=}CHCHO$
C_5H_6O 82.102
Flavouring ingredient.

(E)-form [20432-40-0]
Bp_{10} 30°. λ_{max} 250 (ε 34400) (no solvent reported).

2,4-Dinitrophenylhydrazone:
Mp 176-177°.

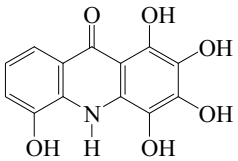
(Z)-form [37918-47-1]
Bp_{10} 29-30°. λ_{max} 260 (ε 19100) (no solvent reported).

2,4-Dinitrophenylhydrazone:
Orange-red needles. Mp 150-151°.

Woods, G.F. *et al., J.A.C.S.*, 1946, **68**, 2483 (*synth*)
Cookson, R.C. *et al., Chem. Comm.*, 1978, 924 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 637
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2114-2115

1,2,3,4,5-Pentahydroxyacridone P-89

*1,2,3,4,5-Pentahydroxy-9*H*-acridin-9-one*



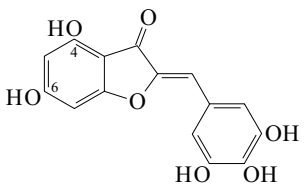
$C_{13}H_9NO_6$ 275.217

2,3,4-Tri-Me ether, N*-Me:* [86680-34-4] *1,5-Dihydroxy-2,3,4-trimethoxy-10-methylacridone.* ***Citbrasine***
$C_{17}H_{17}NO_6$ 331.324
Alkaloid from the root bark of *Citrus sinensis* var. *brasiliensis* (navel orange). Red plates (Et_2O). Mp 154-156°.

Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1983, **31**, 901 (*isol, uv, ir, pmr, ms, struct*)

3′,4,4′,5′,6-Pentahydroxyaurone P-90

[3260-50-2]
*4,6-Dihydroxy-2-(3,4,5-trihydroxybenzylidene)-3(*2H*)-benzofuranone, 8CI.* ***Bracteatin***



$C_{15}H_{10}O_7$ 302.24
Orange needles (MeOH aq.). Mp 350° dec. approx.

Penta-Ac:
Pale-yellow needles (MeOH). Mp 225-235° dec.

4-O-β-D-Glucopyranoside: [22684-08-8] ***Bractein***
$C_{21}H_{20}O_{12}$ 464.382
Mp 245° dec.

6-O-β-D-Glucopyranoside: [7056-91-9] ***Bracteatin 6-glucoside***
$C_{21}H_{20}O_{12}$ 464.382

4-Me ether: [66274-46-2] *3′,4′,5′,6-Tetrahydroxy-4-methoxyaurone. Subulaurone*
$C_{16}H_{12}O_7$ 316.267
Cryst. (EtOAc/EtOH). Mp 320° dec.

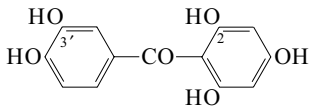
4-Me ether, 6-O-[α-L-rhamnopyranosyl(1→4)-β-D-glucopyranoside]: [66274-45-1] ***Subulin***
$C_{28}H_{32}O_{16}$ 624.551
Isol. from seeds of *Amomum subulatum* (Nepal cardamom). Yellow cryst. ($EtOAc/Et_2O$). Mp 178°.

Hänsel, R. *et al., Tet. Lett.*, 1962, 599 (*struct, uv*)
Hänsel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1963, **296**, 619 (*synth, ir, uv*)
Harborne, J.B. *et al., Phytochemistry*, 1963, **2**, 237; 1966, **5**, 111 (*isol*)
Huke, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1969, **302**, 401; 423 (*pmr, synth, uv*)
Gilbert, R.I. *et al., Phytochemistry*, 1975, **14**, 1461 (*6-Glucoside*)

Lakshmi, V. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 814 (*Subulin*)
Weitz, S. *et al., Phytochemistry*, 1977, **16**, 1108 (*isol*)

2,3′,4,4′,6-Pentahydroxybenzophenone, 8CI P-91

[519-34-6]
(3,4-Dihydroxyphenyl)(2,4,6-trihydroxyphenyl)methanone, 9CI. ***Maclurin***. *Moringerbic acid*. *Laguncurin*



$C_{13}H_{10}O_6$ 262.218
Extract from heartwood of *Garcinia mangostana* (mangosteen). Also from *Morus alba* (white mulberry). Yellowish prisms (H_2O). Mp 222-222.5°.

2,4,6-Tri-Me ether:3′,4′-Dihydroxy-2,4,6-trimethoxybenzophenone. ***Cotogenin***
$C_{16}H_{16}O_6$ 304.299
Leaflets (EtOH). Mp 217°.

Penta-Me ether: [58262-60-5] *2,3′,4,4′,6-Pentamethoxybenzophenone*
$C_{18}H_{20}O_6$ 332.352
Pale-yellow needles (MeOH). Mp 165-166° (156.8-157.2°).

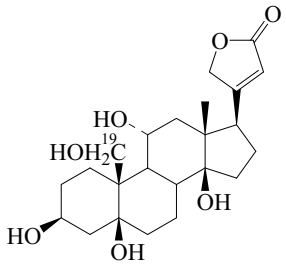
3′,4′-Methylene, 2,4-di-Me ether:2-Hydroxy-4,6-dimethoxy-3′,4′-methylenedioxybenzophenone. ***Protocotoin***
$C_{16}H_{14}O_6$ 302.283
Prisms (MeOH). Mp 141-142°.

3′,4′-Methylene, 2,4,6-tri-Me ether:2,4,6-Trimethoxy-3′,4′-methylenedioxybenzophenone. ***Methylprotocotoin***. *Oxyleucotin*
$C_{17}H_{16}O_6$ 316.31
Prisms (EtOH). Mp 133-135°.

2,3′,4-Tri-Me ether: [156640-26-5] *2,4′-Dihydroxy-3′,4,6-trimethoxybenzophenone*
$C_{16}H_{16}O_6$ 304.299

Ciamician, G. *et al., Ber.*, 1892, **25**, 1119; 1124 (*Protocotoin*)
Späth, E. *et al., Monatsh. Chem.*, 1928, **49**, 429 (*synth*)
Houben, J. *et al., J. Prakt. Chem.*, 1929, **123**, 89 (*synth*)
Haley, T.J. *et al., J. Am. Pharm. Assoc.*, 1951, **40**, 111 (*isol*)
Jefferson, A. *et al., Nature (London)*, 1965, **207**, 1193
Locksley, H.D. *et al., Tetrahedron*, 1967, **23**, 2229 (*isol*)
Atkinson, J.E. *et al., J.C.S.(C)*, 1969, 281 (*uv, ir*)
Holloway, D.M. *et al., Phytochemistry*, 1975, **14**, 2517 (*isol*)
Minami, H. *et al., Phytochemistry*, 1994, **36**, 501 (*2,3′,4-tri-Me ether*)

3,5,11,14,19-Pentahydroxycard-20(22)-enolide P-92

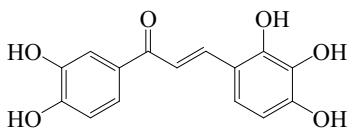


$C_{23}H_{34}O_7$ 422.517
(3β,5β,11α,14β)-*form*
3-O-(6-Deoxy-β-D-gulopyranoside): [82228-15-7] ***Canesceol***
$C_{29}H_{44}O_{11}$ 568.66
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA.
19-Aldehyde, 3-O-(6-deoxy-β-D-gulopyranoside): [22333-73-9] ***Canescein***
$C_{29}H_{42}O_{11}$ 566.644
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Amorph. Mp 192-194°. $[\alpha]_D^{24}$ +4.6 (MeOH).

Buchvarov, Y. *et al., CA*, 1985, **102**, 42839k (*Canesceol*)
Ankli, A. *et al., Phytochemistry*, 2000, **54**, 531-537 (*Canescein*)

2,3,3′,4,4′-Pentahydroxychalcone P-93

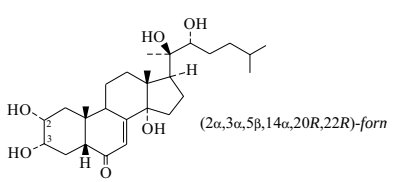
1-(3,4-Dihydroxyphenyl)-3-(2,3,4-trihydroxyphenyl)-2-propen-1-one



$C_{15}H_{12}O_6$ 288.256
(*E*)-*form*
2-Me ether: [197227-39-7] *3,3′,4,4′-Tetrahydroxy-2-methoxychalcone*
$C_{16}H_{14}O_6$ 302.283
Constit. of licorice (*Glycyrrhiza* sp.). Yellow needles. Mp 196°. λ_{max} 208 (log ε 4.43); 258 (log ε 3.97); 367 (log ε 4.27) (MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1485-1492

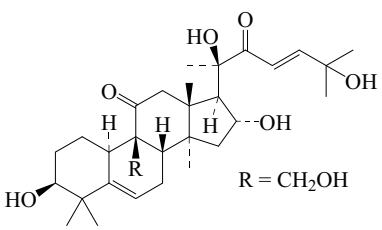
2,3,14,20,22-Pentahydroxycholest-7-en-6-one P-94



$C_{27}H_{44}O_6$ 464.641
(2α,3α,5β,14α,20*R*,22*R*)-*form* [19338-77-3]
Ponasterone B
Noncryst.
2,3,22-Tri-Ac:
Cryst. Mp 128-130°.
(2β,3β,5β,14α,20*R*,22*R*)-*form* [13408-56-5]
Ponasterone A
Cryst. (EtOH). Mp 259-260° dec. $[\alpha]_D^{15}$ +90 (MeOH). λ_{max} 244 (ε 12400); 326 (ε 130) (MeOH) (Berdy).
3-O-β-D-Xylopyranoside: ***Limnantheoside B***
$C_{32}H_{52}O_{10}$ 596.757
Gum. λ_{max} 242 (log ε 4) (no solvent reported).
3-O-β-D-Glucopyranoside: [20117-33-3] ***Ponasteroside A***. *Warabisterone*
$C_{33}H_{54}O_{11}$ 626.783
Isol. from *Pteridium aquilinum* (bracken fern). Cryst. Mp 278-279.5°. $[\alpha]_D$ +28.5 (Py).

Hüppi, G. *et al., Tet. Lett.*, 1968, 1113 (*synth*)
Nakanishi, K. *et al., Bull. Soc. Chim. Fr.*, 1969, 3475
Hikino, H. *et al., Phytochemistry*, 1970, **9**, 367 (*biosynth*)
Koreeda, M. *et al., J.A.C.S.*, 1971, **93**, 4085 (*abs config*)
Takemoto, T. *et al., Chem. Pharm. Bull.*, 1973, **21**, 2336 (*isol*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 125 (*cmr*)
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*occur*)
Sarker, S.D. *et al., Phytochemistry*, 1997, **44**, 513 (*Limnatheoside B*)
Vokác, K. *et al., Phytochemistry*, 1998, **49**, 2109-2114 (*Ponasterone A, pmr, cmr*)

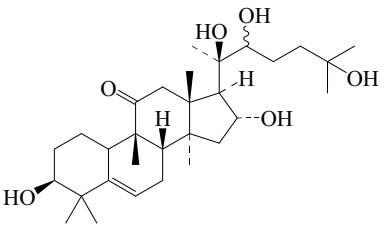
3,16,19,20,25-Pentahydroxycucurbita-5,23-diene-11,22-dione P-95



$C_{30}H_{46}O_7$ 518.689
λ_{max} 231 (ε 11000); 298 (ε 11310) (MeOH) (Berdy).
▶ RC6160000
(3β,16α,20*R*,23*E*)-*form*
25-Ac: [5988-76-1] ***Cucurbitacin C***
$C_{32}H_{48}O_8$ 560.726
Constit. of Cucurbitaceae, e.g. *Cucumis sativus* (cucumber). Cryst. (EtOAc). Mp 207.5°. $[\alpha]_D$ +95.2 (EtOH).

de Kock, W.T. *et al., J.C.S.*, 1963, 3828 (*struct*)
Audier, H.E. *et al., Tet. Lett.*, 1966, 2205 (*ms*)
Bull, J.R. *et al., S. Afr. J. Chem.*, 1979, **32**, 27 (*cmr*)
Che, C.-T. *et al., J. Nat. Prod.*, 1985, **24**, 429 (*pmr*)

3,16,20,22,25-Pentahydroxy-5-cucurbiten-11-one P-96



$C_{30}H_{50}O_6$ 506.721

(3β,16α,20*R*)-*form*

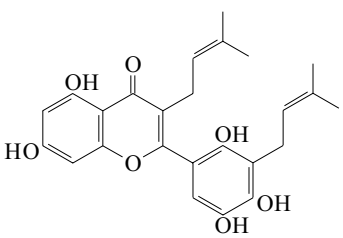
3-O-*[α-L-Rhamnopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]:* [251102-63-3]
$C_{48}H_{80}O_{20}$ 977.148
Constit. of *Cyclanthera pedata* (achoccha).

3-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [178062-94-7]
$C_{42}H_{70}O_{16}$ 831.005
Constit. of *Cyclanthera pedata* (achoccha). $[\alpha]_D^{25}$ +25 (c, 1 in MeOH).

25-Ac, 3-O-*β-D-glucopyranoside:* [178062-95-8]
$C_{38}H_{62}O_{12}$ 710.901
Constit. of *Cyclanthera pedata* (achoccha). $[\alpha]_D^{25}$ +3 (c, 1 in MeOH).

De Tommasi, N. *et al., J. Agric. Food Chem.*, 1996, **44**, 2020-2025; 1999, **47**, 4512-4519 (*isol, pmr, cmr*)

2′,4′,5,5′,7-Pentahydroxy-3,3′-diprenylflavone P-97



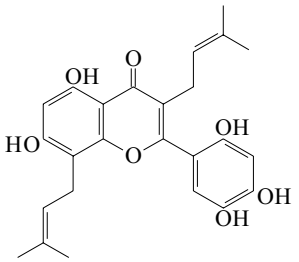
$C_{25}H_{26}O_7$ 438.476

4′-Me ether: [170894-23-2] *2′,5,5′,7-Tetrahydroxy-4′-methoxy-3,3′-diprenylflavone.* ***Heteroartonin A***
$C_{26}H_{28}O_7$ 452.503
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Yellow plates (C_6H_6). Mp 206-208°.

Chung, M.-I. *et al., Phytochemistry*, 1995, **40**, 1279 (*isol, pmr, cmr*)

2′,4′,5,5′,7-Pentahydroxy-3,8-diprenylflavone P-98

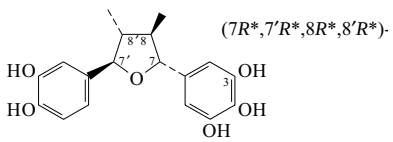
[158642-43-4]
*5,7-Dihydroxy-3,8-bis(3-methyl-2-butenyl)-2-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Artonin V***



$C_{25}H_{26}O_7$ 438.476
Constit. of the root bark of *Artocarpus altilis* (breadfruit). Pale yellow needles (hexane/Et_2O). Mp 85-87°. λ_{max} 206 ; 263 ; 301 ; 341 (MeOH).

Hano, Y. *et al., J. Chem. Res., Synop.*, 1994, 348 (*isol, ir, uv, pmr, cmr*)

3,3′,4,4′,5-Pentahydroxy-7,7′-epoxylignan P-99



$C_{18}H_{20}O_6$ 332.352

(7*R,7′*R**,8*R**,8′*R**)-*form***

3,3′,5-Tri-Me ether: [112572-54-0] ***Fragransin C2***
$C_{21}H_{26}O_6$ 374.433
Isol. from *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +20.2 (c, 0.11 in $CHCl_3$).

(7*R,7′*S**,8*S**,8′*S**)-*form***

3,3′,4′,5-Tetra-Me ether: [114422-24-1] ***Fragransin D3***
$C_{22}H_{28}O_6$ 388.46
Constit. of *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +11.45 (c, 0.262 in $CHCl_3$).

3,3′,5-Tri-Me ether: [112503-91-0] ***Fragransin C3b***
From *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +7.2 (c, 0.24 in $CHCl_3$).

(7*R,7′*S**,8*S**,8′*R**)-*form***

3,3′,4,5-Tetra-Me ether: [114422-23-0] ***Fragransin D2***
$C_{22}H_{28}O_6$ 388.46
Constit. of *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +30.49 (c, 0.106 in $CHCl_3$).

(7*R,7′*S**,8*R**,8′*R**)-*form***

3,3′,5-Tri-Me ether: [112572-53-9] ***Fragransin C3a***
$C_{21}H_{26}O_6$ 374.433
From *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +19.6 (c, 0.29 in $CHCl_3$).

(7*R,7′*S**,8*R**,8′*S**)-*form***

3,3′,5-Tri-Me ether: [112572-57-3] *4,4′-Dihydroxy-3,3′,5-trimethoxy-7,7′-epoxylignan.* ***Fragransin C1****. Machilin H*
$C_{21}H_{26}O_6$ 374.433
Isol. from *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +3.8 (c, 0.60 in $CHCl_3$). $[\alpha]_D$ +8.8 (c, 0.37 in $CHCl_3$).

3,3′,4,5-Tetra-Me ether: [114394-21-7] *4′-Hydroxy-3,3′,4,5-tetramethoxy-7,7′-epoxylignan.* ***Fragransin D1***
$C_{22}H_{28}O_6$ 388.46
Constit. of *Myristica fragrans* (nutmeg). Oil. $[\alpha]_D$ +18.38 (c, 0.136 in $CHCl_3$).

(7*S*,7′*R*,8*S*,8′*S*)-*form*

Penta-Me ether:3,3′,4,4′,5-Pentamethoxy-7,7′-epoxylignan
$C_{23}H_{30}O_6$ 402.486
Yellow oil. $[\alpha]_D$ +16 (c, 0.1 in $CHCl_3$).

(7*S*,7′*S*,8*S*,8′*S*)-*form*

3,4,5-Tri-Me, 3′,4′-methylene ether:3,4,5-Trimethoxy-3′,4′-methylenedioxy-7,7′-epoxylignan
$C_{22}H_{26}O_6$ 386.444
Yellow oil. $[\alpha]_D$ -10 (c, 0.02 in $CHCl_3$).

Penta-Me ether:
$C_{23}H_{30}O_6$ 402.486
Oil. $[\alpha]_D$ -12.6 (c, 0.1 in $CHCl_3$).

(7*R,7′*R**,8*R**,8′*S**)-*form***

3,4,5-Tri-Me, 3′,4′-methylene ether: [107783-46-0] ***Henricine***
$C_{22}H_{26}O_6$ 386.444
Cryst. Mp 73-75°. $[\alpha]_D^{21}$ +102 ($CHCl_3$).

Lian-niang, L. *et al., Planta Med.*, 1986, 493-494 (*Henricine*)

Hattori, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3315

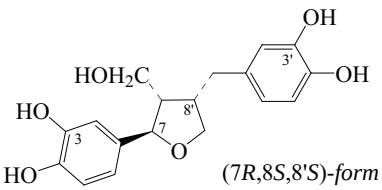
Hada, S. *et al., Phytochemistry*, 1988, **27**, 563

Shimomura, H. *et al., Phytochemistry*, 1988, **27**, 634

Lopes, N.P. *et al., Phytochemistry*, 1996, **43**, 1089

3,3′,4,4′,9-Pentahydroxy-7,9′-epoxylignan P-100

Tetrahydro-2-(3,4-dihydroxyphenyl)-4-[(3,4-dihydroxyphenyl)methyl]-3-furanmethanol, 9CI



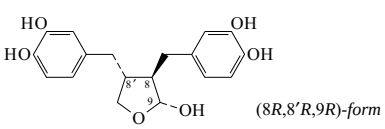
$C_{18}H_{20}O_6$ 332.352

(7ξ,8ξ,8′ξ)-*form*

3′,4′-Methylene, 3-Me ether: [54854-91-0] *4,9-Dihydroxy-3-methoxy-3′,4′-methylenedioxy-7,9′-epoxylignan.* ***Sanshodiol***
$C_{20}H_{22}O_6$ 358.39
Isol. from bark of *Zanthoxylum piperitum* (Japanese pepper tree). Needles. Mp 140-141°. $[\alpha]_D$ -14.4 (c, 1.0 in $CHCl_3$).

Abe, F. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2650 (*Sanshodiol*)

3,3′,4,4′,9-Pentahydroxy-9,9′-epoxylignan P-101



$C_{18}H_{20}O_6$ 332.352

(8*R*,8′*R*,9*R*)-*form*

3,4-Methylene, 3′,4′-di-Me ether: [67533-86-2] *9-Hydroxy-3′,4′-dimethoxy-3,4-methylenedioxy-9,9′-epoxylignan. 3′,4′-*

Dimethoxy-3′,4′-desmethylenecubebin
$C_{21}H_{24}O_6$ 372.417
Constit. of *Piper nigrum* (pepper). Cryst. (C_6H_6/hexane). Mp 66°. $[\alpha]_D^{25}$ -15.9 (c, 0.2 in $CHCl_3$).

3′,4′-Methylene, 3,4-di-Me ether: [77533-71-2]

[210161-38-9] *3,4-Dimethoxy-3,4-desmethylenecubebin*
$C_{21}H_{24}O_6$ 372.417
Constit. of *Piper chaba* (Javanese long pepper), *Piper nigrum* (pepper). Needles (C_6H_6/hexane). Mp 89-91°. $[\alpha]_D^{25}$ -52.9 (c, 0.3 in $CHCl_3$).

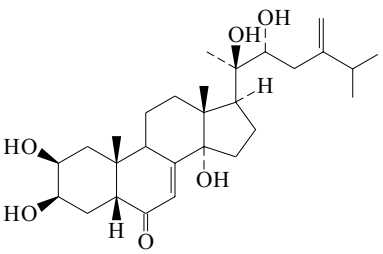
(8R,8′R,9S)-form

3′,4′-Methylene, 3,4-di-Me ether:
Constit. of *Piper chaba* (Javanese long pepper).

Ruecker, G. *et al., Planta Med.*, 1981, **41**, 143-149 (*Dimethoxydesmethylenecubebins*)
Sumathykutty, M.A. *et al., Indian J. Chem., Sect. B*, 1988, **27**, 388-389 (*Dimethoxydesmethylenecubebins*)
Conserva, L.M. *et al., Phytochemistry*, 1990, **29**, 257 (*isol*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1994, **57**, 713
Vidigal, M.C.S. *et al., Phytochemistry*, 1995, **40**, 1259 (*isol*)
Bhandari, S.P.S. *et al., Phytochemistry*, 1998, **47**, 1435-1436 (*3,4-di-Me 3′,4′-methylene ether*)
Da Silva, A.P.F. *et al., J. Braz. Chem. Soc.*, 1999, **10**, 122-126

2,3,14,20,22-Pentahydroxyergosta-7,24(28)-dien-6-one P-102

2,3,14,20,22-Pentahydroxy-24-methylenecholest-7-en-6-one



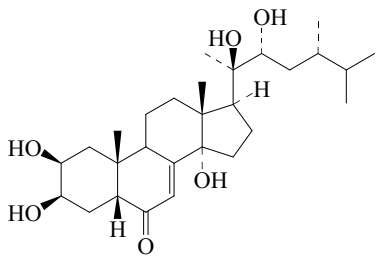
$C_{28}H_{44}O_6$ 476.652

(2β,3β,5β,14α,20*R*,22*R*)-*form* [141360-89-6]
Polyporusterone B
Constit. of *Polyporus umbellatus* (zhu ling). Needles (MeOH). Mp 250°. $[\alpha]_D^{20}$ +56.1 (c, 0.46 in EtOH).

Ohsawa, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 143 (*isol, pmr, cmr*)

2,3,14,20,22-Pentahydroxyergost-7-en-6-one P-103

2,3,14,20,22-Pentahydroxy-24-methylcholest-7-en-6-one



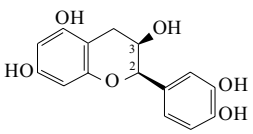
$C_{28}H_{46}O_6$ 478.668

(2β,3β,5β,14α,20*R*,22*R*,24*S*)-*form* [141360-88-5]
Polyporusterone A
Constit. of *Polyporus umbellatus* (zhu ling). Needles (MeOH). Mp 261.5°. $[\alpha]_D^{20}$ +52.9 (c, 0.61 in EtOH).

Ohsawa, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 143-147 (*isol, pmr, cmr*)
Ishida, H. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1626-1628 (*isol, pmr, cmr, cryst struct*)

3,3′,4′,5,7-Pentahydroxyflavan P-104

[13392-26-2]
2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol, 9CI. 3′,4′,5,7-Tetrahydroxyflavanol



(2*R*,3*R*)-*form*

$C_{15}H_{14}O_6$ 290.272

(2*R*,3*R*)-*form* [490-46-0]

[321-01-7]
(-)-cis-*form*. ***Epicatechin***. *Epicatechol. Teacatechin I. Acacatechin. Kakaol. Colatein*
Widespread flavanol found in a variety of foodstuffs esp. apples, apricots, blackberries, broad beans, cherries, chocolate, grapes, raspberries, red wine, strawberries and tea. Cryst. Mp 242°. $[\alpha]_D$ -68 (EtOH). Log P 0.38 (uncertain value) (calc). λ_{max} 281 (MeOH) (Berdy).

▶ KB3745000

3-O-β-D-Glucopyranoside: [103303-00-0] *Epicatechin 3-glucoside*
$C_{21}H_{24}O_{11}$ 452.414
Isol. from Chinese cinnamon (*Cinnamomum cassia*) bark. Off-white powder + $1H_2O$. $[\alpha]_D$ -71.5 (c, 1 in MeOH).

3-O-(4-Hydroxybenzoyl): [108907-45-5] *3-(4-Hydroxybenzoyl)epicatechin*
$C_{22}H_{18}O_8$ 410.379
Isol. from oolong tea (*Camellia sinensis* var. *assamica*). Off-white powder + $1H_2O$. $[\alpha]_D^{21}$ -144.4 (c, 1 in Me_2CO).

3-O-(3,4,5-Trihydroxybenzoyl): [1257-08-5]

[863-03-6] *3-O-Galloylepicatechin. Epicatechin gallate. Teatannin*
$C_{22}H_{18}O_{10}$ 442.378
Isol. from tea and numerous other plant spp. inc. rhubarb and grapes. Mp 257-258° (253°). $[\alpha]_D$ -190 (EtOH). $[\alpha]_D^{23}$ -160.6 (c, 0.22 in Me_2CO). Log P 1.83 (uncertain value) (calc).

▶ DH9030000

3-O-(3,4-Dihydroxy-5-methoxybenzoyl): [83104-86-3] *3-O-(3-Methylgalloyl)epicatechin*
$C_{23}H_{20}O_{10}$ 456.405
Isol. from green China tea (*Camellia sinensis*) leaves. $[\alpha]_D^{14}$ -168 (c, 1 in EtOH).

3-O-(3,5-Dihydroxy-4-methoxybenzoyl): [108907-44-4] *3-O-(4-Methylgalloyl)epicatechin*
$C_{23}H_{20}O_{10}$ 456.405
Isol. from *Camellia sinensis* var. *assamica* (coml. oolong tea). Off-white powder + $^2/_3H_2O$. $[\alpha]_D^{22}$ -160.1 (c, 1.1 in Me_2CO).

3,5-Bis(3,4,5-trihydroxybenzoyl): [37484-74-5] *3,5-Digalloylepicatechin*
$C_{29}H_{22}O_{14}$ 594.484
Constit. of green tea leaves. Amorph. powder. $[\alpha]_D$ -9 (EtOH).

(2*R*,3*S*)-*form* [154-23-4]
(+)-trans-*form*. ***Catechin***†. *Catechol*†. *Cianidanol, INN, JAN. Dexcyanidanol. Cianidol. Catergen. Drenoliver. Biocatechin. Tanningenic acid. Cyanidol*†. *Gambircatechin. Catechuic acid*
Present in red wine. Widespread in plants; found in a variety of foodstuffs esp. apricots, broad beans, cherries, chocolate, grapes, nectarines, red wine, rhubarb, strawberries and tea. Cryst. + $4H_2O$ (AcOH aq.). Mp 93-96° Mp 175-177° (anhyd.). $[\alpha]_D$ +17. Log P 0.38 (uncertain value) (calc). Not to be confused with 1,2-Benzenediol.

▶ Severe and occasionally fatal haemolytic anaemia reported when used therapeutically. LD_{50} (mus, ipr) 1000 mg/kg. Exp. reprod. and teratogenic effects. DJ3450000

5-O-β-D-Glucopyranoside: [88126-53-8] *Catechin 5-glucoside*
$C_{21}H_{24}O_{11}$ 452.414
Isol. from commercial rhubarb *Rheum* spp.. Needles + $2H_2O$ (MeOH aq.). Mp 203-204°. $[\alpha]_D$ -28.8 (c, 1 in MeOH).

7-O-β-D-Glucopyranoside: [65597-47-9] *Catechin 7-glucoside*
$C_{21}H_{24}O_{11}$ 452.414
Isol. from commercial rhubarb (*Rheum* spp.,) and azuki bean (*Vigna angularis*). Needles + $1^1/_2H_2O$ ($CHCl_3$/MeOH). Mp 214-216°. $[\alpha]_D^{32}$ -33.4 (c, 1 in MeOH).

3′-O-β-D-Glucopyranoside: [105330-51-6] *Catechin 3′-glucoside*
$C_{21}H_{24}O_{11}$ 452.414
Isol. from *Rheum* spp. roots. Powder + $1H_2O$. $[\alpha]_D^{23}$ -39.3 (c, 0.6 in MeOH).

4′-O-β-D-Glucopyranoside: [105330-52-7] *Catechin 4′-glucoside*
$C_{21}H_{24}O_{11}$ 452.414
Isol. from commercial rhubarb (*Rheum* spp.). Powder + $1H_2O$. $[\alpha]_D^{22}$ -34 (c, 0.59 in MeOH).

3′,4′-Di-O-β-D-glucopyranoside: [105330-

55-0] *Catechin 3′,4′-diglucoside*
$C_{27}H_{34}O_{16}$ 614.556
Isol. from commercial rhubarb *Rheum* spp.. Powder + 1½H_2O. $[\alpha]_D^{29}$ -48.2 (c, 0.53 in MeOH).

3′,5-Di-O-*β-D-glucopyranoside:* [105330-54-9] *Catechin 3′,5-diglucoside*
$C_{27}H_{34}O_{16}$ 614.556
Isol. from commercial rhubarb *Rheum* spp.. Powder + 1½H_2O. $[\alpha]_D^{29}$ -48.2 (c, 0.53 in MeOH).

3′,7-Di-O-*β-D-glucopyranoside:* [105330-53-8] *Catechin 3′,7-diglucoside*
$C_{27}H_{34}O_{16}$ 614.556
Isol. from commercial rhubarb *Rheum* spp.. Powder + 1½H_2O. $[\alpha]_D^{29}$ -67.4 (c, 0.63 in MeOH).

4′,5-Di-O-*β-D-glucopyranoside:* [105330-56-1] *Catechin 4′,5-diglucoside*
$C_{27}H_{34}O_{16}$ 614.556
Isol. from commercial rhubarb (*Rheum* spp.). Powder + 3½H_2O. $[\alpha]_D^{18}$ -46.8 (c, 0.19 in MeOH).

3-O-*(3,4,5-Trihydroxybenzoyl):* [25615-05-8] *3-Galloylcatechin*
$C_{22}H_{18}O_{10}$ 442.378
Constit. of *Bergenia crassifolia* (Siberian tea). Amorph. Sol. MeOH. $[\alpha]_D^{26}$ +56 (c, 0.9 in EtOH). λ_{max} 278 (MeOH) (Berdy).

7-O-*(3,4,5-Trihydroxybenzoyl):* [89702-01-2] *7-Galloylcatechin*
$C_{22}H_{18}O_{10}$ 442.378
Isol. from roots of great burnet (*Sanguisorba officinalis*). Needles + 1½H_2O (H_2O). Mp 165-168°. $[\alpha]_D$ +38.9 (c, 0.81 in Me_2CO).

3-O-*(1,6-Dihydroxy-2-cyclohexene-1-carboxylate):* [99257-73-5]
$C_{22}H_{22}O_9$ 430.41
Powder. $[\alpha]_D^{26}$ -87.1 (c, 0.9 in Me_2CO).

3′-Me ether: ***3′-O-Methylcatechin***
$C_{16}H_{16}O_6$ 304.299
Constit. of *Pinus sylvestris* (Scotch pine). $[\alpha]_D$ +21.4 (c, 0.3 in Me_2CO aq.).

4′-Me ether: [69912-75-0] *3,3′,5,7-Tetrahydroxy-4′-methoxyflavan.* ***4′-O-Methylcatechin***
$C_{16}H_{16}O_6$ 304.299
Constit. of Chinese cinnamon (*Cinnamomum cassia*). Needles (H_2O). Mp 152°. $[\alpha]_D^{26}$ +6.7 (c, 0.85 in Me_2CO).

4′,7-Di-Me ether: [105330-66-3] *3,3′,5-Trihydroxy-4′,7-dimethoxyflavan.* ***4′,7-Di-O-methylcatechin***
$C_{17}H_{18}O_6$ 318.326
Constit. of Chinese cinnamon (*Cinnamomum cassia*). Prisms (EtOH). Mp 142-144°. $[\alpha]_D^{26}$ -3.8 (c, 0.87 in MeOH).

4′,5,7-Tri-Me ether: [105330-59-4] *3,3′-Dihydroxy-4′,5,7-trimethoxyflavan.* *4′,5,7-Tri*-O-*methylcatechin*
$C_{18}H_{20}O_6$ 332.352
Constit. of Chinese cinnamon (*Cinnamomum cassia*) and commercial rhubarb. Needles (hexane/EtOAc). Mp 125°. $[\alpha]_D$ -8.2 (c, 1.03 in Me_2CO).

*6-Chloro:6-Chloro-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2*H-*1-benzopyran-3,5,7-triol, 9CI. 6-Chloro-3′,4′,5,7-tetrahydroxyflavanol.* ***6-Chlorocatechin***
$C_{15}H_{13}ClO_6$ 324.717
Constit. of the roots of *Rumex patientia* (patience dock). Amorph. $[\alpha]_D^{20}$ +50 (c, 0.16 in DMSO).

(2*S*,3*R*)-*form* [18829-70-4]
(-)-trans-*form.* ent-*Catechin*
Isol. in small amt. from *Acacia catechu* (black catechu), prob. as artifact of epimerisation. Needles (H_2O). Mp 175-176°. $[\alpha]_D^{20}$ -16 (c, 2 in Me_2CO aq.).

(2*RS*,3*RS*)-*form* [17334-50-8]
(±)-Epicatechin
Prisms + 4H_2O or needles + 1H_2O. Mp 224-226°.

3′,4′-Methylene, 5,7-di-Me ether: [87562-72-9]
Isol. from bark of Chinese cinnamon (*Cinnamomum cassia*). Needles (Me_2CO/hexane). Mp 162-164°. $[\alpha]_D$ -39.3 (c, 0.84 in $CHCl_3$).

[72690-97-2, 88191-48-4, 88191-49-5, 90276-13-4, 99367-40-5]

Bokaida, M.M. *et al., Proc. Chem. Soc., London*, 1960, 280 (*stereochem*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Clark-Lewis, J.W. *et al., Aust. J. Chem.*, 1968, **21**, 3025 (*ms*)
Haslam, E. *et al., J.C.S.(C)*, 1969, 1824 (*isol*)
Weinges, K. *et al., Annalen*, 1970, **234**, 46 (*deriv*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1762-1764 (*occur*)
Markham, K.R. *et al., Tetrahedron*, 1976, **32**, 2607 (*cmr*)
Takani, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 3388 (*7-glucoside*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3904-3906 (*hydroxybenzoyl derivs, oolong tea*)
Miyamura, M. *et al., Phytochemistry*, 1983, **22**, 215 (*3-Hydroxy-5,7-dimethoxy-3′,4′-methylenedioxyflavan*)
Tanaka, T. *et al., Phytochemistry*, 1983, **22**, 2575 (*7-Galloylcatechin*)
Spek, A.L. *et al., Acta Cryst. C*, 1984, **40**, 2068 (*cryst struct, Epicatechin*)
Singh, J. *et al., J. Indian Chem. Soc.*, 1984, **61**, 1044 (*props*)
Delgado, G. *et al., Phytochemistry*, 1984, **23**, 675; 1986, **34**, 633; 643 (*derivs*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2281 (*deriv*)
Elliger, C.A. *et al., Synth. Commun.*, 1985, **15**, 1315 (*synth*)
Miyata, T. *et al., Yakugaku Zasshi*, 1985, **105**, 59 (*cryst struct*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 633-642 (*cinnamon glycosides*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3208 (*glucosides*)
Porter, L.J. *et al., J. Chem. Res., Synop.*, 1986, 86 (*pmr, conformn*)
Perrissoud, D. *et al., Prog. Clin. Biol. Res.*, 1986, **213**, 559 (*rev, pharmacol*)
Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1987, **35**, 611 (*Epicatechin derivs, oolong tea*)
Ishimaru, K. *et al., Phytochemistry*, 1987, **26**, 1167 (*3-glucoside, 3-rhamnoside*)
Malan, E. *et al., Phytochemistry*, 1987, **26**, 2049; 1990, **29**, 1334; 1991, **30**, 2737 (*gallates*)
Kiehlmann, E. *et al., Magn. Reson. Chem.*, 1988, **26**, 204 (*cmr*)
Nakane, H. *et al., Biochemistry*, 1990, **29**, 2841 (*Epicatechin gallate, anti-HIV activity*)
Rossouw, W. *et al., Tetrahedron*, 1990, **50**, 12477 (*pmr, abs config*)
Urano, M. *et al., J. Het. Chem.*, 1991, **28**, 1845 (*synth*)
Lee, M.W. *et al., Phytochemistry*, 1992, **31**, 2117 (*gallates*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1353
Shen, C.-C. *et al., Phytochemistry*, 1993, **34**, 843 (*pmr, cmr*)
Mukherjee, R.K. *et al., Phytochemistry*, 1994, **37**, 1641 (*5,7-di-Me, 3′,4′-methylene ether*)
Pan, H. *et al., Phytochemistry*, 1995, **39**, 1423; 1996, **42**, 1185 (*3′-O-Methylcatechin 7-glucoside, 3′-O-Methylcatechin*)
Seto, R. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1434-1439 (*isol, pmr, cmr*)
Van Rensberg, H. *et al., Tet. Lett.*, 1997, **38**, 3089 (*synth*)
Miketova, P. *et al., J. Nat. Prod.*, 1998, **61**, 461-467 (*ms*)
Demirezer, L.O. *et al., Phytochemistry*, 2001, **58**, 1213-1217 (*6-chloro*)

3′,4,4′,5,7-Pentahydroxyflavan P-105

[24897-98-1]
*2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H-*1-benzopyran-4,5,7-triol, 9CI.* ***Luteoforol***

$C_{15}H_{14}O_6$ 290.272
Constit. of *Zea mays* (sweet corn) and *Sorghum vulgare* (sorghum).

Bate-Smith, E.C. *et al., J. Food Sci.*, 1969, **34**, 203 (*isol*)
Bate-Smith, E.C. *et al., Phytochemistry*, 1969, **8**, 1803; 1811 (*isol, synth*)
Styles, E.D. *et al., Phytochemistry*, 1975, **14**, 413 (*isol*)
Stich, K. *et al., Z. Naturforsch., C*, 1988, **43**, 311 (*isol*)

3′,4′,5′,7,8-Pentahydroxyflavan P-106

*5-(3,4-Dihydro-7,8-dihydroxy-2*H-*1-benzopyran-2-yl)-1,2,3-benzenetriol, 9CI*

$C_{15}H_{14}O_6$ 290.272

(*S*)-*form*

3′,4′,7-Tri-Me ether: [133342-96-8] *5′,8-Dihydroxy-3′,4′,7-trimethoxyflavan*
$C_{18}H_{20}O_6$ 332.352
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Needles (MeOH). Mp 153°. $[\alpha]_D^{20}$ -45.5 (c, 0.2 in $CHCl_3$). λ_{max} 245 (ε 5250); 270 (ε 1820) (MeOH) (Berdy).

3′,4′,5′,7-Tetra-Me ether: [133342-94-6] *8-Hydroxy-3′,4′,5′,7-tetramethoxyflavan*
$C_{19}H_{22}O_6$ 346.379
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Prisms (MeOH). Mp 154°. $[\alpha]_D^{20}$ -48.5 (c, 0.38 in $CHCl_3$). λ_{max} 246 (ε 6360); 271 (ε 1830) (MeOH) (Berdy).

3′,4′,7,8-Tetra-Me ether: [133342-93-5] *5′-Hydroxy-3′,4′,7,8-tetramethoxyflavan*
$C_{19}H_{22}O_6$ 346.379
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Oil. $[\alpha]_D^{20}$ -59.2 (c, 0.26 in $CHCl_3$). λ_{max} 229 (ε 14450); 274 (ε 2300) (MeOH) (Berdy).

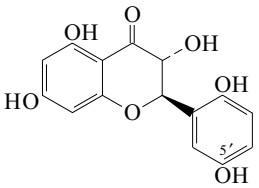
Penta-Me ether: [133342-91-3] *3′,4′,5′,7,8-Pentamethoxyflavan*
$C_{20}H_{24}O_6$ 360.406
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Oil. $[\alpha]_D^{20}$ -75 (c, 0.3 in $CHCl_3$). λ_{max} 229 (ε 15000); 274 (ε 2320) (MeOH) (Berdy).

Kaneda, N. *et al., J. Nat. Prod.*, 1991, **54**, 196

(*isol, derivs*)

2′,3,5,5′,7-Pentahydroxyflavanone P-107

*2-(2,5-Dihydroxyphenyl)-2,3-dihydro-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, 9CI. 2′,5,5′,7-Tetrahydroxydihydroflavonol*



$C_{15}H_{12}O_7$ 304.256

(2*R*,3*R*)-*form* [160389-08-2]
Needles (MeOH). Mp 242-244° (dec.). λ_{max} 211 (sh) (log ε 4.46); 292 (log ε 4.38) (MeOH).

5′-Me ether:2′,3,5,7-Tetrahydroxy-5′-methoxyflavanone
$C_{16}H_{14}O_7$ 318.282
Cryst. (EtOAc). Mp 98-100°. $[\alpha]_D^{22}$ -4.7 (c, 0.068 in MeOH). Shows unusual subn. pattern.

5′,7-Di-Me ether: [74175-80-7] *2′,3,5-Trihydroxy-5′,7-dimethoxyflavanone*
$C_{17}H_{16}O_7$ 332.309
Isol. from *Blumea balsamifera* (sambong). Cryst. ($CHCl_3$/petrol). Mp 158°.

3-O-α-L-*Rhamnopyranoside:* [157072-27-0]
$C_{21}H_{22}O_{11}$ 450.398Config. not detd..

Baruah, N.C. *et al., Phytochemistry*, 1979, **18**, 2003
Barua, N.C. *et al., Phytochemistry*, 1992, **31**, 4040 (*5′7-di-Me ether*)
Zhang, Y.Y. *et al., Chin. Chem. Lett.*, 1994, **5**, 851-854 (*isol, pmr, cmr*)
Mendez, J. *et al., Phytochemistry*, 1994, **36**, 1087 (*3-rhamnoside*)
Zhang, Y.Y. *et al., Planta Med.*, 1997, **63**, 536-539 (*isol, uv, ir, cd, pmr, cmr, ms*)

2′,4′,5,6′,7-Pentahydroxyflavanone P-108

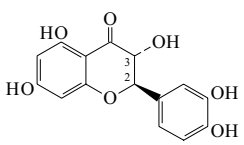
$C_{15}H_{12}O_7$ 304.256

2′,4′,6′,7-Tetra-Me ether: [151171-28-7] *5-Hydroxy-2′,4′,6′,7-tetramethoxyflavone.* ***Heteroflavanone A***
$C_{19}H_{20}O_7$ 360.363
Isol. from the root bark of *Artocarpus heterophyllus* (jackfruit). Needles. Mp 184°. $[\alpha]_D^{25}$ +7 (c, 0.1 in $CHCl_3$).

Lu, C. *et al., Phytochemistry*, 1993, **33**, 909

3,3′,4′,5,7-Pentahydroxyflavanone P-109

[98006-93-0]
*2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,5,7-Tetrahydroxydihydroflavonol. Dihydroquercetin*



(2*R*,3*R*)-*form*

$C_{15}H_{12}O_7$ 304.256Log P 0.25 (uncertain value) (calc).

▶ LK6920000

(2*R*,3*R*)-*form* [480-18-2]
(+)-trans-*form.* ***Taxifolin.*** *Taxifoliol. Distylin*
Cryst. (EtOH or H_2O). Mp 240-242° (221-222°). $[\alpha]_D^{24}$ +44 (c, 1.03 in 50% Me_2CO aq.). Log P 0.25 (uncertain value) (calc).

▶ LD_{50} (rat, ipr) 1200 mg/kg. LK6920000

3-O-α-L-*Arabinofuranoside:*
$C_{20}H_{20}O_{11}$ 436.371
Constit. of the roots of *Fragaria* x *ananassa* (strawberry). Amorph. powder. $[\alpha]_D^{25}$ -32 (c, 0.4 in MeOH).

3-O-α-L-*Rhamnopyranoside:* [29838-67-3] ***Astilbin***
$C_{21}H_{22}O_{11}$ 450.398
Constit. of *Vitis vinifera* (wine grape). Needles (EtOH). Mp 179-180°. $[\alpha]_D^{25}$ +4 (50% Me_2CO aq.).

3′-Me ether: [55812-91-4] *3,4′,5,7-Tetrahydroxy-3′-methoxyflavanone. 4′,5,7-Trihydroxy-3′-methoxydihydroflavonol.* ***Dihydroisorhamnetin***
$C_{16}H_{14}O_7$ 318.282
Isol. from *Dillenia indica* (elephant apple). Pale yellow cryst. (EtOH aq.). Mp 230°. $[\alpha]_D^{27}$ +25 (EtOH).

4′-Me ether: [70411-27-7] *3,3′,5,7-Tetrahydroxy-4′-methoxyflavanone. 3′,5,7-Trihydroxy-4′-methoxydihydroflavonol*
$C_{16}H_{14}O_7$ 318.282
Isol. from *Blumea balsamifera* (sambong). Amorph. powder. Mp 181.5-182.5°. $[\alpha]_D$ +20.4 (c, 0.75 in MeOH).

3′,7-Di-Me ether: [37971-67-8] *3,4′,5-Trihydroxy-3′,7-dimethoxyflavanone. 4′,5-Dihydroxy-3′,7-dimethoxydihydroflavonol*
$C_{17}H_{16}O_7$ 332.309
Isol. from *Blumea balsamifera* (sambong). Cryst. (Me_2CO/petrol). Mp 184-186°.

4′,7-Di-Me ether: [79995-67-8] *3,3′,5-Trihydroxy-4′,7-dimethoxyflavanone. 3′,5-Dihydroxy-4′,7-dimethoxydihydroflavonol*
$C_{17}H_{16}O_7$ 332.309
Isol. from *Blumea balsamifera* (sambong). Needles (EtOAc). Mp 184-186°. $[\alpha]_D^{29}$ +32.8 (c, 0.015 in MeOH).

[5117-01-1, 17654-26-1, 63393-40-8, 64191-31-7, 64191-33-9, 82517-11-1, 83680-48-2, 117894-18-5]

Pavanasasivam, G. *et al., J.C.S. Perkin 1*, 1975, 612 (*Dihydroisorhamnetin*)
The Flavonoids, (Eds. Harborne, J.B. *et al*), Chapman and Hall, London, 1975, 585 (*occur*)
Chauhan, J.S. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 169 (*deriv*)
The Flavonoids: Advances in Research, (Eds. Harborne, J.B. *et al*), Chapman and Hall, London, 1982, 375 (*occur*)
Balza, F. *et al., Phytochemistry*, 1984, **23**, 2333 (*3,4′,5-Trihydroxy-3′,7-dimethoxyflavanone*)
Timmermann, B.N. *et al., Phytochemistry*, 1986, **25**, 723 (*3′,7-di-Me ether*)
Zdero, C. *et al., Phytochemistry*, 1986, **25**, 2841 (*3-Ac, 3′-Me ether*)
Sakushima, A. *et al., Phytochemistry*, 1988, **27**, 948 (*3-arabinoside*)
De Britto, J. *et al., Chem. Pharm. Bull.*, 1995, **43**, 338 (*Astilbin, Neoastilbin, Neoisoastilbin*)
Ishimaru, K. *et al., Phytochemistry*, 1995, **40**, 345 (*Taxifolin 3-arabinofuranoside*)
Gaffield, W. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1102 (*Astilbins*)
Islam, M.T. *et al., Phytochemistry*, 2000, **54**, 901-907 (*4′-Me ether, 4′,7-di-Me ether*)
Ohmori, K. *et al., Tet. Lett.*, 2000, **41**, 5537-5541 (*synth, Astilbin*)

3,4′,5,6,7-Pentahydroxyflavanone P-110

*2,3-Dihydro-3,5,6,7-tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{12}O_7$ 304.256

4′,6-Di-Me ether: [143114-81-2] *3,5,7-Trihydroxy-4′,6-dimethoxyflavanone*
$C_{17}H_{16}O_7$ 332.309
Constit. of the heartwood of *Prunus domestica* (plum). Yellow solid. Mp 164°.

Parmar, V.S. *et al., Phytochemistry*, 1992, **31**, 2185

3′,4′,5,7,8-Pentahydroxyflavanone P-111

*2-(3,4-Dihydroxyphenyl)-2,3-dihydro-5,7,8-trihydroxy-4*H*-1-benzopyran-4-one.* ***8-Hydroxyeriodictyol***

$C_{15}H_{12}O_7$ 304.256

(*S*)-*form* [188590-64-9]

Penta-Me ether:3′,4′,5,7,8-Pentamethoxyflavanone
$C_{20}H_{22}O_7$ 374.39
Constit. of a *Citrus* sp. (Dancy tangerine). Pale yellow needles (MeOH). Mp 177-178°.

Chen, J. *et al., J. Agric. Food Chem.*, 1998, **46**, 1235-1238 (*Pentamethoxyflavanone*)

3,4′,5,7,8-Pentahydroxyflavanone P-112

*2,3-Dihydro-3,5,7,8-tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one. 4′,5,7,8-Tetrahydroxydihydroflavonol*

$C_{15}H_{12}O_7$ 304.256

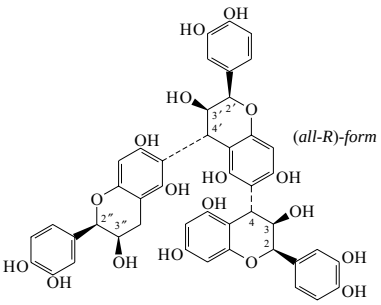
(2*R*,3*R*)-*form* [73249-37-3]
Pale yellow needles (EtOH aq.). Mp 230-231°.

4′,8-Di-Me ether, 7-O-β-D-*glucopyranoside:* [24512-61-6] ***Dihydroprudomenin***
$C_{23}H_{26}O_{12}$ 494.451
Isol. from wood of *Prunus mume* (Japanese apricot). Stereochem. not. det..

Hasegawa, M. *et al., Shokubutsugaku Zasshi*, 1969, **82**, 148; *CA*, **71**, 67946x
Jalal, M.A.F. *et al., Phytochemistry*, 1982, **21**, 1397
Proksch, P. *et al., Planta Med.*, 1987, **53**, 334 (*derivs*)

[3,3′,4′,5,7-Pentahydroxyflavan(4→6)]$_2$-3,3′,4′,5,7-pentahydroxyflavan P-113

2,2′,2″-Tris(3,4-dihydroxyphenyl)-3,3′,3″,4,4′,4″-hexahydro-[4,6′:4′,6″-ter-2H-1-benzopyran]-3,3′,3″,5,5′,5″,7,7′,7″-nonol, 9CI



(*all-R*)-form

$C_{45}H_{38}O_{18}$ 866.784

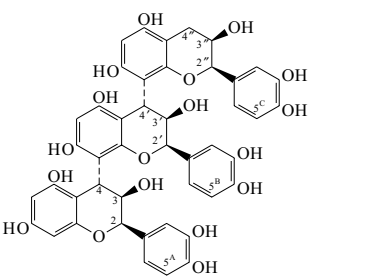
(all-R)-form [101401-64-3]
[Epicatechin(4β→6)]$_2$epicatechin
Off-white powder +3H$_2$O. $[\alpha]_D^{20}$ +127.8 (c, 0.5 in Me$_2$CO).

3,3′,3″-Tris(3,4,5-trihydroxybenzoyl): [106548-98-5] *Epicatechin 3-O-gallate(4β→6)-epicatechin 3-O-gallate(4β→6)-epicatechin 3-O-gallate*
$C_{66}H_{50}O_{30}$ 1323.103
Isol. from *Rheum* sp.. Tan amorph. powder +2H$_2$O. $[\alpha]_D^{28}$ +51 (c, 0.58 in Me$_2$CO).

Hsu, F.L. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3142 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4083 (*deriv*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4717 (*isol*)

[3,3′,4′,5,7-Pentahydroxyflavan(4→8)]$_2$-3,3′,4′,5,7-pentahydroxyflavan P-114

[37064-30-5]
2,2′,2″-Tris(3,4-dihydroxyphenyl)-3,3′,3″,4,4′,4″-hexahydro-[4,8′:4′,8″-ter-2H-1-benzopyran]-3,3′,3″,5,5′,5″,7,7′,7″-nonol, 9CI



(2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*R*,4*R*,4′*R*)-form

$C_{45}H_{38}O_{18}$ 866.784

►WY9070000

(2R,2′R,2″R,3R,3′R,3″R,4R,4′R)-form [65085-09-8]
[Epicatechin(4β→8)]$_2$epicatechin. ***Proanthocyanidin C$_1$.*** *Procyanidin C$_1$*
$[\alpha]_D$ +102 (H$_2$O).

3′,3″-Bis(3,4,5-trihydroxybenzoyl): [106533-61-3] *Procyanidin C1 3′,3″-di-O-gallate*
$C_{59}H_{46}O_{26}$ 1170.997
Isol. from *Rheum* sp. (commercial rhubarb). Tan amorph. powder + 4H$_2$O. $[\alpha]_D^{28}$ -5.5 (c, 0.64 in Me$_2$CO).

3,3′,3″-Tris(3,4,5-trihydroxybenzoyl): [106533-62-4] *Procyanidin C1 3,3′,3″-tri-O-gallate*
$C_{66}H_{50}O_{30}$ 1323.103
Isol. from *Rheum* sp.. Tan amorph. powder + 3H$_2$O. $[\alpha]_D^{28}$ +13.4 (c, 0.93 in Me$_2$CO).

(2R,2′R,2″R,3R,3′R,3″S,4R,4′R)-form [79813-67-5]
[Epicatechin(4β→8)]$_2$-catechin. ***Arecatannin A$_1$***
$[\alpha]_D$ +74 (H$_2$O).

3,3′-Bis(3,4,5-trihydroxybenzoyl): [106533-63-5] *[Epicatechin 3-O-gallate(4β→8)]$_2$-catechin*
$C_{59}H_{46}O_{26}$ 1170.997
Isol. from *Rheum* sp.. Tan amorph. powder + 3H$_2$O. $[\alpha]_D^{28}$ +19.4 (c, 0.95 in Me$_2$CO).

(2R,2′R,2″R,3S,3′S,3″S,4S,4′S)-form [37064-31-6]
[Catechin(4α→8)]$_2$catechin. ***Procyanidin C$_2$***

5^A-Hydroxy: [79127-37-0] ***Gallocatechin(4α→8)catechin(4α→8)catechin***
$C_{45}H_{38}O_{19}$ 882.784
Isol. from barley (*Hordeum vulgare*) seeds.

5^B-Hydroxy: [87421-89-4] ***Catechin(4α→8)gallocatechin(4α→8)catechin***
$C_{45}H_{38}O_{19}$ 882.784
Isol. from barley (*Hordeum vulgare*) seeds.

5^A,5^B-Dihydroxy: [79136-97-3] ***[Gallocatechin(4α→8)]$_2$catechin***
$C_{45}H_{38}O_{20}$ 898.783
Isol. from barley grains *Hordeum vulgare*.

(2R,2′S,2″S,3R,3′S,3″S,4R,4′S)-form *Epicatechin(4β→8)*-ent-*epicatechin(4α→8)*-ent-*epicatechin*

3,3′-Bis(3,4,5-trihydroxybenzoyl):
$C_{59}H_{46}O_{26}$ 1170.997
Constit. of *Byrsonima crassifolia* (nance) bark. $[\alpha]_D^{26}$ -56 (c, 1 in Me$_2$CO).

(2S,2′S,2″S,3S,3′S,3″S,4S,4′S)-form ent-*Epicatechin(4α→8)*-ent-*epicatechin(4α→8)*-ent-*epicatechin*

3,3′-Bis(3,4,5-Trihydroxybenzoyl):
$C_{59}H_{46}O_{26}$ 1170.997
Constit. of *Byrsonima crassifolia* (nance) bark. $[\alpha]_D^{26}$ -42 (c, 1 in Me$_2$CO).

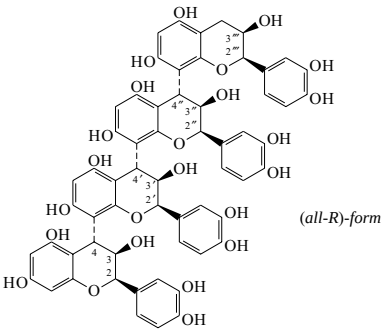
[23459-99-6, 78655-09-1, 80823-25-2]

Brandon, M.J. *et al., Phytochemistry*, 1982, **21**, 2953-2957 (*5-hydroxy, 5,5-dihydroxy*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4083 (*Rheum gallates*)
Delcour, J.A. *et al., J. Inst. Brewing*, 1986, **92**, 244 (*5-hydroxy, 5,5-dihydroxy*)

[3,3′,4′,5,7-Pentahydroxyflavan(4→8)]$_3$-3,3′,4′,5,7-pentahydroxyflavan P-115

[102491-63-4]

2,2′,2″,2‴-Tetrakis(3,4-dihydroxyphenyl)-3,3′,3″,3‴,4,4′,4″,4‴-octahydro-[4,8′:4′,8″:4″,8‴-quater-2H-1-benzopyran]-3,3′,3″,3‴,5,5′,5″,5‴,7,7′,7″,7‴-dodecol, 9CI



(*all-R*)-form

$C_{60}H_{50}O_{24}$ 1155.041

(all-R)-form [86631-38-1]
[Epicatechin(4β→8)]$_3$epicatechin. ***Cinnamtannin A$_1$.*** *Cinnamtannin I*
Isol. from *Cinnamomum cassia* (Chinese cinnamon). Pale brown amorph. powder + 3H$_2$O. $[\alpha]_D$ +89.2 (c, 0.9 in Me$_2$CO).

(3‴S)-form [79763-29-4]
[Epicatechin(4β→8)]$_3$catechin. ***Arecatannin A$_2$***
$[\alpha]_D$ +98.6 (Me$_2$CO).

(3S,3′S,3″S,4S,4′S,4‴S)-form [97233-68-6]
[Catechin(4α→8)]$_3$epicatechin
Hexadeca-Me ether, 3,3′,3″,3‴-tetra-Ac: Amorph. solid.

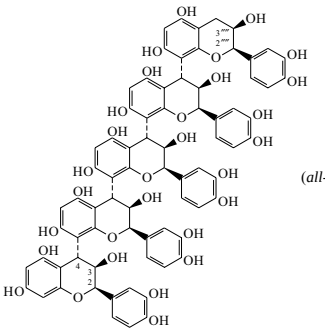
(3S,3′S,3″S,3‴S,4S,4′S,4″S)-form [88244-66-0]
[Catechin(4α→8)]$_3$catechin
Hexadeca-Me ether, 3,3′,3″,3‴-tetra-Ac: Amorph. solid.

[89396-12-3, 93781-31-8, 102130-87-0, 112294-88-9]

Nonaka, G. *et al., Chem. Comm.*, 1981, 781 (*isol*)
Delcour, J.A. *et al., J.C.S. Perkin 1*, 1983, 1711; 1985, 669 (*synth*)
Kolodziej, H. *et al., J.C.S. Perkin 1*, 1984, 343 (*isol*)
Ezaki-Furuichi, E. *et al., Agric. Biol. Chem.*, 1986, **50**, 2061 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 633 (*isol*)

[3,3′,4′,5,7-Pentahydroxyflavan(4→8)]$_4$-3,3′,4′,5,7-pentahydroxyflavan P-116

[103729-51-7]
2,2′,2″,2‴,2⁗-Pentakis(3,4-dihydroxyphenyl)-3,3′,3″,3‴,3⁗,4,4′,4″,4‴,4⁗-decahydro-[4,8′:4′,8″:4″,8‴:4‴,8⁗-quinque-2H-1-benzopyran]-3,3′,3″,3‴,3⁗,5,5′,5″,5‴,5⁗,7,7′,7″,7‴,7⁗-pentadecol, 9CI. *[Epicatechin-(4β→8)]$_4$catechin*



(*all-R*)-*form*

$C_{75}H_{62}O_{30}$ 1443.297

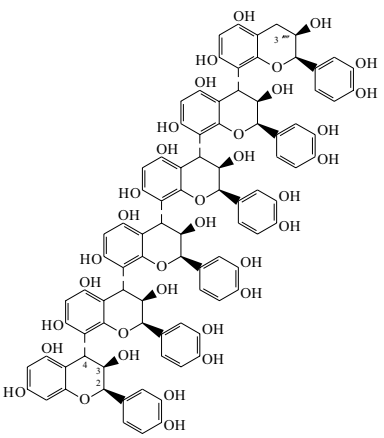
(*all-R*)-*form* [86631-39-2]
[Epicatechin(4β→8)]$_4$epicatechin. ***Cinnamtannin II***. *Cinnamtannin A$_3$*
Isol. from *Cinnamomum cassia* (Chinese cinnamon). Pale brown amorph. powder + 3H_2O. $[\alpha]_D^{24}$ +102.1 (c, 1 in Me_2CO).

(3′′′′*S*)-*form* [86588-85-4]
[Epicatechin(4β→8)]$_4$catechin. ***Arecatannin A$_3$***
Isol. from *Areca catechu* (betel nut). No phys. props. reported.

Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 633 (*isol*)
Gujer, R. *et al., Phytochemistry*, 1986, **25**, 1431 (*isol*)
Foo, L.Y. *et al., Phytochemistry*, 1991, **30**, 667 (*isol*)

[3,3′,4′,5,7-Pentahydroxyflavan(4→8)]$_5$-3,3′,4′,5,7-pentahydroxyflavan P-117

2,2′,2′′,2′′′,2′′′′,2′′′′′-Hexakis(3,4-dihydroxyphenyl)-3,3′,3′′,3′′′,3′′′′,3′′′′′,4,4′,4′′,4′′′,4′′′′,4′′′′′-dodecahydro-[4,8′:4′,8′′:4′′,8′′′:4′′′,8′′′′:4′′′′,8′′′′′-sexi-2H-1-benzopyran]-3,3′,3′′,3′′′,3′′′′,3′′′′′,5,5′,5′′,5′′′,5′′′′,5′′′′′-′′,5′′′′′,7,7′,7′′,7′′′,7′′′′,7′′′′′-octadecol, 9CI

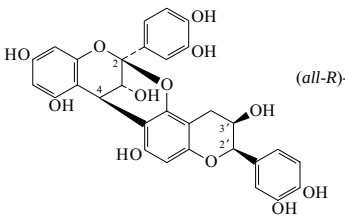


$C_{90}H_{74}O_{36}$ 1731.553

(*all-R*)-*form* [88847-05-6]
[Epicatechin(4β→8)]$_5$epicatechin. ***Cinnamtannin III***. *Cinnamtannin A$_4$*
Isol. from the bark of *Cinnamomum cassia* (Chinese cinnamon). Pale brown amorph. powder + 3H_2O. $[\alpha]_D^{22}$ +112.5 (c, 0.9 in Me_2CO).

Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 633 (*isol*)

3,3′,4′,5,7-Pentahydroxyflavan(2→5,4→6)-3,3′,4′,5,7-pentahydroxyflavan P-118



(*all-R*)-*form*

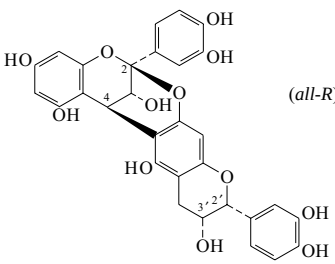
$C_{30}H_{24}O_{12}$ 576.512

(*all-R*)-*form* [114569-32-3]
Epicatechin-(2β→5,4β→6)-epicatechin. ***Proanthocyanidin A$_7$***
Needles + 2½H_2O (H_2O). Mp 300°. $[\alpha]_D^{21}$ +35.9 (c, 1.2 in Me_2CO).

(2*R***,2′***S***,3***R***,3′***S***,4***R***)-*form*** [135095-75-9]
*Epicatechin-(2β→5,4β→6)*ent-*epicatechin*
Isol. from *Theobroma cacao* (cocoa). $[\alpha]_{578}$ +20.5 (c, 0.1 in MeOH). There is a discrepancy in the journal between text and diagrams, as to the C-2′ and C-3′ configs..

Morimoto, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4717 (*Proanthocyanidin A$_7$*)
Porter, L.J. *et al., Phytochemistry*, 1991, **30**, 1657 (*isol*)

3,3′,4′,5,7-Pentahydroxyflavan(2→7,4→6)-3,3′,4′,5,7-pentahydroxyflavan P-119



(*all-R*)-*form*

$C_{30}H_{24}O_{12}$ 576.512

(*all-R*)-*form* [114569-31-2]
Epicatechin-(2β→7,4β→6)-epicatechin. ***Proanthocyanidin A$_6$***
Needles + 2H_2O (H_2O). Mp 300°. $[\alpha]_D^{21}$ +22.4 (c, 1.2 in Me_2CO).

(2*R***,2′***R***,3***R***,3′***S***,4***R***)-*form***
Epicatechin-(2β→7,4β→6)-catechin
Constit. of the skins of peanuts (*Arachis hypogaea*). Needles + 1H_2O (H_2O). Mp 271-273° dec.

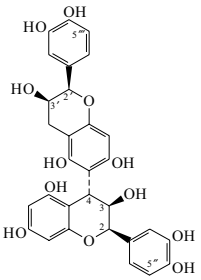
(2*R***,2′***S***,3***R***,3′***R***,4***R***)-*form***
Epicatechin-(2β→7,4β→6)-ent-*catechin*
Constit. of the skins of peanuts (*Arachis hypogaea*). Amorph. powder + 2H_2O (H_2O). Mp 262°.

(2*R***,2′***S***,3***R***,3′***S***,4***R***)-*form***
*Epicatechin-(2β→7,4β→6)*ent-*epicatechin*
Constit. of the skins of peanuts (*Arachis hypogaea*). Amorph. powder + 2H_2O (H_2O). Mp 280° dec.

Morimoto, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4717
Lou, H. *et al., Phytochemistry*, 1999, **51**, 297-308 (*isol, cd, pmr, cmr*)
Kamiya, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 551-557 (*Proanthocyanidin A$_6$, isol, pmr, cmr*)

3,3′,4′,5,7-Pentahydroxyflavan-(4→6)-3,3′,4′,5,7-pentahydroxyflavan P-120

[123051-09-2]



(2*R*,2′*R*,3*R*,3′*R*,4*R*)-*form*

$C_{30}H_{26}O_{12}$ 578.528

(2*R***,2′***R***,3***R***,3′***R***,4***R***)-*form*** [12798-57-1]
Procyanidin B$_5$. *Epicatechin(4β→6)epicatechin*. *Proanthocyanidin B$_5$*
Isol. from cacao *Theobroma cacao*. $[\alpha]_D$ +102 (H_2O).

▶ DT4325000

3′-(3,4,5-Trihydroxybenzoyl):3′-O-*Galloylprocyanidin B$_5$*
$C_{37}H_{30}O_{16}$ 730.634
Off-white powder. $[\alpha]_D^{22}$ +61 (c, 0.12 in MeOH). λ_{max} 211 (log ε 4.95); 279 (log ε 4.2) (MeOH).

3,3′-Bis(3,4,5-trihydroxybenzoyl): [106533-60-2] *3,3′-Di*-O-*galloylprocyanidin B$_5$*
$C_{44}H_{34}O_{20}$ 882.741
Constit. of commercial rhubarb (*Rheum* spp.). Tan amorph. powder + 4H_2O. $[\alpha]_D^{28}$ +31.3 (c, 0.16 in Me_2CO).

5′′-Hydroxy, 3,3′-bis(3,4,5-trihydroxybenzoyl): [126715-92-2] *Epigallocatechin 3*-O-*gallate(4β→6)-epicatechin 3*-O-*gallate*
$C_{44}H_{34}O_{21}$ 898.74
Tannin constit. of oolong tea *Camellia sinensis* var. *viridis*. Tan amorph. powder. $[\alpha]_D^{21}$ +14.5 (c, 0.7 in Me_2CO).

5′′′-Hydroxy, 3,3′-bis(3,4,5-trihydroxybenzoyl): [126715-91-1] *Epicatechin 3*-O-*gallate (4β→6)epigallocatechin 3*-O-*gallate*
$C_{44}H_{34}O_{21}$ 898.74
Isol. from oolong tea *Camellia sinensis* var. *viridis*. Tan amorph. powder + 3½H_2O. $[\alpha]_D^{26}$ +12.8 (c, 0.7 in Me_2CO).

5′′,5′′′-Dihydroxy: [87338-95-2] *Epigallocatechin(4β→6)epigallocatechin*. ***Prodelphinidin B$_5$***
$C_{30}H_{26}O_{14}$ 610.527
Off-white amorph. powder. $[\alpha]_D^{14}$ +112 (c, 0.56 in Me_2CO).

5′′,5′′′-Dihydroxy, 3′-(3,4,5-trihydroxybenzoyl):Epigallocatechin(4β→6)-epigallocatechin 3-O-*gallate*

$C_{37}H_{30}O_{18}$ 762.633

5″,5‴-Dihydroxy, 3,3′-bis(3,4,5-trihydroxybenzoyl): [86588-87-6] *3,3′-Di*-O-*galloylprodelphinidin B5*
$C_{44}H_{34}O_{22}$ 914.739
Isol. from bark of *Myrica rubra* (Chinese bayberry). Off-white amorph. powder. $[\alpha]_D^{18}$ +57.4 (c, 1.01 in Me_2CO).

3″-Deoxy, 5‴-hydroxy, 3,3′-bis(3,4,5-trihydroxybenzoyl): [126715-93-3] *Epiafzelechin 3*-O-*gallate-(4β→6)-epigallocatechin 3*-O-*gallate*
$C_{44}H_{34}O_{20}$ 882.741
Isol. from commercial oolong tea (*Camellia sinensis* var. *viridis*). Tan amorph. powder. $[\alpha]_D^{21}$ +22.2 (c, 1.2 in Me_2CO).

(2*R*,2′*R*,3*S*,3′*S*,4*S*)-*form* [12798-58-2]
Procyanidin B6*. Catechin(4α→6)catechin*
Isol. from leaves and fruit of cowberry *Vaccinium vitis-idaea* and other plants. Powder + $1H_2O$. $[\alpha]_D$ -130 (EtOH).

(2*R*,2′*R*,3*R*,3′*S*,4*R*)-*form* [12798-59-3]
Procyanidin B7*. Epicatechin(4β→6)catechin*
Isol. from unripe fruits of cowberry *Vaccinium vitis-idaea*. $[\alpha]_D$ +142 (H_2O).

(2*R*,3′*R*,3*S*,3′*R*,4*S*)-*form* [12798-60-6]
Procyanidin B8*. Catechin(4α→6) epicatechin*
Present in fruit and leaves of blackberry (*Rubus fruticosus*), raspberry (*Rubus idaeus*) and cowberry (*Vaccinium vitis idaea*). $[\alpha]_D$ -160 (MeOH).

(2*R*,2′*S*,3*R*,3′*S*,4*R*)-*form* [88314-65-2]
*Epicatechin(4β→6)*ent-*epicatechin*
Powder. $[\alpha]_D^{30}$ +77 (Me_2CO).

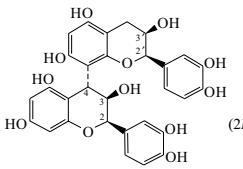
(2*S*,2′*S*,3*S*,3′*S*,4*S*)-*form*
ent-*Epicatechin(4α→6)*-ent-*epicatechin*
Constit. of *Byrsonima crassifolia* (nance). $[\alpha]_D^{26}$ -105 (c, 1 in Me_2CO).

[99685-01-5, 121842-81-7]

Thompson, R.S. *et al., J.C.S. Perkin 1*, 1972, 1387 (*isol, cd, bibl*)
Fletcher, A.C. *et al., J.C.S. Perkin 1*, 1977, 1628 (*conformn, config*)
Foo, L.Y. *et al., J.C.S. Perkin 1*, 1983, 1535 (*synth, pmr, cmr*)
Delcour, J.A. *et al., J.C.S. Perkin 1*, 1983, 1711; 1985, 669 (*synth*)
Nonaka, G. *et al., Phytochemistry*, 1983, **22**, 237 (*derivs*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4083 (*gallates*)
Viswanadham, V.K.N. *et al., J.C.S. Perkin 2*, 1987, 739 (*conformn*)
Newman, R.H. *et al., Magn. Reson. Chem.*, 1987, **25**, 118 (*cmr*)
Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3255 (*derivs*)
Cui, C.-B. *et al., Chem. Pharm. Bull.*, 1992, **40**, 889 (*isol, pmr, cmr*)
Balas, L. *et al., Magn. Reson. Chem.*, 1994, **32**, 386 (*pmr*)
Danne, A. *et al., Phytochemistry*, 1994, **37**, 533 (*deriv*)
Greiss, F. *et al., Phytochemistry*, 1995, **39**, 635 (*isol*)
Wang, J.-N. *et al., Phytochemistry*, 2000, **53**, 1097-1102 (*3′-Galloylprocyanidin B5*)

3,3′,4′,5,7-Pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan P-121

[35356-33-3]
Procyanidin C. Proanthocyanidin C. Leucocyanidin 1



(2R,2′R,3R,3′R,4R)-form

$C_{30}H_{26}O_{12}$ 578.528
The (*RS*) config. at C-4 is difficult to assign. Given here as (4*R*) for Procyanidin B_1, following Barrett *et al*. Confusingly, the name Procyanidin C has been used for this group of compounds having unspecified stereochem., but the individual stereoisomers are called Procyanidins B. Procyanidin D has also been named as a stereoisomer.Poorly sol. hexane.

3-(3,4,5-Trihydroxybenzoyl): [82916-01-6]
Proanthocyanidin B6
$C_{37}H_{30}O_{16}$ 730.634Contains isomers with (2*R*,3*R*) and (2′,3′*R*) configs. with unknown config. of flavonoid linkage.

(2*R*,2′*R*,3*R*,3′*R*,4*R*)-*form* [29106-49-8]
Procyanidin B2*. Epicatechin(4β→8)epicatechin. Proanthocyanidin B2*
Present in red wine. $[\alpha]_D$ +26 (H_2O).

*3′-(3,4,5-Trihydroxybenzoyl):****3′-Galloylprocyanidin B2***
$C_{37}H_{30}O_{16}$ 730.634
Isol. from *Thea sinensis* (tea). $[\alpha]_D$ -45.8 (c, 0.72 in Me_2CO).

3,3′-Bis(3,4,5-trihydroxybenzoyl): [79907-44-1] ***3,3′-Digalloylprocyanidin B2***
$C_{44}H_{34}O_{20}$ 882.741
Isol. from *Rheum* rhizome and *Thea sinensis* (tea). Pale brown amorph. powder + $1^1/_2H_2O$. $[\alpha]_D^{22}$ -95.2 (c, 1.1 in Me_2CO).

(2*R*,2′*R*,3*R*,3′*S*,4*R*)-*form* [20315-25-7]
Procyanidin B1*. Epicatechin(4β→8)catechin. Proanthocyanidin B1*
Present in red wine. Cryst. (MeOH) (as deca-Ac). Mp 231-232° (deca-Ac). $[\alpha]_D^{25}$ +110.9 (c, 2 in Me_2CO) (deca-Ac).

*3-(3,4,5-Trihydroxybenzoyl):****3-Galloylprocyanidin B1***
$C_{37}H_{30}O_{16}$ 730.634
Isol. from *Rheum* rhizome. $[\alpha]_D^{21}$ -21 (Me_2CO).

3′-(1-Hydroxy-6-oxo-2-cyclohexene-1-carboxylate):
$C_{37}H_{32}O_{15}$ 716.651
Off-white amorph. powder + $2H_2O$. $[\alpha]_D^{18}$ -62.6 (c, 1 in Me_2CO).

*3′-*O*-(4-Hydroxybenzoyl):3′-(4-Hydroxybenzoyl)procyanidin B1*
$C_{37}H_{30}O_{14}$ 698.636

(2*R*,2′*R*,3*S*,3′*S*,4*S*)-*form* [23567-23-9]
Procyanidin B3*. Catechin(4α→8)catechin. Proanthocyanidin B3*
Present in red wine. Occurs in *Fragaria* spp.. Amorph. (as deca-Ac). $[\alpha]_D$ -235 (MeOH aq.).

*3-*O*-β-D-Glucopyranoside:* [155260-74-5]
Procyanidin B3 3-glucoside
$C_{36}H_{36}O_{17}$ 740.67
Light tan amorph. solid.

*3-*O*-α-L-Rhamnopyranoside:* [109194-84-5]
Procyanidin B3 3-rhamnoside
$C_{36}H_{36}O_{16}$ 724.671
$[\alpha]_D^{22}$ -110.2 (c, 0.6 in Me_2CO).

*3′-*O*-β-D-Glucopyranoside:* [118627-69-3]
Procyanidin B3 3′-O-*glucoside*
$C_{36}H_{36}O_{17}$ 740.67
Brown amorph. powder. $[\alpha]_D^{18}$ -166.5 (c, 1 in Me_2CO aq.).

*3′-*O*-α-L-Rhamnopyranoside:* [109194-83-4] ***Procyanidin B3 3′-rhamnoside***
$C_{36}H_{36}O_{16}$ 724.671
$[\alpha]_D$ -203 (c, 0.8 in Me_2CO).

*7-*O*-β-D-Glucopyranoside:* [105330-57-2]
Procyanidin B3 7-glucoside
$C_{36}H_{36}O_{17}$ 740.67
Isol. from *Rheum* spp.. Tan powder + $1H_2O$. $[\alpha]_D^{19}$ -197.5 (c, 0.69 in MeOH).

*3-(3,4,5-Trihydroxybenzoyl):****3-Galloylprocyanidin B3***
$C_{37}H_{30}O_{16}$ 730.634
Isol. from *Sanguisorba officinalis* (burnet bloodwort). Off-white amorph. powder + $1^1/_2H_2O$. $[\alpha]_D^{23}$ -170.1 (c, 0.72 in Me_2CO).

(2*R*,2′*R*,3*S*,3′*R*,4*S*)-*form* [29106-51-2]
Procyanidin B4*. Catechin(4α→8)epicatechin*
Occurs in *Rubus fruticosus* (blackberry) and *Rubus idaeus* (raspberry). Cryst. (EtOH) (as deca-Ac). Mp 172-173° (deca-Ac). $[\alpha]_D$ -194 (EtOH).

*3-(3,4,5-Trihydroxybenzoyl):****3′-Galloylprocyanidin B4***
$C_{37}H_{30}O_{16}$ 730.634
Isol. from *Thea sinensis* (tea). Pale brown amorph. powder + $1^1/_2H_2O$. $[\alpha]_D^{22}$ -255.7 (c, 0.56 in Me_2CO).

(2*R*,2′*S*,3*R*,3′*S*,4*R*)-*form* [82262-99-5]
*Epicatechin(4β→8)*ent-*epicatechin*
Powder. $[\alpha]_D^{30}$ +187 (c, 0.24 in MeOH aq.).

(2*R*,2′*R*,3*R*,3′*R*,4*S*)-*form* [67253-04-7]
Epicatechin(4α→8)epicatechin

(2*R*,2′*S*,3*S*,3′*R*,4*S*)-*form* [88314-66-3]
*Catechin(4α→8)*ent-*catechin*
Powder. $[\alpha]_D^{30}$ -234 (c, 0.26 in MeOH aq.).

(2*S*,2′*R*,3*S*,3′*R*,4*S*)-*form* [82262-98-4]
ent-*Epicatechin(4α→8)epicatechin*

(2*S*,2′*R*,3*S*,3′*S*,4*S*)-*form* [121842-80-6]
ent-*Epicatechin(4α→8)catechin*
Isol. from the pith of *Metroxylon sagu* (sago palm). Amorph. powder + $2^1/_2H_2O$. $[\alpha]_D^{24}$ -115.7 (c, 0.5 in Me_2CO).

(2*S*,2′*S*,3*S*,3′*S*,4*S*)-*form* [88314-64-1]
ent-*Epicatechin(4α→8)*ent-*epicatechin*
$[\alpha]_D^{30}$ -23.9 (c, 0.2 in MeOH aq.).

3-(3,4,5-Trihydroxybenzoyl):
$C_{37}H_{30}O_{16}$ 730.634
Constit. of *Byrsonima crassifolia* (nance). $[\alpha]_D^{26}$ +18 (c, 1 in Me_2CO).

3′-(3,4,5-Trihydroxybenzoyl):
$C_{37}H_{30}O_{16}$ 730.634
Constit. of *Byrsonima crassifolia* (nance). $[\alpha]_D^{26}$ +12.5 (c, 1 in Me_2CO).

3,3′-Bis(3,4,5-trihydroxybenzoyl):
$C_{44}H_{34}O_{20}$ 882.741

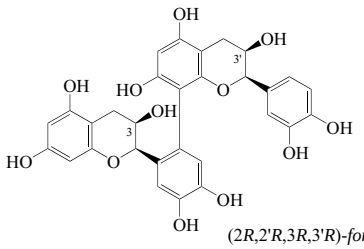
Constit. of *Byrsonima crassifolia* (nance). $[\alpha]_D^{26}$ +13.4 (c, 1 in Me_2CO).

(all-ξ)-*form* [41365-27-9]
Auricassidin

[15514-06-4, 20555-01-5, 35356-34-4, 61505-38-2, 86631-41-6, 89064-33-5]

Weinges, K. *et al., Annalen*, 1968, **711**, 184; **715**, 164 (*isol, props*)
Reddy, K.R.S. *et al., Indian J. Chem.*, 1972, **10**, 956 (*Auricassidin*)
Haslam, E. *et al., J.C.S. Perkin 1*, 1974, 2663; 1977, 1628; 1637
Fletcher, A.C. *et al., J.C.S. Perkin 1*, 1977, 1628 (*conformn, config*)
Barrett, M.W. *et al., J.C.S. Perkin 1*, 1979, 2375 (*cd*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2862; 1983, **31**, 3906 (*gallates*)
Porter, L.J. *et al., J.C.S. Perkin 1*, 1982, 1217 (*cmr*)
Nonaka, G. *et al., Phytochemistry*, 1982, **21**, 429 (*deriv*)
Foo, L.Y. *et al., J.C.S. Perkin 1*, 1983, 1535 (*isol, synth, pmr, cmr*)
Delcour, J.A. *et al., J.C.S. Perkin 1*, 1983, 1711; 1985, 669 (*synth*)
Tanaka, T. *et al., Phytochemistry*, 1983, **22**, 2575 (*3-Galloylprocyanidin B_3*)
Kulodziej, H. *et al., Phytochemistry*, 1984, **23**, 1745 (*isol, struct*)
Hsu, F.L. *et al., Phytochemistry*, 1985, **24**, 2089 (*2-cyclohexene-1-carboxylates*)
Viswanadhan, V.K.N. *et al., J.C.S. Perkin 2*, 1987, 739 (*conformn*)
Ishimaru, K. *et al., Phytochemistry*, 1987, **26**, 1167 (*glycosides*)
Zhang, B. *et al., Phytochemistry*, 1988, **27**, 3277 (*3′-glucoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Saijo, R. *et al., Phytochemistry*, 1989, **28**, 2443 (*pmr, gallates*)
Ozawa, T. *et al., Agric. Biol. Chem.*, 1990, **54**, 217 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 888 (*isol, pmr*)
Kolodziej, H. *et al., Phytochemistry*, 1991, **30**, 1255 (*3-rhamnoside*)
Balas, L. *et al., Magn. Reson. Chem.*, 1994, **32**, 386 (*pmr*)
Bae, Y.-S. *et al., Phytochemistry*, 1994, **35**, 473 (*Procyanidin B_3 3-glucoside*)
Geiss, F. *et al., Phytochemistry*, 1995, **39**, 635 (*trihydroxybenzoyl derivs*)
Hartisch, C. *et al., Phytochemistry*, 1996, **42**, 191 (*4-Hydroxybenzoylprocyanidin B_1*)
De Bruyne, T. *et al., Phytochemistry*, 1996, **43**, 265 (*pmr*)
Hatano, T. *et al., J.C.S. Perkin 2*, 1997, 1035-1043 (*pmr, conformn*)
Khan, M.L. *et al., Magn. Reson. Chem.*, 1997, **35**, 854-858 (*pmr, cmr, conformn*)
De Bruyne, T. *et al., J. Nat. Prod.*, 1999, **62**, 954-958 (*activity*)
Abe, I. *et al., Planta Med.*, 2000, **66**, 753-756 (*activity*)
Kozikowski, A.P. *et al., J.O.C.*, 2001, **66**, 1287-1296; 2003, **68**, 1641-1658 (*synth*)
Weinges, K. *et al., Tetrahedron*, 2001, **57**, 2327-2330 (*Procyanidin B_1,cryst struct*)
Saito, A. *et al., Tetrahedron*, 2002, **58**, 7829-7837 (*Procyanidin B_3, synth*)

3,3′,4′,5,7-Pentahydroxyflavan(6′→8)-3,3′,4′,5,7-pentahydroxyflavan P-122



(2*R*,2′*R*,3*R*,3′*R*)-*form*

$C_{30}H_{26}O_{12}$ 578.528

(2*R*,2′*R*,3*R*,3′*R*)-*form*
Epicatechin(6′→8)epicatechin
Isol. from Chardonnay grape pomace. Powder.

(2*R*,2′*R*,3*R*,3′*S*)-*form*
Epicatechin(6′→8)catechin
Isol. from Chardonnay grape pomace. Powder.

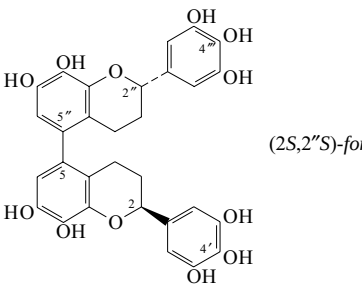
(2*R*,2′*R*,3*S*,3′*S*)-*form*
Catechin(6′→8)catechin

3,3′-Di-O-*β*-D-*glucopyranoside:* [118555-81-0] ***Potentillanin***
$C_{42}H_{46}O_{22}$ 902.812
Off-white powder. $[\alpha]_D^{18}$ -80 (c, 1 in Me_2CO aq.).

Zhang, B. *et al., Phytochemistry*, 1988, **27**, 3277 (*Potentillanin*)
Foo, L.Y. *et al., Phytochemistry*, 1998, **47**, 1137-1140 (*isol, pmr, cmr*)

3′,4′,5′,7,8-Pentahydroxyflavan(5→5)-3′,4′,5′,7,8-pentahydroxyflavan P-123

3′,3‴,4′,4‴,5′,5‴,7,7″,8,8″-Decahydroxy-5,5″-biflavan



(2*S*,2″*S*)-*form*

$C_{30}H_{26}O_{12}$ 578.528

(2*S*,2″*S*)-*form*

3′,3‴,4′,4‴,7,7″-Hexa-Me ether:5′,5‴,8,8″-Tetrahydroxy-3′,3‴,4′,4‴,7′,7″-hexamethoxy-5,5″-biflavan
$C_{36}H_{38}O_{12}$ 662.689
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Prisms (MeOH). Mp 211° dec. $[\alpha]_D^{22}$ +18.9 (c, 0.22 in $CHCl_3$). λ_{max} 244 (ε 19000); 268 (ε 7000) (MeOH) (Berdy).

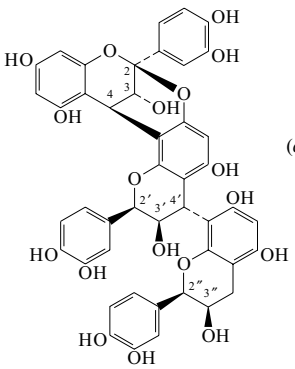
3′,3‴,4′,4‴,5‴,7,7″-Hepta-Me ether:5′,8,8″-Trihydroxy-3′,3‴,4′,4‴,5‴,7′,7″-heptamethoxy-5,5″-biflavan
$C_{37}H_{40}O_{12}$ 676.716
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Prisms (MeOH). Mp 228° dec. $[\alpha]_D^{22}$ +11.3 (c, 0.31 in $CHCl_3$). λ_{max} 247 (ε 15520); 269 (ε 7100) (MeOH) (Berdy).

[133342-99-1, 133343-10-9, 133398-97-7, 133442-48-5]

Kaneda, N. *et al., J. Nat. Prod.*, 1991, **54**, 196

3,3′,4′,5,7-Pentahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan P-124

*2,8-Bis(3,4-dihydroxyphenyl)-4-[2-(3,4-dihydroxyphenyl)-3,4-dihydro-3,5,7-trihydroxy-2*H*-1-benzopyran-8-yl]-3,4-dihydro-8,14-methano-2*H*,14*H*-1-benzopyrano[7,8-*d*][1,3]benzodioxocin-3,5,11,13,15-pentol, 9CI*



(all-*R*)-*form*

$C_{45}H_{36}O_{18}$ 864.769

(all-R)-form [88082-60-4]
Epicatechin(2β→7,4β→8)epicatechin(4β→8)epicatechin
Isol. from cinnamon bark (*Cinnamomum zeylanicum*) and from cowberry (*Vaccinium vitis-idaea*). Off-white amorph. powder + $2H_2O$. $[\alpha]_D^{25}$ +70.3 (c, 1.1 in Me_2CO).

(2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*S*,4*R*,4′*R*)-*form*
[97233-06-2]
Epicatechin(2β→7,4β→8)epicatechin(4β→8)catechin. ***Cinnamtannin D_1***
Isol. from cowberry (*Vaccinium vitis-idaea*). Needles + $2H_2O$ (H_2O). Mp 300°. $[\alpha]_D^{22}$ +102.3 (c, 0.9 in Me_2CO).

3‴,3⁗,3⁗′-Trideoxy: [152378-18-2]
Epiafzelechin(2β→7,4β→8)epiafzelechin(4β→8)afzelechin. ***Sellegueain A***
$C_{45}H_{36}O_{15}$ 816.77
Light brown cryst. (MeOH). $[\alpha]_D^{25}$ +103.6 (c, 1.3 in Me_2CO). Mp > 300°.

(2*R*,2′*S*,2″*R*,3*R*,3′*R*,3″*R*,4*R*,4′*R*)-*form*
[114612-77-0]
Epicatechin(2β→7,4β→8)-ent-*catechin(4β→8)epicatechin*. ***Aesculitannin B***
Off-white amorph. powder + $2H_2O$. $[\alpha]_D^{21}$ +52.8 (c, 1.2 in Me_2CO).

(2*R*,2′*S*,2″*R*,3*R*,3′*S*,3″*S*,4*R*,4′*S*)-*form*
[86631-43-8]
Catechin(2β→7,4β→8)-ent-*epicatechin(4α→8)catechin*. ***Pavetannin B_6***

Isol. from cinnamon bark (*Cinnamomum zeylanicum*).

(2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*R*,4*R*,4′*S*)-*form*
[139975-02-3]
Epicatechin(2β→7,4β→8)epicatechin(4α→8)epicatechin. ***Cinnamtannin B$_1$.*** *Pavetannin B$_2$*
Isol. from a cinnamon bark (*Cinnamomum zeylanicum*). Brown amorph. solid.

3-O-α-L-*Arabinopyranoside:3*-O-α-L-*Arabinopyranosylcinnamtannin B$_1$*
$C_{50}H_{44}O_{22}$ 996.884
Constit. of cocoa liquor (*Theobroma cacao*). Light brown amorph. powder. $[\alpha]_D$ +12.6 (c, 1 in MeOH). λ_{max} 280 (log ϵ 4.2) (MeOH).

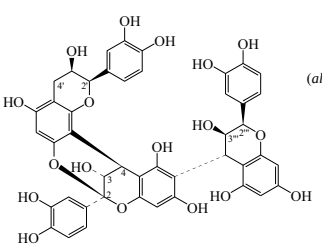
3-O-β-D-*Galactopyranoside:3*-O-β-D-*Galactopyranosylcinnamtannin B$_1$*
$C_{51}H_{46}O_{23}$ 1026.911
Constit. of cocoa liquor (*Theobroma cacao*). Light brown amorph. powder. $[\alpha]_D$ +17.1 (c, 1 in MeOH). λ_{max} 281 (log ϵ 5.02) (MeOH).

(2*R*,2′*R*,2″*S*,3*R*,3′*R*,3″*S*,4*R*,4′*S*)-*form*
[139975-01-2]
Epicatechin(2β→7,4β→8)epicatechin(4α→8)-ent-*epicatechin.* ***Pavetannin B$_1$***
Light brown powder.

(2*R*,2′*R*,2″*R*,3*R*,3′*S*,3″*R*,4*R*,4′*R*)-*form*
[162300-82-5]
Epicatechin(2β→7,4β→8)catechin(4β→8)epicatechin

Nonaka, G. *et al., J.C.S. Perkin 1*, 1983, 2139 (*isol*)
Hsu, F.L. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3142 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4338; 1987, **35**, 4717; 1988, **36**, 33 (*isol*)
Ezaki, N. *et al., Planta Med.*, 1985, 34 (*isol*)
Baldé, A.M. *et al., Phytochemistry*, 1991, **30**, 4129 (*Pavetannins*)
Balde, A.M. *et al., J. Nat. Prod.*, 1993, **56**, 1079 (*Pavetannins*)
Baek, N.-I. *et al., J. Nat. Prod.*, 1993, **56**, 1532 (*Selligueain A*)
Santos-Buelga, C. *et al., Phytochemistry*, 1995, **38**, 499 (*isol*)
Kamiya, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 551-557 (*Aesculitannin B, Cinnamtannin A$_2$, isol, pmr, cmr*)
Hatano, T. *et al., Phytochemistry*, 2002, **59**, 749-758 (*3-Glycosylcinnamtannin B$_1$*)

3,3′,4′,5,7-Pentahydroxyflavan(4→6)-3,3′,4′,5,7-pentahydroxyflavan(2→7,4→8)-pentahydroxyflavan P-125


(*all-R*)-*form*

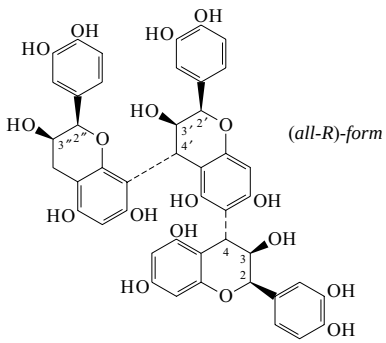
$C_{45}H_{36}O_{18}$ 864.769

(all-R)*-*form
Epicatechin-(4β→6)-epicatechin-(2β→7,4β→8)-epicatechin
Constit. of the fruit of *Vaccinium macrocarpon* (cranberry). Powder. $[\alpha]_D$ +105 (c, 0.15 in MeOH). λ_{max} 282 (log ϵ 4.1) (MeOH).

Foo, L.Y. *et al., J. Nat. Prod.*, 2000, **63**, 1225-1228

3,3′,4′,5,7-Pentahydroxyflavan(4→6)-3,3′,4′,5,7-pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan P-126

2,2′,2″-Tris(3,4-dihydroxyphenyl)-3,3′,3″,4,4′,4″-hexahydro-[4,6′:4′,8″-ter-2H-1-benzopyran]-3,3′,3″,5,5′,5″,7,7′,7″-nonol, 9CI


(*all-R*)-*form*

$C_{45}H_{38}O_{18}$ 866.784

(all-R)*-*form [101469-10-7]
Epicatechin-(4β→6)-epicatechin-(4β→8)-epicatechin
Off-white amorph. powder + 2½H_2O. $[\alpha]_D^{28}$ +138 (c, 1 in Me_2CO).

3,3′,3″-Tris(3,4,5-trihydroxybenzoyl):
[106533-64-6] *Epicatechin 3*-O-*gallate-(4β→6)-epicatechin 3*-O-*gallate-(4β→6)-epicatechin 3*-O-*gallate*
$C_{66}H_{50}O_{30}$ 1323.103
Isol. from *Rheum* sp.. Tan amorph. powder + 3H_2O. $[\alpha]_D^{28}$ -40.7 (c, 0.88 in Me_2CO).

(2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*S*,4*R*,4′*R*)-*form*
[82801-35-2]
Epicatechin-(4β→6)-epicatechin-(4β→8)-catechin
Off-white amorph. powder. $[\alpha]_D^{21}$ +138.2 (c, 0.5 in Me_2CO).

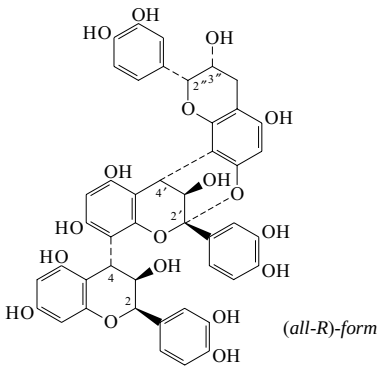
3,3′-Bis(3,4,5-trihydroxybenzoyl):
[106548-99-6] *Epicatechin 3*-O-*gallate-(4β→6)-epicatechin-3*-O-*gallate-(4β→8)-catechin*
$C_{59}H_{46}O_{26}$ 1170.997
Isol. from *Rheum* sp.. Pale brown powder +3½H_2O. Mp 204-205°. $[\alpha]_D^{28}$ +66.1 (c, 0.66 in Me_2CO).

(2*R*,2′*R*,2″*R*,3*S*,3′*R*,3″*R*,4*S*,4′*R*)-*form*
[128779-44-2]
Catechin-(4α→6)-epicatechin-(4β→8)-epicatechin
Pale brown amorph. powder + 1½H_2O. $[\alpha]_D^{21}$ -38 (c, 0.76 in Me_2CO).

[99297-47-9, 106533-66-8]

Porter, L.J. *et al., J.C.S. Perkin 1*, 1982, 1217 (*cmr*)
Hsu, F.L. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3142; 3293 (*isol*)
Ezaki-Furuichi, E. *et al., Agric. Biol. Chem.*, 1986, **50**, 2061 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4083 (*derivs*)
Foo, L.Y. *et al., Phytochemistry*, 1989, **28**, 1743 (*isol*)
Kolodziej, H. *et al., Phytochemistry*, 1990, **29**, 955 (*isol*)

3,3′,4′,5,7-Pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan P-127


(*all-R*)-*form*

$C_{45}H_{36}O_{18}$ 864.769

(all-R)*-*form [114613-62-6]
Epicatechin-(4β→8)-epicatechin-(2β→7,4β→8)-epicatechin. ***Aesculitannin A***
Off-white powder + 2H_2O. $[\alpha]_D^{23}$ +133.6 (c, 0.9 in Me_2CO).

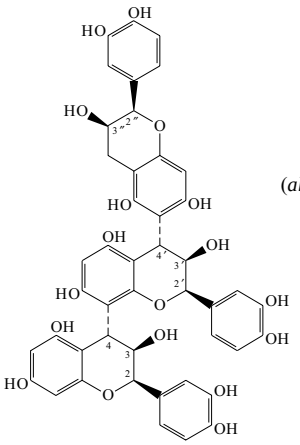
(2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*S*,4*R*,4′*R*)-*form*
[114637-81-9]
Epicatechin-(4β→8)-epicatechin-(2β→7,4β→8)-catechin
Isol. from *Vaccinium vitis-idaea* (cowberry). Off-white powder + 2H_2O. $[\alpha]_D^{18}$ +38.2 (c, 1 in Me_2CO).

(2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*R*,4*S*,4′*R*)-*form*
[162300-83-6]
Epicatechin(4α→8)epicatechin(2β→7,4β→8)epicatechin

Morimoto, S. *et al., Chem. Pharm. Bull.*, 1988, **35**, 4717; **36**, 33 (*isol, struct*)
Santos-Buelga, C. *et al., Phytochemistry*, 1995, **38**, 499 (*isol*)

3,3′,4′,5,7-Pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan(4→6)-3,3′,4′,5,7-pentahydroxyflavan P-128

2,2′,2″-Tris(3,4-dihydroxyphenyl)-3,3′,3″,4,4′,4″-hexahydro-[4,8′:4′,6″-ter-2H-1-benzopyran]-3,3′,3″,5,5′,5″,7,7′,7″-nonol, 9CI



(*all-R*)-form

$C_{45}H_{38}O_{18}$ 866.784

(all-R)-form [88903-74-6]
Epicatechin(4β→8)epicatechin(4β→6)epicatechin
Pale brown amorph. powder + $1H_2O$. $[\alpha]_D$ +126.8 (c, 1.15 in Me_2CO).

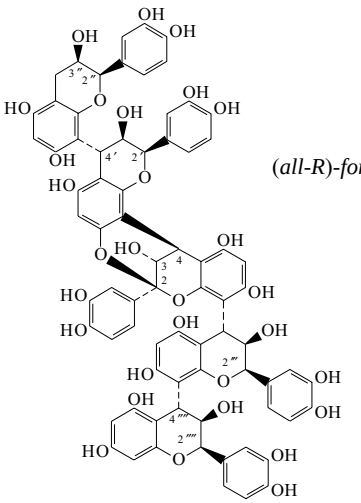
(2R,2′R,2″R,3R,3′R,3″S,4R,4′R)-form [79763-28-3]
Epicatechin (4β→8)epicatechin(4β→6)catechin. ***Arecatannin B1***
Off-white amorph. solid + $^1/_2H_2O$. $[\alpha]_D$ +207 (c, 0.11 in H_2O).

3,3′-Bis(3,4,5-trihydroxybenzoyl): [106533-65-7]
$C_{59}H_{46}O_{26}$ 1170.997
Isol. from *Rheum* sp.. Tan amorph. powder + $4H_2O$. $[\alpha]_D^{28}$ +81.2 (c, 1.09 in Me_2CO).

(2R,2′R,2″R,3S,3′S,3″S,4S,4′S)-form [88244-65-9]
Catechin(4α→8)catechin(4α→6)catechin

Nonaka, G. *et al., Chem. Comm.*, 1981, 781 (*isol*)
Hemingway, R.W. *et al., J.C.S. Perkin 1*, 1982, 1209 (*isol*)
Porter, L.J. *et al., J.C.S. Perkin 1*, 1982, 1217 (*cmr*)
Delcour, J.A. *et al., J.C.S. Perkin 1*, 1983, 1711 (*synth*)
Ezaki-Furuichi, E. *et al., Agric. Biol. Chem.*, 1986, **50**, 2061 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 4083 (*deriv*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1105 (*isol*)
Kolodziej, H. *et al., Phytochemistry*, 1989, **28**, 3487; 1990, **29**, 955 (*isol*)
Cui, C.-B. *et al., Chem. Pharm. Bull.*, 1992, **40**, 889 (*isol, pmr, cmr*)

[3,3′,4′,5,7-Pentahydroxyflavan(4→8)]2-3,3′,4′,5,7-pentahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan P-129



(*all-R*)-form

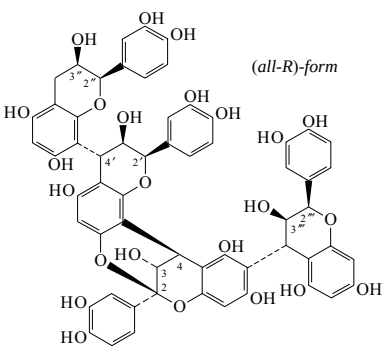
$C_{75}H_{60}O_{30}$ 1441.281

(all-R)-form [88057-90-3]
[Epicatechin(4β→8)]2epicatechin(2β→7,4β→8)epicatechin(4β→8)epicatechin. ***Pavetannin D1***
Isol. from *Cinnamomum zeylanicum* (cinnamon). Pale brown amorph. powder + $3H_2O$. $[\alpha]_D^{25}$ +70.8 (c, 1.1 in Me_2CO).

(3″S)-form [100163-71-1]
[Epicatechin(4β→8)]2epicatechin(2β→7,4β→8)epicatechin(4β→8)catechin
Tan amorph. powder + $3H_2O$. $[\alpha]_D^{24}$ +115.9 (c, 1.1 in Me_2CO).

Nonaka, G. *et al., J.C.S. Perkin 1*, 1983, 2139 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4338 (*isol*)
Balde, A.M. *et al., Phytochemistry*, 1995, **38**, 719 (*Pavetannin D1*)

3,3′,4′,5,7-Pentahydroxyflavan(4→6)-3,3′,4′,5,7-pentahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan P-130



(*all-R*)-form

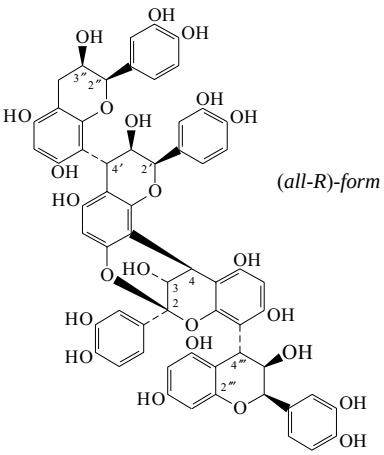
$C_{60}H_{48}O_{24}$ 1153.025

(all-R)-form [88038-15-7]
Epicatechin(4β→6)epicatechin(2β→7,4β→8)epicatechin(4β→8)epicatechin(4β→8)epicatechin. ***Pavetannin C1***
Isol. from *Cinnamomum zeylanicum* (cinnamon). Pale brown amorph. powder + $3H_2O$. $[\alpha]_D$ +93.4 (c, 1.2 in Me_2CO).

(3″S)-form [100163-70-0]
Epicatechin(4β→6)epicatechin(2β→7,4β→8)epicatechin(4β→8)catechin
Tan amorph. powder + $3H_2O$. $[\alpha]_D$ +110.6 (c, 1.1 in Me_2CO).

Nonaka, G. *et al., J.C.S. Perkin 1*, 1983, 2139 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4338 (*isol*)
Balde, A.M. *et al., Phytochemistry*, 1995, **38**, 719 (*Pavetannin C1*)

3,3′,4′,5,7-Pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan P-131



(*all-R*)-form

$C_{60}H_{48}O_{24}$ 1153.025

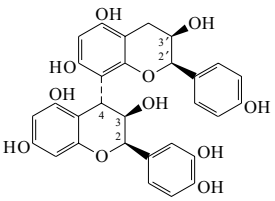
(all-R)-form [88038-12-4]
Epicatechin(4β→8)epicatechin(2β→7,4β→8)epicatechin(4β→8)epicatechin(4β→8)epicatechin. ***Cinnamtannin B2***
Isol. from *Cinnamomum zeylanicum* (cinnamon) and *Vaccinium vitis-idaea* (cowberry). Pale brown amorph. powder + $3H_2O$. $[\alpha]_D$ +51.1 (c, 1 in Me_2CO).

(3″S)-form [97233-47-1]
Epicatechin(4β→8)epicatechin(2β→7,4β→8)epicatechin(4β→8)epicatechin(4β→8)catechin. ***Cinnamtannin D2***
Isol. from *Vaccinium vitis-idaea* (cowberry). Tan amorph. powder + $3H_2O$. $[\alpha]_D^{24}$ +85.6 (c, 1.1 in Me_2CO).

Nonaka, G. *et al., J.C.S. Perkin 1*, 1983, 2139 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4338; 1987, **35**, 4717; 1988, **36**, 33 (*isol*)
Ezaki, N. *et al., Planta Med.*, 1985, 34 (*isol*)
Balde, A.M. *et al., Phytochemistry*, 1995, **38**, 719 (*isol*)

3,3′,4′,5,7-Pentahydroxyflavan(4→8)-3,4′,5,7-tetrahydroxyflavan P-132

[80685-13-8]
[4′,8″-Biflavan]-3,3′,3″,4′,4‴,5,5″,7,7″-nonol, 8CI


(*all-R*)-*form*

$C_{30}H_{26}O_{11}$ 562.529
Isol. from azuki bean (*Vigna angularis*) seeds.

(*all-R*)-*form* [98104-38-2]
Epicatechin(4β→8)epiafzelechin
Powder + $2H_2O$. $[\alpha]_D^{20}$ +32.3 (c, 0.6 in MeOH).

(2*R*,2′*R*,3*S*,3′*R*,4*S*)-*form*
Catechin(4α→8)epiafzelechin
Nona-Ac: [21179-24-8]
Cryst. (EtOH). Mp 166-167°. $[\alpha]_D^{25}$ -179.6 (c, 2 in Me_2CO).

(2*R*,2′*S*,3*R*,3′*S*,4*R*)-*form* [130981-96-3]
*Epicatechin(4β→8)*ent-*epiafzelechin*

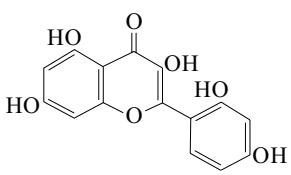
(2*S*,2′*R*,3*S*,3′*R*,4*S*)-*form* [130982-00-2] ent-*Epicatechin(4α→8)epiafzelechin*

(all-*S*)-*form* [130982-03-5] ent-*Epicatechin(4α→8)*ent-*epiafzelechin*

Weinges, K. *et al., Annalen*, 1968, **715**, 164 (*isol*)
Ariga, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 2709 (*isol*)
Middelkoop, T.B. *et al., Z. Naturforsch., B*, 1985, **40**, 855 (*isol*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 39 (*isol*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 888 (*isol, pmr*)

2′,3,4′,5,7-Pentahydroxyflavone P-133

[480-16-0]
*2-(2,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one, 9CI. 2′,4′,5,7-Tetrahydroxyflavonol. **Morin**. 2′-Hydroxypelargidenolon 1522. C.I. Natural yellow 8. C.I. Natural yellow 11. C.I. 75660*



$C_{15}H_{10}O_7$ 302.24
Constit. of various woods, e.g. *Morus alba* (white mulberry). First isol. in 1830. Pale yellow needles + $1H_2O$ (AcOH aq.). Sol. EtOH, alkalis; sl. sol. Et_2O, H_2O. Mp 303-304°. Log P -0.36 (calc).

► LD_{50} (mus, ipr) 555 mg/kg. LK8749000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 96C (*ir*)
Perkin, W.H. *et al., J.C.S.*, 1895, **67**, 649; 1896, **69**, 792 (*isol, struct*)
von Kostanecki, S. *et al., Ber.*, 1906, **39**, 625; 4014; 4022 (*synth*)
Robinson, R. *et al., J.C.S.*, 1929, 61
Perkins, R.W. *et al., Anal. Chem.*, 1956, **28**, 1898 (*detn, Th*)
Dave, K.G. *et al., Tet. Lett.*, 1962, 9 (*isol*)
Kovalev, I.P. *et al., Zh. Obshch. Khim.*, 1963, **33**, 1670 (*ir*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Paris, R. *et al., Ann. Pharm. Fr.*, 1966, **24**, 745 (*isol, Moroside*)
Sasaki, S. *et al., Yakugaku Zasshi*, 1966, **86**, 869 (*isol*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 20
Mirenskaya, I.I. *et al., Khim. Prir. Soedin.*, 1970, **6**, 767; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 781 (*uv, purifn*)
Shnaiderman, S.Ya. *et al., Zh. Anal. Khim.*, 1970, **25**, 2368 (*detn, V*)
Blank, A.B. *et al., Zh. Anal. Khim.*, 1973, **28**, 1331; 1976, **31**, 703; 1978, **33**, 65 (*detn, Zr, rare earths*)
Olenovich, N.L. *et al., Zh. Anal. Khim.*, 1974, **29**, 47 (*detn, In*)
Chang, C.-J. *et al., J. Nat. Prod.*, 1978, **41**, 17 (*cmr*)
Yinon, J. *et al., Org. Mass Spectrom.*, 1978, **13**, 167 (*ms*)
Cody, V. *et al., Plant Flavonoids in Biology and Medicine II*, A.R. Liss, N.Y., 1988, (*biochem*)
Onishi, H. *et al., Photometric Determination of Traces of Metals, Part IIb: Individual Metals. Magnesium to Zinc*, John Wiley, New York, 4th Ed., 1989, 765
Ono, K. *et al., Eur. J. Biochem.*, 1990, **190**, 469 (*anti-HIV activity*)
Cody, V. *et al., J. Mol. Struct.*, 1994, **317**, 89 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MRN500

3,3′,4′,5,7-Pentahydroxyflavone P-134

[117-39-5]
*2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one, 9CI. 3′,4′,5,7-Tetrahydroxyflavonol. **Quercetin**. Sophoretin. Meletin. Quercetol. Quertin. Ericin*†

$C_{15}H_{10}O_7$ 302.24
Many methyl ethers and common glycosides have individual entries. Isol. from many plants, esp. fruits, such as *Helichrysum*, *Euphorbia* and *Karwinskia* spp. Present in the Solanaceae, Rhamnaceae, Passifloraceae and many other families. For example detected in almost all studied Umbelliferae. Nutriceutical with antiinflammatory props. and a positive influence on the blood lipid profile. Found in a wide variety of foodstuffs esp. apples, bee pollen, blackcurrants, capers, cocoa, cranberries, dock leaves, elderberries, fennel, lovage, red onions, ancho peppers, dill weed and tarragon. Yellow cryst. + $2H_2O$ (EtOH aq.). Sol. EtOH, Et_2O, bases; poorly sol. H_2O, hexane, $CHCl_3$. Mp 313-314° dec. Log P -0.29 (calc). λ_{max} 258 (ε 20900); 375 (ε 20900) (EtOH) (Berdy).

► LD_{50} (mus, orl) 159 mg/kg. Exp. reprod. effects. LK8750000

3-O-α-L-Arabinopyranoside: [22255-13-6] ***Guaijaverin***. *Foeniculin*†. *Guaiaverin*
$C_{20}H_{18}O_{11}$ 434.356
Obt. from leaves of guava (*Psidium guajava*) and from other plants. Bright yellow needles + H_2O (EtOH aq.). Sol. EtOH, Et_2O, bases; poorly sol. H_2O, hexane. Mp 256° (anhyd.) Mp 239° (hydrate). λ_{max} 256 ; 260 (ε 28200); 269 ; 358 ; 360 (ε 24000) (EtOH) (Berdy).

7-O-β-D-Xylopyranoside: [82178-32-3]
$C_{20}H_{18}O_{11}$ 434.356
Isol. from the famine food *Adansonia digitata* (baobab). Mp 245-247°.

3-O-β-D-Glucuronopyranoside: [22688-79-5] *Quercetin 3-glucuronide*. ***Miquelianin***. *Querciturone*
$C_{21}H_{18}O_{13}$ 478.365
Present in red wine. Yellow needles (MeOH aq.). Mp 193-195° (190-191°). $[\alpha]_D^{30}$ -48.2 (c, 0.835 in Py aq.).

3-O-[3,4-Dihydroxycinnamoyl-(→2)-β-D-glucuronopyranoside]:Quercetin 3-(2-caffeoylglucuronoside)
$C_{30}H_{24}O_{16}$ 640.51
Constit. of Spanish oysterplant (*Scolymus hispanicus*).

4′-O-β-D-Glucuronopyranoside: [201463-36-7] *Quercetin 4′-glucuronide*
$C_{21}H_{18}O_{13}$ 478.365
Constit. of guava.

3-O-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside]: [83048-35-5] *Quercetin 3-(2-xylosylglucoside). Quercetin 3-sambubioside*
$C_{26}H_{28}O_{16}$ 596.498
Isol. from *Actinidia arguta* (tara vine). $[\alpha]_D^{20}$ -65 (c, 0.38 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranoside]: [86749-52-2]
$C_{26}H_{28}O_{15}$ 580.498
Isol. from seeds of black mustard (*Brassica nigra*). Yellow needles + $4H_2O$ (MeOH aq.). Mp 194-195°.

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [32453-36-4] ***Calendoflavobioside***. *Quercetin 3-neohesperidoside*
$C_{27}H_{30}O_{16}$ 610.524
Isol. from some *Solanum* spp..

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [147714-62-3] *Quercetin 7-rutinoside*
$C_{27}H_{30}O_{16}$ 610.524
Isol. form *Capparis spinosa* (caper). Yellow cryst.(MeOH aq.). Mp 218-222° (178-179). $[\alpha]_D$ -48.5 (c, 0.65 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 7-O-β-D-glucuronopyranoside: [140163-57-1] *Quercetin 7-glucuronoside 3-sophoroside*
$C_{33}H_{38}O_{23}$ 802.649
Isol. from the leaves of onion (*Allium cepa*). Yellow-green powder.

3-O-[β-D-Glucopyranosyl-(1→?)-β-D-glucuronopyranoside]: [93252-57-4] ***Nelumboside***
$C_{27}H_{28}O_{18}$ 640.507
Isol. from leaves of fennel (*Foeniculum vulgare*). Yellow needles (H_2O). Mp 174-175°. $[\alpha]_D^{26}$ -21.1 (H_2O).

3-O-[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]: [55780-29-5]
$C_{33}H_{40}O_{21}$ 772.666
Isol. from soya bean leaves (*Glycine*

max).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]:* [55696-56-5]
$C_{33}H_{40}O_{22}$ 788.666
Isol. from soya bean leaves (*Glycine max*).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [38681-85-5] *Quercetin 3-sophorotrioside*
$C_{33}H_{40}O_{22}$ 788.666
Isol. from *Pisum sativum* (pea).

3-O-*[3,4-Dihydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:Quercetin 3-(6″-caffeoylsophorotrioside)*
$C_{42}H_{46}O_{25}$ 950.81
Constit. of pea (*Pisum sativum*).

3-O-*[4-Hydroxy-3,5-dimethoxy*-E-*cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:Quercetin 3-(6″-sinapoylsophorotrioside)*
$C_{44}H_{50}O_{26}$ 994.863
Constit. of pea (*Pisum sativum*).

3-O-*[4-Hydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{42}H_{46}O_{24}$ 934.811
Isol. from pea (*Pisum sativum*).

3-O-*[4-Hydroxy-3-methoxy*-E-*cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:Quercetin 3-(feruloylsophorotrioside)*
$C_{43}H_{48}O_{25}$ 964.837
Isol. from pea (*Pisum*) spp..

3,7-Di-Me ether, 5-O-*β-D-glucopyranoside:* [128388-46-5] *3′,4′,5-Trihydroxy-3,7-dimethoxyflavone 5-glucoside*
$C_{23}H_{24}O_{12}$ 492.435
Isol. from maize (*Zea mays*) whorl tissue.

3′,4′,5,7-Tetra-Me ether, 3-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [58528-03-3]
$C_{31}H_{38}O_{16}$ 666.632
Isol. from tartary buckwheat (*Fagopyrum tataricum*) leaves.

[6151-25-3, 6743-88-0, 7215-44-3, 7678-36-6, 27214-55-7, 90332-36-8, 103666-99-5, 116097-14-4, 120537-33-9]

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3′,4′,5,5′,7-Pentahydroxyflavone P-135

[520-31-0]
5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Tricetin***

$C_{15}H_{10}O_7$ 302.24
Constit. of the seed coat of lentil (*Lens culinaris*). Yellow needles + H_2O (EtOH aq.). Mp 310° Mp 330°.

3′-O-*Sulfate:* [59176-59-9]
$C_{15}H_{10}O_{10}S$ 382.304

3′,7-Di-O-*sulfate:* [59176-60-2]
$C_{15}H_{10}O_{13}S_2$ 462.368

3′-O-*β-D-Xylopyranoside:* [117247-36-6]
$C_{20}H_{18}O_{11}$ 434.356

3′-O-*β-D-Glucopyranoside:* [22149-72-0]
$C_{21}H_{20}O_{12}$ 464.382
Needles (Me_2CO aq.). Mp 284-285°.

3′-O-*β-D-Glucopyranoside, 5′*-O-*α-L-rhamnopyranoside:* [261912-74-7] *Tricetin 3′-glucoside 5′-rhamnoside*
$C_{27}H_{30}O_{16}$ 610.524
λ_{max} 255 ; 270 ; 347 (MeOH).

7-O-*β-D-Glucopyranoside:* [77298-67-0]
$C_{21}H_{20}O_{12}$ 464.382

7-O-*β-D-Glucopyranoside, 3′*-O-*[3-hydroxy-3-methylglutaroyl-(→6)-β-D-glucopyranoside]:* [151750-87-7]
$C_{33}H_{38}O_{21}$ 770.651

3′,5′-Di-O-*β-D-glucopyranoside:* [93373-19-4]
$C_{27}H_{30}O_{17}$ 626.524

3′,7-Di-O-*β-D-glucuronopyranoside:* [107721-49-3]
$C_{27}H_{26}O_{19}$ 654.491

3′-O-*[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranoside]:* [261912-75-8]
$C_{27}H_{30}O_{15}$ 594.525
λ_{max} 255 ; 270 ; 347 (MeOH).

7-O-*[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:* [80668-06-0]
$C_{27}H_{30}O_{17}$ 626.524

Penta-Ac: [86918-84-5]
$C_{25}H_{20}O_{12}$ 512.426
No. phys. props. reported.

3′-Me ether: [60303-28-8] *3′,4′,5,7-Tetrahydroxy-5′-methoxyflavone.* ***Selagin****. Selgin*
$C_{16}H_{12}O_7$ 316.267
Cryst. (MeOH). Mp 320-325° dec.

3′-Me ether, 7-O-*β-D-glucopyranoside:* [73413-70-4]
$C_{22}H_{22}O_{12}$ 478.409
Small needles (MeOH aq.). Mp 265-270°.

3′-Me ether, 7-O-*β-D-glucuronopyranoside:*
$C_{22}H_{20}O_{13}$ 492.392
Constit. of the aerial parts of alfalfa (*Medicago sativa*). Amorph. yellow powder. Mp 219-220°. $[\alpha]_D^{24}$ -27.6 (c, 0.1 in MeOH/DMSO aq.).

*3′-Me ether, 5′,7-di-*O*-β-D-glucuronopyranoside:* [107668-77-9]
$C_{28}H_{28}O_{19}$ 668.518

4′-Me ether: [90745-22-5] *3′,5,5′,7-Tetrahydroxy-4′-methoxyflavone*
$C_{16}H_{12}O_7$ 316.267

*4′-Me ether, 7-*O*-[β-D-apiofuranosyl-(1→2)-6-*O*-acetyl-β-D-glucopyranoside]:*
$C_{29}H_{32}O_{17}$ 652.562
Pale yellow powder. Mp 230-232°. λ_{max} 267 (log ε 4.34); 334 (log ε 4.32) (MeOH).

*7-Me ether, 3′-*O*-β-D-glucopyranoside, 5′-*O*-α-L-rhamnopyranoside:* [261912-73-6]
$C_{28}H_{32}O_{16}$ 624.551
λ_{max} 250 ; 270 ; 350 (MeOH).

3′,4′-Di-Me ether: [76900-87-3] *3′,5,7-Trihydroxy-4′,5′-dimethoxyflavone.* ***Apometzgerin***
$C_{17}H_{14}O_7$ 330.293
No phys. props. reported.

*3′,4′-Di-Me ether, 7-*O*-β-D-glucuronopyranoside:* [107668-76-8]
$C_{23}H_{22}O_{13}$ 506.419
Cryst.

3′,5-Di-Me ether: [188885-68-9] *3′,4′,7-Trihydroxy-5,5′-dimethoxyflavone.* ***Gramrione***
$C_{17}H_{14}O_7$ 330.293

3′,5′-Di-Me ether: 4′,5,7-Trihydroxy-3′,5′-dimethoxyflavone, T-549

3′,4′,5′-Tri-Me ether: [18103-42-9] *5,7-Dihydroxy-3′,4′,5′-trimethoxyflavone*
$C_{18}H_{16}O_7$ 344.32
Isol. from leaves of barley (*Hordeum vulgare*). Cryst. (AcOH). Mp 272-274°.

*3′,4′,5′-Tri-Me ether, 7-*O*-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [289915-88-4]
$C_{30}H_{36}O_{16}$ 652.605
Constit. of wheat (*Triticum aestivum*) leaves. λ_{max} 270 ; 311 (sh) ; 331 (MeOH).

3′,4′,7-Tri-Me ether: [178664-72-7] *3′,5-Dihydroxy-4′,5′,7-trimethoxyflavone.* ***Lethedocin***
$C_{18}H_{16}O_7$ 344.32
Yellow needles (MeOH). Mp 194-195°. λ_{max} 210 (log ε 4.6); 240 (log ε 4.2); 270 (log ε 4.1); 334 (log ε 4.2) (EtOH).

*3′,4′,7-Tri-Me ether, 5-*O*-β-D-glucopyranoside:* ***Lethedoside C***
$C_{24}H_{26}O_{12}$ 506.462
Amorph. solid. $[\alpha]_D^{20}$ -61.6 (c, 0.36 in Py). λ_{max} 207 (log ε 4.7); 239 (log ε 4.4); 263 (log ε 4.1); 330 (log ε 4.3) (MeOH).

3′,5′,7-Tri-Me ether: [107316-94-9] *4′,5-Dihydroxy-3′,5′,7-trimethoxyflavone*
$C_{18}H_{16}O_7$ 344.32
Yellow cryst. (EtOH). Mp 218-220°.

3′,4′,5′,7-Tetra-Me ether: [18103-41-8] *5-Hydroxy-3′,4′,5′,7-tetramethoxyflavone.* ***Corymbosin***†
$C_{19}H_{18}O_7$ 358.347
Mp 188-189°.

*3′,4′,5′,7-Tetra-Me ether, 5-*O*-β-D-glucopyranoside:* ***Lethedoside B***
$C_{25}H_{28}O_{12}$ 520.489
Amorph. solid. $[\alpha]_D^{20}$ -33.4 (c, 0.32 in Py). λ_{max} 207 (log ε 4.6); 237 (log ε 4.4); 265 (log ε 4.1); 323 (log ε 4.2) (MeOH).

*3′,4′,5′,7-Tetra-Me ether, 5-*O*-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Lethedioside B***
$C_{30}H_{36}O_{16}$ 652.605
Amorph. solid. $[\alpha]_D^{20}$ -51.5 (c, 0.34 in Py). λ_{max} 213 (log ε 4.8); 239 (log ε 4.5); 262 (log ε 4.4); 325 (log ε 4.5) (MeOH).

Penta-Me ether: [53350-26-8] *3′,4′,5,5′,7-Pentamethoxyflavone*
$C_{20}H_{20}O_7$ 372.374
Needles (MeOH), prisms ($CHCl_3$). Mp 196-197° (193°).

*4′-*O*-(3-Methyl-2-butenyl), 3′,5′,7-tri-Me ether:5-Hydroxy-3′,5′,7-trimethoxy-4′-prenyloxyflavone*
$C_{23}H_{24}O_7$ 412.438
Brown oil. λ_{max} 245 (log ε 3.97); 333 (log ε 3.98); 380 (sh) (log ε 3.43) (MeOH).

3′,4′-Methylene, 5,5′,7′-tri-Me ether: [89029-11-8] *5,5′,7-Trimethoxy-3′,4′-methylenedioxyflavone*
$C_{19}H_{16}O_7$ 356.331
Prisms (MeOH). Mp 244-246°.

4′,5′-Methylene, 3′,7-di-Me ether:5-Hydroxy-3′,7-dimethoxy-4′,5′-methylenedioxyflavone
$C_{18}H_{14}O_7$ 342.304
Brown oil. λ_{max} 260 (log ε 3.32); 332 (log ε 3.09); 380 (sh) (log ε 2.98) (MeOH).

[28472-41-5]

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Harder, L.H. *et al., Z. Naturforsch., C*, 2000, **55**, 337-340 (*3′,4′,5′-tri Me 7-rutinoside*)
Stochmal, A. *et al., J. Agric. Food Chem.*, 2001, **49**, 5310-5314 (*3′-Me 7-glucuronide*)
Amaral, D.F. *et al., J. Braz. Chem. Soc.*, 2001, **12**, 538-541 (*Ficus gomelleira derivs*)

3,4′,5,6,7-Pentahydroxyflavone P-136

[4324-55-4]
*3,5,6,7-Tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 4′,5,6,7-Tetrahydroxyflavonol.* ***Galetin****. 6-Hydroxykaempferol*

$C_{15}H_{10}O_7$ 302.24
Yellow cryst. (EtOH/Me_2CO). Mp 328-330°.

*7-*O*-β-D-Allopyranoside:* [205496-87-3]
$C_{21}H_{20}O_{12}$ 464.382
Constit. of the flowers of *Tagetes erecta* (African marigold).

*3-*O*-β-D-Glucopyranoside:* [145134-61-8]
$C_{21}H_{20}O_{12}$ 464.382
Isol. from the dried petals of *Carthamus tinctorius* (safflower). Yellow needles (MeOH). Mp 263-265°.

*7-*O*-β-D-Glucopyranoside:* [70056-55-2]
$C_{21}H_{20}O_{12}$ 464.382
Isol. from *Tagetes erecta* (African marigold). No phys. props. reported.

*3,6-Di-*O*-β-D-glucopyranoside, 7-*O*-β-D-glucuronopyranoside:*
$C_{33}H_{38}O_{23}$ 802.649
Constit. of fresh florets of *Carthamus tinctorius* (safflower). Amorph. powder. λ_{max} 268 (log ε 4.33); 340 (log ε 4.32) (MeOH).

*6,7-Di-*O*-β-D-glucopyranoside:*
$C_{27}H_{30}O_{17}$ 626.524
Constit. of the flowers of *Carthamus tinctorius* (safflower). Light yellow prisms. Mp 187° dec. $[\alpha]_D^{25}$ -66.2 (c, 0.08 in MeOH). λ_{max} 257 ; 269 ; 365 (MeOH).

*6,7-Methylene, 3-Me ether, 4′-*O*-β-D-glucuronopyranoside:*
$C_{23}H_{20}O_{13}$ 504.403
Constit. of spinach (*Spinacia oleracea*).

Bacon, J.D. *et al., Phytochemistry*, 1978, **17**, 1939 (*7-glucoside*)
Ulubelen, A. *et al., J. Nat. Prod.*, 1981, **44**, 457 (*7-glucoside*)

The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Hattori, M. *et al., Phytochemistry*, 1992, **31**, 4001 (*isol, pmr, cmr, glycosides*)
Das, K.C. *et al., Fitoterapia*, 1997, **68**, 477 (*7-alloside*)
Kazuma, K. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1588-1599 (*3,6-diglucoside 7-glucuronide*)
Bergman, M. *et al., Phytochemistry*, 2001, **58**, 143-152 (*6,7-methylene 3-Me 4′-glucuronide*)
Li, F. *et al., Chin. J. Chem.*, 2002, **20**, 699-702 (*6,7-diglucoside*)

3′,4′,5,6,7-Pentahydroxyflavone P-137

[18003-33-3]
*2-(3,4-Dihydroxyphenyl)-5,6,7-trihydroxy-4*H*-1-benzopyran-4-one.* ***6-Hydroxyluteolin***

$C_{15}H_{10}O_7$ 302.24
Isol. from *Valerianella eriocarpa* (Italian corn salad). Plates (EtOAc). Mp 284°.

6-O-*β*-D-*Xylopyranoside:* [65876-67-7]
$C_{20}H_{18}O_{11}$ 434.356
Isol. from *Juniperus communis* (juniper).

3′,4′,5,6-Tetra-Me ether: [40983-99-1] *7-Hydroxy-3′,4′,5,6-tetramethoxyflavone*
$C_{19}H_{18}O_7$ 358.347
Isol. from *Citrus reticulata* (manadarin orange). Needles ($CHCl_3$/hexane). Mp 205-208°.

Penta-Me ether: [2306-27-6] *3′,4′,5,6,7-Pentamethoxyflavone.* ***Sinensetin***
$C_{20}H_{20}O_7$ 372.374
Found in orange peel and other plant sources. Pale yellow prisms (Me_2CO), cryst. (EtOH). Mp 179° (172-173°).

Farkas, L. *et al., Chem. Ber.*, 1969, **102**, 112 (*synth, derivs*)
Greger, H. *et al., Phytochemistry*, 1973, **12**, 1693-1699 (*isol*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 708 (*cmr, derivs*)
Lamer-Zorawska, E. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1980, **54**, 213-219 (*6-xylopyranoside*)
Laux, D.O. *et al., Phytochemistry*, 1985, **24**, 1081 (*7-Hydroxy-3′,4′,5,6-tetramethoxyflavone, Bausplendin*)
Horie, T. *et al., Yakugaku Zasshi*, 1985, **105**, 232 (*synth, derivs*)
Mizuno, M. *et al., J. Nat. Prod.*, 1987, **50**, 751 (*7-Hydroxy-3′,4′,5,6-tetramethoxyflavone*)
Kraut, L. *et al., Phytochemistry*, 1993, **34**, 211; 1999, **52**, 749 (*isol, derivs*)

3,4′,5,6,8-Pentahydroxyflavone P-138

*3,5,6,8-Tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one. 4′,5,6,8-Tetrahydroxyflavonol*

$C_{15}H_{10}O_7$ 302.24
Bright yellow prisms. Mp 258-260°.

3,4′,8-Tri-Me ether:5,6-Dihydroxy-3,4′,8-trimethoxyflavone
$C_{18}H_{16}O_7$ 344.32
Orange-yellow needles (MeOH). Mp 188.5-189.5°. Formerly thought to occur in *Conyza stricta*; however, this compd. was shown to be the 5,7-dihydroxy isomer.

3,6,8-Tri-Me ether: [112667-10-4] *4′,5-Dihydroxy-3,6,8-trimethoxyflavone*
$C_{18}H_{16}O_7$ 344.32
Needles (MeOH). Struct. formerly allocated to Candirone see 3,4′,5,6,7-Pentahydroxyflavone, P-136.

Penta-Me ether: [62953-03-1] *3,4′,5,6,8-Pentamethoxyflavone*
$C_{20}H_{20}O_7$ 372.374
Constit. of *Citrus reticulata* (mandarin) leaves. Needles (EtOH). Mp 142-144°.

Balakrishna, K.J. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1948, **27**, 260 (*synth*)
Horie, T. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2933 (*synth, struct*)
Horie, T. *et al., Phytochemistry*, 1994, **37**, 1189 (*synth, deriv*)
Abdel-Alim, M.A. *et al., Egypt. J. Pharm. Sci.*, 1997, **38**, 131-136 (*Pentamethoxyflavone, isol*)

3,4′,5,7,8-Pentahydroxyflavone P-139

[527-95-7]
*3,5,7,8-Tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7,8-Tetrahydroxyflavonol.* ***Herbacetin****. Isoarticulatidin. 8-Hydroxykaempferol*

$C_{15}H_{10}O_7$ 302.24
Yellow cryst. + $1H_2O$ (EtOH aq.). Mp 280-283°.

3,8-Di-O-*β*-D-*glucopyranoside:* [99224-12-1] *Herbacetin 3,8-diglucoside*
$C_{27}H_{30}O_{17}$ 626.524
Constit. of the leaves of *Linum usitatissimum* (flax).

7-Me ether: [24487-56-7] *3,4′,5,8-Tetrahydroxy-7-methoxyflavone. 4′,5,8-Trihydroxy-7-methoxyflavonol.* ***Pollenitin***
$C_{16}H_{12}O_7$ 316.267
Isol. from the pollen of *Camellia sinensis* (tea). Yellow needles (AcOH). Mp 285°.

7-Me ether, 3-O-*β*-D-*glucopyranoside:* [30484-94-7] ***Pollenin B***
$C_{22}H_{22}O_{12}$ 478.409
Isol. from the pollen of *Camellia sinensis* (tea). Pollenin C also isol. (struct. not deriv.).

7-Me ether, 3-O-*[α-L-rhamnopyranosyl-(1→?)-β-D-glucopyranoside]:* [25134-24-1] ***Pollenin A***
$C_{28}H_{32}O_{16}$ 624.551
Isol. from pollen of *Camellia sinensis* (tea). Yellow cryst. Mp 154-155°.

Sakamoto, Y. *et al., Agric. Biol. Chem.*, 1969, **33**, 818 (*Pollenitin*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1978, **33**, 831-835 (*Pollenitin*)
Ross, S.A. *et al., Herba Pol.*, 1984, **30**, 91-95 (*3,8-diglucoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Hussein, S.A.M. *et al., Phytochemistry*, 1997, **45**, 1529-1532 (*3-rhamnoside 8-glucoside, Pollenitin, cmr*)

3′,4′,5′,7,8-Pentahydroxyflavone P-140

$C_{15}H_{10}O_7$ 302.24

3′-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 8*-O-*β*-D-*glucopyranoside:* [219135-83-8]
$C_{33}H_{40}O_{21}$ 772.666

3′,4′,5′-Tri-Me ether: [79492-68-5] *7,8-Dihydroxy-3′,4′,5′-trimethoxyflavone.* ***Isoprosogerin E***
$C_{18}H_{16}O_7$ 344.32
Mp 275-276°.

4′,5′,7-Tri-Me ether: [133343-00-7] *3′,8-Dihydroxy-4′,5′,7-trimethoxyflavone*
$C_{18}H_{16}O_7$ 344.32
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Pale yellow prisms (MeOH). Mp 225-227° dec. λ_{max} 242 (ϵ 16600); 269 (ϵ 19200); 310 (ϵ 19200) ($CHCl_3$) (Berdy).

4′,5′,7,8-Tetra-Me ether: [133342-98-0] *3′-Hydroxy-4′,5′,7,8-tetramethoxyflavone*
$C_{19}H_{18}O_7$ 358.347
Constit. of the roots of *Muntingia calabura* (Jamaican cherry). Needles (MeOH). Mp 212-213°. λ_{max} 242 (ϵ 20000); 253 (ϵ 15900); 263 (ϵ 14800); 312 (ϵ 24000) ($CHCl_3$) (Berdy).

Penta-Me ether: [133342-97-9] *3′,4′,5′,7,8-Pentamethoxyflavone*
$C_{20}H_{20}O_7$ 372.374
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Prisms (MeOH). Mp 206°. λ_{max} 241 (ϵ 22000); 316 (ϵ 25000) ($CHCl_3$) (Berdy).

Bhardwaj, D.K. *et al., Proc. Indian Natl. Sci. Acad., Part A*, 1982, **48**, 257 (*Isoprosogerin E*)
Kaneda, N. *et al., J. Nat. Prod.*, 1991, **54**, 196 (*derivs*)
Cushman, M. *et al., J. Nat. Prod.*, 1991, **54**, 1345 (*synth, derivs*)
Kandil, F.E. *et al., Orient. J. Chem.*, 1998, **14**, 215-216 (*8-glucoside-3′-rutinoside*)

3′,4′,5,7,8-Pentahydroxyflavone P-141

[27696-41-9]
*2-(3,4-Dihydroxyphenyl)-5,7,8-trihydroxy-4*H*-1-benzopyran-4-one, 9CI.* ***Hypoletin****. Hypolaetin. 8-Hydroxyluteolin*

$C_{15}H_{10}O_7$ 302.24
Deep yellow microneedles or yellow cryst. Mp 243-245° Mp 296°.

8-O-*Sulfate:*
$C_{15}H_{10}O_{10}S$ 382.304
Isol. from annatto (*Bixa orellana*).

8-O-*β*-D-*Glucopyranoside, 3′*-O-*sulfate:* [63109-34-2]
$C_{21}H_{20}O_{15}S$ 544.446
Isol. from high mallow (*Malva sylvestris*). CAS no. refers to K salt.

8-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [115921-09-0] *Hypoletin 8-gentiobioside*
$C_{27}H_{30}O_{17}$ 626.524
Isol. from *Althaea officinalis* (marsh mallow).

3′,7-Di-Me ether, 8-O-*β*-D-*glucopyranoside:* [100997-33-9]
$C_{23}H_{24}O_{12}$ 492.435
Constit. of sugar cane syrup.

3′,8-Di-Me ether, 7-O-*β*-D-*glucopyranoside:* [135043-85-5]
$C_{23}H_{24}O_{12}$ 492.435
Isol. from Italian millet (*Setaria italica*) leaves. Yellow needles. Mp 325° dec.

3′,4′,7,8-Tetra-Me ether: [13003-74-2] *5-Hydroxy-3′,4′,7,8-tetramethoxyflavone*

$C_{19}H_{18}O_7$ 358.347
Constit. of bergamot oil. Mp 210-212°.

Penta-Me ether: [17290-70-9] *3′,4′,5,7,8-Pentamethoxyflavone.* ***Isosinensetin***
$C_{20}H_{20}O_7$ 372.374
Isol. from *Citrus* spp. and the round kumquat (*Fortunella japonica*). Cryst. (EtOH). Mp 206-207°.

[63109-34-2]

Harborne, J.B. *et al., Phytochemistry*, 1969, **8**, 2071 (*isol, uv*)
Harborne, J.B. *et al., Phytochemistry*, 1975, **14**, 1331 (*8-sulfate*)
Nawwar, M.A.M. *et al., Phytochemistry*, 1977, **16**, 145 (*8-glucoside 3′-sulfate*)
Iinuma, M. *et al., Yakugaku Zasshi*, 1980, **100**, 657 (*Isosinensetin*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1984, **32**, 551 (*Isosinensetin, ms*)
Patron, N.H. *et al., Int. Sugar J.*, 1985, **87**, 213-215 (*3′,7-di-Me ether 8-glucoside*)
Jain, N. *et al., Phytochemistry*, 1991, **30**, 1345 (*3′,8-di-Me ether 7-glucoside*)

3,4′,6,7,8-Pentahydroxyflavone P-142

[4443-08-7]
3,6,7,8-Tetrahydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 4′,6,7,8-Tetrahydroxyflavonol. Norauranetin

$C_{15}H_{10}O_7$ 302.24
Yellow cryst. (EtOH). Mp 360° (dec. from 270-280°).

Penta-Me ether: [522-16-7] *3,4′,6,7,8-Pentamethoxyflavone.* ***Auranetin***. *Aurantin*†
$C_{20}H_{20}O_7$ 372.374
Isol. from orange peel (*Citrus aurantium*). Colourless to pale yellow needles (EtOH). Mp 141°.
► LK9225000

Sarin, P.S. *et al., Tetrahedron*, 1960, **8**, 64 (*Auranetin*)

4′,5,6,7,8-Pentahydroxyflavone P-143

[577-26-4]
5,6,7,8-Tetrahydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI

$C_{15}H_{10}O_7$ 302.24
Cryst. (EtOAc/hexane). Mp 330°.

6,8-Di-O-β-D-glucopyranoside: [90456-53-4] ***Vicinin 2***
$C_{27}H_{30}O_{17}$ 626.524
Constit. of lemon (*Citrus limon*) peel and sugar cane syrup.

4′,6-Di-Me ether:5,7,8-Trihydroxy-4′,6-dimethoxyflavone. ***Pilosin***
$C_{17}H_{14}O_7$ 330.293
Constit. of *Ocimum americanum* var. *pilosum* and *Ocimum* x *citriodorum* (lemon basil). Amorph. yellow-brown solid. λ_{max} 287 (sh) ; 299 ; 332 (MeOH).

6,8-Di-Me ether: [4323-80-2] *4′,5,7-Trihydroxy-6,8-dimethoxyflavone.* ***Desmethoxysudachin***. *Demethoxysudachitin*
$C_{17}H_{14}O_7$ 330.293
Isol. from *Citrus sudachi* and *Mentha piperita*. Cryst. (EtOH). Mp 277-279°.

6,7,8-Tri-Me ether: [16545-23-6] *4′,5-Dihydroxy-6,7,8-trimethoxyflavone.* ***Xanthomicrol***
$C_{18}H_{16}O_7$ 344.32
Isol. from *Citrus sudachi*, *Mentha piperita*, *Sideritis* spp. and *Thymus* spp.. Yellow cryst. (MeOH). Mp 227-230°. λ_{max} 282 (ε 18900); 296 (ε 18000); 336 (ε 24700) (MeOH) (Berdy). λ_{max} 276 (ε 15100); 402 (ε 32500) (MeOH-NAOH) (Berdy).

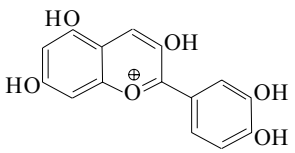
5,6,7,8-Tetra-Me ether: [36950-98-8] *4′-Hydroxy-5,6,7,8-tetramethoxyflavone*
$C_{19}H_{18}O_7$ 358.347
Constit. of mandarin orange (*Citrus reticulata*). Needles (C_6H_6). Mp 196-198°.

Stout, G.H. *et al., Tetrahedron*, 1961, **14**, 296 (*Xanthomicrol*)
Lee, H.H. *et al., J.C.S.*, 1964, 6255 (*Desmethoxysudachin*)
Thomas, M.B. *et al., Phytochemistry*, 1968, **7**, 787 (*Desmethoxysudachin*)
Chhabra, S.C. *et al., Indian J. Chem., Sect. B*, 1971, **14**, 651 (*Desmethoxysudachin*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 708; 717 (*cmr, Gardenin B, 4′-Hydroxy-5,6,7,8-tetramethoxyflavone*)
Patron, N.H. *et al., Int. Sugar J.*, 1985, **87**, 213-215 (*6,8-diglycoside, isol*)
Barberan, F.A.T. *et al., Phytochemistry*, 1985, **24**, 1285 (*Xanthomicrol*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1986, **41**, 87 (*Xanthomicrol*)
Grayer, R.J. *et al., Phytochemistry*, 2001, **56**, 559-567 (*Pilosin, Nevadensin*)

3,3′,4′,5,7-Pentahydroxyflavylium(1+) P-144

[13306-05-3]

[528-58-5]
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-1-benzopyrylium(1+), 9CI. ***Cyanidin***. *Cyanidol*†



$C_{15}H_{11}O_6^{\oplus}$ 287.248
Various methyl ethers have separate entries. Widely distributed anthocyanidin, found esp. in *Vaccinium* spp. (blueberries, bilberries, whortleberries), cherries, raspberries, red onions, red wine and black tea. Chocolate-brown cryst. (EtOH/HCl) or red-brown needles (as chloride). Dec. >200° (chloride).

3-O-β-L-Arabinoside: [27214-72-8] *Cyanidin 3-arabinoside*
$C_{20}H_{19}O_{10}^{\oplus}$ 419.364
Isol. from numerous plant spp. including red pears and apples. Almost black prisms (as chloride).

7-O-Arabinoside: [28985-03-7] *Cyanidin 7-arabinoside*
$C_{20}H_{19}O_{10}^{\oplus}$ 419.364
Isol. from the apple tree *Malus* sp..

3-O-Xyloside: [29761-24-8] *Cyanidin 3-xyloside*
$C_{20}H_{19}O_{10}^{\oplus}$ 419.364
Isol. from apples.

3-O-(O-Malonyl-β-D-xylopyranoside): [156736-60-6] *Cyanidin 3-(malonylxyloside)*
$C_{23}H_{21}O_{13}^{\oplus}$ 505.411
Constit. of red hulled sunflower seeds (*Helianthus annuus*).

3-O-β-D-Galactopyranoside: [27661-36-5]

[60562-64-3] *Cyanidin 3-galactoside.* ***Idein***. *Idaein*
$C_{21}H_{21}O_{11}^{\oplus}$ 449.39
Isol. from numerous plants including cranberry (*Vaccinium vitis-idaea*), red pears and pistachio (*Pistacia vera*). Red-brown prisms with green reflex (as chloride). The earlier-isolated Idein (stereochem. of galactosyl residue not fully defined) was presumably identical with the later isolates.

3-O-β-D-Glucopyranoside: [7084-24-4] ***Chrysanthemin***. *Asterin*†. *Chrysontemin. Kuromamine. Cyanidin 3-glucoside*
$C_{21}H_{21}O_{11}^{\oplus}$ 449.39
Found in many plants and fruits, e.g. cherries, olives and grapes. Bronze-red prisms + $1.5H_2O$ (as chloride).

3-O-(4-O-Acetyl-β-D-glucopyranoside): [88395-42-0] *Cyanidin 3-(4-acetylglucoside)*
$C_{23}H_{23}O_{12}^{\oplus}$ 491.427
Isol. from oranges.

3-O-(Cinnamoyl-β-D-glucopyranoside): [87245-35-0] *Cyanidin 3-(cinnamoylglucoside)*
$C_{30}H_{27}O_{12}^{\oplus}$ 579.536
Isol. from raspberry fruits (*Rubus idaeus*).

3-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside]: [56767-17-0] ***Hyacinthin***
$C_{30}H_{27}O_{13}^{\oplus}$ 595.535
Isol. from grapes.

3-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside], 5-O-β-D-glucopyranoside: [23410-80-2] ***Perillanin***. *Shisonin. Shisonin B*
$C_{36}H_{37}O_{18}^{\oplus}$ 757.677
Isol. from leaves of *Perilla nankinensis*. Dark red-brown plates (dil. HCl) (as chloride).

3-O-[3,4-Dihydroxycinnamoyl-(→6)-β-D-glucopyranoside], 5-O-β-D-glucopyranoside: [68341-44-6] *Cyanidin 3-(6-caffeoylglucoside) 5-glucoside*
$C_{36}H_{37}O_{19}^{\oplus}$ 773.677
Isol. from mature dark red leaves of *Perilla frutescens* var. *crispa*.

3-O-[3,4-Dihydroxycinnamoyl-(→?)-β-D-glucopyranoside]: [28983-74-6] *Cyanidin 3-(caffeoylglucoside)*
$C_{30}H_{27}O_{14}^{\oplus}$ 611.535
Isol. from grapes and other plant spp..

3-O-[4-Hydroxy-3-methoxycinnamoyl-(1→?)-β-D-glucopyranoside]: [96916-71-1] *Cyanidin 3-feruloylglucoside*
$C_{31}H_{29}O_{14}^{\oplus}$ 625.562
Isol. from orange (*Citrus sinensis*).

3-O-[4-Hydroxy-3-methoxycinnamoyl-(→?)-β-D-glucopyranoside], 5-O-β-D-glucopyranoside: [79410-82-5]
$C_{37}H_{39}O_{19}^{\oplus}$ 787.704
Isol. from perilla *Perilla frutescens* var. crispa.

3-O-[4-Hydroxy-3-methoxycinnamoyl-(

*→6)-β-D-glucopyranoside], 5-*O*-(6-*O*-malonyl-β-D-glucopyranoside):* [123453-03-2] *Cyanidin 3-(6-feruloylglucoside) 5-(6-malonylglucoside)*
$C_{40}H_{41}O_{22}^{\oplus}$ 873.751
Isol. from perilla (*Perilla frutescens* var. *crispa*).

*3-*O*-[4-Hydroxy-3,5-dimethoxycinnamoyl-(1→?)-β-D-glucopyranoside]:* [96916-69-7] *Cyanidin 3-(sinapoylglucoside)*
$C_{32}H_{31}O_{15}^{\oplus}$ 655.588
Isol. from orange (*Citrus sinensis*).

*3-*O*-[4-Hydroxycinnamoyl-(→?)-4-hydroxy-3-methoxycinnamoyl-(→?)-β-D-glucopyranoside]:* [96916-70-0] *Cyanidin 3-(*p*-coumaroylferuloylglucoside)*
$C_{40}H_{35}O_{16}^{\oplus}$ 771.707
Isol. from orange (*Citrus sinensis*).

*3-*O*-(3-*O*-Malonyl-β-D-glucopyranoside):*
$C_{24}H_{23}O_{14}^{\oplus}$ 535.437
Constit. of caucus (*Allium victorialis*) (Liliaceae).

*3-*O*-(6-*O*-Malonyl-β-D-glucopyranoside):* [94977-38-5] *Cyanidin 3-(6″-malonylglucoside)*
$C_{24}H_{23}O_{14}^{\oplus}$ 535.437
Isol. from red chicory leaves (*Cichorium intybus*).

*3-*O*-(3,6-Di-*O*-malonyl-β-D-glucopyranoside):*
$C_{27}H_{25}O_{17}^{\oplus}$ 621.484
Constit. of caucus (*Allium victorialis*) (Liliaceae).

*4′-*O*-β-D-Glucopyranoside:* [27459-77-4] *Cyanidin 4′-glucoside*
$C_{21}H_{21}O_{11}^{\oplus}$ 449.39
Isol. from okra petals (*Hibiscus esculentus*).

*7-*O*-β-D-Glucopyranoside:* [64963-51-5] *Cyanidin 7-glucoside*
$C_{21}H_{21}O_{11}^{\oplus}$ 449.39
Isol. from blackberry (*Rubus fruticosus*).

*3,3′-Di-*O*-β-D-glucopyranoside:* [64963-54-8] *Cyanidin 3,3′-diglucoside*
$C_{27}H_{31}O_{16}^{\oplus}$ 611.532
Isol. from plants in the Bromeliaceae.

*3,4′-Di-*O*-β-D-glucopyranoside:* [27459-78-5] *Cyanidin 3,4′-diglucoside*
$C_{27}H_{31}O_{16}^{\oplus}$ 611.532
Isol. from okra petals (*Hibiscus esculentus*).

*3,3′,5-Tri-*O*-β-D-glucopyranoside:* [88110-66-1] *Cyanidin 3,3′,5-triglucoside*
$C_{33}H_{41}O_{21}^{\oplus}$ 773.674
Isol. from the Bromeliaceae, e.g. pineapple (*Ananas comosus*).

*3-*O*-[Arabinosyl-(1→?)-glucoside]:* [36473-49-1] *Cyanidin 3-(arabinosylglucoside)*
$C_{26}H_{29}O_{15}^{\oplus}$ 581.506
Isol. from *Viburnum trilobum* (American cranberry bush).

*3-*O*-[Arabinosyl-(1→?)-galactoside]:* [26856-99-5] *Cyanidin 3-(arabinosylgalactoside)*
$C_{26}H_{29}O_{15}^{\oplus}$ 581.506
Isol. from apples.

*3-*O*-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside]:* [33012-73-6] ***Sambicyanin***. *Cyanidin 3-sambubioside. Sambucicyanin*
$C_{26}H_{29}O_{15}^{\oplus}$ 581.506
Isol. from *Rubus* spp., *Sambucus* spp. and other plant spp.. Brown-yellow prisms + $4H_2O$ (as chloride).

*3-*O*-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:* [53925-33-0] *Cyanidin 5-glucoside 3-sambubioside*
$C_{32}H_{39}O_{20}^{\oplus}$ 743.648
Isol. from American elder fruits (*Sambucus canadensis*) and other plant spp..

*3-*O*-[β-D-Xylopyranosyl-(1→2)-(4-hydroxycinnamoyl)-(→6)-β-D-glucopyranoside](*E*)-:* [162972-64-7]
$C_{35}H_{35}O_{17}^{\oplus}$ 727.651
Constit. of American elder fruits (*Sambucus canadensis*).

*3-*O*-[β-D-Xylopyranosyl-(1→2)-(4-hydroxycinnamoyl)-(→6)-β-D-glucopyranoside](*E*-), 5-*O*-β-D-glucopyranoside:* [139906-05-1]
$C_{41}H_{45}O_{22}^{\oplus}$ 889.793
Constit. of American elder fruits (*Sambucus canadensis*).

*3-*O*-[β-D-Xylopyranosyl-(1→2)-(4-hydroxycinnamoyl)-(→6)-β-D-glucopyranoside](*Z*-), 5-*O*-β-D-glucopyranoside:* [163060-00-2]
$C_{41}H_{45}O_{22}^{\oplus}$ 889.793
Constit. of the fruit of American elder (*Sambucus canadensis*).

*3-*O*-[α-L-Rhamnopyranosyl-(1→?)-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:Cyanidin 5-glucoside 3-rhamnoglucoside*
$C_{33}H_{41}O_{20}^{\oplus}$ 757.675
Isol. from blackberry (*Rubus fruticosus*).

*3-*O*-(4-Hydroxycinnamoylrutinoside), 5-*O*-β-D-glucopyranoside:**Cyananin***
$C_{42}H_{47}O_{22}^{\oplus}$ 903.82
Present in cultivated red potatoes (*Solanum phureja*).

*3-*O*-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:Cyanidin 5-glucoside 3-sophoroside*
$C_{33}H_{41}O_{21}^{\oplus}$ 773.674
Present in acylated form in red cabbage (*Brassica oleracea*).

*3-*O*-(4-Hydroxycinnamoylsophoroside), 5-*O*-β-D-glucopyranoside:* [28880-85-5]
$C_{42}H_{47}O_{23}^{\oplus}$ 919.819
Isol. from red cabbage (*Brassica oleracea*).

*3-*O*-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:*
$C_{42}H_{47}O_{23}^{\oplus}$ 919.82
Constit. of the deep purple callus derived from the storage root of *Ipomoea batatas* (sweet potato).

*3-*O*-(Di-*O*-4-hydroxycinnamoylsophoroside), 5-*O*-β-D-glucopyranoside:* [63642-56-8]
$C_{51}H_{53}O_{25}^{\oplus}$ 1065.965
Isol. from red cabbage (*Brassica oleracea*).

*3-*O*-[4-Hydroxybenzoyl-(→6)-β-D-glucopyranosyl-(1→2)-[3,4-dihydroxy-*E*-cinnamoyl-(→6)]-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:YGM 1A*
$C_{49}H_{51}O_{26}^{\oplus}$ 1055.926
Constit. of the storage roots of sweet potato (*Ipomoea batatas*).

*3-*O*-[3,4-Dihydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-[3,4-dihydroxy-*E*-cinnamoyl-(→6)]-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:YGM 1B*
$C_{51}H_{53}O_{27}^{\oplus}$ 1097.964
Constit. of the storage roots of sweet potato (*Ipomoea batatas*).

*3-*O*-[β-D-Glucopyranosyl-(1→2)-[3,4-dihydroxy-*E*-cinnamoyl-(→6)]-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:*
$C_{42}H_{47}O_{24}^{\oplus}$ 935.819
Constit. of purple sweet potato tubers (*Ipomoea batatas* var. *yamagawmurasaki*).

*3-*O*-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-[3,4-dihydroxy-*E*-cinnamoyl-(→6)]-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside:YGM 3*
$C_{52}H_{55}O_{27}^{\oplus}$ 1111.99
Constit. of the storage roots of sweet potato (*Ipomoea batatas*).

*3-*O*-(Caffeoylsophoroside):* [81360-20-5] *Cyanidin 3-(caffeoylsophoroside)*
$C_{36}H_{37}O_{19}^{\oplus}$ 773.677
Isol. from artichoke (*Cynara scolymus*).

*3-*O*-(Di-*O*-caffeoylsophoroside):* [83574-31-6] *Cyanidin 3-(dicaffeoylsophoroside)*
$C_{45}H_{43}O_{22}^{\oplus}$ 935.821
Isol. from artichoke (*Cynara scolymus*).

*3-*O*-(Feruloylsophoroside), 5-*O*-β-D-glucopyranoside:* [29013-15-8]
$C_{43}H_{49}O_{24}^{\oplus}$ 949.846
Isol. from red cabbage (*Brassica oleracea*).

*3-*O*-(Di-*O*-feruloylsophoroside), 5-*O*-β-D-glucopyranoside:* [29223-00-5]
$C_{53}H_{57}O_{27}^{\oplus}$ 1126.017
Isol. from red cabbage (*Brassica oleracea*).

*3-*O*-(O-Sinapoylsophoroside), 5-*O*-β-D-glucopyranoside:* [63003-10-1]
$C_{44}H_{51}O_{25}^{\oplus}$ 979.872
Isol. from red cabbage (*Brassica oleracea*).

*3-*O*-[4-Hydroxycinnamoyl-(→6)-[4-hydroxy-3,5-dimethoxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside], 5-*O*-(6-*O*-malonyl-β-D-glucopyranoside):*
$C_{56}H_{59}O_{30}^{\oplus}$ 1212.064
Constit. of *Brassica campestris* var. *chinensis*.

*3-*O*-[[4-Hydroxy-3,5-dimethoxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→2)]-[4-hydroxy-3-methoxycinnamoyl-(→6)]-β-D-glucopyranoside], 5-*O*-(6-*O*-malonyl-β-D-glucopyranoside):*
$C_{57}H_{61}O_{31}^{\oplus}$ 1242.09
Constit. of *Brassica campestris* var. *chinensis*.

*3-*O*-(Di-*O*-sinapoylsophoroside), 5-*O*-β-D-glucopyranoside:*
$C_{55}H_{61}O_{29}^{\oplus}$ 1186.069
Isol. from red cabbage (*Brassica oleracea*).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]:* [53696-63-2] *Cyanidin 3-laminaribioside*
$C_{27}H_{31}O_{16}^{\oplus}$ 611.532
Isol. from red onions (*Allium cepa*).

3-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [131189-50-9] *Cyanidin 3-(4-sinapoylgentiobioside)*. ***Alatanin 1***
$C_{38}H_{41}O_{20}^{\oplus}$ 817.73
Isol. from purple yam tubers (*Dioscorea alata*). Purple-red powder (as chloride).

3-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(→6)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside], 3′*-O-*β-D-glucopyranoside, 7*-O-*[4-hydroxy-3,5-dimethoxycinnamoyl-(→6)-β-D-glucopyranoside]:* [139610-21-2] ***Alatanin A***
$C_{67}H_{81}O_{39}^{\oplus}$ 1510.353
Isol. from purple yam tubers (*Dioscorea alata*).

3-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [138688-63-8] ***Alatanin C***. *Cyanidin 3-(6-sinapoylgentiobioside)*
$C_{38}H_{41}O_{20}^{\oplus}$ 817.73
Isol. from tubers of purple yam (*Dioscorea alata*). Dark red solid (as trifluoroacetate).

3-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside], 3′*-O-*β-D-glucopyranoside, 7*-O-*[4-hydroxy-3,5-dimethoxycinnamoyl-(→6)-β-D-glucopyranoside]:* [139610-20-1] ***Alatanin B***
$C_{61}H_{71}O_{34}^{\oplus}$ 1348.211
Isol. from purple yam tubers (*Dioscorea alata*).

3-O-*(6*-O-*4-Hydroxycinnamoyl-2′*-O-*sinapoylsophoroside), 5*-O-*β-D-glucopyranoside:* [110219-77-7] *Cyanidin 3-(6-coumaryl-2′-sinapoylsophoroside) 5-glucoside*
$C_{53}H_{57}O_{27}^{\oplus}$ 1126.017
Isol. from red cabbage (*Brassica oleracea*). Dark red powder (as chloride).

3-O-*[6*-O-*(4-Hydroxy-3-methoxycinnamoyl)(2′*-O-*sinapoylsophoroside)], 5*-O-*β-D-glucopyranoside:* [110202-92-1] *Cyanidin 3-(6-feruloyl-2′-sinapoylsophoroside) 5-glucoside*
$C_{54}H_{59}O_{28}^{\oplus}$ 1156.043
Isol. from red cabbage (*Brassica oleracea*). Dark red powder (as chloride).

3-O-*(Malonylsophoroside), 5*-O-*β-D-glucopyranoside:* [63003-09-8]
$C_{36}H_{43}O_{24}^{\oplus}$ 859.721
Isol. from red cabbage (*Brassica oleracea*).

3-O-*[β-D-Xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-galactopyranoside]:* [142561-98-6]
$C_{32}H_{39}O_{20}^{\oplus}$ 743.648
Isol. from carrot (*Daucus carota*).

3-O-*[β-D-Xylopyranosyl-(1→2)-[(4-hydroxy-3-methoxycinnamoyl)-(→6)-β-D-glucopyranosyl-(1→6)]-β-D-galactopyranoside]:* [142561-99-7]
$C_{42}H_{47}O_{23}^{\oplus}$ 919.819
Isol. from carrot (*Daucus carota*).

3-O-*[β-D-Xylopyranosyl-(1→2)-[(4-hydroxybenzoyl)-(→6)-β-D-glucopyranosyl-(1→6)]-β-D-galactopyranoside]:* [142506-20-5]
$C_{39}H_{43}O_{22}^{\oplus}$ 863.755
Isol. from carrot (*Daucus carota*).

3-O-*[β-D-Xylopyranosyl-(1→2)-[4-hydroxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→6)]-β-D-galactopyranoside]:* [142506-21-6]
$C_{41}H_{45}O_{22}^{\oplus}$ 889.793
Isol. from carrot (*Daucus carota*).

3-O-*[α-L-Rhamnopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranoside]:* [38226-79-8] *Cyanidin 2^G-(xylosylrutinoside)*
$C_{32}H_{39}O_{19}^{\oplus}$ 727.649
Isol. from redcurrants, cherries and other plant spp..

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [55028-57-4] *Cyanidin 3-(2^G-glucosylrutinoside)*
$C_{33}H_{41}O_{20}^{\oplus}$ 757.675
Isol. from redcurrant berries (*Ribes rubrum*). λ_{max} 283 ; 530 (MeOH/HCl).

3-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(→?)-β-D-glucopyranosyl-(1→6)[β-D-xylopyranosyl-(1→2)]-β-D-galactopyranoside]:* [88902-81-2] ***Carrot anthocyanin***
$C_{39}H_{49}O_{24}^{\oplus}$ 901.802
Isol. from carrot (*Daucus carota*).

3-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-galactopyranoside]:* [142630-71-5]
$C_{43}H_{49}O_{24}^{\oplus}$ 949.846
Isol. from carrot (*Daucus carota*).

3-O-*[(2*-O-*Caffeoylglucosyl)rutinoside]:* [61317-10-0]
$C_{42}H_{47}O_{23}^{\oplus}$ 919.819
Isol. from fruits of olive (*Olea europaea*).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:Cyanidin 3-sophorotrioside*
$C_{33}H_{41}O_{21}^{\oplus}$ 773.674
Isol.from red cabbage (*Brassica oleracea*).

3-O-*[2*-O-*β-D-Glucopyranosyl-6*-O-*[3-[4-(β-D-glucopyranosyloxy)cinnamoyl]]-β-D-glucopyranoside], 5*-O-*β-D-glucopyranoside:* [107480-92-2] *Cyanidin 3-[6-(4-glucosylcoumaryl)sophoroside] 5-glucoside*
$C_{48}H_{57}O_{28}^{\oplus}$ 1081.961
Isol. from red cabbage (*Brassica oleracea* var. Red Danish). Dark red powder (as chloride).

3-O-*[2*-O-*β-D-Glucopyranosyl-[3-[4-(β-D-glucopyranosyloxy)-3-methoxycinnamoyl]]-(→6)-β-D-glucopyranoside], 5*-O-*β-D-glucopyranoside:* [107500-83-4] *Cyanidin 3-[6-(4-glucosylferuloyl)sophoroside] 5-glucoside*
$C_{49}H_{59}O_{29}^{\oplus}$ 1111.988
Isol. from red cabbage (*Brassica oleracea*). Dark red powder (as chloride).

3-O-*(6*-O-*Oxalyloxalyl-β-D-glucopyranoside):Cyanidin 3-(6-dioxalylglucoside)*
$C_{25}H_{20}O_{17}$ 592.423
Constit. of the fruit of *Rubus laciniatus* (cutleaf blackberry). Zwitterionic.

[18376-31-3, 39030-77-8, 124168-01-0, 141891-42-1, 142354-29-8, 142354-30-1, 142631-48-9, 142631-49-0]

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Hrazdina, G. *et al., Phytochemistry*, 1977, **16**, 297 (*3-sophoroside, 5-glucosides, Brassica glycosides*)
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Maccarone, E. *et al., Ann. Chim. (Rome)*, 1985, **75**, 79-86 (*3-feruloylglycoside, 3-cinnamoylglycoside, 3-sinapoylglycoside, isol, orange*)
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Saito, N. *et al., Phytochemistry*, 1995, **40**, 1283; 1998, **49**, 875-880 (*Ipomoea purpurea anthocyanins*)
Andersen, O.M. *et al., Phytochemistry*, 1995, **40**, 1809 (*Allium malonylglucosides*)
Suzuki, M. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1929-1930 (*Brassica anthocyanins*)
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Stintzing, F.C. *et al., J. Agric. Food Chem.*, 2002, **50**, 396-399 (*3-6-dioxalylglucoside*)
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3′,4′,5,5′,7-Pentahydroxyflavylium(1+) P-145

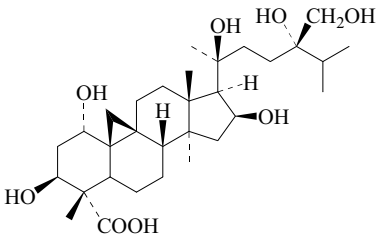
[65618-21-5]
5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)-1-benzopyrylium(1+), 9CI. ***Tricetanidin***

$C_{15}H_{11}O_6^{\oplus}$ 287.248
Isol. from black tea (*Thea sinensis*). CAS no. refers to chloride λ_{max} 281 ; 513 (MeOH/HCl). λ_{max} 564 (MeOH/NaOH).

Roberts, E.A.H. *et al., J. Sci. Food Agric.*, 1957, **8**, 72; 1958, **9**, 217
Harborne, J.B. *et al., Phytochemistry*, 1966, **5**, 589
Ozawa, T. *et al., Agric. Biol. Chem.*, 1982, **46**, 1079 (*isol*)
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1,3,16,20,24-Pentahydroxy-24-(hydroxymethyl)cycloartan-28-oic acid P-146

1,3,16,20,24,31-Hexahydroxy-24-methylcycloartan-28-oic acid



$C_{31}H_{52}O_8$ 552.747

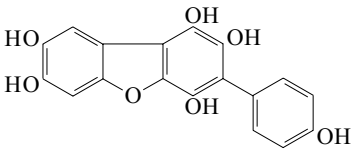
(1α,3β,16β,20*S*,24*S*)-*form* [301540-74-9] ***Cyclopassifloic acid E***
Constit. of *Passiflora edulis* (passion fruit). Needles. Mp 227-228°. $[\alpha]_D^{25}$ +41.2 (0.9 in MeOH).

28-O-β-D-Glucopyranosyl ester: [301540-80-7] ***Cyclopassifloside VII***
$C_{37}H_{62}O_{13}$ 714.889
Constit. of *Passiflora edulis* (passion fruit). Needles. Mp 163-165°. $[\alpha]_D^{25}$ +35.6 (c, 1.5 in MeOH).

Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 1377-1380 (*isol, pmr, cmr*)

1,2,4,7,8-Pentahydroxy-3-(4-hydroxyphenyl)dibenzofuran P-147

3-(4-Hydroxyphenyl)-1,2,4,7,8-dibenzofuranpentol, 9CI



$C_{18}H_{12}O_7$ 340.289

1,2-Di-Ac:BL V
$C_{22}H_{16}O_9$ 424.363
Constit. of the kurukawa mushroom (*Boletopsis leucomelas*) (edibility not reported). Amorph. brown powder.

1,2,4-Tri-Ac: [112209-53-7] *BL IV*
$C_{24}H_{18}O_{10}$ 466.4
Constit. of the kurukawa mushroom (*Boletopsis leucomelas*) (edibility not reported). Pale brown needles. Mp 242-245° dec.

1,2,4,7-Tetra-Ac: [112209-52-6]
$C_{26}H_{20}O_{11}$ 508.437
Constit. of the kurukawa mushroom (*Boletopsis leucomelas*) (edibility not reported).

1,2,4,8-Tetra-Ac: [112209-54-8]
$C_{26}H_{20}O_{11}$ 508.437
Constit. of the kurukawa mushroom (*Boletopsis leucomelas*) (edibility not reported).

1,2,4,4′-Tetra-Ac:BL III
$C_{26}H_{20}O_{11}$ 508.437
Constit. of the kurukawa mushroom (*Boletopsis leucomelas*) (edibility not reported). Pale purple needles. Mp 194-196°.

1,2,4,7,8-Penta-Ac:BL II
$C_{28}H_{22}O_{12}$ 550.475
Constit. of the kurukawa mushroom (*Boletopsis leucomelas*) (edibility not reported). Needles. Mp 130-131°.

Hexa-Ac: [112209-51-5] ***Protoleucomelone. BL I***
$C_{30}H_{24}O_{13}$ 592.512
Constit. of the kurukawa mushroom (*Boletopsis leucomelas*) (edibility not reported). Needles. Mp 203-204°. Originally descr. as a benzoquinone.

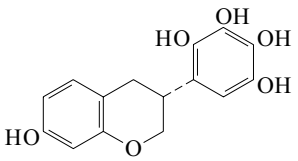
1,2,4-Tris(phenylacetyl): ***Ganbajunin B***
$C_{42}H_{30}O_{10}$ 694.693
Needles (MeOH aq.). Mp 197-198°. λ_{max} 207 (log ε 4.73); 220 (log ε 4.54); 251 (log ε 4.25); 264 (log ε 4.24); 303 (log ε 4.2); 329 (log ε 4.28); 344 (log ε 4.02) (MeOH).

3′-Hydroxy, 2-deoxy, 4-Me ether:3-(3,4-Dihydroxyphenyl)-4-methoxy-1,7,8-dibenzofurantriol. 3-(3,4-Dihydroxyphenyl)-1,7,8-trihydroxy-4-methoxydibenzofuran
$C_{19}H_{14}O_7$ 354.315
Pale yellow oil. λ_{max} 240 (ε 6700); 281 (sh) (ε 5200); 299 (ε 5700); 331 (ε 6400) (MeOH).

3′-Hydroxy, 4-deoxy, 2-Me ether:3-(3,4-Dihydroxyphenyl)-2-methoxy-1,7,8-dibenzofurantriol. 3-(3,4-Dihydroxyphenyl)-1,7,8-trihydroxy-2-methoxydibenzofuran
$C_{19}H_{14}O_7$ 354.315
Off-white gum. λ_{max} 239 (ε 13000); 274 (ε 11000); 303 (ε 14000); 323 (ε 14000) (MeOH).

Jägers, E. *et al., Z. Naturforsch., B*, 1987, **42**, 1349 (*acetates, isol*)
Takahashi, A. *et al., Chem. Pharm. Bull.*, 1992, **40**, 3194 (*isol, struct*)
Belofsky, G.N. *et al., J. Nat. Prod.*, 1998, **61**, 1115-1119 (*Penicillium raistrickii derivs*)
Hu, L. *et al., Helv. Chim. Acta*, 2001, **84**, 3342-3349 (*Ganbajunin B*)

2′,3′,4′,5′,7-Pentahydroxyisoflavan P-148



$C_{15}H_{14}O_6$ 290.272

(*R*)-*form*

3′,4′-Di-Me ether, 2′,5′-di-O-β-D-glucopyranoside: [137217-85-7] *2′,5′,7-Trihydroxy-3′,4′-dimethoxyisoflavan 2′,5-di-O-β-D-glucopyranoside*
$C_{29}H_{38}O_{16}$ 642.61
Needles. Mp 160-162°. $[\alpha]_D$ -17.7 (c, 0.3 in MeOH).

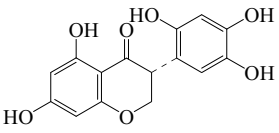
2′,3′,4′-Tri-Me ether: [139906-02-8] *5′,7-Dihydroxy-2′,3′,4′-trimethoxyisoflavan.* ***5′-Hydroxy-3′-methoxysativan***
$C_{18}H_{20}O_6$ 332.352
Constit. of *Medicago sativa* (alfalfa). Mp 137-138°. $[\alpha]_D^{27}$ +7.5 (c, 0.48 in $CHCl_3$).

2′,4′,7-Tri-Me ether:3′,5′-Dihydroxy-2′,4′,7-trimethoxyisoflavan. ***Coluteol***
$C_{18}H_{20}O_6$ 332.352
Pale brown resin. λ_{max} 207 (log ε 4.59); 219 (sh) (log ε 4.13); 282 (log ε 3.63) (MeOH). λ_{max} 207 (ε 38900); 282 (ε 4265) (MeOH) (Berdy).

3′,4′,7-Tri-Me ether: [181311-16-0] *2′,5′-Dihydroxy-3′,4′,7-trimethoxyisoflavan.* ***Colutehydroquinone***
$C_{18}H_{20}O_6$ 332.352
Yellow-tinged amorph. solid (Me_2CO). Mp 103-106° (dec.) Mp 166-167° (as di-Ac). λ_{max} 207 (log ε 4.84); 284 (sh) (log ε 3.916); 289 (log ε 3.922) (EtOH).

Subarnas, A. *et al., Phytochemistry*, 1991, **30**, 2777
Spencer, G.F. *et al., Phytochemistry*, 1991, **30**, 4147 (*5′-Hydroxy-3′-methoxysativan*)
Grosvenor, P.W. *et al., Phytochemistry*, 1996, **43**, 375 (*Colutehydroquinone*)
Grosvenor, P.W. *et al., J. Nat. Prod.*, 1998, **61**, 99-101 (*Coluteol*)

2′,4′,5,5′,7-Pentahydroxyisoflavanone P-149



(*R*)-*form*

$C_{15}H_{12}O_7$ 304.256

(*R*)-*form*

2′,4′,5′-Tri-Me ether:5,7-Dihydroxy-2′,4′,5′-trimethoxyisoflavanone. ***2,3-Dihydro-7-O-demethylrobustigenin***
$C_{18}H_{18}O_7$ 346.336
Amorph. powder. $[\alpha]_D$ -28 (c, 0.1 in MeOH). λ_{max} 291 ; 334 (MeOH).

(±)-*form*

2′,4′,5′-Tri-Me ether:
Cryst. (Me_2CO). Mp 188-190°. λ_{max} 204 (log ϵ 4.02); 225 (log ϵ 3.82); 289 (log ϵ 3.77) (MeOH).

(ξ)-*form*

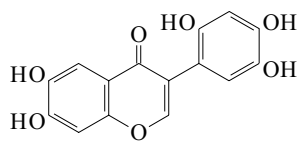
4′,5′-Methylene, 2′-Me ether: [12751-00-7] *5,7-Dihydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavanone.* ***Cicerin***
$C_{17}H_{14}O_7$ 330.293
Constit. of *Cicer arietinum* (chickpea).

4′,5′-Methylene, 2′-Me ether, 7-O-(6-O-malonyl-β-D-glucopyranoside): [146367-93-3]
$C_{26}H_{26}O_{15}$ 578.482
Constit. of *Cicer arietinum* (chickpea).

Mackenbrock, U. *et al., Z. Naturforsch., C*, 1992, **47**, 815
Wanjala, C.C.W. *et al., Fitoterapia*, 2000, **71**, 400-405 (±-*form tri-Me ether*)
Yenesew, A. *et al., Phytochemistry*, 2000, **55**, 457-459 (*Dihydrodemethylrobustigenin*)

2′,4′,5′,6,7-Pentahydroxyisoflavone P-150

6,7-Dihydroxy-3-(2,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one, 9CI



$C_{15}H_{10}O_7$ 302.24

4′,6-Di-Me ether, 2′-O-β-D-glucopyranoside: ***Licoagroside A***
$C_{23}H_{24}O_{12}$ 492.435
Isol. from hairy root cultures of *Glycyrrhiza glabra* (licorice). Powder. $[\alpha]_D^{24}$ +75.1 (c, 0.37 in MeOH). λ_{max} 218 (log ϵ 4.3); 250 (log ϵ 4.07); 294 (log ϵ 3.85); 324 (log ϵ 3.84) (MeOH).

Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Li, W. *et al., Phytochemistry*, 2000, **55**, 447-456 (*Licoagroside A*)

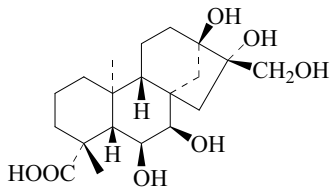
2′,4′,5,5,7,8-Pentahydroxyisoflavone P-151

[104363-16-8]
3-(2,4-Dihydroxyphenyl)-5,7,8-trihydroxy-4H-1-benzopyran-4-one, 9CI

$C_{15}H_{10}O_7$ 302.24
Constit. of *Phaseolus lunatus* (butter bean).

O'Neill, M.J. *et al., Phytochemistry*, 1986, **25**, 1315

6,7,13,16,17-Pentahydroxy-19-kauranoic acid P-152



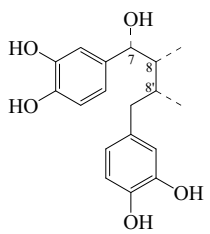
$C_{20}H_{32}O_7$ 384.469

(ent*-6α,7α,13α,16β)-*form [316141-32-9] *Canavaliol*
Powder. $[\alpha]_D^{25}$ -30.5 (c, 1.1 in MeOH).

17-O-β-D-Glucopyranoside: [316141-31-8] ***Canavalioside***
$C_{26}H_{42}O_{12}$ 546.611
Constit. of *Canavalia gladiata* (sword bean). Powder. $[\alpha]_D^{26}$ -43 (c, 1.9 in MeOH).

Murakami, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1673-1680 (*isol, pmr, cmr*)

3,3′,4,4′,7-Pentahydroxylignan P-153



(7*R*,8*R*,8′*R*)-*form*

$C_{18}H_{22}O_5$ 318.369
Lignan numbering shown.

(7*R,8*R**,8′*R**)-*form***

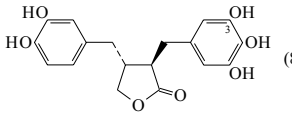
Bis(methylene) ether: ***7-Hydroxyaustrobailignan 5***
$C_{20}H_{22}O_5$ 342.391
Isol. from *Myristica fragrans* (nutmeg). $[\alpha]_D$ -24.7 (c, 0.47 in $CHCl_3$).

(7*R,8*R**,8′*S**)-*form***

3,4:3′,4′-Bis(methylene) ether: [169873-76-1] ***Saururinol***. *7-Hydroxyaustrobailignan 5*
$C_{20}H_{22}O_5$ 342.391
Constit. of *Myristica fragrans* (nutmeg). $[\alpha]_D$ -24.7 (c, 0.47 in $CHCl_3$).

Hattori, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 648-653 (*7-Hydroxyaustrobailignan 5*)
Martinez, V. *et al., Rev. Colomb. Quim.*, 1994, **23**, 9-16; *CA*, **123**, 310319 (*Saururinol*)

3,3′,4,4′,5-Pentahydroxylignan-9,9′-olide P-154



(8*R*,8′*R*)-*form*

$C_{18}H_{18}O_7$ 346.336
Isomeric with 3,3′,4,4′,5′-Pentahydroxylignan-9,9′-olide, P-155.

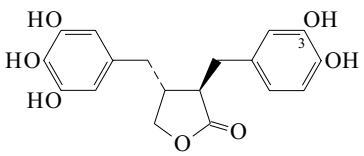
(8*R*,8′*R*)-*form*

3,4:3′,4′-Bis(methylene), 5-Me ether: [112448-63-2] *5-Methoxy-3,4:3′,4′-bis(methylenedioxy)lignan-9,9′-olide.* ***5-Methoxyhinokinin***
$C_{21}H_{20}O_7$ 384.385
Isol. from fruits of *Piper cubeba* (cubeb pepper). Viscous mass. $[\alpha]_D^{25}$ -37 (c, 0.15 in $CHCl_3$).

Maclean, H. *et al., Can. J. Chem.*, 1966, **44**, 1541
Harmatha, J. *et al., Coll. Czech. Chem. Comm.*, 1982, **47**, 644 (*isol, uv, cd, pmr, ms*)
Badheka, L.P. *et al., Phytochemistry*, 1986, **25**, 487
Tanoguchi, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4162 (*isol*)
Badheka, L.P. *et al., Phytochemistry*, 1987, **26**, 2033 (*5-Methoxyhinokinin*)
Kato, M.J. *et al., Phytochemistry*, 1990, **29**, 1799

3,3′,4,4′,5′-Pentahydroxylignan-9,9′-olide P-155

4,5-Dihydro-3-(3,4-dihydroxybenzyl)-4-(3,4,5-trihydroxybenzyl)-2(3H)-furanone



$C_{18}H_{18}O_7$ 346.336
Isomeric with 3,3′,4,4′,5-Pentahydroxylignan-9,9′-olide, P-154.

(8*R*,8′*R*)-*form*

3,4-Methylene ether, 3′,4′,5′-tri-Me ether: [101751-72-8] ***Isoyatein***
$C_{22}H_{24}O_7$ 400.427
Constit. of *Piper cubeba* (cubeb pepper). Viscous mass. $[\alpha]_D^{25}$ -49.6 (c, 0.035 in $CHCl_3$).

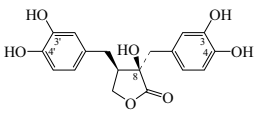
3,3′,4′,5′-Tetra-Me ether: [79288-73-6] ***Traxillagenin***
$C_{22}H_{26}O_7$ 402.443
Syrup. $[\alpha]_D$ -33 (c, 0.5 in EtOH) (synthetic). $[\alpha]_D$ -25.1 (c, 0.55 in EtOH) (nat. prod.).

3,3′,4′,5′-Tetra-Me ether, 4-O-β-D-glucopyranoside: [149415-62-3] ***Traxillaside***
$C_{28}H_{36}O_{12}$ 564.585
Amorph. powder. Mp 88-92°. $[\alpha]_D^{20}$ -71.3 (c, 0.13 in MeOH).

Nishibe, S. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2078 (*Traxillagenin*)
Badheka, L.P. *et al., Phytochemistry*, 1986, **25**, 487
Lalami, K. *et al., Heterocycles*, 1988, **27**, 1131 (*synth*)

Lalami, K. *et al., J. Nat. Prod.*, 1991, **54**, 119 (*synth*)
Nishibe, S. *et al., Phytochemistry*, 1993, **32**, 1579 (*Traxillaside*)

3,3′,4,4′,8-Pentahydroxylignan-9,9′-olide P-156



(8*R*,8′*R*)-*form*

$C_{18}H_{18}O_7$ 346.336
Lignan numbering shown.

(8*R*,8′*R*)-*form*

3,3′,4′-Tri-Me ether, 4-O-β-D-glucopyranoside: [177930-79-9] ***Saussurenoside***
$C_{27}H_{34}O_{12}$ 550.558
Amorph. solid (as tetra-Ac). $[\alpha]_D$ -35.2 (c, 0.9 in $CHCl_3$) (tetra-Ac). λ_{max} 226 (log ε 4.37); 279 (log ε 3.93) (MeOH).

(8*R*,8′*S*)-*form*

3,3′,4,4′-Tetra-Me ether, 8-Ac: [235743-17-6]
$C_{24}H_{28}O_8$ 444.48
Amorph. powder. $[\alpha]_D^{25}$ -19.3 (c, 1 in $CHCl_3$).

(8*S*,8′*S*)-*form*

3,3′-Di-Me ether: Wikstromol, W-3

3′,4′-Di-Me ether:
$C_{20}H_{22}O_7$ 374.39
$[\alpha]_D^{25}$ -39.1 (c, 0.5 in MeOH). λ_{max} 233 (log ε 4.15); 282 (log ε 3.75) (MeOH).

3′,4′-Di-Me ether, 4-O-β-D-glucopyranoside:
$C_{26}H_{32}O_{12}$ 536.532
$[\alpha]_D^{25}$ -57.5 (c, 0.5 in MeOH).

3,3′,4′-Tri-Me ether: [34209-69-3] ***Trachelogenin***
$C_{21}H_{24}O_7$ 388.416
Needles. Mp 139-141°. $[\alpha]_D^{23}$ -43.5 (c, 0.25 in EtOH). Log P 1.12 (calc). λ_{max} 229 (ε 8300); 280 (ε 4700) (MeOH) (Berdy).

3,3′,4′-Tri-Me ether, 4-O-β-D-glucopyranoside: [33464-71-0] ***Trachelosside***
$C_{27}H_{34}O_{12}$ 550.558
Constit. of *Carthamus tinctorius* (safflower). Cryst. (EtOAc). Mp 168-170°. $[\alpha]_D^{20}$ -60 (EtOH).

3,3′,4,4′-Tetra-Me ether: [33464-73-2]

[41328-83-0] *8-Hydroxy-3,3′,4,4′-tetramethoxylignan-9,9′-olide. Methyltrachelogenin*
Mp 97-98.5°. $[\alpha]_D^{28}$ -46.9 (c, 1.4 in EtOH).

3,4-Methylene, 3′,4′-di-Me ether, 8-O-angeloyl: [18884-21-4] ***Helianthoidin***
$C_{26}H_{28}O_8$ 468.502
Mp 134-135°. $[\alpha]_D^{25}$ -145.4 (c, 1.52 in $CHCl_3$).

3′,4′-Methylene, 3-Me ether: [222849-85-6] ***8-Hydroxypluviatolide***
$C_{20}H_{20}O_7$ 372.374
$[\alpha]_D^{25}$ -32.1 (c, 0.6 in $CHCl_3$). λ_{max} 232 (ε 17500); 285 (ε 9240) (MeOH).

3′,4′-Methylene, 3,4-di-Me ether: [150448-65-0] ***Benchequiol***
$C_{21}H_{22}O_7$ 386.401
$[\alpha]_D^{20}$ -8 (c, 1.5 in $CHCl_3$).

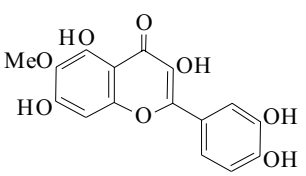
Bis(methylene) ether: [120051-54-9] *8-Hydroxy-3,4:3′,4′-bis(methylenedioxy)-lignan-9,9′-olide.* ***Meridinol***
Needles (EtOAc/petrol). Mp 122-123° Mp 126.5° (synthetic). $[\alpha]_D^{25}$ -30 (c, 0.1 in $CHCl_3$). $[\alpha]_D^{20}$ -38.6 (c, 0.09 in $CHCl_3$) (synthetic).

[131351-77-4]

Burden, R.S. *et al., Chem. Comm.*, 1969, 693 (*Helianthoidin*)
Nishibe, S. *et al., Chem. Pharm. Bull.*, 1971, **19**, 866; 1972, **20**, 2075; 1973, **21**, 674; 1108 (*isol, struct*)
Inagaki, I. *et al., Phytochemistry*, 1971, **10**, 211 (*isol*)
Inagaki, I. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2710 (*Trachelogenin*)
Vanhaelen, M. *et al., Phytochemistry*, 1975, **14**, 2709 (*isol*)
Amaro-Luis, J.M. *et al., Phytochemistry*, 1988, **27**, 3933 (*Meridinol*)
Schröder, H.C. *et al., Z. Naturforsch., C*, 1990, **45**, 1215 (*HIV activity*)
Khamlach, K. *et al., Tetrahedron*, 1992, **48**, 10115-10126 (*Trachelogenin*)
Estevez-Reyes, R. *et al., J. Nat. Prod.*, 1993, **56**, 1177-1181 (*Benchequiol*)
Kuo, Y.H. *et al., J. Nat. Prod.*, 1996, **59**, 622 (*Saussurenoside*)
Moritani, Y. *et al., J.O.C.*, 1996, **61**, 6922-6930 (*synth, Trachelogenin*)
Takano, D. *et al., J. Het. Chem.*, 1999, **36**, 221-224 (*Meridinol, synth, abs config*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1999, **62**, 946-948 (*tetra-Me 8-Ac*)
Lin, W. *et al., Phytochemistry*, 1999, **50**, 653-658 (*8-Hydroxypluviatolide*)
Rastrelli, L. *et al., J. Nat. Prod.*, 2001, **64**, 79-81 (*3′,4′-di-Me and 4-glucoside*)

3,3′,4′,5,7-Pentahydroxy-6-methoxyflavone P-157

[519-96-0]
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-6-methoxy-4H-1-benzopyran-4-one, 9CI. 3′,4′,5,7-Tetrahydroxy-6-methoxyflavonol. ***Patuletin****. 6-O-Methylquercetagetin*



$C_{16}H_{12}O_8$ 332.266
Pigment from flowers of French marigold *Tagetes patula*. Pale yellow needles (EtOH aq.). Mp 262-264°.

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [101021-28-7] *Patuletin 3-gentiobioside*
$C_{28}H_{32}O_{18}$ 656.55
Isol. from spinach (*Spinacea oleracea*) leaves. Yellow needles + $1H_2O$ (MeOH aq.). Mp 220-222°. $[\alpha]_D^{27}$ -22.3 (c, 0.1 in MeOH).

3-O-[β-D-Apiofuranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]: [101021-30-1]
$C_{33}H_{40}O_{22}$ 788.666
Isol. from spinach (*Spinacia oleracea*) leaves. Yellow powder. $[\alpha]_D^{25}$ -77.3 (c, 0.14 in MeOH).

3-O-[β-D-Apiofuranosyl-(1→2)-[4-hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]:
$C_{43}H_{48}O_{25}$ 964.837
Constit. of spinach (*Spinacea oleracea*) leaves. λ_{max} 255 ; 274 ; 295 (sh) ; 337 ; 371 (sh) (MeOH).

[33530-69-7, 35399-34-9, 73202-46-7]

Nielsen, J.G. *et al., Acta Chem. Scand.*, 1970, **24**, 724 (*pmr, ms*)
Smith, D.M. *et al., Phytochemistry*, 1971, **10**, 3115 (*3-diglucoside*)
Bhardwaj, D.K. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 338 (*synth*)
Mues, R. *et al., Phytochemistry*, 1979, **18**, 1379 (*uv, ms*)
Bhardwaj, D.K. *et al., Phytochemistry*, 1980, **19**, 713 (*isol*)
Proksch, P. *et al., Phytochemistry*, 1984, **23**, 679 (*isol*)
Ferreres, F. *et al., Phytochemistry*, 1997, **45**, 1701 (*apiosylglucosylglucoside*)

3,3′,4′,5,8-Pentahydroxy-7-methoxyflavone P-158

[18799-01-4]
2-(3,4-Dihydroxyphenyl)-3,5,8-trihydroxy-7-methoxy-4H-1-benzopyran-4-one. 3′,4′,5,8-Tetrahydroxy-7-methoxyflavonol. ***Ranupenin****. Gossypetin 7-methyl ether*

$C_{16}H_{12}O_8$ 332.266
Yellow cryst. (MeOH aq.). Mp 303-305°.

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [85122-22-1] *Ranupenin 3-rutinoside*
$C_{28}H_{32}O_{17}$ 640.551
Isol. from *Ruta graveolens* (rue).

Harborne, J.B. *et al., Phytochemistry*, 1965, **4**, 647; 1969, **8**, 177; 1978, **17**, 589 (*glycosides*)
Harborne, J.B. *et al., Z. Naturforsch., C*, 1983, **38**, 148 (*3-rutinoside*)

3,3′,5,5′,7-Pentahydroxy-4′-methoxyflavone P-159

[16805-10-0]
2-(3,5-Dihydroxy-4-methoxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one, 9CI. 3′,5,5′,7-Tetrahydroxy-4′-methoxyflavonol. ***Mearnsetin****. Myricetin 4′-methyl ether*

$C_{16}H_{12}O_8$ 332.266
Yellow needles (EtOH). Mp 208-210°.

3-O-(4-O-Acetyl-α-L-rhamnopyranoside): ***Eujambolin***
$C_{24}H_{24}O_{13}$ 520.446
Constit. of *Eugenia jambolana* (jambolan). Amorph. yellow powder.

Mahmoud, I.I. *et al., Phytochemistry*, 2001, **58**, 1239-1244 (*Eujambolin*)

3,4′,5,6,7-Pentahydroxy-3′-methoxyflavone P-160

[57093-48-8]
3,5,6,7-Tetrahydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI. Quercetagetin 3′-methyl ether

$C_{16}H_{12}O_8$ 332.266

3-O-β-D-Galactopyranoside: [128351-80-4]

$C_{22}H_{22}O_{13}$ 494.408

3-O-β-D-Glucopyranoside: [128351-79-1]
$C_{22}H_{22}O_{13}$ 494.408

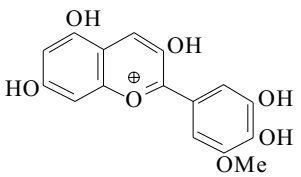
7-O-β-D-Glucopyranoside: [29741-08-0]
$C_{22}H_{22}O_{13}$ 494.408
Isol. from *Chrysanthemum coronarium* (chop-suey greens).

Harborne, J.B. *et al., Phytochemistry*, 1970, **9**, 2011 (*7-glucoside*)
D'Agostino, M. *et al., Phytochemistry*, 1990, **29**, 353 (*3-glycosides*)
El-Lakany, A.M. *et al., Pharmazie*, 1996, **51**, 435 (*isol*)

3,3′,4′,5,7-Pentahydroxy-5′-methoxyflavylium(1+) P-161

[13270-60-5]

[1429-30-7]
2-(3,4-Dihydroxy-5-methoxyphenyl)-3,5,7-trihydroxy-1-benzopyrylium(1+), 9CI. ***Petunidin****. Myrtillidin. Petunidol*



$C_{16}H_{13}O_7^{\oplus}$ 317.274
Isol. from bilberries (*Vaccinium myrtillus*), giant granadilla (*Passiflora quadrangularis*), *Amonum subulatum* (Nepal cardamon) and other plants. Also found in red table wine and red wine vinegar. Glycosides also widely distributed. Grey-brown leaflets or prisms (HCl aq.)(as chloride). Forms several hydrates.

3-O-Arabinoside: [28500-03-0] *Petunidin 3-arabinoside*
$C_{21}H_{21}O_{10}^{\oplus}$ 433.391
Isol. from *Vaccinium* spp. and other plant spp..

3-O-α-L-Rhamnopyranoside, 5-O-β-D-glucopyranoside: [53925-30-7]
$C_{28}H_{33}O_{16}^{\oplus}$ 625.559
Isol. from the Leguminosae.

3-O-β-D-Galactopyranoside: [28500-02-9] *Petunidin 3-galactoside*
$C_{22}H_{23}O_{12}^{\oplus}$ 479.416
Pigment from whortleberry, blackberry, etc.. Dark bronze-brown flat prisms + $4H_2O$ (MeOH/HCl) (as chloride).

3-O-β-D-Glucopyranoside: [6988-81-4] *Petunidin 3-glucoside*
$C_{22}H_{23}O_{12}^{\oplus}$ 479.416
Present in red wine. Dark red cryst. with green metallic lustre (as chloride).

3-O-[4-Hydroxycinnamoyl-(→?)-β-D-glucopyranoside]: [71991-89-4]
$C_{31}H_{29}O_{14}^{\oplus}$ 625.562
Isol. from grapes.

3-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside], 5-O-β-D-glucopyranoside: [51939-66-3]
$C_{37}H_{39}O_{19}^{\oplus}$ 787.704
Isol. from grapes.

3,5-Di-O-β-D-glucopyranoside: [25846-73-5] ***Petunin****. Muscadinin*
$C_{28}H_{33}O_{17}^{\oplus}$ 641.558
Isol. from muscat grapes (*Vitis vinifera*), muscadine grapes (*Vitis rotundifolia*) and other plants. Copper-coloured cryst. + $2H_2O$ (as chloride). Mp 179° approx Mp 300°.

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [39824-84-5] *Petunidin 3-rutinoside*
$C_{28}H_{33}O_{16}^{\oplus}$ 625.559
Isol. from *Morus* sp..

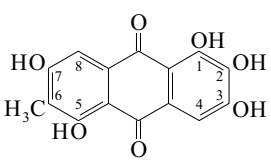
3-O-[4-Hydroxycinnamoyl-(→4)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 5-O-β-D-glucopyranoside: [69915-09-9] ***Petanin***
$C_{43}H_{49}O_{23}^{\oplus}$ 933.846
Isol. from *Solanum* spp..

3-O-[4-Hydroxycinnamoyl-(→6)-α-L-rhamnopyranosyl-(→?)-β-D-glucopyranoside]: Petunidin 3-[6-(coumaroylrhamnosyl)glucoside]
$C_{37}H_{39}O_{18}^{\oplus}$ 771.704
Isol. from tubers of potato (*Solanum tuberosum*).

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [39814-18-1] *Petunidin 3-gentiobioside*
$C_{28}H_{33}O_{17}^{\oplus}$ 641.558
Isol. from *Eugenia jambolana* (jambolan).

Robinson, G.M. *et al., Biochem. J.*, 1931, **25**, 1687 (*struct*)
Bell, J.C. *et al., J.C.S.*, 1934, 1604 (*isol*)
do Vale, J.C. *et al., CA*, 1964, **61**, 7356 (*rhamnosylglucoside*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1742 (*occur*)
Billot, J. *et al., Phytochemistry*, 1974, **13**, 2886 (*isol*)
Bombardelli, E. *et al., J. Chromatogr.*, 1976, **120**, 115 (*glc, ms*)
Iacobucci, G.A. *et al., Tetrahedron*, 1983, **39**, 3005 (*rev*)
Hoshino, T. *et al., Phytochemistry*, 1986, **25**, 829 (*cd*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Merlin, J.-C. *et al., Phytochemistry*, 1994, **35**, 227 (*Raman*)
Hosokawa, K. *et al., Phytochemistry*, 1995, **38**, 1293 (*derivs, ir, uv, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PCU000

1,2,3,5,7-Pentahydroxy-6-methylanthraquinone P-162



$C_{15}H_{10}O_7$ 302.24

2,3-Di-Me ether: [38934-17-7] *1,3,5-Trihydroxy-6,7-dimethoxy-2-methylanthraquinone*
$C_{17}H_{14}O_7$ 330.293
Isol. from roots of *Cassia tora* (charota). Mp 210° dec. Struct. not fully established.

Tiwari, R.D. *et al., Planta Med.*, 1972, **21**, 393-397

1,2,3,7,8-Pentahydroxy-6-methylanthraquinone P-163

$C_{15}H_{10}O_7$ 302.24
Cryst. (MeOH/$CHCl_3$). Mp 273-274°.

1,2,3,8-Tetra-Me ether: [70588-06-6] *2-Hydroxy-1,6,7,8-tetramethoxy-3-methylanthraquinone.* ***Chrysoobtusin***
$C_{19}H_{18}O_7$ 358.347
Isol. from seeds of *Cassia tora* (charota). Yellow needles. Mp 219-220°.

Shibata, S. *et al., Chem. Pharm. Bull.*, 1969, **17**, 454 (*isol, Chrysoobtusin*)

1,3,5,6,8-Pentahydroxy-2-methylanthraquinone P-164

[99499-84-0]

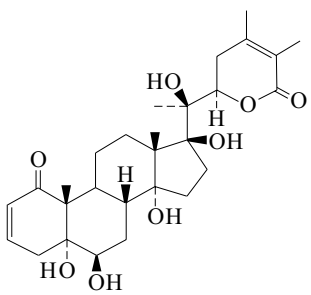
$C_{15}H_{10}O_7$ 302.24

6-Me ether: [101508-13-8] *1,3,5,8-Tetrahydroxy-6-methoxy-2-methylanthraquinone*
$C_{16}H_{12}O_7$ 316.267
Isol. from *Diospyros discolor* (mabolo). Mp 150-153° dec.

6-Me ether, 8-O-β-D-glucopyranoside: [101508-15-0]
$C_{22}H_{22}O_{12}$ 478.409
Isol. from *Diospyros discolor* (mabolo). Brown needles (Me_2CO/MeOH). Mp 255-256°.

Srivastava, S.K. *et al., Planta Med.*, 1985, 537
Singh, J. *et al., Indian J. Chem., Sect. B*, 1988, **27**, 858

5,6,14,17,20-Pentahydroxy-1-oxowitha-2,24-dienolide P-165



$C_{28}H_{40}O_8$ 504.619

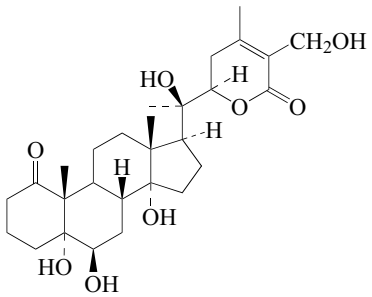
(5α,6β,17βOH,20*S*,22*R*)-*form*

5-Et ether: [79710-17-1] *5α-Ethoxy-6β,14α,17β,20-tetrahydroxy-1-oxowitha-2,24-dienolide*
$C_{30}H_{44}O_8$ 532.673
Cryst. (EtOAc). Mp 167°. $[\alpha]_D$ +62.7 (c, 0.11 in $CHCl_3$).

5-Butyl ether, 6-Ac: ***Physapruin B***
$C_{34}H_{50}O_9$ 602.764
Constit. of *Physalis pruinosa* (strawberry tomato). Amorph. powder. $[\alpha]_D$ +47 (c, 0.47 in MeOH).

Velde, V.V. *et al., Phytochemistry*, 1981, **20**, 1359
Shingu, K. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1873 (*Physapruin B*)

5,6,14,20,27-Pentahydroxy-1-oxowith-24-enolide P-166

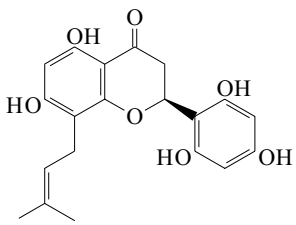


$C_{28}H_{42}O_8$ 506.635

(5α,6β,14α,20*R*,22*R*)-*form* [222609-97-4]
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D$ +72.5 (c, 0.23 in MeOH). λ_{max} 215 (log ϵ 3.99) (MeOH).

Ahmad, S. *et al., Phytochemistry*, 1999, **50**, 647-651 (*isol, pmr, cmr*)

2′,4′,5,6′,7-Pentahydroxy-8-prenylflavanone P-167



$C_{20}H_{20}O_7$ 372.374

(*S*)-*form*

4′-Me ether: [144161-81-9] *2′,5,6′,7-Tetrahydroxy-4′-methoxy-8-prenylflavanone.* ***Kenusanone D***
$C_{21}H_{22}O_7$ 386.401
Amorph. powder.

4′,7-Di-Me ether: [144161-82-0] *2′,5,6′-Trihydroxy-4′,7-dimethoxy-8-prenylflavanone.* ***Kenusanone E***
$C_{22}H_{24}O_7$ 400.427
Powder.

2′,4′,6′-Tri-Me ether: [156127-36-5] *5,7-Dihydroxy-2′,4′,6′-trimethoxy-8-prenylflavanone.* ***Heteroflavanone C***
$C_{23}H_{26}O_7$ 414.454
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Needles ($CHCl_3$/MeOH). Mp 155-156°. $[\alpha]_D^{24}$ +71.4 (c, 0.07 in $CHCl_3$).

2′,4′,6′,7-Tetra-Me ether: [151171-29-8] *5-Hydroxy-2′,4′,6′,7-tetramethoxy-8-prenylflavanone.* ***Heteroflavanone B***
$C_{24}H_{28}O_7$ 428.481
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Needles. Mp 145-147°. $[\alpha]_D^{25}$ +64 (c, 0.1 in $CHCl_3$). Tentative config. given.

Iinuma, M. *et al., Phytochemistry*, 1992, **31**, 2855

Lu, C.-M. *et al., Phytochemistry*, 1993, **33**, 909; 1994, **34**, 781 (*Heteroflavanone B, Heteroflavanone C*)

3′,4′,5,5′,7-Pentahydroxy-6-prenylflavanone P-168

*2,3-Dihydro-5,7-dihydroxy-6-(3-methyl-2-butenyl)-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one*

$C_{20}H_{20}O_7$ 372.374

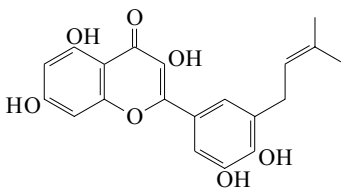
3′,4′,5′,7-Tetra-Me ether: [55303-95-2] *5-Hydroxy-3′,4′,5′,7-tetramethoxy-6-prenylflavanone.* ***Artoflavanone***
$C_{24}H_{28}O_7$ 428.481
Constit. of *Artocarpus heterophyllus* (jackfruit). Needles (petrol). Mp 141-142°. $[\alpha]_D$ +52 (c, 0.5 in $CHCl_3$).

Dayal, R. *et al., Indian J. Chem.*, 1974, **12**, 895 (*isol*)

Dayal, R. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 612 (*synth*)

3,3′,4′,5,7-Pentahydroxy-5′-prenylflavone P-169

[139163-15-8]
3′,4′,5,7-Tetrahydroxy-5′-prenylflavonol. ***Uralenol***



$C_{20}H_{18}O_7$ 370.358
Constit. of the leaves of *Glycyrrhiza uralensis* (Chinese licorice). Yellow cryst. Mp 170.5-172.5°.

3-Me ether: [150853-98-8] *3′,4′,5,7-Tetrahydroxy-3-methoxy-5′-prenylflavone.* ***3-O-Methyluralenol***
$C_{21}H_{20}O_7$ 384.385
Constit. of the leaves of *Glycyrrhiza uralensis* (Chinese licorice). Yellow cryst. Mp 104-109°.

Jia, S.S. *et al., Yaoxue Xuebao*, 1991, **25**, 758-762 (*isol*)

Jia, S. *et al., Chin. Chem. Lett.*, 1992, **3**, 189 (*3-Me ether*)

Jia, S.S. *et al., Yaoxue Xuebao*, 1993, **28**, 28-31 (*3-O-Methyluralenol*)

3,3′,4′,5,7-Pentahydroxy-6-prenylflavone P-170

[129145-54-6]
*2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Gancaonin P***

$C_{20}H_{18}O_7$ 370.358
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Yellow needles (Me_2CO). Mp 238-240°.

3-Me ether: [151649-34-2] *3′,4′,5,7-Tetrahydroxy-3-methoxy-6-prenylflavone.* ***3-O-Methylgancaonin P***
$C_{21}H_{20}O_7$ 384.385

3′-Me ether: [151776-21-5] *3,4′,5,7-Tetrahydroxy-3′-methoxy-6-prenylflavone.* ***3′-O-Methylgancaonin P***
$C_{21}H_{20}O_7$ 384.385
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Yellow cryst. Mp 160-162°.

3,7-Di-Me ether: [151649-35-3] *3′,4′,5-Trihydroxy-3,7-dimethoxy-6-prenylflavone.* ***3,7-Di-O-methylgancaonin P***
$C_{22}H_{22}O_7$ 398.412

4′,7-Di-Me ether: [101770-13-2] *3,3′,5-Trihydroxy-4′,7-dimethoxy-6-prenylflavone.* ***Isorhyncospermin***
$C_{22}H_{22}O_7$ 398.412
Pale yellow needles (MeOH). Mp 190°.

Adinarayana, D. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 880 (*Isorhyncospermin*)

Fukai, T. *et al., Heterocycles*, 1990, **31**, 370 (*isol, pmr, cmr*)

Nia, M.A. *et al., J. Nat. Prod.*, 1992, **55**, 1152 (*Isorhyncospermin*)

Harborne, J.B. *et al., Phytochemistry*, 1993, **34**, 219 (*derivs*)

Jia, S.S. *et al., Yaoxue Xuebao*, 1993, **28**, 623 (*3′-O-Methylgancaonin P*)

3,3′,4′,6,7-Pentahydroxy-2′-prenylflavone P-171

[139163-16-9]
3′,4′,6,7-Tetrahydroxy-2′-prenylflavonol. ***Neouralenol***

$C_{20}H_{18}O_7$ 370.358
Constit. of the leaves of *Glycyrrhiza uralensis* (Chinese licorice). Dark yellow cryst. Mp 229-231°.

Jia, S.S. *et al., Yaoxue Xuebao*, 1991, **25**, 758-762 (*isol, struct*)

3,4′,5,5′,6-Pentahydroxy-2′-prenylflavone P-172

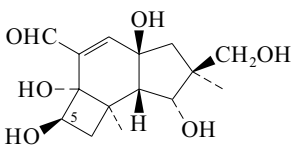
4′,5,5′,6-Tetrahydroxy-2′-prenylflavonol

$C_{20}H_{18}O_7$ 370.358

3-Me ether: [150853-99-9] *4′,5,5′,6-Tetrahydroxy-3-methoxy-2′-prenylflavone.* ***Uralene***
$C_{21}H_{20}O_7$ 384.385
Constit. of the leaves of *Glycyrrhiza uralensis* (Chinese licorice). Light yellow cryst. Mp 216-218°.

Jia, S.S. *et al., Chin. Chem. Lett.*, 1992, **3**, 189
Jia, S.S. *et al., Yaoxue Xuebao*, 1993, **28**, 28-31

1,5,6,9,13-Pentahydroxy-7-protilluden-14-al P-173



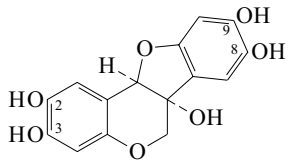
$C_{15}H_{22}O_6$ 298.335

(1α,5β)-*form*

5-O-(2-Hydroxy-4-methoxy-6-methylbenzoyl): [112471-06-4] ***13-Hydroxy-5′-O-methylmelledonal***. *15-Hydroxy-5′-O-methylmelledonal*
$C_{24}H_{30}O_9$ 462.496
Metab. of *Armillaria mellea* (honey mushroom). Cryst. Mp 174-176°. $[\alpha]_D^{25}$ +77.3 (c, 0.22 in MeOH).

Donnelly, D.M.X. *et al., Phytochemistry*, 1987, **26**, 3075

2,3,6*a*,8,9-Pentahydroxypterocarpan P-174



$C_{15}H_{12}O_7$ 304.256

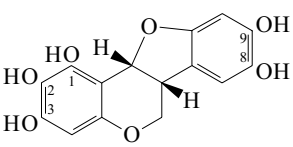
2-Me, 8,9-methylene ether: [99624-64-3] *3,6a-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan*. ***Hildecarpin***
$C_{17}H_{14}O_7$ 330.293
Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O. λ_{max} 208 (ϵ 25800); 297 (ϵ 18200) (EtOH) (Berdy). λ_{max} 214 ; 252 ; 305 (EtOH-NaOH) (Berdy). λ_{max} 208 ; 292 ; 305 ; 321 ; 352 (EtOH-HCl) (Berdy).

3-Me, 8,9-methylene ether: [147821-58-7] *2,6a-Dihydroxy-3-methoxy-8,9-methylenedioxypterocarpan*. ***2-Hydroxypisatin***
$C_{17}H_{14}O_7$ 330.293
$[\alpha]_D^{28}$ +216 (c, 0.3 in EtOH).

2,3-Di-Me, 8,9-methylene ether: [83159-18-6] *6a-Hydroxy-2,3-dimethoxy-8,9-methylenedioxypterocarpan*. ***Lathycarpin***
$C_{18}H_{16}O_7$ 344.32
Phytoalexin from leaves of *Lathyrus sativus* (chickling pea). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. $[\alpha]_D^{21}$ +232 (c, 0.012 in MeOH). λ_{max} 212 ; 303 (MeOH) (Berdy). λ_{max} 212 ; 303 (MeOH-NaOH) (Berdy). λ_{max} 303 ; 368 (MeOH-HCl) (Berdy).

Ingham, J.L. *et al., Z. Naturforsch., C*, 1982, **37**, 724 (*isol, uv, pmr, struct, abs config, Lathycarpin*)
Lwande, W. *et al., Insect Sci. Its Appl.*, 1985, **6**, 537; 1986, **7**, 501; *CA*, **104**, 31710; **106**, 15746 (*Hildecarpin*)
Kobayashi, A. *et al., Phytochemistry*, 1993, **22**, 77 (*2-Hydroxypisatin*)

1,2,3,8,9-Pentahydroxypterocarpan P-175



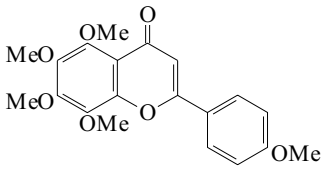
$C_{15}H_{12}O_7$ 304.256
(6α*R*,11α*R*)-form

2-Me, 8,9-methylene ether: [73520-83-9] *1,3-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan*. ***Trifolian***
$C_{17}H_{14}O_7$ 330.293
Isol. from roots of *Trifolium pratense* (red clover). Cryst. (MeOH). Mp 132-134°. $[\alpha]_D$ -240 (c, 0.5 in MeOH). λ_{max} 302 (ϵ 30000) (EtOH) (Berdy).

Fraishtat, P.D. *et al., Bioorg. Khim.*, 1979, **5**, 1879; 1981, **7**, 927

4′,5,6,7,8-Pentamethoxyflavone P-176

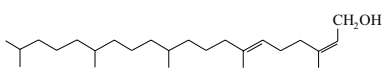
[481-53-8]
5,6,7,8-Tetramethoxy-2-(4-methoxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Tangeritin***. *Ponkanetin. Tangeretin*



$C_{20}H_{20}O_7$ 372.374
Formerly assigned the 3,4′,5,6,7-pentamethoxy struct.. Isol. from tangerine peel and *Fortunella japonica* (round kumquat). Potential nutriceutical. Rods or needles (EtOAc). Mp 154°.
▶ DJ3102725

Sehgal, J.M. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1955, **42**, 252 (*synth*)
Goldsworthy, L.J. *et al., Chem. Ind. (London)*, 1957, 47 (*struct*)
Okigawa, M. *et al., J.C.S. Perkin 1*, 1975, 1563 (*pmr*)
Talapatra, S.K. *et al., Phytochemistry*, 1975, **14**, 309 (*isol*)
Matsuura, S. *et al., Chem. Pharm. Bull.*, 1978, **26**, 305 (*synth*)
Tatum, J.H. *et al., Phytochemistry*, 1978, **17**, 447 (*isol*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 708 (*cmr*)
Rizzi, G.P. *et al., J. Agric. Food Chem.*, 1984, **32**, 551 (*ms*)
Elgamal, M.H.A. *et al., J. Prakt. Chem.*, 1986, **328**, 893 (*ms*)

3,7,11,15,19-Pentamethyl-2,6-eicosadien-1-ol P-177

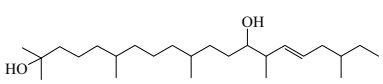


$C_{25}H_{48}O$ 364.654
(2*Z*,6*E*)-form [26549-03-1]
Constit. of the leaves of *Solanum tuberosum* (potato). Pale yellow oil.

Toyoda, M. *et al., Tet. Lett.*, 1969, 4879

2,6,10,14,18-Pentamethyl-15-eicosene-2,13-diol P-178

[255833-55-7]
Lepidiumsesterterpenol

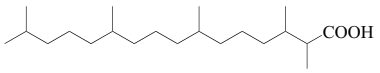


$C_{25}H_{50}O_2$ 382.669
Constit. of *Lepidium sativum* (garden cress). Cryst. ($CHCl_3$). Mp 200-201°. λ_{max} 205 (log ϵ 1.5) (MeOH).

Pande, S.D. *et al., Pharmazie*, 1999, **54**, 851-853 (*isol, pmr, cmr*)

2,3,7,11,15-Pentamethylhexadecanoic acid P-179

[122706-68-7]

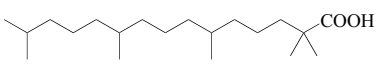


$C_{21}H_{42}O_2$ 326.562
Isol. from the oil of the redfish (*Sebastes* sp.).

Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630 (*isol*)

2,2,6,10,14-Pentamethylpentadecanoic acid P-180

[122706-67-6]



$C_{20}H_{40}O_2$ 312.535
Isol. from the oil of the redfish (*Sebastes* sp.).

Ratnayake, W.M.N. *et al., Lipids*, 1989, **24**, 630 (*isol*)

Pentanal, 9CI P-181

[110-62-3]
n-*Valeraldehyde, 8CI. Valeric aldehyde. FEMA 3098*

$H_3CCH_2CH_2CH_2CHO$

$C_5H_{10}O$ 86.133
Found in olive oil and several essential oils. Also present in Bantu beer, plum brandy, cardamom, coriander leaf, rice, Bourbon vanilla, clary sage, cooked shrimps, scallops, apple, banana, sweet cherry, blackcurrant and other foods. Liq. d_4^{20} 0.81. Fp -92. Bp 102.5-103°. n_D^{20} 1.3947.
▶ Highly flammable, fl. p. 12°, autoignition temp. 222°. Eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 3200 mg/kg. LD_{50} (rbt, skn) 4857 mg/kg. YV3600000

Oxime: [628-79-5]
$C_5H_{11}NO$ 101.148
Cryst. Mp 52°.

2,4-Dinitrophenylhydrazone: [2057-84-3]
Yellow cryst. Mp 106-107°.

Di-Me acetal: [26450-58-8] *1,1-Dimethoxypentane*
$C_7H_{16}O_2$ 132.202
Liq. Bp 120-129°.

Di-Et acetal: [3658-79-5] *1,1-Diethoxypentane*
$C_9H_{20}O_2$ 160.256
Volatile component of strawberries and other fruits. Liq. d_4^{22} 0.83. Bp 162.5-163.5° Bp_{12} 59°. n_D^{23} 1.4029.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 729C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 467B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 553B (*ir*)
Blaise, E.E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1904, **138**, 698 (*synth*)
Bruylants, P. *et al., CA*, 1932, **26**, 3232 (*synth*)
Org. Synth., 1971, **51**, 31 (*synth*)
Zeidler, U. *et al., CA*, 1974, **81**, 91007 (*synth*)

Roberts, J.D. *et al., J.O.C.*, 1974, **39**, 1017 (*cmr*)
Savoia, D. *et al., J.O.C.*, 1978, **43**, 2907; 1980, **45**, 3227 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 919 (*rev, tox*)
Maccoll, A. *et al., Org. Mass Spectrom.*, 1986, **21**, 251 (*ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VAG000
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1312

Pentane, 9CI P-182

[109-66-0]

$H_3CCH_2CH_2CH_2CH_3$

C_5H_{12} 72.15

Present in hop oil. Volatile liq. Sl. sol. H_2O. d_4^{20} 0.63. Fp -129. Bp 36°. n_D^{20} 1.3577.

▶ Extremely flammable, fl. p. -49°, autoignition temp. 243°. High conc. narcotic. OES: long-term 600 ppm; short-term 750 ppm. RZ9450000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 2A (*ir*)
Shepard, A.F. *et al., J.A.C.S.*, 1931, **53**, 1948-1958 (*props*)
Org. Synth., Coll. Vol., 2, 1943, 478-480 (*synth*)
Buttery, R.G. *et al., Nature (London)*, 1963, **200**, 435 (*isol*)
Gallant, R.W. *et al., Hydrocarbon Process.*, 1967, **46**, 121-129 (*props*)
Svec, H.J. *et al., J.C.S. Faraday 2*, 1973, **69**, 1187-1199 (*ms*)
Kondo, M. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 589-592 (*pmr*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313-321 (*cmr*)
Flurry, R.L. *et al., J. Phys. Chem.*, 1983, **87**, 1753-1757 (*ir, Raman*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PBK250
Boese, R. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 988-992 (*cryst struct.*)
Low, L.K. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 279 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1878
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 970
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Pentanedial, 9CI P-183

[111-30-8]

Glutaraldehyde. ***Glutaral, INN, USAN.*** *Aldesan. Alhydex. Bactron K31. Cidex. Diswart. Gludesin. Glutaclean. Glutarex 28. Glutarol. Hospex. Sonacide. Sporicidin. Ucarcide. Verucasep. Virsal*

$OHCCH_2CH_2CH_2CHO$

$C_5H_8O_2$ 100.117

Exists mainly as cyclic hemiacetal and linear dihydrate forms in 25% aq. soln.. Used as an antimicrobial agent in sugar mills and as a fixing agent in the immobilisation of glucose isomerase enzyme preparations for use in the manuf. of high fructose corn syrup. Oil. Sol. H_2O, EtOH. Mp -14°. Bp 188° dec. Bp_{10} 71-72°. n_D^{20} 1.4200. Log P -0.61 (calc). Polymerises in presence of H_2O → glassy polymer which on dist. *in vacuo* regenerates the dialdehyde. Usually sold as a 50% or 25% aq. soln. Vp 17 mmHg (20°). Spontaneous or catalytic polym. gives a copolymer of a cyclic struct. and an open chain struct..

▶ Symptoms from prolonged or repeated (occup.) exposure incl. nausea, headache, eye, skin and respiratory tract irritation. Can cause asthma and dermatitis. LD_{50} (rat, orl) 134 mg/kg. OES: short-term 0.2 ppm. MA2450000

Dioxime: [6635-57-0]
$C_5H_{10}N_2O_2$ 130.146
Needles (H_2O). Mp 178°. Subl. without dec..

Mono-2,4-dinitrophenylhydrazone: [81591-72-2]
Mp 193.7-194.7°.

Bis-2,4-dinitrophenylhydrazone: [5085-07-4]
Mp 185°.

Di-Me acetal: [50789-30-5] *5,5-Dimethoxypentanal, 9CI*
$C_7H_{14}O_3$ 146.186
Liq. Bp_5 80-82°.

Di-Et acetal: [79893-96-2] *5,5-Diethoxypentanal, 9CI*
$C_9H_{18}O_3$ 174.239
Liq. Bp_2 53-57°.

Bis(di-Me acetal): [4454-02-8] *1,1,5,5-Tetramethoxypentane, 9CI*
$C_9H_{20}O_4$ 192.255
Liq. Bp_5 87-91° Bp_1 70-72°.

Bis(di-Et acetal): [4454-01-7] *1,1,5,5-Tetraethoxypentane, 9CI*
$C_{13}H_{28}O_4$ 248.362
Liq. Bp_2 97° $Bp_{0.3}$ 85-86°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 480C (*ir*)
U.S. Pat., 1951, 2 546 018; *CA*, **45**, 7589 (*synth*)
Stoll, A. *et al., Helv. Chim. Acta*, 1953, **36**, 268 (*synth*)
Aso, C. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 1426 (*polym*)
Meyersen, K. *et al., Makromol. Chem.*, 1962, **58**, 204 (*polym*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 411
Whipple, E.B. *et al., J.O.C.*, 1974, **39**, 1667 (*cmr, pmr*)
Russell, A.D. *et al., Prog. Med. Chem.*, 1976, **13**, 271 (*rev, use*)
Gray, K.G. *et al., Aust. J. Hosp. Pharm.*, 1980, **10**, 139 (*rev, pharmacol*)
Haley, T.J. *et al., Dangerous Prop. Ind. Mater. Rep.*, 1981, **1**, 2 (*rev, props, tox*)
Griesbaum, K. *et al., Chem. Ber.*, 1982, **115**, 2697 (*ms*)
Boeckman, R.K. *et al., J.A.C.S.*, 1982, **104**, 1033 (*synth, pmr, acetal*)
Griesbaum, K. *et al., J.O.C.*, 1990, **55**, 6024 (*acetals*)
Beauchamp, R.O. *et al., Crit. Rev. Toxicol.*, 1992, **22**, 143 (*rev, tox*)
Russell, A.D. *et al., Principles and Practice of Disinfection, Preservation and Sterilization*, 2nd Ed., Blackwell, 1992, (*uses*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 796
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2607-2608 (*use*)
Wanner, M.J. *et al., J.O.C.*, 1995, **60**, 5634 (*acetal, synth, pmr, cmr, ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1216-1217
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 647
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GFQ000

2,3-Pentanedione, 9CI P-184

[600-14-6]

Ethyl methyl diketone. FEMA 2841

$H_3CCOCOCH_2CH_3$

$C_5H_8O_2$ 100.117

Flavour ingredient. Present in peach, wheat bread, yoghurt, cocoa, coffee, black tea, roasted barley, roasted filbert and other foodstuffs. Yellow liq. Sol. H_2O. d_4^{19} 0.96. Mp -52°. Bp 108°. n_D^{19} 1.4014.

▶ Skin irritant. SA1850000

2-Oxime: [32818-79-4]
$C_5H_9NO_2$ 115.132
Leaflets. Mp 69-71°.

▶ LD_{50} (mus, ipr) 350 mg/kg. SA2300000

3-Oxime: [609-29-0]
$C_5H_9NO_2$ 115.132
Leaflets. Mp 58-59°. Bp 183-187° part. dec..

▶ LD_{50} (mus, ipr) 601 mg/kg. SA2350000

Dioxime: [4775-86-4] *Ethylmethylglyoxime*
$C_5H_{10}N_2O_2$ 130.146
Needles (EtOH). Mp 172-173° part. subl. pK_{a2} 12.02.

3-Phenylhydrazone: [58120-93-7]
Cryst. (EtOH). Mp 115°.

2-(4-Nitrophenylhydrazone), 3-oxime:
$C_{11}H_{14}N_4O_3$ 250.257
Yellow cryst. (EtOH). Mp 235-236°.

Bis-2,4-dinitrophenylhydrazone: [1180-59-2]
Orange cryst. (nitrobenzene). Mp 280-281° Mp 306°.

Disemicarbazone:
Mp 251-252°.

2,2-Di-Me acetal: [21983-78-8] *2,2-Dimethoxy-3-pentanone*
$C_7H_{14}O_3$ 146.186
Liq. Bp 162-163°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 660B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 424A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 510A (*ir*)
U.K. Pat., 1947, 586 754; *CA*, **41**, 6894 (*synth*)
Anand, V.D. *et al., Mikrochim. Acta*, 1961, 650 (*synth, detn, Co*)
Reusch, W. *et al., Tetrahedron*, 1967, **23**, 2893 (*ms*)
Egneus, B. *et al., Anal. Chim. Acta*, 1968, **43**, 53; 1969, **48**, 291 (*use, dioxime, detn, Ni*)
Yamashita, M. *et al., Chem. Comm.*, 1977, 691 (*synth*)
Bartnik, R. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1988, **62**, 433 (*cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBL350

2,4-Pentanedione, 9CI, 8CI P-185

[123-54-6]

Acetylacetone. Diacetylmethane. 4-Hydroxy-3-penten-2-one

$H_3CCOCH_2COCH_3 \Leftrightarrow H_3CC(OH)=CHCOCH_3$

$C_5H_8O_2$ 100.117

Tautomeric. Enol-form predominates in pure liq., vapour and most solvs., oxo-form predominates (84%) in aq. soln.. Isol. from ethereal oil of *Pinus sylvestris* (Scotch pine). Liq. Sol. dil. HCl; spar. sol. hot H_2O; misc. org. solvs. d_4^{25} 0.93. Bp_{746} 139°.

▶ Flammable, fl. p. 34°, autoignition temp. 340°. Skin and severe eye irritant. LD_{50} (rat, orl) 55 mg/kg. Exp. neurotoxic. Repeated exposure to low concs. may be cumulative. SA1925000

[10556-94-2, 17272-66-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 425A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 661B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 511B (*ir*)
Org. Synth., Coll. Vol., 3, 1955, 16 (*synth*)
Cameron, D.W. *et al., CA*, 1959, **53**, 16476 (*isol*)
Bowie, J.H. *et al., J.O.C.*, 1966, **31**, 1384 (*ms*)
Chalmers, R.A. *et al., Analyst (London)*, 1968, **93**, 629 (*use, Al*)
Koshimura, H. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 632 (*pmr*)
Soendergaard, N.C. *et al., Acta Chem. Scand., Ser. A*, 1975, **29**, 709 (*tautom*)
Grens, E. *et al., Spectrochim. Acta A*, 1975, **31**, 555 (*ir*)
Vallarino, L.M. *et al., Inorg. Chim. Acta*, 1985, **105**, 135 (*cmr, pmr, props*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH Weinheim, 1985, **A15**, 89 (*rev*)
Hush, N.S. *et al., Aust. J. Chem.*, 1987, **40**, 599 (*pe, tautom*)
Meany, J.E. *et al., J. Chem. Educ.*, 1988, **65**, 461 (*uv*)
Tobita, S. *et al., Int. J. Mass Spectrom. Ion Processes*, 1991, **105**, 101 (*ms*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3928-3930 (*use*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4773
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 971
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABX750

1-Pentanesulfenothioic acid, 9CI P-186

[86849-52-7]

Pentyl hydrodisulfide

$H_3C(CH_2)_4SSH$

$C_5H_{12}S_2$ 136.282

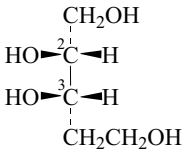
Constit. of chives (*Allium schoenoprasum*). Liq. with sweet onion smell.

S-*Me:* [72437-68-4] *Methyl pentyl disulfide, 9CI*
$C_6H_{14}S_2$ 150.309
Constit. of chives (*Allium schoenoprasum*). Liq. with sweet onion smell.

Kameoka, H. *et al., Phytochemistry*, 1983, **22**, 294

1,2,3,5-Pentanetetrol P-187

2-Deoxypentitol, 9CI



$C_5H_{12}O_4$ 136.147

The pentitol numbering starts at the other end of the chain.

(2*R*,3*S*)-*form*

2-Deoxy-D-ribitol

Constit. of the fruit of *Foeniculum vulgare* (fennel). Syrup. $[\alpha]_D^{22}$ -20 (c, 0.3 in H_2O). $[\alpha]_D$ -17 (c, 0.3 in MeOH).

Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)

1,2,4,5-Pentanetetrol P-188

[89617-06-1]

3-Deoxypentitol, 9CI

$C_5H_{12}O_4$ 136.147

(2*S*,4*S*)-*form* [92691-36-6]

D-threo-form. 3-Deoxy-D-arabinitol

Constit. of the fruit of *Foeniculum vulgare* (fennel). Cryst. (EtOH/Et_2O) or syrup. Mp 73-75° Mp 102° (dimorph.). $[\alpha]_D^{18}$ +31 (c, 0.4 in H_2O) (synthetic). $[\alpha]_D^{22}$ -46 (c, 1.03 in EtOH) (synthetic). $[\alpha]_D^{22}$ -11 (c, 0.1 in H_2O) (nat.). $[\alpha]_D$ -34.5 (c, 0.1 in MeOH) (nat.).

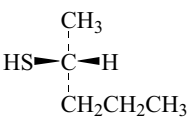
[124867-27-2]

Tsuda, Y. *et al., Chem. Pharm. Bull.*, 1980, **28**, 920-925 (*synth, derivs*)
Witczak, Z.J. *et al., Carbohydr. Res.*, 1982, **110**, 326-329 (*synth*)
Katajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988 (*isol*)

2-Pentanethiol, 9CI P-189

[2084-19-7]

2-Mercaptopentane. sec-*Amyl mercaptan*



(*R*)-*form*

$C_5H_{12}S$ 104.216

(*R*)-*form* [212195-83-0]
Bp 112°. $[\alpha]_D^{20}$ -4.7 (c, 17 in Et_2O).

(*S*)-*form* [212195-84-1]
Component of guava flavour (*Psidium guajava*). $[\alpha]_D^{20}$ +7.9 (c, 12 in Et_2O).

(±)-*form* [110503-18-9]
Flavouring material. Liq. d^{25} 0.83. Bp 112°. n_D^{25} 1.4386.

S-*Me:* [13286-91-4] *2-(Methylthio)pentane*
$C_6H_{14}S$ 118.243
Bp 138.9° Bp_{60} 63-64°. n_D^{20} 1.4468.

S-*Me,* S,S-*dioxide:* [101944-72-3] *2-(Methylsulfonyl)pentane*
$C_6H_{14}O_2S$ 150.241
Bp_2 101-102°. n_D^{20} 1.4602.

Levene, P.A. *et al., J. Biol. Chem.*, 1927, **75**, 593 (*abs config*)
Reid, L.M. *et al., J.A.C.S.*, 1932, **54**, 1685 (*synth*)
Brown, H.C. *et al., J.A.C.S.*, 1956, **78**, 2199 (*S-Me, dioxide*)
Levy, E.J. *et al., Anal. Chem.*, 1961, **33**, 707 (*ms*)
Bassols, F. *et al., J. Essent. Oil Res.*, 1994, **6**, 481-483 (*occur*)
Koenig, T. *et al., CA*, 1998, **129**, 200547c (*isol, abs config*)
Koenig, T. *et al., J. High Resol. Chromatogr.*, 1998, **21**, 371-372 (*occur, config*)

Pentanoic acid, 9CI P-190

[109-52-4]

Valeric acid, 8CI. FEMA 3101

$H_3CCH_2CH_2CH_2COOH$

$C_5H_{10}O_2$ 102.133

Minor constit. of biological systems e.g. yeast fat, some plant oils. Also present in blue cheeses, wines, apple, banana, morello cherry, cooked shrimp, scallop, roasted peanut, roasted filberts and other foodstuffs. Flavouring agent. Liq. with unpleasant rancid odour. Sol. EtOH, Et_2O; spar. sol. H_2O. d_4^{20} 0.95. Fp -34.5. Bp 186° Bp_{15} 86-88°. n_D^{23} 1.4075. pK_a 4.81. Log P 1.35 (calc).

▶ Fl. p. 89°, autoignition temp. 400°. Corrosive and irritating to skin, eyes and mucous membranes. LD_{50} (mus, orl) 600 mg/kg. YV6100000

Me ester: [624-24-8] *Methyl pentanoate. Methyl valerate. FEMA 2752*
$C_6H_{12}O_2$ 116.16
Present in baked potato, red chilli (*Capsicum frutescens*), wines, coffee, black tea, honey, olive, Bourbon vanilla, melon, papaya, pineapple and other fruits. Flavouring agent. Liq. with green-fruity apple- and pineapple-like taste and odour. d_4^{20} 0.89. Bp 127.3° Bp_{130} 74-79°. n_D^{20} 1.3969.

▶ Flammable, fl. p. < 25°. YV7750500

Et ester: [539-82-2] *Ethyl pentanoate. Ethyl valerate. FEMA 2462*
$C_7H_{14}O_2$ 130.186
Present in wines, Bantu beer, sake, honey, apple, banana, morello cherry, guava and other fruits. Flavouring agent. Liq. with fruity, apple-like odour. d_4^{20} 0.87. Bp 145.1°. n_D^{20} 1.4004.

Propyl ester: [141-06-0] *Propyl pentanoate. Propyl valerate*
$C_8H_{16}O_2$ 144.213
Used in pineapple flavours. Liq. Bp 167.4°.

Butyl ester: [591-68-4] *Butyl pentanoate. Butyl valerate. FEMA 2217*
$C_9H_{18}O_2$ 158.24
Present in apple, banana, blackberry, plum, jackfruit (*Artocarpus heterophyllus*), malt whisky and Bourbon vanilla. Flavouring agent. Liq. with apple-raspberry odour and sweet taste. d_4^{20} 0.87. Bp 186.5° (175°). n_D^{20} 1.4118.

3-Methylbutyl ester: [2050-09-1] *3-Methylbutyl pentanoate, 9CI. Isoamyl valerate. Isopentyl valerate, 8CI*
$C_{10}H_{20}O_2$ 172.267
Found in various fruits and cider. No synth. or phys. props. reported.

Nitrile: [110-59-8] *Pentanenitrile, 9CI. Valeronitrile, 8CI. Butyl cyanide. 1-Cyano-*

butane
C_5H_9N 83.133
Constit. of various *Brassica* spp.. Liq. Bp 138-140°.
▶ YV8195000

[6106-41-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 482B; 605C; 712A; 728C; 839C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 752C; 913A; 913B; 1166C; 1193C; 1352B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 574B; 618C; 618D; 769B; 797A (*ir*)
Ivanoff, D. *et al., Bull. Soc. Chim. Fr.*, 1925, **37**, 287 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 361 (*synth*)
Boudet, R. *et al., Bull. Soc. Chim. Fr.*, 1948, 390 (*synth, derivs*)
Geyer, R.P. *et al., J. Biol. Chem.*, 1950, **184**, 641 (*metab*)
Scheuerman, R.F. *et al., Acta Cryst.*, 1962, **15**, 1244 (*cryst struct*)
Brett, D. *et al., J.O.C.*, 1967, **32**, 855 (*nitrile*)
Miyazaki, S. *et al., J. Am. Oil Chem. Soc.*, 1978, **55**, 536 (*synth*)
Couperus, P.A. *et al., Org. Magn. Reson.*, 1978, **11**, 590 (*cmr*)
Dillon, K.B. *et al., J. Magn. Reson.*, 1980, **39**, 499 (*pmr*)
Hulkenberg, A. *et al., Tet. Lett.*, 1982, **23**, 1505 (*nitrile*)
Takahashi, K. *et al., J.O.C.*, 1983, **48**, 3566 (*synth, pmr*)
Hsiu, S.L. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2091 (*cmr, nitrile*)
Zav'yalov, S.I. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1985, 1071; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1985, 975 (*synth*)
Maccoll, A. *et al., Int. J. Mass Spectrom. Ion Processes*, 1988, **86**, 227 (*ms*)
Jursic, B. *et al., J. Chem. Res., Synop.*, 1988, 168; 336 (*nitrile*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, VAQ000
Huang, B. *et al., Synth. Commun.*, 1996, **26**, 165 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 358; 1047; 1881; 2887 (*occur, props, esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VAQ000; VBA000

1-Pentanol, 9CI P-191

[71-41-0]

[30899-19-5]
n-*Amyl alcohol. Pentyl alcohol. FEMA 2056*

$H_3CCH_2CH_2CH_2CH_2OH$
$C_5H_{12}O$ 88.149
Widely distributed in plant sources, e.g. peppermint oil, tomatoes, tea, potatoes. Flavouring ingredient. Liq. Sl. sol. H_2O. d_4^{20} 0.82. Mp -79°. Bp 137° Bp_{13} 49-50°. n_D^{20} 1.4103.
▶ Flammable, fl. p. 33/38°, autoignition temp. 300°. Eye, skin and respiratory tract irritant. Adverse CNS effects from prolonged exposure. SB9800000

Formyl: [638-49-3] *Pentyl formate. Amyl formate. FEMA 2068*
$C_6H_{12}O_2$ 116.16
Found in strawberry fruit, tomato, fried cured pork, cognac and honey. Used in fruit food flavouring. Liq. d 0.9. Bp 130-131°. n_D^{20} 1.3988.
▶ LQ9370000

Ac: [628-63-7] *Pentyl acetate.* n-*Amyl acetate*
$C_7H_{14}O_2$ 130.186
Flavouring agent. Liq. d_0^0 0.9. Fp -70.8. Bp 149.2°. n_D^{20} 1.4023.
▶ Eye irritant. Inhalation causes conjunctiva irritation, headache, somnolence. AJ1925000

Butanoyl: [540-18-1] *Pentyl butanoate, 9CI.* n-*Amyl butyrate, 8CI. FEMA 2059*
$C_9H_{18}O_2$ 158.24
Found in banana, apple and apricot fruits. Used in food flavouring. Liq. with apricot-like odour. d_4^{18} 0.87. Mp -73.2°. Bp 185°. n_D^{20} 1.4123.

Benzoyl: [2049-96-9] *Pentyl benzoate*
$C_{12}H_{16}O_2$ 192.257
Liq. Bp_{44} 167°.
▶ DH6276000

4-Nitrobenzoyl: [14309-42-3]
Mp 8.5-10.5°.

4-Nitrophenylurethane: [90429-36-0]
Mp 86°.

Me ether: [628-80-8] *1-Methoxypentane, 9CI. Methyl pentyl ether. Amyl methyl ether*
$C_6H_{14}O$ 102.176
Liq. d_4^{22} 0.76. Bp 99-100°. n_D^{22} 1.3862.
▶ KO2200000

Et ether: [17952-11-3] *1-Ethoxypentane, 9CI. Ethyl pentyl ether. Amyl ethyl ether*
$C_7H_{16}O$ 116.203
Liq. Bp 119-120°.
▶ KO0350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 110B; 602B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 164B; 901B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 156C (*ir*)
Gartenmeister, R. *et al., Annalen*, 1886, **233**, 254 (*formyl*)
Blaise, E.E. *et al., Ann. Chim. Phys.*, 1912, **25**, 253
Brown, H.C. *et al., J.A.C.S.*, 1959, **81**, 6434 (*synth*)
Johnson, D.E. *et al., Anal. Chem.*, 1961, **33**, 669 (*use*)
Schollkopf, U. *et al., Chem. Ber.*, 1964, **97**, 636 (*synth, deriv*)
Darbre, A. *et al., J. Chromatogr.*, 1965, **17**, 31 (*use*)
Blau, K. *et al., J. Chromatogr.*, 1965, **17**, 445; 1967, **26**, 35 (*use*)
Hikino, H. *et al., Tetrahedron*, 1976, **32**, 325 (*cmr*)
Bieber, H. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 278 (*rev*)
Borchers, F. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1979, **31**, 247-256 (*butanoyl, ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1980, **18**, 649-650 (*rev, formyl*)
Holmes, J.L. *et al., Org. Mass Spectrom.*, 1990, **25**, 381 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 709 (*rev*)
Yang, H. *et al., Synth. Commun.*, 1994, **24**, 3269-3275 (*butanoyl, synth, ir, pmr*)
Food Chemicals Codex, 4th edn., National Academy Press, 1996, 454-455 (*butanoyl, props*)
Merck Index, 12th edn., 1996, No. 645 (*butanoyl*)
Tiers, G.V.D. *et al., Acta Chem. Scand.*, 1998, **52**, 1223-1233 (*Me ether*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 97
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 75
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOD725; AOE000; AOJ500

2-Pentanol, 9CI P-192

[6032-29-7]

[30899-19-5]
sec-*n-Amyl alcohol. FEMA 3316*

$C_5H_{12}O$ 88.149
Flavouring ingredient. Chiral form not specified by FEMA.
▶ Flammable, fl. p. 40/49°. Eye and skin irritant. LD_{50} (rat, orl) 1470 mg/kg. High vapour conc. narcotic. SA4900000

(±)-*form* [13403-73-1]
Liq. Sol. H_2O. d_4^{20} 0.83. Bp 118-119°. n_D^{25} 1.4041.

Butanoyl: [60415-61-4] *1-Methylbutyl butanoate. 2-Pentyl butyrate. FEMA 3893*
$C_9H_{18}O_2$ 158.24
Food flavourant. Present in bananas, passion fruit and strawberry.

(ξ)-*form*
Present in many foodstuffs, e.g. fruits, alcoholic beverages and cheeses.

[116783-17-6]

Pickard, R.H. *et al., J.C.S.*, 1911, **99**, 65 (*resoln*)
Brunel, R.F. *et al., J.A.C.S.*, 1923, **45**, 1337 (*synth*)
Lemieux, R.U. *et al., Can. J. Chem.*, 1951, **29**, 678 (*abs config*)
Adembri, G. *et al., Ann. Chim. (Rome)*, 1956, **46**, 62; *CA*, **50**, 13714 (*synth*)
Brown, H.C. *et al., J.A.C.S.*, 1964, **86**, 1397 (*synth*)
Vigneron, J.P. *et al., Tetrahedron*, 1976, **32**, 939 (*synth*)
Bieber, H. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 278 (*rev*)
Herman, J.A. *et al., Can. J. Chem.*, 1981, **59**, 2125 (*ms*)
Ejchart, A. *et al., Org. Magn. Reson.*, 1981, **15**, 22 (*cmr*)
Thomas, E.J. *et al., J.C.S. Perkin 1*, 1989, 1529 (*resoln*)
Cheskis, B.A. *et al., Zh. Org. Khim.*, 1990, **26**, 1864; *J. Org. Chem. USSR (Engl. Transl.)*, 1990, **26**, 1613 (*synth, pmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 709
Morgan, B. *et al., J.O.C.*, 1992, **57**, 3231 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2116-2117
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1415; 1422 (*use, occur, butanoyl*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 136
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 75

2-Pentanone, 9CI P-193

[107-87-9]
Methyl propyl ketone. FEMA 2842

$H_3CCH_2CH_2COCH_3$
$C_5H_{10}O$ 86.133
Isol. from soya oil (*Glycine max*), pine-

apple and a few other plant sources. Liq. d_{15}^{15} 0.81. Bp 102°. n_D^{20} 1.3895.

▶ Highly flammable, fl. p. 7°, autoignition temp. 452/505°. Eye, skin and respiratory tract irritant. Inhalation also causes headache and nausea. LD_{50} (rat, orl) 3730 mg/kg. OES: long-term 200 ppm; short-term 250 ppm. SA7875000

Oxime: [623-40-5]
$C_5H_{11}NO$ 101.148
Bp 167°.

2,4-Dinitrophenylhydrazone: [1636-82-4]
Orange cryst. Mp 141°.

Dimethylhydrazone: [28236-86-4]
$C_7H_{16}N_2$ 128.217
Oil. Bp 134°.

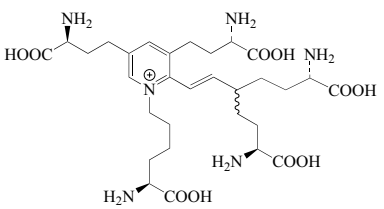
Semicarbazone: [3622-62-6]
Mp 110°.

Di-Et acetal: [80359-80-4] *2,2-Diethoxypentane, 9CI*
$C_9H_{20}O_2$ 160.256
Liq. Bp 151-153° $Bp_{18.5}$ 57.4°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 406A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 632C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 488A (*ir*)
Meerwein, H. *et al., Annalen*, 1913, **398**, 242 (*synth*)
U.K. Pat., 1928, 318 124; *CA*, **24**, 2140 (*synth*)
Yakovlev, I.P. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1954, **24**, 1163; *CA*, **50**, 4773 (*synth*)
Kawai, S. *et al., Chem. Pharm. Bull.*, 1966, **14**, 618 (*use*)
Harrison, A.G. *et al., Org. Mass Spectrom.*, 1986, **21**, 557 (*ms*)
Rittner, R. *et al., Magn. Reson. Chem.*, 1988, **26**, 51 (*cmr*)
Pande, P.P. *et al., Synth. Commun.*, 1998, **28**, 4193-4200 (*synth, ir, pmr*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 972
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBN250

Pentasine P-194

[108133-63-7]



$C_{30}H_{49}N_6O_{10}^{\oplus}$ 653.751
Cross-linking amino acid isol. from bovine ligament elastin.

Starcher, B. *et al., Connect. Tissue Res.*, 1987, **16**, 15-25; *CA*, **106**, 191359p

2,3,5,7,9-Pentathiadecane 2,2-dioxide, 9CI P-195

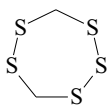
[156430-94-3]
SE-3
Me-S-S-$CH_2SCH_2SCH_2SO_2$Me
$C_5H_{12}O_2S_5$ 264.479
Revised struct.. Isol. from the shiitake mushroom (*Lentinus edodes*). Needles (Me_2CO). Mp 80-82° (79-80.5°).

[17135-23-8]

Morita, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 988
Block, E. *et al., J.O.C.*, 1994, **59**, 2273 (*synth, struct*)

1,2,3,5,6-Pentathiepane, 9CI, 8CI P-196

[292-46-6]
1,2,3,5,6-Pentathiacycloheptane. ***Lenthionine***

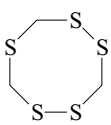


$C_2H_4S_5$ 188.384
Constit. of the edible mushroom Shiitake (*Lentinus edodes*), responsible for its characteristic odour. Also a volatile prod. of cooked mutton. Also isol. from petai (*Parkia speciosa*). Cryst. (CH_2Cl_2). Prac insol. H_2O, polar org. solvs.; sol. oils. Mp 60-61°.

Morita, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 988 (*synth, isol, ms*)
Wada, S. *et al., J. Food Sci.*, 1967, **32**, 559 (*isol, synth*)
Wratten, S.J. *et al., J.O.C.*, 1976, **41**, 2465 (*isol*)
Iwami, K. *et al., CA*, 1978, **89**, 161546 (*rev, bibl*)
Nixon, L.N. *et al., J. Agric. Food Chem.*, 1979, **27**, 355 (*isol*)
Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521 (*isol, props*)
Still, I.W.J. *et al., Tet. Lett.*, 1981, 1939 (*synth*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)
Bannister, R.M. *et al., J.C.S. Perkin 1*, 1990, 509 (*synth*)
Ritzau, M. *et al., Annalen*, 1993, 871 (*isol*)

1,2,4,5,7-Pentathiocane, 9CI P-197

[81531-39-7]
1,2,4,5,7-Pentathiacyclooctane



$C_3H_6S_5$ 202.41
Constit. of the seeds of petai (*Parkia speciosa*) and the shiitake mushroom (*Lentinus edodes*). Prisms ($CHCl_3$/hexane). Mp 102-104°. Prod. from *Parkia* sp. may be the 1,2,3,5,7-Pentathiocane isomeric compd. Data given above.

[81531-40-0]

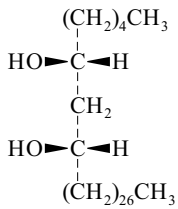
Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521 (*isol*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)
Chen, C.C. *et al., J. Agric. Food Chem.*, 1986, **34**, 830 (*occur*)

1,7-Pentatriacontadien-11-ol P-198

[151454-18-1]
$H_3C(CH_2)_{23}CH(OH)CH_2CH_2CH=CH(CH_2)_4CH=CH_2$
$C_{35}H_{68}O$ 504.922
Incorr. descr. as the 12-ol in the ref.. Constit. of the tubers of *Colocasia esculenta* (taro). Mp 68-69°.

Ali, M. *et al., J. Indian Chem. Soc.*, 1992, **69**, 887 (*isol*)

6,8-Pentatriacontanediol P-199



$C_{35}H_{72}O_2$ 524.953
(6*R,8*S**)-*form*** [155800-92-3]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 85-87°. $[\alpha]_D$ +1.9 (c, 0.14 in $CHCl_3$).

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

8,10-Pentatriacontanediol P-200

$C_{35}H_{72}O_2$ 524.953
(8*R,10*S**)-*form*** [193419-80-6]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 75-78°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

2-Pentenal, 9CI P-201

[764-39-6]
FEMA 3218
$H_3CCH_2CH=CHCHO$
C_5H_8O 84.118
Found in peas, cooked potato, French fries, wheat bread, caviar, black tea, fish oils, raspberries, strawberries and other foods. Flavouring ingredient.

▶ SB1550000

(E)*-form [1576-87-0]
Bp_{160} 80-81° Bp_{80} 62-64°.

▶ SB1560000

2,4-Dinitrophenylhydrazone:
Orange-red needles ($CHCl_3$/MeOH). Mp 163-165°.

Semicarbazone:
Mp 177-178°.

(Z)*-form [1576-86-9]
Bp_{85} 58-60°. Forms 2,4-dinitrophenylhydrazone of (*E*)-form.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 735C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 559C (*ir*)
Prévost, C. *et al., Bull. Soc. Chim. Fr.*, 1944, **11**, 218 (*synth*)
Thomas, D.A. *et al., J.C.S.*, 1965, 2988 (*synth*)

Jaenicke, L. *et al., Chem. Ber.*, 1975, **108**, 225 (*synth*)
Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2118-2119 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBP500

4-Pentenoic acid, 9CI P-202

[591-80-0]
Allylacetic acid. 3-Butene-1-carboxylic acid. FEMA 2843
$H_2C{=}CHCH_2CH_2COOH$
$C_5H_8O_2$ 100.117
Flavouring ingredient. Liq. Sl. sol. H_2O; sol. EtOH, Et_2O. d_4^{18} 0.98. Mp -22.5°. Bp 188-189° Bp_4 70-72°. n_D^{20} 1.4280.
▶ LD_{50} (rat, orl) 470 mg/kg. SB2800000

Me ester: [818-57-5]
$C_6H_{10}O_2$ 114.144
Liq. Bp 128-129° Bp_{22} 42°.

Et ester: [1968-40-7]
$C_7H_{12}O_2$ 128.171
Bp 144-146°.

2-Propenyl ester: [75265-78-0]
$C_8H_{12}O_2$ 140.182
d_{20}^{20} 0.99. Bp_{12} 83-84°. n_D^{20} 1.4280.

Benzyl ester: [113882-48-7]
$C_{12}H_{14}O_2$ 190.241
Liq. Bp_{25} 137° Bp_4 105-106°.

Chloride: [39716-58-0]
C_5H_7ClO 118.562
Liq. Bp 128°.

Amide: [6852-94-4]
C_5H_9NO 99.132
Cryst. (toluene). Mp 104.5-105.5° (94°). Bp 230° Subl.0.1 80.

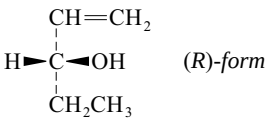
Nitrile: [592-51-8] *4-Cyano-1-propene. Allylacetonitrile*
C_5H_7N 81.117
Liq. Insol. H_2O; misc. EtOH, Et_2O. d^{24} 0.82. Bp 140° Bp_{40} 60-61°. n_D^{14} 1.4213.

Anhydride: [63521-92-6]
$C_{10}H_{14}O_3$ 182.219
$Bp_{0.4}$ 78-81°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 499B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 778A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 584A (*ir*)
Sadtler Standard NMR Spectra, 14093 (*pmr*)
Fittig, R. *et al., Annalen*, 1881, **208**, 37 (*synth*)
Croxall, W.J. *et al., J.A.C.S.*, 1950, **72**, 803-808 (*2-propenyl ester*)
Ragazzini, M. *et al., Eur. Polym. J.*, 1970, **6**, 1331 (*amide*)
Ireland, R.E. *et al., J.A.C.S.*, 1976, **98**, 2868 (*synth*)
Eisch, J.J. *et al., J.A.C.S.*, 1979, **101**, 1148 (*synth*)
Günther, H.J. *et al., Annalen*, 1984, 15 (*synth, cmr*)
Maillard, B. *et al., Nouv. J. Chim.*, 1987, **11**, 7 (*esters, synth*)
Glover, S.A. *et al., Aust. J. Chem.*, 1993, **46**, 1213 (*nitrile*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 640
Madsen, R. *et al., J.O.C.*, 1995, **60**, 7920-7926 (*anhydride, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2119-2120
Iyer, R.P. *et al., Tetrahedron*, 1997, **53**, 2731-2750 (*anhydride, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBQ750

1-Penten-3-ol, 9CI P-203

[616-25-1]
Ethylvinylcarbinol. FEMA 3584



(R)-form

$C_5H_{10}O$ 86.133
Isol. from soya (*Glycine max*), banana, orange juice or peel oil, raspberries, asparagus, shallot, crispbread, smoked fatty fish, scallops, roasted peanut, black and green tea (*Thea sinensis*) and other foods. Flavouring ingredient.

(R)-form [93222-01-6]
Liq. $[\alpha]_D^{25}$ -24.3 (c, 1.6 in EtOH) (90% ee).

(±)-form [67928-92-1]
Liq. d_4^0 0.86. Bp 114-116° Bp_{20} 37°. $n_D^{27.5}$ 1.4182.

4-Nitrobenzoyl:
Mp 53°.

Me ether: [107847-09-6] *3-Methoxy-1-pentene, 9CI*
$C_6H_{12}O$ 100.16
Liq. Bp 73-85°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 140D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 212A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 203B (*ir*)
Hunsdiecker, H. *et al., Ber.*, 1942, **75**, 460 (*synth*)
Winter, M. *et al., Helv. Chim. Acta*, 1962, **45**, 2212; 1964, **47**, 1215 (*isol*)
Org. Synth., 1972, **52**, 19 (*synth*)
Seo, S. *et al., Org. Magn. Reson.*, 1984, **22**, 428 (*cmr*)
Harrison, A.G. *et al., Org. Mass Spectrom.*, 1984, **19**, 573 (*ms*)
Lodge, E.P. *et al., J.A.C.S.*, 1987, **109**, 3353 (*Me ether, synth, ir, pmr, cmr*)
Denmark, S.E. *et al., J.O.C.*, 1987, **52**, 4031 (*synth*)
Paquette, L.A. *et al., Tetrahedron*, 1990, **46**, 4487 (*resoln*)
Oguni, N. *et al., J.C.S. Perkin 1*, 1991, 25 (*synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2120-2121

2-Penten-1-ol, 9CI P-204

[20273-24-9]
$H_3CCH_2CH{=}CHCH_2OH$
$C_5H_{10}O$ 86.133

(E)-form [1576-96-1]
Isol. from grapes and fruits of *Vaccinium* spp.. Liq. Bp 137-139° Bp_{15} 45-46°. n_D^{20} 1.4335.

Me ether: [57648-46-1] *1-Methoxy-2-pentene, 9CI*
$C_6H_{12}O$ 100.16
Liq. Bp 101°.

(Z)-form [1576-95-0]
Isol. from green and black tea (*Thea sinensis*). Liq. Bp 137-139° Bp_{15} 50°. n_D^{20} 1.4360.

2,4-Dinitrobenzoyl:
Mp 60°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 210C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 141A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 203D (*ir*)
Prévost, C. *et al., Ann. Chim. (Paris)*, 1928, **10**, 113 (*synth*)
Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1955, 953 (*synth*)
Kobayashi, A. *et al., Agric. Biol. Chem.*, 1965, **29**, 488 (*isol*)
Johnson, C.R. *et al., J.O.C.*, 1973, **38**, 4263 (*pmr*)
Alexakis, A. *et al., J. Mol. Catal.*, 1975, **1**, 43 (*Me ether*)
Duboudin, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1977, **284**, 351 (*synth*)
Barabas, A. *et al., Tetrahedron*, 1978, **34**, 2191 (*cmr*)
Gastaminza, A.E. *et al., J.O.C.*, 1984, **49**, 3859 (*synth*)
Zaidlewicz, M. *et al., J. Organomet. Chem.*, 1985, **293**, 139 (*synth, pmr*)

1-Penten-3-one, 9CI P-205

[1629-58-9]
Ethyl vinyl ketone. Propionylethylene. FEMA 3382
$H_2C{=}CHCOCH_2CH_3$
C_5H_8O 84.118
Present in banana, orange peel oil, grapefruit juice, wine grape, peach, fish oil, chicken fat, black tea, soybean, lovage leaf, endive, oyster, clam and cooked beef. Liq. d_4^{20} 0.85. Bp_{740} 102° Bp_{90} 44°. n_D^{20} 1.4192. Undergoes radical polym..
▶ Lachrymator. SB3800000

2,4-Dinitrophenylhydrazone: [21454-46-6]
Mp 125-127°.

Dimethylhydrazone: [96546-66-6]
$C_7H_{14}N_2$ 126.201
Liq. Bp 139-141°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 414A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 644A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 499D (*ir*)
McMahon, E.M. *et al., J.A.C.S.*, 1948, **70**, 2971 (*synth*)
Woodward, R.B. *et al., J.A.C.S.*, 1952, **74**, 4239 (*synth*)
Archer, A. *et al., J.O.C.*, 1957, **22**, 92 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 388
Grieco, P.A. *et al., Chem. Comm.*, 1974, 497 (*synth*)
Allio, A. *et al., Helv. Chim. Acta*, 1974, **57**, 616 (*polym*)
Floyd, J.C. *et al., Tet. Lett.*, 1974, 2877 (*synth*)
Delseth, C. *et al., Helv. Chim. Acta*, 1980, **63**, 498 (*cmr*)
Konoshita, A. *et al., J. Appl. Polym. Sci.*, 1983, **28**, 3093 (*ir*)
Byrne, B. *et al., Synthesis*, 1986, 870 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2121-2122 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBR250

3-Penten-2-one, 9CI P-206

[625-33-2]
Methyl propenyl ketone. FEMA 3417
$H_3CCH{=}CHCOCH_3$
C_5H_8O 84.118
Flavouring ingredient. Found in roasted peanuts, roasted filbert, cranberry, bilberry, coca, tea and other foods.
▶SB3850000
(E)-form [3102-33-8]
Oil with fruity odour. Bp 121.5-124° Bp_{26} 37°. n_D^{20} 1.4367.
▶Skin and eye irritant. LD_{50} (rbt, skn) 500 mg/kg.
2,4-Dinitrophenylhydrazone:
Mp 155°.
Semicarbazone:
Mp 142°.
(Z)-form [3102-32-7]
Oil. Bp_{740} 130° (111°). n_D^{20} 1.4242.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 414B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 644B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 500A (*ir*)
Claisen, L. *et al., Annalen*, 1899, **306**, 322 (*synth*)
Heilmann, R. *et al., Bull. Soc. Chim. Fr.*, 1957, 119 (*synth, ir, uv*)
Dubois, J.E. *et al., Bull. Soc. Chim. Fr.*, 1965, 2199 (*synth*)
Org. Synth., 1971, **51**, 115 (*synth*)
Sváta, V. *et al., Coll. Czech. Chem. Comm.*, 1976, **41**, 1194 (*synth*)
Vondrák, T. *et al., Coll. Czech. Chem. Comm.*, 1982, **48**, 82 (*glc, isom*)
Müllen, K. *et al., Tet. Lett.*, 1984, **25**, 5623 (*cmr*)
Arseniyadis, S. *et al., Org. Mass Spectrom.*, 1989, **24**, 909 (*ms*)
McEwen, I. *et al., J.A.C.S.*, 1993, **115**, 3989 (*synth, pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3930-3931 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 644
Arisawa, M. *et al., Synthesis*, 1995, 1371 (*E-form, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2122-2123
Chiu, P. *et al., Synth. Commun.*, 1998, **28**, 4513-4516 (*E-form, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PBR500

4-Penten-2-one, 9CI P-207

[13891-87-7]
Allyl methyl ketone. Vinylacetone
$H_3CCOCH_2CH{=}CH_2$
C_5H_8O 84.118
Constit. of *Tamarindus indica* (tamarind). Liq. with unpleasant odour. Bp 107-108° Bp_{130} 56.5-57°. n_D^{20} 1.4145.
Oxime: [68843-70-9]
C_5H_9NO 99.132
Liq. $Bp_{0.25}$ 35°. Mixt. containing *ca.* 12.5% (*E*)-isomer, 87% (*Z*)-.
Semicarbazone:
Mp 144-145°.
2,4-Dinitrophenylhydrazone: [32520-71-1]
Cryst. Mp 157.5-158.5°.
Di-Me acetal: [98429-28-8] *4,4-Dimethoxy-1-pentene, 9CI*
$C_7H_{14}O_2$ 130.186
Liq. Bp_{75} 66°.
Et-Me acetal: [25400-67-3] *4-Ethoxy-4-methoxy-1-pentene*
$C_8H_{16}O_2$ 144.213
Liq. Bp_{44} 60-62°.
Gaudemar, M. *et al., Bull. Soc. Chim. Fr.*, 1962, 974 (*synth*)
Mikhailov, B.M. *et al., J. Organomet. Chem.*, 1971, **27**, 165 (*synth, derivs*)
Djerassi, C. *et al., J.O.C.*, 1972, **37**, 776 (*ms*)
Scarborough, R.M. *et al., Tet. Lett.*, 1977, 4361 (*synth*)
Rousseau, G. *et al., Tet. Lett.*, 1981, **22**, 649 (*synth*)
Kosugi, M. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 767 (*synth*)

1-Pentenyl glucosinolate P-208

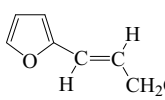
*1-Thio-β-D-glucopyranose 1-[*N*-(sulfooxy)-2-hexenimidate], 9CI*
$H_3CCH_2CH_2CH{=}CHC(SGlc){=}NOSO_3H$
$C_{12}H_{21}NO_9S_2$ 387.431
Present in brassicas.
Daxenbichler, M.E. *et al., Phytochemistry*, 1991, **30**, 2623-2628

4-Pentenyl glucosinolate P-209

[19041-10-2]
*1-Thio-β-D-glucopyranose 1-[*N*-(sulfooxy)-5-hexenimidate], 9CI. **Glucobrassicanapin***
$H_2C{=}CH(CH_2)_3C(SGlc){=}NOSO_3H$
$C_{12}H_{21}NO_9S_2$ 387.431
Isol. from rape (*Brassica napus*) and other *Brassica* sp..
[37491-62-6]
Kjaer, A. *et al., Acta Chem. Scand.*, 1956, **10**, 1365 (*isol*)
Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, D.H.), CRC Press, 1998, 29-53 (*rev*)

2-(1-Pentenyl)furan, 9CI P-210

[81677-78-3]
1-(2-Furanyl)-1-pentene



(*E*)-*form*

$C_9H_{12}O$ 136.193
Component of reversion flavour in soybean oil. Aroma volatile of cooked pork and boiled potato. Bp_{14} 64-67°.
(E)-form [20992-69-2] Characterised spectroscopically. Higher Bp isomer.
(Z)-form [20992-60-3]
Bp_6 44.2°.
[55810-12-3]
Buddrus, J. *et al., Chem. Ber.*, 1974, **107**, 2050-2061 (*synth, pmr*)
Ho, C.-T. *et al., J. Am. Oil Chem. Soc.*, 1978, **55**, 233-237; 1983, **60**, 553-557 (*synth, ir, pmr, ms, occur*)
Elmore, J.S. *et al., J. Chromatogr., A*, 2001, **905**, 233-240 (*occur*)

Pentigetide, INN, USAN P-211

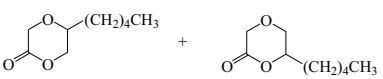
[62087-72-3]
Hamburger pentapeptide. Human IgE pentapeptide. Aspartylserylaspartylprolylarginine. Pentyde. HEPP
H-Asp-Ser-Asp-Pro-Arg-OH
$C_{22}H_{36}N_8O_{11}$ 588.573
Immunoglobulin E fragment. Immunoglobulin E fragment. Mp 185-200° dec. $[\alpha]_D$ -87.7 (c, 0.5 in H_2O).
Hamburger, R.N. *et al., Science (Washington, D.C.)*, 1975, **189**, 389
Suzuki, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 3025; 1978, **26**, 2269 (*synth*)
Hamburger, R.N. *et al., New Trends Allergy, [Pap. Int. Symp.], 1980 (1981)*, 1980, 311 (*rev*)

Pentyl glucosinolate P-212

[127929-24-2]
*1-Thio-β-D-glucopyranose 1-[*N*-(sulfooxy)hexanimidate], 9CI*
$H_3C(CH_2)_4C(SGlc){=}NOSO_3H$
$C_{12}H_{23}NO_9S_2$ 389.447
Present in radish (*Raphanus sativus*) and in kohlrabi aroma.
Kjaer, A. *et al., Agric. Biol. Chem.*, 1978, **42**, 1715 (*occur*)
Macleod, G. *et al., Phytochemistry*, 1990, **29**, 1183 (*occur*)

5(6)-Pentyl-1,4-dioxan-2-one P-213

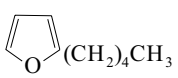
[65504-96-3]
FEMA 2076



$C_9H_{16}O_3$ 172.224
Mixed isomers used in food flavouring. Liq. with fruity-winey, somewhat ethereal odour.
Belg. Pat., 1963, 628 078; *CA*, **60**, 12021f (*synth, use, glc, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 42 (*props, use*)

2-Pentylfuran P-214

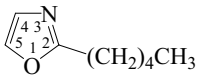
[3777-69-3]
FEMA 3317



$C_9H_{14}O$ 138.209
Occurs in many foods including coffee, potatoes, tomatoes, roasted filberts and soybean oil and is a component of aroma of these foods. Flavouring ingredient. Oil. Bp_{10} 57-59°. Probably results from oxidn. of an unsaturated fatty acid.
▶LD_{50} (mus, orl) 1200 mg/kg. LU5187000
Chang, S.S. *et al., Chem. Ind. (London)*, 1966, 1926 (*ir, ms*)
Ibrayimov, I.I. *et al., Khim. Geterotsikl. Soedin.*, 1973, 1434 (*synth*)
Schmidt, B. *et al., Eur. J. Org. Chem.*, 2000, 3145-3163 (*synth, pmr, cmr*)

2-Pentyloxazole, 9CI P-215

[77311-05-8]

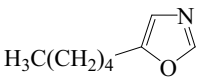


$C_8H_{13}NO$ 139.197
Constit. of roasted peanut volatiles. Characterised spectroscopically.

Lee, M.-H. *et al., J. Agric. Food Chem.*, 1981, **29**, 686-688 (*occur, ms*)
Ho, C.-T. *et al., J. Food Sci.*, 1981, **47**, 127-133 (*occur, ms*)

5-Pentyloxazole P-216

[84027-84-9]



$C_8H_{13}NO$ 139.197
Not reported in mature. Liq. (?) with fatty bacon-green odour. Characterised spectroscopically.

Ho, C.-T. *et al., J. Agric. Food Chem.*, 1983, **31**, 180-181 (*synth, ms*)
Jin, Q.Z. *et al., Perfum. Flavor.*, 1984, **9(4)**, 25-28

2-Pentyl-3-phenyl-2-propenal P-217

[122-40-7]

[78605-96-6]
2-(Phenylmethylene)heptanal, 9CI. α-Pentylcinnamaldehyde, 8CI. α-Pentyl-β-phenylacrolein. Amylcinnamic aldehyde. 2-Benzylideneheptanal. Jasmine aldehyde. α-Amylcinnamaldehyde. FEMA 2061

$PhCH{=}C(CHO)(CH_2)_4CH_3$

$C_{14}H_{18}O$ 202.296
Flavouring ingredient. Liq. with flowery, jasmine-type odour. d^{15} 0.97. Bp_{20} 174-175°. n_D^{20} 1.5552. Relatively unstable, requires stabilising with antioxidants. *E*,*Z*-composition of coml. prod. is not clear.

▶ Skin irritant. LD_{50} (rat, orl) 3730 mg/kg. GD6825000

Oxime: [13372-82-2]
$C_{14}H_{19}NO$ 217.31
Mp 72.5-73°.

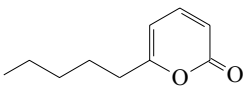
2,4-Dinitrophenylhydrazone:
Scarlet solid. Mp 164°.

Di-Me acetal: [91-87-2] *[2-(Dimethoxymethyl)-1-heptenyl]benzene, 9CI. 2-(Dimethoxymethyl)-1-phenyl-1-heptene. FEMA 2062*
$C_{16}H_{24}O_2$ 248.364
Flavouring ingredient.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 927B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1281D (*ir*)
Rutowski, B.N. *et al., J. Prakt. Chem.*, 1928, **119**, 272 (*synth*)
Backes, M. *et al., Bull. Soc. Chim. Fr.*, 1942, 60 (*synth*)
Brittain, E.F.H. *et al., Org. Mass Spectrom.*, 1969, **2**, 325 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AOG500
Abenhaim, D. *et al., Synth. Commun.*, 1994, **24**, 1199 (*synth, ms, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 37
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 154-156
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOG500

6-Pentyl-2*H*-pyran-2-one P-218

[27593-23-3]
2,4-Decadien-5-olide. 6-Pentyl-α-pyrone. 5-Hydroxy-2,4-decadienoic acid δ-lactone. FEMA 3696

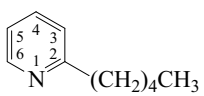


$C_{10}H_{14}O_2$ 166.219
Present in peach (*Prunus persica*) and heated beef. Comly. available flavour/aroma modifier; FDA approved flavouring. Shows antibacterial and antifugal props.. Liq. d^{25} 1.01. $Bp_{0.35}$ 92-93°. n_D^{25} 1.5071. λ_{max} 218 (ϵ 2920); 301 (ϵ 6320) (MeOH).

Nobuhara, A. *et al., Agric. Biol. Chem.*, 1969, **33**, 1264 (*synth*)
Collins, R.P. *et al., J. Agric. Food Chem.*, 1972, **20**, 437 (*struct, isol, ir, ms, pmr*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1946 (*struct*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1975, **23**, 1189 (*synth, ir, ms, pmr*)
Jones, T.H. *et al., Tet. Lett.*, 1983, **24**, 5439 (*synth*)
Cutler, H.G. *et al., Agric. Biol. Chem.*, 1986, **50**, 2943 (*isol, pmr, cmr, props*)
Dieter, R.K. *et al., J.O.C.*, 1988, **53**, 2031 (*synth*)
Benoni, H. *et al., Naturwissenschaften*, 1990, **77**, 539 (*isol, uv, ir, pmr, ms*)
Almassi, F. *et al., J. Nat. Prod.*, 1991, **54**, 396 (*isol*)
Dickinson, J.M. *et al., Nat. Prod. Rep.*, 1993, 71 (*rev, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 361
Morimitsu, Y. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1428-1433 (*isol, pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1366-1367
Parker, S.R. *et al., J. Agric. Food Chem.*, 1997, **45**, 2774-2776 (*use*)

2-Pentylpyridine, 9CI P-219

[2294-76-0]
FEMA 3383



$C_{10}H_{15}N$ 149.235
Maillard prod. formed by thermal interaction of 2,4-Decadienal and aminoacids. A major contributor to the unpalatable taste of soy flour and protein isolates. The major odour active basic compd. in roast lamb fat. Also present in aroma of grilled/fried chicken, pork and beef, roasted sesame seeds, roasted peanuts roasted filbert, ambrette seed oil, bell pepper and coriander oil. Flavouring ingredient. Oil with fatty tallow-like odour and throat-catching greasy taste. d_4^{20} 0.88. Bp_{12} 86-88° $Bp_{8.5}$ 82.5-84.5°. n_D^{16} 1.4890. n_D^{20} 1.4834. Flavour threshold 1.2×10^{-5} ppm in H_2O.

Picrate: [23692-26-4]
Mp 73°.

[65307-85-9]

Osuch, C. *et al., J.A.C.S.*, 1956, **78**, 1723-1725 (*synth*)
Cuvigny, T. *et al., Bull. Soc. Chim. Fr.*, 1964, 2000-2009; 1965, 1881-1888 (*synth*)
Miyadera, T. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1344-1351 (*synth*)
Waldradt, J.P. *et al., J. Agric. Food Chem.*, 1971, **19**, 972-979 (*occur, peanuts*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1977, **25**, 1227-1229 (*occur, glc, ms, lamb fat*)
Tang, J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1287-1292 (*occur*)
Mottram, D.S. *et al., J. Sci. Food Agric.*, 1985, **36**, 377-382 (*detn, pork*)
Lamparsky, D. *et al., Perfum. Flavor.*, 1988, **13**, 17-18 (*occur, coriander oil*)
Sutherland, M.M. *et al., J. Sci. Food Agric.*, 1995, **69**, 403-413 (*occur*)
Takeoka, G. *et al., J. Agric. Food Chem.*, 1996, **44**, 654-660 (*occur*)
Kim, Y.-S. *et al., J. Agric. Food Chem.*, 1996, **44**, 3906-3908 (*formn*)
Lambrechts, S. *et al., Flavour Fragrance J.*, 1997, **12**, 439-442 (*synth, props*)
Boatright, W.L. *et al., J. Am. Oil Chem. Soc.*, 1997, **74**, 1575-1581; 1998, **75**, 1379-1383 (*occur, glc, soybean*)
Kim, Y.-S. *et al., J. Food Lipids*, 1997, **4**, 239-244; 1998, **5**, 173-182 (*occur*)

3-Pentylpyridine, 9CI P-220

[1802-20-6]

$C_{10}H_{15}N$ 149.235
Minor constit. of roast lamb fat. Present in tobacco smoke condensate. d_4^{20} 0.91. Bp_1 51.5-52°. n_D^{20} 1.4925.

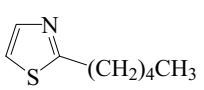
Picrate: [2296-03-9]
Mp 107.8-108°.

[65307-85-9]

Buttery, R.G. *et al., J. Agric. Food Chem.*, 1977, **25**, 1227-1229 (*occur, glc, ms*)
Heckman, R.A. *et al., Tob. Int.*, 1981, **183**, 83-89 (*occur*)
Tsuge, O. *et al., Clin. Allergy*, 1984, 1255-1258 (*synth*)
Chumakov, Y.I. *et al., CA*, **71**, 61162s (*synth, props*)

2-Pentylthiazole P-221

[37645-62-8]



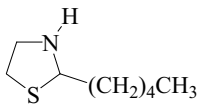
$C_8H_{13}NS$ 155.263
Flavour enhancer for tomato products; flavour component of roast cocoa beans.

U.S. Pat., 1972, 3 660 112; *CA*, **77**, 33120g (*use*)

Ho, C.T. *et al., J. Food Sci.*, 1983, **48**, 1570-1571 (*synth, ms*)
Ho, C.T. *et al., Perfum. Flavor.*, 1984, **9**, 15-18 (*synth, odour*)
Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur, cocoa*)

2-Pentylthiazolidine, 9CI P-222

[41204-65-3]
Tetrahydro-2-pentylthiazole



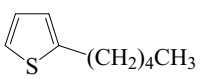
$C_8H_{17}NS$ 159.295

(±)-*form*
Flavouring ingredient. Bp_4 92°.

Ger. Pat., 1974, 2 333 581; *CA*, **80**, 95930s (*use*)
U.S. Pat., 1977, 4 011 233; *CA*, **87**, 23264z (*use*)
Yasuhara, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 2273-2274 (*synth*)

2-Pentylthiophene P-223

[4861-58-9]

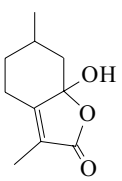


$C_9H_{14}S$ 154.276
Cysteine-derived Maillard product. Constit. of cooked pork, beef or lamb, yeast extract and ripe bell peppers. d_4^{20} 0.94. Bp_8 74.5°.

Grey, T.F. *et al., J.C.S.*, 1960, 1502-1508 (*synth*)
Jeffery, G.H. *et al., J.C.S.*, 1961, 570-575 (*synth*)
Elmore, J.S. *et al., J. Agric. Food Chem.*, 2000, **48**, 2420-2424 (*occur*)
Elmore, J.S. *et al., J. Chromatogr., A*, 2001, **905**, 233-240 (*occur*)

Peperinic acid P-224

[514-93-2]
*2,4,5,6,7,7*a-*Hexahydro-7*a-*hydroxy-3,6-dimethyl-2-benzofuranone. 3-Hydroxy*-p-*menth-4(8)-en-9,3-olide*



$C_{10}H_{14}O_3$ 182.219
Isol. from aged peppermint oil. Cryst. (MeOH or C_6H_6). Mp 191° (188-189°). $[\alpha]_D^{21}$ +60.7. Prob. artifact of oxidn. of Menthofuran, M-189.

Fester, G.A. *et al., An. Asoc. Quim. Argent.*, 1949, **37**, 197; 1952, **40**, 246; *CA*, **40**, 4636; **48**, 1974 (*isol*)
Woodward, R.B. *et al., J.A.C.S.*, 1950, **72**, 399 (*isol*)
Crowley, K.J. *et al., J.C.S.*, 1964, 4254 (*isol*)

Pepsin P-225

[9001-75-6]
Pepsina. Pepsini pulvis. Puerzym. E.C. 3.4.23.1 (pepsin A). E.C. 3.4.23.2 (pepsin B). E.C. 3.4.23.3 (pepsin C)

Enzyme. A mixt. of pepsins A-C with pepsin A as the major component. Used in the preparation of fish meal and other protein hydrolysates and in the manuf. of cheese as a milk-clotting agent. Cryst. or amorph. powder. V. sol. H_2O; prac. insol. EtOH, $CHCl_3$, Et_2O.
►SC6132000

pro-*form* [9001-10-9]
Pepsinogen. Propepsin

[9012-71-9, 9025-48-3, 9074-32-2, 61536-72-9]

Ryle, A.P. *et al., Methods Enzymol.*, 1970, **19**, 316-336 (*rev*)
Fruton, J.S. *et al., The Enzymes*, Academic, New York, 1971, **4**, 119 (*rev*)
Clement, G.E. *et al., Prog. Bioorg. Chem.*, 1973, **2**, 177 (*rev*)
Merck Index, 11th edn., 1989, No. 7103
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2133-2134
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, No. 616
Fruton, J.S. *et al., Q. Rev. Biol.*, 2002, **77**, 127-147 (*rev*)

Peracetic acid P-226

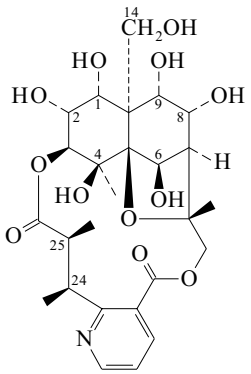
[79-21-0]
Ethaneperoxoic acid, 9CI. Acetyl hydroperoxide. Peroxyacetic acid. Estosteril. Osbon AC

$H_3CCOOOH$
$C_2H_4O_3$ 76.052
Bleaching agent for food starch. Component of antimicrobial washes for poultry carcasses and fruit. Liq. with unpleasant odour. Sol. H_2O, EtOH, Et_2O. Fp 0.1. Bp 105°. pK_a 8.2 (20°).
►Explodes violently above 110°. Corrosive and irritating to skin, eyes, and mucous membranes. Na salt is explosive when dry. LD_{50} (rat, orl) 1540 mg/kg. SD8750000

tert-*Butyl ester:* [107-71-1] tert-*Butyl peracetate. Kayabutyl A. Perbutyl A*
$C_6H_{12}O_3$ 132.159
Liq. $Bp_{1.5}$ 27°.
►Shock-sensitive explosive in solid state, detonates on rapid heating, flammable, fl. p. < 27°. Skin and eye irritant. LD_{50} (rat, orl) 675 mg/kg. SD8925000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 481C (*ir*)
Greenspan, F.P. *et al., J.A.C.S.*, 1946, **68**, 907 (*synth*)
Bunton, C.A. *et al., Chem. Ind. (London)*, 1954, 191 (*synth*)
Giguère, P.A. *et al., Can. J. Chem.*, 1956, **34**, 689 (*uv*)
Phillips, B. *et al., J.O.C.*, 1958, **23**, 1823 (*synth*)
Muecke, H. *et al., Pharmazie*, 1967, **22**, 444 (*synth, use*)
Lewis, S.N. *et al., Oxidation*, Rohm and Haas Co., Philadelphia, 1969, **1**, 213 (*rev*)
Emken, E.A. *et al., Lipids*, 1971, **6**, 686; 1972, **7**, 459 (*use*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **17**, 60 (*peroxyacids, rev*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 386
Beckwith, A.L.J. *et al., J.A.C.S.*, 1986, **108**, 8230 (*tert-butyl ester*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 801
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 3933-3937 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2136-2137
Osvath, R. *et al., Food Chem. News*, 2001, **43**, 11 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0732; 0785; 2355
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 207; 976; 1148
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSC250; PCL500

Perdeacyleuojaponin P-227



$C_{26}H_{35}NO_{12}$ 553.562

8-Epimer, 1,6,9,14-tetra-Ac: ***Aquifoliunine EII***
$C_{34}H_{43}NO_{16}$ 721.711
Alkaloid from the root bark of *Maytenus aquifolium* (tea). Amorph. $[\alpha]_D$ -17.2 (c, 3 in $CHCl_3$).

8-Epimer, 1,2,6,9,14-penta-Ac: [220751-20-2] ***Aquifoliunine EIII***
$C_{36}H_{45}NO_{17}$ 763.748
Alkaloid from *Maytenus aquifolium* (tea). Amorph. solid. $[\alpha]_D$ -20.8 (c, 3.3 in $CHCl_3$).

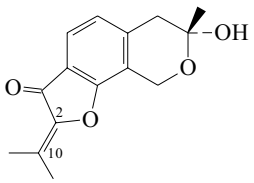
8-Epimer, 8-benzoyl, 1,2,6,9,14-penta-Ac: ***Aquifoliunine EI***
$C_{43}H_{49}NO_{18}$ 867.856
Alkaloid from the root bark of *Maytenus aquifolium* (tea). Amorph. solid. $[\alpha]_D$ -3.1 (c, 3.2 in $CHCl_3$).

8-Epimer, 8-(3-pyridinecarbonyl), 1,2,6,9,14-penta-Ac: [220751-22-4] ***Aquifoliunine EIV***
$C_{42}H_{48}N_2O_{18}$ 868.844
Alkaloid from *Maytenus aquifolium* (tea). $[\alpha]_D$ -15.2 (c, 2.9 in $CHCl_3$).

Corsino, J. *et al., Phytochemistry*, 1998, **48**, 137-140; **49**, 2181-2183 (*Aquifoliunines*)
Gonzaler, A.G. *et al., Bioorg. Med. Chem.*, 2000, **8**, 1773-1778 (*activity, Euonymine*)
Duan, H. *et al., J. Nat. Prod.*, 2000, **63**, 357 (*isol, activity*)

Pergillin P-228

[74798-20-2]
*6,9-Dihydro-7-hydroxy-7-methyl-2-(1-methylethylidene)-7*H-*furo[3,2-*h*][2]benzopyran-3(2*H*)-one, 9CI*



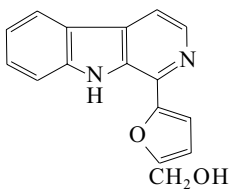
$C_{15}H_{16}O_4$ 260.289
Prod. by *Aspergillus ustus* growing on seeds of *Pisum sativum* (pea).

2,10-Dihydro: [81118-18-5] ***Dihydropergillin***
$C_{15}H_{18}O_4$ 262.305C-2 config. not determined.

Cutler, H.G. *et al., J. Agric. Food Chem.*, 1980, **28**, 989 (*isol*)

Perlolyrine P-229

[29700-20-7]
5-(9H-Pyrido[3,4-b]indol-1-yl)-2-furanmethanol, 9CI. 2-(β-Carbolin-1-yl)-5-hydroxymethylfuran. Alkaloid YS



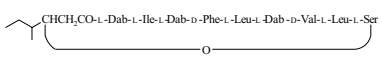
$C_{16}H_{12}N_2O_2$ 264.283
Alkaloid from Korean ginseng and Japanese soy sauce. Yellow cryst. Mp 183°.

Hydrochloride:
Yellow needles. Mp 204-233° dec.

Jeffreys, J.A.D. *et al., J.C.S.(C)*, 1970, 1091 (*isol, uv, ir, pmr, ms, cryst struct, synth*)
Nakatsuka, S. *et al., Tet. Lett.*, 1986, **27**, 3399 (*isol, pmr*)
Gessner, W.P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1988, **321**, 95 (*synth, uv*)
Bracher, F. *et al., Annalen*, 1992, 1315 (*synth, ir, pmr, cmr, ms*)

Permetin A P-230

[71888-70-5]
9-L-Serinepolypeptin A, 9CI. Permycin A. NLF-II. Antibiotic NLF-II



$C_{54}H_{92}N_{12}O_{12}$ 1101.394
Cyclic depsipeptide antibiotic. Animal food additive. Amorph. powder (as hydrochloride). Sol. H_2O, MeOH; poorly sol. Me_2CO, Et_2O. Mp 210-220° dec. (hydrochloride). Related to Polypeptin A and Polypeptin B λ_{max} 252 (ϵ 145); 258 (ϵ 142); 264 (ϵ 118); 268 (ϵ 100) (MeOH/HCl) (Derep). λ_{max} 258 (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 36 mg/kg , LD_{50} (mus, orl) 2100 mg/kg. SD6785000

Takahara, Y. *et al., J. Antibiot.*, 1979, **32**, 115; 121 (*isol, struct, uv, ir, ms, pmr, cmr*)
Murai, A. *et al., J. Antibiot.*, 1985, **38**, 1610 (*config*)

Peroxydisulfuric acid ($[(HO)S(O)_2]_2O_2$), 11CI P-231

[13445-49-3]
Persulfuric acid. Hypersulfuric acid. Marshall's acid
$HO(O)_2SOOS(O)_2OH$
$H_2O_8S_2$ 194.143
Interatomic distances: O–O 131, S–O 150 pm.Colourless monoclinic cryst., stable for weeks at 20°, smelling of ozone. Dec. into $SO_4^{\ominus}$. Sol. H_2O (dec.); sol. EtOH; sl. sol. Et_2O. Mp 65° dec.
▶ Strong oxidant.

Di-NH_4 salt: [7727-54-0] *Ammonium peroxydisulfate. Diammonium peroxodisulfate. Ammonium persulfate. Diammonium peroxydisulfate*
$H_8N_2O_8S_2$ 228.204
Bleaching agent for food starch. Colourless monoclinic cryst. Stable as dry solid. Dec. in H_2O forming O_2.
▶ SE0350000

[14149-70-3, 15092-81-6]

Simon, A. *et al., Z. Anorg. Allg. Chem.*, 1962, **315**, 196 (*di-NH_4 salt, ir, Raman*)
Sivertsen, B.K. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1969, **130**, 449 (*di-NH_4 salt, cryst struct*)
House, J.E. *et al., Thermochim. Acta*, 1978, **24**, 117 (*di-NH_4 salt, tga, dsc*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 139-140 (*di-NH_4 salt*)

Peroxyoctanoic acid, 8CI P-232

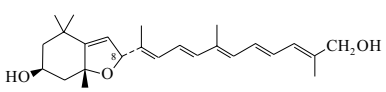
[33734-57-5]
Octaneperoxoic acid, 9CI. Peroctanoic acid
$H_3C(CH_2)_6COOOH$
$C_8H_{16}O_3$ 160.213
Component of antimicrobial washes for poultry carcasses. Mp 31-32°.

tert-*Butyl ester:* [13467-82-8]
$C_{12}H_{24}O_3$ 216.32
No phys. props. reported.

Parker, W.E. *et al., J.A.C.S.*, 1955, **77**, 4037-4041 (*synth*)
Madhusudanan, K.P. *et al., Indian J. Chem., Sect. B*, 1988, **27**, 398-401 (*tert-butyl ester, synth, ms*)
Bjorkling, F. *et al., Tetrahedron*, 1992, **48**, 4587-4592 (*synth*)
Osvath, R. *et al., Food Chem. News*, 2001, **43**, 11 (*use*)

Persicachrome P-233

[80931-31-3]
5,8-Epoxy-5,8-dihydro-12′-apo-β-carotene-3,12′-diol



(3*S*,5*R*,8*R*)-*form*

$C_{25}H_{36}O_3$ 384.558
Yellow pigment from plums *Prunus domestica*. Yellow pigment.

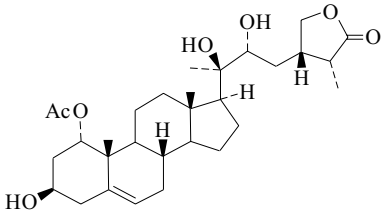
(3*S*,5*R*,8*R*)-*form*
Constit. of peach (*Prunus persica*).

(3*S*,5*R*,8*S*)-*form*
Constit. of flesh of cling peaches (*Prunus persica*).

Gross, J. *et al., Phytochemistry*, 1981, **20**, 2267
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1988, **71**, 1689 (*isol, pmr, uv, cd, abs config*)

Perulactone P-234

[76994-38-2]

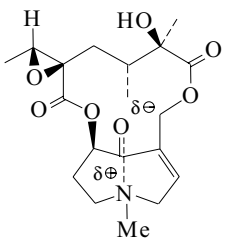


$C_{30}H_{46}O_7$ 518.689
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. (MeOH). Mp 214-215° Mp 239-240° (dimorph.).

Gottlieb, H.E. *et al., J.C.S. Perkin 1*, 1980, 2700

Petasitenine P-235

[60102-37-6]
Fukinotoxin



$C_{19}H_{27}NO_7$ 381.425
Cyclic ester of Otonecine and Petasinecic acid. Stereoisomer of Otosenine. Alkaloid from *Petasites japonicus* (sweet coltsfoot). Cryst. (C_6H_6/hexane or Me_2CO). Mp 129-130°. $[\alpha]_D$ +63.8 ($CHCl_3$).
▶ Carcinogen, hepatotoxin. SE5085000

Ac: [60409-51-0]

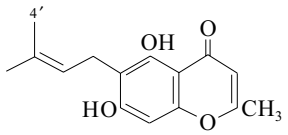
[61303-14-8] ***Neopetasitenine***
$C_{21}H_{29}NO_8$ 423.462
Alkaloid from *Petasites japonicus* (sweet coltsfoot). Amorph. solid; cryst. (as hydrochloride). Mp 212° (as hydrochloride). $[\alpha]_D^{19}$ +49 (c, 1.19 in EtOH).

[60132-19-6, 60409-53-2]

Yamada, K. *et al., Chem. Lett.*, 1976, 461 (*isol, struct*)
Furuya, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1120 (*isol, ir, pmr, cd, cryst struct*)
Iwao, H. *et al., J. Natl. Cancer Inst.*, 1977, **58**, 1155; *CA*, **87**, 976u (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PCQ750

Peucenin P-236

[578-72-3]
5,7-Dihydroxy-2-methyl-6-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI. 5,7-Dihydroxy-2-methyl-6-prenylchromone



$C_{15}H_{16}O_4$ 260.289
Plates (Et_2O). Mp 212°.

7-Me ether: [13544-40-6] *7*-O-*Methylpeucenin*. *5-Hydroxy-7-methoxy-2-methyl-6-prenylchromone.* ***7*-O-*Methylpeucenin***
$C_{16}H_{18}O_4$ 274.316
Needles (MeOH). Mp 108.5-109.5°.

4′-Hydroxy: [103629-80-7] ***Cnidimol A***
$C_{15}H_{16}O_5$ 276.288
Mp 203-204°.

4′-Hydroxy, 7-O-*β*-D-*glucopyranoside:* [121748-72-9] *Cnidimol 7-glucoside*
$C_{21}H_{26}O_{10}$ 438.43
Constit. of *Angelica archangelica* (angelica). C-2′ config. not known.

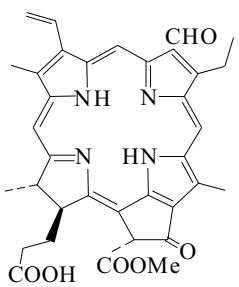
4′-β-D-*(Glucopyranosyloxy):* [155112-93-9] ***Cnidimoside A***
$C_{21}H_{26}O_{10}$ 438.43
Cryst. powder. Mp 137-139°. $[\alpha]_D^{24}$ -13.8 (c, 0.6 in MeOH). Possesses (*Z*)-config..

4′-(β-D-*Glucopyranosyloxy), 7-Me ether,:* [155112-94-0] ***Cnidimoside B***
$C_{22}H_{28}O_{10}$ 452.457
Cryst. powder. Mp 197-200°. $[\alpha]_D^{24}$ -7.8 (c, 0.5 in dioxane). Possesses (*Z*)-config..

Späth, E. *et al., Ber.*, 1941, **74**, 1851
Bolleter, A. *et al., Helv. Chim. Acta*, 1951, **34**, 186 (*synth, uv*)
McCabe, P.H. *et al., J.C.S.(C)*, 1967, 145 (*ir, pmr, ms*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 1815 (*7-Methylpeucenin*)
Baba, K. *et al., Shoyakugaku Zasshi*, 1985, **39**, 282; *CA*, **105**, 85018w (*Cnidimol A*)
Cisowski, W. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1988, **62**, 135 (*Cnidimol 7-glucoside*)
Baba, K. *et al., Phytochemistry*, 1992, **31**, 1367 (*Cnidimol A*)
Baba, K. *et al., Phytochemistry*, 1994, **35**, 221 (*Cnidimosides*)

Phaeophorbide b P-237

[20239-99-0]
Pheophorbide b



$C_{35}H_{34}N_4O_6$ 606.677
Constit. of various plant spp. incl. *Brassica* spp.. Grey-black cryst. (CH_2Cl_2/petrol). Sol. $CHCl_3$. Mp 220-223°. λ_{max} 439 (ϵ 154000); 530 (ϵ 12300); 553 (ϵ 9320); 602 (ϵ 9270); 653 (ϵ 39800) (Me_2CO).

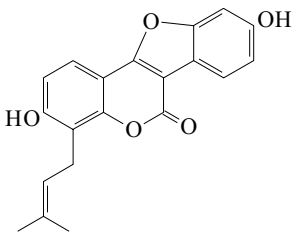
Me ester: [5522-71-4] *Methyl phaeophorbide b*
$C_{36}H_{36}N_4O_6$ 620.704
Grey plates (CH_2Cl_2/MeOH). Mp 269°. $[\alpha]_{Hg}^{20}$ -128 (c, 1.56 in Me_2CO).

[92935-95-0]

Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (ii), 1940, 245-249 (*rev*)
Kenner, G.W. *et al., J.C.S. Perkin 1*, 1973, 2517-2523 (*synth*)
Smith, K.M. *et al., Porphyrins and Metalloporphyrins*, (ed. Smith, K.M.), Elsevier Elsevier, Amsterdam, 1975, 776 (*synth*)
Smith, K.M. *et al., Tetrahedron*, 1975, **31**, 367-375 (*cmr*)
Wasielewski, M.R. *et al., J.O.C.*, 1980, **45**, 1969-1974 (*synth, uv, pmr*)
Nakamura, Y. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1028-1030 (*isol*)

Phaseol P-238

[88478-02-8]
*3,9-Dihydroxy-4-(3-methyl-2-butenyl)-6*H-*benzofuro[3,2-*c*][1]benzopyran-6-one, 9CI. 3,9-Dihydroxy-4-prenylcoumestan*



$C_{20}H_{16}O_5$ 336.343
Isol. from *Phaseolus aureus* (mung bean). No phys. props. reported. λ_{max} 254 ; 305 ; 345 (MeOH) (Berdy). λ_{max} 280 ; 384 (MeOH/NaOH) (Berdy).

O'Neill, M.J. *et al., Z. Naturforsch., C*, 1983, **38**, 698 (*isol*)

Phaseolamin, 9CI P-239

[56996-83-9]
Carbo-Lite

Protein. Isol. from kidney bean seeds (*Phaseolus vulgaris* var. Great Northern).

Marshall, J.J. *et al., J. Biol. Chem.*, 1975, **250**, 8030 (*isol*)

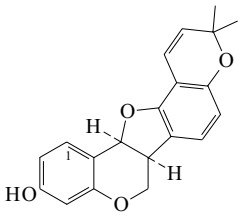
Phaseolic acid P-240

[29533-15-1]
5,8(9),12-Trihydroxy-2-oxododecanoic acid
$HOCH_2(CH_2)_3CH(OH)CH_2CH_2$-$CH(OH)CH_2CH_2COCOOH$ + $HOCH_2CH_2CH_2CH(OH)(CH_2)_3$-$CH(OH)CH_2CH_2COCOOH$
$C_{12}H_{22}O_6$ 262.302
Isol. from dry bean seeds (*Phaseolus* sp.). Amorph. solid.

Redemann, C.T. *et al., CA*, 1970, **73**, 129780r (*isol*)

Phaseollin P-241

[13401-40-6]
*6*b,*12*b-*Dihydro-3,3-dimethyl-3*H,*7*H-*furo[3,2-*c:*5,4-*f*]bis[1]benzopyran-10-ol, 9CI. Phaseolin*



Absolute configuration

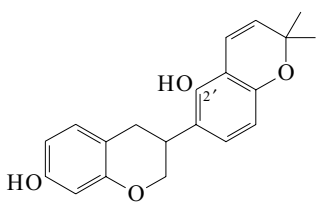
$C_{20}H_{18}O_4$ 322.36
Isol. from *Phaseolus vulgaris* (kidney bean) and *Vigna unguiculata*. Sol. MeOH, Et_2O, bases; fairly sol. H_2O. Mp 177-178°. $[\alpha]_D$ -145 (c, 0.17 in EtOH). pK_a 9.13. Log P 3.96 (uncertain value) (calc). λ_{max} 207 (ϵ 47900); 230 (ϵ 25100); 280 (ϵ 9330); 286 (ϵ 7940); 315 (ϵ 2190) (MeOH) (Derep). λ_{max} 279 (ϵ 9120); 286 (ϵ 7940); 315 (ϵ 2190) (EtOH) (Berdy). λ_{max} 281 (ϵ 11480); 292 (ϵ 10960); 377 (ϵ 2880) (EtOH/NaOH) (Berdy).

1-Methoxy: [157226-48-7] ***1*-Methoxyphaseollin**
$C_{21}H_{20}O_5$ 352.386
Constit. of the roots of *Glycyrrhiza glabra* (licorice). Yellowish oil. $[\alpha]_D^{25}$ -16.7 (c, 0.91 in MeOH).

Perrin, O.R. *et al., Tet. Lett.*, 1964, 438 (*isol*)
Cruickshank, I. *et al., Phytopathol. Z.*, 1971, **70**, 209 (*isol*)
Perrin, O.R. *et al., Tet. Lett.*, 1972, 1673 (*pmr, ms, uv*)
DeMartinis, C. *et al., Tetrahedron*, 1978, **34**, 1849 (*cryst struct*)
Kamat, V.S. *et al., Heterocycles*, 1981, **15**, 1163 (*isol*)
Dewick, P.M. *et al., Phytochemistry*, 1982, **21**, 1599 (*biosynth*)
Thomas, P. *et al., Tet. Lett.*, 1984, **25**, 1099 (*synth*)
Mohamed, S.E.N. *et al., J.C.S. Perkin 1*, 1987, 431 (*synth*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1056 (*1-Methoxyphaseollin*)

Phaseollinisoflavan P-242

[40323-57-7]
*3,4-Dihydro-2,2-dimethyl[3,6′-bi-2*H-*1-benzopyran]-5′,7-diol, 9CI*



$C_{20}H_{20}O_4$ 324.376
Isoflavanoid numbering shown. Phytoalexin from *Phaseolus vulgaris* (kidney bean), other *Phaseolus* spp. and *Glycyrrhiza glabra* (licorice). $[\alpha]_D$ -9 (c, 0.1 in MeOH).

2′-Me ether: [49594-01-6] ***2′*-O-*Methylphaseollinisoflavan***. *2′-Methoxyphaseollinisoflavan (incorr.)*
$C_{21}H_{22}O_4$ 338.402
From *Phaseolus vulgaris* (kidney bean). $[\alpha]_D^{24}$ +19.5 (EtOH). λ_{max} 228 (ϵ 39800);

271 (ε 9120); 280 (ε 9330); 313 (ε 2040) (EtOH) (Berdy).

Burden, R.S. *et al., Tet. Lett.*, 1972, 4175 (*isol, struct, uv, pmr*)
v. Etten, H.D. *et al., Phytochemistry*, 1973, **12**, 1791 (*deriv*)
Seifert, K. *et al., Z. Naturforsch., C*, 1993, **48**, 550 (*isol, pmr, cmr*)
Tanaka, H. *et al., Phytochemistry*, 1998, **47**, 1397-1400 (*isol, cd, pmr, cmr*)

Phaseoloside A P-243

Triterpene glycoside of unknown struct.. Constit. of *Phaseolus vulgaris* (kidney bean). No phys. props. given.

Chirva, V.Y. *et al., Khim. Prir. Soedin.*, 1970, **6**, 377; *Chem. Nat. Compd. (Engl. Transl.)*, 386

Phaseoloside B P-244

Triterpene glycoside of unknown struct.. Constit. of *Phaseolus vulgaris* (kidney bean). No phys. props. given.

Chirva, V.Y. *et al., Khim. Prir. Soedin.*, 1970, **6**, 377; *Chem. Nat. Compd. (Engl. Transl.)*, 386

Phaseoloside C P-245

Triterpene glycoside of unknown struct.. Constit. of *Phaseolus vulgaris* (kidney bean). No phys. props. given.

Chirva, V.Y. *et al., Khim. Prir. Soedin.*, 1970, **6**, 377; *Chem. Nat. Compd. (Engl. Transl.)*, 386

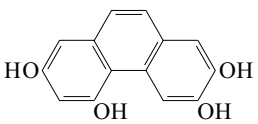
Phaseothione P-246

Mercaptopeptide of unknown struct.. Constit. of *Glycine max* (soybean), *Phaseolus vulgaris* (kidney bean) and *Trifolium repens* (white clover).

Price, C.A. *et al., Nature (London)*, 1957, **180**, 148 (*isol*)

2,3,5,7-Phenanthrenetetrol P-247

2,3,5,7-Tetrahydroxyphenanthrene



$C_{14}H_{10}O_4$ 242.231

3,5-Di-Me ether: [108352-70-1] *3,5-Dimethoxy-2,7-phenanthrenediol. 2,7-Dihydroxy-3,5-dimethoxyphenanthrene*
$C_{16}H_{14}O_4$ 270.284
Found in *Dioscorea batatas* (Chinese yam) inoculated with *Pseudomonas cichorii*. Mp 193-194° (173-174° subl.). λ_{max} 261 (ε 83000); 284 (ε 14200); 295 (ε 11200); 347 (ε 4360); 364 (ε 5620) (EtOH) (Berdy).

2,5,7-Tri-Me ether: [51415-00-0] *3-Hydroxy-2,5,7-trimethoxyphenanthrene.* ***Batatasin I***
$C_{17}H_{16}O_4$ 284.311
Constit. of *Dioscorea batatas* (Chinese yam). Mp 148.5-149.6°. λ_{max} 252 (sh) (ε); 256 (sh) (ε); 264 (ε); 283 (sh) (ε); 292 (sh) (ε); 304 (sh) (ε); 328 (ε); 344 (ε); 361 (ε) (EtOH) (Derep).

9,10-Dihydro: [22318-82-7]
$C_{14}H_{12}O_4$ 244.246
Isol. from *Dioscorea bulbifera* (air potato). Needles (C_6H_6/AcOH). Mp 291-292°.

Erdtman, H. *et al., Acta Chem. Scand.*, 1969, **23**, 249 (*synth, deriv*)
Letcher, R.M. *et al., J.C.S.(C)*, 1971, 3070 (*synth, deriv, uv, pmr*)
Letcher, R.M. *et al., J.C.S. Perkin 1*, 1972, 2941; 1973, 1179 (*isol, struct*)
Hasegawa, K. *et al., Planta*, 1972, **108**, 369 (*isol*)
Reisch, J. *et al., Phytochemistry*, 1973, **12**, 228
Letcher, R.M. *et al., Phytochemistry*, 1973, **12**, 2789 (*synth*)
Hasegawa, K. *et al., Phytochemistry*, 1974, **13**, 2849 (*synth, struct*)
Wij, M. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 643 (*isol, deriv*)
Hata, K. *et al., Chem. Pharm. Bull.*, 1979, **27**, 984 (*isol, ir, pmr, deriv*)
Coxon, D.T. *et al., Phytochemistry*, 1982, **21**, 1389 (*deriv, pmr*)
Juneja, R.K. *et al., Phytochemistry*, 1987, **26**, 1123 (*isol*)
Leong, Y.-W. *et al., Phytochemistry*, 1997, **44**, 157; 1999, **50**, 1237-1241 (*isol, derivs*)

2,4,5,6-Phenanthrenetetrol P-248

[68570-34-3]
2,4,5,6-Tetrahydroxyphenanthrene

$C_{14}H_{10}O_4$ 242.231
Isol. from rhizomes of *Dioscorea bulbifera* (air potato). Mp 220°.

Tetra-Ac: [68570-35-4]
$C_{22}H_{18}O_8$ 410.379
Cryst. Mp 160-161°.

Tetra-Me ether:2,4,5,6-Tetramethoxyphenanthrene
$C_{18}H_{18}O_4$ 298.338
Cryst. Mp 92-93°.

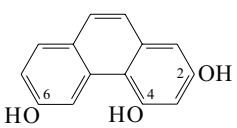
9,10-Dihydro, 2,4-di-Me ether: [58115-33-6] *9,10-Dihydro-5,7-dimethoxy-3,4-phenanthrenediol, 9CI. 9,10-Dihydro-5,6-dihydroxy-2,4-dimethoxyphenanthrene*
$C_{16}H_{16}O_4$ 272.3
Needles. Mp 144-145°.

9,10-Dihydro, 2,6-di-Me ether: [83016-16-4] *9,10-Dihydro-2,6-dimethoxy-4,5-phenanthrenediol, 9CI. 9,10-Dihydro-4,5-dihydroxy-2,6-dimethoxyphenanthrene.* ***Cannithrene 2***
$C_{16}H_{16}O_4$ 272.3
Cryst. (Et_2O/petrol). Mp 170-172°.

Kondo, H. *et al., CA*, 1955, **49**, 1076a (*synth, deriv*)
Wij, M. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 643 (*isol, deriv, uv, pmr*)
Ines, B. *et al., J.O.C.*, 1985, **50**, 2236 (*synth, deriv*)

2,4,6-Phenanthrenetriol P-249

2,4,6-Trihydroxyphenanthrene



$C_{14}H_{10}O_3$ 226.231

2-O-β-D-Glucopyranoside:
$C_{20}H_{20}O_8$ 388.373
Isol. from Riesling wine.

2,6-Di-Me ether: [55806-42-3] *2,6-Dimethoxy-4-phenanthrenol. 4-Hydroxy-2,6-dimethoxyphenanthrene*
$C_{16}H_{14}O_3$ 254.285
Found in opium extracts.

Baderschneider, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 2681-2686 (*2-glucoside*)

3,4,6-Phenanthrenetriol P-250

3,4,6-Trihydroxyphenanthrene, 9CI

$C_{14}H_{10}O_3$ 226.231

3,6-Di-Me ether: [481-81-2] *3,6-Dimethoxy-4-phenanthrenol, 9CI. Thebaol*
$C_{16}H_{14}O_3$ 254.285
Found in opium. Plates and columns (AcOH). Mp 94°.

Tri-Me ether: [96253-84-8] *3,4,6-Trimethoxyphenanthrene.* ***O-Methylthebaol***
$C_{17}H_{16}O_3$ 268.312
Viscous oil.

Pschorr, R. *et al., Ber.*, 1902, **35**, 4400; 1912, **45**, 2212
Vongerichten, E. *et al., Ber.*, 1902, **35**, 4410
Bergten, C. *et al., Chem. Ber.*, 1967, **100**, 3002 (*deriv*)
Reisch, J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 814 (*deriv*)
Theuns, H.G. *et al., Phytochemistry*, 1985, **24**, 163-169 (*O-Methylthebaol*)

Phenol P-251

[108-95-2]
Hydroxybenzene. Carbolic acid. Benzenol. FEMA 3223

PhOH

C_6H_6O 94.113
Used as a flavouring agent in a few foods, at maximum levels below 10 ppm. Deliquescent needles with a characteristic odour. Sol. H_2O, EtOH, Et_2O, Me_2CO, C_6H_6. Mp 43° Fp 41. Bp 181.8° Bp_{25} 90.2°. Log P 1.47 (calc). Steam-volatile. Also used as sodium salt (Phenolate sodium, USAN).

▶ Fl. p. 75/79°, autoignition temp. 605/715°. OES: long-term 5 ppm; short-term 10 ppm (Sk). Violent reactions with a variety of substances. Vapour irritates respiratory system and eyes. Contact with solid or conc. solns. causes chemical burns of the skin and severe eye damage. Readily absorbed through skin and can cause headache, dizziness, respiratory distress, liver and kidney injury, and other effects. Fatalities recorded from skin absorption or ingestion. SJ3325000

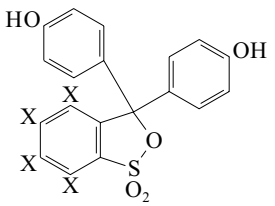
[100-67-4, 2122-46-5, 3229-70-7, 5793-84-0, 13127-88-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1052B; 1069A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 207A; 243A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 984D; 1001A (*ir*)
Kueding, W.W. *et al., J.O.C.*, 1965, **30**, 3756 (*synth*)
Houben-Weyl, *et al., Methoden Org. Chem. (Houben-Weyl), 4th edn.*, Vol. I, 1976, (*bibl*)
Thurman, C. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **17**, 373 (*rev*)
IARC Monog., 1989, **47**, 263; 1990, **50**, 385 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 654

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2171-2173
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 468
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2187
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 994
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGR000; PDO000; SJF000; PEL500; PDN750; PDY750

Phenoltetrabromosulfonephthalein P-252

*4,4′-(4,5,6,7-Tetrabromo-3*H*-2,1-benzoxathiol-3-ylidene)bisphenol* S,S*-dioxide*



X = Br

$C_{19}H_{10}Br_4O_5S$ 669.967
Reddish-black cryst. Sol. EtOH, Me_2CO, EtOAc, alkalis; spar. sol. H_2O. pK_{a1} 7.03 (25°).

Harden, W.C. *et al., J.A.C.S.*, 1929, **51**, 562 (*synth*)
Boyd, W.M. *et al., J.A.C.S.*, 1930, **52**, 4954 (*synth*)
Haring, M.M. *et al., J.A.C.S.*, 1941, **63**, 1024 (*synth*)
Lippi, U. *et al., CA*, 1967, **66**, 45549q (*detn, proteins*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, (*use, ind*)

Phenoxyacetic acid, 9CI P-253

[122-59-8]
Glycollic acid phenyl ether. FEMA 2872
$PhOCH_2COOH$
$C_8H_8O_3$ 152.149
Flavouring ingredient. Present in cocoa beans. Needles (H_2O) with sour, sweet odour and honey-like taste. Mp 98-99°. Bp 285° dec.. pK_{a1} 3.16 (25°). pK_a 5.12.
▶ Skin irritant. LD_{50} (rat, orl) 1500 mg/kg. AJ2230000

2-Propenyl ester: [7493-74-5] *Allyl phenoxyacetate. FEMA 2038*
$C_{11}H_{12}O_3$ 192.214
Flavouring ingredient. Liq. with honey and pineapple-like aroma. Bp_1 100-102°. $n_D^{25.5}$ 1.5131.
▶ LD_{50} (rat, orl) 475 mg/kg. LD_{50} (rbt, skn) 820 mg/kg. AJ2240000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 142C; 338C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 990C; 1213A; 1334A (*nmr*)
Brettle, R. *et al., J.C.S.*, 1956, 1891 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 703 (*rev, tox, allyl ester*)
Junghens, P. *et al., Z. Chem.*, 1975, **15**, 153 (*pmr*)
Kennard, C.H.L. *et al., Acta Cryst. B*, 1982, **38**, 868 (*cryst struct*)
Nair, M.G. *et al., Phytochemistry*, 1988, **27**, 3169-3173 (*isol*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AGQ750
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ; PDR100

2-Phenoxyethanol, 9CI P-254

[122-99-6]
Phenylcellosolve. 2-Hydroxyethyl phenyl ether. 1-Hydroxy-2-phenoxyethane. Ethylene glycol monophenyl ether. Phenoxetol. Ethylene glycol phenyl ether. Newpol EFP. Dalpad A
$PhOCH_2CH_2OH$
$C_8H_{10}O_2$ 138.166
Yellow-brown liq. d_{20}^{20} 1.11. Fp 11-13. Bp 245.2° $Bp_{12.5}$ 116°. n_D^{20} 1.5370. pK_{a1} 15.1 (25°).
▶ Skin and severe eye irritant. LD_{50} (rat, orl) 1260 mg/kg. Fl. p. 121°. KM0350000

Ac: [6192-44-5] *2-Phenoxyethyl acetate*
$C_{10}H_{12}O_3$ 180.203
Liq. d_{25}^{25} 1.1. Mp -20°. Bp 231° (243°) $Bp_{3.2}$ 140.2°.
▶ Mod. toxic. KM0525000

Benzoyl: [4173-59-5] *2-Phenoxyethyl benzoate*
$C_{15}H_{14}O_3$ 242.274
Cryst. Mp 60° (57-58°). $Bp_{0.27}$ 143-146°.

2-Methylpropanoyl: [103-60-6] *2-Phenoxyethyl isobutyrate. FEMA 2873*
$C_{12}H_{16}O_3$ 208.257
Flavouring ingredient. Liq. with sweet floral odour and fruity (peach-like) taste. Sl. sol. H_2O. Bp 265°.
▶ UA2470910

4-Methylbenzenesulfonyl: [43224-81-3]
$C_{15}H_{16}O_4S$ 292.355
Mp 82°.

Me ether: [41532-81-4] *(2-Methoxyethoxy)benzene, 9CI. 1-Methoxy-2-phenoxyethane*
$C_9H_{12}O_2$ 152.193
Liq. Bp_9 96-97°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1157A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 395B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1080A (*ir*)
Rindfusz, R.E. *et al., J.A.C.S.*, 1919, **41**, 665 (*synth*)
Becker, B. *et al., Monatsh. Chem.*, 1947, **77**, 80 (*synth*)
Yoshino, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 553 (*synth*)
Taylor, R. *et al., J.C.S. Perkin 2*, 1976, 280 (*acetate*)
Gilbert, P. *et al., Microbios*, 1977, **19**, 125; *CA*, **89**, 158025 (*use*)
Funanshi, K. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 1488 (*synth, ir, pmr*)
Krabbenhoff, H.O. *et al., J.O.C.*, 1979, **44**, 4285 (*synth, cmr, ir, pmr*)
Bangov, I.P. *et al., Org. Magn. Reson.*, 1983, **21**, 443 (*cmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 338-339
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1142
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2171 (*2-Methylpropanoyl*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 3943
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PER000

Phenyl acetate, 9CI, 8CI P-255

[122-79-2]
Acetoxybenzene. FEMA 3958
$H_3CCOOPh$
$C_8H_8O_2$ 136.15
Flavouring ingredient in baked goods and candies. Liq. with offensive odour. d_4^4 1.09. Bp 196°.
▶ AJ2800000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1285B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 312B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1379B (*ir*)
Crymble, C.R. *et al., J.C.S.*, 1911, **99**, 451 (*synth, uv*)
Schulman, E.M. *et al., J.A.C.S.*, 1972, **94**, 5972 (*cmr*)

Phenyl vinyl sulfide, 8CI P-256

[1822-73-7]
(Ethenylthio)benzene, 9CI. Phenylthioethene
$PhSCH{=}CH_2$
C_8H_8S 136.217
Component of beef aroma. Bp 201° Bp_{25} 94-97°. n_D^{20} 1.5883. Undergoes radical polym. Q/e values for copolym., Q 0.33, e -0.99.

S-*Oxide:* [20451-53-0] *(Ethenylsulfinyl)benzene, 9CI. Phenyl vinyl sulfoxide*
C_8H_8OS 152.217
d^{20} 1.14. $Bp_{1.5}$ 105-110°. n_D^{20} 1.5865. Stable for several days at 180°. Opt. active forms known. Undergoes anionic homopolym. and copolym., e.g. with Styrene, S-255.

S,S-*Dioxide:* [5535-48-8] *(Ethenylsulfonyl)benzene, 9CI. Phenyl vinyl sulfone*
$C_8H_8O_2S$ 168.216
Cryst. (hexane). Mp 66-67°.

[88180-53-4, 89299-85-4, 89299-86-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1176A; **2**, 483C; 485A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 432C; 1578B; 1579C (*nmr*)
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Montanari, F. *et al., CA*, 1957, **51**, 5723b (*synth, uv*)
Tsuda, K. *et al., J. Macromol. Sci., Part A: Chem.*, 1967, **1**, 1025-1037 (*polym*)
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Barbieri, G. *et al., J.C.S.(C)*, 1968, 659-663 (*sulfoxide, synth*)
Weringa, W.D. *et al., Tet. Lett.*, 1969, 273-276 (*ms*)
Ceccarelli, G. *et al., Org. Magn. Reson.*, 1970, **2**, 409-421 (*pmr*)
Paquette, L.A. *et al., J.A.C.S.*, 1978, **100**, 1597-1599 (*sulfoxide, use*)

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Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427-443 (*Qle values*)
Koizumi, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 4198-4201 (*oxide*)
Carr, R.V.C. *et al., J.O.C.*, 1983, **48**, 4976-4986 (*sulfone, synth, pmr, ir, use*)
Smith, M.B. *et al., Synth. Commun.*, 1986, **16**, 85-90 (*synth, pmr*)
Lee, J.W. *et al., Synth. Commun.*, 1989, **19**, 2209-2212 (*sulfone*)
Kanga, R.S. *et al., Macromolecules*, 1990, **23**, 4235-4240 (*polym, oxide*)
Brace, N.O. *et al., J.O.C.*, 1993, **58**, 4506-4508 (*sulfone, synth*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4030-4033 (*S-oxide, use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4041-4045 (*S,S-dioxide, use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4102-4104 (*use*)
Davies, H.M.L. *et al., J.O.C.*, 1995, **60**, 7529-7534 (*sulfone synth, pmr, ms*)
Cossu, S. *et al., Synth. Commun.*, 1996, **26**, 211-216 (*sulfone, synth, bibl*)
Org. Synth., 1997, **74**, 124-129 (*synth, pmr, cmr*)

Phenylacetaldehyde P-257

[122-78-1]
Benzeneacetaldehyde, 9CI. α-Toluic aldehyde. Phenylethanal. FEMA 2874
$PhCH_2CHO$
C_8H_8O 120.151
Found in some essential oils, e.g. *Citrus* spp., *Tagetes minuta* (Mexican marigold) and in the mushroom *Phallus impudicus* (common stinkhorn). Flavouring ingredient. Liq. with hyacinth odour. $d_4^{19.6}$ 1.03. Bp 195° Bp_{10} 78°. n_D^{20} 1.5290. Forms complexes with metals. Polym. on standing to odourless trimer.
▶ Fl. p. 68° (71°,88°). Human skin irritant. LD_{50} (rat, orl) 1550 mg/kg. CY1420000

Oxime: [7028-48-0]
C_8H_9NO 135.165
Testosterone-dependent urinary metab. of phenylalanine isol. from guinea pigs Cryst. (MeOH). Mp 98.5°.
▶ CY1462000

2,4-Dinitrophenylhydrazone: [2074-04-6]
Light-yellow needles (EtOH). Mp 189-190°.

Di-Me acetal: [101-48-4] *(2,2-Dimethoxyethyl)benzene, 9CI. 1,1-Dimethoxy-2-phenylethane. Viridine. FEMA 2876*
$C_{10}H_{14}O_2$ 166.219
Flavouring ingredient. Oil. d_0^{18} 1. Bp_{754} 219-221°.
▶ AB3040000

Di-Et acetal: [6314-97-2] *(2,2-Diethoxyethyl)benzene, 9CI. 1,1-Diethoxy-2-phenylethane. Alleglal*
$C_{12}H_{18}O_2$ 194.273
Oil. Bp 245-246° Bp_8 91-92°.

Ethylene acetal: [101-49-5] *2-(Phenylmethyl)-1,3-dioxolane, 9CI. 2-Benzyl-1,3-dioxolane*
$C_{10}H_{12}O_2$ 164.204
Oil. d_4^{20} 1.09. Bp_1 98-99° Bp_{12} 115-120°. n_D^{20} 1.5220.
▶ JH6768000

Bis(2-methylpropyl) acetal: [68345-22-2] *[2,2-Bis(2-methylpropoxy)ethyl]benzene, 9CI. FEMA 3384*
$C_{16}H_{26}O_2$ 250.38
Flavouring ingredient. Liq. Bp 240°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1066C; **2**, 101A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 230A; 239A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 998A; 998B; 1279A (*ir*)
CRC Atlas of Spectral Data and Physical Constants, 937 (*uv, ir, ms*)
Erlenmeyer, E. *et al., Annalen*, 1883, **219**, 179 (*synth*)
Naidan, V.M. *et al., Zh. Org. Khim.*, 1965, **1**, 1377-1383; *J. Org. Chem. USSR (Engl. Transl.)*, 1965, **1**, 1395-1400 (*ethylene acetal, synth, uv*)
Attaway, J.A. *et al., Phytochemistry*, 1966, **5**, 1273 (*isol*)
Hawkes, G.E. *et al., J.O.C.*, 1974, **39**, 1017 (*cmr*)
Pritchard, J.G. *et al., Org. Mass Spectrom.*, 1974, **8**, 103 (*ms*)
Org. Synth., 1974, **54**, 42 (*synth*)
Smith, A.B. *et al., J. Chem. Ecol.*, 1977, **3**, 309
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 377 (*rev, tox*)
Schaefer, T. *et al., Can. J. Chem.*, 1985, **63**, 2597 (*conformn, pmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BBL500
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Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2177-2181
Katritzky, A.R. *et al., J.O.C.*, 2000, **65**, 1886-1888 (*ethylene acetal, synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ; PDX000; BEN250

Phenylacetic acid P-258

[103-82-2]
Benzeneacetic acid, 9CI. Phenylethanoic acid. α-Toluic acid. FEMA 2878
$PhCH_2COOH$
$C_8H_8O_2$ 136.15
Found in essential oils, e.g. neroli, rose oil, free and as esters. Also present in grapes, raspberry, strawberry, cherimoya, other fruits, cheddar cheese, Swiss cheese, wine, black tea, peated malt and other foodstuffs. Flavouring ingredient. Plates (petrol) with sweet taste at low conc. and rose-like odour. Mp 77-78.5°. Bp 265.5° $Bp_{0.01}$ 65-70°. pK_a 4.31 (H_2O).
▶ Fl. p. 102°. LD_{50} (rat, orl) 2250 mg/kg. Exp. teratogenic effects. AJ2430000

Me ester: [101-41-7] *Methyl phenylacetate. FEMA 2733*
$C_9H_{10}O_2$ 150.177
Flavouring ingredient. Odoriferous constit. of many plants. Present in cocoa, coffee and strawberry. Liq. with sweet honey-like flavour. d_{16}^{16} 1.06. Bp 215° Bp_{50} 131-132°.
▶ Skin irritant. LD_{50} (rat, orl) 2550 mg/kg. AJ3175000

Et ester: [101-97-3] *Ethyl phenylacetate. FEMA 2452*
$C_{10}H_{12}O_2$ 164.204
Odoriferous constit. of many plants. Present in apple, grapefruit, guava fruit, papaya, melon, pineapple, wheat bread, crispbread, wines, fruit brandies, shoyu, bael (*Aegle marmelos*), sake, and ceriman (*Monstera deliciosa*). Flavouring ingredient. Liq. with honey and bittersweet flavour. d_4^{20} 1.03. Bp 227-227.6° $Bp_{17.5}$ 120-125° (lit. gives a pressure range). n_D^{20} 1.4955.
▶ AJ2824000

Propyl ester: [4606-15-9] *Propyl phenylacetate. FEMA 2955*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient. Liq. with sweet honey-like flavour. d_4^{20} 1.01 $d_4^{15.5}$ 0.99. Bp 253°. n_D^{20} 1.4960.

Isopropyl ester: [4861-85-2] *Isopropyl phenylacetate. FEMA 2956*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient. Liq. with sweet honey-like flavour and wine undertone. d_4^{20} 1.01. Bp 253° Bp_{12} 157-165°.

Butyl ester: [122-43-0] *Butyl phenylacetate. FEMA 2209*
$C_{12}H_{16}O_2$ 192.257
Flavouring agent. Present in mountain papaya (*Carica pubescens*). Liq. d_4^{25} 0.99. Bp 260°. n_D^{20} 1.4880. n_D^{20} 1.4910.
▶ AJ2480000

2-Methylpropyl ester: [102-13-6] *2-Methylpropyl phenylacetate. Isobutyl phenylacetate. Eglantine. Iphaneine. Phenysol. FEMA 2210*
$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Liq. with sweet, honey-like flavour. d 0.98. Bp 247° (253°).

Pentyl ester: [5137-52-0] *Pentyl phenylacetate. Amyl phenylacetate*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. Liq. Bp 266-269°.

3-Methylbutyl ester: [102-19-2] *3-Methylbutyl phenylacetate. Isoamyl phenylacetate. FEMA 2081*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. Liq. with a sweet pleasant odour. Bp_{723} 265-266° Bp_3 103°.

Hexyl ester: [5421-17-0] *Hexyl phenylacetate. FEMA 3457*
$C_{14}H_{20}O_2$ 220.311
Flavouring ingredient. Bp 47° 10.

Octyl ester: [122-45-2] *Octyl phenylacetate. FEMA 2812*
$C_{16}H_{24}O_2$ 248.364
Flavouring ingredient. Viscous liq. $d^{15.5}$ 0.98. Bp 315° Bp_3 165-166°.

2-Propenyl ester: [1797-74-6] *2-Propenyl phenylacetate. Allyl phenylacetate. FEMA 2039*
$C_{11}H_{12}O_2$ 176.215
Flavouring ingredient. Oil with honey-like aroma and flavour. Bp 239-240.5° Bp_3 89-93°. $n_D^{13.5}$ 1.5122.

Benzyl ester: [102-16-9] *Phenylmethyl benzeneacetate, 9CI. Benzyl phenylacetate. FEMA 2149*
$C_{15}H_{14}O_2$ 226.274
Used in food flavouring. Liq. with floral odour and slight honey-like taste. d^{17} 1.09. Bp 318-320° Bp_4 165-166°. n_D^{20} 1.5530. n_D^{20} 1.5580.

4-Methylphenyl ester: [101-94-0] *4-Methylphenyl phenylacetate. p-Tolyl phenylacetate. FEMA 3077*
$C_{15}H_{14}O_2$ 226.274
Flavouring ingredient. Cryst. with floral odour and sweet honey-like taste. Mp 76° (EtOH). Bp 310°.

2-Phenylethyl ester: [102-20-5] *Phenethyl phenylacetate. 2-Phenylethyl benzeneacetate. FEMA 2866*
$C_{16}H_{16}O_2$ 240.301
Imitation fruit flavouring ingredient. Needles (MeOH) with hyacinth-like odour and sweet honey-like taste. Mp 28°. Bp 325° Bp_{28} 210°.

Diethylamide: [2431-96-1] N,N-*Diethylbenzeneacetamide, 9CI*
$C_{12}H_{17}NO$ 191.272
Found in various plant oils, e.g. garden cress (*Lepidium sativum*). Mp 86°. Bp 297°.

▶AB7410000

Nitrile: [140-29-4] *Benzeneacetonitrile, 9CI. Benzyl cyanide. Benzyl nitrile. (Cyanomethyl)benzene. Cyanophenylmethane. Phenylacetonitrile*
C_8H_7N 117.15
Isol. from oil of garden cress (*Lepidium sativum*) and other plant oils. Liq. d_{15}^{15} 1.02. Bp 234° Bp_{12} 107°. n_D^{25} 1.5211.

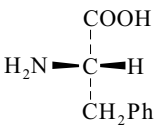
▶Explosive reaction with NaOCl + $H^{\oplus}$. Skin irritant. LD_{50} (rat, orl) 270 mg/kg. LD_{50} (rbt, skn) 270 mg/kg. AM1400000

[114-70-5]

Sadtler Standard C-13 NMR Spectra, 4213 (*cmr*)
Hodgkinson, W.R. *et al., J.C.S.*, 1880, **37**, 485 (*benzyl ester*)
Autenrieth, W. *et al., Ber.*, 1924, **57**, 435 (*4-methylphenyl ester*)
Hibbert, H. *et al., J.A.C.S.*, 1925, **47**, 2242 (*2-phenylethyl ester*)
Org. Synth., Coll. Vol., 1, 1932, 436 (*synth*)
Cogan, M. *et al., Bull. Soc. Chim. Fr.*, 1941, **8**, 157-164 (*benzyl ester*)
Johns, S.R. *et al., Aust. J. Chem.*, 1969, **22**, 1315 (*isol*)
El-Bayoumi, M.A. *et al., J.A.C.S.*, 1971, **93**, 6396 (*uv*)
Scott, K.N. *et al., J. Magn. Reson.*, 1972, **6**, 55 (*pmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1977, **15**, 621; Suppl 1, 1978, **16**, 791 (*2-propenyl ester, 3-methylbutyl ester, rev*)
Larson, R.A. *et al., J. Chromatogr.*, 1977, **138**, 186 (*glc*)
Crew, R.M. *et al., J. Chem. Ecol.*, 1979, **5**, 861
Bakke, J.M. *et al., J. Chem. Ecol.*, 1983, **9**, 513
Harrison, A.G. *et al., J.O.C.*, 1984, **49**, 4993 (*ms*)
Probst, B. *et al., J. Chem. Ecol.*, 1987, **13**, 851
Murahashi, S. *et al., J.O.C.*, 1987, **52**, 4319 (*2-phenylethyl ester, synth, ir, pmr, ms*)
Hodgson, D.J. *et al., Acta Cryst. C*, 1991, **47**, 1986 (*cryst struct*)
Seebach, D. *et al., Helv. Chim. Acta*, 1991, **74**, 1102 (*2-propenyl ester*)
Bhawal, B.M. *et al., Synthesis*, 1991, 112 (*esters, synth, ir, pmr*)
Hirota, A. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 492-494 (*isol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1415
Okano, T. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 2339 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 30; 64; 93; 263; 354; 382; 396; 420; 546; 629; 652; 659; 762 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 99; 274-275; 351-352; 1032-1033; 1336-1337; 1431-1432; 1458-1459; 1498-1499; 1833-1834; 2038-2039; 2166; 2814-2815 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2181-2182 (*occur, props*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2747
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 997; 998
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BQJ350; EOH000; MHA500; PDX750; PEA750; PDY850

Phenylalanine, 9CI, USAN P-259

[3617-44-5]
α-Aminobenzenepropanoic acid. 2-Amino-3-phenylpropanoic acid. β-Phenylalanine. α-Aminohydrocinnamic acid. FN 1636. Antibiotic FN 1636. Phe



(S)-form

$C_9H_{11}NO_2$ 165.191
Log P -1.56 (uncertain value) (calc).

(*R*)-*form* [673-06-3]
D-form
Leaflets (H_2O). Mp 196° dec Mp 283-284° dec. $[\alpha]_D^{25}$ +34.5 (c, 1 in H_2O). $[\alpha]_D$ +4.47 (c, 1 in 5*M* HCl).

▶Human systemic effects by ingestion reported (gastrointestinal). LD_{50} (rat, ipr) 5452 mg/kg. AY7533000

Me ester: [21685-51-8]

[13033-84-6]
$C_{10}H_{13}NO_2$ 179.218
Liq. $Bp_{0.1}$ 95°. $[\alpha]_D^{20}$ -26 (c, 2.2 in EtOH) (>95% ee).

Et ester: [63060-94-6]
$C_{11}H_{15}NO_2$ 193.245
Cryst. (EtOH/Et_2O) (as hydrochloride). Mp 156-158° (hydrochloride). $[\alpha]_D^{21}$ -36.5 (c, 4.8 in EtOH).

tert-*Butyl ester:* [6404-30-4]
$C_{13}H_{19}NO_2$ 221.299
Liq. d_4^{20} 1.02. $Bp_{0.75}$ 115°. $[\alpha]_D^{25}$ -23.4 (c, 1.95 in MeOH). n_D^{20} 1.5006.

Amide: [5241-59-8] *α-Aminobenzenepropanamide, 9CI. Phenylalanine amide*
$C_9H_{12}N_2O$ 164.207
Cryst. (C_6H_6). Mp 91-93°. $[\alpha]_D^{24}$ -13.41 (MeOH).

N-*Formyl:* [59366-89-1]
$C_{10}H_{11}NO_3$ 193.202
Plates (H_2O). Mp 167°. $[\alpha]_D^{20}$ -75.2 (EtOH).

N-*Ac:* [10172-89-1]
Mp 170-171°. $[\alpha]_D$ -49.3.

N-*Ac, Me ester:* [21156-62-7]
$C_{12}H_{15}NO_3$ 221.255
Prisms (Et_2O). Mp 90-91°. $[\alpha]_D^{25}$ -19 (c, 2 in MeOH).

N-*Ac, Et ester:* [20918-84-7]
$C_{13}H_{17}NO_3$ 235.282
Cryst. Mp 93.5-94.5°. $[\alpha]_D^{25}$ -61.8 (c,1 in $CHCl_3$) (72% ee).

N-*Benzoyl:* [37002-52-1]
$C_{16}H_{15}NO_3$ 269.299
Needles (H_2O). Mp 154-155° (146-148°). $[\alpha]_D^{25}$ -6.8 (c, 1.0 in MeOH).

N-*Benzenesulfonyl:* [40279-94-5]
$C_{15}H_{15}NO_4S$ 305.354
Mp 133°. $[\alpha]_D$ +6.7.

N-*(4-Methylbenzenesulfonyl):* [86117-53-5]
$C_{16}H_{17}NO_4S$ 319.381
Cryst. (EtOH aq.). Mp 164-165°. $[\alpha]_D^{29}$ +2.4 (Me_2CO).

N-*Chloroacetyl:* [137503-97-0]
$C_{11}H_{12}ClNO_3$ 241.673
Mp 125°. $[\alpha]_D$ -50.8 (c, 2 in EtOH).

N-*Carboxyacetyl:***N-*Carboxyacetyl-D-phenylalanine***. N-*Malonyl-D-phenylalanine*
$C_{12}H_{13}NO_5$ 251.238
Isol. from pea seedlings.

N-*Me:* [56564-52-4] N-*Methylphenylalanine, 9CI. 2-Methylamino-3-phenylpropanoic acid*
$C_{10}H_{13}NO_2$ 179.218
Needles (H_2O). Mp 250-253° subl. $[\alpha]_D^{25}$ -24.7 (c, 1.6 in 1*M* HCl).

N-*Et:* [105806-84-6]
$C_{11}H_{15}NO_2$ 193.245
Mp 238-240° dec. $[\alpha]_D^{20}$ -53 (c, 1 in 0.1*M* NaOH).

(*S*)-*form* [63-91-2] *L-form. L-Phenylalanine, JAN. FEMA 3585*
Found in many foods. Used in cocoa substitutes. Flavouring ingredient; dietary supplement. Needles (H_2O). Spar. sol. H_2O (2.97 g/100 g at 25°). Mp 283-284° (rapid heat). $[\alpha]_D^{20}$ -34.3 (c, 1 in H_2O) (98% op). pK_{a1} 1.83; pK_{a2} 9.13 (NH_2). Isoelectric point 5.48. Bitter taste.

▶LD_{50} (rat, ipr) 5287 mg/kg. AY7535000

Me ester, hydrochloride: [7524-50-7]

[2577-90-4]
Mp 159-161°. $[\alpha]_D^{25}$ -4.6 (c, 5 in H_2O).

Et ester, hydrochloride: [3182-93-2]

[3081-24-1]
Cryst. (EtOH/Et_2O). Mp 159-161°. $[\alpha]_D^{25}$ -4.6 (c, 5 in H_2O). $[\alpha]_D^{21}$ +36.8 (c, 4.8 in EtOH).

tert-*Butyl ester:* [16874-17-2]
Liq. d_4^{20} 1.02. $Bp_{0.25}$ 107°. $[\alpha]_D^{25}$ +24.6 (neat). n_D^{20} 1.4970.

tert-*Butyl ester, hydrochloride:* [15100-75-1]
Cryst. Mp 207-208° dec. $[\alpha]_D^{25}$ +45.2 (c, 2 in EtOH).

Benzyl ester: [962-39-0]
$C_{16}H_{17}NO_2$ 255.316

Benzyl ester, hydrochloride: [2462-32-0]
Cryst. (H_2O). Mp 208° (203°). $[\alpha]_D^{25}$ -23 (c, 2.0 in 0.25 *M* HCl).

Amide: [5241-58-7]
Mp 81-83°.

N-*Formyl:* [13200-85-6]
Plates (H_2O). Mp 167°. $[\alpha]_D^{20}$ +75.1 (c, 1 in EtOH).

N-*Formyl, Me ester:* [2311-21-9]
$C_{11}H_{13}NO_3$ 207.229
Yellow oil. $[\alpha]_D$ +84.9 (c, 1 in CH_2Cl_2).

N-*Ac:* [2018-61-3]
Cryst. (H_2O). Mp 170-171°. $[\alpha]_D^{26}$ +50.4 (c, 0.5 in EtOH) (98% op).

N-*Ac, Me ester:* [3618-96-0]
Viscous oil ($CHCl_3$); needles (petrol); prisms (Et_2O). Mp 91-92°. $[\alpha]_D$ +101.5 (c, 1 in $CHCl_3$). $[\alpha]_D^{25}$ +19.5 (c, 2 in MeOH).

N-*Ac, Et ester:* [2361-96-8]
Cryst. (EtOH aq.). Mp 93-94°. Subl. 89-92. $[\alpha]_D^{25}$ +85.9 (c, 1 in $CHCl_3$) (100% ee).

N-*Benzoyl:* [2566-22-5] N-*Benzoylphenylalanine*
Mp 142-143°. $[\alpha]_D$ +19.8.

N-*Methanesulfonyl:* [42361-65-9]
$C_{10}H_{13}NO_4S$ 243.283
Needles ($CHCl_3$). Mp 105-107°. $[\alpha]_D^{20}$ -16.7 (c, 4.2 in $CHCl_3$).

N-*Methanesulfonyl, chloride:* [63640-54-0]
$C_{10}H_{12}ClNO_3S$ 261.728
Needles (hexane/Et_2O) or fine powder. Mp 85-86°. $[\alpha]_D^{20}$ +4.3 (c, 1.6 in THF).

N-*Benzenesulfonyl:* [40279-95-6]
Mp 133°. $[\alpha]_D$ -7.

N-*(4-Methylbenzenesulfonyl):* [13505-32-3]
$C_{16}H_{17}NO_4S$ 319.381
Mp 163-164°.

N-*(4-Methylbenzenesulfonyl), chloride:* [29739-88-6]
$C_{16}H_{16}ClNO_3S$ 337.826
Mp 132° dec. $[\alpha]_D^{22}$ +9.38 (c, 2.97 in $CHCl_3$).

4-Methylbenzenesulfonyl, benzyl ester: [1738-78-9]
$C_{23}H_{23}NO_4S$ 409.505
Cryst. (Et_2O/petrol). Mp 170.5-171.5° (164-165.5°). $[\alpha]_D^{20}$ +7.8 (c, 2 in DMF). $[\alpha]_D^{25}$ -7.2 (c, 1 in MeOH).

N-*4-Nitrobenzenesulfonyl:* [64501-87-7]
$C_{15}H_{14}N_2O_6S$ 350.351
Cryst. (EtOAc/petrol). Mp 166-169°.

N-*(3,4-Dihydroxycinnamoyl)*(E-*):* [170663-16-8] **N-*Caffeoylphenylalanine***
$C_{18}H_{17}NO_5$ 327.336
Light yellow powder. $[\alpha]_D^{20}$ -20 (c, 0.7 in MeOH).

N-*Me:* [2566-30-5]
Mp 260° subl. (243-246° dec.). $[\alpha]_D^{20}$ 0 (c, 0.5 in H_2O). $[\alpha]_D^{20}$ +21.8 (c, 0.9 in 1*M* HCl).

N-*Me,* N-tert-*butyloxycarbonyl:* [37553-65-4]
$C_{15}H_{21}NO_4$ 279.335
Cryst. (EtOAc/hexane). Mp 85°. $[\alpha]_D^{20}$ -84.9 (c, 1 in MeOH).

N-*Me,* N-*benzyloxycarbonyl:* [2899-07-2]
$C_{18}H_{19}NO_4$ 313.352
Cryst. (EtOAc/hexane). Mp 67-71°. $[\alpha]_D^{28}$ -67 (c, 1.8 in EtOH).

N,N-*Di-Me:* [17469-89-5] N,N-*Dimethylphenylalanine*
$C_{11}H_{15}NO_2$ 193.245

N,N,N-*Tri-Me, betaine:* [125982-49-2] α-*Carboxy*-N,N,N-*trimethylbenzeneethanaminium, 9CI. α-Trimethyl-β-phenylpropiobetaine. Phenylalanine betaine*
$C_{12}H_{17}NO_2$ 207.272
Mp 240-242° dec.

N-*Hydroxy:* See *N*-Hydroxyphenylalanine in *The Combined Chemical Dictionary.*

N-*2,4-Dinitrophenyl:* [1655-54-5]
$C_{15}H_{13}N_3O_6$ 331.284
Cryst. (MeOH aq.). Mp 189°.

4-Nitroanilide, N-*Ac:* [17682-83-6]
Mp 244-246°. $[\alpha]_D^{20}$ +97.9 (MeOH).

(±)-*form* [150-30-1] *FEMA 3726*
Flavouring ingredient. Prisms (H_2O). Spar. sol. H_2O, EtOH; insol. Et_2O. Mp 271-273° Mp 284-288° dec Mp 318-320° dec. pK_{a1} 2.16; pK_{a2} 9.15 (25°,$NH_3^{\oplus}$, 0.1*M* NaCl).

Hydrochloride: [27172-85-6]
Cryst. (EtOH/Et_2O). Mp 234-235°.

Me ester: [15028-44-1]
Liq. Bp_{12} 141°.

Me ester, hydrochloride: [5619-07-8]
Needles. Mp 158° dec.

Et ester: [1795-96-6]
Bp_{10} 143°.

Et ester, hydrochloride: [19881-53-9]
Mp 127°.

tert-*Butyl ester:* [16367-71-8]
Liq. d_4^{20} 1.01. $Bp_{0.35}$ 96°. n_D^{20} 1.4536.

Benzyl ester: [25282-53-5]
Mp 196° (as hydrochloride).

Amide: [17193-31-6]
Prisms ($CHCl_3$). Mp 138-140°.

Nitrile: α-Aminobenzenepropanenitrile, 9CI. 1-Cyano-2-phenylethylamine. 2-Amino-3-phenylpropionitrile
$C_9H_{10}N_2$ 146.191
Mp 39.5-40.5°.

N-*Formyl:* [4289-95-6]
Cryst. (H_2O). Mp 168-169°.

N-*Ac:* [2901-75-9] ***Afalanine, INN***
$C_{11}H_{13}NO_3$ 207.229
Plates (Me_2CO). Mp 152-153°.

N-*Ac, Me ester:* [62436-70-8]
Cryst. (Et_2O/petrol). Mp 62-63°.

N-*Ac, Et ester:* [4134-09-2]
Cryst. (petrol). Mp 69-70°. Bp_2 155-157°.

N-*Benzoyl:* [2901-76-0] *α-Benzoylaminobenzenepropanamide, 9CI.* N-*Benzoylphenylalanine*
$C_{16}H_{15}NO_3$ 269.299
Cryst. (EtOH). Mp 185-187°.

N-*Benzoyl, Et ester:* [19817-70-0]
$C_{18}H_{19}NO_3$ 297.353
Needles (petrol). Mp 95°.

▶AY3276140

N-*Benzoyl, amide:* [24250-72-4]
$C_{16}H_{16}N_2O_2$ 268.315
Needles ($CHCl_3$). Mp 198°.

N-*Me:* [2566-35-0]
Plates (H_2O). Mp 252-254° subl.

N,N-*Di-Me:* [24268-81-3]
Cryst. (MeOH). Mp 228°.

N-*(4-Methylbenzenesulfonyl), benzyl ester:* [119290-61-8]
Cryst. (H_2O). Mp 149°.

4-Nitroanilide, N-*Ac:* [19746-42-0] *α-Acetamido-4′-nitrohydrocinnamanilide. α-(Acetylamino)*-N-*(4-nitrophenyl)benzenepropanamide, 9CI*
$C_{17}H_{17}N_3O_4$ 327.339
Mp 266-268° dec.

[60058-39-1, 65864-22-4, 146815-23-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 250C; 250D; 251A; 260B; 283C; 283D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1181B; 1181C; 1182A; 1182B; 1225B; 1225C (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 489 (*synth*)
Huang, H.T. *et al., J.A.C.S.*, 1952, **74**, 105-109 (*N-Ac, Me ester, synth*)
Ronwin, E. *et al., J.O.C.*, 1953, **18**, 1546-1553 (*N-benzoyl*)
Zervas, L. *et al., J.O.C.*, 1957, **22**, 1515-1521 (*4-methylbenzenesulfonyl, benzyl ester*)
Anderson, G.W. *et al., J.A.C.S.*, 1960, **82**, 3359-3363 (tert-*butyl ester*)
Vanderhaeghe, H. *et al., J.A.C.S.*, 1960, **82**, 4414-4422 (*N-Me*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2156 (*rev*)
Halpern, B. *et al., Chem. Ind. (London)*, 1963, 1399-1400 (*resoln*)
Fujiwara, S. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 344-349 (*pmr*)
Sokolovsky, M. *et al., J.A.C.S.*, 1964, **86**, 1202-1206 (*benzyl ester*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679-681 (*cd*)
Cavanaugh, R. *et al., J.A.C.S.*, 1967, **89**, 1558-1564 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2355 (*occur*)
Al-Karaghouli, A.R. *et al., Acta Cryst. B*, 1975, **31**, 2461-2465 (*cryst struct*)
Oguri, T. *et al., Chem. Pharm. Bull.*, 1975, **23**, 167-172 (*synth*)
Kasai, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 2489-2490 (*L-Phenylalanine amide*)
Glaser, R. *et al., J. Organomet. Chem.*, 1976, **121**, 249-260 (*N-Ac, Me ether, N-Ac, Et ester, tert-butyl ester, synth, ir, pmr*)
Okogun, J.I. *et al., Phytochemistry*, 1976, **15**, 826-827 (*betaine*)
Ogawa, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 1811-1812 (*N-Carboxyacetyl-D-phenylalanine*)
Smith, C.D. *et al., Biochem. J.*, 1977, **165**, 121 (*N-4-nitrobenzenesulfonyl*)
Jones, J.H. *et al., J.C.S. Perkin 1*, 1979, 3203-3206 (*N-Ac nitroanilide*)
Glaser, R. *et al., Tetrahedron*, 1979, **35**, 2381-2387 (*N-Ac, Et ester*)
Kasafirek, E. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 442-451 (*N-Ac nitroanilide*)
Nara, M. *et al., Tetrahedron*, 1980, **36**, 3161-3170; 3171-3175 (*N-tosyl derivs, N-methanesulfonyl chloride*)
Doerfler, D.L. *et al., Phytochemistry*, 1981, **20**, 2303-2304 (*isol, Benzoylphenylalanine*)
Roper, J.M. *et al., Synthesis*, 1983, 1041-1043 (*resoln, Ac*)
Sinha, B.K. *et al., Acta Cryst. C*, 1984, **40**, 166-168 (*N-Ac nitroanilide*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH, Weinheim, 1985, **A2**, 72 (*manuf*)
Eur. Pat., 1986, 178 911, (*Sankyo*); *CA*, **106**, 55906n (*Afalanine*)
Van Fleteren, L. *et al., Bull. Soc. Chim. Belg.*, 1988, **97**, 505-517 (*N-Me N-tert-butyloxycarbonyl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PEC500; PEC750
Portelli, M. *et al., Gazz. Chim. Ital.*, 1989, **119**, 215-216 (*synth*)
Adamczeski, M. *et al., J.A.C.S.*, 1989, **111**, 647-654 (*isol, Me ester N-Ac*)

Hashimoto, S. *et al., Synth. Commun.*, 1991, **21**, 833-839 (*N-4-methylbenzenesulfonyl chloride, synth, use*)
Oppolzer, W. *et al., Helv. Chim. Acta*, 1992, **75**, 1965-1978; 1993, **76**, 187-196 (*N-alkyl derivs*)
Lagriffoul, P. *et al., J.C.S. Perkin 2*, 1992, 1279-1284 (*nitrile*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1046
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 663-664
Adam, K.-P. *et al., Phytochemistry*, 1995, **40**, 1577-1578 (*N-Caffeoylphenylalanine*)
Ager, D.J. *et al., Synth. Commun.*, 1996, **26**, 3865-3868 (*amide, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2182-2185
Giard, T. *et al., Synthesis*, 1998, 297-300 (*N-formyl Me ester*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1462-1463
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PEC500; PEC750

4-Phenylbutanoic acid P-260

[1821-12-1]
Benzenebutanoic acid, 9CI
$PhCH_2CH_2CH_2COOH$
$C_{10}H_{12}O_2$ 164.204
Leaflets (H_2O). Mp 52°. Bp 290° Bp_1 120-125°. pK_a 4.76 (25°). Approved for clinical use in the European Union (1999)

Na salt: [1716-12-7] ***Sodium phenylbutyrate, BAN, USAN.*** *TriButyrate. Ammonaps*
Prodrug of Phenylacetic acid, P-258.

Me ester: [2046-17-5] *FEMA 2739*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient. Liq. with a sweet fruity flavour.

Et ester: [10031-93-3] *FEMA 2453*
$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Liq. with a sweet fruity odour. Bp_{10} 130-131°.

Chloride: [18496-54-3]
$C_{10}H_{11}ClO$ 182.649
Bp_9 119°.

Amide: [1199-98-0]
$C_{10}H_{13}NO$ 163.219
Plates (H_2O). Mp 84.5°.

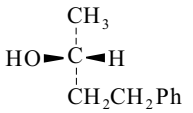
Hydrazide: [39181-61-8]
$C_{10}H_{14}N_2O$ 178.233
Needles ($CHCl_3$). Mp 78-79°.

Nitrile: [2046-18-6] *1-Cyano-3-phenylpropane*
$C_{10}H_{11}N$ 145.204
Bp_{10} 129-131°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 141A; 424D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 988B; 1481B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1317D (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 499 (*synth*)
Stuckwisch, C.G. *et al., J.O.C.*, 1963, **28**, 2362 (*synth*)
Quillet, J.P. *et al., Bull. Soc. Chim. Fr.*, 1967, 255 (*synth*)
Dover, G.J. *et al., N. Engl. J. Med.*, 1992, **327**, 569 (*Na salt*)
Fibach, E. *et al., Blood*, 1993, **82**, 2203 (*pharmacol, Na salt, bibl*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 549; **2**, 263 (*Me ester, Et ester*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1755
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1033-1034; 1839 (*Et ester*)

4-Phenyl-2-butanol P-261

[2344-70-9]
α-Methylbenzenepropanol, 9CI. FEMA 2879


(*R*)-*form*

$C_{10}H_{14}O$ 150.22

(R)-form [39516-03-5]
Liq. Bp_{14} 132°. $[\alpha]_D^{26}$ -32 (c, 6.2 in C_6H_6). Steam-volatile.

Phenylurethane:
Mp 113-114°.

(S)-form [22148-86-3]
Bp_{14} 132°. $[\alpha]_D^{25}$ +12.3 (c, 6.05 in $CHCl_3$). $[\alpha]_D^{20}$ +13.8 (c, 3.8 in $CHCl_3$) (98% ee).

Ac: [109431-71-2]
$C_{12}H_{16}O_2$ 192.257
Bp_{15} 130°.

(±)-form [14786-43-7]
Flavouring ingredient. Oil with aromatic odour. $d_4^{16.5}$ 0.99. Bp 238°. $n_D^{16.5}$ 1.5170.

Phenylurethane:
Mp 116-117°.

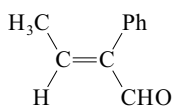
Ac: [59960-25-7]

[10415-88-0] *FEMA 2882*
Flavouring ingredient. Liq. with a mild, green, fruity odour and sweet, fruity taste. d^{16} 0.99. Bp_{15} 123-124°. n_D^{16} 1.4895.

Packendorff, K. *et al., Ber.*, 1934, **67**, 906 (*synth*)
Mozingo, R. *et al., J.A.C.S.*, 1944, **66**, 1860 (*synth*)
Yamamoto, Y. *et al., J.O.C.*, 1976, **41**, 303 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 660; 662
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2185-2186; 2189
Aleu, J. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 1589-1596 (*S-form, synth, pmr, ms*)
Kuwano, R. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 485-496 (*S-form, synth, pmr*)
Nakamura, K. *et al., J.C.S. Perkin 1*, 2000, 3205-3211 (*S-form, synth, ir, pmr*)

2-Phenyl-2-butenal P-262

[4411-89-6]
α-Ethylidenebenzeneacetaldehyde, 9CI. 2-Phenylcrotonaldehyde. FEMA 3224


(*E*)-*form*

$C_{10}H_{10}O$ 146.188

(E)-form [54075-09-1]
Flavouring ingredient. Odorous component of black tea. d^{18} 1.05. $Bp_{0.1}$ 68-70°. n_D^{18} 1.5605.

(Z)-form [54075-10-4] Characterised spectroscopically.

Iliceto, A. *et al., Gazz. Chim. Ital.*, 1960, **90**, 262; *CA*, **55**, 11336 (*synth*)
Dana, G. *et al., Bull. Soc. Chim. Fr.*, 1974, 2089
Clinch, K. *et al., Tetrahedron*, 1989, **45**, 239 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 660
Newcomb, M. *et al., J.A.C.S.*, 1995, **117**, 12085 (*Z-form, synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2186-2187

4-Phenyl-2-butenal, 9CI P-263

[13910-23-1]
4-Phenylcrotonaldehyde
$PhCH_2CH{=}CHCHO$
$C_{10}H_{10}O$ 146.188
Odorous component of *Phallus impudicus* (common stinkhorn).

(E)-form [55177-35-0]

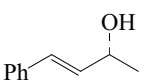
Semicarbazone:
Mp 210°.

2,4-Dinitrophenylhydrazone:
Mp 172-174°.

Prévost, C. *et al., Bull. Soc. Chim. Fr.*, 1944, **11**, 218 (*synth*)
List, P.H. *et al., Naturwissenschaften*, 1966, **53**, 585 (*isol*)
Nakai, T. *et al., Tet. Lett.*, 1974, 3625 (*synth*)
Wada, M. *et al., Chem. Lett.*, 1977, 345 (*synth*)

4-Phenyl-3-buten-2-ol, 9CI P-264

[17488-65-2]
Methylstyrylcarbinol. α-Methylcinnamyl alcohol. FEMA 2880


(*R*)-(*E*)-*form*

$C_{10}H_{12}O$ 148.204

(R)-(E)-form [62413-47-2]
Bp_5 150°. $[\alpha]_D$ +24.5 (c, 3.0 in $CHCl_3$) (99% ee). $[\alpha]_D^{20}$ +20.9 (c, 5.04 in $CHCl_3$) (53% ee).

Ac: [84519-63-1]
$C_{12}H_{14}O_2$ 190.241
Oil. $[\alpha]_D^{20}$ +142.2 (c, 1.0 in $CHCl_3$) (99% ee).

(R)-(Z)-form [92075-80-4]

Ac: [100017-26-3]
$C_{12}H_{14}O_2$ 190.241
Oil. $[\alpha]_D^{20}$ -34.5 (c, 1.1 in $CHCl_3$) (99% ee).

(R)-form [32271-52-6]
Cryst. (petrol). Mp 39-41°. $[\alpha]_D^{20}$ +9.73 (c, 1.5 in MeOH). Geom. isom. not defined.

(S)-(E)-form [81176-43-4]
Plates (hexane). Mp 58-59°. $[\alpha]_D$ -35 (c, 5 in $CHCl_3$).

(±)-(E)-form
No phys. props. reported.

(±)-(Z)-form [31915-95-4]

[104974-60-9]

Flavouring ingredient. Thick oil with a floral odour. d^{22} 1.01. Bp_{21} 144°. λ_{max} 240 (ϵ 12000) (no solvent reported).

[31915-95-4, 36004-04-3, 76946-09-3, 84519-62-0]

Braude, E.A. *et al., J.C.S.*, 1951, 2085-2092 (*synth*)
Pocker, Y. *et al., J.A.C.S.*, 1971, **93**, 691-697 (*synth*)
Thummel, R.P. *et al., J.O.C.*, 1972, **37**, 3919-3923 (*pmr*)
Červinka O., *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 294-297 (*synth, abs config*)
Kawasaki, M. *et al., Chem. Pharm. Bull.*, 1985, **33**, 347-350 (*isomers, synth*)
Schenck, T.G. *et al., J.A.C.S.*, 1985, **107**, 2058-2066 (*synth, resoln, bibl*)
Sato, T. *et al., Tet. Lett.*, 1989, **30**, 2959-2962 (*use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1992, **16**, 216 (*use*)
Stary, I. *et al., Tetrahedron*, 1992, **48**, 7229-7250 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 661
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2187-2188
Tietze, L.F. *et al., Chem. Eur. J.*, 1999, **5**, 297-304 (*synth, uv, pmr, ms*)
Kuwano, R. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 485-496 (*synth, pmr*)
Clausen, R.P. *et al., J.O.C.*, 2000, **65**, 2797-2801 (*synth, pmr, cmr*)
Kazmaier, U. *et al., Eur. J. Org. Chem.*, 2001, 4067-4076 (*S-E-form, synth, pmr, cmr, Ac*)

4-Phenyl-3-buten-2-one, 9CI P-265

[122-57-6]
Benzylideneacetone. Methyl styryl ketone. Benzalacetone. FEMA 2881

$PhCH{=}CHCOCH_3$

$C_{10}H_{10}O$ 146.188
Flavouring ingredient. Present in hydrolysed soy protein.

▶Fl. p. 66°. Mild skin irritant. LD_{50} (rat, orl) 2031 mg/kg. EN0330000

(*E*)-*form* [1896-62-4]
Lustrous plates. Mp 42°. Bp 260-262° Bp_9 126-128°.

▶EN0330050

Oxime: [1721-83-1]

[21613-44-5, 21613-45-6]
$C_{10}H_{11}NO$ 161.203
Needles. Mp 116°.

Phenylhydrazone:
Yellow needles. Mp 156-157°.

Semicarbazone: [1722-63-0]
Mp 187°.

Ethylene dithioacetal: [107389-59-3] *2-Methyl-2-(2-phenylethenyl)-1,3-dithiolane*
$C_{12}H_{14}S_2$ 222.375
Solid. Mp 52-53°. $Bp_{0.16}$ 109-112°.

(*Z*)-*form* [937-53-1]
Liq. Mp -21.5°. $Bp_{0.2}$ 67-68°.

Semicarbazone: [1722-65-2]
Mp 177.5°.

[2887-98-1, 5468-31-5, 13387-22-9, 22921-89-7, 61210-87-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 7C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 799C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1227D (*ir*)
Grignard, V. *et al., Ann. Chim. (Paris)*, 1928, **9**, 5-54 (*synth*)
Schinz, H. *et al., CA*, 1955, **49**, 6874 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1011-1081 (*rev, tox*)
Baas, P. *et al., Tetrahedron*, 1977, **33**, 1509-1511 (*conformn, pmr*)
Ravi, B.N. *et al., J.O.C.*, 1979, **44**, 3109-3113 (*isol, ir, pmr*)
Fischer, H. *et al., Chem. Ber.*, 1990, **123**, 399-404 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 661
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2188-2189
Org. Synth., Coll. Vol., 9, 1998, 649-652
Tietze, L.F. *et al., Angew. Chem., Int. Ed.*, 1999, **5**, 297-304 (*synth, ir, uv, pmr, ms*)
Zhong, P. *et al., Synth. Commun.*, 2000, **30**, 3245-3253 (*synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SMS500

4-Phenylbutyl glucosinolate P-266

[76265-26-4]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)benzenepentanimidate], 9CI

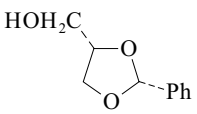
$Ph(CH_2)_4C(SGlc){=}NOSO_3H$

$C_{17}H_{25}NO_9S_2$ 451.518
Present in horseradish (*Armoracia lapathifolia*).

Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)

2-Phenyl-1,3-dioxolane-4-methanol, 9CI P-267

1,2-O-Benzylideneglycerol. Glycerol 1,2-benzylidene ether. 4-Hydroxymethyl-2-phenyl-1,3-dioxolane



(2*R*,4*S*)-*form*

$C_{10}H_{12}O_3$ 180.203
Benzaldehyde glyceryl acetal comprising this compd. and/or 5-Hydroxy-2-phenyl-1,3-dioxane, H-721, is used as a food flavouring agent (FEMA 2128)..

(2*R*,4*S*)-*form* [61688-52-6]
(+)-cis-*form*
Oil. Bp_2 140°. $[\alpha]_D^{20}$ +18 (EtOH aq.).

(2*S*,4*S*)-*form* [61688-53-7]
(+)-trans-*form*
Mp 32-33°. $[\alpha]_D^{20}$ +50 (EtOH aq.).

(2*RS*,4*SR*)-*form* [25687-68-7]
(±)-cis-*form*

4-Methylbenzenesulfonyl:
$C_{17}H_{18}O_5S$ 334.392
Mp 62°.

(2*RS*,4*RS*)-*form* [25687-63-2] *(±)*-trans-*form*

4-Methylbenzenesulfonyl:
Mp 72°.

Serdarevich, B. *et al., J. Am. Oil Chem. Soc.*, 1967, **44**, 381 (*synth, pmr*)
Inch, T.D. *et al., J.C.S.(C)*, 1970, 263 (*synth, pmr*)
Carman, R.M. *et al., Aust. J. Chem.*, 1976, **29**, 1761 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 128
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 246

1-Phenyl-1,3-docosanedione P-268

1-Benzoyl-2-heneicosanone

$H_3C(CH_2)_{18}COCH_2COPh$

$C_{28}H_{46}O_2$ 414.67
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Phenyl-1,3-dodecanedione P-269

1-Benzoyl-2-undecanone

$H_3C(CH_2)_8COCH_2COPh$

$C_{18}H_{26}O_2$ 274.402
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Phenyl-1,3-eicosanedione, 9CI P-270

[58446-52-9]
1-Benzoyl-2-nonadecanone

$PhCOCH_2CO(CH_2)_{16}CH_3$

$C_{26}H_{42}O_2$ 386.617
Constit. of the pollen of *Helianthus annuus* (sunflower).

3-Alcohol:3-Hydroxy-1-phenyl-1-eicosanone
$C_{26}H_{44}O_2$ 388.632
Constit. of the pollen of *Helianthus annuus* (sunflower).

Ger. Pat., 1975, 2 439 282; *CA*, **84**, 109019y (*synth*)
Ger. Pat., 1975, 2 600 516; *CA*, **85**, 125135j (*use*)
Eur. Pat., 1995, 658 592; *CA*, **123**, 288308k (*synth, use*)
Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

2-Phenylethanethiol P-271

[4410-99-5]
Benzeneethanethiol, 9CI. β-Phenylethylmercaptan. 1-Mercapto-2-phenylethane. Phenethyl mercaptan. FEMA 3894

$PhCH_2CH_2SH$

$C_8H_{10}S$ 138.233
Food flavouring. Bp_{23} 105°.

S-*Ph:* [13865-49-1] *(2-Phenylethyl)thiobenzene, 9CI. Phenythyl phenyl sulfide*
$C_{14}H_{14}S$ 214.331
Oil.

S-*(2,4-Dinitrophenyl):*
Mp 89-90°.

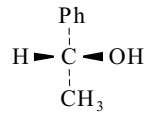
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 416C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1089D (*ir*)
v. Braun, J. *et al., Ber.*, 1912, **45**, 1564 (*synth*)
Bost, R.W. *et al., J.A.C.S.*, 1932, **54**, 1985 (*deriv, synth*)
Katritzky, A.R. *et al., J.C.S. Perkin 1*, 1987, 769 (*synth*)

Hudlicky, T. *et al., J.C.S. Perkin 1*, 1996, 2187 (*S-Ph, synth, pmr*)

1-Phenylethanol P-272

[98-85-1]

α-Methylbenzenemethanol, 9CI. α-Methylbenzyl alcohol, 8CI. Methylphenylcarbinol. α-Hydroxyethylbenzene. sec*-Phenethyl alcohol. 1-(Phenylethyl) alcohol. Styrallyl alcohol. FEMA 2685*



(*R*)-*form*

$C_8H_{10}O$ 122.166

Flavouring agent. Present in tea aroma, mushroom volatiles, European cranberry, chive, Scotch spearmint oil, cheeses, spirits, white wine, cocoa and roasted filbert.

▶ Skin and eye irritant. LD_{50} (rat, orl) 400 mg/kg. LD_{50} (rbt, skn) 2500 mg/kg. DO9275000

(*R*)-*form* [1517-69-7]

Oil. $d_4^{13.3}$ 1.02. Bp 202-204° Bp_1 75°. $[\alpha]_D^{25}$ +54.8 (c, 0.9 in $CHCl_3$) (97% ee). n_D^{20} 1.5270.

(*S*)-*form* [1445-91-6]

Oil. Bp_{17} 97-98°. $[\alpha]_D^{20}$ -41.6 (c, 0.75 in MeOH) (91% op). $[\alpha]_D^{26}$ -38.1 (neat) (94.3% ee). n_D^{20} 1.5270.

(±)-*form* [13323-81-4]

Flavouring agent. Liq. with dry floral odour. d_4^{20} 1.01. Mp 20°. Bp 203.6° Bp_7 85-86°.

▶ Fl. p. 86°.

Formyl: [7775-38-4] *1-Phenylethyl formate. α-Methylbenzyl formate. FEMA 2688*
$C_9H_{10}O_2$ 150.177
Flavouring ingredient. Liq.

Ac: [50373-55-2]

[93-92-5] *1-Phenylethyl acetate. FEMA 2684*
Flavouring ingredient. Present in gardenia flower oil. Oil. Bp 222° Bp_4 72-73°.

Propanoyl: [120-45-6] *1-Phenylethyl propanoate. FEMA 2689*
$C_{11}H_{14}O_2$ 178.23
Flavouring agent. Bp 91-92°.

▶ DP0620000

Butanoyl: [3460-44-4] *1-Phenylethyl butyrate. α-Methylbenzyl butyrate. FEMA 2686*
$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Oil.

2-Methylpropanoyl: [7775-39-5] *1-Phenylethyl isobutyrate. α-Methylbenzyl isobutyrate. FEMA 2687*
$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Liq.

[3299-05-6, 4013-34-7]

Registry of Mass Spectral Data, Wiley-Interscience, 186 (*ms*)
Sadtler Standard Ultraviolet Spectra, 582 (*uv*)
McKenzie, A. *et al., J.C.S.*, 1913, **103**, 695 (*synth*)
Ashworth, F. *et al., J.C.S.*, 1928, 1798 (*synth*)
Houssa, A.J.H. *et al., J.C.S.*, 1930, 2261 (*resoln*)
Adv. Chem. Ser., 1955, **15**, 348 (***props***)
Eliel, E.L. *et al., J.O.C.*, 1956, **21**, 596 (*synth, abs config*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 611 (*rev, tox, Ac*)
Brienne, M.-J. *et al., Synthesis*, 1983, 704 (*resoln*)
Givens, R.S. *et al., J.A.C.S.*, 1984, **106**, 1779 (*synth, R-form, S-form*)
Sheo, S. *et al., Org. Magn. Reson.*, 1984, **22**, 428 (*cmr*)
Stein, A.R. *et al., Can. J. Chem.*, 1985, **63**, 3442 (*synth, resoln*)
Blagg, J. *et al., J.C.S. Perkin 1*, 1986, 1581 (*synth, deriv, ir, pmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PDE000
Radhakrishna, A.S. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 373 (***synth***)
Zwanenburg, B. *et al., Tetrahedron*, 1991, **47**, 7645 (*synth, R-form, S-form*)
Danda, H. *et al., Tetrahedron*, 1991, **47**, 8701 (*synth, S-form*)
Mathre, D.J. *et al., J.O.C.*, 1993, **58**, 2880 (*synth*)
Ohkuma, T. *et al., J.O.C.*, 1994, **59**, 217 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 473-476 (*acyl derivs*)
Reyes, A. *et al., Synth. Commun.*, 1995, **25**, 1053 (*resoln*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1719-1726 (*acyl derivs*)
Lutz, C. *et al., Synthesis*, 1999, 312-316 (*S-form, synth*)
Kuwano, R. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 485-496 (*S-form, synth, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PDE000; PFR000

2-Phenylethanol P-273

[60-12-8]

Benzeneethanol, 9CI. ***Phenethyl alcohol, 8CI, BAN.*** *Benzylcarbinol. β-Hydroxyethylbenzene. Phenylethyl alcohol, USAN. FEMA 2858*

$PhCH_2CH_2OH$

$C_8H_{10}O$ 122.166

Flavouring ingredient. Component of ylang-ylang oil. Liq. with mild rose odour and peach-like taste (initially slightly bitter). Mod. sol. H_2O. d_4^{20} 1.02. Mp -25.8°. Bp 221-222° Bp_{10} 99.5°. n_D^{20} 1.5170. n_D^{20} 1.5325. Log P 1.18 (calc).

▶ Fl. p. 96°. Skin and eye irritant. LD_{50} (rat, orl) 1790 mg/kg. LD_{50} (rbt, skn) 790 mg/kg. Exp. reprod. and teratogenic effects. SG7175000

O-*α-D-Glucopyranoside:* [105088-18-4] *2-Phenylethyl α-D-glucopyranoside. Phenethyl α-D-glucoside*
$C_{14}H_{20}O_6$ 284.308
Isol. from Riesling grapes. Constit. of *Rosa damascena bulgaria* (damask rose) and *Vitis vinifera* (wine grape).

O-*β-D-Glucopyranoside:* [18997-54-1]
$C_{14}H_{20}O_6$ 284.308
Isol. from and *Citrus unshiu* (satsuma mandarin). Mp 38-39°. $[\alpha]_D$ -28.8 (c, 0.4 in MeOH). $[\alpha]_D^{20}$ -33.5 (c, 3.0 in H_2O).

O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:* ***Phenethyl 6-galloyl-glucoside***
$C_{21}H_{24}O_{10}$ 436.415
Isol. from *Rosa damascena* (damask rose).

O-*β-D-Galactopyranoside:* [14861-16-6]

[55520-11-1] *2-Phenylethyl galactopyranoside. Phenethyl galactoside*
$C_{14}H_{20}O_6$ 284.308
Isol. from Riesling grapes. Constit. of *Rosa damascena bulgaria* (damask rose var.) and *Vitis vinifera* (wine grape).

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [129932-48-5] *Phenylethyl primeveroside*
$C_{19}H_{28}O_{10}$ 416.424
Constit. of *Camellia sinensis* (oolong tea), *Jasminum sambac* (Arabian Jasmine). $[\alpha]_D$ -63.2 (c, 1.5 in MeOH) (-29).

O-*[β-D-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [88510-08-1] *Phenethyl rutinoside*
$C_{20}H_{30}O_{10}$ 430.451
Isol. from *Citrus unshiu* (Satsuma mandarin). Amorph. powder + $1H_2O$. $[\alpha]_D$ -101.2 (c, 0.1 in MeOH).

Formyl: [104-62-1] *2-Phenylethyl formate, 9CI. Phenethyl formate. FEMA 2864*
$C_9H_{10}O_2$ 150.177
Flavouring ingredient. Liq. with bittersweet plum taste. Bp 226° Bp_3 73-75°.

▶ LQ9400000

Ac: [103-45-7] *2-Phenylethyl acetate, 9CI. Phenethyl acetate. FEMA 2857*
$C_{10}H_{12}O_2$ 164.204
Flavouring ingredient. Oil with raspberry-like taste. Mp -31.1°. Bp 232° Bp_{13} 118-120°.

▶ AJ2220000

Propanoyl: [122-70-3] *2-Phenylethyl propanoate. Phenethyl propionate. FEMA 2867*
$C_{11}H_{14}O_2$ 178.23
Found in guava *Pisidium guajava*, cheeses, peanut and brandy. Food flavour. Liq. with rose/fruity flavour. d_{25}^{25} 1.012. Bp 244°. n_D^{20} 1.4950.

Butanoyl: [103-52-6] *2-Phenylethyl butanoate. Phenethyl butyrate. FEMA 2861*
$C_{12}H_{16}O_2$ 192.257
Food flavouring. Liq. with sweet honey taste and rose odour. d 1. Bp 238°. n_D^{20} 1.4897.

2-Methylpropanoyl: [103-48-0] *2-Phenylethyl 2-methylpropanoate. Phenethyl isobutyrate. FEMA 2862*
$C_{12}H_{16}O_2$ 192.257
Found in *Mentha* spp., olive (*Olea europea*), beer and other beverages. Food flavouring. Liq. with bittersweet fruity odour. d 1. Bp 230°. n_D^{20} 1.4870.

Pentanoyl: [7460-74-4] *2-Phenylethyl pentanoate. Phenethyl valerate*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. d 0.98. Bp 268°. n_D^{20} 1.4854.

2-Methylbutanoyl: [24817-51-4] *2-Phenylethyl 2-methylbutanoate. Phenethyl 2-methylbutyrate. FEMA 3632*
$C_{13}H_{18}O_2$ 206.284
Isol. from *Mentha cardiaca*, *Alpinia officinarum* (lesser galangal) and cider. Food flavouring ingredient. Liq. with

sweet, fruity taste.

3-Methylbutanoyl: [140-26-1] *2-Phenylethyl 3-methylbutanoate. Phenethyl isovalerate. FEMA 2871*
$C_{13}H_{18}O_2$ 206.284
Food flavour. Found in mint oils, alcoholic beverages and other sources. Liq. with peach-like taste. d^{15} 0.98. Bp 263°. n_D^{20} 1.4855.

Hexanoyl: [6290-37-5] *2-Phenylethyl hexanoate. Phenethyl caproate. FEMA 3221*
$C_{14}H_{20}O_2$ 220.311
Found in alcoholic drinks, fruit juices and other natural sources. Food flavour. Oil with fresh pineapple taste. d 0.98. Bp 263°.

Octanoyl: [5457-70-5] *2-Phenylethyl octanoate. Phenethyl caprylate. FEMA 3222*
$C_{16}H_{24}O_2$ 248.364
Found in wine and spirits. Oil with mild, fruity odour. d^{20} 0.947. $Bp_{1.5}$ 143.5°. n_D^{20} 1.4801.

3-Methyl-2-butenoyl: [42078-65-9] *2-Phenylethyl 3-methyl-2-butenoate. Phenethyl senecioate. FEMA 2869*
$C_{13}H_{16}O_2$ 204.268
Food flavour. Oil with fruity taste.

Benzoyl: [94-47-3] *2-Phenylethyl benzoate, 9CI. Phenethyl benzoate. FEMA 2860*
$C_{15}H_{14}O_2$ 226.274
Flavouring ingredient. Oil with a sweet, rose-honey odour. Bp_8 177-178°.

► DH6288000

2-Hydroxybenzoyl: [87-22-9] *Phenethyl salicylate. FEMA 2868*
$C_{15}H_{14}O_3$ 242.274
Used imitation fruit flavours. Mp 44°. Bp 370°.

Cinnamoyl: [103-53-7] *2-Phenylethyl 3-phenyl-2-propenoate. Phenethyl cinnamate. FEMA 2863*
$C_{17}H_{16}O_2$ 252.312
Food flavour. Isol. from the buds of *Populus balsamifera* (balsam poplar). Cryst. with sweet rose/plum taste. Mp 57-59°. Bp >300°.

Me ether: [3558-60-9] *(2-Methoxyethyl)-benzene, 9CI. 1-Methoxy-2-phenylethane. Methyl phenethyl ether. Kewda ether. FEMA 3198*
$C_9H_{12}O$ 136.193
Flavouring ingredient. Isol. from the famine food *Pandanus odoratissimus*. Fragrant liq. Bp 189-190° Bp_{25} 100-105°.

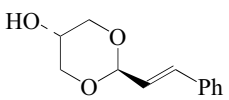
► KO2230000

[40356-59-0, 126199-49-3]

Registry of Mass Spectral Data, Wiley-Interscience, 187 (*ms*)
Reclaire, A. *et al., Chem. Zentralbl.*, 1924, **II**, 2616 (*esters*)
Leonard, C.S. *et al., J.A.C.S.*, 1925, **47**, 1774 (*synth*)
Burger, A.M. *et al., Chem. Zentralbl.*, 1926, **II**, 2124; 1928, **I**, 2466 (*esters*)
Albert, O. *et al., Z. Phys. Chem., Abt. A*, 1938, **182**, 421 (*cinnamoyl*)
Kland-English, M.J. *et al., J.A.C.S.*, 1953, **75**, 3709 (*uv*)
Adv. Chem. Ser., 1955, **15**, 349 (***props***)
Kaul, C.L. *et al., CA*, 1958, **52**, 20017a (*synth, Me ether*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 251 (*occur*)
Mel'nikov, V.N. *et al., Khim. Prir. Soedin.*, 1976, **11**, 807; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **11**, 822 (*glucoside*)
Bangov, I.P. *et al., Org. Magn. Reson.*, 1983, **21**, 443 (*cmr*)
Kitamura, T. *et al., Mol. Cryst. Liq. Cryst.*, 1985, **130**, 231 (*Ac*)
Umehara, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 5004 (*glycosides*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PDD750
Nishimura, H. *et al., Phytochemistry*, 1990, **29**, 3303 (*xylosylglucosides*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 340-341
Shu, C.-K. *et al., J. Agric. Food Chem.*, 1994, **42**, 1732-1733 (*α-glucoside, synth*)
Inagaki, J. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 738 (*primeveroside, rutinoside*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 545; 645-654 (*esters, Me ether*)
Mahmood, N. *et al., Biochem. Biophys. Res. Commun.*, 1996, **229**, 73-79 (*6-galloylglucoside*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1140
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1832-1833; 2152-2171 (*Me ether, esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IHV050; PFB250; PFC250; PFD325; PDD750; PFB750

2-(2-Phenylethenyl)-1,3-dioxan-5-ol, 9CI P-274

5-Hydroxy-2-styryl-1,3-dioxan. Cinnamaldehyde 1,3-glycerol acetal



(2RS,5RS)-form

$C_{12}H_{14}O_3$ 206.241

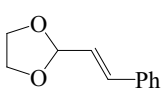
(2*RS*,5*RS*)-(*E*)-*form* [87562-73-0]
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Leaflets. Mp 106-109°.

(2*RS*,5*SR*)-(*E*)-*form* [87562-74-1]
Constit. of *Cinnamomum cassia* (Chinese cinnamon). Amorph. powder.

Miyamura, M. *et al., Phytochemistry*, 1983, **22**, 215-218

2-(Phenylethenyl)-1,3-dioxolane, 9CI P-275

[5660-60-6]
2-Styryl-1,3-dioxolane, 8CI. Cinnamaldehyde ethylene acetal. FEMA 2287. Cinncloval



(E)-form

$C_{11}H_{12}O_2$ 176.215

Protected form of cinnamaldehyde which liberates cinnamaldehyde flavour on oral contact. Used in products such as chewing gum.

(*E*)-*form* [83977-12-2]
trans-*form*
Needles (petrol). Mp 29.5-31°. $Bp_{0.1}$ 84°. n_D^{24} 1.5625.

Davis, H.A. *et al., Can. J. Chem.*, 1971, **49**, 2563-2577 (*synth*)
Eur. Pat., 1992, 466 450; *CA*, **116**, 172693 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 114 (*use, props*)
Lu, T.-J. *et al., J.O.C.*, 1995, **60**, 2931-2934 (*E-form, synth, pmr*)

2-Phenylethyl glucosinolate P-276

[499-30-9]
*1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)benzenepropanimidate], 9CI. **Gluconasturtiin**. Phenethyl glucosinolate. Gluconasturiin*

$PhCH_2CH_2C(SGlc)=NOSO_3H$

$C_{15}H_{21}NO_9S_2$ 423.464
Isol. from *Nasturtium officinale* (water cress), *Barbarea vulgaris* (winter cress) and other crucifers. Off-white cryst. (MeOH/EtOH) (as K salt). Mp 171° (K salt). $[\alpha]_D^{20}$ -20.7 (c, 1.0 in H_2O).

Tetra-Ac: [75347-10-3]
Needles (EtOH aq.) (as K salt). Mp 198-200° dec. (K salt). $[\alpha]_D^{24}$ -11 (c, 1 in 50% EtOH aq.).

[18425-76-8]

Benn, M.H. *et al., J.C.S.*, 1964, 4072 (*synth*)
Doernemann, D. *et al., Can. J. Biochem.*, 1974, **52**, 916 (*biosynth*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Gil, V. *et al., Tetrahedron*, 1980, **36**, 779 (*synth*)

2-Phenylethylamine P-277

[64-04-0]
Benzeneethanamine, 9CI. Phenethylamine, 8CI. β-Aminoethylbenzene. FEMA 3220

$PhCH_2CH_2NH_2$

$C_8H_{11}N$ 121.182
Present in cooked cabbage, cheeses, sherry, wine, processed lean fish, cocoa, raw cauliflower, raw beetroot and raw radish. Flavouring ingredient. Liq. with a fish odour. d_4^{24} 0.96. Bp 197-198° Bp_7 70-71°. n_D^{25} 1.5290. Absorbs CO_2 from air.

► Fl. p. 84°. Skin irritant and possible sensitiser. SG8750000

[1077-11-8, 6068-85-5, 62510-53-6, 75337-06-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1269D; 1270A; 1275D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 570C; 571A; 583C; 584A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1164C; 1166D (*ir*)
Sadtler Standard C-13 NMR Spectra, 68 (*cmr*)
Org. Synth., Coll. Vol., 3, 1955, 720 (*synth*)
Fitzgerald, J.S. *et al., Aust. J. Chem.*, 1964, **17**, 160 (*isol, pmr*)
Mosnaim, A. *et al., Clin. Chim. Acta*, 1973, **46**, 407 (*ir, ms*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*occur*)

Doetsch, P.W. *et al., J. Chromatogr.*, 1980, **189**, 79 (*occur*)
Purchase, C.F. *et al., J.O.C.*, 1991, **56**, 457 (*synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 648
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2155-2156
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PDE250; PDE500

N-2-Phenylethylcinnamamide P-278

[55030-23-4]
3-Phenyl-N-*(2-phenylethyl)-2-propenamide, 9CI*. N-*Cinnamoylphenethylamine*
PhCH=CHCONHCH$_2$CH$_2$Ph
$C_{17}H_{17}NO$ 251.327

(*E*)-*form* [103188-43-8]
Needles (cyclohexane). Mp 125-126°.

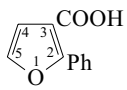
N-*Me:* [121817-38-7] ***Lansiumamide C***. N-*Methyl*-N-*phenylethylcinnamamide*
$C_{18}H_{19}NO$ 265.354
Alkaloid from seeds of *Clausena lansium* (wampee). Yellowish plates (Et_2O). Mp 58-59°.

2,3-Dihydro: [10264-31-0] *3-Phenyl*-N-*(2-phenylethyl)propanamide*
$C_{17}H_{19}NO$ 253.343
Cryst. Mp 94-96°.

Borges-del-Castillo, J. *et al., Phytochemistry*, 1984, **23**, 2671 (*isol, ir, pmr, cmr, ms, struct*)
Huneck, S. *et al., Fitoterapia*, 1986, **57**, 523 (*isol*)
Lin, J.H. *et al., Phytochemistry*, 1989, **28**, 621 (*Lansiumamide C*)
Maldonado, E. *et al., Phytochemistry*, 1992, **31**, 1413 (*3-Phenyl-N-(2-phenylethyl)propanamide*)
Riemer, B. *et al., Phytochemistry*, 1997, **45**, 337 (*isol, uv, ir, pmr*)
Stefanuti, I. *et al., Tet. Lett.*, 2000, **41**, 3735-3738 (*synth, Lansiumamide C*)

2-Phenyl-3-furancarboxylic acid, 9CI P-279

[57697-76-4]
2-Phenyl-3-furoic acid



$C_{11}H_8O_3$ 188.182
Cryst. (diisopropyl ether). Mp 186°.

Et ester: [50626-02-3] *FEMA 3468*
$C_{13}H_{12}O_3$ 216.236
Flavouring ingredient. Bp_6 148-154°.

Novak, J.J.K. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 2855 (*synth, pmr*)
Tius, M.A. *et al., Tet. Lett.*, 1985, **26**, 3635 (*synth*)
Jurášek, A. *et al., Coll. Czech. Chem. Comm.*, 1989, **54**, 215 (*synth, uv*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 662 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2190 (*Et ester*)

1-Phenyl-1,3-heneicosanedione P-280

1-Benzoyl-2-eicosanone
$H_3C(CH_2)_{17}COCH_2COPh$
$C_{27}H_{44}O_2$ 400.643
Constit. of the pollen of *Helianthus annuus* (sunflower).

3-Alcohol:3-Hydroxy-1-phenyl-1-heneicosanone. 1-Benzoyl-2-eicosanol
$C_{27}H_{46}O_2$ 402.659
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Phenyl-1,3-heptadecanedione P-281

1-Benzoyl-2-hexadecanone
$H_3C(CH_2)_{13}COCH_2COPh$
$C_{23}H_{36}O_2$ 344.536
Constit. of the pollen of *Helianthus annuus* (sunflower).

3-Alcohol:3-Hydroxy-1-phenyl-1-heptadecanone. 1-Benzoyl-2-hexadecanol
$C_{23}H_{38}O_2$ 346.552
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Phenyl-1,3-hexadecanedione P-282

1-Benzoyl-2-pentadecanone
$H_2C(CH_2)_{12}COCH_2COPh$
$C_{22}H_{34}O_2$ 330.509
Constit. of the pollen of *Helianthus annuus* (sunflower).

1-Alcohol:1-Hydroxy-1-phenyl-3-hexadecanone
$C_{22}H_{36}O_2$ 332.525
Constit. of the pollen of *Helianthus annuus* (sunflower).

3-Alcohol:3-Hydroxy-1-phenyl-1-hexadecanone. 1-Benzoyl-2-pentadecanol
$C_{22}H_{36}O_2$ 332.525
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

6-Phenyl-3,5-hexadien-2-one, 9CI P-283

[4173-44-8]
Cinnamylideneacetone
PhCH=CHCH=CHCOCH$_3$
$C_{12}H_{12}O$ 172.226
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002).

(3*E*,5*E*)-*form* [29179-13-3]
Leaflets (Et_2O). Mp 68° (66°).

Oxime: [56672-25-4]
$C_{12}H_{13}NO$ 187.241
Needles. Mp 153°.

Semicarbazone:
Mp 193-195°.

Phenylhydrazone:
Mp 180°.

[29246-55-7]

Jossang, P. *et al., J. Chromatogr.*, 1967, **31**, 375 (*isol*)
Leraux, Y. *et al., Ann. Chim. (Paris)*, 1968, **3**, 133 (*synth*)
Kluge, A.F. *et al., J.O.C.*, 1971, **36**, 1977 (*uv, ir, pmr, conformn*)
Alper, H. *et al., Tet. Lett.*, 1979, 2665 (*synth*)
Font, J. *et al., Tetrahedron*, 1981, **37**, 2391 (*synth*)
Shi, L. *et al., Tet. Lett.*, 1987, **28**, 2155 (*synth*)
Ogima, M. *et al., Chem. Lett.*, 1989, 1959 (*synth*)
Huang, Y.Z. *et al., Synth. Commun.*, 1989, **19**, 501 (*synth*)
Moriarty, R.M. *et al., J.A.C.S.*, 1991, **113**, 6315 (*synth*)

1-Phenyl-2,4-hexadiyne P-284

[520-74-1]
2,4-Hexadiynylbenzene, 9CI. ***Capillene***. *Agropyrene. Capilline*
PhCH$_2$C≡CC≡CCH$_3$
$C_{12}H_{10}$ 154.211
Isol. from oil of *Artemisia dracunculus* (tarragon). Oil. d_0^{22} 0.98. Fp 0. Bp_1 101-103°. n_D^{22} 1.5810. Log P 3.47 (calc).

Harada, R. *et al., Nippon Kagaku Kaishi*, 1957, **78**, 415; 1031; *CA*, **54**, 347 (*struct, synth*)
Cymerman-Craig, J. *et al., Chem. Ind. (London)*, 1959, 952
Bohlmann, F. *et al., Chem. Ber.*, 1962, **95**, 39 (*isol*)
Yano, K. *et al., Phytochemistry*, 1994, **37**, 689 (*isol*)

1-Phenyl-2,4-hexadiyn-1-one, 9CI P-285

[495-74-9]
2,4-Hexadiynophenone, 8CI. 1-Benzoyl-1,3-pentadiyne. ***Capillin***
PhCOC≡CC≡CCH$_3$
$C_{12}H_8O$ 168.195
Constit. of essential oil from *Artemisia dracunculus* (tarragon). Pale cream needles (hexane). Mp 82-83°. Log P 2.48 (calc).

▶ MM3622000

2,4-Dinitrophenylhydrazone:
Orange needles (EtOH). Mp 225° dec. (214°).

2′-Methoxy: [209972-80-5] *1-(2-Methoxyphenyl)-2,4-hexadiyn-1-one*. ***Capillaridin E***
$C_{13}H_{10}O_2$ 198.221
Yellow oil. λ_{max} 269 (sh) ; 280 ; 294 (sh) ; 337 (MeOH).

Bohlmann, F. *et al., Chem. Ber.*, 1963, **96**, 226; 1964, **97**, 1179; 1966, **99**, 995 (*isol, biosynth*)
Reisch, J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1964, **297**, 628 (*synth*)
Nash, B.W. *et al., J.C.S.*, 1965, 2983 (*synth, bibl*)
Hearn, M.T.W. *et al., J. Magn. Reson.*, 1975, **19**, 401 (*cmr*)
De Pascual, T.J. *et al., CA*, 1982, **96**, 109953 (*isol*)
Jones, G.E. *et al., Tet. Lett.*, 1982, **23**, 3203 (*synth, bibl*)
Wu, T.-S. *et al., Phytochemistry*, 1998, **47**, 1645-1648 (*Capillaridin E*)

6-Phenyl-3-hexen-2-one, 9CI P-286

[33046-41-2]
$H_3CCOCH=CHCH_2CH_2Ph$
$C_{12}H_{14}O$ 174.242

Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Oil. Bp_{19} 153° $Bp_{0.2}$ 100°.

Semicarbazone:
Mp 139°.

(E)-form [56161-62-7]
$Bp_{0.5}$ 98-100°.

Cornubert, R. *et al., Bull. Soc. Chim. Fr.*, 1954, 531 (*synth*)
Liedtke, R.J. *et al., J.O.C.*, 1972, **37**, 776 (*ms*)
Reich, H.J. *et al., J.O.C.*, 1975, **40**, 2570 (*synth*)
Kondo, K. *et al., Tet. Lett.*, 1975, 1007
Sato, A. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1509 (*synth, pmr*)
Lidgard, R.O. *et al., Biomed. Environ. Mass Spectrom.*, 1986, **13**, 305; 1988, **17**, 371 (*occur*)
Fischer, H. *et al., Chem. Ber.*, 1990, **123**, 399 (*synth*)
Barton, D.H.R. *et al., Tet. Lett.*, 1990, **31**, 1965 (*synth*)

Phenylmethanethiol P-287

[100-53-8]
Benzenemethanethiol, 9CI. α-Toluenethiol, 8CI. Benzyl mercaptan. Thiobenzyl alcohol. Benzyl thiol. (Mercaptomethyl)benzene. (Thiomethyl)benzene. FEMA 2147

$PhCH_2SH$

C_7H_8S 124.206
Flavouring agent. Liq. with a repulsive, garlic-like odour. d^{20} 1.06. Bp 194-195°. n_D^{20} 1.5748. pK_{a1} 9.43 (25°).

▶ Fl. p. 70°. Eye irritant. LD_{50} (rat, orl) 493 mg/kg. XT8650000

S-*Me:* Benzyl methyl sulfide, B-51

S-*Et:* [6263-62-3] *[(Ethylthio)methyl]benzene. Benzyl ethyl sulfide*
$C_9H_{12}S$ 152.26
Bp 214-216°.

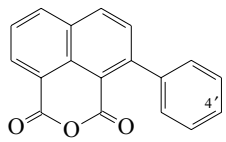
S-*Et,* S,S-*dioxide:* [772-47-4] *Benzyl ethyl sulfone*
$C_9H_{12}O_2S$ 184.259
Cryst. Mp 83°.

[3492-64-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1173C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 415C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1089C (*ir*)
Sadtler Standard C-13 NMR Spectra, 1022 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 1822 (*uv*)
Tatematsu, A. *et al., Tet. Lett.*, 1966, 4609 (*ms*)
Bittel, J.E. *et al., J.O.C.*, 1978, **43**, 1687 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 62
Choi, J. *et al., Synthesis*, 1995, 373 (*synth, ir, pmr, ms*)
Bandaranayake, W.M. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1996, **113**, 499 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 272
Aitken, R.A. *et al., Synthesis*, 1997, 787-791 (*benzyl ethyl sulfone*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGO750

4-Phenyl-1*H*,3*H*-naphtho[1,8-*cd*]pyran-1,3-dione, 9CI P-288

[56252-04-1]
2-Phenylnaphthalic anhydride



$C_{18}H_{10}O_3$ 274.275
Constit. of banana (*Musa acuminata*). Fine needles (Me_2CO/petrol). Mp 241-243°. λ_{max} 240 (log ε 5.9); 339 (log ε 1.8) (MeOH).

4′-Hydroxy: [158922-28-2] *2-(4-Hydroxyphenyl)naphthalic anhydride*
$C_{18}H_{10}O_4$ 290.275
Isol. from the unripe banana fruit (*Musa acuminata*) infected with *Colletotrichum musae*. Yellow needles. Mp 278-281°.

*4′-Hydroxy, 1-alcohol:3-Hydroxy-9-(4-hydroxyphenyl)-1*H,*3*H-*naphtho[1,8-cd]pyran-1-one*
$C_{18}H_{12}O_4$ 292.29
Isol. from *Musa acuminata* infected with *Colletotrichum musae*. Powder. Racemic λ_{max} 227 (ε 19000); 245 (ε 14000); 290 (ε 5300); 303 (ε 4700); 332 (ε 4100) (MeOH).

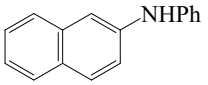
*4′-Hydroxy, 3-alcohol:3-Hydroxy-4-(4-hydroxyphenyl)-1*H,*3*H-*naphtho[1,8-cd]pyran-1-one*
$C_{18}H_{12}O_4$ 292.29
Isol. from *Musa acuminata* infected with *Colletotrichum musae*. Powder. Racemic λ_{max} 228 (ε 17000); 245 (ε 11000); 274 (ε 6700); 308 (ε 3300); 319 (ε 3400); 340 (ε 2800) (MeOH).

4′-Methoxy:2-(4-Methoxyphenyl)naphthalic anhydride
$C_{19}H_{12}O_4$ 304.301
Isol. from the unripe banana fruit (*Musa acuminata*) infected with *Colletotrichum musae*. λ_{max} 237 ; 317 ; 339 ; 377 (MeOH).

Cook, R.G. *et al., Aust. J. Chem.*, 1975, **28**, 1053 (*isol, synth*)
Hirai, N. *et al., Phytochemistry*, 1994, **37**, 383 (*isol, deriv*)
Kamo, T. *et al., Phytochemistry*, 1998, **49**, 1617-1621 (*isol, uv, ir, pmr, ms*)
Takikawa, H. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1834-1836 (*synth*)
Kamo, T. *et al., Tetrahedron*, 2001, **57**, 7649-7656 (*derivs, isol*)

N-Phenyl-2-naphthylamine P-289

[135-88-6]
2-Anilinonaphthalene. Antioxidant 116. Antioxidant D. Antioxidant PBN



$C_{16}H_{13}N$ 219.285
Constit. of *Daucus carota* (carrot). Needles (MeOH). Mod. sol. EtOH, Et_2O, AcOH, C_6H_6. Mp 108° (103-104°). Bp 395-399.5° Bp_{13} 237°. Solns. show blue fluor. Natural occurrence appears doubtful. Probable contaminant.

▶ Exp. carcinogenic data. LD_{50} (rat, orl) 8730 mg/kg. QM4550000

N-*Ac:* [74495-79-7] N-*2-Naphthalenyl*-N-*phenylacetamide, 9CI*
$C_{18}H_{15}NO$ 261.323
Cryst. (Et_2O). Sol. EtOH, Et_2O, AcOH, C_6H_6. Mp 93°.

N-*Benzoyl:*
$C_{23}H_{17}NO$ 323.393
Needles (EtOH). Sol. C_6H_6, spar. sol. EtOH. Mp 147-148° (136°).

N-*Me:* [6364-05-2]
$C_{17}H_{15}N$ 233.312
Mp 52-53°.

N-*Et:*
$C_{18}H_{17}N$ 247.339
Leaflets. Mp 58°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 553A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1159D (*ir*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 748F (*ir*)
Aldrich Library of NMR Spectra, **5**, 88D (*pmr*)
Sadtler Standard C-13 NMR Spectra, 4804 (*cmr*)
Streiff, J. *et al., Annalen*, 1881, **209**, 151 (*synth, N-Ac, N-benzoyl*)
Knoevenagel, E. *et al., J. Prakt. Chem.*, 1914, **89**, 1 (*synth*)
Gershzon, G.I. *et al., CA*, 1944, **38**, 1479 (*synth*)
Salimov, M.A. *et al., Dokl. Akad. Nauk SSSR*, 1957, **112**, 890 (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 846
IARC Monog., 1978, **16**, 325; *Suppl.* 7, 318; *Suppl.* 6, 461 (*rev, tox*)
Riepe, W. *et al., Org. Mass Spectrom.*, 1978, **13**, 57 (*ms*)
Mallabaev, A. *et al., Khim. Prir. Soedin.*, 1982, **18**, 123 (*isol*)
Sultankhodzhaev, M.N. *et al., Khim. Prir. Soedin.*, 1982, **18**, 660 (*isol*)
Papanov, G.Y. *et al., Phytochemistry*, 1985, **24**, 3045-3046 (*isol, synth, pmr, cmr, ms*)
Li, Y. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 302-304 (*isol, pmr, cmr, cryst struct*)
Likhitwitayawuid, K. *et al., Planta Med.*, 2000, **66**, 275-276 (*isol, pmr, cmr, ms*)
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 473
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1006
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PFT500

1-Phenyl-1,3-nonadecanedione P-290

1-Benzoyl-2-octadecanone
$H_3C(CH_2)_{15}COCH_2COPh$

$C_{25}H_{40}O_2$ 372.59
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Phenyl-1,3-octadecanedione P-291

1-Benzoyl-2-heptadecanone
$H_3C(CH_2)_{14}COCH_2COPh$

$C_{24}H_{38}O_2$ 358.563

Constit. of the pollen of *Helianthus annuus* (sunflower).

1-Alcohol:1-Hydroxy-1-phenyl-3-octadecanone
$C_{24}H_{40}O_2$ 360.579
Constit. of the pollen of *Helianthus annuus* (sunflower).

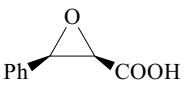
3-Alcohol:3-Hydroxy-1-phenyl-1-octadecanone. 1-Benzoyl-2-heptadecanol
$C_{24}H_{40}O_2$ 360.579
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

3-Phenyloxiranecarboxylic acid, 9CI P-292

[5694-02-0]

[121-39-1]
2,3-Epoxy-3-phenylpropanoic acid. β-Phenylglycidic acid



(2*R*,3*R*)-*form*

$C_9H_8O_3$ 164.16

(2*R*,3*R*)-*form* [99528-64-0]

Me ester: [99528-65-1]
$C_{10}H_{10}O_3$ 178.187
$[\alpha]_D^{25}$ +11 (c, 4.4 in $CHCl_3$).

(2*R*,3*S*)-*form* [79898-19-4] *(-)*-trans-*form*
$[\alpha]_D^{25}$ -154 (c, 1.03 in H_2O) (as NH_4 salt).

(2*S*,3*R*)-*form* [79898-17-2] *(+)*-trans-*form*
$[\alpha]_D^{25}$ +153.5 (c, 1.1 in H_2O) (as NH_4 salt).

(2*S*,3*S*)-*form* [54323-79-4]
Mp 203-204° dec. (as K salt). $[\alpha]_D^{25}$ +4.4 (c, 0.98 in H_2O). CAS no. refers to K salt.

(2*RS*,3*RS*)-*form* [54265-93-9] *(±)*-trans-*form*
Mp 82-83°.

(2*RS*,3*SR*)-*form* [54265-95-1] *(±)*-cis-*form*
Prisms. Mp 83-84°. $Bp_{4.5}$ 128-130° (lit. gives a pressure range).

Et ester: [54276-44-7]

[121-39-1] *Ethyl phenylglycidate. Aldehyde C_{16} special (misleading). FEMA 2454*
$C_{11}H_{12}O_3$ 192.214
Flavouring ingredient. Liq. with strawberry odour. Bp_{18} 162-164°. The coml. prod. is likely to be a mixt. of stereoisomers.

Anilide:
$C_{15}H_{13}NO_2$ 239.273
Needles (EtOH). Mp 142°.

(2ξ,3ξ)-*form*

Methylamide: [189315-54-6] N-*Methyl-3-phenyloxiranecarboxamide, 9CI.* ***Clausamide II***
$C_{10}H_{11}NO_2$ 177.202

N-*Methyl*-N-*(2-phenylethenyl)amide:* [189315-53-5]

[183812-57-9, 183812-58-0] ***Clausamide I***
$C_{18}H_{17}NO_2$ 279.338

[1566-68-3, 73610-79-4]

Darzens, G. *et al., C. R. Hebd. Seances Acad. Sci.*, 1937, **204**, 272 (*synth*)
Harada, K. *et al., J.O.C.*, 1966, **31**, 1407 (*synth, abs config, trans-form*)
Harada, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 2911 (*synth, abs config, cis-form*)
Edwards, J.O. *et al., Photochem. Photobiol.*, 1979, **30**, 63 (*synth, pmr, racemates*)
Denis, J.-N. *et al., J.O.C.*, 1986, **51**, 46 (*synth, ir, pmr*)
Thijs, L. *et al., Tetrahedron*, 1990, **46**, 2611 (*resoln*)
Takahashi, T. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1821 (*synth, abs config*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 264 (*Et ester*)
Li, S.H. *et al., Chin. Pharm. J. (Taipei)*, 1996, **48**, 367-373 (*Clausamides*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1034-1035 (*Et ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EOK600

1-Phenyl-1,3-pentadecanedione P-293

1-Benzoyl-2-tetradecanone
$H_3C(CH_2)_{11}COCH_2COPh$
$C_{21}H_{32}O_2$ 316.483
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

5-Phenyl-1,3-pentadiyne P-294

[41268-41-1]
2,4-Pentadiynylbenzene, 9CI. Benzyldiacetylene
$PhCH_2C{\equiv}CC{\equiv}CH$
$C_{11}H_8$ 140.184
Isol. from roots of *Artemisia dracunculus* (tarragon). Oil. $Bp_{0.001}$ 45-50°. n_D^{22} 1.5726.

Bohlmann, F. *et al., Chem. Ber.*, 1962, **95**, 39; 1963, **96**, 226 (*isol, uv, ir, struct*)
Klein, J. *et al., J.C.S. Perkin 2*, 1973, 599 (*nmr*)
Harada, R. *et al., Phytochemistry*, 1982, **21**, 2009 (*isol, ir, uv, nmr*)

1-Phenyl-2,4-pentadiyn-1-one, 9CI P-295

[29743-36-0]
Benzoylbutadiyne. Demethylcapillone. Desmethylcapillone
$PhCOC{\equiv}CC{\equiv}CH$
$C_{11}H_6O$ 154.168
Isol. from *Chrysanthemum coronarium* (chop-suey greens). Cryst. (petrol). Mp 106°.

Bohlmann, F. *et al., Chem. Ber.*, 1963, **96**, 226; 1964, **97**, 1179 (*isol, uv, ir, synth*)
Walton, D.R.M. *et al., J. Organomet. Chem.*, 1972, **37**, 45 (*synth*)

1-Phenyl-2-pentanol P-296

[705-73-7]
α-Propylbenzeneethanol, 9CI. Benzylpropylcarbinol. α-Propylphenethyl alcohol. FEMA 2953
$H_3CCH_2CH_2CH(OH)CH_2Ph$
$C_{11}H_{16}O$ 164.247
Bp 247°.

(±)-*form*

Flavouring agent. Bp 247° Bp_{15} 127°.

Phenylurethane:
Needles (petrol). Mp 80°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1153D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 387B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1075C (*ir*)
Roblin, R.O. *et al., J.A.C.S.*, 1935, **57**, 151 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 705
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2370-2371

5-Phenyl-1-pentanol P-297

[10521-91-2]
Benzenepentanol, 9CI. FEMA 3618
$Ph(CH_2)_4CH_2OH$
$C_{11}H_{16}O$ 164.247
Flavouring ingredient. Liq. with a floral odour. d^{20} 0.98. Bp_{20} 155°. n_D^{20} 1.5156.

Ac: [75553-28-5]
$C_{13}H_{18}O_2$ 206.284
Bp_{12} 155°.

Ph ether:1-Phenoxy-5-phenylpentane
$C_{17}H_{20}O$ 240.344
Viscous liq. Bp_{14} 198°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1156C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 391C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1078A (*ir*)
Roblin, R.O. *et al., J.A.C.S.*, 1935, **57**, 151 (*synth*)
Hornfeldt, A.B. *et al., Ark. Kemi*, 1963, **21**, 239; *CA*, **59**, 13917 (*synth*)
Hubert, A.J. *et al., J.C.S.(C)*, 1967, 235 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 666
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2192-2193

1-Phenyl-1-pentanone, 9CI P-298

[1009-14-9]
Valerophenone, 8CI. n-*Butyl phenyl ketone. 1-Benzoylbutane*
$PhCOCH_2CH_2CH_2CH_3$
$C_{11}H_{14}O$ 162.231
Found in celery. Liq. Bp_{25} 135-140°.

Oxime: [69060-55-5]
$C_{11}H_{15}NO$ 177.246
Needles (EtOH aq. or petrol). Sol. EtOH, C_6H_6, spar. sol. petrol. Mp 52-52.5°. Bp_{13} 163-165°.

Semicarbazone:2-(1-Phenylpentylidene)-hydrazinecarboxamide
Needles (EtOH). Mp 166° (157-157.5°).

2,4-Dinitrophenylhydrazone:
Orange-red cryst. (EtOH). Mp 123-124° (166°).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 803B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 9C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1229C (*ir*)
Pfeiffer, P. *et al., J. Prakt. Chem.*, 1924, **108**, 341 (*oxime*)

Shriner, R.L. *et al., J.A.C.S.*, 1930, **52**, 1267 (*synth*)
Milstein, D. *et al., J.A.C.S.*, 1978, **100**, 3636 (*synth*)
Yamashita, M. *et al., Tet. Lett.*, 1978, 761 (*synth*)

2-Phenyl-4-pentenal P-299

[24401-36-3]
α-2-Propenylbenzeneacetaldehyde, 9CI. FEMA 3519
$H_2C{=}CHCH_2CHPhCHO$
$C_{11}H_{12}O$ 160.215

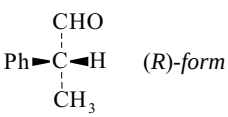
(±)-*form*
Flavouring ingredient. Oil. $Bp_{0.35}$ 77-78° (lit. gives a pressure range) $Bp_{0.7}$ 57°.
4-Methylbenzenesulfonylhydrazone: Cryst. Mp 109-111°.
2,4-Dinitrophenylhydrazone: Cryst. Mp 106°.
Elhik, E. *et al., Bull. Soc. Chim. Fr.*, 1969, 903 (*synth, ir, uv, pmr*)
Corey, E.J. *et al., J.A.C.S.*, 1970, **92**, 5522 (*synth*)
Takahashi, K. *et al., Tetrahedron*, 1988, **44**, 4737 (*synth, pmr*)
Bloodworth, A.J. *et al., J.C.S. Perkin 1*, 1990, 2951 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 665
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2193

3-Phenyl-4-pentenal, 9CI P-300

[939-21-9]
3-Phenyl-3-vinylpropionaldehyde. FEMA 3318
$H_2C{=}CHCHPhCH_2CHO$
$C_{11}H_{12}O$ 160.215
Flavouring ingredient. Liq. with cocoa odour. Bp_{25} 120-121°.
2,4-Dinitrophenylhydrazone: Yellow plates (EtOH). Mp 105-107°.
Di-Me acetal:5,5-Dimethoxy-3-phenyl-1-pentene
$C_{13}H_{18}O_2$ 206.284
Oil. $Bp_{0.5}$ 72-73°.
Burgstahler, A.W. *et al., J.C.S.*, 1963, 4986-4989 (*synth*)
Schreiber, W.L. *et al., J. Agric. Food Chem.*, 1974, **22**, 269-273 (*acetal*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1472-1473 (*use, props*)

2-Phenylpropanal P-301

[93-53-8]
α-Methylbenzeneacetaldehyde, 9CI. Hydratropaldehyde, 8CI. Hydratropic aldehyde. 2-Phenylpropionaldehyde. FEMA 2886



(R)-form

$C_9H_{10}O$ 134.177
Found in various mushrooms.
► LD_{50} (rat, orl) 2800 mg/kg. CY1460000

(*R*)-*form* [38235-74-4]
Liq. Bp_5 85°. $[\alpha]_D^{25}$ -238 (neat) (100% op). $[\alpha]_D^{20}$ -288.3 (c, 0.5 in C_6H_6) (91% ee).

(*S*)-*form* [33530-47-1]
Liq. Bp_5 85°. $[\alpha]_D^{20}$ +314.6 (c, 0.45 in C_6H_6) (99.4% ee).

Di-Me acetal: [103593-60-8] *(2,2-Dimethoxy-1-methylethyl)benzene, 9CI. 1,1-Dimethoxy-2-phenylpropane*
$C_{11}H_{16}O_2$ 180.246
Oil. $[\alpha]_D^{22}$ +3.3 (c, 1.01 in $CHCl_3$).

(±)-*form* [34713-70-7]
Flavour ingredient. Liq. with sweet pungent taste apricot-like taste. Bp 202-205° Bp_{12} 92-92.5°. n_D^{20} 1.5170.
Oxime: [54667-62-8]
$C_9H_{11}NO$ 149.192
Oil. Bp_7 124°.
2,4-Dinitrophenylhydrazone: [5530-36-9] Mp 136-137°.
Semicarbazone: [1567-36-8] Plates (EtOH). Mp 153-154°.
Di-Me acetal: [130605-86-6] *1,1-Dimethoxy-2-phenylpropane. FEMA 2888* Flavouring agent. Oil with mushroom-like odour and taste. Bp 240-241° $Bp_{3.2}$ 82-83.2°.
Di-Et acetal: [130605-87-7] *1,1-Diethoxy-2-phenylpropane*
$C_{13}H_{20}O_2$ 208.3
Oil. Bp_3 92-93°.

[90-87-9, 59647-78-8]
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 925C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 101C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 998C; 1279D (*ir*)
Org. Synth., Coll. Vol., 3, 1955, 733 (*synth*)
Botteghi, C. *et al., Annalen*, 1974, 864 (*synth*)
Cornils, B. *et al., Chem.-Ztg.*, 1974, **98**, 596 (*rev*)
Fetizon, M. *et al., Org. Mass Spectrom.*, 1974, **8**, 201 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 548 (*rev, tox*)
Matsushita, H. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 201 (*synth*)
Zushi, S. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 3631 (*cmr, pmr, conformn*)
Enders, D. *et al., Chem. Comm.*, 1984, 1221 (*resoln*)
Maruoka, K. *et al., Synthesis*, 1986, 130 (*synth*)
Org. Synth., Coll. Vol., 6, 1988, 905; 1028 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, COF000
Jones, D.M. *et al., J.O.C.*, 1993, **58**, 2286 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COF000; HII600

3-Phenylpropanal P-302

[104-53-0]
Benzenepropanal, 9CI. Hydrocinnamaldehyde. 3-Phenylpropionaldehyde. FEMA 2887
$PhCH_2CH_2CHO$
$C_9H_{10}O$ 134.177
Present in cinnamon, tomato, gruyere de comte cheese, beer, cooked trassi, origanum (Spanish) and strawberry. Flavour ingredient. Liq. with hyacinth odour and green, warm flavour. d_4^{15} 1.02. Bp 221-224° Bp_{13} 104-105°. n_D^{20} 1.5230.
► Skin irritant. MW4890000
Oxime: [1197-50-8]
$C_9H_{11}NO$ 149.192
Prisms (EtOH). Mp 93-94.5°.
2,4-Dinitrophenylhydrazone: [1237-68-9] Yellow solid. Mp 151-151.5° (146-148°).
Semicarbazone: [27843-08-9] Plates or needles (EtOH aq.). Mp 127°.
Di-Me acetal: [30076-98-3] *(3,3-Dimethoxypropyl)benzene, 9CI. 1,1-Dimethoxy-3-phenylpropane*
$C_{11}H_{16}O_2$ 180.246
Liq. Bp 240° Bp_{15} 114°.
Di-Et acetal: [6956-37-2] *(3,3-Diethoxypropyl)benzene, 9CI. 1,1-Diethoxy-3-phenylpropane*
$C_{13}H_{20}O_2$ 208.3
Liq. $Bp_{2.7}$ 103-104°.
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 925B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 101B (*ir*)
Sadtler Standard C-13 NMR Spectra, 2211 (*cmr*)
Sadtler Standard Proton NMR Spectra, 17199 (*pmr*)
Heck, R.F. *et al., J.A.C.S.*, 1968, **90**, 5526 (*synth*)
Org. Synth., 1971, **51**, 17; 31 (*synth*)
Cornils, B. *et al., Chem.-Ztg.*, 1974, **98**, 596 (*rev*)
Mizoroki, T. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 2148 (*synth*)
Nibbering, N.M.M. *et al., J.A.C.S.*, 1978, **100**, 541 (*ms*)
Hanna, P.E. *et al., J. Med. Chem.*, 1982, **25**, 1189 (*synth, oxime*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HHP000
Curran, D.P. *et al., Synthesis*, 1992, 123 (*synth, 2,4-DNP, pmr, ir*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HHP000

1-Phenyl-1,2-propanedione, 8CI P-303

[579-07-7]
Methyl phenyl diketone. Acetylbenzoyl. FEMA 3226
$Ph^{\alpha}CO^{\beta}COCH_3$
$C_9H_8O_2$ 148.161
Present in coffee aroma. Flavouring ingredient. Yellow oil with a pungent odour. V. spar. sol. H_2O. d_4^{20} 1.01. Bp 222° Bp_{12} 102°. Steam-volatile.
► Highly flammable, fl. p. < 21°.
α-Oxime: [25355-34-4] *α-Isonitroso-α-phenylacetone. Phenyl acetyl ketoxime*
$C_9H_9NO_2$ 163.176
Yellow needles (AcOH). Mp 166-167°.
α-Oxime, Ac:
$C_{11}H_{11}NO_3$ 205.213
Leaflets (EtOH aq.). Mp 61-62°.
β-Oxime: [119-51-7] *α-Isonitrosopropiophenone. Methyl benzoyl ketoxime*
$C_9H_9NO_2$ 163.176
Needles (H_2O). Mp 114-115°.
► LD_{50} (rat, orl) 4240 mg/kg. UH2975000
Dioxime: [4937-86-4] *Methyl phenyl glyoxime*
$C_9H_{10}N_2O_2$ 178.19

Needles (EtOH aq.). Mp 238-240°.

Disemicarbazone: [30911-80-9]
Mp 229-232°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 53B; 924D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 876B; **3**, 491C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1264C (*ir*)
Org. Synth., Coll. Vol., 3, 1955, 20 (*synth*)
Bestmann, H.-J. *et al., Chem. Ber.*, 1969, **102**, 2259 (*synth*)
U.S. Pat., 1978, 4 107 210; *CA*, **90**, 87047 (*synth*)
Davis, F.A. *et al., J.O.C.*, 1990, **55**, 360 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 666
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2194-2195
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ILI000; PGA500

3-Phenylpropanoic acid P-304

[501-52-0]
Benzenepropanoic acid, 9CI. Benzylacetic acid. Hydrocinnamic acid. Homotoluic acid. Dihydrocinnamic acid

$PhCH_2CH_2COOH$

$C_9H_{10}O_2$ 150.177
Prisms (petrol). V. spar. sol. H_2O. Mp 48.5°. Bp 280° Bp_6 125-129°. pK_a 4.66 (H_2O). Steam-volatile.

► LD_{50} (mus, ivn) 3000-5000 mg/kg. DA8600000

Me ester: [103-25-3] *FEMA 2741*
$C_{10}H_{12}O_2$ 164.204
Flavouring ingredient. Liq. with a strong floral-fruity odour. Bp 238-239°.

Et ester: [2021-28-5] *FEMA 2455*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient. Liq. with a floral odour. d^{20} 1.015. Bp 247-248°. n_D^{20} 1.4940.

Chloride: [645-45-4]
C_9H_9ClO 168.622
Bp_{10} 105°.

Amide: [102-93-2]
$C_9H_{11}NO$ 149.192
Needles (H_2O). Mp 105°.

► MW4905500

Hydrazide: [3538-68-9]
$C_9H_{12}N_2O$ 164.207
Mp 103°.

Nitrile: [645-59-0] *Benzenepropanenitrile. Hydrocinnamonitrile. 1-Cyano-2-phenylethane*
C_9H_9N 131.177
Constit. of *Brassica napus* (rape seed) and *Nasturtium officinale* (water cress). Bp 261° Bp_{18} 114-118°.

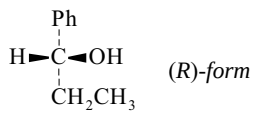
► LD_{50} (mus, orl) 116 mg/kg. MW5604750

Anhydride: [15781-96-1]
$C_{18}H_{18}O_3$ 282.338
Bp_{14} 216-217°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 139C; 337B; 424C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 985A; 1214C; 1331B; 1481A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1348A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 311 (*synth*)
Schwenk, E. *et al., J.O.C.*, 1946, **11**, 798 (*synth*)
Walter, M. *et al., Helv. Chim. Acta*, 1961, **44**, 1546 (*synth*)
Oki, M. *et al., Bull. Chem. Soc. Jpn.*, 1962, **35**, 283 (*ir*)
Bestmann, H.J. *et al., Chem. Ber.*, 1962, **95**, 2921 (*synth*)
Berenfeld, V.M. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1965, **162**, 1300 (*uv*)
Grimmer, G. *et al., Biochem. Z.*, 1966, **346**, 186 (*isol*)
Fritig, B. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1966, **263**, 860 (*isol*)
Bakke, J.M. *et al., J. Chem. Ecol.*, 1983, **9**, 513
Gould, S.J. *et al., J. Nat. Prod.*, 1993, **56**, 1239-1245 (*nitrile, isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 264; 552 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1035-1036; 1842 (*esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HHP100

1-Phenyl-1-propanol P-305

[93-54-9]
α-Ethylbenzenemethanol, 9CI. Ethylphenylcarbinol. α-Hydroxypropylbenzene. α-Ethylbenzyl alcohol. Ejibil. Felicur. Livonal. Phenycholon. FEMA 2884. SH 261. Other proprietary names



(*R*)-*form*

$C_9H_{12}O$ 136.193

► LD_{50} (rat, orl) 1600 mg/kg. DO5470000

(*R*)-*form* [1565-74-8]
Bp_{10} 98.5°. $[\alpha]_D^{22}$ +28.1 (neat). $[\alpha]_D^{20}$ +47 (c, 5 in $CHCl_3$) (98% ee).

(*S*)-*form* [613-87-6]
Bp_{10} 94-95°. $[\alpha]_D^{20}$ -27.73 (neat). $[\alpha]_D^{25}$ -48.5 (c, 1.2 in $CHCl_3$).

(±)-*form* [613-86-5]
Flavouring ingredient. Oil with a balsamic, floral fragrance and a sweet honey-like taste. Insol. H_2O; sol. EtOH. d_0^{23} 0.99. Bp 217-221° Bp_{11} 100-101°. n_D^{20} 1.5204.

Ac: [2114-29-6]
$C_{11}H_{14}O_2$ 178.23
Bp 227-228°.

Butanoyl: [10031-86-4] *1-Phenylpropyl butyrate. α-Ethylbenzyl butyrate. FEMA 2424*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. Liq. with sweet, plum-like taste.

4-Nitrobenzoyl:
Mp 59-60°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1123B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 330A; 330B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1048B; 1048C; 1048D (*ir*)
MacLeod, R. *et al., J.A.C.S.*, 1960, **82**, 876 (*abs config*)
Linet, O. *et al., Arzneim.-Forsch.*, 1962, **12**, 347-352 (*pharmacol*)
Landor, S.R. *et al., J.C.S.(C)*, 1966, 2280 (*synth*)
Cervinka, O. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 441 (*synth*)
Kuchar, M. *et al., Coll. Czech. Chem. Comm.*, 1976, **41**, 633 (*synth*)
Vigneron, J.P. *et al., Tetrahedron*, 1976, **32**, 939 (*synth*)
Yamaguchi, S. *et al., Tetrahedron*, 1976, **32**, 1363 (*synth*)
Krishnamurthy, S. *et al., J.O.C.*, 1977, **42**, 2534 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 219; **2**, 667
Wirth, T. *et al., J.O.C.*, 1996, **61**, 2686 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 953-954; 2195-2196
Lutz, C. *et al., Synthesis*, 1999, 312-316 (*S-form, synth*)
Kuwano, R. *et al., Bull. Chem. Soc. Jpn.*, 2000, **73**, 485-496 (*S-form, synth, pmr*)
Spieler, J. *et al., Eur. J. Org. Chem.*, 2000, 391-399 (*R-form, synth, pmr*)
Org. Synth., 2002, **79**, 139-145 (*S-form, synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EGQ000

1-Phenyl-2-propanol P-306

[698-87-3]
α-Methylbenzeneethanol, 9CI. α-Methylphenethyl alcohol, 8CI. Benzylmethylcarbinol

$C_9H_{12}O$ 136.193

► SG8589500

(*R*)-*form* [1572-95-8]
Bp_{25} 125° Bp_{13} 84-86.5°. $[\alpha]_D^{20}$ -41 (c, 5.3 in C_6H_6). Steam-volatile.

Me ether:2-Methoxy-1-phenylpropane
$C_{10}H_{14}O$ 150.22
Bp_{12} 85°.

(*S*)-*form* [1517-68-6]
Bp_{10} 100° (bulb). $[\alpha]_D^{20}$ +40.7 (c, 5 in C_6H_6) (98.4% ee).

(±)-*form* [14898-87-4]
Bp 219-221° $Bp_{7.5}$ 116°.

Phenylurethane:
Mp 92°.

Butanoyl: [68922-11-2] *α-Methylphenethyl butyrate. FEMA 3197*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient.

4-Methylbenzenesulfonyl:
Mp 93.7-94°.

Et ether: [17953-97-8] *2-Ethoxy-1-phenylpropane*
$C_{11}H_{16}O$ 164.247
Bp 205-206°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1152D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 385B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1074A (*ir*)
Arcus, C.L. *et al., J.C.S.*, 1956, 2987 (*resoln*)
Witkop, B. *et al., J.A.C.S.*, 1957, **79**, 197 (*abs config*)
Eliel, E.L. *et al., J.A.C.S.*, 1957, **79**, 5986 (*synth*)
Cervinka, O. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 1684 (*synth*)
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Koga, K. *et al., Chem. Lett.*, 1980, 981 (*synth*)

Masuda, S. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 1089 (*synth*)
Tripathy, P.B. *et al., Synthesis*, 1990, 200 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 545 (*butanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1832 (*butanoyl*)
D'Arrigo, P. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 4021-4026 (*S-form, synth, pmr*)
Nakamura, K. *et al., J.C.S. Perkin 1*, 2000, 3205-3211 (*S-form, synth, pmr, ir*)

2-Phenyl-1-propanol P-307

[1123-85-9]
β-Methylbenzeneethanol, 9CI. β-Hydroxycumene. Hydratropic alcohol. β-Methylphenethyl alcohol. FEMA 2732

$C_9H_{12}O$ 136.193

►LD_{50} (rat, orl) 2300 mg/kg. SG8590000

(*R*)-*form* [19141-40-3]
Bp_{19} 112-113°. $[\alpha]_D^{34}$ +13.28 (neat).

(*S*)-*form* [37778-99-7]
$[\alpha]_D$ -17.4 (neat).

(±)-*form*
Flavouring agent. d^0 1.02. Bp_{14} 114° (Bp_4 88°).

Butanoyl: [80866-83-7]

[132316-78-0] *2-Phenylpropyl butyrate. FEMA 2891*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. Liq. with a fruity odour and sweet plum-like flavour. d 0.99. n_D^{20} 1.4880.

2-Methylpropanoyl: [65813-53-8] *2-Phenylpropyl isobutyrate. FEMA 2892*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. Liq. with a fruity odour and taste. d 0.97. n_D^{20} 1.4860.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1153A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 385C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1074B (*ir*)
Nakajima, T. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 2980 (*synth*)
Watson, M.B. *et al., J.C.S. Perkin 1*, 1972, 1597 (*abs config*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 1923 (*synth*)
Cornils, B. *et al., Chem.-Ztg.*, 1974, **98**, 596 (*rev*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 547 (*rev, tox*)
Brown, H.C. *et al., J.O.C.*, 1977, **42**, 2533 (*synth*)
Cook, M.J. *et al., Tetrahedron*, 1986, **42**, 249 (*synth*)
Harada, T. *et al., J.A.C.S.*, 1987, **109**, 527 (*synth*)
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Behrens, K. *et al., Eur. J. Org. Chem.*, 1998, 2397-2403 (*R-form, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PGB750

2-Phenyl-2-propanol P-308

[617-94-7]
α,α-Dimethylbenzenemethanol, 9CI. α,α-Dimethylbenzyl alcohol, 8CI. Dimethylphenylcarbinol. Cumyl alcohol

$(H_3C)_2C(OH)Ph$

$C_9H_{12}O$ 136.193
Prisms. Mp 35-37°. Bp 202° Bp_{14} 98°.

►Skin irritant. LD_{50} (rat, orl) 1300 mg/kg. DO4562000

Ac: [3425-72-7]
$C_{11}H_{14}O_2$ 178.23
Bp 231-233° Bp_{15} 124-125°.

2-Methylpropanoyl: [7774-60-9] *1-Methyl-1-phenylethyl isobutyrate. α,α-Dimethylbenzyl isobutyrate. FEMA 2388*
$C_{13}H_{18}O_2$ 206.284
Flavouring ingredient. Liq.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1122D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 328B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1048A (*ir*)
Capp, C.W. *et al., J.C.S.*, 1953, 4106 (*synth*)
Viehe, H.G. *et al., Chem. Ber.*, 1962, **95**, 2557 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 75 (*2-methylpropanoyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 849-850 (*2-methylpropanoyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DTN100

3-Phenyl-1-propanol P-309

[122-97-4]
Benzenepropanol, 9CI. Hydrocinnamic alcohol. Hydrocinnamyl alcohol. FEMA 2885

$PhCH_2CH_2CH_2OH$

$C_9H_{12}O$ 136.193
Occurs in storax and fern balsam. Also present in *Vaccinium* spp. fruits, guava fruit and peel, blackberry, other fruits, rum, white wine, shiitake mushroom, matsutake mushroom and peated malt. Flavouring ingredient. Oil with pleasant odour and apricot-like sweet, pungent taste. d_4^{24} 1.006. Bp 235° (219°) Bp_{12} 119° $Bp_{0.4}$ 95-97°. n_D^{23} 1.5351.

►Fl.p. 100°. Skin irritant. LD_{50} (rat, orl) 2300 mg/kg. UB8970000

Carbamate: [673-31-4] ***Phenprobamate, BAN, INN.*** *Gamaquil. Actiphan. Nelaxan*
Leaflets (EtOH aq.). Mp 101-104°. Log P 1.77 (calc).

►LD_{50} (rat, orl) 1110 mg/kg. UB9275000

Phenylurethane:
Mp 47°.

Formyl: [104-64-3] *3-Phenylpropyl formate. Hydrocinnamyl formate. FEMA 2895*
$C_{10}H_{12}O_2$ 164.204
Used in food flavouring. d 1.04. Bp 238°.

Ac: [122-72-5] *3-Phenylpropyl acetate. 1-Acetoxy-3-phenylpropane. Hydrocinnamyl acetate. FEMA 2890*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient. Present in guava fruit and peel, melon, rum and cassia leaf. Liq. with spicy odour and bittersweet, currant flavour. d_4^{25} 1.01. Bp 244-245° $Bp_{0.05}$ 74°. n_D^{20} 1.4990.

Propanoyl: [122-74-7] *3-Phenylpropyl propanoate. FEMA 2897*
$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Liq. with a sweet, fruity taste. $d^{15.5}$ 1.01. Bp 265°. n_D^{20} 1.5125.

Butanoyl: [7402-29-1] *3-Phenylpropyl butanoate*
$C_{13}H_{18}O_2$ 206.284
d 0.99. Bp 258°.

2-Methylpropanoyl: [103-58-2] *FEMA 2893. 3-Phenylpropyl 2-methylpropanoate. Hydrocinnamyl isobutyrate*
$C_{13}H_{18}O_2$ 206.284
d 0.99. Bp 252°. n_D^{20} 1.4864.

3-Methylbutanoyl: [5452-07-3] *3-Phenylpropyl isovalerate. FEMA 2899*
$C_{14}H_{20}O_2$ 220.311
Flavouring ingredient. Liq. with a sweet, fruity taste. Bp 280°.

Hexanoyl: [6281-40-9] *3-Phenylpropyl hexanoate*
$C_{15}H_{22}O_2$ 234.338
Flavouring ingredient. Liq. Bp 292°.

4-Nitrobenzoyl:
Cryst. (EtOH). Mp 45-46°.

Cinnamoyl: [122-68-9] *3-Phenylpropyl cinnamate. FEMA 2894*
$C_{18}H_{18}O_2$ 266.339
Flavouring ingredient. Liq. with cocoa-like sweet flavour. Bp >300° dec..

Me ether: [2046-33-5] *3-Methoxypropylbenzene, 9CI. 1-Methoxy-3-phenylpropane*
$C_{10}H_{14}O$ 150.22
Bp 206.5° Bp_{12} 92-94°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1154A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 387C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1076A (*ir*)
Ruegheimer, L. *et al., Annalen*, 1874, **172**, 122-131 (*Ac*)
Burger, A.M. *et al., Chem. Zentralbl.*, 1928, **1**, 2466; **2**, 338; 1317 (*butanoyl*)
Huston, R.C. *et al., J.O.C.*, 1941, **6**, 123-133 (*synth*)
Jacobs, M.B. *et al., Am. Perfumer Essent. Oil Rev.*, 1948, **51**, 350 (*formyl*)
Org. Synth., Coll. Vol., 4, 1963, 798-801 (*bibl, synth*)
Swiss Pat., 1968, 451 114; *CA*, **69**, 96193 (*synth, pharmacol, Phenprobamate*)
Snyder, E.I. *et al., J.A.C.S.*, 1969, **91**, 2579-2582 (*conformn*)
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Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, HHP 050
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 610
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 670-674 (*esters*)
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Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HHP050; PGA750

1-Phenyl-1-propanone, 9CI P-310

[93-55-0]

Propiophenone. Propionylbenzene. Ethyl phenyl ketone. Benzoylethane. FEMA 3469

$PhCOCH_2CH_3$

$C_9H_{10}O$ 134.177

Present in Camembert cheese, coffee, tea and roasted nuts. Flavouring ingredient. d_{25}^{25} 1.01. Mp 19-20°. Bp_{764} 218° Bp_8 84-85°. n_D^{20} 1.5268.

► Fl. p. 88°. Low acute mammalian toxicity. UG7175000

Oxime: [2157-50-8]
$C_9H_{11}NO$ 149.192
Plates (petrol). Mp 53-54°. Bp 245-246° dec. Bp_{38} 165°.

2,4-Dinitrophenylhydrazone: [3375-37-9]
Red leaflets (EtOH). Mp 187-189°.

Semicarbazone:
Needles (EtOH). Spar. sol. EtOH, Et_2O. Mp 182-184°.

Anil:
$C_{15}H_{15}N$ 209.29
Pale yellow needles (hexane). Mp 50°. Bp_{11} 169°.

Azine:
$C_{18}H_{20}N_2$ 264.369
Yellow needles. Mp 79-80° (68°).

Di-Me acetal: [25310-92-3] *1,1-Dimethoxy-1-phenylpropane. (1,1-Dimethoxypropyl)benzene, 9CI*
$C_{11}H_{16}O_2$ 180.246
Oil. Bp 206-208° Bp_{27} 82-83°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 8C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 802B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1228D (*ir*)
Shriner, R.L. *et al., J.A.C.S.*, 1930, **52**, 1267-1269 (*synth*)
Hauser, C.R. *et al., J.A.C.S.*, 1948, **70**, 426 (*synth*)
Adv. Chem. Ser., 1955, **15**, 356 (***props***)
Schultz, H.P. *et al., J.O.C.*, 1963, **28**, 879 (*synth, uv*)
Levine, R. *et al., J.O.C.*, 1975, **40**, 1770 (*synth*)
Hunig, S. *et al., Synthesis*, 1975, 180 (*synth*)
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Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2335-2336
Verevkin, S.P. *et al., Eur. J. Org. Chem.*, 1998, 2323-2332 (*di-Me acetal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EOL500

3-Phenyl-2-propenal, 9CI P-311

[104-55-2]

Cinnamaldehyde, 8CI. Cinnamal. Cinnamic aldehyde. 3-Phenylacrolein. FEMA 2286

$PhCH{=}CHCHO$

C_9H_8O 132.162

Fairly sol. H_2O; poorly sol. hexane. Log P 1.9 (calc).

► Severe human skin irritant. LD_{50} (rat, orl) 2220 mg/kg. GD6475000

(E)-form [14371-10-9]
Constit. of cinnamon and cassia oils. Used in perfumery and flavour industries. Liq. with cinnamon odour. d_4^{20} 1.05. Fp -7.5. Bp *ca.*° 250 part. dec. Bp_{20} 130°. Steam-volatile. Forms bisulfite compd. Base-labile.

► GD6476000

(Z)-form [57194-69-1]
Liq. d^{20} 1.04. $Bp_{0.4}$ 67-69°.

[3839-82-5, 4364-06-1, 7148-78-9, 132200-89-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 102A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 926C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1281A (*ir*)
Andrews, L.J. *et al., J.A.C.S.*, 1947, **69**, 3062 (*uv*)
Jun, N. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 1512 (*pmr*)
Hayes, W.P. *et al., Spectrochim. Acta A*, 1968, **24**, 323 (*ir*)
Org. Synth., 1971, **51**, 11; 20; 1974, **54**, 42 (*synth*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Mikaya, A.I. *et al., Org. Mass Spectrom.*, 1983, **18**, 99 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, 969
Laihia, K. *et al., Magn. Reson. Chem.*, 1990, **28**, 541 (*cmr*)
Shudo, K. *et al., J.A.C.S.*, 1991, **113**, 1364 (*oximes*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 347 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1350; 1354
Daubresse, N. *et al., Synthesis*, 1994, 369 (*synth*)
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Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 338
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMP969

3-Phenyl-2-propenoic acid, 9CI P-312

[621-82-9]

Cinnamic acid, 8CI. 3-Phenylacrylic acid. FEMA 2288

$PhCH{=}CHCOOH$

$C_9H_8O_2$ 148.161

Sol. MeOH, Et_2O; fairly sol. H_2O. Log P 2.09 (calc).

► GD7800000

(E)-form [140-10-3]
Occurs as free acid and esters in storax, Peruvian balsam and other resins. Also present in tomato, pepper, red or white wine, porcini (*Boletus edulis*), peated malt, guava fruit, grapes, pineapple, raspberry, blackberry and other fruits. Flavouring agent. Needles or prisms (EtOH). Insol. H_2O; sol. C_6H_6, Et_2O, Me_2CO, AcOH. Mp 133°. Bp 300°. pK_a 4.46 (25°). Steam-volatile. Resistant to radical homopolym. but copolym. to some extent with vinyl monomers.

► Skin irritant. LD_{50} (rat, orl) 2500 mg/kg. GD7850000

Me ester: [103-26-4]

[1754-62-7] *Methyl cinnamate. FEMA 2698*
$C_{10}H_{10}O_2$ 162.188
Occurs in essential oils e.g. from *Ocimum* and *Alpinia* spp. Also present in various fruits, e.g. guava, feijoa, strawberry. Flavouring agent. Cryst. (EtOH). Mp 36°. Bp 263°.

► LD_{50} (rat, orl) 2610 mg/kg. GE0190000

Et ester: [4192-77-2] *Ethyl cinnamate. FEMA 2430*
$C_{11}H_{12}O_2$ 176.215
Occurs in storax. Also present in many fruits, e.g. cherry, American cranberry, pineapple, blackberry and passion fruit. Oil with sweet peach/apricot taste. d_{25}^{25} 1.05. Fp 6.5 Mp 12°. Bp 271-272° Bp_{24} 159°. n_D^{20} 1.5590.

► Fl. p. >82°.

Propyl ester: [7778-83-8]

[74513-58-9] *Propyl cinnamate. FEMA 2938*
$C_{12}H_{14}O_2$ 190.241
Flavouring ingredient. Viscous liq. with peach-apricot flavour and wine-like odour. d_0^0 1.04. Mp 13°. Bp 283-284°. n_D^{20} 1.5510.

Isopropyl ester: [7780-06-5]

[60512-85-8] *Isopropyl cinnamate. FEMA 2939*
$C_{12}H_{14}O_2$ 190.241
Flavouring ingredient. Viscous liq.with sweet amber-like odour and fresh, fruity flavour; solidifies when cold. Bp 268-270°.

Butyl ester: [538-65-8]

[52392-64-0] *Butyl cinnamate. FEMA 2192*
$C_{13}H_{16}O_2$ 204.268
Flavouring ingredient. Liq. d^{18} 1.01. Bp 295°. n_D^{20} 1.5470.

2-Methylpropyl ester: [122-67-8]

[31416-74-7] *Isobutyl cinnamate. Labdanol. FEMA 2193*
$C_{13}H_{16}O_2$ 204.268
Flavouring ingredient. Liq. with sweet, fruity, balsamic odour and a sweet currant-like taste. Bp_{13} 145°.

3-Methylbutyl ester: [7779-65-9]

[85180-66-1] *Isoamyl cinnamate. FEMA 2063*
$C_{14}H_{18}O_2$ 218.295
Flavouring ingredient. Liq.

Heptyl ester: [10032-08-3] *Heptyl cinnamate. FEMA 2551*
$C_{16}H_{22}O_2$ 246.349
Flavouring ingredient. Liq.

2-Propenyl ester: [56289-56-6] *Allyl cinnamate. FEMA 2022*
$C_{12}H_{12}O_2$ 188.226
Flavouring agent. Liq. with peach/apricot aroma. d_4^{23} 1.05. Bp_{15} 150-152°. n_D^{20} 1.5300. Readily polym..

Cyclohexyl ester: [7779-17-1]

[138964-30-4] *Cyclohexyl cinnamate. FEMA 2352*
$C_{15}H_{18}O_2$ 230.306
Flavouring ingredient. Liq. with fruity odour and flavour. Mp 28°. Bp_{12} 195°.

Benzyl ester: [103-41-3] *FEMA 2142*

$C_{16}H_{14}O_2$ 238.285
Isol. from various plant spp.. Present in Sumatra and Penang benzoin, Peru and tolu balsams, main constit. of copaiba balsam. Flavouring agent. Cryst. or liq. with sweet balsamic odour and honey-like taste. Mp 37-39°. Bp_5 195-200°.

► GD8400000

Cinnamyl ester: [122-69-0] *Cinnamyl cinnamate. Styracin. FEMA 2298*
$C_{18}H_{16}O_2$ 264.323
Occurs in storax and Peruvian balsam. Flavouring agent. Needles or prisms with characteristic sweet resinous odour. Mp 44°.

► GD8562000

(*Z*)-*form* [102-94-3]
Cryst. in three forms. Mp 42° Mp 58° Mp 68° (trimorph.). Bp 95° (high vac.). pK_a 3.85 (25°). The highest-melting (*Z*)-form has been known as Allocinnamic acid. The other two forms have both been referred to as Isocinnamic acid.

[102-92-1, 103-36-6, 538-42-1, 621-79-4, 1866-31-5, 3098-92-8, 4360-47-8, 39124-46-4, 59015-50-8]

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Mendez, J. *et al., Microchem. J.*, 1968, **13**, 232 (*uv*)
Analyst (London), 1972, **97**, 740 (*microanal*)
v. Massow, F. *et al., J.C.S. Perkin 2*, 1973, 1480 (*cmr*)
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Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 687 (*rev, tox*)
Marco, J.A. *et al., Phytochemistry*, 1978, **17**, 1438 (*isol*)
Schaldach, B. *et al., Org. Mass Spectrom.*, 1980, **15**, 175 (*ms*)
Ripperger, H. *et al., Phytochemistry*, 1981, **20**, 1453 (*isol, ir, pmr, ms*)
Brunet, J.-J. *et al., Tet. Lett.*, 1981, **22**, 1013 (*synth*)
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Wierda, D.A. *et al., Acta Cryst. C*, 1989, **45**, 338 (*cryst struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CMP975; MIO500
Hon, Y.-S. *et al., Heterocycles*, 1991, **32**, 1089 (*synth, ir, pmr, cmr, ms, allyl ester*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 344 (*rev*)
Reed, G.A. *et al., J.O.C.*, 1993, **58**, 6364 (*synth, ir, pmr, cmr, ms*)
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Lee, H.H. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 1475; 2574 (*cryst struct, Z-form*)
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3-Phenyl-2-propen-1-ol, 9CI P-313

[104-54-1]
Cinnamyl alcohol, 8CI. Cinnamic alcohol. 3-Phenylallyl alcohol. Styrone. Styryl alcohol. FEMA 2294

PhCH=CHCH$_2$OH

$C_9H_{10}O$ 134.177
Flavouring ingredient.

► Fl. p. >106°. Skin irritant. LD_{50} (rat, orl) 2000 mg/kg. GE2200000

(*E*)-*form* [4407-36-7]
Constit. of storax and Peruvian balsam, mainly as ester of Cinnamic acid. Flavouring. Stabiliser. Needles with attractive mild odour. Sol. H_2O. d_4^{20} 1.04. Mp 33°. Bp 258° Bp_{14} 142-145°.

Formyl: [23510-72-7]

[104-65-4] *Cinnamyl formate. FEMA 2299*
$C_{10}H_{10}O_2$ 162.188
Flavouring ingredient. Liq. with balsamic, fruital-floral odour and bitter-sweet apple-like taste. Bp 250°.

Ac: [21040-45-9] *Cinnamyl acetate. FEMA 2293*
$C_{11}H_{12}O_2$ 176.215
Constit. of Cassia and basil oils. Also present in guava fruit and peel, starfruit, melon and strawberry jam. Flavouring ingredient. Liq. with sweet, woody odour. d_4^{12} 1.06. Bp 265° Bp_{18} 141°. n_D^{12} 1.5442.

Propanoyl: [103-56-0] *Cinnamyl propionate. FEMA 2301*
$C_{12}H_{14}O_2$ 190.241
Used in fruit food flavouring. Bp 289°.

Butanoyl: [103-61-7] *Cinnamyl butyrate. FEMA 2296*
$C_{13}H_{16}O_2$ 204.268
Used in orange and citrus food flavouring. Present in apple. Bp 300°.

2-Methylpropanoyl: [103-59-3] *Cinnamyl isobutyrate. FEMA 2297*
$C_{13}H_{16}O_2$ 204.268
Used in food flavouring. Liq. with sweet taste reminiscent of apple and banana. Bp 254°.

3-Methylbutanoyl: [140-27-2] *Cinnamyl isovalerate. FEMA 2302*
$C_{14}H_{18}O_2$ 218.295
Used in food flavouring. Liq. with rose-like odour and apple-like taste. Bp 313°.

Phenylacetyl: [7492-65-1] *Cinnamyl phenylacetate. FEMA 2300*
$C_{17}H_{16}O_2$ 252.312
Flavouring ingredient. Liq. with spicy, honey-like flavour. $d^{15.5}$ 1.09. Bp 333-335°.

Benzoyl: [50555-04-9]
$C_{16}H_{14}O_2$ 238.285
Flavouring ingredient. Liq. or cryst. with balsamic odour. Mp 38.5°. Bp 335°.

2-Aminobenzoyl: [87-29-6] *Cinnamyl anthranilate. FEMA 2295*
$C_{16}H_{15}NO_2$ 253.3
Prohibited from use in food. Mp 64°. Bp 332°.

► Experimental neoplastigen LD_{50} (rat, orl) 5000 mg/kg.

[103-54-8, 5320-75-2, 77134-01-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1124A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 392C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1078D (*ir*)
Bert, L. *et al., C. R. Hebd. Seances Acad. Sci.*, 1930, **191**, 332 (*synth*)
Young, W.G. *et al., J.A.C.S.*, 1936, **58**, 100 (*synth*)
Campbell, T.W. *et al., J.A.C.S.*, 1947, **69**, 880 (*uv*)
Scipioni, A. *et al., Gazz. Chim. Ital.*, 1951, **81**, 654 (*synth*)
Minyard, J.P. *et al., J. Chromatogr.*, 1967, **29**, 88 (*chromatog*)
Overman, L. *et al., Tet. Lett.*, 1979, 321 (*synth*)
Mikaya, A.I. *et al., Org. Mass Spectrom.*, 1983, **18**, 99 (*ms*)
Pritzkow, W. *et al., J. Prakt. Chem.*, 1984, **326**, 73 (*cmr*)
Lakshmy, K.V. *et al., Org. Prep. Proced. Int.*, 1985, **17**, 251 (*synth*)
Denis, J.-N. *et al., J.O.C.*, 1986, **51**, 46 (*synth, ir, pmr*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1988, **A11**, 185 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CMQ740
Pelter, A. *et al., J.C.S. Perkin 1*, 1990, 2775 (*synth, ir, pmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 344 (*rev*)
Davis, F.A. *et al., J.O.C.*, 1992, **57**, 2599 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 119 (*phenylacetate*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 600-604; 606; 608-609 (*occurs, props, esters, phenylacetate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMQ740; CMQ750

3-Phenylpropyl glucosinolate P-314

[76265-25-3]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)benzenebutanimidate], 9CI

Ph(CH$_2$)$_3$C(SGlc)=NOSO$_3$H

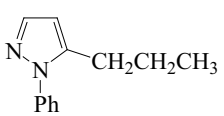
$C_{16}H_{23}NO_9S_2$ 437.491
Present in horseradish (*Armoracia lapathifolia*).

Grob, K. *et al., Phytochemistry*, 1980, **19**, 1789 (*occur*)

1-Phenyl-5-propyl-1*H*-pyrazole P-315

[91565-82-1]

[65504-93-0]
FEMA 3727

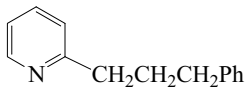


$C_{12}H_{14}N_2$ 186.256
FEMA 3727 refers to a mixt. with the isomeric 3-propyl compd., which has not been individually characterised. Flavouring ingredient. Bp_{15} 156° $Bp_{0.2}$ 85-90°.

Benary, E. *et al., Ber.*, 1926, **59**, 2198-2201 (*synth*)
Menozzi, G. *et al., J. Het. Chem.*, 1987, **24**, 1669-1675 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 656 (*use*)

2-(3-Phenylpropyl)pyridine, 9CI, 8CI P-316

[2110-18-1]
FEMA 3751



$C_{14}H_{15}N$ 197.279
Flavouring ingredient. Liq. d_4^{20} 1.01. Bp_{16} 170-171°. n_D^{20} 1.5142.

Wegler, R. *et al., Chem. Ber.*, 1950, **83**, 6-10 (*synth*)
Pines, H. *et al., J.O.C.*, 1969, **34**, 2113-2118 (*synth, pmr*)
Budzikiewicz, H. *et al., Org. Mass Spectrom.*, 1976, **11**, 398-405 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 674 (*use*)

2-(3-Phenylpropyl)tetrahydrofuran P-317

[3208-40-0]
Tetrahydro-2-(3-phenylpropyl)furan, 9CI. FEMA 2898

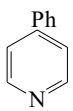


$C_{13}H_{18}O$ 190.285
Flavouring ingredient. Liq. with honey-like, sweet flavour. d_4^{20} 0.99. Bp_3 124-126°. n_D^{20} 1.5140.

Burdick, H.E. *et al., J.A.C.S.*, 1934, **56**, 438-442 (*synth*)
Ponomarev, A.A. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1953, **93**, 297-300; *CA*, **48**, 12731f (*synth*)

4-Phenylpyridine, 9CI P-318

[939-23-1]



$C_{11}H_9N$ 155.199
Occurs in tea and peppermint. Plates (H_2O). Sol. hot H_2O. Mp 77-78°. Bp 274-275°. pK_a 5.35 (25°).
► LD_{50} (mus, ivn) 89 mg/kg. UT7141000

Picrate:
Orange needles. Mp 195-196°.

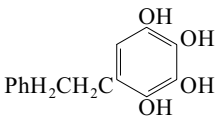
1-Oxide: [1131-61-9]
$C_{11}H_9NO$ 171.198
Prisms (C_6H_6). Mp 152°.

1-Me: See 1-Methyl-4-phenylpyridinium(1+) in *The Combined Chemical Dictionary.*

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 249B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 739A; 917B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1519B (*ir*)
Elks, J. *et al., J.C.S.*, 1943, 441
Saeki, S. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1780 (*synth*)
Snyder, S.H. *et al., Nature (London)*, 1985, **317**, 198 (*tox*)
Godin, C.S. *et al., Drug Metab. Dispos.*, 1989, **17**, 180 (*metab*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PGE750

1-Phenyl-2-(2,3,4,5-tetrahydroxyphenyl)ethane P-319

5-(2-Phenylethyl)-1,2,3,4-benzenetetrol. 2,3,4,5-Tetrahydroxybibenzyl



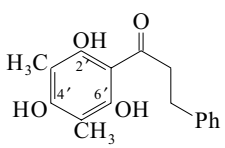
$C_{14}H_{14}O_4$ 246.262

4,5-Di-Me ether: [39354-56-8] *2,3-Dihydroxy-4,5-dimethoxybibenzyl. 1-(2,3-Dihydroxy-4,5-dimethoxyphenyl)-2-phenylethane.* ***Batatasin II***
$C_{16}H_{18}O_4$ 274.316
Constit. of *Dioscorea batatas* (Chinese yam).

Hashimoto, T. *et al., Planta*, 1972, **108**, 369 (*isol, props*)
Hashimoto, T. *et al., Egypt. J. Pharm. Sci.*, 1980, **21**, 249 (*struct, isol, uv, ir, pmr, ms*)
Ireland, C.R. *et al., Phytochemistry*, 1981, **20**, 1569 (*rev*)

3-Phenyl-1-(2,4,6-trihydroxy-3,5-dimethylphenyl)-1-propanone P-320

[70155-37-2]
2′,4′6′-Trihydroxy-3′,5′-dimethyldihydrochalcone



$C_{17}H_{18}O_4$ 286.327
Cryst.(Et_2O/hexane). Mp 122-123°.

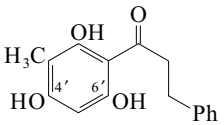
4′-Me ester: [34328-55-7] *1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone. 2′,6′-Dihydroxy-4′-methoxy-3′,5′-dimethyldihydrochalcone.* ***Myrigalon B***
$C_{18}H_{20}O_4$ 300.354
Isol. from *Myrica gale* (bog myrtle). Yellow needles (Et_2O/petrol). Mp 121° (116-117°).

6′-Me ether: [76444-55-8] *1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone, 9CI. 2′,4′-Dihydroxy-6′-methoxy-3′,5′-dimethyldihydrochalcone.* ***Angoletin****. Myrigalon D*
$C_{18}H_{20}O_4$ 300.354
Cryst. ($CHCl_3$/hexane). Poorly sol. hexane. Mp 74-76°.

Anthonsen, T. *et al., Acta Chem. Scand.*, 1971, **25**, 1929 (*deriv*)
Uyar, T. *et al., Phytochemistry*, 1978, **17**, 2011
Misurlioglu, H. *et al., Phytochemistry*, 1978, **17**, 2015 (*synth, deriv*)
Hufford, C.D. *et al., Phytochemistry*, 1980, **19**, 2036 (*isol, uv, pmr, cmr, struct, Angoletin*)
Hufford, C.D. *et al., J. Nat. Prod.*, 1982, **45**, 337 (*synth*)
Wollenweber, E. *et al., J. Plant Physiol.*, 1985, **117**, 423 (*isol*)
Tanrisevar, N. *et al., Phytochemistry*, 1986, **26**, 175 (*isol*)

3-Phenyl-1-(2,4,6-trihydroxy-3-methylphenyl)-1-propanone P-321

[70155-33-8]
2′,4′,6′-Trihydroxy-3′-methyldihydrochalcone



$C_{16}H_{16}O_4$ 272.3

4′,6′-Di-Me ether: [65349-37-3] *1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-phenyl-1-propanone. 2′-Hydroxy-4′,6′-dimethoxy-3′-methyldihydrochalcone.* ***Myrigalone E***
$C_{18}H_{20}O_4$ 300.354
Constit. of *Myrica gale* (bog myrtle). Needles (MeOH). Mp 146-147°.

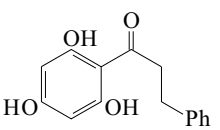
4′-Me ether: [83247-38-5] *1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-phenyl-1-propanone. 2′,6′-Dihydroxy-4′-methoxy-3′-methyldihydrochalcone.* ***Myrigalone G***
$C_{17}H_{18}O_4$ 286.327
Constit. of the fruit of *Myrica gale* (bog myrtle). Light yellow cryst. (MeOH aq.). Mp 169-171° (synthetic).

6′-Me ether: [143502-00-5] *1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-3-phenyl-1-propanone. 2′,4′-Dihydroxy-6′-methoxy-3′-methyldihydrochalcone.* ***Myrigalone H***
$C_{17}H_{18}O_4$ 286.327
Constit. of the fruit of *Myrica gale* (bog myrtle).

Anthonsen, T. *et al., Phytochemistry*, 1977, **16**, 1805 (*isol, struct*)
Misirlioglu, H. *et al., Phytochemistry*, 1978, **17**, 2015 (*synth*)
Schiemenz, G.P. *et al., Annalen*, 1982, 1509 (*synth, deriv*)
Malterud, K.E. *et al., Acta Pharm. Nord.*, 1992, **4**, 65; *CA*, **117**, 157491t (*4′-Me ether, 6′-Me ether, isol*)
Japan. Pat., 1999, 99 80 012; *CA*, **130**, 247022p (*Myrigalone G, activity*)

3-Phenyl-1-(2,4,6-trihydroxyphenyl)-1-propanone P-322

[1088-08-0]
2′,4′,6′-Trihydroxydihydrochalcone



$C_{15}H_{14}O_4$ 258.273
Prisms. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 138-139° (134-135°). λ_{max} 212 (ϵ

13800); 222 (ϵ 13200); 286 (ϵ 15700) (EtOH) (Berdy).

2′-O-β-D-Glucopyranoside: [31018-48-1]
$C_{21}H_{24}O_9$ 420.415
Occurs in *Malus* spp.. No phys. props. reported.

4′-O-β-D-Glucopyranoside: [73519-16-1]
$C_{21}H_{24}O_9$ 420.415
Occurs in *Malus* spp.. No phys. props. reported.

2′-Me ether: [76444-56-9] *1-(2,4-Dihydroxy-6-methoxyphenyl)-3-phenyl-1-propanone, 9CI. 2′,4′-Dihydroxy-6′-methoxydihydrochalcone.* ***Uvangoletin***
Needles (EtOAc/petrol). Mp 189-190°.

4′-Me ether: [35241-55-5] *1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-1-propanone. 2′,6′-Dihydroxy-4′-methoxydihydrochalone. 2′,6′-Dihydroxy-4′-methoxy-β-phenylpropiophenone*
$C_{16}H_{16}O_4$ 272.3
Isol. from *Populus balsamifera* (balsam poplar) oil. Plates (CH_2Cl_2). Mp 174-175° (168°).

2′,4′-Di-Me ether: [3791-76-2] *1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-phenyl-1-propanone. 2′-Hydroxy-4′,6′-dimethoxydihydrochalcone.* ***Dihydroflavokawin B.*** *Lapathone*
$C_{17}H_{18}O_4$ 286.327
Needles. Mp 106-106.5°.

Tri-Me ether:3-Phenyl-1-(2,4,6-trimethoxyphenyl)-1-propanone. ***2′,4′,6′-Trimethoxydihydrochalcone***
$C_{18}H_{20}O_4$ 300.354
Cryst. ($CHCl_3$/hexane). Mp 74-76°.

4′-O-(3-Methyl-2-butenyl): [77129-37-4] ***2′,6′-Dihydroxy-4′-prenyloxydihydrochalcone***
$C_{20}H_{22}O_4$ 326.391
Oil.

2′-Me ether, 4′-O-(3-methyl-2-butenyl): ***2′-Hydroxy-6′-methoxy-4′-prenyloxydihydrochalcone***
$C_{21}H_{24}O_4$ 340.418

Goris, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1935, **20**, 1435; 1520 (*isol, synth*)
Nilsson, M. *et al., Acta Chem. Scand.*, 1961, **15**, 154 (*isol*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1977, **32**, 1013; 1980, **35**, 36
Williams, C.A. *et al., Phytochemistry*, 1979, **18**, 803 (*glucosides*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 839; 1980, **19**, 873
Hufford, C.D. *et al., Phytochemistry*, 1980, **19**, 2036 (*Uvangoletin*)
Itokawa, H. *et al., Phytochemistry*, 1981, **20**, 2503 (*Dihydroflavokawin B*)
Bhardwaj, D.K. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 476 (*synth*)
Hufford, C.D. *et al., J. Nat. Prod.*, 1982, **45**, 337 (*isol*)
Tanaka, H. *et al., Phytochemistry*, 1984, **23**, 1198 (*isol*)
Burke, B. *et al., Phytochemistry*, 1986, **25**, 1427-1430 (*isol*)
Ahmed, M. *et al., Phytochemistry*, 1990, **29**, 2009 (*isol*)
Zdero, C. *et al., Phytochemistry*, 1990, **29**, 2179 (*isol, derivs*)
Orjala, J. *et al., J. Nat. Prod.*, 1994, **57**, 18-26 (*isol, activity*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1997, **60**, 65 (*cmr*)
Juliawaty, L.D. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1726-1728 (*isol, activity*)

Phlean, 11CI P-323

[39289-27-5]
Phlein, 9CI

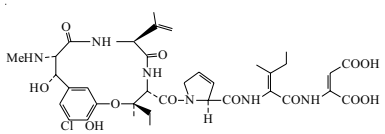
A β-D(2→6)-linked fructan.Mp 220°. $[\alpha]_D$ -50 (c, 1.0 in H_2O). The old isolates Poan from *Poa trivialis* and Graminin from rye are prob. coterminous with phlean.

[55466-18-7]

McDonald, E.J. *et al., Adv. Carbohydr. Chem.*, 1946, **2**, 253 (*rev*)
Schlubach, H.H. *et al., Annalen*, 1950, **544**, 101; 111
Yamamoto, S. *et al., Plant Physiol.*, 1985, **78**, 591 (*isol*)

Phomopsin A P-324

[64925-80-0]



Absolute configuration

$C_{36}H_{45}ClN_6O_{12}$ 789.237

Peptide antibiotic. Mycotoxin produced by *Phomopsis leptostromiformis*. Cryst. (MeOH/EtOH/H_2O). Sol. MeOH. Dec. at 205° without melting λ_{max} 209 (ϵ 52300); 222 (sh) (ϵ 24500); 288 (ϵ 13900) (MeOH) (Derep).

►SY2593000

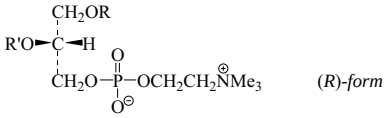
Dechloro: [64925-81-1] ***Phomopsin B***
$C_{36}H_{46}N_6O_{12}$ 754.792
Mycotoxin from *Phomopsis leptostromiformis*. Sol. MeOH. λ_{max} 209 ; 288 (MeOH) (Berdy).

[121128-31-2]

Frahn, J.L. *et al., Toxicon*, (Suppl. 3), 1983, 149 (*props*)
Edgar, J.A. *et al., Bioact. Mol.*, 1986, **1**, 169 (*rev*)
Mackay, M.F. *et al., Chem. Comm.*, 1986, 1219 (*cryst struct*)
Allen, J.G. *et al., J. Appl. Toxicol.*, 1989, **9**, 83 (*isol*)
Culvenor, C.C.J. *et al., Tetrahedron*, 1989, **45**, 2351 (*isol, pmr, cmr, ms, cryst struct, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PGR775

Phosphatidylcholine P-325

[8002-43-5]
1,2-Diacylglycero-3-phosphocholine. Lecithin. Vitellin. Kelecin. Granulestin. Lecithol. Diacyllecithin. Diacylphosphatidylcholine. E322



(*R*)-form

R, R' = acyl groups

The naturally occurring (*R*)-form is equivalent to 1,2-diacyl-*sn*-glycero-3-phosphocholine (*sn*-3-phosphatidylcholine). See also Phosphatidylcholine, P-325. First identified in egg yolk, ox brain and soybean oil. Present throughout the animal and vegetable kingdoms. Used in food processing as an emulsifier and anti-sticking agent. The degree of unsaturation and chain length result in distinct physical and biol. props. Mammalian phosphatidylcholine usually has a saturated acyl group at *sn*-1 and and an unsaturated group at *sn*-2. The term lecithin is also used to describe a mixture of phosphatidyl esters isolated from vegetable oils and consisting mainly of phosphatidylcholine, -serine, -ethanolamine and -inositols with some triglycerides, fatty acids and carbohydrates. There is extensive proliferation of CAS numbers for phosphatidylcholines owing to specification of stereochemistry at different levels of precision in the literature.

Glycerol 1,2-dihexanoate 3-phosphocholine
[34506-67-7]
*4-Hydroxy-*N,N,N-*trimethyl-10-oxo-7-[(1-oxohexyl)oxy]-3,5,9-trioxa-4-phosphapentadecan-1-aminium inner salt 4-oxide, 9CI. Choline phosphate ester with 1,2-dihexanoin, 8CI*
$C_{20}H_{40}NO_8P$ 453.512
Hygroscopic powder. $[\alpha]_D$ +10.9 (c, 4.6 in H_2O).

Glycerol 1,2-didecanoate 3-phosphocholine
[13699-47-3]
[3436-44-0, 63700-87-8]
Didecanoylphosphatidylcholine. Dicaproylphosphatidylcholine
$C_{28}H_{56}NO_8P$ 565.726

Glycerol 1,2-didodecanoate 3-phosphocholine
[18194-25-7]
[18285-71-7, 18656-40-1, 127641-86-5]
Didodecanoylphosphatidylcholine. Dilauroylphosphatidylcholine
$C_{32}H_{64}NO_8P$ 621.833
Cryst. $[\alpha]_D$ +6.1 (c, 1.5 in $CHCl_3$/MeOH 1:1).

Glycerol 1,2-ditridecanoate 3-phosphocholine
[71242-28-9]
[75340-69-1]
Ditridecanoylphosphatidylcholine
$C_{34}H_{68}NO_8P$ 649.887
No phys. props. reported. CAS no. refers to the *R*-enantiomer.

Glycerol 1,2-ditetradecanoate 3-phosphocholine [18194-24-6]
[13699-48-4, 18656-38-7]
Dimyristoylphosphatidylcholine. 1,2-Ditetradecanoylglycero-3-phosphocholine

$C_{36}H_{72}NO_8P$ 677.94
Cryst. Mp 236-237°. $[\alpha]_D^{22}$ +7 (c, 10 in $CHCl_3$/MeOH 1:1). CAS no. and props. refer to *R*-enantiomer.

Glycerol 1,2-dipentadecanoate 3-phosphocholine [3355-27-9]

[67896-63-3]
Dipentadecanoylphosphatidylcholine

$C_{38}H_{76}NO_8P$ 705.994
No phys. props. reported. CAS no. refers to the *R*-enantiomer.

Glycerol 1-hexadecanoate 2-tetradecanoate 3-phosphocholine [63119-37-9]

[69441-09-4, 118043-53-1]
Palmitoylmyristoylphosphatidylcholine. 1-Hexadecanoyl-2-tetradecanoylglycero-3-phosphocholine

$C_{38}H_{76}NO_8P$ 705.994
No phys. props. reported.

Glycerol 2-hexadecanoate 1-tetradecanoate 3-phosphocholine [10589-50-1]

[69525-80-0, 102059-25-6]
Myristoylpalmitoylphosphatidylcholine. 1-Tetradecanoyl-2-hexadecanoylglycero-3-phosphocholine

$C_{38}H_{76}NO_8P$ 705.994
No phys. props. reported.
Launched 1994 (UK)

Glycerol 1,2-dihexadecanoate 3-phosphocholine [2644-64-6]

[63-89-8, 2797-68-4, 35418-55-4]
Dipalmitoylphosphatidylcholine. 1,2-Dihexadecanoylglycero-3-phosphocholine. 1,2-Dipalmitoylglycero-3-phosphocholine. ***Colfosceril palmitate, BAN, INN, USAN****. Exosurf. Surfexo. Dipalmitoyllecithin. BW 129Y83*

$C_{40}H_{80}NO_8P$ 734.048
Mp 235-236°. $[\alpha]_D^{25}$ +7 (c, 5.6 in $CHCl_3$). Props. refer to the *R*-enantiomer. Mixt. with palmitoyloleoylphosphatidylcholine (see below) also used (Pumactant, BAN), (ALEC).

Glycerol 1,2-diheptadecanoate 3-phosphocholine [70897-27-7]

[67896-64-4]
Diheptadecanoylphosphatidylcholine

$C_{42}H_{84}NO_8P$ 762.101

Glycerol 1-octadecanoate 2-dodecanoate 3-phosphocholine [82181-14-4]

[7276-39-3, 15071-88-2]
Octadecanoyldodecanoylphosphatidylcholine. Stearoyllauroylphosphatidylcholine

$C_{38}H_{76}NO_8P$ 705.994
Powder (Et_2O). Mp 211-212°.

Glycerol 2-octadecanoate 1-dodecanoate 3-phosphocholine [15071-88-2]

[127912-48-5]
Dodecanoyloctadecanoylphosphatidylcholine. Lauroylstearoylphosphatidylcholine

$C_{38}H_{76}NO_8P$ 705.994
Mp 225°. Mp refers to the racemate. The *R*-enantiomer has also been synthesised. The CAS no. was originally assigned to the 2-dodecanoyl 1-octadecanoyl isomer.

Glycerol 1-octadecanoate 2-hexadecanoate 3-phosphocholine [10589-48-7]

[59403-53-1]
Stearoylpalmitoylphosphatidylcholine. 2-Hexadecanoyl-1-octadecanoylglycero-3-phosphocholine

$C_{42}H_{84}NO_8P$ 762.101
No phys. props. reported.

Glycerol 2-octadecanoate 1-hexadecanoate 3-phosphocholine [10589-47-6]

[59403-51-9]
1-Hexadecanoyl-2-octadecanoylglycero-3-phosphocholine. Palmitoylstearoylphosphatidylcholine

$C_{42}H_{84}NO_8P$ 762.101
No phys. props. reported.

Glycerol 1,2-dioctadecanoate 3-phosphocholine [4539-70-2]

[816-93-3, 816-94-4, 66701-63-1]
1,2-Dioctadecanoylglycero-3-phosphocholine. Distearoylphosphatidylcholine

$C_{44}H_{88}NO_8P$ 790.155
Mp 231-232°. $[\alpha]_D^{29}$ +6.2 (c, 10 in $CHCl_3$/MeOH). Props. refer to the *R*-enantiomer.

Glycerol 2-(6-octadecenoate) 1-hexadecanoate 3-phosphocholine

[89187-00-8, 89187-01-9]
1-Hexadecanoyl-2-(6-octadecenoyl)glycero-3-phosphocholine. Palmitoylpetroselinoylphosphatidylcholine

$C_{42}H_{82}NO_8P$ 760.085
Cryst. ($Me_2CO/CHCl_3$).

Glycerol 1-(9-octadecenoate) 2-hexadecanoate 3-phosphocholine [59491-62-2]

[17118-56-8]
2-Hexadecanoyl-1-(9-octadecenyl)glycero-3-phosphocholine. Oleoylpalmitoylphosphatidylcholine

$C_{42}H_{82}NO_8P$ 760.085
No phys. props. reported. The oleoyl synonym refers to the biol. important *Z*-isomer. The CAS no. refers to the (*R,Z*)-form.

Glycerol 2-(9-octadecenoate)1-hexadecanoate 3-phosphocholine [26853-31-6]

[6753-55-5, 26662-91-9, 67738-47-0]
1-Hexadecanoyl-2-octadec-9-enoylglycero-3-phosphocholine. Palmitoyloleoylphosphatidylcholine

$C_{42}H_{82}NO_8P$ 760.085
No phys. props. reported. The oleoyl synonym refers to the biol. important *Z*-isomer. CAS no. refers to the (*R,Z*)-isomer.

Glycerol 1-(9-octadecenoate) 2-octadecanoate 3-phosphocholine [7319-55-3]

[7276-38-2]
2-Octadecanoyl-1-octadec-9-enoylglycero-3-phosphocholine. Oleoylstearoylphosphatidylcholine

$C_{44}H_{86}NO_8P$ 788.139
Mp 235°. $[\alpha]_D^{20}$ +6.2 (c, 10 in $CHCl_3$). The oleoyl synonym refers to the biol. important *Z*-isomer. CAS no. and phys. props. refer to the (*R,Z*)-enantiomer.

Glycerol 2-(9-octadecenoate) 1-octadecanoate 3-phosphocholine [6753-56-6]

[56421-10-4]
1-Octadecanoyl-2-octadec-9-enoylglycero-3-phosphocholine. Stearoyloleoylphosphatidylcholine

$C_{44}H_{86}NO_8P$ 788.139
Mp 230-231°. $[\alpha]_D^{20}$ +6 (c, 9 in $CHCl_3$). The oleoyl synonym refers to the biol. important *Z*-isomer.

Glycerol 1,2-di-9-octadecenoate 3-phosphocholine [4235-95-4]

[10015-85-7, 68737-67-7, 84366-67-6]
1,2-Di-9-octadecenoylglycerol-3-phosphocholine. Dioleoylphosphatidylcholine

$C_{44}H_{84}NO_8P$ 786.123
$[\alpha]_D$ +6.1 (c, 1.0 in $CHCl_3$/MeOH). CAS no. and oleoyl synonym refer to the biol. important (*R*)-(*Z,Z*)-isomer.

Glycerol 2-(11-octadecenoate) 1-hexadecanoate 3-phosphocholine [132295-25-1]

[128163-05-3]
Palmitoylvaccenoylphosphatidylcholine

$C_{42}H_{82}NO_8P$ 760.085
Cryst. ($Me_2CO/CHCl_3$).

Glycerol 1,2-di-(2*E*,4*E*-octadecadienoate) 3-phosphocholine [89617-87-8]

[76282-07-0, 77074-06-7, 107382-50-3, 123672-50-4]

$C_{44}H_{80}NO_8P$ 782.092
Mp 200-205°. Racemate.

Glycerol 1-(9,12-octadecadienoate) 2-hexadecanoate 3-phosphocholine [40541-15-9]

[61616-80-6]
2-Hexadecanoyl-1-(9,12-octadecadienoyl)-glycero-3-phosphocholine. Linoleoylpalmitoylphosphatidylcholine

$C_{42}H_{80}NO_8P$ 758.07
No phys. props. reported. The linoleoyl-palmitoyl synonym refers to the biol. important (*R*)-(*all-Z*)-isomer.

Glycerol 2-(9,12-octadecadienoate) 1-hexadecanoate 3-phosphocholine [17708-90-6]

[6931-84-6, 40811-94-7, 128114-92-1]
1-Hexadecanoyl-2-octadeca-9,12-dienoyl-glycero-3-phosphocholine. Palmitoyllinoleoylphosphatidylcholine

$C_{42}H_{80}NO_8P$ 758.07The palmitoyl synonym refers to (*Z,Z*)-geometry. The CAS no refers to the biol. important (*R*)-(*Z,Z*)-isomer.

Glycerol 1-(9,12-octadecadienoate) 2-octadecanoate 3-phosphocholine [85046-21-5]
1-Octadeca-9,12-dienoyl-2-octadecanoyl-glycero-3-phosphocholine. Linoleoyl-stearoylphosphatidylcholine

$C_{44}H_{84}NO_8P$ 786.123
Hygroscopic powder ($EtOH/Me_2CO$) (racemate).

Glycerol 2-(9,12-octadecadienoate) 1-octadecanoate 3-phosphocholine [27098-24-4]

[6753-53-3]
1-Octadecanoyl-2-octadeca-9,12-dienoyl-glycero-3-phosphocholine. Stearoyllinoleoylphosphatidylcholine

$C_{44}H_{84}NO_8P$ 786.123
Gelatinous. $[\alpha]_D^{20}$ +5.02. The linoleoyl synonym refers to the biol. important (*Z,Z*)-isomer. Phys. props. and CAS no. refer to the (*R*)-(*Z,Z*)-enantiomer.

Glycerol 1-(9,12-octadecadienoate) 2-(9-octadecenoate) 3-phosphocholine [816-95-5]

[17589-33-2]
1-Octadeca-9,12-dienoyl-2-octadec-9-enoylglycero-3-phosphocholine. Linoleoyloleoylphosphatdiylcholine

$C_{44}H_{82}NO_8P$ 784.107
Gelatinous. $[\alpha]_D^{20}$ +6.12. The linoleoyl synonym refers to the biol. important (*all-Z*)-isomer. Phys. props. and CAS no. refer to the (*R*)-(*all-Z*)-enantiomer.

Glycerol 1,2-di-9,12-octadecadienoate 3-phosphocholine [998-06-1]

[1188-55-2, 6542-05-8, 123672-49-1]
1,2-Dioctadeca-9,12-dienoylglycero-3-phosphocholine. Dilinoleoylphosphatidylcholine

$C_{44}H_{80}NO_8P$ 782.092
Gelatinous. Mp 232°. $[\alpha]_D^{20}$ +6.02. CAS no. and props. refer to the *R*-enantiomer.

Glycerol 2-(9,12,15-octadecatrienoate) 1-hexadecanoate 3-phosphocholine [17118-61-5]

[35418-56-5, 128114-93-2]
Palmitoyllinolenoylphosphatidylcholine

$C_{42}H_{78}NO_8P$ 756.054
No phys. props. reported. The linolenoyl synonym refers to the biol. significant (*all-Z*)-isomer.

Glycerol 2-(9,12,15-octadecatrienoate) 1-octadecanoate 3-phosphocholine [35418-57-6]
Octadecanoyl-9,12,15-octadecatrienoylphosphatidylcholine. Stearoyllinolenoylphosphatidylcholine

$C_{44}H_{82}NO_8P$ 784.107
No phys. props. reported. The linoleoyl synonym refers to the biol. important (*all-Z*)-isomer. The CAS no. refers to the (*R*)-(*all-Z*)-isomer.

Glycerol 1,2-di-9,12,15-octadecatrienoate 3-phosphocholine [2701-19-1]

[40811-59-4]
Dilinolenoylphosphatidylcholine

$C_{44}H_{76}NO_8P$ 778.06
No phys. props. reported. The synonym refers to the biologically important (*all-Z*)-isomer.

Glycerol 1,2-dinonadecanoate 3-phosphocholine [95416-27-6]
Dinonadecanoylphosphatidylcholine
$C_{46}H_{92}NO_8P$ 818.208
No phys. props. reported.

Glycerol 2-(8,11,14-eicosatrienoate) 1-hexadecanoate 3-phosphocholine [131907-73-8]
1-O-*Hexadecyl-2*-O-*dihomogammalinolenoylglycero-3-phosphocholine*
$C_{44}H_{84}NO_7P$ 770.124
Isol. from the Japanese oyster *Crassostrea gigas*.

Glycerol 2-(5,8,11,14-eicosatetraenoate) 1-hexadecanoate 3-phosphocholine [35418-58-7]

[6931-56-2, 68883-73-8]
1-Hexadecanoyl-2-eicosa-5,8,11,14-tetraenoylglycero-3-phosphocholine. Palmitoylarachidonoylphosphatidylcholine

$C_{44}H_{80}NO_8P$ 782.092CAS no. refers to (*R*)-(*all-Z*)-form which is the biol. significant one. The arachidonoyl synonym refers to (*all-Z*)-geometry.

Glycerol 2-(5*Z*,8*Z*,11*Z*,14*Z*-eicosatetraenate) 1-hexadecanoate 3-phosphocholine-*form* [86288-11-1]
2-O-*Arachidonoyl-1*-O-*hexadecylglycero-3-phosphocholine. Arachidonyl-PAF*

Glycerol 1,2-di-5,8,11,14-eicosatetraenoate 3-phosphocholine [17688-29-8]

[56782-48-0, 97334-99-1, 99782-35-1]
1,2-Diicosa-5,8,11,14-tetraenoylglycero-3-phosphocholine. Diarachidonoylphosphatidylcholine

$C_{48}H_{80}NO_8P$ 830.136
No phys. props. reported. Incorr. named in 9CI. The arachidonyl synonym refers to the biologically preferred (*all-Z*)-form, to which the CAS no. refers.

Glycerol 2-(5,8,11,14,17-eicosapentaenoate) 1-hexadecanoate 3-phosphocholine-*form* [132196-28-2]
2-O-*(5,8,11,14,17-Eicosapentaenoyl)-1*-O-*hexadecylglycero-3-phosphocholine*
Isol. from the Japanese oyster *Crassostrea gigas*.

Glycerol 2-(5,8,11,14-eicosatetraenoate) 1-octadecanoate 3-phosphocholine [35418-59-8]

[18892-74-5, 128114-96-5]
4-Hydroxy-N,N,N-*trimethyl-9-oxo-7-[[(1-oxooctadecyl)oxy]methyl]-3,5,8-trioxa-4-phosphaoctacosa-13,16,19,22-tetraen-1-aminiumhydroxide, inner salt, 4-oxide, 9CI. Arachidonoylstearoylphosphocholine*

$C_{46}H_{84}NO_8P$ 810.145The arachidonoyl synonym refers to the biol. important (*all-Z*)-form. The CAS no. refers to the (*R*)-(*all-Z*)-enantiomer.

Glycerol 2-(4,7,10,13,16,19-docosahexaenoate) 1-hexadecanoate 3-phosphocholine-*form* [97717-93-6]
2-O-*(4,7,10,13,16,19-Docosahexaenoyl)-1*-O-*hexadecylglycero-3-phosphocholine*
Isol. from the Japanese oyster *Crassostrea gigas*.

Glycerol 1,2-di-(10,12-tricosadiynoate) 3-phosphocholine [75898-24-7]

[76078-28-9, 116661-14-4]

$C_{54}H_{92}NO_8P$ 914.297

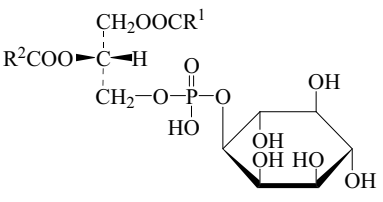
[70094-88-1]

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3-Phosphatidylinositol P-326

1,2-Diacylglycerol-3-phosphoinositol



Naturally occurring phosphatidylinositol is a 1,2-diacyl-*sn*-glycerol derivative of myoinositol 1-phosphate having various alkyl groups R^1 and R^2 which may be the same or different and may be saturated or unsaturated. The abs. config. of the natural form is *R*-glycero, D-myoinositol as illus. and the props given for individual members of the series refer to this isomer unless otherwise stated. Isol. from peas. Comprise about 5% of membrane phospholipid content of eukaryotes.

Glycerol 1,2-dihexadecanoate 3-phosphoinositol [86747-32-2]

[28154-40-7, 28366-80-5, 30595-06-3, 62742-56-7]
Dipalmitoylphosphatidylinositol

$C_{41}H_{79}O_{13}P$ 811.041
Solid ($CHCl_3$/Me_2CO) (as NH_4 salt). Mp 169-172° (NH_4 salt). $[\alpha]_D^{20}$ +7.48 (c, 0.3 in $CHCl_3$).

3-Phosphate: [165689-81-6]
$C_{41}H_{80}O_{16}P_2$ 891.021
Powder. $[\alpha]_D^{23}$ -1.2 (c, 0.4 in $CHCl_3$).

4-Phosphate: [57606-15-2]
$C_{41}H_{80}O_{16}P_2$ 891.021
Solid (as tri-NH_4 salt). Mp 197-205° (tri-NH_4 salt).

3,4-Diphosphate: [165883-85-2]
$C_{41}H_{81}O_{19}P_3$ 971.001
Powder. $[\alpha]_D^{23}$ +1.9 (c, 0.5 in $CHCl_3$).

4,5-Diphosphate: [120595-88-2]
$C_{41}H_{81}O_{19}P_3$ 971.001
No phys. props. reported.

3,4,5-Triphosphate: [165689-82-7]

[55093-25-9]
$C_{41}H_{82}O_{22}P_4$ 1050.981
Powder. $[\alpha]_D^{23}$ +3.7 (c, 0.5 in $CHCl_3$).

Glycerol 1,2-dioctadecanoate 3-phosphoinositol [73208-79-4]

[142128-86-7] *Inositol 1-[2,3-bis(1-oxooctadecyl)oxy]propyl hydrogen phosphate. Distearoylphosphatidylinositol*
$C_{45}H_{87}O_{13}P$ 867.148
Cryst. (butanol). Mp 135-137°.

NH_4 salt:
Solid ($CHCl_3$/Me_2CO). Mp 180-182° (softens at 92°). $[\alpha]_D^{20}$ +7.1 (c, 0.025 in $CHCl_3$/MeOH).

3,4,5-Triphosphate: [154115-24-9]

[155239-93-3]
$C_{45}H_{90}O_{22}P_4$ 1107.088
Waxy solid. $[\alpha]_D^{21}$ +30.4 (c, 0.7 in $CHCl_3$) (as triethylammonium salt).

Glycerol 1,2-di-9*Z*,12*Z*-octadecadienoate 3-phosphoinositol [122921-66-8]

[106140-13-0, 119479-58-2, 120574-70-1] *Dilinoleoylphosphatidylinositol*
$C_{45}H_{79}O_{13}P$ 859.085
No phys. props. reported.

Glycerol 1-dodecanoate 2-(9*Z*-octadecenoate) 3-phosphoinositol [182509-32-6]

[34290-58-9] myo-*Inositol 1-[2-[(1-oxo-9-octadecenyl)oxy]]-3-[(1-oxododecyl)oxy]propyl hydrogen phosphate. Lauroyloleoylphosphatidylinositol*
$C_{39}H_{73}O_{13}P$ 780.972
No phys. props. reported.

Glycerol 1-hexadecanoate 2-(9*Z*-octadecenoate) 3-phosphoinositol [51547-49-0]

[50730-13-7, 58958-02-4] *Palmitoyloleoylphosphatidylinositol*
$C_{43}H_{81}O_{13}P$ 837.079
Cryst. ($CHCl_3$/EtOH) (as NH_4 salt). Mp 172-174° (NH_4 salt). $[\alpha]_D$ +9.2 (c, 0.4 in $CHCl_3$) (NH_4 salt). Other stereoisomers known.

4-Phosphate: [58956-15-3]

[60873-63-4]
$C_{43}H_{82}O_{16}P_2$ 917.059
Cryst. ($CHCl_3$/MeOH) (as tri-NH_4 salt). Mp 187° (tri-NH_4 salt). $[\alpha]_D$ +1.8 (c, 0.3 in $CHCl_3$). Props. refer to the synthetic DL-myoinositol isomer.

Glycerol 1-octadecanoate 2-(9-octadecenoate) 3-phosphoinositol [58116-17-9]

[55093-27-1, 58165-70-1, 83709-18-6, 99147-36-1] *Stearoyloleoylphosphatidylinositol*
$C_{45}H_{85}O_{13}P$ 865.132
Mp 174-176° (as Na salt). $[\alpha]_D^{20}$ +6.4 (c, 0.1 in $CHCl_3$).

Glycerol 1-(9,12-octadecadienoate) 2-(9-octadecenoate) 3-phosphoinositol
$C_{45}H_{81}O_{13}P$ 861.101

Glycerol 2-(5*Z*,8*Z*,11*Z*,14*Z*-eicosatetraenoate) 1-octadecanoate 3-phosphoinositol
[64681-91-0] *Stearoylarachidonoylphosphatidylinositol*
$C_{47}H_{83}O_{13}P$ 887.139

3,4,5-Triphosphate: [194924-60-2]

[227957-76-8]
$C_{47}H_{86}O_{22}P_4$ 1127.078

[119943-95-2]

Davies, J.H. *et al., Chem. Ind. (London)*, 1959, 1155-1156 (*dioctadecanoyl*)
Ansell, G.B. *et al., Phospholipids: Chemistry, Metabolism and Function*, Elsevier, 1964, 85-113 (*bibl, isol*)
Klyashchitskii, B.A. *et al., Tet. Lett.*, 1970, 587-590 (*dihexadecanoyl*)
Gent, P.A. *et al., Tet. Lett.*, 1970, 2575-2578 (*dihexadecanoyl*)
Zhelvakova, E.G. *et al., Zh. Obshch. Khim.*, 1970, **40**, 248; *J. Gen. Chem. USSR (Engl. Transl.)*, 1970, **40**, 227 (*dihexadecanoyl*)
Molotkovsky, J.G. *et al., Chem. Phys. Lipids*, 1973, **11**, 135-147 (*dodecanoyloleoyl, hexadecanoyloleoyl*)
Form and Function of Phospholipids, (eds. Ansell, G.B. *et al*), Elsevier, 1973, (*book*)
Lyutik, A.Y. *et al., Zh. Obshch. Khim.*, 1974, **44**, 2573-2576; 2595-2596; *J. Gen. Chem. USSR (Engl. Transl.)*, 1974, **44**, 2530-2533; 2559 (*dihexadecanoyl, octadecanoyloleoyl*)
Sadovnikova, M.S. *et al., Bioorg. Khim.*, 1975, **1**, 17-24; *CA*, **83**, 131855 (*dihexadecanoyl*)
Shevchenko, V.P. *et al., Chem. Phys. Lipids*, 1975, **15**, 95-104 (*hexadecanoyloleoyl*)
Lyutik, A.Y. *et al., CA*, 1976, **84**, 59900 (*octadecanoyloleoyl*)
Sadovnikova, M.S. *et al., Zh. Obshch. Khim.*, 1976, **46**, 1389-1394; *J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 1365-1370 (*hexadecanoyloleoyl*)
Shevchenko, V.P. *et al., CA*, 1977, **86**, 190385 (*dioctadecanoyl*)
Sukhanov, V.A. *et al., Zh. Obshch. Khim.*, 1977, **47**, 2130-2136; *J. Gen. Chem. USSR (Engl. Transl.)*, 1977, **47**, 1943-1974 (*dihexadecanoyl*)
Krylova, V.N. *et al., Zh. Org. Khim.*, 1979, **15**, 2323-2326; *J. Org. Chem. USSR (Engl. Transl.)*, 1979, **15**, 2104-2106 (*dioctadecanoyl*)

Ansell, G.B. *et al., Phospholipids*, (eds. Hawthorne, J.N. *et al*), Elsevier, 1982, 1-49 (*rev*)
Cevc, G. *et al., Phospholipid Bilayers*, Wiley-Interscience, 1987, (*book*)
Japan. Pat., 1988, 88 185 990; *CA*, **110**, 135643x (*dilinoleoyl*)
Martin, S.F. *et al., Tet. Lett.*, 1988, **29**, 3631-3634 (*synth*)
Ward, J.G. *et al., Tet. Lett.*, 1988, **29**, 6013-6016; 1989, **30**, 5353-5356 (*dihexadecanoyl*)
Dreef, C.E. *et al., Tet. Lett.*, 1988, **29**, 6513-6516 (*dihexadecanoyl*)
Phospholipids: Biochemical, Pharmaceutical and Analytical Considerations, (eds. Hanin, I. *et al*), Plenum Press, 1990, (*synth, anal, biochem, use, rev*)
Olsson, N.U. *et al., J. Chromatogr.*, 1992, **600**, 257-266 (*gc*)
Phospholipids Handbook, (ed. Cevc, G.), M. Dekker, 1993, (*book*)
Young, R.C. *et al., Eur. J. Med. Chem. (Chim. Ther.)*, 1994, **29**, 538-549 (*dihexadecanoyl*)
Paltauf, F. *et al., Prog. Lipids Res.*, 1994, **33**, 239-328 (*synth, rev*)
Kent, C. *et al., Annu. Rev. Biochem.*, 1995, **64**, 315-343 (*biosynth, rev*)
Watanabe, Y. *et al., Tetrahedron*, 1995, **51**, 8969-8976 (*dioctadecanoyl*)
Biochemistry of Lipids, Lipoproteins and Membranes, (eds. Vance, D.E. *et al*), Elsevier, 1996, (*biochem, rev*)
Tolibaev, I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 7-10 (*occur*)
Wang, D.-S. *et al., J.O.C.*, 1996, **61**, 5905-5910 (*dihexadecanoyl*)
Desai, T. *et al., Synthesis in Lipid Chemistry*, (ed. Tyman, J.H.P.), Royal Society of Chemistry, 1996, 67-92 (*phosphates, synth, rev*)
Biochim. Biophys. Acta, 1997, **1348**, 1-256 (*biochem, biosynth, rev*)
Grove, S.J.A. *et al., Chem. Comm.*, 1997, 1635-1636 (*dihexadecanoyl*)
McKeone, B.J. *et al., J. Lipid Res.*, 1997, **38**, 429-436 (*hplc, bibl*)
Stokoe, D. *et al., Science (Washington, D.C.)*, 1997, **277**, 567-570; 1998, **279**, 710-714 (*3,4,5-triphosphate, occur, activity*)
Aneja, S.G. *et al., Tet. Lett.*, 1997, **38**, 803-806 (*dihexadecanoyl*)
Watanabe, Y. *et al., Tetrahedron*, 1999, **55**, 9743 (*3,4,5-triphosphate, synth*)
Gaffney, P.R.J. *et al., J.C.S. Perkin 1*, 2001, 192-205 (*3,4,5-triphosphate, synth*)
Kubiak, R.J. *et al., J.O.C.*, 2003, **68**, 960-968 (*synth*)

Phosphine, 9CI, 8CI P-327

[7803-51-2]

Hydrogen phosphide. Phosphorus trihydride. Phosphorus hydride (PH_3). Phosphane

PH_3

H_3P 33.997

Interatomic distances: P–H 141.5, 143.7 pm, angle: 93.3-93.8° (gas). At -140°, has f.c.c. struct.. Fumigant for cereals, flour, packaged foods. Colourless gas with garlic-like odour. Extremely weak base. V. sol. H_2O (giving neutral soln.). d_4^{-135} 0.9 d_4^{-90} 0.75. Mp -132.5°. Bp -87°. Dec. noticeably only at >550°. Forms complexes with boron hydrides and halides. Solid form exhibits transitions at -263°, -243°, -224°, -185°.

► Extremely poisonous. Ignites in dry air at *ca*. 150° or spont. at r.t. if P_2H_4 present. SY7525000

BH_3 adduct (1:1): See Trihydro(phosphine)boron in *The Combined Chemical Dictionary.*

$BHCl_2$ adduct (1:1):
BCl_2H_4P 116.722
Cryst. Mp 68°.

BCl_3 adduct (1:1):
BCl_3H_3P 151.167
Colourless, well-defined cryst.

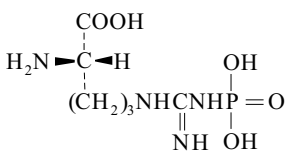
BBr_3 adduct (1:1):
BBr_3H_3P 284.52
Solid.

[13967-14-1, 16749-13-6]

Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, 7 (*rev, bibl*)
Fluck, E. *et al., Fortschr. Chem. Forsch.*, 1969, **13**, 125; 1973, **35**, 1 (*rev, bibl*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1971, **8/III**, 272 (*rev*)
Francia, M.D. *et al., J. Chem. Phys.*, 1973, **58**, 1061 (*ir*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 510 (*synth*)
Huang, T.H. *et al., J. Phys. Chem. Solids*, 1977, **38**, 897 (*ir, Raman*)
Jameson, A.K. *et al., J. Magn. Reson.*, 1978, **32**, 455 (*P-31 nmr*)
Friedrich, H. *et al., Chem. Phys. Lett.*, 1979, **64**, 360 (*pe*)
Dolenko, G.N. *et al., Zh. Strukt. Khim.*, 1979, **20**, 334; *J. Struct. Chem. (Engl. Transl.)*, 1979, **20**, 279 (*x-ray fluorescence*)
Baldacca, A. *et al., J. Mol. Spectrosc.*, 1980, **81**, 179 (*ir*)
Tarrago, G. *et al., J. Mol. Spectrosc.*, 1981, **88**, 311 (*ir*)
Ishiguro, E. *et al., J. Phys. B: At., Mol. Opt. Phys.*, 1987, **20**, 4725 (*photoabs spectrum*)
Gassmann, G. *et al., Angew. Chem., Int. Ed.*, 1993, **32**, 761 (*synth*)
Pharmaceutical Manufacturing Encyclopaedia, 1997, No. 574 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PGY000

Phosphoarginine P-328

N^5-*[Imino(phosphonoamino)methyl]ornithine, 9CI.* N^5-*(Phosphonoamidino)ornithine, 8CI.* N-*Phosphonoarginine*



$C_6H_{15}N_4O_5P$ 254.182
Mp 175-180°.

(*S*)-*form* [1189-11-3]
L-form
Constit. of crayfish muscle. Cryst. + $2H_2O$ (Me_2CO aq.). Mp 175-180°. Stored as Ba salt; rapidly dec. at -10° in free state.

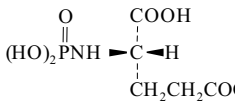
P,P-*Dibenzyl ester,* C-*Me ester:Dibenzyl [[[(4-amino-4-methoxycarbonyl)butyl]amino](imino)methyl]phosphoramidate*
$C_{21}H_{29}N_4O_5P$ 448.458
Solid. Mp 91-93°.

(±)-*form*
Cryst. (Me_2CO aq.). Mp 175-180°.

Si-Oh, L. *et al., J.A.C.S.*, 1955, **77**, 1866 (*ester*)
Cramer, F. *et al., Chem. Ber.*, 1962, **95**, 1670 (*synth*)
Marcus, F. *et al., Biochem. J.*, 1964, **92**, 429 (*isol, synth*)
Poat, P.C. *et al., Biochim. Biophys. Acta*, 1980, **613**, 410 (*synth*)

N-Phosphoglutamic acid P-329

2-[(Dihydroxyphosphinyl)amino]pentanedioic acid. 2-Phosphoramidopentanedioic acid. 2-Phosphoramidoglutaric acid. Phaseotoxin A. N-*Phosphonoglutamic acid*



(*S*)-*form*

$C_5H_{10}NO_7P$ 227.11

(*S*)-*form* [59360-03-1]
L-form

P,P-*Di-Me ester,* C,C-*diamide:2-[(Dimethoxyphosphinyl)amino]pentanedioic diamide*
$C_7H_{16}N_3O_5P$ 253.194
Solid. Mp 117-120° dec.

P,P-*Dibenzyl ester,* C,C-*di-Me ester:Dimethyl 2-[(dibenzyloxyphosphinyl)amino]pentanedioate*
$C_{21}H_{26}NO_7P$ 435.413
Viscous oil.

Tetrabenzyl ester:Dibenzyl 2-[(dibenzyloxyphosphinyl)amino]pentanedioate
$C_{33}H_{34}NO_7P$ 587.608
Waxy solid. Mp 45-47°.

(±)-*form*

P,P-*Diphenyl ester,* C,C-*di-Et ester:Diethyl 2-[(diphenoxyphosphinyl)amino]pentanedioate*
$C_{21}H_{26}NO_7P$ 435.413
Solid. Mp 73.5-74°.

Sciarini, L.J. *et al., J.A.C.S.*, 1949, **71**, 2940 (*synth*)
Li, S.-O. *et al., J.A.C.S.*, 1955, **77**, 1866 (*synth*)
Patil, S.S. *et al., Biochem. Biophys. Res. Commun.*, 1976, **69**, 1019-1027 (*isol, synth*)
Smith, A.G. *et al., Physiol. Plant Pathol.*, 1979, **15**, 269-278 (*synth, ir, props*)

Phospholipase A_2 P-330

[81317-15-9]

Human pancreatic juice activation peptide

H-Asp-Ser-Gly-Ile-Ser-Pro-Arg-OH

$C_{29}H_{50}N_{10}O_{12}$ 730.774

Grataroli, R. *et al., Eur. J. Biochem.*, 1982, **122**, 111 (*struct*)

Phosphoric acid, 9CI, 8CI, USAN P-331

[7664-38-2]

Orthophosphoric acid. Trihydroxo oxophosphorus(V). E338. FEMA 2900

$(HO)_3P{=}O$

H_3O_4P 97.995

A strong tribasic acid. Possesses a H-bonded layer struct. in which each molecule is linked to six others. Found in fruit juices. Used in foods as an acidulant for drinks and candies, pH control agent, buffering agent, flavour

enhancer, flavouring agent, sequestrant, stabiliser and thickener, and synergist. Colourless cryst. or syrup. Misc. H_2O, many org. solvs. d 1.86. Mp 42.3°. n_D^{20} 1.4503. pK_{a1} 2.15; pK_{a2} 7.2; pK_{a3} 12.4 (H_2O). Melts to a syrup and may be supercooled to a glass which yields a second cryst. form at -54°, reverting at -6° to the form stable at r.t. Complexes with a wide variety of compds. e.g. ketones and ethers. When heated strongly partial dehydration → Diphosphoric acid.

► OES: long-term 1 mg m^{-3}; short-term 3 mg m^{-3}. Eye, skin and respiratory tract irritant. Conc. solns. corrosive. LD_{50} (rat, orl) 1530 mg/kg. TB6300000

[14066-19-4, 14066-20-7, 14335-33-2, 39456-59-2]

Inorg. Synth., 1939, **1**, 101 (*synth*)
Beveridge, G.S.G. *et al., Chem. Process. Eng. (Bombay)*, 1968, **49**, 6; 63 (*manuf*)
Slack, A.V. *et al., Phosphoric Acid*, E. Arnold, London, 1968, (*rev*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 528 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **17**, 426
Blessing, R.H. *et al., Acta Cryst. B*, 1988, **44**, 334; 1989, **45**, 200 (*cryst struct*)
Hayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 2429 (*P-31 nmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1401
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2211-2215
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1492
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 4190
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 478
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1015
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PHB250

Phosphoryl chloride, 9CI, 8CI P-332

[10025-87-3]
Trichlorophosphine oxide. Trichlorooxophosphorus(V). Phosphorus oxychloride

$P(O)Cl_3$

Cl_3OP 153.331

Pyramidal. In solid, forms infinite chains through Cl–O bonding. Interatomic distances: P–Cl 198, P=O 146 (solid); P–Cl 199.3, P=O 144.6 pm (vapour); angles: OPCl 114.9°, ClPCl 103.3°. Etherification and esterification agent for modification of food starch. Colourless mobile fuming liq. d_4^0 1.71 d_4^{25} 1.67. Mp 1-1.5°. Bp 107-107.5°. ΔH_{298}° -561(g), -601(l) kJ mol^{-1} V. reactive to nucleophiles. Hydrolysed rapidly by H_2O at r.t. Readily complexes through P=O bond.

► V. pungent vapour. Lachrymator. TH4897000

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1691C (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 16, 1965, 458 (*rev, bibl*)
Olie, K. *et al., Acta Cryst. B*, 1971, **27**, 1459 (*cryst struct*)
Moritani, T. *et al., Inorg. Chem.*, 1971, **10**, 344 (*ed, struct*)
Burgos, A. *et al., J. Mol. Struct.*, 1971, **9**, 283 (*ir, Raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1971, **8/III**, 458; 1153 (*rev*)
Li, Y.S. *et al., J. Mol. Struct.*, 1972, **14**, 261 (*microwave*)
Cavell, R.G. *et al., Inorg. Chem.*, 1975, **14**, 2828 (*pe*)
Grossman, G. *et al., Z. Chem.*, 1976, **16**, 362 (*O-17 nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **17**, 511 (*rev*)
Barlos, K. *et al., Chem. Ber.*, 1980, **113**, 3716 (*Cl-35 nmr*)
Filguiera, R.R. *et al., Spectrochim. Acta A*, 1980, **36**, 745 (*ir, Raman*)
Carpenter, J.H. *et al., J. Mol. Spectrosc.*, 1983, **101**, 306 (*microwave*)
Gupta, S.R. *et al., Spectrochim. Acta A*, 1983, **39**, 529 (*Raman*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 249 (*use*)
Nefedov, V.I. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1988, **46**, 381 (*pe, Auger*)
Firth, S. *et al., J. Mol. Spectrosc.*, 1988, **127**, 209 (*microwave*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2215-2216
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1042
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PHQ800

Phosvitin P-333

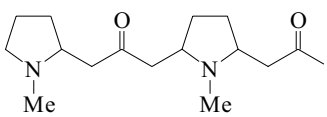
[9008-96-2]

Phosphoprotein. Isol. from egg yolk.

Mecham, D.K. *et al., J.A.C.S.*, 1949, **71**, 3670-3679 (*isol*)
Sato, K. *et al., Am. J. Physiol.*, 1962, **203**, 1170-1172 (*pharmacol*)
Belitz, H.D. *et al., Angew. Chem., Int. Ed.*, 1964, **3**, 645 (*amino acid sequence*)
Grizzuti, K. *et al., J. Biol. Chem.*, 1970, **245**, 2573-2578 (*conformn*)
Kuksis, A. *et al., Biochim. Biophys. Acta*, 1992, **1124**, 205-222 (*rev*)

Phygrine P-334

[148139-97-3]



$C_{16}H_{28}N_2O_2$ 280.409

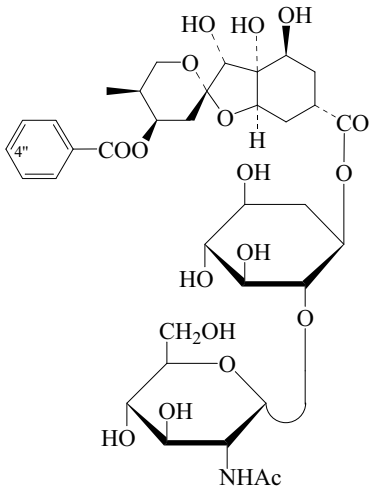
Alkaloid from roots and aerial parts of *Physalis alkekengi* (winter cherry), the famine food *Physalis angulata* (cutleaf ground cherry), *Physalis philadelphica* (tomatillo), *Physalis peruviana* (Cape gooseberry), *Physalis pubescens* (ground cherry) and *Physalis pruinosa* (strawberry tomato). Gum.

Dipicrate: [148218-52-4]
Mp 189° dec.

Basey, K. *et al., Phytochemistry*, 1992, **31**, 4173 (*isol, ir, pmr, cmr, ms, struct*)

Phyllanthusol B P-335

[294864-89-4]



$C_{35}H_{49}NO_{18}$ 771.768

Constit. of *Phyllanthus acidus* (otaheite gooseberry). Amorph. solid. Mp 183-185°. $[\alpha]_D^{28}$ -18.4 (c, 0.77 in H_2O). λ_{max} 200 (log ϵ 4.1); 231 (log ϵ 4) (H_2O).

4''-Hydroxy: [294864-88-3] ***Phyllanthusol A***

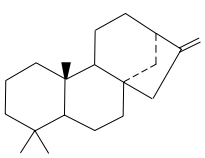
$C_{35}H_{49}NO_{19}$ 787.767

Constit. of *Phyllanthus acidus* (otaheite gooseberry). Amorph. solid. Mp 187-191°. $[\alpha]_D^{28}$ -7.4 (c, 1.82 in H_2O). λ_{max} 202 (log ϵ 4.2); 257 (log ϵ 4.1) (H_2O).

Vongvanich, N. *et al., J.O.C.*, 2000, **65**, 5420-5423 (*isol, pmr, cmr*)

16-Phyllocladene P-336

[20070-61-5]
Phyllocladene. *Dacrene. Sciadopitene*



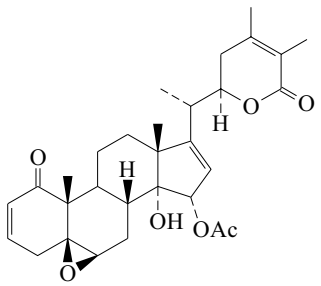
$C_{20}H_{32}$ 272.473

Constit. of sunflower oil. Cryst. (MeOH). Mp 98°. $[\alpha]_D^{25}$ +15.8 ($CHCl_3$).

Kitahara, Y. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 890 (*pmr*)
Shimagaki, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1209 (*synth, bibl*)
Manh, D.K. *et al., J. Chem. Res., Synop.*, 1978, 22 (*synth, bibl*)

Physagulin A P-337

[146713-98-6]

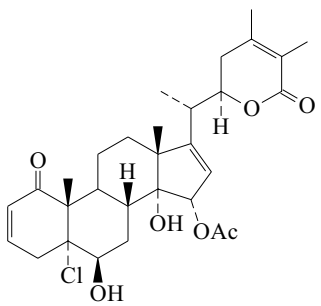


$C_{30}H_{38}O_7$ 510.626
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Powder. $[\alpha]_D$ +134.9 (c, 0.56 in MeOH).

Shingu, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2088 (*isol, pmr, cmr*)

Physagulin B P-338

[146713-97-5]

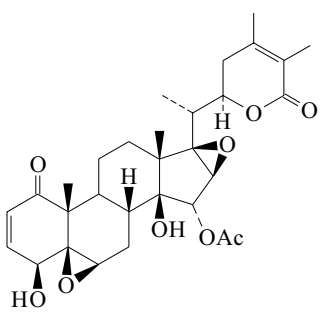


$C_{30}H_{39}ClO_7$ 547.087
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Powder. $[\alpha]_D$ +159.5 (c, 0.87 in $CHCl_3$).

Shingu, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2088 (*isol, pmr, cmr*)

Physagulin C P-339

[136997-67-6]

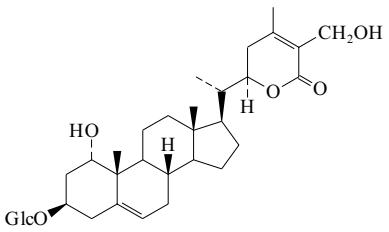


$C_{30}H_{38}O_9$ 542.625
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (butanol aq.). Mp 242.5-243°. $[\alpha]_D^{31}$ +105.8 (c, 0.52 in MeOH).

Shingu, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1591 (*isol, pmr, cmr, cryst struct*)

Physagulin D P-340

[146713-92-0]

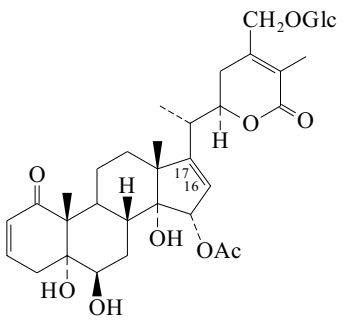


$C_{34}H_{52}O_{10}$ 620.779
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Powder. $[\alpha]_D$ +21 (c, 0.8 in MeOH).

Shingu, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2088 (*isol, pmr, cmr*)

Physagulin E P-341

[148054-13-1]



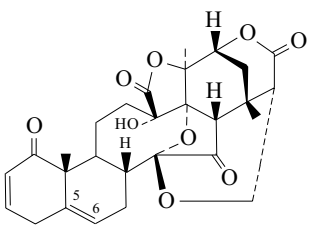
$C_{36}H_{50}O_{14}$ 706.783
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Powder. $[\alpha]_D$ +56.7 (c, 0.66 in MeOH).

16β,17β-Epoxide: [148076-22-6] ***Physagulin G***
$C_{36}H_{50}O_{15}$ 722.782
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Powder. $[\alpha]_D$ +31.3 (c, 0.76 in MeOH).

Shinga, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2448 (*isol, pmr, cmr*)

Physalin B P-342

[23133-56-4]



$C_{28}H_{30}O_9$ 510.54
Constit. of *Physalis alkekengi* (winter cherry). Cryst. (MeOH). Poorly sol. hexane. Mp 271°. Log P -0.67 (uncertain value) (calc). λ_{max} 222 (ϵ 10000) (EtOH) (Berdy).

5α,6α-Epoxide: [57517-46-1] ***Physalin J***
$C_{28}H_{30}O_{10}$ 526.539
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. ($CHCl_3$/MeOH). Mp 268-270°. $[\alpha]_D$ -60 (c, 0.5 in Me_2CO).

5β,6β-Epoxide: [57423-71-9] ***Physalin F***
$C_{28}H_{30}O_{10}$ 526.539
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH/Me_2CO). Mp 295-296° (262-264°). $[\alpha]_D$ -60.7 (c, 0.17 in $CHCl_3$). $[\alpha]_D$ -20 (c, 0.5 in Me_2CO). λ_{max} 218 (MeOH) (Berdy).

7α-Hydroxy: [70286-65-6] ***Physalin N***
$C_{28}H_{30}O_{10}$ 526.539
Constit. of *Physalis alkekengi* (winter cherry). Prisms (2-propanol). Mp 252-254°. $[\alpha]_D^{24}$ -124 (c, 0.14 in Me_2CO).

5,6-Dihydro, 5α-chloro, 6β-hydroxy: [70241-09-7] ***Physalin H***
$C_{28}H_{31}ClO_{10}$ 563
From the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH). Mp 238-240°. Struct. revised in 1995. Formerly assigned as $C_{28}H_{30}O_{10}$ (7β-hydroxyphysalin B) λ_{max} 226 (ϵ 6918) (MeOH) (Berdy).

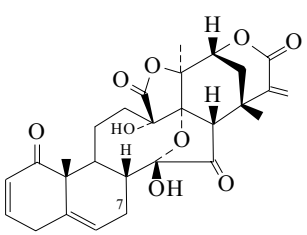
5,6-Dihydro, 6β-hydroxy, 5α-ethoxy:
$C_{30}H_{36}O_{11}$ 572.608
Artifact isol. from *Physalis alkekengi* (winter cherry). Needles (MeOH). Mp 224-226°. $[\alpha]_D^{25}$ -88 (c, 0.15 in Me_2CO).

5,6-Dihydro, 5α-hydroxy, 6β-ethoxy: Physalin L (incorr.)
$C_{30}H_{36}O_{11}$ 572.608
Needles (MeOH/Me_2CO). Mp 193-197°. $[\alpha]_D^{20}$ -70 (c, 0.14 in MeOH).

Matsuura, T. *et al., J.C.S.(C)*, 1970, 664 (*struct*)
Glotter, E. *et al., J.C.S. Perkin 1*, 1975, 1370 (*isol*)
Row, L.R. *et al., Phytochemistry*, 1978, **17**, 1641; 1647 (*isol, struct*)
Antoun, M.D. *et al., J. Nat. Prod.*, 1981, **44**, 579 (*isol*)
Kawai, M. *et al., Phytochemistry*, 1992, **31**, 4299 (*Physalin N*)
Makino, B. *et al., J. Nat. Prod.*, 1995, **58**, 1668 (*Physalin H, struct*)
Kawai, M. *et al., Phytochemistry*, 1996, **43**, 661 (*artifacts*)
Karikas, G.A. *et al., Fitoterapia*, 1998, **69**, 468-469 (*Physalin B, pmr*)

Physalin C P-343

[27503-33-9]



$C_{28}H_{30}O_9$ 510.54
Constit. of the winter cherry (*Physalis alkekengi*). Cryst. (EtOAc). Mp 274-277°. λ_{max} 218 (ϵ 8000) (MeOH) (Berdy).

25α,27-Dihydro: [80154-53-6] ***25,27-Dihydrophysalin C***

$C_{28}H_{32}O_9$ 512.555
Cryst. (MeOH). Poorly sol. hexane. Mp 230-234°. $[\alpha]_D$ -114 (c, 0.057 in EtOH). λ_{max} 220 (ϵ 7100) (EtOH) (Berdy).

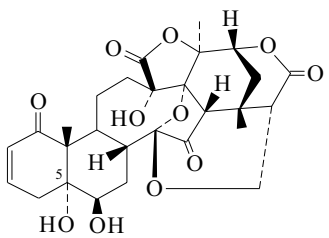
7α-Hydroxy: [23027-91-0] ***Physalin A***
$C_{28}H_{30}O_{10}$ 526.539
From *Physalis alkekengi* (winter cherry). Cryst. ($CHCl_3$/MeOH). Mp 266°. $[\alpha]_D$ -173 (c, 0.2 in EtOH). λ_{max} 218 (ϵ 10000) (MeOH) (Berdy).

7α-Hydroxy, 25α,27-dihydro: [120849-18-5] ***Physalin O***
$C_{28}H_{32}O_{10}$ 528.555
Constit. of *Physalis alkekengi* (winter cherry). Needles (Me_2CO). Mp 272-273°. $[\alpha]_D^{24}$ -115 (c, 0.1 in Me_2CO).

Kawai, M. *et al., J.C.S.(B)*, 1970, 812 (*deriv, cryst struct*)
Matsuura, T. *et al., J.C.S.(C)*, 1970, 664 (*deriv*)
Kawai, M. *et al., Tetrahedron*, 1970, **26**, 1743 (*isol*)
Antoun, M.D. *et al., J. Nat. Prod.*, 1981, **44**, 579 (*25,27-dihydro*)
Kawai, M. *et al., Phytochemistry*, 1992, **31**, 4299 (*Physalin O*)
Sunayama, R. *et al., Phytochemistry*, 1993, **34**, 529 (*Physalin A, pmr, cmr*)

Physalin D P-344

[54980-22-2]



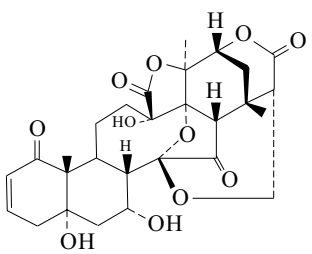
$C_{28}H_{32}O_{11}$ 544.554
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (Me_2CO/MeOH). Poorly sol. hexane. Mp 286-287°. $[\alpha]_D$ -68 (MeOH). Log P -2.61 (uncertain value) (calc).

5-Me ether: ***Physalin I***
$C_{29}H_{34}O_{11}$ 558.581
From the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH). Mp 305-307°. $[\alpha]_D$ +12 (c, 0.5 in Me_2CO).

Alluri, R.R. *et al., J. Nat. Prod.*, 1976, **39**, 405
Row, L.R. *et al., Phytochemistry*, 1980, **19**, 1175

Physalin E P-345

[70241-10-0]



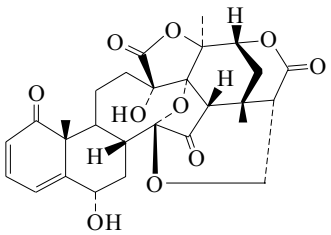
$C_{28}H_{32}O_{11}$ 544.554
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH). Mp 305-307°. $[\alpha]_D$ -83 (c, 0.5 in $CHCl_3$).

7-Ac: [70255-21-9] *Physalin E acetate*
$C_{30}H_{34}O_{12}$ 586.591
Constit. of *Physalis pubescens* (ground cherry).

Row, L.R. *et al., Phytochemistry*, 1978, **17**, 1641; 1984, **23**, 427

Physalin G P-346

[76045-38-0]

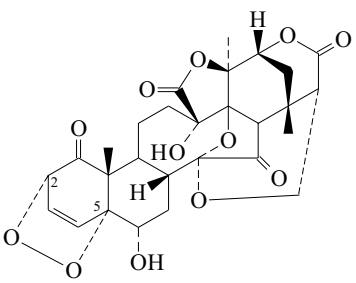


$C_{28}H_{30}O_{10}$ 526.539
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (Me_2CO). Mp 295-296°. $[\alpha]_D$ +17 (c, 0.5 in Me_2CO).

Row, L.R. *et al., Phytochemistry*, 1980, **19**, 1175

Physalin K P-347

[76045-35-7]



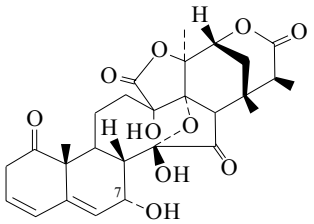
$C_{28}H_{30}O_{12}$ 558.538
Struct. revised in 1995. Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (Me_2CO/MeOH). Mp 280-282°. $[\alpha]_D$ -224 (c, 0.04 in MeOH).

2,5-Diepimer: [161407-65-4] ***Physalin Q***
$C_{28}H_{30}O_{12}$ 558.538
Constit. of *Physalis alkekengi* (winter cherry). Needles (Me_2CO). Mp 300°. $[\alpha]_D^{20}$ +38 (c, 0.06 in MeOH).

Row, L.R. *et al., Phytochemistry*, 1980, **19**, 1175 (*isol*)
Makino, B. *et al., Bull. Chem. Soc. Jpn.*, 1995, **68**, 219 (*isol, struct*)

Physalin L P-348

[113146-74-0]



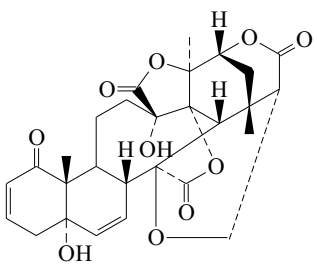
$C_{28}H_{32}O_{10}$ 528.555
Constit. of *Physalis alkekengi* (winter cherry). Cryst. (propan-2-ol). Mp 248-249°. $[\alpha]_D^{24}$ -118 (c, 0.3 in Me_2CO). λ_{max} 226 (ϵ 10300) (MeOH) (Berdy).

7-Deoxy: [117591-92-1] ***Physalin M***
$C_{28}H_{32}O_9$ 512.555
Constit. of *Physalis alkekengi* (winter cherry). Cryst. (propan-2-ol). Mp 224-227°. $[\alpha]_D^{24}$ -106 (c, 0.34 in Me_2CO). λ_{max} 228 (ϵ 11000) (MeOH) (Berdy).

Kawai, M. *et al., Phytochemistry*, 1987, **26**, 3313 (*Physalin L*)
Kawai, M. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 2696 (*Physalin M*)
Sunayama, R. *et al., Phytochemistry*, 1993, **34**, 529 (*pmr, cmr*)

Physalin P P-349

[149204-27-3]

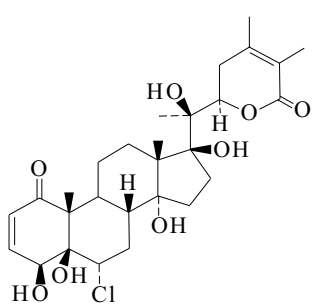


$C_{28}H_{30}O_{10}$ 526.539
Constit of *Physalis alkekengi* (winter cherry). Needles ($EtOAc/C_6H_6$). Mp 272-273°. $[\alpha]_D^{24}$ +54 (c, 0.25 in Me_2CO).

Kawai, M. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 1299 (*isol, pmr, cmr*)

Physalolactone P-350

[71339-25-8]
*6α-Chloro-4β,5,14,17β,20*S*-pentahydroxy-1-oxo-5β,22*R*-witha-2,24-dienolide*



$C_{28}H_{39}ClO_8$ 539.064

Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 227-228°. $[\alpha]_D$ +29.4 (c, 0.2 in Py). λ_{max} 220 (ϵ 17900) (EtOH) (Derep).

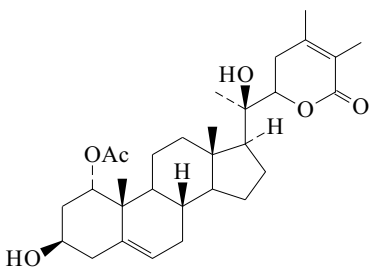
4-Deoxy: [78286-00-7] ***4-Deoxyphysalolactone.*** *6-Chloro-5,14,17,20-tetrahydroxy-1-oxowitha-2,24-dienolide*
$C_{28}H_{39}ClO_7$ 523.065
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. (EtOAc). Mp 207-208°. $[\alpha]_D$ +103 (c, 0.1 in $CHCl_3$). λ_{max} 220 (ϵ 17900) (EtOH) (Derep).

23α-Hydroxy: [118194-16-4] *6-Chloro-4,5,14,17,20,23-hexahydroxy-1-oxowitha-2,24-dienolide.* ***23-Hydroxyphysalolactone***
$C_{28}H_{39}ClO_9$ 555.063
Constit. of *Physalis peruviana* (Cape gooseberry). Needles (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 202-204°. $[\alpha]_D^{25}$ +60 (c, 1.4 in MeOH). λ_{max} 216 (ϵ 16000) (MeOH).

Ray, A.B. *et al., J. Indian Chem. Soc.*, 1978, **55**, 1175
Frolow, F. *et al., J.C.S. Perkin 1*, 1981, 1029
Nittala, S.S. *et al., Phytochemistry*, 1981, **20**, 2549 (*cryst struct, deriv*)
Eguchi, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2897 (*23-Hydroxyphysalolactone*)

Physalolactone B P-351

[78916-78-6]



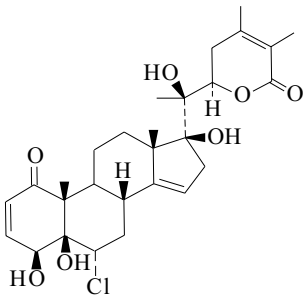
$C_{30}H_{44}O_6$ 500.674
Isol. from roots and leaves of *Physalis peruviana* (Cape gooseberry). Prisms. Mp 252-254°. $[\alpha]_D$ +14.2 (MeOH).

3-O-β-D-Glucopyranoside: [82087-30-7]
$C_{36}H_{54}O_{11}$ 662.816
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D$ +3.7 (c, 0.2 in Py).

Ray, A.B. *et al., Chem. Ind. (London)*, 1981, 62 (*isol*)
Kirson, I. *et al., J. Chem. Res., Synop.*, 1983, 120 (*deriv*)

Physalolactone C P-352

[92594-02-0]

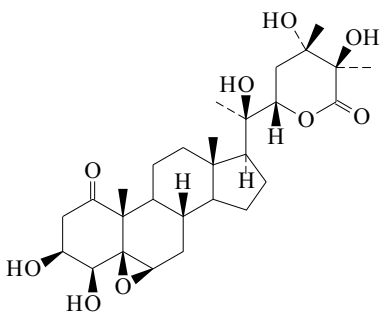


$C_{28}H_{37}ClO_7$ 521.049
Constit. of *Physalis peruviana* (Cape gooseberry). Needles (MeOH). Mp 271°. $[\alpha]_D^{25}$ +174 (c, 0.2 in DMSO).

Ali, A. *et al., J. Nat. Prod.*, 1984, **47**, 648

Physangulide P-353

[131749-58-1]
*5β,6β-Epoxy-3β,4β,20*R,*24*S,*25*R*-pentahydroxy-1-oxo-22*S*-withanolide*

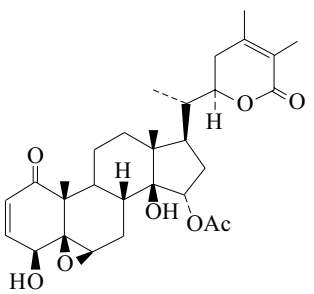


$C_{28}H_{42}O_9$ 522.634
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH). Mp 265-270°.

Vasina, O.E. *et al., Khim. Prir. Soedin.*, 1990, **26**, 366; *Chem. Nat. Compd. (Engl. Transl.)*, 304 (*isol, pmr, cmr*)

Physapubenolide P-354

[100217-92-3]
*15α-Acetoxy-5β,6β-epoxy-4β,14β-dihydroxy-1-oxo-20*S,*22*R*-witha-2,24-dienolide*

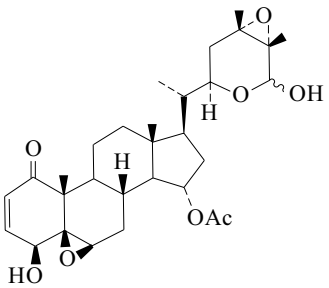


$C_{30}H_{40}O_8$ 528.641
Constit. of *Physalis pubescens* (ground cherry). Cryst. ($CHCl_3/C_6H_6$). Mp 144-145°. $[\alpha]_D$ +76 (c, 0.16 in $CHCl_3$).

Glotter, E. *et al., J.C.S. Perkin 1*, 1985, 2241

Physapubescin P-355

[74747-52-7]
15-Acetoxy-5,6:22,26:24,25-triepoxy-4,26-dihydroxyergost-2-en-1-one, 9CI

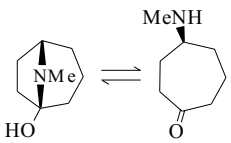


$C_{30}H_{42}O_8$ 530.657
Constit. of *Physalis pubescens* (ground cherry). Gum.

Kirson, I. *et al., J. Chem. Res., Synop.*, 1980, 125

Physoperuvine P-356

[60723-27-5]
8-Methyl-8-azabicyclo[3.2.1]octan-1-ol, 9CI. 4-(Methylamino)cycloheptanone, 9CI. 1-Hydroxytropane. 1-Tropanol



Absolute configuration

$C_8H_{15}NO$ 141.213
Free base tautomeric. Alkaloid from *Physalis peruviana* (Cape gooseberry). Mp 47-48° Mp 68-70°. May be a partial racemate.
▶ Mod. toxic.

Hydrochloride:
Mp 153°. $[\alpha]_D$ -0.8 (c, 1 in MeOH). Tropane bicyclic struct..

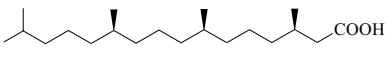
N-*Benzoyl:*
$C_{15}H_{19}NO_2$ 245.321
Mp 136-137°. Monocyclic struct..

[82748-86-5]

Ray, A.B. *et al., Heterocycles*, 1982, **19**, 1233 (*cryst struct, cmr, pmr, cd, abs config*)
McPhail, A.T. *et al., Tetrahedron*, 1984, **40**, 1661 (*cryst struct, synth, resoln*)
Boyer, F.-D. *et al., Synlett*, 1992, 357 (*synth*)
Justice, D.E. *et al., J.C.S. Perkin 1*, 1994, 2559 (*synth*)
Hiroya, K. *et al., Chem. Comm.*, 1995, 2205 (*synth*)
Majewski, M. *et al., Synlett*, 1996, 785 (*synth*)
Hodgson, D.M. *et al., Tet. Lett.*, 1999, **40**, 8637-8640 (*synth*)

1-Phytanoic acid P-357

3,7,11,15-Tetramethylhexadecanoic acid.
Phytanic acid



(3*R*,7*R*,11*R*)-*form*

$C_{20}H_{40}O_2$ 312.535

(3*R*,7*R*,11*R*)-*form* [18654-64-3]
Constit. of butter. Oil. Sol. MeOH, Et_2O. $Bp_{7.5}$ 221°. $[\alpha]_{500}^{20}$ -3.8 (c, 4 in MeOH/$CHCl_3$). λ_{max} 215 (ϵ 28400); 231 (ϵ 28300); 420 (ϵ 7660) (MeOH) (Berdy).

Kates, M. *et al., Biochemistry*, 1967, **6**, 3329 (*struct*)
Cox, R.E. *et al., Chem. Comm.*, 1970, 1639 (*isol, struct*)
Lough, A.K. *et al., Prog. Chem. Fats Other Lipids*, Part 1, 1973, **14**, (*rev*)
Sita, L.R. *et al., J.O.C.*, 1993, **58**, 5285 (*synth*)

3-Phytase P-358

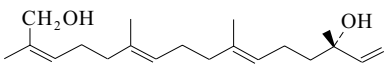
[37288-11-2]
Phytate 3-phosphatase, 9CI. Phytase. E.C. 3.1.3.8

Enzyme. Used in soy protein isolate production. Hydrolyses, Hexaphosphate to D-*myo*-inositol 1,2,4,5,6-pentakisphosphate + orthophosphate; animal feed supplement.

Howson, S.J. *et al., Enzyme Microb. Technol.*, 1983, **5**, 377-382 (*isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2216 (*use*)

1,6,10,14-Phytatetraene-3,17-diol P-359

2,6,10,14-Tetramethyl-2,6,10,15-hexadecatetraene-1,14-diol



$C_{20}H_{34}O_2$ 306.487

(3*S*,6*E*,10*E*,14*Z*)-*form*
20-Hydroxygeranyllinalool
Oil. $[\alpha]_D$ +9 (c, 1 in $CHCl_3$).

3,17-Di-O-*β*-D-*glucopyranoside:* [150396-00-2] ***Lyciumoside I***
$C_{32}H_{54}O_{12}$ 630.771
Constit. of *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D^{27}$ -21 (c, 0.5 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 17*-O-*[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [121961-81-7] ***Capsianoside III***. *Capsianside III*
$C_{50}H_{84}O_{26}$ 1101.198
Constit. of fruits of *Capsicum annuum*. Powder. $[\alpha]_D^{20}$ -26.4 (c, 1 in MeOH). CAS structure and name incorrect.

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 17*-O-*[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranosyl(1→3)-α-L-rhamnopyranoside]:* [121961-80-6] ***Capsianoside II***. *Capsianside II*
$C_{50}H_{84}O_{25}$ 1085.199
Constit. of fruits of *Capsicum annuum*. Powder. $[\alpha]_D^{20}$ -35.5 (c,1 in MeOH).

3-O-*[6*-O-*Malonyl-β-D-glucopyranoside], 17*-O-*β-D-glucopyranoside:* [212773-48-3] ***Lyciumoside IX***
$C_{35}H_{56}O_{15}$ 716.818
Constit. of *Lycium chinense* (Chinese boxthorn).

17-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 3*-O-*β-D-glucopyranoside:* [150396-01-3] ***Lyciumoside II***
$C_{38}H_{64}O_{17}$ 792.913
Constit. of *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D^{26}$ -19.6 (c, 0.49 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside], 17*-O-*β-D-glucopyranoside:* [212773-31-4] ***Lyciumoside IV***
$C_{38}H_{64}O_{16}$ 776.914
Constit. of *Lycium chinense* (Chinese boxthorn).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside], 17*-O-*[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [212773-42-7] ***Lyciumoside VI***
$C_{44}H_{74}O_{20}$ 923.057
Constit. of *Lycium chinense* (Chinese boxthorn).

17-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 3*-O-*β-D-glucopyranoside:* [212773-32-5] ***Lyciumoside V***
$C_{38}H_{64}O_{16}$ 776.914

17-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside], 3*-O-*β-D-glucopyranoside:* [212773-44-9] ***Lyciumoside VII***
$C_{44}H_{74}O_{21}$ 939.056
Constit. of *Lycium chinense* (Chinese boxthorn).

(3ξ,6*E*,10*E*,14*Z*)-*form*

3-O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside], 17*-O-*[α-L-rhamnopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [159721-35-4]
$C_{50}H_{84}O_{24}$ 1069.199
$[\alpha]_D$ -58.8 (c, 1.1 in MeOH).

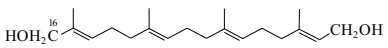
17-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-α-L-rhamnopyranoside], 3*-O-*β-D-glucopyranoside:* ***Capsianoside VI***. *Capsianside VI*
$C_{44}H_{74}O_{20}$ 923.057
Constit. of *Capsicum annuum*. Powder. $[\alpha]_D^{18}$ -36.2 (c, 0.55 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside], 17*-O-*[β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [159721-34-3]
$C_{50}H_{84}O_{25}$ 1085.199
$[\alpha]_D$ -42.7 (c, 0.56 in MeOH).

Wallin, I. *et al., Acta Chem. Scand., Ser. B*, 1980, **34**, 391-396 (Nicotiana sylvestri *constit.*)
Izumitani, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1299-1307 (*Capsianosides*)
Yahara, S. *et al., Chem. Pharm. Bull.*, 1991, **39**, 3258-3260 (*Capsianoside VI*)
Yahara, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 703 (*Lyciumosides*)
Shinozaki, Y. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 903-905 (*glycosides, pmr, cmr*)
Terauchi, M. *et al., Nat. Med. (Tokyo)*, 1998, **52**, 167-171; *CA*, **129**, 228074v (*Lyciumosides*)

2,6,10,14-Phytatetraene-1,16-diol P-360

2,6,10,14-Tetramethyl-2,6,10,14-hexadecatetraene-1,16-diol



$C_{20}H_{34}O_2$ 306.487

(2*E*,6*E*,10*E*,14*E*)-*form* [79577-80-3]
16-Hydroxygeranylgeraniol
Gum.

Difumaroyl: [128530-03-0] ***Cavipetin B***
$C_{28}H_{38}O_8$ 502.603
Constit. of the edible mushroom (*Boletinus cavipes*). Mp 86-87°. λ_{max} 210 (ϵ 37150) (MeOH) (Berdy).

1-O-*(2-Methylfumaroyl):* [128530-04-1] ***Cavipetin D***
$C_{25}H_{38}O_5$ 418.572
Constit. of the edible mushroom (*Boletinus cavipes*). Oil. Incorrect struct. assigned in CA λ_{max} 208 (ϵ 22390) (MeOH) (Berdy).

O-*(2-Methylfumaroyl)*, O-*fumaroyl:*

[128530-05-2, 128552-91-0] ***Cavipetin E***
$C_{29}H_{40}O_8$ 516.63
Constit. of the edible mushroom (*Boletinus cavipes*). Oil. A mixture of the two isomeric esters λ_{max} 210 (ϵ 20900) (MeOH) (Berdy).

Bis(2-methylfumaroyl): [128530-02-9] ***Cavipetin A***
$C_{30}H_{42}O_8$ 530.657
Constit. of the edible mushroom *Boletinus cavipes*. Powder. Mp 137-138°. λ_{max} 209 (ϵ 19050) (MeOH) (Berdy).

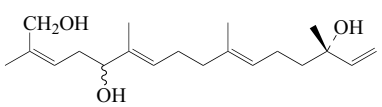
16-Aldehyde, 1-O-*(3-hydroxy-2-methyl-2-propenoyl)(Z-):* [128552-90-9] ***Cavipetin C***
$C_{24}H_{36}O_4$ 388.546
Constit. of the edible mushroom *Boletinus cavipes*. Oil. λ_{max} 208 (ϵ 20900) (MeOH) (Berdy).

16-Carboxylic acid, 1-Ac: [80368-54-3] *1-Acetoxy-2,6,10,14-phytatetraen-16-oic acid*. ***Koanoadmantic acid***
$C_{22}H_{34}O_4$ 362.508
Gum (as Me ester).

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1903; 1982, **21**, 1349
Kramp, W. *et al., Annalen*, 1986, 226 (*synth*)
Toyota, M. *et al., Phytochemistry*, 1990, **29**, 1485 (*Cavipetins*)
Peng, L.Z. *et al., Chin. Chem. Lett.*, 2003, **14**, 249-250 (*synth*)

1,6,10,14-Phytatetraene-3,12,17-triol P-361

2,6,10,14-Tetramethyl-2,6,10,15-hexadecatetraene-1,5,14-triol



$C_{20}H_{34}O_3$ 322.487

(3*S*,6*E*,10*E*,12ξ,14*Z*)-*form*

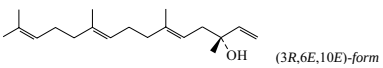
3,17-Di-O-*β*-D-*glucopyranoside:* [212773-47-2] ***Lyciumoside VIII***

$C_{32}H_{54}O_{13}$ 646.771
Constit. of *Lycium chinense* (Chinese boxthorn).

Terauchi, M. *et al., Nat. Med. (Tokyo)*, 1998, **52**, 167-171; *CA*, **129**, 228074v (*Lyciumoside VIII, isol, pmr, cmr*)

1,6,10,14-Phytatetraen-3-ol P-362

[1113-21-9]
3,7,11,15-Tetramethyl-1,6,10,14-hexadecatetraen-3-ol



(3*R*,6*E*,10*E*)-*form*

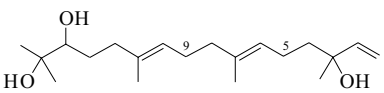
$C_{20}H_{34}O$ 290.488
► MM0335000
(3*R*,6*E*,10*E*)-*form*
Geranyllinalool
Oil. $Bp_{0.005}$ 115°. $[\alpha]_D$ -14.1 (c, 0.34 in $CHCl_3$) (-10.1). n_D^{24} 1.4878.
(3*S*,6*E*,10*E*)-*form*
Constit. of Jasmine oil. $Bp_{0.005}$ 115°. $[\alpha]_D$ +14.5.

[2211-30-5]

Demole, E. *et al., Bull. Soc. Chim. Fr.*, 1958, 1128 (*synth, ir*)
Kimland, B. *et al., Acta Chem. Scand.*, 1967, **21**, 825 (*pmr*)
Vig, O.P. *et al., Indian J. Chem.*, 1969, **7**, 574
Avdyukova, N.V. *et al., Khim. Prir. Soedin.*, 1971, **7**, 839; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 820 (*isol*)

1,6,10-Phytatriene-3,14,15-triol P-363

2,6,10,14-Tetramethyl-6,10,15-hexadecatriene-2,3,14-triol, 9CI



$C_{20}H_{36}O_3$ 324.503
(3ξ,6*E*,10*E*,14ξ)-*form* [84093-67-4]
14,15-Dihydro-14,15-dihydroxygeranyllinalool
Gum.

5-Hydroxy: [84093-68-5] ***1,6,10-Phytatriene-3,5,14,15-tetrol***. *2,6,10,14-Tetramethyl-6,10,15-hexadecatriene-2,3,12,14-tetrol*
$C_{20}H_{36}O_4$ 340.502
Gum.

9-Acetoxy: [84093-69-6]
$C_{22}H_{38}O_5$ 382.539
Gum.
(3*S*,6*E*,10*E*,14ξ)-*form*

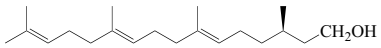
3,14-Di-O-β-D-glucopyranoside: ***Lyciumoside III***
$C_{32}H_{56}O_{13}$ 648.787
Constit. of *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D^{26}$ -31.1 (c, 0.48 in MeOH).

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1739
Yahara, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 703 (*Lyciumoside III*)

6,10,14-Phytatrien-1-ol P-364

[88882-26-2]

[36237-65-7, 51446-64-1, 51606-80-5]
3,7,11,15-Tetramethyl-6,10,14-hexadecatrien-1-ol

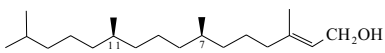


$C_{20}H_{36}O$ 292.504
(3*R*,6*E*,10*E*)-*form* [36237-66-8]
Geranylcitronellol
Isol. from *Zizyphus jujuba* (Chinese date). $[\alpha]_D$ +5.2 (c, 0.2 in $CHCl_3$).
Ac:
$C_{22}H_{38}O_2$ 334.541

Ahlquist, L. *et al., Chem. Scr.*, 1971, **1**, 237-246 (*synth*)
Valterova, I. *et al., Coll. Czech. Chem. Comm.*, 1996, **61**, 1501-1508 (*isol, synth, pmr, cmr, ir, ms*)

2-Phyten-1-ol P-365

[7541-49-3]
3,7,11,15-Tetramethyl-2-hexadecen-1-ol. ***Phytol***



(2*E*,7*R*,11*R*)-*form*

$C_{20}H_{40}O$ 296.535
(2*E*,7*R*,11*R*)-*form* [150-86-7]
Oil. $Bp_{0.02}$ 132°. $[\alpha]_D^{18}$ +0.2. λ_{max} 240 (MeOH) (Berdy).
► Skin irritant. LD_{50} (rat, orl) >5000 mg/kg. TJ3490000

1-Aldehyde: [13754-69-3] *2-Phyten-1-al. 3,7,11,15-Tetramethyl-2-hexadecenal.* ***Phytal***
$C_{20}H_{38}O$ 294.52
Constit. of *Tetragonia tetragonoides* (New Zealand spinach). Oil.

Burrell, J.W.K. *et al., J.C.S.(C)*, 1966, 2144 (*Phytal, synth, abs config*)

Phytosulfokine α P-366

[179667-62-0]
H-Tyr(SO_3H)-Ile-Tyr(SO_3H)-Thr-Gln-OH
$C_{33}H_{46}N_6O_{16}S_2$ 846.889
Constit. of asparagus spears (*Asparagus officinalis*).

Matsubayashi, Y. *et al., Biochem. Biophys. Res. Commun.*, 1996, **225**, 209 (*activity*)
Matsubayashi, Y. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 7623 (*isol, ms, struct*)

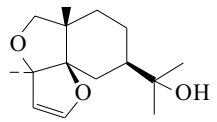
Phytosulfokine β P-367

[179667-63-1]
H-Tyr(SO_3H)-Ile-Tyr(SO_3H)-Thr-OH
$C_{28}H_{38}N_4O_{14}S_2$ 718.759
Constit. of asparagus spears (*Asparagus officinalis*).

Matsubayashi, Y. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 7623 (*isol, ms, struct*)

Phytuberol P-368

[56857-64-8]



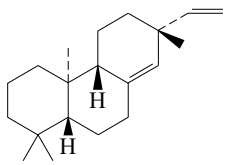
$C_{15}H_{24}O_3$ 252.353
Oil.

Ac: [37209-50-0] ***Phytuberin***
$C_{17}H_{26}O_4$ 294.39
Phytoalexin of potato tubers infected with *Erwinia carotovora*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. $[\alpha]_D$ -35.9 (c, 1.34 in $CHCl_3$).

Coxon, D.T. *et al., J.C.S. Perkin 1*, 1977, 53
Takagi, Y. *et al., Agric. Biol. Chem.*, 1979, **43**, 2395
Caine, D. *et al., J.A.C.S.*, 1980, **102**, 7568 (*synth*)
Findlay, J.A. *et al., Can. J. Chem.*, 1980, **58**, 2827 (*synth*)
Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1202 (*synth*)

8(14),15-Pimaradiene P-369

[19882-10-1]
Pimaradiene

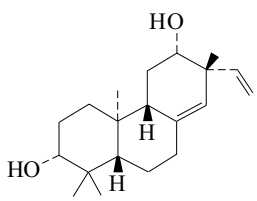


$C_{20}H_{32}$ 272.473
***ent*-form**
Constit. of *Aralia racemosa* (American spikenard). Oil. $[\alpha]_D^{20}$ -115.5 ($CHCl_3$).

[1686-61-9]

Ireland, R.E. *et al., J.O.C.*, 1963, **28**, 6 (*synth*)
Shibata, S. *et al., Tet. Lett.*, 1967, 5241 (*isol*)
Hanson, J.R. *et al., Phytochemistry*, 1970, **9**, 1359
Dell, B. *et al., J. Exp. Bot.*, 1978, **29**, 89 (*biosynth*)

8(14),15-Pimaradiene-3,12-diol P-370



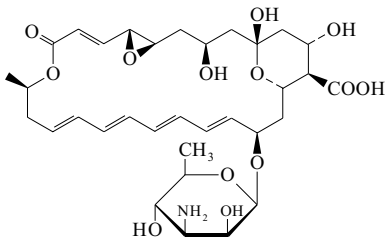
$C_{20}H_{32}O_2$ 304.472
(*ent*-3β,12β)-*form* [119626-54-9]
Yucalexin P21
Constit. of cassava roots (*Manihot esculenta*). Needles ($CHCl_3$/hexane). Mp 169°. $[\alpha]_D$ -91 ($CHCl_3$).

Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769 (*Yucalexins*)

Pimaricin P-371

[7681-93-8]

Natamycin, BAN, INN, USAN. *Antibiotic A 5283. Delvolan. Delvocid. Delvopos. Mycophyt. Myprozine. Natacyn. Natafucin. Pimafucin. Pimafugin. Synogil. Tennecetin. Tymasil. A 5283. CL 12625. E235*



$C_{33}H_{47}NO_{13}$ 665.733

Polyene antibiotic. Primarily used as a surface treatment to prevent growth of yeasts and moulds, esp. on cheese. Permitted agent in USA for surface treatment of cheeses as mould-inhibitor. No reported allergic reactions and it has GRAS status. Cryst. (MeOH aq.). Mp 200°. Log P -5.75 (uncertain value) (calc). Acid hydrol. → 3-Amino-3,6-dideoxymannose λ_{max} 279 (ϵ 35000); 289 (ϵ 55000); 303 (ϵ 78000); 318 (ϵ 76000) (MeOH) (Derep).

▶ LD_{50} (rat, orl) 2730 mg/kg. TK3325000

Me ester: [52555-04-1]
Mp 270-280°. $[\alpha]_D^{26}$ +94 (DMF).

Amide: ***Antibiotic AB 400***. *AB 400*
$C_{33}H_{48}N_2O_{12}$ 664.748
Yellow powder. Stereochem. not confirmed λ_{max} 290 ; 304 ; 318 (no solvent reported).

N-*Ac:*
Mp 200°. $[\alpha]_D^{25}$ +230.

Struyk, A.P. *et al., Antibiot. Annu.*, 1957, 878 (*isol*)
Brik, H. *et al., J. Antibiot.*, 1976, **29**, 632
Pandey, R.C. *et al., J. Antibiot.*, 1977, **30**, 158 (*synth*)
Ceder, O. *et al., Tetrahedron*, 1977, **33**, 2703 (*struct, config*)
Bogan, J.A. *et al., Drugs of Today (Barcelona)*, 1978, **14**, 254 (*rev*)
Hempel, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1978, **146**, 315 (*cryst struct*)
Brik, H. *et al., Anal. Profiles Drug Subst.*, 1981, **10**, 513; 1994, **23**, 399 (*rev*)
Radics, L. *et al., Tetrahedron*, 1982, **38**, 183 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PIF750
Lancelin, J.-M. *et al., J.A.C.S.*, 1990, **112**, 4060; 6749 (*pmr, struct, abs config*)
Duplantier, A.J. *et al., J.A.C.S.*, 1990, **112**, 7079 (*abs config*)
Pesticide Manual, 9th edn., 1991, No. 9760
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A480
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 329
Canedo, L.M. *et al., J. Antibiot.*, 2000, **53**, 623-626 (*AB 400*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PIF750

Pimpinellidine P-372

$C_{27}H_{45}NO_3$ 431.657

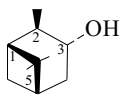
Steroidal alkaloid, prob. of Solanum type. Struct. unknown but may be 23-Hydroxytomatidine. Aglycone from hydrol. of leaves and stems of *Lycopersicon pimpinellifolium* (currant tomato). Needles (MeOH aq.). Mp 172-173°. $[\alpha]_D^{20}$ +14.3 (c, 0.7 in MeOH).

Schreiber, K. *et al., Phytochemistry*, 1966, **5**, 707 (*isol, ir*)

3-Pinanol, 8CI P-373

[473-61-0]

[25465-65-0, 25465-95-6, 27779-29-9, 51152-11-5, 73366-08-2, 125473-76-9]
2,6,6-Trimethylbicyclo[3.1.1]heptan-3-ol, 9CI



(1*R*,2*R*,3*R*,5*S*)-*form*

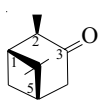
$C_{10}H_{18}O$ 154.252

(1*S*,2*R*,3*R*,5*R*)-*form* [35997-96-7]
(-)-Pinocampheol
Occurs in oils of *Hyssopus officinalis* (hyssop). Cryst. (hexane). Mp 67°. Bp 217°. $[\alpha]_D^{25}$ -57.2 (c, 0.33 in MeOH).

Hückel, W. *et al., Annalen*, 1966, **697**, 69-99 (*synth, config, bibl*)
Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643-656 (*rev*)
Teisseire, P. *et al., Recherches*, 1967, 59-67 (*struct*)
Hirata, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 599-603 (*synth, ir, pmr*)
Coxon, J.M. *et al., J.C.S. Perkin 2*, 1984, 1351-1355 (*cmr*)
Wang, Z.-M. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 667-670 (*synth*)

3-Pinanone P-374

[15358-88-0]
2,6,6-Trimethylbicyclo[3.1.1]heptan-3-one, 9CI



(1*R*,2*R*,5*S*)-*form*

$C_{10}H_{16}O$ 152.236

(1*R*,2*R*,5*S*)-*form* [473-62-1]
(+)-Isopinocamphone
Oil. Bp 213°. $[\alpha]_D^{20}$ +10.5.

Semicarbazone:
Cryst. Mp 219-220°.

(1*R*,2*S*,5*S*)-*form* [18492-59-6] *(+)-Pinocamphone*
Oil. Bp 211-211.5°. $[\alpha]_D^{20}$ +21.3.

Semicarbazone:
Cryst. Mp 227°.

(1*S*,2*R*,5*R*)-*form* [22339-21-5] ***(-)-Pinocamphone***
Constit. of the oils of *Hyssopus officinalis* (hyssop). Oil. Bp 212-214°. $[\alpha]_D^{25}$ -15.2 (c, 0.42 in MeOH).

Semicarbazone:
Cryst. (MeOH aq.). Mp 227.5-228°.

(1*S*,2*S*,5*R*)-*form* [14575-93-0] ***(-)-Isopinocamphone***
Constit. of *Mentha aquatica* (water mint). Oil. Bp 211-211.5°. $[\alpha]_D^{15}$ -7.3.

Semicarbazone:
Cryst. Mp 232°.

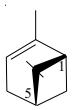
[547-60-4]

Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643 (*rev*)
Hückel, W. *et al., Annalen*, 1966, **697**, 69 (*synth, config, bibl*)
Brown, H.C. *et al., J.O.C.*, 1971, **36**, 387 (*synth*)

α-Pinene P-375

[80-56-8]

[1330-16-1]
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene, 9CI. 2-Pinene, 8CI. Australene. Firpene. Terebenthene. FEMA 2902



(−)-*form*

$C_{10}H_{16}$ 136.236

V. widely distributed in plants; reported in over 400 essential oils. Flavouring ingredient.

▶ Skin, eye and respiratory tract irritant. LD_{50} (rat, orl) 3700 mg/kg. Flammable, fl. p. 33/34°, autoignition temp. 255°. DT7000000

(+)-*form* [7785-70-8]
Oil. Mp -50°. Bp 155-156°. $[\alpha]_D$ +51.4 (neat) (99.6% ee).

(-)-*form* [7785-26-4]
Oil. Bp 155-156°. $[\alpha]_D^{23}$ -51.5 (neat) (99.8% ee).

(±)-*form* [2437-95-8]
Oil. Insol. H_2O. d_4^{20} 0.86. Mp -50°. Bp 156.2°. n_D^{20} 1.4658.

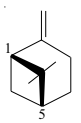
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 50A; 50B; 50C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 72C; 73A; 73B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 74D; 75A; 75B (*ir*)
Roberts, W.J. *et al., J.A.C.S.*, 1950, **72**, 1226 (*polym*)
Ryhage, R. *et al., Acta Chem. Scand.*, 1963, **17**, 2025 (*ms*)
Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643 (*rev*)
Bates, R.B. *et al., J.O.C.*, 1968, **33**, 1730 (*pmr*)
Sakota, N. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 485 (*abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 62 (*occur*)
Abraham, R.J. *et al., Org. Magn. Reson.*, 1972, **4**, 489 (*pmr*)
Wilson, H.W. *et al., Appl. Spectrosc.*, 1976, **30**, 209 (*ir, Raman*)
Thomas, M.T. *et al., J.A.C.S.*, 1976, **98**, 1227 (*synth*)
Mason, S.F. *et al., Tetrahedron*, 1977, **33**, 937 (*cd, uv*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 853 (*rev, tox*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 709 (*rev*)
Stenstrom, Y. *et al., Acta Chem. Scand., Ser. B*, 1980, **34**, 131 (*synth*)
Klimetzek, D. *et al., Experientia*, 1980, **36**, 1343 (*isol*)

Gleizes, M. *et al., Phytochemistry*, 1982, **21**, 2641 (*biosynth*)
Banthorpe, D.V. *et al., Phytochemistry*, 1984, **23**, 291 (*biosynth*)
Org. Synth., 1987, **65**, 224 (*synth*)
Brown, H.C. *et al., J.O.C.*, 1988, **53**, 4059; 1989, **54**, 1764 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PIH250
Lindstrom, M. *et al., J. Chem. Ecol.*, 1989, **15**, 541
Wainhouse, D. *et al., J. Chem. Ecol.*, 1992, **18**, 1693
Denisor, A.Y. *et al., Magn. Reson. Chem.*, 1992, **30**, 95; 886 (*pmr, cmr*)
Meklati, B.Y. *et al., Magn. Reson. Chem.*, 1992, **30**, 807 (*cmr, pmr*)
Bond, A.D. *et al., Acta Cryst. E*, 2001, **57**, o1039-o1040 (*cryst struct*)
Lee, S.G. *et al., Magn. Reson. Chem.*, 2002, **40**, 311-312 (*pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PIH250

β-Pinene P-376

[127-91-3]

[1330-16-1]
6,6-Dimethyl-2-methylenebicyclo[3.1.1]-heptane, 9CI. 2(10)-Pinene. Nopinene. Pseudopinene. Orthodene. FEMA 2903



(+)-*form*

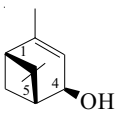
$C_{10}H_{16}$ 136.236
Widely distributed in plants, usually associated with α-Pinene, P-375 but in smaller amounts. Found in lime peel oil, ginger, nutmeg, mace, bitter fennel, rosemary and sage. Flavour ingredient.
▶ Skin irritant. LD_{50} (rat, orl) 4700 mg/kg.
DT5077000
(+)-*form* [19902-08-0]
Oil. Bp 163-164°. $[\alpha]_D^{23}$ +22.7 (neat) (99.6% ee).
(-)-*form* [18172-67-3]
Flavouring ingredient. Oil. d_4^{20} 0.87. Bp 163-164°. $[\alpha]_D^{25}$ -22.8 (neat) (100% op). n_D^{20} 1.4780.
(±)-*form* [23089-32-9]
Oil. Bp 166°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 50D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 77B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 75D (*ir*)
Sakota, N. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 485 (*abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 63
Richards, G.F. *et al., J.O.C.*, 1974, **39**, 86 (*cryst struct*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Wilson, H.W. *et al., Appl. Spectrosc.*, 1976, **30**, 209 (*ir, Raman*)
Thomas, M.T. *et al., J.A.C.S.*, 1976, **98**, 1227 (*synth, pmr*)
Mason, S.F. *et al., Tetrahedron*, 1977, **33**, 937 (*cd, uv*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 859 (*rev, tox*)
Midland, M.M. *et al., J.A.C.S.*, 1982, **104**, 528 (*synth*)
Gleizes, M. *et al., Phytochemistry*, 1982, **21**, 2641 (*biosynth*)
Andricanome, M. *et al., Chem. Comm.*, 1985, 1203 (*synth*)
Kulkarni, Y.S. *et al., J.O.C.*, 1987, **52**, 1568 (*synth*)
Brown, H.C. *et al., J.O.C.*, 1988, **53**, 4059; 1989, **54**, 1764 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, POH750
Meklati, B.Y. *et al., Magn. Reson. Chem.*, 1992, **30**, 807 (*cmr, pmr*)
Brophy, J.J. *et al., Org. Mass Spectrom.*, 1992, **27**, 1042 (*ms*)
Kolehmainen, E. *et al., Magn. Reson. Chem.*, 1997, **35**, 463-467 (*pmr*)
Bond, A.D. *et al., Acta Cryst. E*, 2001, **57**, o1041-o1042 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, POH750

2-Pinen-4-ol P-377

[473-67-6]

[1820-09-3, 1845-30-3, 5416-53-5, 80795-83-1]
*4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-ol, 9CI. **Verbenol**. FEMA 3594*



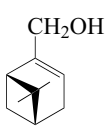
(1*R*,4*R*,5*R*)-*form*

$C_{10}H_{16}O$ 152.236
Flavouring ingredient.
▶ YX7525000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 265B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 246D (*ir*)
Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643-656 (*rev*)
Holden, C.M. *et al., Org. Magn. Reson.*, 1975, **7**, 125-127 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 795
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2907
Harper, J.K. *et al., Acta Cryst. C*, 2000, **56**, 451-452 (*cryst struct, cis-verbenol*)
Harper, J.K. *et al., J.A.C.S.*, 2000, **122**, 3708-3714 (*cmr*)

2-Pinen-10-ol P-378

[515-00-4]
6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-methanol, 9CI. Myrtenol. FEMA 3439



(+)-*form*

$C_{10}H_{16}O$ 152.236
Flavouring ingredient. Present in mandarin peel oil, raspberry, blackberry, strawberry, ginger, hop oil, black tea, peppermint oil, pepper (*Piper nigrum*), myrtle leaf or berry, summer savoury (*Satureja hortensis*) and other foodstuffs.
(+)-*form* [6712-78-3]
Darwinol
Isol. from oil of myrtle (*Myrtus communis*). Oil. Bp_{11} 103-104°. $[\alpha]_D^{22}$ +44.3 (c, 3.21 in $CHCl_3$).
Formyl: [72928-52-0]

[167611-55-4] *FEMA 3405*
$C_{11}H_{16}O_2$ 180.246
Flavouring ingredient. Present in hyssop oil (*Hyssopus officinalis*). Liq. with strong pine/linseed odour. d^{20} 1.01. Bp_{10} 93-97°. $[\alpha]_D^{25}$ -55 (c, 1.5 in $CHCl_3$). n_D 1.4794.

10-Aldehyde: [23727-16-4]

[564-94-3] ***Myrtenal**. FEMA 3395*
$C_{10}H_{14}O$ 150.22
Occurs in orange, lemon, spearmint, pepper, thyme, juniper, calamus, ginger, myrtle, lemon balm, calabash, nutmeg, parsley seed and other plant oils. Unstable oil with cinnamon odour. Bp_{15} 99-100°. $[\alpha]_D^{20}$ +14.75.

10-Carboxylic acid: [601-74-1] *2-Pinen-10-oic acid*. ***Myrtenic acid***
$C_{10}H_{14}O_2$ 166.219
Cryst. Mp 53.5-55°. $[\alpha]_D^{20}$ +55 (c, 0.8 in EtOH).
(-)-*form* [19894-97-4]
Bp_{11} 101-102°. $[\alpha]_D^{20}$ -47.1 (EtOH).
O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]*:***Sacranoside A***
$C_{21}H_{34}O_{10}$ 446.494
Powder. $[\alpha]_D^{25}$ -33.9 (c, 0.1 in MeOH).
*Ac:**Myrtenyl acetate***
$C_{12}H_{18}O_2$ 194.273
Isol. from valerian (*Valeriana officinalis*).
3-Methylbutanoyl:(-)-Myrtenyl isovalerate
$C_{15}H_{24}O_2$ 236.353
Isol. from oil of *Valeriana officinalis* (valerian).
10-Aldehyde: [18486-69-6]
Unstable oil. Bp 220-221°. $[\alpha]_D$ -15.3.
(±)-*form* [111957-74-5]
Flavouring ingredient. Oil. n_D^{20} 1.4963.
Hydrogen phthalate:
Mp 120.5°.
Ac: [35670-93-0] *FEMA 3765*
$C_{12}H_{18}O_2$ 194.273
Flavouring ingredient. d^{20} 0.99. Bp_9 105-107°. n_D 1.4784.
3-Methylbutanoyl: [29021-37-2]
$C_{15}H_{24}O_2$ 236.353
d 0.96.
(ξ)-*form*
O-*(6-O-Acetyl-β-D-glucopyranoside)*:
$C_{18}H_{28}O_7$ 356.415
Oil.

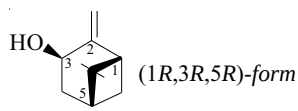
[19250-17-0, 117872-96-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 155D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 264C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 228C (*ir*)
Semmler, F.W. *et al., Ber.*, 1907, **40**, 1374 (*formyl, Ac*)

Stoll, A. *et al., Helv. Chim. Acta*, 1957, **40**, 1205 (*acetate, isovalerate*)
Couchman, F.M. *et al., Tetrahedron*, 1964, **20**, 2037 (*isol*)
Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643 (*rev*)
Bates, R.B. *et al., J.O.C.*, 1968, **33**, 1730 (*pmr*)
Borowiecki, L. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1971, **45**, 573 (*Myrtenic acid*)
Kergomard, A. *et al., Bull. Soc. Chim. Fr.*, 1974, 2572 (*synth*)
Rauchschwalbe, G. *et al., Helv. Chim. Acta*, 1975, **58**, 1094 (*synth*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Harwood, L.M. *et al., Synthesis*, 1980, 456 (*synth*)
Maheshwari, M.L. *et al., Dev. Food Sci.*, 1988, **18**, 171-176 (*S-form, formyl, isol*)
Maheshwari, M.L. *et al., Dev. Food Sci.*, 1988, **18**, 171-176 (*S-form formyl, isol*)
Rustaiyan, A. *et al., Phytochemistry*, 1990, **29**, 985 (*glucoside*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 935 (*rev, tox*)
Shibuya, K. *et al., Synth. Commun.*, 1994, **24**, 2923 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 365; 586
Rashid, M.A. *et al., Fitoterapia*, 1995, **66**, 473 (*Myrtenyl acetate, pmr, cmr*)
Shibuya, K. *et al., Synth. Commun.*, 1995, **25**, 431-449 (*S-form formyl, synth*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1498-1503 (*Sacranoside A*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1126-1127; 1376-1377; 1930-1932 (*props, occur, use*)
Lee, S.G. *et al., Magn. Reson. Chem.*, 2000, **40**, 311-312 (*pmr*)

2(10)-Pinen-3-ol P-379

[5947-36-4]
6,6-Dimethyl-2-methylenebicyclo[3.1.1]-heptan-3-ol, 9CI. ***Pinocarveol****. Pinyl alcohol. Isocarveol. FEMA 3587*



(1*R*,3*R*,5*R*)-*form*

$C_{10}H_{16}O$ 152.236
Flavouring ingredient.

(1*R*,3*R*,5*R*)-*form* [3917-59-7]

[1674-08-4]
(-)-cis-*form*
Cryst. Mp 49-50°. $[\alpha]_D^{25}$ -37.4 (c, 3.6 in MeOH).

(1*R*,3*S*,5*R*)-*form* [19894-98-5]
(+)-trans-*form*
Oil. $[\alpha]_D^{25}$ +60.7 (c, 1.6 in MeOH).

(1*S*,3*R*,5*S*)-*form* [547-61-5]
(-)-trans-*form*
Constit. of oil of *Eucalyptus globulus* (Tasmanian blue gum). Oil. Mp 5°. Bp 209-210° Bp_1 72°.

(1*S*,3*S*,5*S*)-*form* [19889-99-7]

[1674-08-4]
(+)-cis-*form*
Cryst. Mp 49°. $[\alpha]_D$ +47.

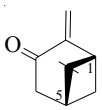
[6712-79-4]

Bose, A.K. *et al., J.O.C.*, 1955, **20**, 1003 (*struct*)
Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643 (*rev*)
Teisseire, P. *et al., Recherches*, 1967, 59 (*synth*)
Hirata, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 3169 (*pmr, synth*)
Org. Synth., 1977, **56**, 25 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 677
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2225-2226

2(10)-Pinen-3-one P-380

[16812-40-1]

[30460-92-5]
6,6-Dimethyl-3-methylenebicyclo[3.1.1]-heptan-3-one, 9CI. ***Pinocarvone****. Carvopinone. Isocarvone. 3-Nopinenone*



(+)-*form*

$C_{10}H_{14}O$ 150.22

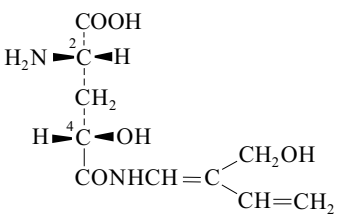
(+)-*form* [34413-88-2]
Oil. Bp_4 84-85°. $[\alpha]_D$ +63.
Oxime:
Cryst. Mp 132-133°.

(-)-*form* [19890-00-7]
Isol. from oil of *Eucalyptus globulus* (Tasmanian blue gum). Oil. Mp -1.8°. Bp_4 67-69°. $[\alpha]_D$ -68.5.
Oxime:
Cryst. Mp 131-132°.

Banthorpe, D.V. *et al., Chem. Rev.*, 1966, **66**, 643 (*rev*)
Bessière-Chrétien, Y. *et al., Bull. Soc. Chim. Fr.*, 1971, 2591 (*synth*)
Jefford, C.W. *et al., Helv. Chim. Acta*, 1973, **56**, 2649 (*synth*)

Pinnatanine P-381

4-Hydroxy-N-*[2-(hydroxymethyl)-1,3-butadienyl]glutamine*



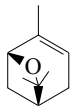
$C_{10}H_{16}N_2O_5$ 244.247

(2*S*,4*S*)-*form* [35214-74-5]
Constit. of *Hemerocallis fulva* (day lily). Mp 175° dec. $[\alpha]_D^{27}$ +3.2 (c, 0.5 in H_2O). Geom. isom. not defined..

Grove, M.D. *et al., Tetrahedron*, 1973, **29**, 2715 (*isol, struct*)
Yoshikawa, K. *et al., Phytochemistry*, 1994, **35**, 1057 (*isol, pmr, cmr*)

Pinol P-382

[2437-97-0]
4,7,7-Trimethyl-6-oxabicyclo[3.2.1]oct-3-ene, 9CI. 6,8-Epoxy-p-*menth-1-ene*



$C_{10}H_{16}O$ 152.236

(+)-*form*
Oil. d^{20} 0.95. Bp 183-184°. $[\alpha]_D^{20}$ +92 (c, 2.5 in EtOH). n_D^{20} 1.4692.

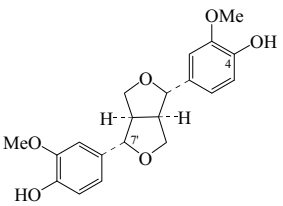
(ξ)-*form*
Isol. from lime oil (*Citrus aurantifolia*).

[497-31-4, 55822-06-5]

Kováts, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2705 (*isol, synth*)
Garver, L. *et al., J.O.C.*, 1976, **41**, 2773 (*synth*)
Bondavalli, F. *et al., J.C.S. Perkin 1*, 1977, 430 (*synth*)

Pinoresinol P-383

*4,4′-(Tetrahydro-1*H*,3*H*-furo[3,4-c]furan-1,4-diyl)bis[2-methoxyphenol], 9CI. 2,6-Bis-(4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo[3.3.0]octane, 9CI. 4,4′-Dihydroxy-3,3′-dimethoxy-7,9′:7′,9-diepoxylignan. Clemaphenol A*



(+)-*form*

$C_{20}H_{22}O_6$ 358.39Lignan numbering shown.

(+)-*form* [487-36-5]
Cryst. (EtOH aq.). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 122°. $[\alpha]_D^{21}$ +84.4 (Me_2CO). λ_{max} 232 (ε 15500); 282 (ε 6300) (MeOH) (Berdy). λ_{max} 230 (ε 14800); 280 (ε 6620) (EtOH) (Berdy).

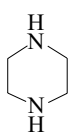
*4-*O*-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]:* [150035-90-8] *KP3*
$C_{38}H_{52}O_{21}$ 844.816
Constit. of sesame seeds. $[\alpha]_D^{25}$ -12 (c, 0.14 in H_2O).

[23171-10-0]

Katsuzaki, H. *et al., Heterocycles*, 1993, **36**, 933 (*KP3*)
Konishi, T. *et al., Yakugaku Zasshi*, 1993, **113**, 670 (*diglucoside*)

Piperazine, 9CI P-384

[110-85-0]
Hexahydropyrazine. 1,4-Diazacyclohexane. Diethylenediamine (obsol.). Vermex. Many other names



$C_4H_{10}N_2$ 86.136
Hygroscopic plates (EtOH) with salty taste. V. sol. H_2O, EtOH; insol. Et_2O. Mp

106°. Bp 146°. pK_{a1} 9.73; pK_{a2} 5.33 (25°). Log P -0.95 (calc). Absorbs CO_2 from the air.

▶ Fl. p. 81° (oc)/88° (oc). High therapeutic doses neurotoxic. Respiratory tract irritant. Corrosive and irritating to eyes and skin. Prolonged or repeated exposure may cause hypersensitivity reactions. LD_{50} (rat, orl) 1900 mg/kg. TK7800000

Hydrochloride (1:2): [142-64-3]
Formerly used as a food additive; now no longer generally recognised as safe. Solid.

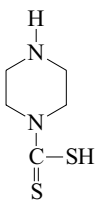
▶ OES: long-term 5 mg m^{-3}. TL4025000

[41372-10-5, 50322-15-1, 55974-34-0, 95356-15-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 371A; 371B; 371C; 371D; 1308B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 581B; 581C; 582A; 582B; 1250A; **2**, 647B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 463B; 463C; 463D; 465D (*ir*)
Kitchen, L.J. *et al., J.A.C.S.*, 1947, **69**, 854 (*synth*)
Martin, W.B. *et al., J.A.C.S.*, 1948, **70**, 1817 (*synth*)
Lanum, W.J. *et al., J. Chem. Eng. Data*, 1969, **14**, 93 (*props*)
Yokozeki, A. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 2352 (*struct*)
Jones, R.G. *et al., J.C.S. Perkin 2*, 1972, 437 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 295 (*rev*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A2**, 15 (*rev*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2690 (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DVF200; HEP000; PIJ000; PIK000; MOD250; PIJ500; PIK500

1-Piperazinecarbodithioic acid, 9CI P-385

[99-00-3]
1-Piperazinedithiocarbamic acid



$C_5H_{10}N_2S_2$ 162.279
Once widely used as an anthelmintic for treatment of roundworm infection in pigs and poultry. Yellow microcryst. powder. Spar. sol. H_2O. Mp 225-227° subl.

▶ TL0650000

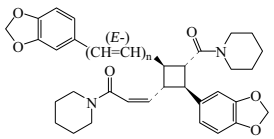
N-*Me:* [5712-49-2] *4-Methyl-1-piperazinecarbodithioic acid, 9CI.* N-*Methylpiperazinedithiocarbamic acid*
$C_6H_{12}N_2S_2$ 176.306
Cryst. (as Na salt). Sol. H_2O (Na salt).

▶ TL0709700

[16909-14-1]

Dunderdale, J. *et al., Chem. Ind. (London)*, 1956, 174 (*synth*)
Macrotrigiano, G.M. *et al., J. Inorg. Nucl. Chem.*, 1974, **36**, 3709 (*synth, deriv*)
Jain, S.K. *et al., Zh. Anal. Khim.*, 1988, **43**, 2164 (*use*)

Pipercyclobutanamide A P-386



$C_{34}H_{38}N_2O_6$ 570.684
Alkaloid from the fruit of *Piper nigrum* (pepper). Amorph. powder. λ_{max} 265 ; 271 ; 289 (hexane).

Fujiwara, Y. *et al., Tet. Lett.*, 2001, **42**, 2497-2499

Pipercyclobutanamide B P-387

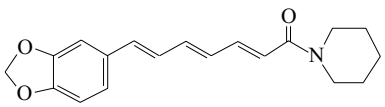
As Pipercyclobutanamide A, P-386 with n = 2

$C_{36}H_{40}N_2O_6$ 596.722
Alkaloid from the fruit of *Piper nigrum* (pepper). Amorph. powder. λ_{max} 285 ; 296 ; 309 (hexane).

Fujiwara, Y. *et al., Tet. Lett.*, 2001, **42**, 2497-2499

Piperettine P-388

[583-34-6]
1-[7-(1,3-Benzodioxol-5-yl)-1-oxo-2,4,6-heptatrienyl]piperidine, 9CI. 1-[7-(3,4-Methylenedioxyphenyl)heptatrienoyl]piperidine



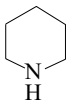
$C_{19}H_{21}NO_3$ 311.38
Alkaloid from the dried fruits of *Piper nigrum* (pepper). Yellow needles (C_6H_6/hexane). Mp 148°.

6,7-Dihydro: [188426-70-2] *1-[7-(1,3-Benzodioxol-5-yl)-1-oxo-2,4-heptadienyl]piperidine, 9CI. 1-[7-(3,4-Methylenedioxyphenyl)heptadienoyl]piperidine.* ***Piperdardine.*** *Piperarboricoline. 6,7-Dihydropiperettine*
$C_{19}H_{23}NO_3$ 313.396
Pale yellow oil. λ_{max} 205 (log ϵ 3.9); 266 (log ϵ 4.04) (EtOH).

Spring, F.S. *et al., J.C.S.*, 1950, 1177 (*isol, struct, synth*)
Rao, J.M. *et al., Curr. Sci.*, 1974, **43**, 76 (*isol*)
Dehmlow, E.V. *et al., J. Chem. Res., Synop.*, 1981, 106 (*synth*)
De Araujo-Junior, J.X. *et al., Phytochemistry*, 1997, **44**, 559 (*Piperdardine*)
De Araujo-Junior, J.X. *et al., Synth. Commun.*, 2001, **31**, 117-123 (*Piperdardine*)

Piperidine, 9CI P-389

[110-89-4]
Hexahydropyridine. Azacyclohexane. FEMA 2908



$C_5H_{11}N$ 85.149
Present in black pepper (*Piper nigrum*). Flavouring agent. Liq. with characteristic odour and a burning, peppery taste. Misc. H_2O; sol. org. solvs. d_4^{20} 0.86. Mp -9°. Bp 106° Bp_{20} 17.7°. n_D^{20} 1.4534. pK_a 11.12 (25°). Forms a hydrate, Mp -14°.

▶ Skin, eye and respiratory tract irritant. LD_{50} (rat, orl) 400 mg/kg. LD_{50} (rbt, skn) 320 mg/kg. Exp. reprod. and teratogenic effects (by inhalation). Highly flammable, fl. p. 3/16°. OES: long-term 1 ppm (Sk). TM3500000

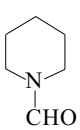
Hydrochloride: [6091-44-7]
Prisms (EtOH). Mp 244-245°.

▶ LD_{50} (rat, orl) 133 mg/kg. TN0400000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 358C; 358D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 563B; **3**, 723B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 449B (*ir*)
Skita, A. *et al., Ber.*, 1912, **45**, 3589; 1916, **49**, 1597 (*synth*)
Org. Synth., Coll. Vol. 1, 1932, 99 (*synth*)
Wojcik, B. *et al., J.A.C.S.*, 1934, **56**, 2419 (*synth*)
Seikel, M.K. *et al., J.A.C.S.*, 1940, **62**, 750 (*use*)
Weitkamp, H. *et al., Chem. Ber.*, 1962, **95**, 2895 (*pmr*)
Daasch, L.W. *et al., J. Phys. Chem.*, 1965, **69**, 3196 (*ms*)
Gupta, J.K.D. *et al., Indian J. Phys.*, 1970, **44**, 561 (*cryst struct*)
Kausch, M. *et al., Org. Magn. Reson.*, 1977, **10**, 208 (*pmr, cmr*)
Lambert, J.B. *et al., J.O.C.*, 1983, **48**, 3982 (*cmr*)
Rubiralta, M. *et al., Piperidine: Structure, Preparation, Reactivity and Synthetic Applications of Piperidine*, (Std. Org. Chem. Vol. 43), Elsevier, Amsterdam, 1991, (*book*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 678
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2227-2228
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2688
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 251
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1037
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADA250; HET000; NLJ500; PIL500

1-Piperidinecarboxaldehyde, 9CI, 8CI P-390

[2591-86-8]
N-*Formylpiperidine*



$C_6H_{11}NO$ 113.159
Present in pepper. Liq. Bp 222° Bp_{10} 97-

100°.

►TN0380000

Hydrobromide:
Mp 103.5°.

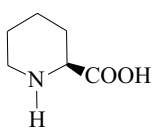
Oxime: [18600-89-0]
$C_6H_{12}N_2O$ 128.174
Mp 49-50°.

Di-Me acetal: [5211-86-9] *1-(Dimethoxymethyl)piperidine*
$C_8H_{17}NO_2$ 159.228
Liq. Bp_{15} 83°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 763D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1248A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 785A (*ir*)
de Benneville, P.L. *et al., J.O.C.*, 1956, **21**, 772 (*synth*)
Nefedov, B.L. *et al., Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1973, 2652 (*synth, bibl*)
De Brauwere, J. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 167-177 (*isol*)
Nair, R.S. *et al., Fundam. Appl. Toxicol.*, 1992, **18**, 96 (*tox*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2599-2600 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FOH000

2-Piperidinecarboxylic acid, 9CI P-391

[535-75-1]
Pipecolic acid. *Hexahydropicolinic acid. Pipecolinic acid. Homoproline*†



(*S*)-*form*

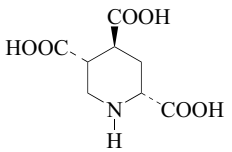
$C_6H_{11}NO_2$ 129.158
►TK6021000
(*R*)-*form* [1723-00-8]
D-form
Plates (EtOH). Mp 270°. $[\alpha]_D^{25}$ +24.5.
(*S*)-*form* [3105-95-1]
L-form
Present in beans and other legumes, and in lesser quantities in other plants including barley, hops, malt and mushrooms. Needles (MeOH/Et_2O). Sol. H_2O. Mp 259-260°. $[\alpha]_D^{20}$ -30.6 (c, 1 in H_2O).
N-*γ-Glutamyl*:***γ-L-Glutamyl-L-pipecolic acid***
$C_{11}H_{18}N_2O_5$ 258.274
Isol. from the seeds of *Gleditisia caspica* (Caspian locust). Cryst. (H_2O). $[\alpha]_D^{20}$ -66.8 (c, 0.5 in H_2O).
(±)-*form* [4043-87-2]
Plates (H_2O). Mp 270°. pK_{a2} 10.77 (20°).
Hydrochloride: [5107-10-8]
Mp 264°.

[41994-45-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 585B; 585C; 585D; 682B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 889A; 889B; 889C; 1085B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 737B (*ir*)
Rodwell, V.W. *et al., Methods Enzymol., Part B*, 1971, **17**, 174 (*rev*)
Dardenne, G. *et al., Phytochemistry*, 1974, **13**, 1515 (*Glutamylpipecolic acid*)
Fujii, T. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 1341 (*synth*)
Aketa, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 621 (*synth*)
Bhattacharjee, S.K. *et al., Acta Cryst. B*, 1979, **35**, 396 (*cryst struct*)
Kisfaludy, L. *et al., Synthesis*, 1982, 163 (*synth*)
Shuman, R.T. *et al., J.O.C.*, 1990, **55**, 738 (*synth*)
Amino, Y. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 620 (*synth, derivs*)
Ng-Youn-Chen, M.C. *et al., J.O.C.*, 1994, **59**, 2075 (*resoln*)
Berrien, J.-F. *et al., J.O.C.*, 1994, **59**, 3769 (*synth*)
Agami, C. *et al., Synth. Commun.*, 2000, **30**, 2565-2572 (*S-form, synth, pmr*)

2,4,5-Piperidinetricarboxylic acid, 9CI P-392

Hexahydroberberonic acid

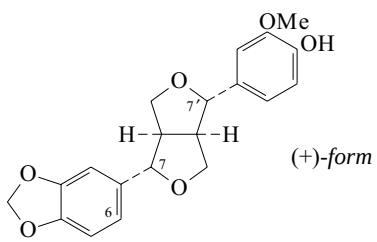


Relative Configuration

$C_8H_{11}NO_6$ 217.178Various stereoisomers have been synthesized.
(2*R,4*S**,5*R**)-*form*** [160699-23-0]
Yamano, K. *et al., Z. Naturforsch., C*, 1994, **49**, 707-711 (*isol, pmr, cmr, struct*)
Hashimoto, K. *et al., Heterocycles*, 1997, **46**, 581-588 (*synth, pmr*)

Piperitol P-393

4-[4-(1,3-Benzodioxol-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan-1-yl]-2-methoxyphenol, 9CI. 2-(4-Hydroxy-3-methoxyphenyl)-6-(3,4-methylenedioxyphenyl)-3,7-dioxabicyclo[3.3.0]octane. 4′-Hydroxy-3′-methoxy-3,4-methylenedioxy-7,9′:7′,9-diepoxylignan. Regiomontanin



(+)-*form*

$C_{20}H_{20}O_6$ 356.374
(-)-*form* [54983-96-9]
Obt. from *Zanthoxylum piperitum* (Japanese pepper tree). Syrup. $[\alpha]_D$ -66.3 ($CHCl_3$).
O-*(3-Methyl-2-butenyl):* [54631-93-5]

[54615-53-1, 157659-20-6]
Constit. of *Zanthoxylum piperitum* (Japanese pepper tree). Needles. Mp 58-59°. $[\alpha]_D^{20}$ -45.7 (c, 5.4 in $CHCl_3$). λ_{max} 234 (log ε 4.26); 284 (log ε 3.95) (MeOH).

7-Epimer: [54983-95-8] ***Xanthoxylol***
$C_{20}H_{20}O_6$ 356.374
Isol. from *Zanthoxylum piperitum* (Japanese pepper tree). Cryst. Mp 140-142°. $[\alpha]_D$ -117 ($CHCl_3$).

[92620-81-0]

Abe, F. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1617; 1974, **22**, 2650 (*Piperitol, Xanthoxylol*)
Dominguez, X. *et al., Rev. Latinoam. Quim.*, 1973, **4**, 155 (*isol*)
Brieskorn, C.H. *et al., Tet. Lett.*, 1976, 2221 (*isol*)
Pelter, A. *et al., Tetrahedron*, 1976, **32**, 2783 (*configs*)
Vaquette, J. *et al., Planta Med.*, 1979, **35**, 42 (*isol*)
Carvalho, M.G. *et al., Phytochemistry*, 1980, **19**, 332; 1987, **26**, 265 (*isol, pmr, pharmacol*)
Pelter, A. *et al., J.C.S. Perkin 1*, 1985, 587 (*synth, nmr*)
Stevens, D.R. *et al., J.C.S. Perkin 1*, 1992, 185 (*synth*)
Kwon, J.C. *et al., Arch. Pharmacal Res.*, 1999, **22**, 417-422 (*isol, activity*)
Roy, S.C. *et al., J.O.C.*, 2002, **67**, 3242-3248 (*synth*)

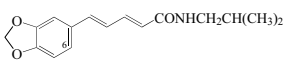
Piperlongine P-394

Struct. unknown. Constit. of *Piper longum* roots (long pepper). Oil. Bp_3 110-115° (lit. gives a pressure range). Not characterized. May not be an alkaloid.

Chatterjee, A. *et al., Tetrahedron*, 1967, **23**, 1769 (*isol*)

Piperlonguminine P-395

5-(1,3-Benzodioxol-5-yl)-N-(2-methylpropyl)-2,4-pentadienamide, 9CI. 5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoic acid isobutylamide



(*E,E*)-form

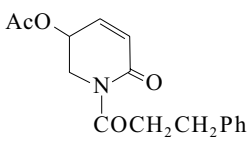
$C_{16}H_{19}NO_3$ 273.331
(*E,E*)-*form* [5950-12-9]
Alkaloid from *Piper longum* (long pepper) and other *Piper* spp.. Cryst. (C_6H_6/petrol). Mp 167-169°.
4,5-Dihydro: [23512-53-0] *5-(1,3-Benzodioxol-5-yl)-N-(2-methylpropyl)-2-pentenamide, 9CI.* N-*Isobutyl-5-(3,4-methylenedioxyphenyl)-2-pentenamide, 8CI.* ***4,5-Dihydropiperlonguminine***. *Δ$^{\alpha,\beta}$-Dihydropiperlonguminine*
$C_{16}H_{21}NO_3$ 275.347
Alkaloid from fruits of *Piper longum* (long pepper). Cryst. (C_6H_6 or C_6H_6/petrol). Mp 90-94° (natural) Mp 110° (synthetic).
6-Methoxy: [102934-25-8] *5-(6-Methoxy-3,4-methylenedioxyphenyl)-2,4-pentadienoic acid isobutylamide.* ***6-Methoxypiperoylisobutylamine***
$C_{17}H_{21}NO_4$ 303.357
(*Z,Z*)-*form* [79097-19-1]
Isopiperlonguminine
Mp 140-143°.

Chatterjee, A. *et al., Tetrahedron*, 1967, **23**, 1769 (*isol, uv, pmr, ms, synth*)

Loder, J.W. *et al., Aust. J. Chem.*, 1969, **22**, 1531 (*synth, 4,5-Dihydropiperlonguminine*)
Gupta, O.P. *et al., Phytochemistry*, 1972, **11**, 2646 (*isol*)
Mahanta, P.K. *et al., J. Pharm. Sci.*, 1974, **63**, 1160 (*uv, ir, pmr*)
Okogun, J.I. *et al., J.C.S. Perkin 1*, 1974, 2195 (*isol, uv, ir, pmr, ms, synth*)
Patra, A. *et al., Phytochemistry*, 1974, **13**, 2889 (*isol*)
Dwuma-Badu, D. *et al., Phytochemistry*, 1976, **15**, 822 (*4,5-Dihydropiperlonguminine*)
Olsen, R.A. *et al., J. Agric. Food Chem.*, 1981, **29**, 942 (*synth, uv, ir, pmr*)
Soares Costa, S. *et al., Phytochemistry*, 1981, **20**, 1305 (*isol, uv, ir, pmr, ms, Piperlonguminine, Isopiperlonguminine*)
Kubo, I. *et al., Experientia*, 1984, **40**, 340 (*4,5-Dihydropiperlonguminine*)
Achenbach, H. *et al., Planta Med.*, 1986, **52**, 12-18 (*6-Methoxy*)
Kaga, H. *et al., Synlett*, 1994, 607 (*synth*)

Pipermethystine P-396

[71627-22-0]
5-Acetoxy-5,6-dihydro-1-(3-phenylpropanoyl)-2(1H)-pyridone

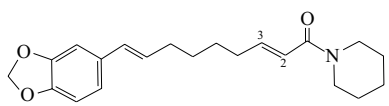


$C_{16}H_{17}NO_4$ 287.315
Alkaloid from the leaves of kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Oil.

Smith, R.M. *et al., Tetrahedron*, 1979, **35**, 437 (*isol, uv, ir, pmr, cmr, ms, struct*)
Gomez, R. *et al., Org. Lett.*, 2001, **3**, 3381-3383 (*synth*)

Pipernonaline P-397

[88660-10-0]
1-[9-(1,3-Benzodioxol-5-yl)-1-oxo-2,8-nonadienyl]piperidine, 9CI. 9-(3,4-Methylenedioxyphenyl)-2,8-nonadienoic acid piperidide



$C_{21}H_{27}NO_3$ 341.449
Alkaloid from the fruits of *Piper longum* (long pepper). Cryst. (EtOAc/hexane). Mp 54-55.5°.

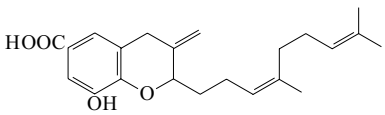
2,3-Dihydro: [30505-89-6] ***Piperolein B***
$C_{21}H_{29}NO_3$ 343.465
Minor constit. of *Piper nigrum* (black pepper). Oil. λ_{max} 214 (ε 28000); 260 (ε 16600); 268 (ε 16100); 305 (ε 10800) (MeOH) (Derep).

4,5-Didehydro: [107584-38-3] ***Dehydropipernonaline***. *9-(3,4-Methylenedioxy)-2,4,8-nonatrienoic acid piperidide*
$C_{21}H_{25}NO_3$ 339.433
Isol. from fruits of *Piper longum* (long pepper). Plates (hexane/Me_2CO). Mp 98-99°.

Grewe, R. *et al., Chem. Ber.*, 1970, **103**, 3752 (*isol, uv, ir, pmr, ms, synth, struct, Piperolein B*)
Tabuneng, W. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3562 (*isol, pmr, cmr, ir, uv, ms, struct*)
Shoji, N. *et al., J. Pharm. Sci.*, 1986, **75**, 1188 (*Dehydropipernonaline*)
Kaga, H. *et al., Synlett*, 1994, 607 (*synth, Pipernonaline, Dehydropipernonaline*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419 (*synth, Dehydropipernonaline*)
Yang, Y.-C. *et al., J. Agric. Food Chem.*, 2002, **50**, 3765-3767 (*isol, pmr, cmr*)

Piperochromanoic acid P-398

[110979-03-8]
2-(4,8-Dimethyl-3,7-nonadienyl)-3,4-dihydro-8-hydroxy-3-methylene-2H-1-benzopyran-6-carboxylic acid, 9CI

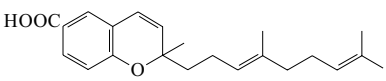


$C_{22}H_{28}O_4$ 356.461
Constit. of the leaves of *Piper auritum* (Veracruz pepper). Green oil. $[\alpha]_D^{34}$ +3 ($CHCl_3$).

Ampofo, S.A. *et al., Phytochemistry*, 1987, **26**, 2367 (*isol, pmr, cmr, ms*)

Piperochromenoic acid P-399

[110979-01-6]
2-(4,8-Dimethyl-3,7-nonadienyl)-2-methyl-2H-1-benzopyran-6-carboxylic acid, 9CI

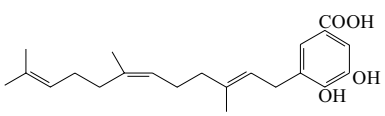


$C_{22}H_{28}O_3$ 340.461
Constit. of the leaves of *Piper auritum* (Veracruz pepper). Brown amorph. solid. $[\alpha]_D^{34}$ +8 (c, 1 in $CHCl_3$).

Ampofo, S.A. *et al., Phytochemistry*, 1987, **26**, 2367 (*isol, pmr, cmr, ms*)

Piperoic acid P-400

[110979-04-9]
3,4-Dihydroxy-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)benzoic acid, 9CI

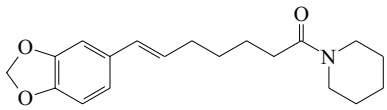


$C_{22}H_{30}O_4$ 358.477
Constit. of the leaves of *Piper auritum* (Veracruz pepper). Oil.

Ampofo, S.A. *et al., Phytochemistry*, 1987, **26**, 2367 (*isol, pmr, cmr, ms*)

Piperolein A P-401

1-[7-(1,3-Benzodioxol-5-yl)-1-oxo-6-heptenyl]piperidine, 9CI. 1-[7-(3,4-Methylenedioxyphenyl)-6-heptenoyl]piperidine



$C_{19}H_{25}NO_3$ 315.411
λ_{max} 214 (ε 28000); 260 (ε 16600); 268 (ε 16100); 305 (ε 10800) (MeOH) (Derep).

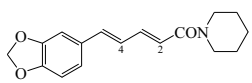
(E)-form [30505-92-1]
Minor constit. of *Piper nigrum* (pepper). Pale yellow oil.

2,3-Didehydro, 6,7-dihydro: [156970-11-5] ***Piperine S***. *1-[7-(1,3-Benzodioxol-5-yl)-1-oxo-2-heptenyl]piperidine. 1-[7-(3,4-Methylenedioxyphenyl)-2-heptenoyl]piperidine*
$C_{19}H_{25}NO_3$ 315.411
Yellow needles. Mp 52-54°. λ_{max} 202 ; 232 (sh) ; 280 (MeOH).

Grewe, R. *et al., Chem. Ber.*, 1970, **103**, 3752 (*isol, synth, struct*)
Wu, Q. L. *et al., Phytochemistry*, 1997, **44**, 727; *CA*, **121**, 104122z (*Piperine S*)

1-Piperoylpiperidine P-402

1-[5-(1,3-Benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]piperidine, 9CI. 1-[5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoyl]-piperidine. 5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoic acid piperidide



(2E,4E)-form

$C_{17}H_{19}NO_3$ 285.342

(2E,4E)-form [94-62-2]
Piperine. *FEMA 2909*
Constit. of pepper (*Piper nigrum*) and many other *Piper* spp. (Piperaceae). Used to impart pungent taste to brandy. Responsible for the hot taste of pepper. Flavour ingredient. Sol. EtOH; poorly sol. H_2O. Mp 129°. pK_a 1.98 (15°). Log P 2.7 (calc).
▶ LD_{50} (rat, orl) 514 mg/kg. Exp. reprod. and teratogenic effects. TN2321500

4,5-Dihydro: [23512-46-1] *1-[5-(1,3-Benzodioxol-5-yl)-1-oxo-2-pentenyl]piperidine. 5-(3,4-Methylenedioxyphenyl)-2-pentenoic acid piperidide.* ***Piperanine***. *β-Hydropiperylpiperidine. $\Delta^{\alpha,\beta}$-Dihydropiperine*
$C_{17}H_{21}NO_3$ 287.358
Isol. from pepper. Cryst. (EtOAc or petrol). Mp 79-80°. λ_{max} 232 (ε 11800); 285 (ε 4350) (MeOH).

(2E,4Z)-form [30511-77-4]
Isochavicine
Constit. of pepper (*Piper nigrum*) (Piperaceae). Cryst. ($CHCl_3$/hexane). Mp 110° (103°).

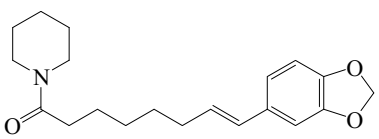
(2Z,4E)-form [30511-76-3]
Isopiperine
Constit. of pepper (*Piper nigrum*) (Piperaceae). Cryst. ($CHCl_3$/hexane). Mp 89° (86°).

(2Z,4Z)-form [495-91-0]
Chavicine
Constit. of pepper (*Piper nigrum*) (Piperaceae). Oil. $Bp_{0.0001}$ 110°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 362C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1379B (*nmr*)
Rügheimer, L. *et al., Ber.*, 1882, **15**, 1390 (*synth, Piperine*)
Loder, J.W. *et al., Aust. J. Chem.*, 1969, **22**, 1531 (*Piperanine*)
Grewe, R. *et al., Chem. Ber.*, 1970, **103**, 3752 (*isol, uv, ir, pmr, synth*)
Traxler, J.T. *et al., J. Agric. Food Chem.*, 1971, **19**, 1135 (*Piperanine*)
Wenkert, E. *et al., J.A.C.S.*, 1971, **93**, 6271 (*pmr, cmr, Piperine*)
Grynpas, M. *et al., Acta Cryst. B*, 1975, **31**, 2663 (*cryst struct, Piperine*)
DeCleyn, R. *et al., Chromatographia*, 1975, **8**, 342 (*isol, uv*)
Addae-Mensah, I. *et al., Phytochemistry*, 1977, **16**, 483 (*Piperanine*)
Tsuboi, S. *et al., Tet. Lett.*, 1979, 1043 (*synth, Piperine, Isochavicine*)
Schulze, A. *et al., Annalen*, 1981, 1725 (*synth*)
Kaga, H. *et al., Synlett*, 1994, 607 (*synth, Piperine*)
De Araujo-Junior, J.X. *et al., Phytochemistry*, 1997, **44**, 559 (*pmr, cmr, Piperine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PIV600

Pipertipine P-403

1-[8-(1,3-Benzodioxol-5-yl)-1-oxo-7-octadecenyl]piperidine, 9CI. 1-[8-(3,4-Methylenedioxyphenyl)-7-octadecenoyl]piperidine

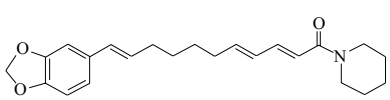


$C_{20}H_{27}NO_3$ 329.438
Alkaloid from the dried seeds of pepper *Piper nigrum*. Yellow wax. λ_{max} 263 (ϵ 13400); 270 (ϵ 12800); 310 (ϵ 5850); 322 (sh) (MeOH).

Siddiqui, B.S. *et al., Heterocycles*, 2002, **57**, 1653-1658 (*isol, pmr, cmr, ms*)

Piperundecalidine P-404

[88660-11-1]
1-[11-(1,3-Benzodioxol-5-yl)-1-oxo-2,4,10-undecatrienyl]piperidine, 9CI. 11-(3,4-Methylenedioxyphenyl)-2,4,10-undecatrienoic acid piperidide

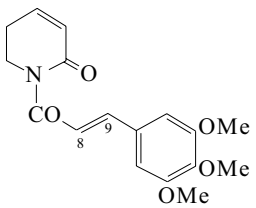


$C_{23}H_{29}NO_3$ 367.487
Alkaloid from the fruits of *Piper longum* (long pepper). Cryst. (EtOAc/hexane). Mp 64.5-65.5°.

Tabuneng, W. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3562 (*isol, uv, ir, pmr, cmr, ms, struct*)

Piplartine P-405

[20069-09-4]
5,6-Dihydro-1-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-propenyl]-2(1H)-pyridinone, 9CI. N-*(3,4,5-Trimethoxycinnamoyl)-Δ^3-piperidin-2-one. 5,6-Dihydro-1-(3,4,5-trimethoxycinnamoyl)-2(1H)-pyridinone. Piperlongumine*



$C_{17}H_{19}NO_5$ 317.341
Alkaloid from the roots of *Piper longum* (long pepper). Needles (EtOH/Et_2O). Mp 124°. Isomeric Δ^5 struct. originally proposed λ_{max} 222 ; 240 ; 325 (MeOH) (Berdy). λ_{max} 225 (ϵ 11000); 324 (ϵ 10000) (EtOH) (Berdy).

Chatterjee, A. *et al., Tetrahedron*, 1967, **23**, 1769 (*isol, uv, ir, pmr*)
Joshi, B.S. *et al., Tet. Lett.*, 1968, 2395 (*pmr, struct*)
Banerji, J. *et al., Phytochemistry*, 1974, **13**, 2327 (*isol*)
Banerjee, T. *et al., Can. J. Chem.*, 1986, **64**, 876 (*cryst struct*)

Piscicolins P-406

Peptides. Prod. by *Carnobacterium piscicola*. Bacteriocins with potential food uses.

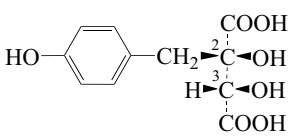
Piscicolin 61 [155808-74-5]
Prod. by *Carnobacterium piscicola* LV61.

Piscicolin 126 [177772-85-9]
Prod. by *Carnobacterium piscicola* JG126. Bacterial control agent in meat paste. Comprises 44 amino acid residues with one intramolecular disulfide bond.

Schillinger, U. *et al., Int. J. Food Microbiol.*, 1993, **20**, 131-147 (*Piscicolin 61*)
Hulck, A. *et al., Curr. Microbiol.*, 1994, **29**, 63-68 (*Piscicolin 61*)
Jack, R.W. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 2887-2903 (*Piscicolin 126*)

Piscidic acid P-407

2,3-Dihydroxy-2-[(4-hydroxyphenyl)-methyl]butanedioic acid, 9CI. p-*Hydroxybenzyltartaric acid*



$C_{11}H_{12}O_7$ 256.212
CAS numbering shown. The chain is frequently numbered from the other end. All 4 stereoisomers have been synthesised.

(2R,3S)-form [35388-57-9]
Isol. from the famine food *Agave americana* and from *Opuntia ficus-indica* (Indian fig). Elongated prisms (EtOAc/$CHCl_3$). Mp 186-187°. $[\alpha]_D$ +42.8 (c, 0.8 in MeOH). λ_{max} 255 (log ϵ 3.88); 277 (log ϵ 3.17) (MeOH).

Di-Me ester:
$C_{13}H_{16}O_7$ 284.265
Cryst. (C_6H_6). Mp 127°. $[\alpha]_D^{19}$ +23.71 (c, 6.37 in EtOH).

*3-O-(3,4-Dihydroxy-*E*-cinnamoyl):*
[219986-51-3] *3-O-Caffeoylpiscidic acid. 2-O-Caffeoylpiscidic acid.* ***Cimicifugic acid D***
$C_{20}H_{18}O_{10}$ 418.356
Pale yellow powder. $[\alpha]_D$ +67.3 (c, 0.34 in MeOH). λ_{max} 248 (sh) (log ϵ 4.02); 291 (log ϵ 4.07); 332 (log ϵ 4.25) (MeOH).

*3-O-(3-Hydroxy-4-methoxy-*E*-cinnamoyl):*
[220618-91-7] *3-O-Isoferuloylpiscidic acid. 2-O-Isoferuloylpiscidic acid.* ***Cimicifugic acid F***
$C_{21}H_{20}O_{10}$ 432.383
Pale yellow powder. $[\alpha]_D$ +37.6 (c, 0.5 in MeOH). λ_{max} 245 (sh) (log ϵ 4.1); 297 (log ϵ 4.19); 326 (log ϵ 4.25) (MeOH).

*3-O-(3-Hydroxy-4-methoxy-*E*-cinnamoyl), 4-Me ester:* [220618-93-9]
$C_{22}H_{22}O_{10}$ 446.41
Pale yellow powder. $[\alpha]_D$ +33.6 (c, 0.2 in MeOH). λ_{max} 245 (sh) (log ϵ 3.92); 295 (log ϵ 3.93); 325 (log ϵ 3.97) (MeOH).

*3-O-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):*
[219986-67-1] *3-O-Feruloylpiscidic acid. 2-O-Feruloylpiscidic acid.* ***Cimicifugic acid E***
$C_{21}H_{20}O_{10}$ 432.383
Pale yellow powder. $[\alpha]_D$ +50.3 (c, 0.2 in MeOH). λ_{max} 291 (log ϵ 3.98); 325 (log ϵ 4.16) (MeOH).

*3-O-(4-Hydroxy-3-methoxy-*E*-cinnamoyl), 4-Me ester:* [220618-92-8]
$C_{22}H_{22}O_{10}$ 446.41
Pale yellow powder. $[\alpha]_D$ +32.8 (c, 0.3 in MeOH). λ_{max} 246 (sh) (log ϵ 4.03); 292 (sh) (log ϵ 4.07); 326 (log ϵ 4.24) (MeOH).

4′-Me ether: [128464-41-5]
$C_{12}H_{14}O_7$ 270.238
Cryst. (EtOAc/$CHCl_3$). Mp 169-170°. $[\alpha]_D^{22.5}$ +41.97 (c, 1.13 in H_2O).

Buckle, A.L.J. *et al., J.C.S.*, 1954, 3981 (*synth*)
Nordal, A. *et al., Acta Chem. Scand.*, 1964, **18**, 1979; 1966, **20**, 1431 (*isol*)
Yoshihara, T. *et al., Tet. Lett.*, 1971, 3809 (*stereochem*)
Takahira, M. *et al., Phytochemistry*, 1998, **49**, 2115-2119 (*isol, uv, pmr, cmr, ms*)
Toshima, H. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 964-967; 1934-1941 (*synth*)
Kruse, S.O. *et al., Planta Med.*, 1999, **65**, 763-764 (*isol*)

Plantacin B P-408

[113956-42-6]
Prod. by *Lactobacillus plantarum* NCDO 1193. Bacteriocin.

West, C.A. *et al., FEMS Microbiol. Lett.*, 1988, **49**, 163-165 (*isol*)

Plantaricin P-409

Polypeptides. Bacteriocins with potential food use.

Plantaricin A

Prod. by *Lactobacillus plantarum* SIK-83. Bioactivity is associated with 2 peptides, α and β.

Plantaricin BN [144377-77-5]
Prod. by *Lactobacillus plantarum* BN.

Plantaricin C [156511-47-6]
Prod. by *Lactobacillus plantarum* LL441.

Plantaricin C19 [153858-63-0]

Plantaricin D [208996-42-3]
Prod. by *Lactobacillus plantarum* BFE 905 isol. from a ready-to-eat salad.

Plantaricin F [159605-63-7]
Prod. by *Lactobacillus plantarum* isol. from processed channel catfish.

Plantaricin KW30 [185915-29-1]
Prod. by *Lactobacillus plantarum* isol. from fermented corn.

Plantaricin LC74 [154303-40-9]
Prod. by *Lactobacillus plantarum* isol. from crude goat's milk.

Plantaricin LP84 [209533-98-2]
Prod. by *Lactobacillus plantarum* NCIM 2084.

Plantaricin S [148937-56-8]
Prod. by *Lactobacillus plantarum* LPCO 10 isol. from green olive fermentation. Bacteriocin activity associated with 2 distinct peptides, α- and β-.

Plantaricin SA6 [154303-54-5]
Prod. by *Lactobacillus plantarum* SA6.

Plantaricin SIK83 [116439-54-4]
Prod. by *Lactobacillus plantarum* SIK-83.

Plantaricin T [148937-57-9]
Prod. by *Lactobacillus plantarum* LPCO 10 isol. from green olive fermentations.

Plantaricin UG1 [160830-12-6]
Prod. by *Lactobacillus plantarum* UG1 isol. from dry sausage.

Plantaricin 1.25 [187285-33-2]

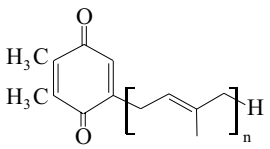
[244277-12-1, 244277-13-2]
Prod. by *Lactobacillus plantarum* TMW 1.25 isol. from fermented dry sausage. Biol. activity associated with 2 peptides, α and β.

Plantaricin 149 [155421-98-0]

Plantaricin 423 [183681-68-7]
Prod. by *Lactobacillus plantarum* 423 isol. from sorghum beer.

Andersson, R.E. *et al., Biochimie*, 1988, **70**, 381-390 (*Plantaricin SIK83*)
Lewis, C.B. *et al., Food Biotechnol.*, 1992, **6**, 153-174 (*Plantaricin BN*)
Nissen-Meyer, J. *et al., J. Gen. Microbiol.*, 1993, **139**, 1973-1978 (*Plantaricin A*)
Gonzalez, B. *et al., Appl. Environ. Microbiol.*, 1994, **60**, 2158-2163 (*Plantaricin C*)
Rekhif, N. *et al., Biotechnol. Lett.*, 1994, **16**, 771-776 (*Plantaricin LC74*)
Kato, T. *et al., J. Ferment. Bioeng.*, 1994, **77**, 277-282 (*Plantaricin 149*)
Fricourt, B.W. *et al., J. Food Prot.*, 1994, **57**, 698-702 (*Plantaricin F*)
Jimenez-Diaz, R. *et al., Appl. Environ. Microbiol.*, 1995, **61**, 4459-4463; 1993, **59**, 1416-1424 (*Plantaricin S, Plantaricin T*)
Rekhif, N. *et al., J. Appl. Bacteriol.*, 1995, **78**, 349-358 (*Plantaricin SA6*)
Evan, G. *et al., Int. J. Food Microbiol.*, 1996, **30**, 189-215 (*Plantaricin UG1*)
Kelly, W.J. *et al., J. Appl. Bacteriol.*, 1996, **81**, 657-662 (*Plantaricin KW30*)
Suma, K. *et al., Int. J. Food Microbiol.*, 1998, **40**, 17-25 (*Plantaricin LP84*)
Van Reenan, C.N. *et al., J. Appl. Microbiol.*, 1998, **84**, 1131-1137 (*Plantaricin 423*)
Franz, C.M.A.P. *et al., Lett. Appl. Microbiol.*, 1998, **26**, 231-235 (*Plantaricin D*)
Remiger, A. *et al., J. Appl. Microbiol.*, 1999, **86**, 1053-1058 (*Plantaricin 1.25*)
Atrih, A. *et al., Int. J. Food Microbiol.*, 2001, **68**, 93-104 (*Plantaricin C19*)

Plastoquinone P-410



A series of homologous prenylated quinones where n defines the plastoquinone number. The side-chain may be unsubstituted (Plastoquinones), monohydroxylated (Plastoquinone C), monoacylated (Plastoquinone B) or monohydroxylated and monoacylated (Plastoquinone Z). The latter classes appear to be confined to higher plant tissues.

Plastoquinone 3 [1168-52-1]
Plastoquinone 15
$C_{23}H_{32}O_2$ 340.505
Constit. of spinach chloroplasts (*Spinacia oleracea*). Yellow oil.

Plastoquinone 4 [4464-99-7]
Plastoquinone 20
$C_{28}H_{40}O_2$ 408.623
Unstable orange oil.

Plastoquinone 8 [28974-95-0]
$C_{48}H_{72}O_2$ 681.096
Isol. from the leaves of *Zea mays* (sweet corn). Oil.

Plastoquinone 9 [4299-57-4]
Plastoquinone 45. Plastoquinone A. Plastoquinone. Q 254. Koflerquinone
$C_{53}H_{80}O_2$ 749.214
Constit. of alfalfa and other plants. Yellow cryst. Mp 48-49°. λ_{max} 254 ; 261 ; 314 (no solvent reported).

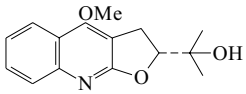
Plastoquinone 10 [4299-58-5]
Plastoquinone 50
$C_{58}H_{88}O_2$ 817.332
Pale yellow leaflets. Mp 46-48°.

[4299-58-5]

Kofler, M. *et al., Helv. Chim. Acta*, 1959, **42**, 1278; 1283; 1960, **43**, 2088 (*Plastoquinone 10*)
Kofler, M. *et al., Helv. Chim. Acta*, 1959, **42**, 2252 (*struct, synth*)
Eck, H. *et al., Z. Naturforsch., B*, 1963, **18**, 446 (*isol, uv, ir, pmr*)
Das, B.C. *et al., Biochem. Biophys. Res. Commun.*, 1965, **21**, 318 (*ms, uv*)
Misiti, D. *et al., J.A.C.S.*, 1965, **87**, 1402; 1407 (*isol, uv, ir, pmr, ms, struct*)
Misiti, D. *et al., J.A.C.S.*, 1965, **87**, 1407 (*struct*)
Whistance, G.R. *et al., Phytochemistry*, 1970, **9**, 213; 737 (*isol*)
Bar, R. *et al., Methods Enzymol.*, 1971, **23**, 372 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 4261 (*bibl*)
Pennock, J.F. *et al., Methods Enzymol.*, 1985, **110**, 313 (*rev, biosynth*)
Okamoto, T. *et al., J. Chromatogr.*, 1988, **430**, 11 (*hplc*)
Boers, R.T. *et al., Eur. J. Org. Chem.*, 2002, 2094-2108 (*Plastoquinone 9, synth, pmr, cmr*)

Platydesmine P-411

2,3-Dihydro-4-methoxy-α,α-dimethyl-furo[2,3-b]quinoline-2-methanol, 9CI



(*R*)-*form*

$C_{15}H_{17}NO_3$ 259.304

Absolute configuration revised in 2000.

(*S*)-*form* [2824-86-4]
Needles (C_6H_6/petrol). Mp 137-138°. $[\alpha]_D$ +47 (c, 0.7 in MeOH).

Ac: **O-*Acetylplatydesmine***
$C_{17}H_{19}NO_4$ 301.341
Prisms (Me_2CO/Et_2O). Mp 126-127°. $[\alpha]_D^{23}$ +23 (c, 1.8 in $CHCl_3$).

N-*Me:* ***Platydesminium***
$C_{16}H_{20}NO_3^{\oplus}$ 274.339
Alkaloid from *Ruta graveolens* (rue). Mp 192-196° (as chloride). $[\alpha]_D$ +31 (c, 0.74 in MeOH) (as iodide).

(*R*)-*form* [318465-89-3]
Mp 137-138°. $[\alpha]_D$ -47 (c, 0.76 in MeOH).

N-*Me:*
$C_{16}H_{20}NO_3^{\oplus}$ 274.339
Mp 180° (as perchlorate). $[\alpha]_D$ -24.3 (c, 0.11 in MeOH) (perchlorate).

(±)-*form* [7764-73-0]
Plates (C_6H_6/petrol). Mp 137-138°.

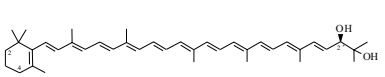
Ac:
Needles (C_6H_6). Mp 126-127°.

N-*Me:*
Prisms (MeOH/diisopropyl ether). Mp 156-158° dec.

Wernhey, F. *et al., Tetrahedron*, 1963, **19**, 1293 (*isol, struct, ir, uv, ms*)
Johns, S.R. *et al., Aust. J. Chem.*, 1966, **19**, 1991 (*isol, pmr*)
Bowman, R.M. *et al., J.C.S.(C)*, 1966, 1504 (*synth, pmr*)
Murphy, S.T. *et al., Aust. J. Chem.*, 1974, **27**, 187 (*isol*)
Rideau, M. *et al., Phytochemistry*, 1979, **18**, 155 (*isol, ms*)
Ramesh, M. *et al., Heterocycles*, 1984, **22**, 125 (*synth, ir, pmr*)
Boyd, D.R. *et al., J.C.S. Perkin 1*, 2000, 3397-3405 (*synth, abs config*)

Plectaniaxanthin P-412

[16795-87-2]
3′,4′-Didehydro-1′,2′-dihydro-β,ψ-carotene-1′,2′-diol



(*R*)-*form*

$C_{40}H_{56}O_2$ 568.881

(*R*)-*form*
Red cryst. (petrol). Mp 172-173°.

2′-Ketone: [16796-12-6] *1′-Hydroxy-3′,4′-didehydro-1′,2′-dihydro-β,ψ-caroten-2′-one.* ***2′-Dehydroplectaniaxanthin***
$C_{40}H_{54}O_2$ 566.865

Isol. from the ascomycete *Aleuria aurantia* (orange cup). Mp 169-170°. Achiral λ_{max} 495 ; 522 (Me_2CO).

2ξ-Hydroxy: [52043-06-8] ***2-Hydroxyplectaniaxanthin***. *3′,4′-Didehydro-1′,2′-dihydro-β,ψ-carotene-1′,2,2′-triol*
$C_{40}H_{56}O_3$ 584.881
Mp 175-177°.

(*S*)-*form*

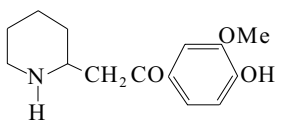
1′-O-β-D-Glucopyranoside: [33762-98-0] ***Phleixanthophyll***
$C_{46}H_{66}O_7$ 731.023
Deep mauve-black cryst. (Py/petrol). Mp 209°.

1′-O-(Hexadecanoyl-β-D-glucopyranoside):Phleixanthophyll palmitate
$C_{62}H_{96}O_8$ 969.436Full struct. not determined.

Hertzberg, S. *et al., Acta Chem. Scand.*, 1967, **21**, 15
Vacheron, M.J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1970, **271**, 881 (*Phleixanthophyll palmitate*)
Bae, M. *et al., Phytochemistry*, 1971, **10**, 625
Shian Liu, I. *et al., Phytochemistry*, 1973, **12**, 2953 (*2-Hydroxyplectaniaxanthin*)
Buchecker, R. *et al., Phytochemistry*, 1976, **15**, 1013 (*isol, Dehydroplectaniaxanthin*)
Rønneberg, H. *et al., Phytochemistry*, 1982, **21**, 2087; 1985, **24**, 309 (*abs config*)
Dumont, R. *et al., Helv. Chim. Acta*, 1984, **67**, 1283 (*synth*)

Pleurospermine P-413

[7363-20-4]
1-(4-Hydroxy-3-methoxyphenyl)-2-(2-piperidinyl)ethanone, 9CI. 4′-Hydroxy-3′-methoxy-2-(2-piperidyl)acetophenone, 8CI. 2-(4-Hydroxy-3-methoxyphenacyl)piperidine



$C_{14}H_{19}NO_3$ 249.309
Cryst. (H_2O). Mp 177° dec. $[\alpha]_D$ +44. pK_a 8 (50% EtOH aq.). The positive opt. rotn. reported could not be substantiated. On reexamination, the original isolate was found to be racemic, and only racemic Pleurospermine could be obt. from fresh plant. This could however, be a case of v. ready racemisation (cf. Isopelleterine).

Hydrochloride:
Cryst. (EtOH). Mp 219-220°.

Picrate:
Cryst. (Me_2CO). Mp 166° dec. Dec. from 150°.

Me ether: [23837-54-9] ***3,4-Dimethoxy-ω-(2-piperidyl)acetophenone***
$C_{15}H_{21}NO_3$ 263.336
Needles (Me_2CO). Poorly sol. hexane. Mp 81-82°. Opt. inactive.

Demethoxy, N-*Me:* [248259-06-5] *4′-Hydroxy-2-(1-methylpiperidin-2-yl)acetophenone.* ***Thalictroidine***
$C_{14}H_{19}NO_2$ 233.31
Alkaloid from the rhizomes of *Caulophyllum thalictroides* (blue cohosh). Glassy solid.

Gellert, E. *et al., Aust. J. Chem.*, 1959, **12**, 90 (*isol, ir*)
Loder, J.W. *et al., Aust. J. Chem.*, 1962, **15**, 296 (*synth, struct*)
Hart, N.K. *et al., Aust. J. Chem.*, 1968, **21**, 1397 (*isol, struct, pmr, deriv*)
Farnsworth, N.R. *et al., Aust. J. Chem.*, 1969, **22**, 1805 (*deriv*)
Al-Shamma, A. *et al., Phytochemistry*, 1982, **21**, 485 (*isol, pharmacol, deriv*)
Kennelly, E.J. *et al., J. Nat. Prod.*, 1999, **62**, 1385-1389 (*Thalictroidine*)

Polacrilin, INN, USAN P-414

[54182-62-6]

[50602-21-6]
Amberlite IRP 64

Copolymer of 2-Methyl-2-propenoic acid and divinylbenzenes. Ion-exchange resin used in food applications.

K salt: ***Polacrilin potassium, USAN***. *Amberlite IRP 88*

[9017-36-1]

Pat. Coop. Treaty (WIPO), 1990, 90 01 926, (*Himedics*); *CA*, **113**, 237831m (*use*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 350-351
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1743
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1687-1688

Polixetonium(1+) P-415

$[OCH_2CH_2N^{\oplus}Me_2CH_2CH_2N^{\oplus}Me_2CH_2CH_2]_n$
$C_{10}H_{24}N_2O^{2\oplus}$ 188.312
Polymer. Minimum formula given.

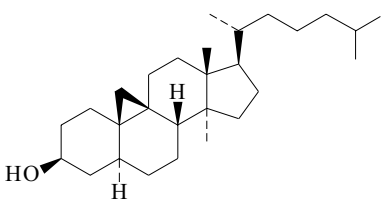
Dichloride: [31512-74-0] *Poly[oxyethylene(dimethyliminio)ethylene(dimethyliminio)ethylene dichloride], 8CI.* ***Polixetonium chloride, INN, USAN***. *Bualta*
$C_{10}H_{24}Cl_2N_2O$ 259.218
Sugarcane ripener. Minimum formula given.

▶ LD_{50} (rat, orl) 1850 mg/kg. TR1650000

U.S. Pat., 1973, 3 771 989, (*Buckman*); *CA*, **80**, 141818m (*synth, use*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **18**, 7; **24**, 431
Bortel, E. *et al., Makromol. Chem.*, 1987, **188**, 2019 (*synth*)

Pollinastanol P-416

[1912-66-9]
9,19-Cyclo-14-methylcholestan-3-ol. Pollinasterol



$C_{28}H_{48}O$ 400.687
Isol. from *Smilax medica* (Sarsaparilla). Cryst. (MeOH). Mp 111-112° (95°). $[\alpha]_D^{20}$ +35 ($CHCl_3$).

Ac: [10376-41-7]
Cryst. (Et_2O). Mp 88-90°. $[\alpha]_D^{20}$ +25 ($CHCl_3$).

Hügel, M.F. *et al., Bull. Soc. Chim. Fr.*, 1964, 2012-2013 (*isol*)
Devys, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1969, **269**, 2033 (*isol*)
Bekaert, A. *et al., Helv. Chim. Acta*, 1975, **58**, 1071-1077 (*synth*)
Khuong-Huu, F. *et al., Tet. Lett.*, 1975, 1787 (*cmr*)
Ducruix, A. *et al., Acta Cryst. B*, 1976, **32**, 76-81 (*cryst struct, Ac*)
Devys, M. *et al., Apidologie*, 1977, **8**, 83 (*rev*)

Polyethylene glycol P-417

[25322-68-3]
α-Hydro-ω-hydroxypoly(oxy-1,2-ethanediyl), 8CI. PEG

$H(OCH_2CH_2)_nOH$ where $n > 4$
Av. MW 200-6000. Diluent in colour additive mixts. for colouring shell eggs; coating, binder, plasticising agent and/or lubricant in tablets used for food; adjuvant to improve flavour and as a bodying agent in non-nutritive sweeteners; adjuvant in dispersing vitamin preparations; defoaming agent; boiler-water additive, etc.. Viscous liq. or solid. Sol. H_2O, org. solv., aromatic hydrocarbons. Mp 4-10°.

▶ Eye irritant. TQ3500000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1166D; 1167A; 1167B; 1167C; 1167D; 1168A; 1168B; 1168C; 1170C; 1170D; 1171A; 1171B; 1171C; 1171D (*ir*)
Fordyce, H. *et al., J.A.C.S.*, 1939, **61**, 1905 (*synth*)
Ziegler, M. *et al., Fresenius' Z. Anal. Chem.*, 1961, **184**, 166 (*detn, Au*)
Chapman, A.H. *et al., Metallurgia*, 1968, **78**, 217 (*detn, Au*)
Davidson, R.L. *et al., Handb. Water-Soluble Gums Resins*, McGraw Hill, N.Y., 1980, (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 355-361
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1722
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2242-2245 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PJT000; PJU000; PJV000; PJT200; PJT225; PJT230; PJT240; PJT250; PJT500; PJT750

Polygalacturonase, 9CI P-418

[9032-75-1]
Poly(1,4-α-D-galacturonide) glycanohydrolase. Pectin depolymerase. Pectinase. E.C. 3.2.1.15

Enzyme. Used in processing apples, lemons and other fruits and in increasing fruit juice yield. Randomly hydrolyses 1,4-α-D-galactosiduronic linkages in pectate and other galacturonans.

Deuel, H. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1958, **20**, 341-382 (*rev*)
Rexova-Benkova, L. *et al., Adv. Carbohydr. Chem. Biochem.*, 1976, **33**, 323-385 (*rev*)
Sakai, T. *et al., Adv. Appl. Microbiol.*, 1993, **39**, 213-214 (*rev*)
Blanco, P. *et al., FEMS Microbiol. Lett.*, 1999, **175**, 1-9 (*rev*)

ϵ-Polylysine P-419

[25104-18-1]

$[-NHCH_2CH_2CH_2CH_2CH(NH_2)CO-]_n$

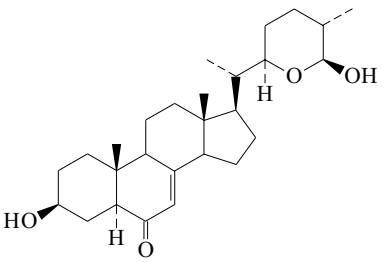
Comprises 25-30 L-lysine residues in an isopeptide linkage. Food additive. Sol. H_2O; poorly sol. Me_2CO, hexane.

Shoji, S. *et al., Agric. Biol. Chem.*, 1981, **45**, 2503-2508 (*isol*)
Kunioka, M. *et al., Appl. Microbiol. Biotechnol.*, 1997, **47**, 469-475 (*rev*)
Kahar, P. *et al., J. Biosci. Bioeng.*, 2001, **91**, 190-194 (*rev*)

Polypodogenin P-420

[33285-07-3]

22,26-Epoxy-3,26-dihydroxycholest-7-en-6-one



$C_{27}H_{42}O_4$ 430.626

Stereochem. revised in 1994. Cryst. (MeOH). Mp 162-164°. $[\alpha]_D^{25}$ +6.6 (c, 0.5 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [33285-16-4] ***Polypodosaponin***
$C_{39}H_{62}O_{13}$ 738.911
Saponin of the licorice fern (*Polypodium vulgare*). Amorph. Mp 198-201° (as 26-Me ether). $[\alpha]_D^{20}$ -14 (c, 0.3 in MeOH) (26-Me ether).

3-O-*β-D-Glucopyranoside, 26*-O-*α-L-rhamnopyranoside:* [120015-16-9] ***Polypodoside B***
$C_{39}H_{62}O_{13}$ 738.911
Constit. of the rhizomes of the licorice fern (*Polypodium glycyrrhiza*). Natural sweetener, 600 times sweeter than sucrose (as mixt. with Polypodoside C).

3-O-*β-D-Glucopyranoside, 26*-O-*(3*-O-*methyl-α-L-rhamnopyranoside):* [120015-17-0] ***Polypodoside C***
$C_{40}H_{64}O_{13}$ 752.938
Constit. of the rhizomes of the licorice fern *Polypodium glycyrrhiza*. Natural sweetener, see above.

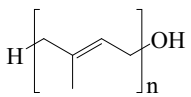
3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 26*-O-*α-L-rhamnopyranoside:* [119784-25-7] ***Polypodoside A***
$C_{45}H_{72}O_{17}$ 885.054
Constit. of rhizomes of the licorice fern (*Polypodium glycyrrhiza*). Intensely sweet substance. Needles (EtOH). Mp 198-200°. $[\alpha]_D$ -37 (c, 0.3 in MeOH).

Jizba, J. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 2867
Jizba, J. *et al., Chem. Ber.*, 1971, **104**, 837
Kim, J. *et al., J. Nat. Prod.*, 1988, **51**, 1166 (*Polypodoside A*)
Kim, J. *et al., Phytochemistry*, 1989, **28**, 1225 (*Polypodosides*)
Nishizawa, M. *et al., Chem. Lett.*, 1994, 1555 (*struct*)

Polyprenol P-421

[10589-57-8]

Betulaprenol. Castaprenol. Albizziaprenol. Cleomeprenol. Cappaprenol. Ficaprenol. Malloprenol. Polyisoprenol. Polyprenyl alcohol. Polyisoprenyl alcohol. Moraprenol



The betulaprenol number indicates the no. of isoprene units. Various geom. isomers isol., although most isolates are of undetd. isomers or mixts. Synonyms for most isolates are given here together regardless of geom. isomerism; Cleomeprenols (Malloprenols, Ficaprenols) appear to be the 3*Z*-isomers.

Dihydro: See Dolichols in *The Combined Chemical Dictionary.*

Betulaprenol 6 [5915-64-0] *Betulahexaprenol. Hexaisoprenol*
$C_{30}H_{50}O$ 426.724
Oil.

Betulaprenol 7 [5905-41-9] *Betulaheptaprenol. Heptaisoprenol*
$C_{35}H_{58}O$ 494.843
Oil.

O-*[β-D-Xylopyranosyl-(1→4)-β-D-xylopyranoside]:* [265658-62-6] ***Plakopolyprenoside***
$C_{45}H_{74}O_9$ 759.074
Amorph. solid. $[\alpha]_D$ -9.

Betulaprenol 8 [5905-42-0] *Betulaoctaprenol. Octaisoprenol*
$C_{40}H_{66}O$ 562.961
Oil.

Betulaprenol 9 [13190-97-1] *Solanesol. Betulanonaprenol. Nonaisoprenol*
$C_{45}H_{74}O$ 631.079
Oil or cryst. Mp 41.5-42.5°.

Betulaprenol 10 [15575-04-9] *Decaprenol. Betuladecaprenol. Decaisoprenol*
$C_{50}H_{82}O$ 699.197
Oil.

(2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z)-isomer:Arachisprenol 10
$C_{50}H_{82}O$ 699.197
Constit. of *Arachis hypogaea* (peanut).
Oil.

Betulaprenol 11 [15575-14-1] *Undecaprenol. Betulaundecaprenol. Undecaisoprenol*
$C_{55}H_{90}O$ 767.315
Oil. Mp 9-10°.

*(2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z,34Z)-isomer:**Arachisprenol 11***
$C_{55}H_{90}O$ 767.315
Constit. of *Arachis hypogaea* (peanut).
Oil.

Betulaprenol 12 [15575-05-0] *Dodecaprenol. Betuladodecaprenol. Dodecaisoprenol*
$C_{60}H_{98}O$ 835.434
Oil. Mp 15-16°.

Ac: [99936-79-5]
$C_{62}H_{100}O_2$ 877.471

*(2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z,34-Z,38Z)-isomer:**Arachisprenol 12***
$C_{60}H_{98}O$ 835.434
Constit. of *Arachis hypogaea* (peanut).
Oil.

Betulaprenol 13 [20741-08-6] *Betulatridecaprenol. Tridecaprenol. Tridecaisoprenol*
$C_{65}H_{106}O$ 903.552
Oil.

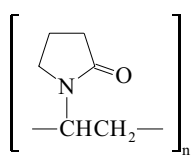
[17093-81-1, 26296-50-4, 28973-73-1, 56453-70-4, 56453-71-5, 59684-99-0, 72690-19-8, 86903-50-6, 96647-64-2]

Rüegg, R. *et al., Helv. Chim. Acta*, 1960, **43**, 1745 (*synth*)
Carruthers, W. *et al., Chem. Ind. (London)*, 1962, 1020 (*ms, Solanesol*)
Wellburn, A.R. *et al., Biochem. J.*, 1966, **102**, 313; 325 (*isol*)
Wellburn, A.B. *et al., Nature (London)*, 1966, **212**, 1364 (*isol*)
Fukawa, H. *et al., Tet. Lett.*, 1966, 6209 (*isol*)
Tabacik-Wlotzku, C. *et al., Phytochemistry*, 1967, **6**, 597 (*isol*)
Gough, D.P. *et al., Biochem. J.*, 1970, **117**, 309 (*biosynth*)
Higashi, Y. *et al., J. Biol. Chem.*, 1970, **245**, 3697 (*isol*)
Morton, R.A. *et al., Biochem. J.*, 1972, **128**, 11P (*rev*)
Suga, T. *et al., J.C.S. Perkin 1*, 1980, 2098 (*Cleomeprenol 12*)
Suga, T. *et al., Phytochemistry*, 1980, **19**, 2327 (*Malloprenol 12*)
Pachaly, P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 615 (*Albizziaprenol*)
Monaco, P. *et al., J. Nat. Prod.*, 1983, **46**, 174
Sato, K. *et al., Chem. Lett.*, 1984, 1105 (*synth*)
Sato, K. *et al., Chem. Comm.*, 1986, 1761 (*synth*)
Suga, T. *et al., J.A.C.S.*, 1986, **108**, 2366 (*biosynth*)
Novikova, M.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1987, 356 (*synth*)
Tanaka, Y. *et al., Chem. Phys. Lipids*, 1989, **51**, 183 (*pmr*)
Suga, T. *et al., J.O.C.*, 1989, **54**, 3390 (*isol, bibl*)
Desoky, E.K. *et al., Phytochemistry*, 1995, **39**, 1383 (*isol, pmr*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1997, **60**, 65 (*Betulaprenol 6, pmr, cmr*)
Aoki, T. *et al., Phytochemistry*, 1997, **46**, 715-720 (*Arachisprenols, Glycinoprenols 7 and 8*)
Costantino, V. *et al., Tetrahedron*, 2000, **56**, 1393-1395 (*Plakopolyprenoside*)

Polyvidone, INN P-422

[9003-39-8]

Povidone, BAN, USAN. *1-Ethenyl-2-pyrrolidinone homopolymer, 9CI. Plasdone. Vinisil. Polyvinylpyrrolidone. Kollidon. Disadine. Many other names*



C_6H_9NO 111.143

Polymer. Monomer formula given. Used as a diluent in colour additive mixtures for marking food; in coatings on fresh citrus fruits; as a clarifying agent for beer, wine and vinegar; as a tableting adjuvant. Faintly yellow solid. The name Crospovidone, INN, USAN also appears to be used.

▶Carcinogen (IARC Group 3). Exp. tumourigenic data. TR8180000

I_2complex: [25655-41-8] ***Povidone-Iodine, BAN, USAN.*** *Betadine. PVP-Iodine. Iodopovidonum. Jodpolyvinylpyrrolidon. Pevidine. Many other names*
Yellowish-brown amorph. powder. ^{125}I and ^{131}I labelled compounds, (Povidone I 125, USAN and Povidone I 131) are used as radioactive agents.

▶Can cause skin haemorrhage and dermatitis. LD_{50} (rat, orl) >8000 mg/kg. LD_{50} (rat, scu) 3450 mg/kg. TR1579600

[92815-93-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1202A; 1202B; 1202C; 1202D; 1203B (*ir*)
U.S. Pat., 1959, 2 900 305, (*General Aniline & Film*); *CA*, **54**, 1811f (*synth*)
Wessel, W. *et al., Arzneim.-Forsch.*, 1971, **21**, 1468 (*rev, pharmacol*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **20**, 220
IARC Monog., 1979, **19**, 461 (*rev, tox*)
Froemming, K.H. *et al., J. Pharm. Sci.*, 1981, **70**, 738 (*props, bibl*)
Horn, D. *et al., J. Pharm. Sci.*, 1982, **71**, 1021 (*props*)
Carli, F. *et al., J. Pharm. Sci.*, 1985, **74**, 963 (*bibl*)
Zamora, J.L. *et al., Am. J. Surg.*, 1986, **151**, 400 (*rev, pharmacol*)
Marshall, P.V. *et al., J. Pharm. Sci.*, 1991, **80**, 899
Adeyeye, C.M. *et al., Anal. Profiles Drug Subst.*, 1993, **22**, 555 (*rev*)
Khattab, I. *et al., J. Pharm. Pharmacol.*, 1993, **45**, 687 (*use*)
Gordon, M.S. *et al., J. Pharm. Sci.*, 1993, **82**, 220
Rahn, R. *et al., J. Postgrad. Med. (Bombay)*, *Suppl.* 3, 1993, **69**, S4 (*povidone-iodine, rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 143-144; 392-399
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 537 (*synonyms*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1143; 1540
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2274-2277
Barabas, E.S. *et al., Anal. Profiles Drug Subst.*, 1998, **25**, 341-462 (*rev, pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKE250; PKR000; PKS000; PKQ250; PKR250; PKQ500; PKR500; PKQ750; PKR750

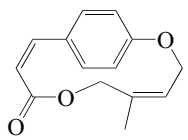
Poly(vinyl alcohol) P-423

[9002-89-5]
Ethenol homopolymer, 9CI. PVA
$[-CH_2CH(OH)-]_n$
Diluent in colour additive mixtures for marking food. White or cream granular powder. Sol. H_2O. Prepd. by hydrolysis of poly(vinyl acetate).

▶TR8100000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1174B; 1174D; 1175A; 1175C; 1175D; 1176A; 1176B; 1176D (*ir*)
Calmé, P. *et al., Mikrochim. Acta*, 1972, 173 (*detn, Cu*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 848 (*rev*)
Dunn, A.S. *et al., Chem. Ind. (London)*, 1980, 801 (*rev*)
Marczenko, Z. *et al., Separation and Spectrophotometric Determination of Elements*, Horwood, Chichester, 1986, (*use*)
Merck Index, 11th edn., 1989, No. 7562
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2272
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKP750

Pondaplin P-424

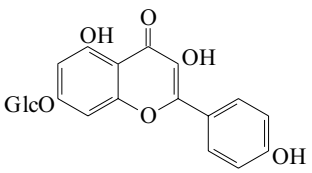


$C_{14}H_{14}O_3$ 230.263
Constit. of the leaves of *Annona glabra* (pond apple). Cryst. Mp 194-195°. λ_{max} 245 (log ϵ 3.05); 295 (sh) (log ϵ 3.03) (no solvent reported). λ_{max} 245 (ϵ 1122); 295 (MeOH) (Berdy).

Liu, X.-X. *et al., Tet. Lett.*, 1999, **40**, 399-402 (*isol, uv, ir, pmr, cmr*)

Populnin P-425

[16290-07-6]
7-O-β-D-Glucopyranosyloxy-3,4′,5-trihydroxyflavone. Kaempferol 7-β-D-glucoside



$C_{21}H_{20}O_{11}$ 448.382
Cryst. (H_2O). Mp 250°. Log P -2.28 (calc).

2″-O-(4-Hydroxy-3-methoxycinnamoyl), 3-O-[α-L-rhamnopyranosyl-(1→2)-D-glucopyranoside]:
$C_{43}H_{48}O_{23}$ 932.838
Constit. of *Allium ursinum* (ramsons). $[\alpha]_D^{25}$ -36 ($CHCl_3$) (as per-Ac).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside]:
$C_{33}H_{40}O_{21}$ 772.666
Constit. of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 220-222°. $[\alpha]_D^{26}$ -37 (c, 0.09 in H_2O). λ_{max} 267 (log ϵ 4.33); 320 (sh) (log ϵ 4.18); 352 (log ϵ 4.25) (MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-6-O-acetyl-β-D-galactopyranoside]:
$C_{35}H_{42}O_{22}$ 814.704
Constit. of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 200-203°. $[\alpha]_D^{26}$ -76 (c, 0.08 in MeOH). λ_{max} 267 (log ϵ 4.35); 321 (sh) (log ϵ 4.17); 350 (log ϵ 4.28) (MeOH).

2″-O-(4-Hydroxycinnamoyl), 3-O-[α-L-rhamnopyranosyl-(1→2)-D-glucopyranoside]:
$C_{42}H_{46}O_{22}$ 902.812
Constit. of *Allium ursinum* (ramsons). $[\alpha]_D^{25}$ -40 ($CHCl_3$) (as per-Ac). λ_{max} 226 ; 266 (sh) ; 300 ; 318 (sh) ; 355 (MeOH).

2″-O-(4-Hydroxycinnamoyl), 3″-O-β-D-glucopyranosyl, 3-O-[α-L-rhamnopyranosyl-(1→2)-D-glucopyranoside]:
$C_{48}H_{56}O_{27}$ 1064.954
Constit. of *Allium ursinum* (ramsons). $[\alpha]_D^{25}$ -45 ($CHCl_3$). λ_{max} 226 ; 267 (sh) ; 301 ; 317 (sh) ; 355 (MeOH).

4″-O-β-D-Glucopyranosyl, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]: [220342-42-7] *Kaempferol 7-cellobioside 3-sophoroside*
$C_{39}H_{50}O_{26}$ 934.808
Constit. of cabbage leaves (*Brassica oleracea*). λ_{max} 265 ; 344 (EtOH aq.).

3-O-[4-Hydroxy-3,5-dimethoxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]: [61042-11-3]
$C_{44}H_{50}O_{25}$ 978.864
Isol. from rape seed (*Brassica napus*). Yellow cryst. (MeOH aq.). Mp 220-225°.

6″-O-(3,4,5-Trihydroxybenzoyl): [85933-23-9]
$C_{28}H_{24}O_{15}$ 600.489
Isol. from *Acacia farnesiana* (sweet acacia).

6″-O-(4-Hydroxycinnamoyl): [142750-32-1] ***Buddlenoid A***. *Biondnoid A*
$C_{30}H_{26}O_{13}$ 594.528
Isol. from *Muntingia calabura* (Jamaica cherry). Powder (MeOH). Mp 173-174°.

*4″-O-β-D-Glucopyranosyl, 3-O-[3,4-dihydroxy-*E*-cinnamoyl-(→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [220342-45-0]
$C_{48}H_{56}O_{29}$ 1096.953
Constit. of cabbage leaves (*Brassica oleracea*). λ_{max} 267 ; 331 (EtOH aq.).

*4″-O-β-D-Glucopyranosyl, 3-O-[(4-hydroxy-3-methoxy-*E*-cinnamoyl)-(→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [220342-44-9]
$C_{49}H_{58}O_{29}$ 1110.98
Constit. of cabbage leaves (*Brassica oleracea*). λ_{max} 268 ; 331 (EtOH aq.).

*4″-O-β-D-Glucopyranosyl, 3-O-[(4-hydroxy-3,5-dimethoxy-*E*-cinnamoyl)-(→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [220342-43-8]
$C_{50}H_{60}O_{30}$ 1141.006
Constit. of cabbage leaves (*Brassica oleracea*). λ_{max} 268 ; 334 (EtOH aq.).

*3-O-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-α-L-rhamnopyranoside]:*
$C_{42}H_{46}O_{22}$ 902.812
Constit. of the leaves of *Ginkgo biloba* (ginkgo). Amorph. yellow powder. λ_{max} 268 ; 316 (MeOH).

[27661-49-0]

Stengel, B. *et al., Z. Naturforsch., C*, 1976, **31**, 622 (*3-sinapoylsophoroside*)
El-Negoumy, S.L. *et al., Egypt. J. Chem.*, 1981, **24**, 471 (*6″-gallate*)
Kubo, I. *et al., Phytochemistry*, 1992, **31**, 1075 (*Buddlenoid A*)
Carotenuto, A. *et al., Phytochemistry*, 1996, **41**, 531 (*Allium ursinum flavonoids*)
Nielsen, J.K. *et al., Phytochemistry*, 1998, **49**, 2171-2176 (*Brassica oleracea glucosides*)
Han, Y. *et al., Phytochemistry*, 2001, **58**, 577-580 (*Trigonella f. graecum glycosides*)

Tang, Y. *et al., Phytochemistry*, 2001, **58**, 1251-1256 (*Ginkgo biloba glycoside*)

Potassium acetate P-426

[127-08-2]

Acetic acid, potassium salt, 8CI. Ethanoic acid, potassium salt. FEMA 2920. E261

KOAc

$C_2H_3KO_2$ 98.143

Flavouring ingredient. Used to modify the flavour of products acidified/preserved with acetic acid. Used in preference to Sodium acetate, S-119 for low-Na foods. White monoclinic powder; deliquescent. Converts to a second monoclinic modification at 76° and undergoes a monoclinic to orthorhombic transition at 140°. Dec. on heating forming $K_2C_2O_4$ as intermed. and K_2CO_3 as final prod. V. sol. H_2O (253 g per 100 cm^3 at 20°; 492 g per 100 cm^3 at 62°), MeOH (24 g per 100 cm^3 at 15°), EtOH; insol. Et_2O, Me_2CO. Mp 292°. ΔH_f° -725 kJ mol^{-1}.

► AJ3325000

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 324G (*ir*)
Grigor'ev, A.I. *et al., Zh. Neorg. Khim.*, 1963, **8**, 802 (*ir*)
Fletton, R.A. *et al., Analyst (London)*, 1971, **96**, 370 (*pmr*)
Hatibarua, J. *et al., Acta Cryst. B*, 1972, **28**, 3100 (*struct, polymorphs*)
Bloor, E.G. *et al., Can. J. Chem.*, 1972, **50**, 3926 (*K-39 nmr*)
Baraldi, P. *et al., Spectrochim. Acta A*, 1982, **38**, 51 (*ir, thermal dec*)
Jenkins, J.E. *et al., J. Phys. Chem. Solids*, 1983, **44**, 565 (*polymorphs, Raman*)
Hofman, A. *et al., Makromol. Chem.*, 1984, **185**, 91 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 15C (*haz*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 2920
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2279-2280
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1161
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKT750

Potassium bromate(*V*) ($KBrO_3$) P-427

[7758-01-2]

Bromic(V) acid, potassium salt, 8CI

$KBrO_3$

$BrKO_3$ 167.001

Dough conditioning agent used in bread making. Normally decomposed during the baking process; also used in barley malting. Colourless hexagonal cryst. Sol. H_2O (13 g per 100 cm^3 at 40°; 50 g per 100 cm^3 at 100°); spar. sol. EtOH; insol. Me_2CO. Mp 434°. ΔH_f -360 kJ mol^{-1}; ΔG_f° -271 kJ mol^{-1}; S° 149 J K^{-1} mol^{-1}. Pyroelectric.

► Oxidiser, toxic, cancer suspect agent. EF8725000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1254B (*ir*)
Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, No. 539, 1957, **7**, 38 (*cryst struct*)
Hird, F.J.B. *et al., Biochem. J.*, 1961, **80**, 612-615 (*use*)
Sterzel, W. *et al., Z. Anorg. Allg. Chem.*, 1971, **383**, 231 (*ir*)
Okado, J. *et al., J. Phys. Soc. Jpn.*, 1972, **32**, 1412 (*K-39 nmr*)
Kondilenko, I.I. *et al., Opt. Spektrosk.*, 1975, **38**, 689 (*Raman*)
Harrison, J.J. *et al., J.O.C.*, 1981, **46**, 2169 (*use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2896A (*haz*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4188-4189 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2284-2285
Himata, K. *et al., Food Addit. Contam.*, 1997, **14**, 809-818 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKY300

Potassium bromide (KBr), 8CI P-428

[7758-02-3]

KBr

BrK 119.002

NaCl struct.. Used in lye peeling or washing of fruits and vegetables. Sl. hygroscopic colourless cubic cryst. V. sol. H_2O (53 g per 100 cm^3 at 0°; 102 g per 100 cm^3 at 100°); spar. sol. EtOH (0.14 g per 100 cm^3 at 25°), Et_2O. Mp 734°. Bp 1435°. ΔH_f° -393.8 kJ mol^{-1}; ΔG_f° -380.4 kJ mol^{-1}; S° 95.9 J K^{-1} mol^{-1}.

► Irritant. TS7650000

Mentzel, A. *et al., Z. Phys.*, 1934, **88**, 178 (*ir*)
Doucet, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1945, **220**, 196 (*uv*)
de Cugnac, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1964, **258**, 4761 (*cryst struct*)
Bonera, G. *et al., Phys. Rev.*, 1968, **165**, 391 (*Br-79 nmr*)
Sahm, W. *et al., Z. Naturforsch., A*, 1974, **29**, 1754 (*K-39 nmr*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 435 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2896B (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2285-2286
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKY500

Potassium carbonate (K_2CO_3) P-429

[584-08-7]

Carbonic acid, dipotassium salt, 8CI. Pearl ash. E501

K_2CO_3

CK_2O_3 138.206

Food flavouring agent and adjuvant, pH control agent and processing aid. Hygroscopic colourless monoclinic cryst. Undergoes polymorphic change at 250°. Dec. on heating with CO_2 loss. V. sol. H_2O (112 g per 100 cm^3 at 20°; 156 g per 100 cm^3); insol. EtOH, Me_2CO. Mp 901°. ΔH_f° -1150 kJ mol^{-1}; ΔG_f° -1065 kJ mol^{-1}; S° 155.5 J K^{-1} mol^{-1}. The name E501 is also used for Potassium hydrogen carbonate, P-433.

► Irritant. TS7750000

Sesquihydrate: [6381-79-9]
$C_2H_6K_4O_9$ 330.457
Colourless monoclinic cryst. Dec. on heating with H_2O loss (-½ H_2O at 235°; -1½ H_2O at 273°). V. sol. H_2O (268 g per 100 cm^3 at 100°); insol. EtOH.

► Irritant.

Duval, C. *et al., Anal. Chem.*, 1959, **20**, 20 (*ir*)
Caranoni, C. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1970, **270**, 1106 (*hydrate, struct*)
Bloor, E.G. *et al., Can. J. Chem.*, 1972, **50**, 3926 (*K-39 nmr*)
Gatehouse, B.M. *et al., J.C.S. Dalton*, 1973, 70 (*struct*)
Becht, H.Y. *et al., Acta Cryst. B*, 1976, **32**, 3344 (*polymorphs*)
Deshpande, D.A. *et al., Thermochim. Acta*, 1983, **66**, 255 (*thermal dehydration, hydrate*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 606 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2896D; 2897A (*haz*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4203-4207 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2287-2288
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLA000

Potassium chloride, 8CI, JAN, USAN P-430

[7447-40-7]

E508

KCl

ClK 74.551

NaCl struct.. Added to food as a flavour enhancer, flavouring agent, nutrient supplement, pH control agent, stabiliser or thickener. Deliquescent colourless cubic cryst. with saline-type taste. V. sol. H_2O (24 g per 100 cm^3 at 20°; 57 g per 100 cm^3 at 100°); sol. Et_2O; spar. sol. EtOH. Mp 771° Mp 773°. Bp 1500°. ΔH_f° -436.7 kJ mol^{-1}; ΔG_f° -408.8 kJ mol^{-1}; S° 82.6 J K^{-1} mol^{-1}. ^{24}K labelled compd. is used as a radioactive agent. Component of Klotrix, Infalyte, Kolyum and Lyteers.

► Eye irritant. TS8050000

Mineral-*form* [14336-88-0]

Sylvite

White, grey or bluish cryst.

Miller, F.A. *et al., Anal. Chem.*, 1952, **24**, 1253 (*ir*)
Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, 1953, **1**, 65 (*cryst struct*)
Sham, W. *et al., Z. Naturforsch., A*, 1974, **29**, 1754 (*K-39 nmr*)
Industrial Chemicals, (Eds. Lowenheim, F.A. *et al*), 4th Ed., Wiley-Interscience, 1975, 666 (*synth*)
Yudasak, M. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 1933 (*Cl-35 nmr*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 753 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2897C (*haz*)
Saxena, K. *et al., Med. Toxicol. Adverse Drug Exper.*, 1989, **4**, 429 (*tox*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 385-387
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1182
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2291-2293
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLA500

Potassium diphosphate ($K_4(P_2O_7)$) P-431

[7320-34-5]

Tetrapotassium pyrophosphate, 8CI. Tetrapotassium diphosphate, 9CI. Potassium pyrophosphate

$K_4(P_2O_7)$

$K_4O_7P_2$ 330.336

The tetrapotassium salt of Diphosphoric acid. Used in foods as a buffering agent, pH control agent, alkalinity source, dispersing agent, protein modifier, coagulant, sequestrant and nutrient source. V. sol. H_2O (187 g per 100 cm^3 at 25°). Dec. v. rapidly at 1300°. Forms adduct with H_2O_2.

▶ JL6735000

Monohydrate:

Trihydrate: [7790-67-2]
Colourless cryst. (elongated rods). Monoclinic cell with anion in staggered conformn. P–O(P) 162.3, 164.9, P $-O_{term.}$ 150.3 pm. POP 130.3°. K 7 or 8 coordinate.

Tetrahydrate: [41159-38-0]
Monoclinic cryst.

α-*form*

High temp.-form

V. hygroscopic, colourless solid. Stable at r.t..

β-*form*

Low temp.-form

V. hygroscopic, colourless solid. Stable at r.t. Transforms into α-form at 500°.

Gofman, I.L. *et al., CA*, 1967, **67**, 110138 (*manuf*)
Bronnikov, A.Kh. *et al., Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1419; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1369 (*synth*)
Shen, C.Y. *et al., J. Am. Oil Chem. Soc.*, 1968, **45**, 510 (*use*)
Mardirosova, I.V. *et al., Zh. Neorg. Khim.*, 1970, **15**, 2507; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1297 (*props*)
Muck, A. *et al., Z. Chem.*, 1971, **11**, 29 (*ir*)
Norbert, A. *et al., Bull. Soc. Fr. Mineral. Cristallogr.*, 1972, **95**, 614 (*cryst struct*)
Bekturov, A.B. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1972, **8**, 303; *Inorg. Mater. (Engl. Transl.)*, 1972, **8**, 266 (*props*)
Frazier, A.W. *et al., J. Agric. Food Chem.*, 1972, **20**, 146 (*synth, props, cryst struct*)
Morgan, W.E. *et al., J.A.C.S.*, 1973, **95**, 751 (*pe*)
Dumas, Y. *et al., Acta Cryst. B*, 1974, **30**, 390 (*cryst struct*)
Yasuda, S. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 1313
Grimmer, A.R. *et al., Chem. Phys. Lett.*, 1983, **99**, 487 (*P-31 nmr*)
Hayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3061 (*P-31 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2317-2318

Potassium disulfite P-432

[16731-55-8]

[23134-05-6]

*Disulfurous acid dipotassium salt, 9CI. Pyrosulfurous acid dipotassium salt, 8CI. Potassium disulfate(*IV*). Potassium pyrosulfite. Potassium metabisulfite. Potassium hypothionate. E224*

$K_2(O_3SSO_s)$

$K_2O_5S_2$ 222.326

Food additive; preservative. Not permitted for meats, food sources of vitamin B_1 or fresh fruit or vegetables. Colourless monoclinic cryst. Dec. on heating to SO_2 and K_2SO_3; some evidence exists for intermediate formation of $SO_2^{\ominus}$. Spar. sol. H_2O, EtOH; insol. Et_2O.

▶ TT4920000

[7773-03-7]

Inorg. Synth., 1946, **2**, 162 (*synth*)
Janzen, E.G. *et al., J. Phys. Chem.*, 1972, **76**, 157 (*thermal dec*)
Jerman, Z. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 2911 (*thermal dec*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 563 (*use*)
Devarajan, V. *et al., Spectrochim. Acta A*, 1977, **33**, 1041 (*ir, Raman*)
Meyer, B. *et al., Spectrochim. Acta A*, 1979, **35**, 345 (*Raman*)
Chen, I.C. *et al., Acta Cryst. C*, 1984, **40**, 1780 (*cryst struct*)
Masson, M.R. *et al., Solubility Data Ser.*, 1986, **26**, 108 (*soly*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLR250

Potassium hydrogen carbonate P-433

[298-14-6]

Potassium bicarbonate, USAN. Potassium carbonate. Carbonic acid, monopotassium salt, 8CI. E501

$K[HCO_3]$

$CHKO_3$ 100.115

Used in foodstuffs as a pH control agent, formulation aid, processing aid and nutrient supplement (potassium). Also used in the production of cacao nibs. Colourless monoclinic cryst. Hygroscopic. Dec. on heating with H_2O and CO_2 loss. V. sol. H_2O (60 g per 100 cm^3 at 60°); insol. EtOH. ΔH_f° -963 kJ mol^{-1}; ΔG_f° -864 kJ mol^{-1}; S° 116 J K^{-1} mol^{-1}. The name E501 is also used for Potassium carbonate (K_2CO_3), P-429.

[71-52-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1273D (*ir*)
Lucienne, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1949, **229**, 1215 (*Raman*)
Nitta, I. *et al., Acta Cryst.*, 1954, **7**, 140 (*cryst struct*)
Zhabrova, G.M. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1959, 596; *CA*, 1960, **54**, 56[3] (*dta*)
Novak, A. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1385 (*ir*)
Feucht, H. *et al., Z. Naturforsch., A*, 1976, **31**, 1173 (*pmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 860
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKX100

Potassium hydrogen sulfate ($KHSO_4$) P-434

[7646-93-7]

[10233-01-9]

Potassium sulfate (KHSO₄). Sulfuric acid, monopotassium salt, 8CI. Potassium bisulfate. Sal enixum. E515

$K[HSO_4]$

HKO_4S 136.17

Food additive (seasoning); acidity regulator. Deliquescent colourless orthorhombic cryst. V. sol. H_2O (36 g per 100 cm^3 at 0°; 122 g per 100 cm^3 at 100°); insol. EtOH, Me_2CO. Mp 214°. The name E515 is also used for Potassium sulfate (K_2SO_4), P-446.

▶ Corrosive. TS7200000

Mineral-*form* [14832-77-0]

Mercallite

Stalactites, white or sky blue.

Mineral-*form*

Misenite

Identity not confirmed.Acicular or lathlike cryst., greyish white.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1265D (*ir*)
Miller, F.A. *et al., Anal. Chem.*, 1952, **24**, 1253 (*ir*)
Thilo, E. *et al., Z. Anorg. Allg. Chem.*, 1963, **319**, 387 (*props*)
Cruickshank, D.W.L. *et al., Acta Cryst.*, 1964, **17**, 682 (*cryst struct*)
Sahm, W. *et al., Z. Naturforsch., A*, 1974, **29**, 1754 (*K-39, K-40 nmr*)
Feucht, H. *et al., Z. Naturforsch., A*, 1976, **31**, 1173 (*pmr*)
Tomishko, M.M. *et al., CA*, 1980, **92**, 153658 (*$KHSO_4$-V_2O_5 catalysts*)
Dey, B. *et al., J. Raman Spectrosc.*, 1982, **13**, 209 (*ir, Raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2904C (*haz*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4245-4247 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKX750

Potassium hydroxide (KOH), 8CI P-435

[1310-58-3]

Potash. E525

KOH

HKO 56.106

Has β-TlI struct.. Added to food as a pH control agent, processing aid, formulation aid, stabiliser or thickener. Colourless orthorhombic cryst.; deliquescent. Undergoes orthorhombic to cubic transition at 243°. V. sol. H_2O (107 g per 100 cm^3 at 15°, 178 g per 100 cm^3 at 100°); sol. EtOH; insol. Et_2O. Mp 406°. Bp 1324°. ΔH_f° -424.7 kJ mol^{-1}; ΔG_f° -378.9 kJ mol^{-1}; S° 78.9 J K^{-1} mol^{-1}. Readily reacts with CO_2 and H_2S to form K_2CO_3 ($KHCO_3$) and K_2S (KSH).

▶ Corrosive, toxic. TT2100000

Monohydrate: [26288-25-5]
Hygroscopic colourless monoclinic cryst. Mp 127°.

Dihydrate: [12306-33-1]
Colourless monoclinic cryst. V. sol. H_2O (195 g per 100 cm^3 at 25°). ΔH_f° -1051 kJ mol^{-1}; ΔG_f° -887 kJ mol^{-1}; S° 151 J K^{-1} mol^{-1}.

Deutero compd.: [24572-01-8] *Potassium deuteroxide*
DKO 57.112
Deliquescent colourless orthorhombic cryst. Mp 406°. Bp 1324°. ΔH_f° -425 kJ mol^{-1}; ΔG_f° -379 kJ mol^{-1}; S° 79 J K^{-1}

mol^{-1}.

▶ Corrosive, toxic.

Teichert, V.W. *et al., Z. Anorg. Allg. Chem.*, 1939, **243**, 138 (*polymorphs*)
Ernst, T. *et al., Angew. Chem.*, 1948, **60A**, 77 (*cryst struct*)
Hoyer, H. *et al., Chem. Ber.*, 1950, **83**, 131 (*deuteroxide, synth, uses*)
Clastre, J. *et al., Cah. Phys.*, 1956, **74**, 24 (*monohydrate, cryst struct*)
Krishnamurti, D. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1959, **50**, 223 (*ir, Raman*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 935 (*uses*)
Ford, J.M. *et al., Encycl. Chem. Process. Des.*, 1978, **7**, 22 (*rev, uses*)
Kanesaka, I. *et al., J. Raman Spectrosc.*, 1984, **15**, 165 (*deuteroxide, Raman*)
Jacobs, H. *et al., Z. Anorg. Allg. Chem.*, 1984, **516**, 67 (*monohydrate, synth, cryst struct, thermal dec*)
Amm, D.T. *et al., Diss. Abstr. Int., B*, 1985, **46**, 1222 (*nmr*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1219 (*thermochem data, polymorphs*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2899B; 2904D (*haz*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4348-4258 (*use*)
Garrett, D.E. *et al., Potash*, Chapman & Hall, 1996, (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2299-2301
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLJ500; PLJ750

Potassium iodate(*V*) (KIO_3) P-436

[7758-05-6]

Iodic acid (HIO₃), potassium salt, 8CI

KIO_3

IKO_3 214.001

Dough strengthener/conditioner used in baking bread. Colourless triclinic cryst. Becomes monoclinic at 72.5°. Also undergoes 2 phase changes below r.t. but remains triclinic. V. sol. H_2O (4.7 g per 100 cm^3 at 0°; 32 g per 100 cm^3 at 100°); insol. EtOH. Mp 560°. ΔH_f° -501 kJ mol^{-1}; ΔG_f° -418 kJ mol^{-1}; S° 152 J K^{-1} mol^{-1}.

▶ Oxidiser, irritant. NN1350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1254D (*ir*)
Timokhina, N.I. *et al., CA*, 1965, **63**, 2604d (*synth*)
Sterzel, W. *et al., Z. Anorg. Allg. Chem.*, 1971, **383**, 231 (*ir*)
Hamid, S.A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1973, **137**, 412 (*polymorphs*)
Kondilenko, I.I. *et al., Zh. Prikl. Spektrosk.*, 1974, **21**, 282 (*Raman*)
Lucas, B.W. *et al., Acta Cryst. C*, 1984, **40**, 1989; 1985, **41**, 1388 (*cryst struct, polymorphs*)
Kamman, P.W. *et al., Baker's Dig.*, 1984, **58**, 18 (*rev, use*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2905C (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2301-2302
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLK250

Potassium iodide, 8CI, JAN, USAN P-437

[7681-11-0]

KI

IK 166.003

NaCl struct.. Nutrient supplement; added to food as a source of iodine. Colourless cubic cryst. V. sol. H_2O (128 g per 100 cm^3 at 0°, 208 g per 100 cm^3 at 100°); mod. sol. EtOH (1.9 g per 100 cm^3 at 25°), Me_2CO (1.3 g per 100 cm^3 at 25°); spar. sol. Et_2O. Mp 681° Mp 723°. Bp 1330°. ΔH_f° -327.9 kJ mol^{-1}; ΔG_f° -323.0 kJ mol^{-1}; S° 106.4 J K^{-1} mol^{-1}. Component of Elixophyllin -KI and Quadrinal.

▶ Human teratogen. TT2975000

Hildebrandt, *et al., Arch. Exp. Pathol. Pharmakol.*, 1923, **96**, 292 (*tox*)
Inorg. Synth., 1939, **1**, 163 (*synth*)
Barr, E.S. *et al., J. Chem. Phys.*, 1939, **7**, 8 (*ir*)
Doucet, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1943, **216**, 198 (*uv*)
Hambling, P.G. *et al., Acta Cryst.*, 1953, **6**, 98 (*cryst struct*)
Kanert, O. *et al., Z. Naturforsch., A*, 1971, **26**, 1435 (*I-127 nmr*)
Shih, J.S. *et al., Inorg. Nucl. Chem. Lett.*, 1977, **13**, 105 (*K-39 nmr*)
Waterfall, W.K. *et al., Br. Med. J.*, 1980, **281**, 988 (*use*)
Vincent, C.A. *et al., Solubility Data Ser.*, 1980, **11**, 39; 123; 198 (*soly*)
Scrosati, B. *et al., Solubility Data Ser.*, 1980, **11**, 251; 278; 329 (*soly*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1335 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2905D (*haz*)
Kirk, K.L. *et al., Biochemistry of the Elemental Halogens and Inorganic Halides*, Plenum Press, 1991, 121 (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 972
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4258-4259 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2302-2303
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLK500

Potassium metaphosphate, 9CI, 8CI P-438

[7790-53-6]

$(KPO_3)_x$

KO_3P 118.07

Generally polymeric; monomeric salt has been matrix-isol. Mp 803-813°.

Polymeric-*form* [29057-10-1]

Consists of PO_4 tetrahedra sharing corners. P–O 144-163 pm. $K^\oplus$ ions are 7- and 8-coordinated. Used as a buffering agent in foods. Undergoes polymorphic transitions at *ca*. 500°, 670° and various forms may resemble the Na Maddrell and Kurrol salts, the latter form being the most characteristic for K salt.

Jost, K.H. *et al., Acta Cryst.*, 1963, **16**, 623 (*cryst struct*)
Bekturov, A.B. *et al., Zh. Neorg. Khim.*, 1968, **13**, 41; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1968, **13**, 20 (*props*)
Jost, K.H. *et al., Acta Cryst. B*, 1971, **27**, 1345 (*struct*)
Vorob'ev, N.I. *et al., CA*, 1972, **77**, 150961 (*manuf*)
Exarhos, G.J. *et al., J. Chem. Phys.*, 1974, **60**, 4145 (*ir, Raman*)
Rat'kovskii, I.A. *et al., Zh. Fiz. Khim.*, 1974, **48**, 230; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1974, **48**, 140 (*ms*)
Steblevskii, A.V. *et al., Zh. Neorg. Khim.*, 1977, **22**, 23; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1977, **22**, 11 (*props, ms*)
Bowling, R.A. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1979, **17**, 25 (*pe*)
Grimmer, A.R. *et al., Chem. Phys. Lett.*, 1983, **99**, 487 (*P-31 nmr*)
Bencivenni, L. *et al., J. Mol. Struct.*, 1983, **98**, 195 (*synth, ir*)
Prabhakar, S. *et al., Chem. Phys. Lett.*, 1987, **139**, 96 (*P-31 nmr*)
Girichov, G.V. *et al., Zh. Strukt. Khim.*, 1987, **28**, 189; *J. Struct. Chem. (Engl. Transl.)*, 1987, **28**, 630 (*ed, struct*)
Chudinova, N.N. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1989, **25**, 459; *Inorg. Mater. (Engl. Transl.)*, 1989, **25**, 399 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2316-2317

Potassium nitrate (KNO_3) P-439

[7757-79-1]

Nitric acid, potassium salt, 8CI. Potassium nitrate. E252

KNO_3

KNO_3 101.103

Preservative for cod roe, cured red meat and poultry products. Colourless orthorhombic cryst. Undergoes orthorhombic (form I) - rhombohedral (form II) transition at 128°; cooling form II gives a metastable rhombohedral polymorph (form III) which exists between 128 and 109°. V. sol. H_2O (13 g per 100 cm^3 at 0°; 247 g per 100 cm^3 at 100°). Mp 334°. ΔH_f° -495 kJ mol^{-1}; ΔG_f° -395 kJ mol^{-1}; S° 133 J K^{-1} mol^{-1}.

▶ Oxidiser, irritant. TT3700000

Mineral-*form* [15621-57-5]

*Nitre. **Niter**. Saltpetre. Saltpeter. Nitratine*

Isotypic with aragonite ($CaCO_3$).Brittle orthorhombic crusts.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1257C (*ir*)
Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, 1954, **3**, 58 (*cryst struct*)
McLaren, A.C. *et al., Rev. Pure Appl. Chem.*, 1962, **12**, 54 (*polymorphs*)
Nakagawa, I. *et al., J. Chem. Phys.*, 1969, **51**, 1389 (*ir, Raman*)
Sahm, W. *et al., Z. Naturforsch., A*, 1974, **29**, 1754 (*K-39, K-40, K-41 nmr*)
Kamada, M. *et al., J. Phys. Soc. Jpn.*, 1975, **35**, 1561 (*uv*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2906B (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2307-2308
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLL500

Potassium nitrite (KNO_2) P-440

[7758-09-0]

Nitrous acid potassium salt, 8CI. Potassium nitrite. E249

KNO_2

KNO_2 85.104

Preservative for red meat and poultry products. Pale yellow hexagonal cryst.; deliquescent. Undergoes rhombohedral to cubic transition at 70°. Disproportionates

on heating in the absence of air forming KNO_3 and K_2O and evolving N_2. V. sol. H_2O (281 g per 100 cm^3 at 0°; 413 g per 100 cm^3 at 100°). Mp 440°. ΔH_f° -370 kJ mol^{-1}; ΔG_f° -307 kJ mol^{-1}; S° 152 J K^{-1} mol^{-1}.

► Oxidiser, toxic. TT3750000

Rodloff, G. *et al., Z. Phys.*, 1934, **91**, 511 (*uv*)
Tanisaki, S. *et al., J. Phys. Soc. Jpn.*, 1965, **20**, 1277 (*cryst struct, polymorphs*)
Patil, K.C. *et al., Inorg. Chim. Acta*, 1967, **1**, 155 (*ir*)
Bloor, E.G. *et al., Can. J. Chem.*, 1972, **50**, 3926 (*K-39 nmr*)
Adams, D.M. *et al., Solid State Commun.*, 1977, **23**, 729 (*Raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2906C (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2308
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLM500

Potassium permanganate, JAN, USAN P-441

[7722-64-7]

*Potassium manganate(*VII*) (KMnO₄)*

$KMnO_4$

$KMnO_4$ 158.034

Mn–O 162.9 pm; isomorphous with $KClO_4$,KBF_4, $BaSO_4$. Bleaching agent for food starch. Air-stable dark bronze-purple cryst. Sol. H_2O; mod. sol. MeOH, AcOH, Me_2CO, Py. Mp 240° dec. Aq. solns. slowly deposit MnO_2. Exhibits positive magnetic susceptibility of *ca.* 70 x 10^{-6} cgs mol^{-1}.

► Corrosive and irritating to all tissues. Dilute solns. stain skin. Ingestion can cause gastrointestinal haemorrhage, liver and kidney damage. Fatal human dose *ca.* 10g. Must be stored away from combustible materials, can explode on contact with AcOH, DMF and other organic compds. LD_{50} (rat, orl) 1090 mg/kg. Neurotoxic (Parkinson-type symptoms) from chronic misuse. SD6475000

18-Crown-6 complex:
Sol. CH_2Cl_2, $CHCl_3$. Mp 50° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1291A (*ir*)
Griffith, W.P. *et al., J.C.S.(A)*, 1966, 1467 (*ir*)
Palenik, G.J. *et al., Inorg. Chem.*, 1967, **6**, 503 (*cryst struct*)
Smyth, H.F. *et al., Am. Ind. Hyg. Assoc. J.*, 1969, **30**, 470 (*tox*)
Johnson, L.W. *et al., J. Chem. Phys.*, 1971, **55**, 2985 (*uv*)
Weinstock, N. *et al., J. Chem. Phys.*, 1973, **59**, 5063 (*Raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 56, 1975, **C2**, 146 (*rev, bibl*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **3**, 1586 (*synth*)
Lowenheim, F.A. *et al., Ind. Chem.*, Eds., 4th Ed., Wiley-Interscience, N.Y., 1975, 679
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **14**, 859
Holzgraefe, M. *et al., J. Toxicol. Clin. Toxicol.*, 1986, **24**, 235 (*tox*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4274-4282 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2310
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1123
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1056
Bretherick's Handbook of Reactive Chemical Hazards, 6th edn., (ed. Urben, P.G.), Butterworth-Heinemann, 1999, 4647
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, PLP000

Potassium persulfate ($K_2S_2O_8$) P-442

[7727-21-1]

*Potassium peroxodisulfate(*VI*). Peroxydisulfuric(*VI*) acid, dipotassium salt, 8CI*

$K_2[O_3S–O–O–SO_3]$

$K_2O_8S_2$ 270.324

Defoamer and dispersing adjuvant for coatings on fresh citrus fruits. Colourless triclinic cryst. Dec. on heating to $K_2S_2O_7$ with loss of O_2. Mod. sol. H_2O (6.2 g per 100 cm^3 at 25°). ΔH_f° -1918 kJ mol^{-1}.

► Oxidiser, irritant. LD_{50} (rat, orl) 802 mg/kg. SE0400000

Keen, R.C. *et al., Z. Kristallogr.*, 1935, **91**, 129 (*cryst struct*)
Sengupta, R. *et al., J.C.S.*, 1951, 3278 (*uses*)
Miller, F.A. *et al., Anal. Chem.*, 1952, **24**, 1253 (*ir*)
Simon, A. *et al., Z. Anorg. Allg. Chem.*, 1962, **315**, 196 (*Raman*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 952 (*uses*)
House, J.E. *et al., Thermochim. Acta*, 1978, **24**, 117 (*stability*)
Thiele, W. *et al., Chem. Technol.*, 1979, **31**, 198 (*synth*)
Vacek, V. *et al., Chem. Prum.*, 1982, **32**, 178 (*props*)
Vacek, V. *et al., Thermochim. Acta*, 1985, **90**, 33 (*props*)
Eysel, H.H. *et al., J. Raman Spectrosc.*, 1987, **18**, 123 (*Raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2908D (*haz*)
Merck Index, 11th edn., 1989, No. 7644
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2310-2311
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DWQ000

Potassium phosphate ($K(H_2PO_4)$) P-443

[7778-77-0]

[16068-46-5]

Potassium dihydrogenphosphate. Monopotassium phosphate, 9CI, 8CI. Potassium phosphate monobasic, USAN

$K(H_2PO_4)$

H_2KO_4P 136.085

Ferroelectric phase is orthorhombic; paraelectric phase (ordinary phase) is tetragonal, becoming monoclinic at 180-192°. Buffering agent; acidulant; leavening agent; nutrient source. White cryst. solid. Sol. H_2O (23 g per 100 cm^3 at 20°, 34 g per 100 cm^3 at 40°). Mp 253° Mp 272°. Exhibits electrooptical and piezooptical props. at high temps.; also thermoluminescence coincident with paraelectric-ferroelectric transition at -150°.

[13761-79-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1267B (*ir*)
Stephenson, C.C. *et al., J.A.C.S.*, 1944, **66**, 1397 (*thermodyn*)
Ubbelohde, A.R. *et al., Proc. R. Soc. London, A*, 1947, **188**, 358 (*cryst struct*)
Steger, E. *et al., Z. Anorg. Allg. Chem.*, 1964, **331**, 169 (*ir, Raman*)
Hill, R.M. *et al., J. Chem. Phys.*, 1968, **48**, 838 (*ir*)
Blinc, R. *et al., J. Chem. Phys.*, 1968, **49**, 4996 (*pmr, ir*)
Tsutsumi, Y. *et al., J. Phys. Soc. Jpn.*, 1968, **24**, 429 (*K-39 nmr*)
Mullin, J.W. *et al., J. Appl. Chem.*, 1970, **20**, 153 (*morphology, props*)
Baldini, G. *et al., Solid State Commun.*, 1972, **11**, 1257 (*uv*)
Blinc, R. *et al., Chem. Phys. Lett.*, 1973, **23**, 486 (*O-17 nqr*)
Anbar, M. *et al., Inorg. Chem.*, 1976, **15**, 727 (*ms*)
Jasiński, A. *et al., Phys. Status Solidi B*, 1976, **74**, K5 (*P-31 nmr*)
Koralewski, M. *et al., Phys. Status Solidi A*, 1980, **58**, K59 (*ord, cd*)
Belouet, C. *et al., Prog. Cryst. Growth Charact.*, 1980, **3**, 121 (*rev*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **42**, 335 (*P-31 nmr*)
Busch, G. *et al., Ferroelectrics*, (*Special Issue*), 1987, **71**, ; **72**, 335
Tun, Z. *et al., J. Phys. C: Solid State Phys.*, 1988, **21**, 245 (*nd, struct*)
Yagi, T. *et al., Ferroelectrics*, 1989, **95**, 249 (*Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 858
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2313-2315

Potassium phosphate (K_3PO_4) P-444

[7778-53-2]

[16068-46-5]

Tripotassium phosphate, 9CI, 8CI. Potassium orthophosphate (K_3PO_4)

K_3PO_4

K_3O_4P 212.266

Exists in low and high temp. form, the latter being stabilised by divalent metal cations. Used in food processing as a source of alkalinity, buffering agent, emulsifier, nutrient, protein modifier and stabiliser. Colourless hygroscopic powder. V. sol. H_2O. ΔH_f° -1949 kJ mol^{-1}.

► TC8450000

Sesquihydrate: [22763-04-8]

Trihydrate: [22763-03-7] *In vacuo* at 20° → 1.5 hydrate. At 300° → anhyd. salt.

Heptahydrate: [22763-02-6] Additionally reported hydrates include the hemihydrate, the monohydrate, and the tetrahydrate.

Tetrakis-H_2O_2 complex: [36563-86-7] Dec. at *ca.* 90°. *In vacuo* over P_4O_{10}r 1:1 and 1:2 complexes.

[27176-09-6, 27176-10-9, 36563-87-8, 36563-88-9, 39041-45-7, 62770-61-0]

Miller, F.A. *et al., Spectrochim. Acta A*, 1960, **16**, 135 (*ir*)
Brauer, G. *et al., Handb. Prep. Inorg. Chem., 2nd edn., Academic Press*, 1965, **1**, 545 (*synth*)

Pinchas, S. *et al., J. Inorg. Nucl. Chem.*, 1968, **30**, 1785 (*ir, Raman*)
Brun, G. *et al., Rev. Chim. Miner.*, 1968, **5**, 823 (*synth, props*)
Morgan, W.E. *et al., J.A.C.S.*, 1973, **95**, 751 (*pe*)
Hoppe, R. *et al., Z. Naturforsch., B*, 1973, **28**, 507 (*synth, cryst struct*)
Lutz, O. *et al., Z. Naturforsch., A*, 1978, **33**, 380 (*O-18 nmr, P-31 nmr*)
Mazghouni, M. *et al., Thermochim. Acta*, 1981, **47**, 125 (*props*)
Gerothanassis, I.P. *et al., J. Magn. Reson.*, 1982, **46**, 423 (*O-17 nmr*)
Taniguchi, K. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 909 (*pe*)
Ger. Pat., 1985, 3 423 071; *CA*, **102**, 115958 (*manuf*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Eysel, H.H. *et al., J. Raman Spectrosc.*, 1988, **19**, 535 (*Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2315-2316

Potassium phosphinate, 9CI P-445

[7782-87-8]
Potassium hypophosphite

KH_2PO_2

H_2KO_2P 104.087

Listed in the EAFUS Food Additive Database (Jan 2001) but with no reported uses. Deliquescent cryst.

Wurtz, A. *et al., Annalen*, 1846, **58**, 51 (*synth*)
Von Wazer, J.R. *et al., J.A.C.S.*, 1956, **78**, 5715-5726 (*nmr*)
Ziomek, J.S. *et al., J. Mol. Spectrosc.*, 1962, **8**, 212-221 (*ir, Raman*)
Lovejoy, R.W. *et al., J. Phys. Chem.*, 1964, **68**, 544-550 (*ir*)

Potassium sulfate (K_2SO_4) P-446

[7778-80-5]

[10233-01-9]
Sulfuric acid, dipotassium salt, 8CI. Sal polychrestum. Arcanum duplicatum. Tartarus vitriolatus. E515

K_2SO_4

K_2O_4S 174.26

Flavouring agent and enhancer. Colourless orthorhombic cryst. Undergoes orthorhombic-hexagonal transition at 584°. Sol. H_2O (12 g per 100 cm^3 at 25°; 24 g per 100 cm^3 at 100°); insol. EtOH, Me_2CO. Mp 1069°. Bp 1689°. ΔH_f° -1438 kJ mol^{-1}; ΔG_f° -1320 kJ mol^{-1}; S° 175.5 J K^{-1} mol^{-1}. Ferroelectric. The name E515 is also used for Potassium hydrogen sulfate ($KHSO_4$), P-434.

▶TT5900000

Mineral-*form* [14293-72-2]
Arcanite
Orthorhombic.Colourless, yellowish, transparent, pseudohexagonal, thin plates.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1263B (*ir*)
Robinson, M.T. *et al., J. Phys. Chem.*, 1958, **62**, 925 (*cryst struct*)
Waggoner, W.H. *et al., Talanta*, 1960, **5**, 121 (*uv*)
Ananthanaryanan, V. *et al., Z. Phys.*, 1961, **163**, 144 (*Raman*)
Steger, E. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1964, **68**, 102 (*ir*)
Pannetier, G. *et al., Bull. Soc. Chim. Fr.*, 1966, 188 (*polymorphs*)
Xie, K.C. *et al., J. Catal.*, 1985, **94**, 323 (*K_2SO_4-V_2O_5 catalysts*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1418 (*polymorphs, thermochem data*)
Eckert, H. *et al., J.A.C.S.*, 1986, **108**, 2140 (*S-33 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2323-2324
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1161
Tomishko, M.M. *et al., CA*, **92**, 153658 (*K_2SO_4-V_2O_5 catalysts*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLT000

Potassium sulfite (K_2SO_3) P-447

[10117-38-1]
Sulfurous acid dipotassium salt, 8CI

K_2SO_3

K_2O_3S 158.261

Food additive listed in the EAFUS Food Additive Database (Jan. 2001). Colourless hexagonal cryst. V. sol. H_2O.

▶Irritant. WT3530000

Dihydrate: [7790-56-9]
$H_4K_2O_5S$ 194.291
Pale yellow hexagonal cryst., dec. on heating with loss of H_2O. V. sol. H_2O.

Inorg. Synth., 1946, **2**, 162 (*synth*)
Seibert, H. *et al., Z. Anorg. Allg. Chem.*, 1954, **275**, 225 (*ir, Raman*)
Rasch, R. *et al., Sprechsaal Keram., Glas, Email, Silik.*, 1970, **103**, 117; *CA*, **72**, 125755 (*thermodyn*)
Archer, C. *et al., Can. J. Chem.*, 1979, **57**, 899 (*cryst struct, synth*)
Peter, L. *et al., Inorg. Chem.*, 1985, **24**, 3071 (*ir, Raman*)
Masson, M.R. *et al., Solubility Data Ser.*, 1986, **26**, 90 (*soly*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 2909C (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PLT500

Potassium tetraborate P-448

[1332-77-0]
Boric acid ($H_2B_4O_7$) dipotassium salt, 9CI, 8CI. Boron potassium oxide ($B_4K_2O_7$), 11CI, 10CI. Potassium biborate. Potassium borate. Dipotassium borate ($B_4O_7^{2\ominus}$)

$K_2B_4O_7$

$B_4K_2O_7$ 233.436

Listed in the EAFUS Food Additive Database (Jan. 2001). Colourless triclinic cryst., hygroscopic. Mp 815°. ΔH_f° -3334.2 kJ mol^{-1}; ΔG_f° -3136.8 kJ mol^{-1}; S° 208 J K^{-1} mol^{-1}.

'Tetrahydrate': See Dipotassium tetraborate dihydrate in *The Combined Chemical Dictionary.*

Miller, F.A. *et al., Anal. Chem.*, 1952, **24**, 1253 (*ir*)
Krogh-Moe, J. *et al., Acta Cryst.*, 1961, **14**, 68 (*cryst struct*)
Tolédano, P. *et al., Rev. Chim. Miner.*, 1964, **1**, 353 (*synth*)
Epperlein, B.W. *et al., Z. Naturforsch., A*, 1975, **30**, 955 (*B-10 nmr, B-11 nmr*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 289 (*thermochem data*)
Skvortsov, V.G. *et al., Zh. Neorg. Khim.*, 1985, **30**, 2341 (*uv*)

Potassium triphosphate ($K_5(P_3O_{10})$) P-449

[13845-36-8]
Potassium tripolyphosphate. Pentapotassium triphosphate, 9CI, 8CI

$K_5(P_3O_{10})$

$K_5O_{10}P_3$ 448.407

Penta potassium salt of Triphosphoric acid. Food contaminant derived from its use as a boiler water additive for the prepn. of steam used in food processing. Texturiser and sequestrant in foods, mainly as the K/Na double salt. Hygroscopic colourless solid. V. sol. H_2O. Mp 625-630° (incongr.). In addition to hydrates, forms adducts with H_2O_2.

Dihydrate (α-form):
Colourless cryst.

Dihydrate (β-form): [66904-52-7]
Colourless cryst.

Tetrahydrate: [53171-31-6] Thought to exist in two (α,β) modifications. Yields the dihydrate when heated and in dry air at 400-450° is completely dehydrated.

[24315-83-1]

U.S. Pat., 1967, 3 309 174; *CA*, **66**, 117480 (*manuf*)
Bronnikov, A.Kh. *et al., Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1419; 1969, **42**, 984; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1369; 1969, **42**, 942 (*synth*)
U.S. Pat., 1971, 3 607 018; *CA*, **75**, 142385 (*manuf*)
Jesson, J.P. *et al., J.A.C.S.*, 1973, **95**, 618 (*P-31 nmr*)
Sotnikova-Yuzhik, V.A. *et al., Zh. Neorg. Khim.*, 1976, **21**, 41; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1976, **21**, 23 (*synth, ir, props*)
Lysutsko, V.A. *et al., Zh. Prikl. Spektrosk.*, 1982, **37**, 415; *J. Appl. Spectrosc. (Engl. Transl.)*, 1982, **37**, 1033 (*ir, Raman*)
Grimmer, A.R. *et al., Chem. Phys. Lett.*, 1983, **99**, 487 (*P-31 nmr*)
Malashonok, I.E. *et al., Zh. Neorg. Khim.*, 1988, **33**, 3049; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1988, **33**, 1758 (*ir, Raman*)
Hayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3061 (*P-31 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2324

Potato carboxypeptidase A inhibitor P-450

[70322-64-4]
Carboxypeptidase inhibitor (potato AP-1-A). PCI

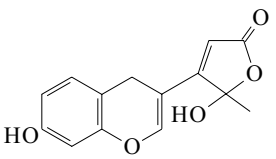
Struct. consists of 39 amino-acid residues with 3 intramolecular disulfide bonds. A 38 amino-acid analogue has also been isol.. Isol. from potato.

[56092-20-7, 56092-22-9]

Ryan, C.A. *et al., J. Biol. Chem.*, 1974, **249**, 5495 (*isol*)
Hass, G.H. *et al., Biochemistry*, 1975, **14**, 1334 (*struct*)
Leary, R.T. *et al., Biochemistry*, 1979, **18**, 2252 (*struct*)

Pratenol A P-451

[147838-41-3]

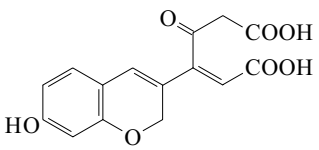


$C_{14}H_{12}O_5$ 260.246
Constit. of *Trifolium pratense* (red clover). Yellow fluorescent cryst. (EtOAc/hexane). Mp 240-250° dec.

Yoshihara, T. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1955 (*isol, uv, ir, pmr*)

Pratenol B P-452

[147710-51-8]



$C_{15}H_{12}O_7$ 304.256
Constit. of *Trifolium pratense* (red clover). Yellow fluorescent powder.

Yoshihara, T. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1955 (*isol, uv, ir, pmr*)

Pratoletin P-453

$C_{15}H_{10}O_6$ 286.24
Struct. unknown. Flavonoid. Has been assigned the struct. 3,4′,5,8-Tetrahydroxyflavone but this is prob. incorrect. Isol. from *Trifolium pratense* (red clover). Dark yellow substance + $2H_2O$. Mp 285°.

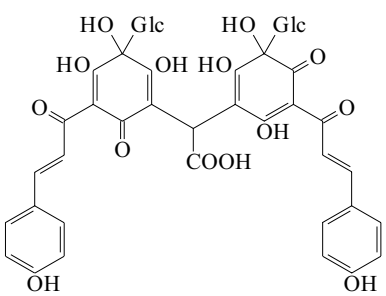
Tri-Me ether:
Mp 154°.

Tetra-Me ether:
Mp 138°.

Hattori, S. *et al., CA*, 1951, **45**, 5156

PRE P-454

[160564-02-3]

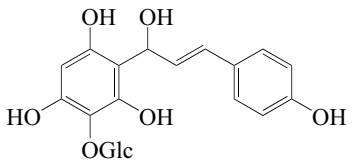


$C_{44}H_{44}O_{24}$ 956.817
Isol. from the flowers of *Carthamus tinctorius* (safflower). Unstable yellow microneedles. Mp 300°.

Kumazawa, T. *et al., Chem. Lett.*, 1994, 2343 (*isol, uv, pmr, cmr, ms*)

Precarthamin P-455

[102716-32-5]
2,4,6-Trihydroxy-3-[1-hydroxy-3-(4-hydroxyphenyl)-2-propenyl]phenyl β-D-glucopyranoside, 9CI

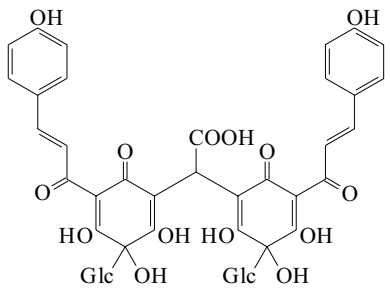


$C_{21}H_{24}O_{11}$ 452.414
Red pigment from the flowers of *Carthamus tinctorius* (safflower).

Saito, K. *et al., Acta Soc. Bot. Pol.*, 1989, **58**, 593
Kazuma, K. *et al., CA*, 1995, **123**, 93009f (*isol, struct*)

Precarthamin P-456

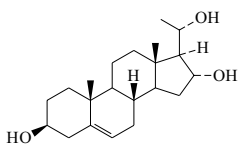
[168216-23-7]



$C_{44}H_{44}O_{24}$ 956.817
Yellow pigment of the flowers of *Carthamus tinctorius* (safflower). Amorph. yellow powder. λ_{max} 238 (ε 23600); 406 (ε 46400) (MeOH).

Kazuma, K. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1588-1590; 2000, **64**, 1588-1599 (*isol, pmr, cmr, struct*)

Pregn-5-ene-3,16,20-triol P-457



(3β,16α,20*S*)-*form*

$C_{21}H_{34}O_3$ 334.498

(3β,16α,20*S*)-*form*

3-O-[2-Acetyl-3-O-methyl-β-D-fucopyranosyl-(1→4)-2,6-dideoxy-3-O-methyl-β-D-ribo-hexopyranoside], 20-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→2)-3-O-methyl-β-D-fucopyranoside]: [73528-21-9] ***Plocoside B***
$C_{56}H_{92}O_{25}$ 1165.328
Amorph. powder. $[\alpha]_D$ +18.5 (c, 0.54 in MeOH).

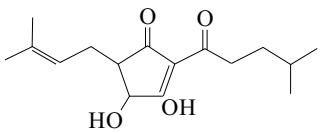
(3β,16β,20*R*)-*form*
Powder. Mp 212-215°. $[\alpha]_D^{23}$ -12.3 (c, 0.15 in MeOH).

3-O-β-D-Glucopyranoside: [171828-53-8]
$C_{27}H_{44}O_8$ 496.64
Constit. of *Balanites aegyptiaca* (soapberry tree fruits). Cryst. Mp 220-222°. $[\alpha]_D^{23}$ +17.5 (c, 0.15 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]: [172046-43-4] ***Balagyptin***
$C_{39}H_{64}O_{16}$ 788.925
Constit. of *Balanites aegyptiaca* (soapberry tree fruits). Powder. Mp 231-233°. $[\alpha]_D^{23}$ +11.3 (c, 0.2 in MeOH).

Umehara, K. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1565 (*Plocoside B, isol, pmr, cmr*)
Kamel, M.-S. *et al., Phytochemistry*, 1995, **40**, 1773 (*isol, pmr, cmr*)

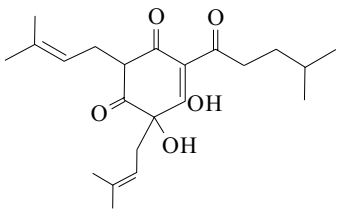
Prehumulinic acid P-458



$C_{16}H_{24}O_4$ 280.363
Constit. of hops. Cryst. Mp 96.5-97.5°.

Rillaers, G. *et al., Bull. Soc. Chim. Belg.*, 1962, **71**, 438

Prehumulone P-459

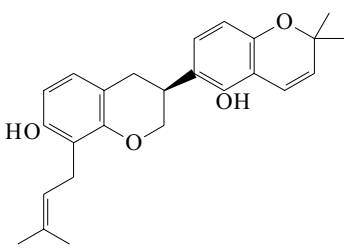


$C_{22}H_{32}O_5$ 376.492
Minor constit. of hops. Oil. $[\alpha]_D^{23}$ -172 (c, 0.12 in 2,2,3-trimethylpentane).

Rillaers, G. *et al., Bull. Soc. Chim. Belg.*, 1962, **71**, 438

8-Prenylphaseollinisoflavan P-460

[175554-12-8]
3,4-Dihydro-2′,2′-dimethyl-8-(3-methyl-2-butenyl)-[3,6′-bi-2H-1-benzopyran]-5,7′-diol



$C_{25}H_{28}O_4$ 392.494

(S)*-*form
Constit. of *Glycyrrhiza glabra* (licorice). Plates (MeOH aq.). Mp 151-152°. $[\alpha]_D^{25}$ -7.6 (c, 2 in $CHCl_3$). Config. assigned tentatively λ_{max} 278 (log ε 4.07); 285 (sh) (log ε 4.05); 310 (log ε 3.54) (MeOH).

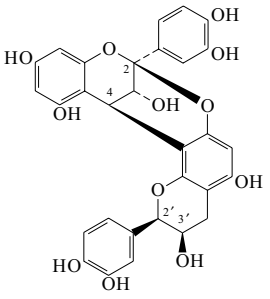
Kinoshita, T. *et al., Heterocycles*, 1996, **43**, 581-

588 (*isol, uv, ir, pmr, cmr, cd, ms*)

Procyanidin A_1 P-461

[12798-56-0]

*2,8-Bis(3,4-dihydroxyphenyl)-3,4-dihydro-8,14-methano-2*H*,14*H*-1-benzopyrano[7,8-d][1,3]benzodioxocin-3,5,11,13,15-pentol, 9CI. 3,3′,4′,5,7-Pentahydroxyflavan-(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan*



(*all-R*)-*form*

$C_{30}H_{24}O_{12}$ 576.512

(all-R)-form [41743-41-3]

[50897-01-3]

Proanthocyanidin A_2. *Procyanidin A_2. Procyanidoepicatechin. Epicatechin-(2β→7,4β→8)-epicatechin*

Isol. from cassia bark (*Cinnamomum aromaticum*). Needles (H_2O). Mp 300°. $[\alpha]_D$ +64 (Me_2CO).

(2R,2′R,3R,3′S,4R)-form [103883-03-0]

Proanthocyanidin A_1. *Epicatechin-(2β→7,4β→8)-catechin*

Isol. from cassia bark (*Cinnamomum aromaticum*). Mp 300°. $[\alpha]_D$ +61 (Me_2CO aq.).

(2S,2′R,3S,3′R,4S)-form [111466-30-9]

Proanthocyanidin $A_{5'}$. ent-*Epicatechin-(2α→7,4α→8)-epicatechin*

Isol. from sloe (*Prunus spinosa*). Fine needles + $2H_2O$ (H_2O). Mp 300°. $[\alpha]_D^{26}$ -111 (c, 1.6 in MeOH).

3-O-α-L-*Arabinopyranoside:3*-O-α-L-*Arabinopyranosylproanthocyanidin $A_{5'}$*

$C_{35}H_{32}O_{16}$ 708.628

Constit. of cocoa beans (*Theobroma cacao*).

3-O-β-D-*Galactopyranoside:3*-O-β-D-*Galactopyranosylproanthocyanidin $A_{5'}$*

$C_{36}H_{34}O_{17}$ 738.654

Constit. of cocoa beans (*Theobroma cacao*).

(2S,2′R′,3S,3′S′,4S)-form [130853-74-6]

Pavetannin A_2. ent-*Epicatechin-(2α→7,4α→8)-catechin. Pavitannin A_2*

Isol. from sloe (*Prunus spinosa*).

3-O-α-L-*Arabinopyranoside:3*-O-α-L-*Arabinopyranosylpavetannin A_2*

$C_{35}H_{32}O_{16}$ 708.628

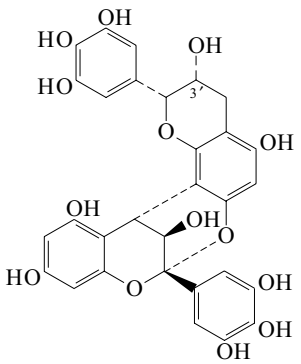
Constit. of cocoa liquor (*Theobroma cacao*).

[17947-28-3, 53585-73-2]

Mayer, W. *et al., Tet. Lett.*, 1966, 429 (*isol*)
Weinges, K. *et al., Annalen*, 1968, **711**, 184
Jacques, D. *et al., J.C.S. Perkin 1*, 1974, 2663 (*cmr, pmr, struct, bibl*)
Ohtsuka, H. *et al., Yakugaku Zasshi*, 1982, **102**, 162 (*cryst struct*)
Nonaka, G. *et al., J.C.S. Perkin 1*, 1983, 2139 (*synth, cmr, bibl*)
Van Rooyen, P.H. *et al., S. Afr. J. Chem.*, 1983, **36**, 49 (*isol, cryst struct*)
Morimoto, S. *et al., Chem. Pharm. Bull.*, 1986, **34**, 633; 643 (*isol*)
Karchesy, J.J. *et al., J. Agric. Food Chem.*, 1986, **34**, 966 (*isol*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1987, **35**, 149 (*isol, cmr, struct*)
Baldé, A.M. *et al., Phytochemistry*, 1991, **30**, 337; 4129 (*isol, Pavetannin A_2*)
Porter, L.J. *et al., Phytochemistry*, 1991, **30**, 1657-1663 (*3-Arabinosylproanthocyanidin $A_{5'}$, 3-Galactopyranosylproanthocyanidin $A_{5'}$*)
Kolodziej, H. *et al., Phytochemistry*, 1991, **30**, 2041 (*isol*)
Crespo Irizar, A. *et al., Spectroscopy (Amsterdam)*, 1992, **10**, 17 (*isol, abs config*)
Vivas, N. *et al., Tet. Lett.*, 1996, **37**, 2015 (*pmr, cmr, conformn*)
De Bruyne, T. *et al., J. Nat. Prod.*, 1999, **62**, 954-958 (*Proanthocyanidin A_2, Proanthocyanidin A_1, activity*)
Kamiya, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 551-557 (*Proanthocyanidin A_2, isol, pmr, cmr*)
Hatano, T. *et al., Phytochemistry*, 2002, **59**, 749-758 (*3-Arabinosylpavetannin A_2*)

Prodelphinidin A_2 P-462

3,3′,4′,5,5′,7-Hexahydroxyflavan-(2→7,4→8)-3,3′,4′,5,5′,7-hexahydroxyflavan. Epigallocatechin-(2β→7,4β→8)-epigallocatechin



$C_{30}H_{24}O_{14}$ 608.511

Off-white powder. $[\alpha]_D^{19}$ +54.3 (c, 0.3 in Me_2CO).

3′-O-*(3,4,5-Trihydroxybenzoyl):* [126715-94-4] ***Prodelphinidin A_2 3′-gallate***

$C_{37}H_{28}O_{18}$ 760.617

Constit. of oolong tea (*Camellia sinensis* var. *viridis*). Tan powder. $[\alpha]_D^{20}$ -60 (c, 0.5 in Me_2CO).

3′-Epimer:Epigallocatechin-(2β→7,4β→8)-gallocatechin. ***Prodelphinidin A_1***

$C_{30}H_{24}O_{14}$ 608.511

Constit. of *Phyllanthus emblica* (emblic). Tan powder + $3H_2O$. $[\alpha]_D^{16}$ +25.3 (c, 0.4 in MeOH).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3255-3263 (*isol, struct*)
Zhang, Y.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1507-1510 (*Prodelphinidin A_1*)

Proflamin P-463

[96231-73-1]

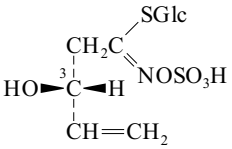
A weakly acidic glycoprotein containing >90% protein and < 10% carbohydrate; MW approx. 13 kD. Isol. from the culture mycelium of *Flammulina velutipes* (velvet shank).

Ikekawa, T. *et al., Jpn. J. Cancer Res.*, 1985, **76**, 142-148 (*isol*)

Progoitrin P-464

[585-95-5]

1-Thio-β-D-glucopyranose 1-[3-hydroxy-N-(sulfooxy)-4-pentenimidate], 9CI. 2-Hydroxy-3-butenyl glucosinolate. Glucorapiferin



$C_{11}H_{19}NO_{10}S_2$ 389.404

Present in red cabbage, Brussel sprouts, savoy cabbage, *Brassica napus* (rape seed) and other *Brassica* spp..

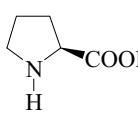
[31362-92-2, 35522-68-0]

Kjaer, A. *et al., Acta Chem. Scand.*, 1956, **10**, 1365; 1959, **13**, 144 (*abs config*)
Kreula, M. *et al., Acta Chem. Scand.*, 1959, **13**, 1375 (*occur*)
Greer, M.A. *et al., Arch. Biochem. Biophys.*, 1962, **99**, 369 (*isol, ir, uv*)
Björkman, R. *et al., Acta Chem. Scand.*, 1972, **26**, 1111 (*isol*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Hanley, A.B. *et al., J. Sci. Food Agric.*, 1983, **34**, 869 (*isol*)
MacLeod, A.J. *et al., J.C.S. Perkin 1*, 1983, 717 (*synth*)
Cox, J.I. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*cmr*)
Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, D.H.) Sheffield Academic Press, 1998, 29-53 (*rev, occur*)
Reichelt, M. *et al., Phytochemistry*, 2002, **59**, 663-671 (*isol, pmr, cmr*)

Proline, 9CI P-465

[7005-20-1]

2-Pyrrolidinecarboxylic acid. Tetrahydro-2-pyrrolecarboxylic acid. Pro



(*S*)-*form*

$C_5H_9NO_2$ 115.132

(R)-form [344-25-2]

D-*form*

Cryst. (EtOH/Et_2O). Mp 206° (215-220° dec.). $[\alpha]_D^{20}$ +86.2 (c, 1.0 in H_2O) (100% op). $[\alpha]_D$ +60.4 (c, 1 in 5*M* HCl).

Me ester: [43041-12-9]

$C_6H_{11}NO_2$ 129.158

Oil. $[\alpha]_D^{25}$ +34.

Et ester: [96163-72-3]

$C_7H_{13}NO_2$ 143.185

Oil. $[\alpha]_D^{20}$ +85.6 (c, 2 in H_2O).

Amide: [62937-45-5] *2-Pyrrolidinecarboxamide, 9CI. Prolinamide*

$C_5H_{10}N_2O$ 114.147

Cryst. Mp 97-98°.

N-tert-*Butyloxycarbonyl:* See *tert*-Butyloxycarbonylproline in *The Combined Chemical Dictionary.*

N-*(3-Nitrobenzoyl):*
Mp 137-140°. $[\alpha]_D^{20}$ +120 (*M* NaOH).

N-*(4-Methylbenzenesulfonyl):* [110771-95-4]
$C_{12}H_{15}NO_4S$ 269.321
Mp 130-133°.

(*S*)-*form* [147-85-3] *L-form. FEMA 3319*
Flavouring ingredient; dietary supplement. Cryst. (EtOH/Et_2O). V. sol. H_2O (162.3g/100g at 25°). Mp 220-222° dec. $[\alpha]_D^{25}$ -86.2 (c, 1 in H_2O). $[\alpha]_D$ -60.4 (c, 1 in 5*M* HCl). pK_{a2} 10.6 (NH_2). Isoelectric point pH 6.30. Sweet taste.

▶ TW3584000

Hydrochloride: [7776-34-3]
Mp 115°.

Me ester: [2577-48-2]
Oil. Bp_{10} 70°.

Me ester, hydrochloride: [2133-40-6]
Hygroscopic cryst. Mp 69-70°. $[\alpha]_D^{24}$ -40.1 (c, 0.5 in H_2O).

Et ester: [5817-26-5]
Oil. $[\alpha]_D^{20}$ -84.5 (c, 6.01 in H_2O).

tert-*Butyl ester:* [2812-46-6]
$C_9H_{17}NO_2$ 171.239
Oil. d_4^{20} 0.97. $Bp_{1.5}$ 57°. $[\alpha]_D^{24}$ -40.5 (c, 0.4 in MeOH). n_D^{20} 1.4421.

tert-*Butyl ester, hydrochloride:* [5497-76-7]
Prisms (Me_2CO/Et_2O or MeOH/Et_2O). Mp 108-111°. $[\alpha]_D^{25}$ -27 (c, 1.036 in MeOH).

Benzyl ester:

[16652-71-4, 41324-66-7]
$C_{12}H_{15}NO_2$ 205.256
Cryst. (EtOH) (as hydrochloride). Mp 148-149° (hydrochloride). $[\alpha]_D^{25}$ -43.3 (c, 1 in MeOH).

Amide: [7531-52-4]
Needles. Mp 104° (100-102°). $[\alpha]_D^{23}$ -106.9 (c, 0.9 in EtOH).

Amide, hydrochloride: [42429-27-6]
Mp 179-181°.

Anilide:
$C_{11}H_{14}N_2O$ 190.244
Fibrous needles (cyclohexane). $[\alpha]_D^{20}$ -71.4 (c, 1.0 in EtOH).

Anhydride:
$C_{10}H_{16}N_2O_3$ 212.248
Mp 149°. $[\alpha]_D^{19}$ -147.2.

N-*Ac:* [68-95-1]
$C_7H_{11}NO_3$ 157.169
Cryst. Mp 118°. $[\alpha]_D^{23}$ -115 (c, 2 in H_2O).

N-*Ac, Me ester:* [27460-51-1]
$C_8H_{13}NO_3$ 171.196
Liq. $Bp_{0.2}$ 100-104°. $[\alpha]_D^{20}$ -105.9 (c, 1.6 in MeOH).

N-*Trifluoroacetyl:*
$C_7H_8F_3NO_3$ 211.14
Needles. Mp 47-48°. $[\alpha]_D^{24}$ -1.6 (c, 1.0 in $CHCl_3$).

N-tert-*Butyloxycarbonyl:* See *tert*-Butyloxycarbonylproline in *The Combined Chemical Dictionary.*

N-*Benzoyl:* [5874-58-8]
$C_{12}H_{13}NO_3$ 219.24
Cryst. (hexane/2-propanol). Mp 158-159° (153-157°). $[\alpha]_D^{21}$ -99 (c, 1.0 in EtOH).

N-*(4-Methylbenzenesulfonyl):* [51077-01-1]
Mp 130-133°.

N-*Me:* See 1-Methyl-2-pyrrolidinecarboxylic acid in *The Combined Chemical Dictionary.*

N-*(2,4-Dinitrophenyl):* [1655-55-6]
$C_{11}H_{11}N_3O_6$ 281.224
Mp 137°.

N-*Nitroso:* [7519-36-0]
$C_5H_8N_2O_3$ 144.13

(±)-*form* [609-36-9]
Hygroscopic needles (EtOH/Et_2O). Mp 205° dec. (213°). pK_{a1} 1.8; pK_{a2} 10.63 (20°).

Monohydrate:
Sol. H_2O, EtOH; insol. Me_2CO, $CHCl_3$, Et_2O. Mp 190-191°.

Hydrochloride: [26166-36-9]
Cryst. (H_2O). Mp 158-159°.

Et ester: [60169-67-7]
Oil. Bp_{13} 80°.

Amide: [38806-33-6]
Cryst. (C_6H_6). Mp 93°.

Anhydride:
Mp 183-184°.

N-*Ac:* [1074-79-9]
$C_7H_{11}NO_3$ 157.169
Mp 106°.

N-*(3-Nitrobenzoyl):*
Prisms (H_2O). Mp 90-92°.

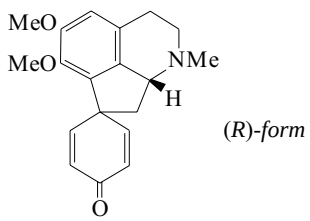
N-*Me:* See 1-Methyl-2-pyrrolidinecarboxylic acid in *The Combined Chemical Dictionary.*

[16395-58-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 583A; 583B; 583C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 886A; 886B; 886C; 1083C; 1246C (*nmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2178 (*rev*)
Rittel, W. *et al., Helv. Chim. Acta*, 1962, **45**, 2473 (*tert-butyl ester*)
Ramachandran, J. *et al., J.O.C.*, 1963, **28**, 173 (*benzyl ester*)
Roeske, R. *et al., J.O.C.*, 1963, **28**, 1251-1253 (*tert-butyl ester*)
Jollés, G. *et al., Bull. Soc. Chim. Fr.*, 1965, 2252-2259 (*tert-butyl ester*)
Buyle, R. *et al., Chem. Ind. (London)*, 1966, 380 (*synth*)
Buckingham, D.A. *et al., Chem. Comm.*, 1969, 581 (*config*)
Campi, E. *et al., Anal. Chim. Acta*, 1972, **58**, 237 (*detn, Cu*)
Verbist, J.J. *et al., Nature (London)*, 1972, **235**, 328 (*cryst struct*)
Monteiro, H.J. *et al., Synthesis*, 1974, 137 (*synth*)
Fermandjian, S. *et al., Biochim. Biophys. Acta*, 1975, **399**, 313 (*cmr*)
Pogliani, L. *et al., Org. Magn. Reson.*, 1975, **7**, 61 (*pmr*)
Schmidt, U. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 777 (*synth*)
Saburi, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 201 (*amide*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 421
Drauz, K. *et al., J.O.C.*, 1986, **51**, 3494 (*synth*)
Kulik, W. *et al., Biomed. Environ. Mass Spectrom.*, 1988, **15**, 419 (*ms*)
Bartsch, H. *et al., Cancer Surv.*, 1989, **8**, 335 (*N-nitrosoproline*)
Shiraiwa, T. *et al., Chem. Lett.*, 1989, 1413 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PMH900
Amino, Y. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 620 (*synth, derivs*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1047
Beak, P. *et al., J.A.C.S.*, 1994, **116**, 3231-3239 (*tert-butyloxycarbonyl*)
Padmanabhan, S. *et al., Acta Cryst. C*, 1995, **51**, 2098 (*cryst struct, DL-form*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 684
O'Brien, P. *et al., J.C.S. Perkin 1*, 1996, 2117 (*anilide, synth, ir, pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2325-2326
Mazzini, C. *et al., J.C.S. Perkin 1*, 1997, 3351-3356 (*R-form, S-form, synth, pmr, cmr, ir*)
Clark, J.S. *et al., J.C.S. Perkin 1*, 2001, 3325-3337 (*N-trifluoroacetyl, synth, ir, pmr, cmr*)
Lesarri, A. *et al., Angew. Chem., Int. Ed.*, 2002, **41**, 4673-4676 (*conformn, struct*)
Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 868

Pronuciferine P-466

Miltanthin. N,O-*Dimethylcrotsparine*



(*R*)-*form*

$C_{19}H_{21}NO_3$ 311.38

(*R*)-*form* [2128-60-1]
Alkaloid from *Nelumbo nucifera* (East India lotus). Mp 127-129°. $[\alpha]_D$ +99 (c, 0.2 in $CHCl_3$). $[\alpha]_D$ +106 (c, 0.41 in EtOH).

▶ WH0167500

N-*De-Me,* N-*methoxycarbonyl:* [275355-87-8] ***Promucosine***
$C_{20}H_{21}NO_5$ 355.39
Alkaloid from *Annona purpurea* (soncoya). Brown powder. Mp 125-127°. $[\alpha]_D^{25}$ +147 (c, 0.07 in $CHCl_3$). λ_{max} 217 (log ϵ 3.78); 267 (log ϵ 4.45); 303 (log ϵ 3.87) (MeOH).

[32410-24-5]

Bernauer, K. *et al., Helv. Chim. Acta*, 1963, **46**, 1783-1785 (*R-form, isol, uv, ir, pmr, struct*)
Baldwin, M. *et al., J.C.S.(C)*, 1967, 154-161 (*ms*)
Ferrari, G. *et al., Farmaco, Ed. Sci.*, 1970, **25**, 449 (*config*)
De Angelis, L. *et al., Drugs of Today (Barcelona)*, 1977, **13**, 22 (*rev, pharmacol*)
Ricca, G.S. *et al., Org. Magn. Reson.*, 1977, **9**, 8 (*cmr*)
Horii, Z. *et al., Chem. Pharm. Bull.*, 1978, **28**, 481-483 (*synth, uv, ir, pmr*)
Kunitomo, J. *et al., Yakugaku Zasshi*, 1981, **101**, 431-436 (*N-Acetylstepharine*)
Fajardo, V. *et al., Chem. Comm.*, 1982, **23**, 1350-1352 (*pmr*)

Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 12785
Chang, F.-R. *et al., J. Nat. Prod.*, 2000, **63**, 746-748 (*Promucosine*)

Propanal, 9CI P-467

[123-38-6]
Propionaldehyde. FEMA 2923
H_3CCH_2CHO
C_3H_6O 58.08
Isol. from various plant sources, e.g. hops, banana, sweet or sour cherry, blackcurrants, melon, pineapple, bread, chesses, coffee, cooked rice and strawberry or apple aroma. Flavouring agent. Liq. with suffocating odour. Mod. sol. H_2O. d_{25}^{25} 0.8. Fp -81 Mp 131°. Bp 47.5-49°. n_D^{20} 1.3636.
▶ Eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 1410 mg/kg. Highly flammable, fl. p. -30/-9°, autoignition temp. 207°. Peroxidizable. UE0350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 215B; 465C (*ir*)
Org. Synth., Coll. Vol., 2, 1943, 541 (*synth*)
Frankiss, S.G. *et al., Spectrochim. Acta A*, 1972, **28**, 2149 (*ir, Raman*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313 (*cmr*)
Bowen, R.D. *et al., Org. Mass Spectrom.*, 1981, **16**, 159 (*ms*)
Randell, J. *et al., Z. Naturforsch., A*, 1987, **42**, 957 (*microwave, struct*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PMT750
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 926 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2331-2332 (*use, occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1150
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1067
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOM200; PMT750

Propane, 9CI P-468

[74-98-6]
E944
$H_3CCH_2CH_3$
C_3H_8 44.096
Propellant and aerating agent in foods. Gas. Fp -189.9. Bp -44.5° Bp_3 -124.2°.
▶ Extremely flammable, fl. p. -104°, autoignition temp. 450°. Asphyxiant. TX2275000

[19252-52-9, 19252-53-0]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1C (*ir*)
Iijima, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1291-1294 (*struct*)
Flesch, G.D. *et al., J.C.S. Faraday 2*, 1973, **69**, 1187-1199 (*ms*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313-321 (*cmr*)
Hamada, K. *et al., Z. Phys. Chem.*, 1975, **97**, 295-299 (*ir, Raman*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 901
Flurry, R.L. *et al., J. Phys. Chem.*, 1983, **87**, 1753-1757 (*ir*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 400-401
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1190
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2327
Boese, R. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 988-992 (*cryst struct*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1, 1987, 261
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1059
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PMJ750

1,3-Propanedial, 9CI P-469

[542-78-9]
Malonaldehyde, 8CI. Malondialdehyde
$OHCCH_2CHO$
$C_3H_4O_2$ 72.063
Used as an indicator of fatty acid and lipid peroxidation, and oxidative changes in foods. Hygroscopic needles. Mp 72-74°.
▶ LD_{50} (rat, orl) 632 mg/kg. TX6475000

Dianil:
$C_{15}H_{14}N_2$ 222.289
Yellow leaflets. Mp 115°.

Di-Me acetal: [19060-10-7] *3,3-Dimethoxypropanal, 9CI*
$C_5H_{10}O_3$ 118.132
Bp_{37} 55°.
▶ ON9103000

Bis(di-Me acetal): [102-52-3] *1,1,3,3-Tetramethoxypropane*
$C_7H_{16}O_4$ 164.201
Liq. d_4^{20} 0.99. Bp 183° Bp_{12} 66°.
▶ Irritant. Fl. p. 77°.

Bis(di-Et acetal): [122-31-6] *1,1,3,3-Tetraethoxypropane*
$C_{11}H_{24}O_4$ 220.308
Liq. d_4^{25} 0.92. Bp_8 92.3°. n_D^{25} 1.4101.
▶ ON8750000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 219A; 219B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 359A; 359B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 288B; 288C (*ir*)
Claisen, L. *et al., Ber.*, 1903, **36**, 3664 (*synth*)
McElvain, S.M. *et al., J.A.C.S.*, 1947, **69**, 2657 (*synth, tetraethoxypropane*)
Arnold, Z. *et al., Chem. Listy*, 1957, **51**, 1082; *CA*, **51**, 13761 (*synth*)
Protopopova, T.V. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1957, **27**, 57 (*acetal*)
Shenyakin, M.M. *et al., Experientia*, 1967, **23**, 428 (*use, tetraethoxypropane*)
George, W.O. *et al., J.C.S.(B)*, 1968, 132 (*synth, pmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 257
Tappel Al, L. *et al., Free Radicals Biol.*, 1980, 1 (*indicator*)
IARC Monog., 1985, **36**, 163; *Suppl.* 7, 65 (*rev, tox*)
Hodgson, S.T. *et al., Tetrahedron*, 1985, **41**, 5871 (*deriv synth, ir, pmr, ms*)
Griesbaum, K. *et al., J.O.C.*, 1990, **55**, 6024 (*synth, pmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **5**, 3211-3213 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PMK000

Propanedioic acid, 9CI P-470

[141-82-2]
Malonic acid, 8CI. Methanedicarboxylic acid
$HOOCCH_2COOH$
$C_3H_4O_4$ 104.062
Cryst. Sol. H_2O, EtOH, Et_2O; mod. sol. Py. Mp 135.6°. pK_{a1} 2.77; pK_{a2} 5.7 (25°,H_2O). Sublimes *in vacuo*.
▶ Skin and eye irritant. LD_{50} (rat, orl) 1310 mg/kg. OO0175000

Butyl Et ester: [17373-84-1] *Butyl ethyl malonate. FEMA 2195*
$C_9H_{16}O_4$ 188.223
Flavouring agent. d^{17} 1.03. Bp 222°.

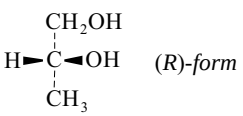
[141-95-7, 156-80-9, 813-56-9, 6148-64-7, 18424-76-5, 36148-03-5, 38330-80-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 490C; 614A; 614C; 740A; 767B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 764C; 935A; 936B; 936C; 1211A; 1252C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 636D; 637B; 637C (*ir*)
Hauser, C.R. *et al., J.A.C.S.*, 1942, **64**, 2714 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 376 (*synth*)
Bentley, L.E. *et al., Nature (London)*, 1952, **170**, 847 (*occur*)
Rodd's Chem. Carbon Compd. (2nd edn.), 1965, **1D**, 293
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 836 (*occur*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **15**, 928 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 84 (*Et butyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 338-339 (*Et butyl ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CCC750; MAO000; DSM200

1,2-Propanediol, 9CI P-471

[57-55-6]

[26264-14-2]
α-Propylene glycol. 3-Deoxyglycerol. E1520. FEMA 2940


(R)-form

$C_3H_8O_2$ 76.095
Anticaking agent, antioxidant, dough strengthener, emulsifier, flavour agent, formulation aid, humectant, solvent, preservative, stabiliser, hog/poultry scald agent, surface active agent and other food uses. Present in roasted sesame seeds, oats, truffle and other mushrooms. pK_{a1} 14.9 (25°).
▶ Skin and eye irritant. Exp. reprod. and teratogenic effects. OES: long-term 150 ppm (total vapour and particulates); long-

term 10 mg m^{-3} (particulates). TY2000000

(±)-*form* [4254-16-4]
Viscous oil with sweet taste. Misc. H_2O, EtOH. $d^{19.4}$ 1.04. Mp -60°. Bp 188-189° Bp_{21} 96-98°. n_D^{20} 1.4320.

1-Octadecanoyl: [1323-39-3] *Propylene glycol stearate. FEMA 2942*
$C_{21}H_{42}O_3$ 342.561
Used as an emulsifier in food processing esp. for margarine. Also as a defoamer and stabiliser. Mp 50°. Commercial material is a mixture of mono- and diesters of stearic and palimitic acids produced by transesterification between propylene glycol and hydrogenated vegetable oils such as soybean oil.

Dibenzoyl: [19224-26-1] *FEMA 3419*
$C_{17}H_{16}O_4$ 284.311
Flavouring ingredient. Mp -3°. Bp_{12} 232°. n_D^{20} 1.5450.

(ξ)-*form*

1-O-β-D-Glucopyranoside:

[162427-75-0, 162601-00-5]
$C_9H_{18}O_7$ 238.237
Constit. of fennel (*Foeniculum vulgare*). Amorph. powder. $[\alpha]_D^{23}$ -21 (c, 0.2 in MeOH).

[4169-04-4, 41593-38-8, 57350-24-0, 105928-08-3, 130879-98-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 128B; 128C; 224B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 192C; 193A; 323C; 340B; **2**, 1241C (*nmr*)
Goldsmith, H.A. *et al., Chem. Ind. (London)*, 1943, **52**, 326 (*octadecanoyl, dodecanoyl*)
Org. Synth., Coll. Vol., 2, 1943, 545-547 (*synth*)
Baer, E. *et al., J.A.C.S.*, 1948, **70**, 609-610 (*abs config*)
Allen, R.J.P. *et al., J.C.S.*, 1957, 524-531 (*synth, dibenzoyl*)
Eisenthal, R. *et al., Biochem. J.*, 1972, **130**, 199-205 (*R-form, S-form, synth, dibenzoyl*)
Guette, J.P. *et al., Bull. Soc. Chim. Fr.*, 1972, 4217-4224 (*synth, props*)
Norula, J.L. *et al., Chem. Era*, 1975, **11**, 21-22 (*resoln*)
Gombos, J. *et al., Chem. Ber.*, 1976, **109**, 2645-2647 (*S-form, synth*)
Melchiorre, C. *et al., Chem. Ind. (London)*, 1976, 218 (*S-form, !synth*)
Pautard, A.M. *et al., J.O.C.*, 1988, **53**, 2300-2303 (*S-form, synth, pmr, cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PML000
Umezawa, H. *et al., J.O.C.*, 1990, **55**, 116-122 (*uv, cd, pmr, dibenzoyl*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **12**, 715 (*rev*)
D'Accorso, N.B. *et al., Org. Mass Spectrom.*, 1991, **26**, 799-803 (*ms, dibenzoyl*)
Poucher, W.A. *et al., Poucher's Perfumes, Cosmetics & Soaps*, 9th edn., Chapman & Hall, London, 1991, **1**, 290; 291
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 407-408
Cotterill, A.S. *et al., J.C.S. Perkin 1*, 1995, 1215-1223 (*S-form, !synth, ir, pmr*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1745
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1643-1646 (*1-glucoside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PML000; PNL250; PNK750

1,2-Propanedithiol, 9CI P-472

[814-67-5]
1,2-Dimercaptopropane. Dithiopropylene glycol. Propylene dithioglycol. FEMA 3520
$H_3CCH(SH)CH_2SH$
$C_3H_8S_2$ 108.228
► LD_{50} (mus, orl) 153 mg/kg. TZ2585000

(±)-*form*
Flavouring ingredient. Oil. Bp 152° Bp_{28} 60°. n_D^{20} 1.5310.

U.K. Pat., 1946, 579 971; *CA*, **41**, 2077 (*synth*)
Fitt, P.S. *et al., J.C.S.*, 1957, 2240 (*synth*)
Iqbal, S.M. *et al., J.C.S.*, 1960, 1030 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 685
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2327-2328

1,3-Propanedithiol, 9CI P-473

[109-80-8]
1,3-Dimercaptopropane. Trimethylene-dithiol. FEMA 3588
$HSCH_2CH_2CH_2SH$
$C_3H_8S_2$ 108.228
Flavouring ingredient. Oil. d^{20} 1.08. Bp 169° Bp_{60} 94°. n_D^{20} 1.5405.
► TZ2585500

Bis-4-methylbenzenesulfonyl: [3866-79-3] *Trimethylene dithiotosylate*
$C_{17}H_{20}O_4S_4$ 416.607
Needles (EtOH). Mp 66-67°.

S,S′-*Di-Me:* [24949-35-7] *1,3-Bis(-methylthio)propane, 9CI*
$C_5H_{12}S_2$ 136.282
Oil. Bp_{15} 92°.

S,S′-*Di-Et:* [33672-52-5] *1,3-Bis(ethylthio)propane, 9CI*
$C_7H_{16}S_2$ 164.335
Oil. Bp 228-231° Bp_7 120°.

S,S′-*Di-Ph:* [28118-53-8] *1,3-Bis(phenylthio)propane*
$C_{15}H_{16}S_2$ 260.423
Bp_{12} 264°. n_D^{20} 1.6281.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 260B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 419A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 342A (*ir*)
Aldrich Library of NMR Spectra, **1**, 165D (*pmr*)
Simpson, S.D. *et al., Can. J. Res., Sect. B*, 1947, **25**, 20
Protiva, M. *et al., Chem. Listy*, 1953, **47**, 580; *CA*, **49**, 155c (*1,3-S-di-Me*)
Cossar, B.C. *et al., J.O.C.*, 1962, **27**, 93 (*synth*)
Griesbaum, K. *et al., J.O.C.*, 1965, **30**, 261 (*derivs, synth*)
Woodward, R.B. *et al., J.O.C.*, 1971, **36**, 1137 (*synth, ir, pmr, use, deriv*)
DeSimone, R.E. *et al., Org. Magn. Reson.*, 1974, **6**, 583 (*cmr*)
Org. Synth., 1974, **54**, 33; 39 (*synth, use*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 493; 1990, **15**, 114; 242; 1988, **13**, 261; 297; 1981, **9**, 308; 1979, **7**, 368; 1981, **9**, 394; 1984, **11**, 404; 1986, **12**, 501; 1977, **6**, 628 (*use*)
Heaton, R.P.R. *et al., J.C.S. Perkin 1*, 1978, 1011 (*synth, deriv*)
Möckel, H.J. *et al., Fresenius' Z. Anal. Chem.*, 1979, **295**, 241 (*ms*)
Jigajinni, V. *et al., J. Chem. Res., Synop.*, 1983, 187 (*1,3-S-di-Ph*)
Gouzoules, F.H. *et al., Tet. Lett.*, 1985, **26**, 3441 (*use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4307-4310 (*use*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **6**, 4310-4312 (*bis-4-methylbenzenesulfonyl, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 685
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2328-2329
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 938

Propanethioic acid, 9CI P-474

[1892-31-5]
Thiopropionic acid
$H_3CCH_2COSH \Leftrightarrow H_3CCH_2CSOH$
C_3H_6OS 90.146
Liq. with pungent sulfuraceous odour.

OH-form

Et ester: [924-45-8]
$C_5H_{10}OS$ 118.199
Insol. H_2O.

Amide: [631-58-3]
C_3H_7NS 89.161
Leaflets (C_6H_6). V. sol. C_6H_6; spar. sol. H_2O, EtOH, Et_2O. Mp 41-43°.

Anilide:
$C_9H_{11}NS$ 165.259
Needles (AcOH aq.). Mp 67-67.5°.

SH-form

Me ester: [5925-75-7]
C_4H_8OS 104.173
Bp 119-120°.

2-Propenyl ester: [41820-22-8] S-*2-Propenyl propanethioate.* S-*Allyl thiopropionate. FEMA 3329*
$C_6H_{10}OS$ 130.21
Flavouring ingredient.

Ph ester: [18245-72-2]
$C_9H_{10}OS$ 166.243
Oil. Bp_{20} 130-131° $Bp_{0.05}$ 62-70°. n_D^{20} 1.5600.

Hubacher, K. *et al., Annalen*, 1890, **259**, 228 (*synth*)
Weigert, F. *et al., Ber.*, 1903, **36**, 1007 (*synth*)
Delépine, M. *et al., Bull. Soc. Chim. Fr.*, 1911, **9**, 907
Caserio, M.C. *et al., J.A.C.S.*, 1983, **105**, 6896 (*ms*)
Fujimoto, K. *et al., Chem. Pharm. Bull.*, 1986, **34**, 999 (*synth*)
Ahmad, S. *et al., Tet. Lett.*, 1986, **27**, 3791 (*S-Ph ester*)
Danheiser, R.L. *et al., J.O.C.*, 1991, **56**, 1176 (*S-Ph ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 3329 (*2-propenyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 101-102 (*2-propenyl ester*)

1-Propanethiol, 9CI P-475

[107-03-9]

[79869-58-2]
Propyl mercaptan. 1-Mercaptopropane.

FEMA 3521

$H_3CCH_2CH_2SH$

C_3H_8S 76.162

Isol. from onion (*Allium cepa*) and other *Allium* ssp. Also present in cooked chicken, beef, beer, American potato chips and durian (*Durio zibethinus*). Liq. with cabbage-like odour and taste. d_4^{25} 0.84. Mp -113.3°. Bp 67°. n_D^{25} 1.4351.

▶ Eye irritant. LD_{50} (rat, orl) 1790 mg/kg. Highly flammable, fl. p. -20°. TZ7300000

3,5-Dinitrobenzoyl:
Cryst. (AcOH aq.). Mp 51-52°.

S-*Me:* [3877-15-4] *1-(Methylthio)propane, 9CI. Methyl propyl sulfide, 8CI*
$C_4H_{10}S$ 90.189
Liq. Bp 95°.

S-*Ph:* See Phenyl propyl sulfide in *The Combined Chemical Dictionary.*

S-*(2,4-Dinitrophenyl):* [7343-56-8]
Mp 85-86°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 255B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 411B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 335D (*ir*)
Ellis, L.M. *et al., J.A.C.S.*, 1932, **54**, 1674 (*synth, props*)
Challenger, F. *et al., Biochem. J.*, 1949, **44**, 87 (*isol*)
Levy, F.J. *et al., Anal. Chem.*, 1961, **33**, 707 (*ms*)
Cossar, B.C. *et al., J.O.C.*, 1962, **27**, 93 (*synth*)
Marcus, S.H. *et al., J. Phys. Chem.*, 1964, **68**, 331 (*pmr*)
Hayashi, M. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 112 (*props*)
Taguchi, T. *et al., Tet. Lett.*, 1969, 3631 (*synth*)
Hall, C.M. *et al., J.O.C.*, 1977, **42**, 2118 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2368-2369 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PML500

2-Propanethiol, 9CI P-476

[75-33-2]

[79869-58-2]
2-Mercaptopropane. Isopropyl mercaptan. Isopropylthiol

$H_3CCH(SH)CH_3$

C_3H_8S 76.162

Food additive listed on the EAFUS Food Additive Database (Jan. 2001). Liq. Mp -130.7°. Bp 58°. n_D^{20} 1.4255. pK_a 10.86 (25°).

▶ Highly flammable, fl. p. -35°. TZ7302000

S-*Me:* [1551-21-9] *2-(Methylthio)propane, 9CI. Isopropyl methyl sulfide, 8CI*
$C_4H_{10}S$ 90.189
Produced by some canned vegetables. Liq. Fp -101.48. Bp 93-95° (84-86°).

S-*2,4-Dinitrophenyl:*
Mp 95°.

[20607-43-6]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 416A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 257D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 339A (*ir*)
Obermeyer, J. *et al., Ber.*, 1887, **20**, 2923 (*S-Me*)
Ellis, L.M. *et al., J.A.C.S.*, 1932, **54**, 1677 (*synth, props*)
McAllan, D.T. *et al., J.A.C.S.*, 1951, **73**, 3627 (*S-Me*)
Leaver, D. *et al., J.C.S.*, 1957, 39 (*S-Me*)
Bacon, E.W. *et al., J.O.C.*, 1960, **25**, 1993 (*synth*)
Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1963, **82**, 68 (*synth*)
Hall, C.M. *et al., J.O.C.*, 1977, **42**, 2118 (*cmr*)
Durig, J.R. *et al., J. Phys. Chem.*, 1980, **84**, 3547 (*ir, Raman*)
Colosimo, M. *et al., Org. Mass Spectrom.*, 1982, **17**, 286 (*ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IMU000

1,2,3-Propanetricarboxylic acid, 9CI, 8CI P-477

[99-14-9]
Tricarballylic acid. 3-Carboxyglutaric acid. Carballylic acid

$HOOCCH_2CH(COOH)CH_2COOH$

$C_6H_8O_6$ 176.126

Isol. from plants e.g. sugarbeet sap, sap of *Acer saccharinum* (maple syrup). Large orthorhombic prisms (H_2O or Et_2O). Sol. H_2O, Et_2O. Mp 166°. pK_{a1} 3.47; pK_{a2} 4.54; pK_{a3} 5.89 (20°, 0.1*M* $NaClO_4$).

Tri-Me ester: [6138-26-7]
$C_9H_{14}O_6$ 218.206
Oil. Bp_{48} 205-208° Bp_{13} 150°.

Tri-Et ester: [1188-22-3]
$C_{12}H_{20}O_6$ 260.286
Oil. Bp_{14} 173-175°.

Trichloride: [23666-71-9]
$C_6H_5Cl_3O_3$ 231.462
Liq. Bp_{14} 140°.

Triamide:
$C_6H_{11}N_3O_3$ 173.171
Prisms (H_2O). Sol. H_2O; insol. EtOH, Et_2O. Mp 205-207° dec.

Trihydrazide: [123277-55-4]
$C_6H_{14}N_6O_3$ 218.215
Cryst. (MeOH aq.). Mp 182.5°.

Trinitrile: [62872-44-0] *1,2,3-Propanetricarbonitrile, 9CI. 1,2,3-Tricyanopropane*
$C_6H_5N_3$ 119.126
Mp 52°.

1,2-Anhydride: [4756-10-9] *Tetrahydro-2,5-dioxo-3-furanacetic acid, 9CI*
$C_6H_6O_5$ 158.11
Needles ($AcOH/CHCl_3$). Sol. H_2O, EtOH, AcOH. Mp 131-132°. Bp_{45} 215-225°.

1,2-Imide: [6324-87-4] *2,5-Dioxo-3-pyrrolidineacetic acid, 9CI*
$C_6H_7NO_4$ 157.126
Prisms (C_6H_6). Sol. H_2O, EtOH. Mp 127-128°.

1,2-Imide, 3-amide:
$C_6H_8N_2O_3$ 156.141
Cryst. (EtOH aq.). Mp 173°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 505B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 775A (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 523 (*synth*)
Feuer, H. *et al., J.O.C.*, 1961, **26**, 1639 (*synth*)
Gelin, R. *et al., Bull. Soc. Chim. Fr.*, 1965, 139 (*synth*)
Martin, R.B. *et al., J. Phys. Chem.*, 1972, **76**, 3073 (*pmr*)
Barnes, J.C. *et al., Acta Cryst. C*, 1988, **44**, 758 (*cryst struct*)
Razynska, A. *et al., J.C.S. Perkin 2*, 1991, 1531 (*conformn, 1,2-anhydride*)

Propanoic acid, 9CI P-478

[79-09-4]
Propionic acid. Ethanecarboxylic acid. Metacetonic acid. E280. FEMA 2924

H_3CCH_2COOH

$C_3H_6O_2$ 74.079

Present in apples, fruit juices, beef, beer, bread, cocoa, dairy products, e.g. ripe Swiss or Jarlsberg cheese, and roasted peanuts. Flavouring ingredient. Preservative used esp. in bread and mould inhibitors. Liq. with acrid odour. Misc. H_2O. d_{15}^{15} 1. Mp -21.5°. Bp 141.1° Bp_{10} 39.7°.

▶ Corrosive and mod. irritating to skin, eyes and respiratory tract. LD_{50} (rat, orl) 3500 mg/kg. OES: long-term 10 ppm; short-term 15 ppm. UE5950000

Na salt: [137-40-6] *Sodium propionate. E281*
Antimicrobial agent used in cheese and other foods. Cryst.

K salt: [327-62-8] *Potassium propionate. E283*
Antimicrobial agent. Plates + $1H_2O$ (EtOH aq.). Mp 300°.

Ca salt: [4075-81-4] *Calcium propionate. E282*
Antimicrobial agent used as preservative in bread, cheese and other foods. Cryst.

Me ester: [554-12-1] *Methyl propionate. FEMA 2742*
$C_4H_8O_2$ 88.106
Flavouring ingredient. Liq. d_4^0 0.94. Bp 79.7°. n_D^{19} 1.3770.

▶ Highly flammable, fl. p. -2°, autoignition temp. 469°. Skin irritant. UF5970000

Et ester: [105-37-3] *Ethyl propionate. FEMA 2456*
$C_5H_{10}O_2$ 102.133
Used in fruity and rum flavour compositions. Liq. with fruity odour. Mod. sol. H_2O. d_4^{20} 0.89. Fp -73. Bp 99°. n_D^{20} 1.3844.

▶ Flammable, fl. p. 12°, autoignition temp. 440/476°. Skin irritant. UF3675000

Propyl ester: [106-36-5] *Propyl propionate. FEMA 2958*
$C_6H_{12}O_2$ 116.16
Flavouring ingredient. Liq. d^0 0.89. Bp 122°. n_D^{20} 1.3910.

▶ Fl. p. 79° (oc). Skin irritant. UF7100000

2-Propenyl ester: [2408-20-0] *Allyl propionate. FEMA 2040*
$C_6H_{10}O_2$ 114.144
Used in fruit flavours. d^{20} 0.91. Bp 123-125°. n_D^{20} 1.4105.

Isopropyl ester: [637-78-5] *Isopropyl propionate. FEMA 2959*
$C_6H_{12}O_2$ 116.16
Flavouring ingredient. Liq. d^0 0.89. Bp_{750} 109-111°. n_D^{20} 1.3872.

▶ Highly flammable, fl. p. 21°. UF5140000

Butyl ester: [590-01-2] *Butyl propionate. FEMA 2211*

$C_7H_{14}O_2$ 130.186
Flavouring ingredient. Liq. d_0^0 0.89. Bp 145.5°. n_D^{20} 1.4010.
▶ Flammable, fl. p. 32°, autoignition temp. 426°. Skin irritant. UE8245000

2-Methylpropyl ester: [540-42-1] *2-Methylpropyl propanoate. Isobutyl propionate. FEMA 2212*
$C_7H_{14}O_2$ 130.186
Flavouring ingredient. Liq. d_4^0 0.89. Bp 137°. n_D^{20} 1.3975.
▶ Highly flammable, fl. p. 18°. UF4930000

Pentyl ester: [624-54-4] *Pentyl propanoate. Amyl propionate*
$C_8H_{16}O_2$ 144.213
Flavouring ingredient. Liq. with an odour of apricot. d_4^{15} 0.88. Fp -73.1. Bp 168.7°. n_D^{15} 1.4096.

Benzyl ester: [122-63-4] *Benzyl propanoate. Benzyl propionate. FEMA 2150*
$C_{10}H_{12}O_2$ 164.204
Used in fruit flavourings. Liq. d 1.03 $d^{15.5}$ 1.04. Bp 222°.

[72-03-7, 16674-79-6, 17448-65-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 27C; 481D; 603D; 604A; 604B; 711B; 724D; 747C; 761A; 837B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 751C; 904A; 904B; 904C; 905A; 905B; 905C; 1165C; 1188B; 1188C; 1219A; 1235A; 1243C; 1244A; 1351B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 573D; 611C; 611D; 612A; 612B; 612C; 612D; 761A; 766D; 777C; 781A; 783C; 783D; 795B (*ir*)
Aldrich Library of NMR Spectra, **2**, 145C (*pmr*)
Hardy, D.V.N. *et al., J.C.S.*, 1936, 358; 364 (*synth*)
Jeffrey, G.H. *et al., J.C.S.*, 1948, 658 (*2-propenyl ester*)
Kirk-Othmer Encycl. Chem. Technol., 2nd edn., Wiley, 1963, **16**, 554 (*rev*)
Williamson, K.L. *et al., J. Magn. Reson.*, 1978, **30**, 367 (*cmr*)
Maccoll, A. *et al., Int. J. Mass Spectrom. Ion Processes*, 1988, **86**, 227 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, EPB500; PMU750
Edwards, H.G.M. *et al., J. Mol. Struct.*, 1991, **248**, 237 (*ir, Raman*)
Yokoyama, I. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 400 (*ir, Raman*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 459-461
Yang, H. *et al., Synth. Commun.*, 1994, **24**, 3269 (*esters*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 31; 65; 94; 139; 151; 265; 355; 412; 421; 553; 630; 652; 688; 706
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 414
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 99-100; 275-276; 353-354; 417-420; 755-756; 785; 1036-1037; 1337-1338; 1459-1460; 1500-1501; 1845-1846; 2039-2040; 2167-2168; 2332-2334; 2373-2374; 2600-2603
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4911
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1092; 1108; 1520; 1849; 2350; 2677
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1068; 1069
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSJ500; MOT000; PMV000; PNU000; PMV250; EPB500; PMW500; PMV500; PMU750; PMV750

1-Propanol, 9CI P-479

[71-23-8]

[62309-51-7]
Propyl alcohol. FEMA 2928

$H_3CCH_2CH_2OH$

C_3H_8O 60.096
Present in the natural odours of apple, cognac and rum. Flavouring agent. Liq. with an alcoholic odour and a characteristic ripe, fruity flavour. Misc. H_2O, EtOH, Et_2O. d_4^{25} 0.8. Mp -127°. Bp 97.4°. n_D^{20} 1.3850. pK_a 16.1 (25°).
▶ Highly flammable, fl. p. 15°, autoignition temp. 405°. Skin and severe eye irritant. LD_{50} (rat, orl) 1870 mg/kg. CNS depressant. OES: long-term 200 ppm; short-term 250 ppm (sk). UH8225000

Ac: [109-60-4] *Propyl acetate. 1-Acetoxypropane. FEMA 2925*
$C_5H_{10}O_2$ 102.133
Flavouring agent. Liq. with a fruity odour. Bp 101.67°.
▶ Highly flammable, fl. p. 13°, autoignition temp. 430°. Eye and respiratory tract irritant. High conc. narcotic. AJ3675000

3,5-Dinitrobenzoyl:
Mp 73°.

4-Nitrophenylurethane:
Mp 115°.

O-*Nitrite:* [543-67-9] *Propyl nitrite*
$C_3H_7NO_2$ 89.094
Bp 48.9-49.4°.
▶ RA1180000

O-*Nitrate:* See Propyl nitrate in *The Combined Chemical Dictionary.*

Me ether: See 1-Methoxypropane in *The Combined Chemical Dictionary.*

Et ether: See 1-Ethoxypropane in *The Combined Chemical Dictionary.*

[4712-36-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 109D; 601A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 163C; 899B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 156A; 607D (*ir*)
Shriner, R.L. *et al., J.A.C.S.*, 1931, **53**, 1602 (*synth, derivs*)
Cowley, E.G. *et al., J.C.S.*, 1933, 1252 (*nitrite*)
Mumford, S.A. *et al., J.C.S.*, 1950, 75 (*props*)
Appleby, A.J. *et al., J. Gas Chromatogr.*, 1967, **5**, 266 (*use*)
Salahub, D.R. *et al., Chem. Phys. Lett.*, 1971, **8**, 71 (*uv*)
Adams, R.F. *et al., J. Chromatogr.*, 1974, **95**, 189 (*use*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 313 (*cmr*)
Harrison, A.G. *et al., Can. J. Chem.*, 1976, **54**, 2029 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 221 (*rev, bibl*)
Merck Index, 11th edn., 1989, No. 7853 (*Ac*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 803
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 690-691
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2336-2339
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4556
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 26 (*tox, rev*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1061; 1071
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PNC250; PND000; PNQ750

2-Propanol, 9CI P-480

[67-63-0]

[62309-51-7]
Isopropanol. 2-Hydroxypropane. Isopropyl alcohol, USAN. Alcojel. Avantin. Bowsteral. Hartasol. Petrohol. Propol. Takineocol. FEMA 2929

$H_3CCH(OH)CH_3$

C_3H_8O 60.096
Present in fruit aromas, e.g. papaya (*Carica papaya*). Used as an extraction solvent in food preparation. Liq. Sol. H_2O. d_4^{20} 0.79. Fp -89.5 Mp -88.5°. Bp 82.5°. n_D^{20} 1.3776. pK_a 17.1. pK_a -4.7 (base). Log P 0.07 (calc). Forms azeotropic mixt. with H_2O ctg. 12.1% H_2O. Can be salted out from aq. solns. Component of Hibistat.
▶ Highly flammable, fl. p. 12°, autoignition temp. 399°. Peroxidizable. Eye, skin and respiratory tract irritant. Contact of the liquid with eyes can cause corneal burns and severe eye damage. Potentiates CCl_4 toxicity. CNS depressant. OES: long-term 400 ppm; short-term 500 ppm (sk). NT8050000

O-*β-D-Glucopyranoside:* [5391-17-3] *Isopropyl β-D-glucoside*
$C_9H_{18}O_6$ 222.238
Present in fennel. Needles (MeOH). Mp 129-131°. $[\alpha]_D^{25}$ -54.9 (Py). $[\alpha]_D^{23}$ -35.6 (c, 1.1 in MeOH).

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:* [147742-24-3]
$C_{14}H_{26}O_{10}$ 354.353
Constit. of the roots of cassava (*Manihot esculenta*). Solid + $\frac{1}{2}H_2O$. Mp 119-120°. $[\alpha]_D^{25}$ -82.7 (c, 0.6 in H_2O).

Formyl: [625-55-8] *Isopropyl formate. FEMA 2944*
Constit. of coffee, plum brandy, various mushrooms and dwarf quince (*Chaenomeles japonica*). Liq. Bp 67.5-68°.
▶ LQ8750000

Ph ether: See Isopropyl phenyl ether in *The Combined Chemical Dictionary.*

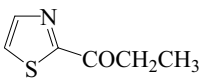
[3979-51-9, 6831-82-9, 15520-32-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 117D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 175B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 166A (*ir*)
Brooks, B.T. *et al., Chem. Rev.*, 1926, **2**, 382 (*rev*)
Brooks, B.T. *et al., J.A.C.S.*, 1934, **56**, 1998 (*synth*)
Hatch, L.F. *et al., Isopropyl Alcohol*, McGraw-Hill, N.Y., 1961, (*bibl*)

Katague, D.B. *et al., J. Pharm. Sci.*, 1965, **54**, 891 (*isol*)
Harrison, A.G. *et al., Org. Mass Spectrom.*, 1974, **9**, 221 (*ms*)
Biondi, P.A. *et al., J. Chromatogr.*, 1975, **109**, 389 (*use*)
Hikino, H. *et al., Tetrahedron*, 1976, **32**, 325 (*cmr*)
IARC Monog., 1977, **15**, 223; *Suppl*. 7, 229; *Suppl*. 6, 351 (*rev, tox*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 198 (*rev, bibl*)
Food Chemicals Codex, 3rd Ed., 1981, 155 (*anal*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, INJ000
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 241-242
Prawat, H. *et al., Phytochemistry*, 1995, **40**, 1167 (*6-apiosylglucoside*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1144
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1483-1496 (*use, esters*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4561
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 291
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1203
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 31
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, INJ000; IPC000; IPY000

2-Propanoylthiazole P-481

[43039-98-1]
1-(2-Thiazolyl)-1-propanone, 9CI. 2-Propionylthiazole. Ethyl 2-thiazolyl ketone. FEMA 3611



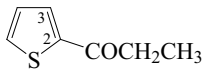
C_6H_7NOS 141.193
Cysteine-derived Maillard product. Reported in lard. Present in cooked spinach leaves. Flavouring ingredient. Light yellow oily liq. Bp_{16} 104-107°. n_D^{20} 1.5305.

2,4-Dinitrophenylhydrazone:
Mp 235°.

Beraud, J. *et al., Bull. Soc. Chim. Fr.*, 1962, 2072-2074 (*synth*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Bird, T.G.C. *et al., J. Med. Chem.*, 1991, **34**, 2176-2188 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 689 (*use*)
Hofmann, T. *et al., J. Agric. Food Chem.*, 1997, **45**, 898-906 (*Maillard product, occur*)
Naf, R. *et al., Flavour Fragrance J.*, 2000, **15**, 329-334 (*occur, spinach*)

2-Propanoylthiophene P-482

[13679-75-9]
1-(2-Thienyl)-1-propanone, 9CI. Propiothienone. Ethyl 2-thienyl ketone



C_7H_8OS 140.206
Maillard product. Pale yellow oil. Bp 228° Bp_{11} 100-101°. n_D^{20} 1.5539.

Oxime:
C_7H_9NOS 155.22
Plates. Mp 55-56°.

Semicarbazone:
Plates (C_6H_6). Mp 167°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 55A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 598A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1474A (*ir*)
Thomas, V. *et al., Bull. Soc. Chim. Fr.*, 1918, **23**, 288
Steinkopf, W. *et al., Annalen*, 1921, **424**, 8
Hartough, H.D. *et al., J.A.C.S.*, 1947, **69**, 3095
Konishi, H. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 957 (*synth*)
Keumi, T. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 455 (*synth*)

2-Propenal, 9CI P-483

[107-02-8]
Acraldehyde. Acrolein, BSI, WSSA. Acrylaldehyde. Formylethylene. Aqualin. Magnacide H

$H_2C{=}CHCHO$

C_3H_4O 56.064
Present in fruit aromas, black tea, carrot, cooked potato, cheeses, white wine, hydrolyzed soy protein, turkey, pork, beef fat and other foods. Used as an etherification agent in the preparation of modified food starches. Herbicide and algicide used in water treatment. Prod. by microorganisms, e.g. *Clostridium perfringens*. Strongly lachrymatory liq. V. sol. H_2O; sol. EtOH, Et_2O, Me_2CO. d_4^{20} 0.84. Mp -87°. Bp 52°. n_D^{20} 1.3998. Vp 220 mmHg (20°). Unstable, polymerises to a white translucent solid Disacryl. Hydroquinone is used as a stabiliser to prevent autoxidn. and polym..
▶ Highly flammable, fl. p. -26°, autoignition temp. 220/235°. Can undergo violent acid- and base-catalysed polym. Irritating to all tissues. Vesicant. Inhalation may cause pulmonary oedema. Potent lachrymator. OES: long-term 0.1 ppm; short-term 0.3 ppm. AS1050000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 220B; 220C; 470D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 349C; 350A; 733B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 289D; 290A (*ir*)
Doebner, O. *et al., Ber.*, 1902, **35**, 1137 (*synth*)
U.K. Pat., 1945, 569 625; *CA*, **41**, 6275 (*synth*)
Bremner, J.G.M. *et al., J.C.S.*, 1946, 1018 (*synth*)
Fischer, R.F. *et al., J.O.C.*, 1960, **25**, 319 (*synth*)
Acrolein, (ed. Smith, C.W.), Wiley, New York, 1962,
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1972, **3**, 5; 1982, **10**, 2; 1984, **11**, 11 (*use*)
Lipnick, R.L. *et al., Tet. Lett.*, 1973, 931 (*struct*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 413 (*cmr*)
Khvostenko, V.I. *et al., Zh. Org. Khim.*, 1975, **11**, 665; *J. Org. Chem. USSR (Engl. Transl.)*, 1975, **11**, 663 (*ms*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Beauchamp, Jr, R.O. *et al., Crit. Rev. Toxicol.*, 1985, **14**, 309 (*tox, rev, acrolein*)
Encyclopaedia of Polymer Science and Engineering, 2nd edn., Wiley-Interscience, New York, 1985, **1**, 160 (*rev, polym*)
IARC Monog., 1985, **36**, 133; *Suppl*. 6, 24, ; *Suppl*. 7, 78, (*rev, tox*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH-Weinheim, 1985, **A1**, 149 (*rev*)
Lou, J.-D. *et al., Chem. Ind. (London)*, 1987, 531 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 232 (*rev, bibl*)
Pesticide Manual, 9th edn., 1991, No. 60
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A2
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1331
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 40-41 (*use, occur*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1076; 1374
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 18; 697
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADR000; HJQ000; DOM600; DHH800
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 307 (*tox*)

1-Propene-1-sulfenic acid, 8CI P-484

[3736-99-0]
Propenylsulfenic acid

$H_3CCH{=}CHSOH$

C_3H_6OS 90.146

(E)-form
Present in onion (*Allium cepa*).
▶ Lachrymator.

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1963, **17**, 461 (*isol, struct, synth*)
Carson, J.F. *et al., J.O.C.*, 1966, **31**, 1634 (*config*)

1-Propene-1-thiol P-485

[16696-81-4]
Thiopropionaldehyde. Propanethial. 1-Mercapto-1-propene. Thiopropanal

$H_3CCH{=}CHSH \Leftrightarrow H_3CCH_2CH{=}S$

C_3H_6S 74.146

Enethiol (*Z*)-form stable in soln. at r.t.. Volatile flavour-component of *Allium* spp.. Bp 65-69° Bp_{165} 28°. n_D^{20} 1.4802.
▶ Lachrymator.

Thial-*form* [56019-38-6]

S-*Oxide:* [32157-29-2]
C_3H_6OS 90.146
Lachrymatory factor of onion (*Allium cepa*). $Bp_{0.5}$ -20°.
▶ Lachrymator.

[56019-37-5, 70565-74-1, 74635-27-1, 122694-34-2]

Strausz, O.P. *et al., Can. J. Chem.*, 1965, **43**, 717 (*synth, pmr, ms, ir*)
Brandsma, L. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1970, **89**, 593 (*synth*)
Block, E. *et al., J.A.C.S.*, 1979, **101**, 2200; 1980, **102**, 2490 (*oxide*)

Block, E. *et al., Tet. Lett.*, 1980, **21**, 1277; 1985, **26**, 1425 (*isom, synth, oxide, dioxide*)
MacDonald, J.N. *et al., J. Mol. Struct.*, 1987, **159**, 229 (*synth, cmr, ir, pmr, E-form*)
Vallée, Y. *et al., Synth. Commun.*, 1993, **23**, 1267
Block, E. *et al., J.A.C.S.*, 1996, **118**, 7492 (*oxide, synth, pmr, cmr, O-17 nmr, microwave*)

2-Propene-1-thiol, 9CI P-486

[870-23-5]
Allyl mercaptan. Allyl thioalcohol. Allylthiol. 3-Mercaptopropene. FEMA 2035
$H_2C{=}CHCH_2SH$
C_3H_6S 74.146
Component of onion flavour (*Allium cepa*) and other *Allium* spp. Flavouring ingredient. Potential nutriceutical. Liq. with strong garlic odour. Bp 68-69°. n_D^{20} 1.4765. pK_{a1} 10 (25°).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 417B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 259C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 341A (*ir*)
v. Braun, J. *et al., Ber.*, 1926, **59**, 1202 (*synth*)
Taguchi, T. *et al., Tet. Lett.*, 1969, 3631 (*synth*)
Boelens, M. *et al., J. Agric. Food Chem.*, 1971, **19**, 984 (*isol*)
Hsu, C.S. *et al., Spectrosc. Lett.*, 1974, **7**, 439 (*ir, Raman*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 84 (*use*)

2-Propenoic acid, 9CI P-487

[79-10-7]
Acrylic acid
$H_2C{=}CHCOOH$
$C_3H_4O_2$ 72.063
Monomer component of packaging materials for food. Corrosive liq. with acrid odour and fumes. Misc. H_2O, EtOH, Et_2O; sol. Me_2CO. d_4^{16} 1.06. Mp 13°. Bp 141° (polymerises). n_D^{20} 1.4424. pK_a 4.25 (25°). Vp 4 mmHg (25°). Polym. readily in the presence of O_2. Acrylic acid and its esters usually contain hydroquinone monomethyl ether as polym. inhibitor. Q/e values for copolym., *Q* 0.83, *e* +0.88. Copolym. with vinyl chloride: r_{AA} 6.8; r_{VC} 0.107 (typical values, 60°); *Q* 1.15; *e* 0.77.
▶ Flammable, fl. p. 52°, autoignition temp. 438°. May polym. exothermically (possibly violently). Irritant to all tissues. LD_{50} (rat, orl) 33.5 mg/kg. LD_{50} (rbt, skn) 280 mg/kg. Exp. teratogen (ipr route). OES: long-term 10 ppm; short-term 20 ppm (Sk). AS4375000

Me ester: [96-33-3] *Methyl acrylate*
$C_4H_6O_2$ 86.09
Liq. Sl. sol. H_2O; sol. EtOH, Et_2O, Me_2CO. d^{20} 0.95. Mp -76.5°. Bp 80.7°. n_D^{20} 1.3984. Vp 68 mmHg (20°). Polym. on long standing.
▶ Highly flammable, fl. p. -3° (oc), autoignition temp. 468°. Can polym. violently if not inhibited. Peroxidisable. Adverse olfactory, eye and respiratory effects by inhalation. Skin and eye irritant. Exp. lung, liver and kidney injury following chronic exposure. OES: long-term 10 ppm. AT2800000

Et ester: [140-88-5] *Ethyl acrylate. FEMA 2418*
$C_5H_8O_2$ 100.117
Flavouring ingredient. Liq. with acid odour. Sl. sol. H_2O; sol. EtOH, Et_2O, $CHCl_3$. d_4^{20} 0.92. Mp -71.2°. Bp 99.8°. n_D^{20} 1.4068. Vp 29 mmHg (20°). Q/e values for copolym., Q 0.41, e +0.55. Rate for radical polym., k_p = 800 L mol^{-1} s^{-1}, k_t = 1.76 × 10^{-6} L mol^{-1} s^{-1}.
▶ Flammable, fl. p. 9/10° (oc), autoignition temp. 372/383°. May polym. exothermically. Eye, skin and respiratory tract irritant. Skin sensitiser. LD_{50} (rat, orl) 800 mg/kg. Exp. carcinogen (v. large doses). OES: long-term 5 ppm; short-term 15 ppm (Sk). AT0700000

Amide: [79-06-1] *Acrylamide. 2-Propenamide, 9CI*
C_3H_5NO 71.079
Polyacrylamides are used as flocculants as a filtration aid in the treatment of waste water and expressed sugar juices and as clarifying agents in a variety of food products. Asparagine-derived Maillard prod. found in trace amounts in a variety of cooked and processed foods. Subject of a 'food scare' in 2001-2 but concern may have been overstated. Leaflets (C_6H_6). Sol. H_2O, EtOH, MeOH, Et_2O, Me_2CO, DMF, DMSO. Mp 85°. Bp 192.6°. Polym. on heating or under uv light. Aq. solns. are stabilised by O_2 and $Cu^{2\oplus}$ ions. Q/e values for copolym., Q 0.23, e +0.54.
▶ Polym. can be violent at Mp. Symptoms of exposure (dermal, inhalation or ingestion) include cold sweating hands and peripheral neuropathies with numbness, paraesthesias and weakness. Dermal absorption can also cause erythema and peeling of the palms. Possible human carcinogen. LD_{50} (rat, orl) 124 mg/kg. LD_{50} (rat, skn) 400 mg/kg. Exp. carcinogen and reprod. effects. Adverse exp. CNS effects. MEL: long-term 0.3 mg m^{-3} (Sk). AS3325000

[6292-01-9, 7446-81-3, 9003-05-8, 9003-06-9, 10192-85-5, 10344-93-1, 14643-87-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 498B; 638B; 638C; 642A; 732A; 749B; 842D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 776A; 973B; 973C; 974A; 974B; 1199A; 1221A; 1244C; 1358B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 583A; 674A; 674B; 674C; 674D; 770D; 778B; 784B; 802B
Wohlk, A. *et al., J. Prakt. Chem.*, 1900, **61**, 200
van der Burg, J.H.N. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1922, **41**, 21 (*synth*)
Ratchford, W.P. *et al., J.A.C.S.*, 1944, **66**, 1864 (*synth*)
Sieburth, J.M. *et al., Science (Washington, D.C.)*, 1960, **132**, 676 (*isol*)
Katayama, T. *et al., CA*, 1966, **65**, 5924 (*isol*)
Bowles, A.J. *et al., Org. Mass Spectrom.*, 1969, **2**, 809 (*ms*)
Katritzky, A.R. *et al., J.A.C.S.*, 1970, **92**, 6861 (*ir*)
Austin, G.T. *et al., Chem. Eng. (N.Y.)*, 1974, **81**, 86 (*rev, manuf*)
Miyajima, G. *et al., Org. Magn. Reson.*, 1974, **6**, 413 (*cmr*)
IARC Monog., 1979, **19**, 47; 73; 1986, **39**, 41; *Suppl.* 6, 27, 41; *Suppl.* 7, 56, 63, 66, 79, 41; 81; 99 (*rev, tox*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH-Weinheim, 1985, **A1**, 161 (*rev*)
Charles, S.W. *et al., J. Mol. Struct.*, 1987, **157**, 17 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 251; 287; 352 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 316 (*Et ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 41-42; 44-45; 945-946; 1709-1710
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4954
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 55; 57; 58; 234; 318
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1039; 1079; 1109; 1433; 1794
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 19; 20; 21; 584; 824
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADS250; ADZ000; EFT000; BPW100; ADX500; MGA500; ADS750; DOP800

2-Propen-1-ol, 9CI P-488

[107-18-6]
Allyl alcohol
$H_2C{=}CHCH_2OH$
C_3H_6O 58.08
Present in garlic (*Allium sativum*). Liq. with pungent mustard-like odour. Misc. H_2O, alcohols, Et_2O; sol. $CHCl_3$. d^{20} 0.85. Mp -129°. Bp 96-97°. n_D^{20} 1.4135. pK_a 15.5 (25°). Vp 24 mmHg (25°). Forms constant-boiling mixt. with H_2O contg. 27.7% H_2O. Homopolym. with difficulty. Q/e values for copolym., Q 0.005, e-1.48.
▶ Extremely flammable, fl. p. 21°, autoignition temp. 375°. Reacts violently with H_2SO_4. Reaction with CCl_4 produces unstable halogenated C_4-epoxides. Skin, severe eye (human), and systemic irritant. LD_{50} (rat, orl) 64 mg/kg. LD_{50} (rbt, skn) 45 mg/kg. Hepatotoxic. OES: long-term 2 ppm; short-term 4 ppm (Sk). BA5075000

Benzoyl: [583-04-0] *Allyl benzoate*
$C_{10}H_{10}O_2$ 162.188
Used in food flavouring. Liq. d 1.06. Bp 230° Bp_{24} 120-122°.

[20907-32-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 138B; 633B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 207B; 333B; 963C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 200C; 663D (*ir*)
Aldrich Library of NMR Spectra, **1**, 100C (*pmr*)
Perkin, W.H. *et al., J.C.S.*, 1896, **69**, 1226 (*allyl benzoate*)
Deulafeu, V. *et al., CA*, 1928, **22**, 4104 (*synth*)
Delaby, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1929, **18**, 710
U.K. Pat., 1947, 577 992; *CA*, **41**, 2067 (*synth*)
Vogel, A.I. *et al., Textbook of Practical Organic Chemistry*, Longmans, London, 1956, (*purifn*)
Boyer-Kawenoki, F. *et al., Bull. Soc. Chim. Fr.*, 1959, 624 (*polym*)
Bernhard, R.A. *et al., Arch. Biochem. Biophys.*, 1964, **107**, 137 (*isol*)
Yonemoto, T. *et al., J. Magn. Reson.*, 1974, **13**, 153 (*cmr*)
Silvi, B. *et al., Spectrochim. Acta A*, 1976, **32**, 11 (*ir, Raman*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, ; 1981, **9**, 10 (*use*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A1**, 431 (*rev*)
Badawi, H. *et al., J. Mol. Struct.*, 1987, **162**, 247 (*microwave, struct*)
Bowen, R.D. *et al., J.C.S. Perkin 2*, 1987, 1019 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 144 (*rev, bibl*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4662
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1149
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 3, 1992, 189 (*tox, rev*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 23; 25
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFU750; AFV500; AGK750

2-Propenyl glucosinolate P-489

[534-69-0]

[3952-98-5]
1-Thio-β-D-glucopyranose 1-[N-(sulfooxy)-3-butenimidate], 9CI. ***Sinigrin***. *Allyl glucosinolate. Myronic acid*

$H_2C{=}CHCH_2C(SGlc){=}NOSO_3H$

$C_{10}H_{17}NO_9S_2$ 359.378

Isol. from seeds of black mustard (*Brassica nigra*) and cabbage, as K salt. Present in many crucifers, major glucosinolate in Brussels sprouts (*Brassica oleraceae*). Cryst. (as K salt). Mp 125-127° (K salt). $[\alpha]_D^{28}$ -17 (c, 0.2 in H_2O).

Tetra-Ac: [5019-27-2]
Cryst. (as K salt). Mp 193-195° (K salt). $[\alpha]_D^{26}$ -16 (c, 0.14 in H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 904D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1456C (*nmr*)
Benn, M.H. *et al., Chem. Comm.*, 1965, 445 (*synth*)
Matsuo, M. *et al., Tet. Lett.*, 1968, 4101 (*biosynth*)
Marsh, R.E. *et al., Acta Cryst. B*, 1970, **26**, 1030 (*cryst struct*)
v. Etten, C.H. *et al., J. Agric. Food Chem.*, 1976, **24**, 452; *CA*, **85**, 3935z
Watson, W.H. *et al., Cryst. Struct. Commun.*, 1977, **6**, 441 (*cryst struct*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Parry, R.J. *et al., J.A.C.S.*, 1982, **104**, 3217 (*biosynth*)
Hanley, A.B. *et al., J. Sci. Food Agric.*, 1983, **34**, 869 (*isol*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*cmr, pmr*)
Mawson, R. *et al., Natural Toxicants - Vol. II, Glycosides*, CRC Press, Boca Raton, 1989, (*glucosinolates, tox, rev*)
Abramski, W. *et al., J. Carbohydr. Chem.*, 1996, **15**, 109 (*synth*)
Olivier, C. *et al., J. Chem. Ecol.*, 1999, **25**, 2687-2701 (*activity, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGH125

1-Propenyl 2-propenyl disulfide, 9CI P-490

[33368-82-0]
Allyl 1-propenyl disulfide. 4,5-Dithia-1,6-octadiene

$H_2C{=}CHCH_2{-}^4S{-}^5S{-}CH{=}CHCH_3$

$C_6H_{10}S_2$ 146.277

(E)-form [122156-02-9]
Constit. of garlic (*Allium sativum*). Oil.

4-Oxide: [134568-42-6] S-*1-Propenyl 2-propenesulfinothioate*
$C_6H_{10}OS_2$ 162.276
Constit. of *Allium* spp..

5-Oxide: [134595-70-3]

[136516-40-0] S-*2-Propenyl 1-propenesulfinothioate*
$C_6H_{10}OS_2$ 162.276
Constit. of *Allium* spp..

(Z)-form [122156-03-0]
Constit. of garlic (*Allium sativum*). Oil.

4-Oxide: [136516-39-7]
Constit. of *Allium* spp..

5-Oxide: [143038-12-4]
Constit. of *Allium* spp..

Block, E. *et al., Pure Appl. Chem.*, 1993, **65**, 625-632 (*derivs, occur*)
Block, E. *et al., J.A.C.S.*, 1996, **118**, 2799 (*synth, pmr, cmr*)

2-Propenyl [3-(2-propenylthio)-2-propenyl] sulfate P-491

$H_2C{=}CHCH_2SCH{=}CHCH_2OSO_2OCH_2CH{=}CH_2$

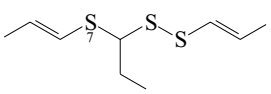
$C_9H_{14}O_4S_2$ 250.339

(E)-form
Constit. of garlic (*Allium sativum*). Oil.

Hu, Q. *et al., J. Agric. Food Chem.*, 2002, **50**, 1059-1062 (*isol, pmr, cmr, ms*)

1-Propenyl 1-(1-propenylthio)propyl disulfide, 9CI P-492

[126876-28-6]
6-Ethyl-4,5,7-trithia-2,8-decadiene



$C_9H_{16}S_3$ 220.423

Isol. from the Welsh onion (*Allium fistulosum*).

7-Oxide:1-Propenyl 1-(1-propenylsulfinyl)propyl disulfide
$C_9H_{16}OS_3$ 236.423
Isol. from onion (*Allium cepa*). Obt. as various isomers.

[125017-86-9, 125224-25-1, 125224-26-2, 125224-27-3]

Bayer, T. *et al., Phytochemistry*, 1989, **28**, 2373-2377 (*7-oxide*)
Kuo, M.C. *et al., J. Agric. Food Chem.*, 1990, **38**, 1378-1381 (*isol*)
Block, E. *et al., J.O.C.*, 1992, **57**, 5815-5817 (*synth*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*isol, ms*)

1-Propenyl 1-(2-propenylthio)propyl disulfide P-493

6-Ethyl-4,5,7-trithia-2,9-decadiene

$H_2C{=}CHCH_2{-}^7S{-}CH(CH_2CH_3){-}S{-}S{-}CH{=}CHCH_3$

$C_9H_{16}S_3$ 220.423

7-Oxide:1-Propenyl 1-(2-propenylsulfinyl)propyl disulfide
$C_9H_{16}OS_3$ 236.423
Constit. of *Allium* sp..

Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422

2-Propenyl 1-(1-propenylthio)propyl disulfide P-494

6-Ethyl-4,5,7-trithia-1,8-decadiene

$H_3CCH{=}CH{-}^7S{-}CH(CH_2CH_3){-}S{-}S{-}CH_2CH{=}CH_2$

$C_9H_{16}S_3$ 220.423

7-Oxide: [138898-92-7] *2-Propenyl 1-(1-propenylsulfinyl)propyl disulfide*
$C_9H_{16}OS_3$ 236.423
Constit. of *Allium* spp..

Morimitsu, Y. *et al., J. Agric. Food Chem.*, 1992, **40**, 368-372 (*synth*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*isol*)

2-Propenyl 1-(2-propenylthio)propyl disulfide P-495

Allyl 1-(allylthio)propyl disulfide. 6-Ethyl-4,5,7-trithia-1,9-decadiene

$H_2C{=}CHCH_2{-}^7SCH(CH_2CH_3){-}S{-}S{-}CH_2CH{=}CH_2$

$C_9H_{16}S_3$ 220.423

7-Oxide:2-Propenyl 1-(2-propenylsulfinyl)propyl disulfide. Allyl 1-(allylsulfinyl)propyl disulfide
$C_9H_{16}OS_3$ 236.423
Constit. of *Allium tricoccum* (wood leek).

[72869-75-1]

Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol, ms*)

1-Propenyl propyl disulfide P-496

[5905-46-4]
4,5-Dithia-2-octene. FEMA 3227

$H_3CCH{=}CH{-}^4S{-}^5S{-}CH_2CH_2CH_3$

$C_6H_{12}S_2$ 148.293

Flavouring ingredient. Bp_{13} 78-80°.

(E)-form [23838-21-3]
Constit. of the essential oils of *Allium* spp.. Oil.

4-Oxide: [119052-98-1]

[121955-54-2] S-*1-Propenyl 1-propanesulfinothioate*
$C_6H_{12}OS_2$ 164.292
Constit. of *Allium* spp..

5-Oxide: [143063-27-8]

[121955-55-3] S-*Propyl 1-propenesulfinothioate*
$C_6H_{12}OS_2$ 164.292
Constit. of *Allium* spp..

(Z)-form [23838-20-2]
Constit. of the essential oils of *Allium* spp.. Oil.

4-Oxide: [119052-97-0]
Constit. of *Allium* spp..

5-Oxide: [143038-13-5]
Constit. of *Allium* spp..

Wijers, H.E. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 519 (*synth*)
Block, E. *et al., Pure Appl. Chem.*, 1993, **65**, 625-632 (*derivs, occur*)
Block, E. *et al., J.A.C.S.*, 1996, **118**, 2799-2810 (*synth, pmr, cmr, ms*)

2-Propenyl propyl disulfide, 9CI P-497

[2179-59-1]
Allyl propyl disulfide, 8CI. APDS. 4,5-Dithia-1-octene

$H_2C{=}CHCH_2$-S-S-$CH_2CH_2CH_3$

$C_6H_{12}S_2$ 148.293
Constit. of *Allium* spp. Flavourant in garlic and onions. Bp_{16} 66-69°. Log P 3.37 (calc).

▶ Powerful irritant. JO0350000

4-Oxide: [136516-42-2] S-*2-Propenyl 1-propanesulfinothioate.* S-*Allyl 1-propanesulfinothioate*
$C_6H_{12}OS_2$ 164.292
Constit. of garlic (*Allium sativum*) and wild leek (*Allium tricoccum*).

5-Oxide: [136516-43-3] S-*Propyl 2-propene-1-sulfinothioate*
$C_6H_{12}OS_2$ 164.292
Constit. of *Allium sativum* (garlic).

Carson, J.F. *et al., J.O.C.*, 1959, **24**, 175-179 (*synth, glc*)
Jacobsen, J.V. *et al., Arch. Biochem. Biophys.*, 1964, **104**, 473-477 (*ir, glc*)
Brodnitz, M.H. *et al., J. Agric. Food Chem.*, 1969, **17**, 760 (*isol, pmr, ir, ms, glc*)
Lawson, L.D. *et al., Planta Med.*, 1991, **57**, 263-270 (*derivs, isol, synth*)
Calvey, E.M. *et al., J. Agric. Food Chem.*, 1997, **45**, 4406-4413 (*derivs, isol, synth, pmr, cmr*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGR500

1-Propenyl propyl sulfide P-498

[33922-70-2]
1-(Propylthio)-1-propene, 9CI. 4-Thia-2-heptene

$H_3CCH_2CH_2$-S-CH$=$$CHCH_3$

$C_6H_{12}S$ 116.227
Volatile constit. of Welsh onion, scallions, leek, garlic and shallots. Usually present as a mixt. of (*E*)- and (*Z*)-isomers.

(*E*)-*form* [37981-35-4]
Bp_{18} 58°.

(*Z*)-*form* [37981-34-3]
Bp_{18} 55°. Undergoes equilibration to a 1:1 mixt. of (*E*)- and (*Z*)-isomers on standing at 0° for 6 weeks.

Wu, J.L. *et al., J. Food Sci.*, 1982, **47**, 606-608 (*occur*)
Kuo, M.C. *et al., J. Agric. Food Chem.*, 1992, **40**, 1906-1910 (*occur*)
Block, E. *et al., J.A.C.S.*, 1996, **118**, 2799-2810 (*synth, pmr, cmr, ms*)

1-Propenyl 1-(propylthio)propyl disulfide, 9CI P-499

[126876-29-7]
6-Ethyl-4,5,7-trithia-2-decene

$H_3CCH_2CH_2^7SCH(CH_2CH_3)$−S−S−CH$=$$CHCH_3$

$C_9H_{18}S_3$ 222.439

(*E*)-*form* [137363-95-2]
Constit. of *Allium fistulosum* (Welsh onion).

7-Oxide:

[138898-88-1] *1-Propenyl 1-(propylsulfinyl)propyl disulfide*
$C_9H_{18}OS_3$ 238.439
Constit. of *Allium tricoccum* (wood leek).

(*Z*)-*form* [137363-92-9]
Constit. of *Allium fistulosum* (Welsh onion).

Kuo, M.C. *et al., J. Agric. Food Chem.*, 1992, **40**, 111-117 (*isol*)
Morimitsu, Y. *et al., J. Agric. Food Chem.*, 1992, **40**, 368-372 (*deriv, synth*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol, ms*)

2-Propenyl 1-(propylthio)propyl disulfide P-500

6-Ethyl-4,5,7-trithia-1-decene
$H_3CCH_2CH_2$-^{7}S-CH(CH_2CH_3)-S-S-$CH_2CH{=}CH_2$

$C_9H_{18}S_3$ 222.439

7-Oxide:2-Propenyl 1-(propylsulfinyl)propyl disulfide
$C_9H_{18}OS_3$ 238.439
Constit. of *Allium* sp..

Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422

S-1-Propenyl thiosulfate P-501

$H_3CCH{=}CH$−S−SO_3H

$C_3H_6O_3S_2$ 154.211

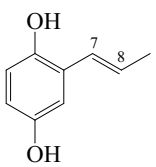
(*E*)-*form*
Constit. of *Allium cepa* (onion). Obt. as Na salt.

(*Z*)-*form*
Constit. of onion (*Allium cepa*). Obt. as Na salt.

[155260-89-2, 155260-90-5]

Yamato, O. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 221 (*isol, pmr, cmr*)

2-(1-Propenyl)-1,4-benzenediol P-502



$C_9H_{10}O_2$ 150.177

(*E*)-*form*
4-Me ether: [98755-22-7]

[98755-19-2] *4-Methoxy-2-(1-propenyl)phenol. Pseudoisoeugenol*
$C_{10}H_{12}O_2$ 164.204Has been synthesised.

4-Me ether, 1-O-*(2-methylbutanoyl):*
[58989-20-1] *Pseudoisoeugenol 2-methylbutanoate*
$C_{15}H_{20}O_3$ 248.321
Constit. of *Pimpinella anisum* (aniseed).

7,8-Epoxide: 2-(3-Methyl-2-oxiranyl)-1,4-benzenediol, M-528

Martin, R. *et al., Planta Med.*, 1985, **51**, 198-202 (*isol*)
Reichling, J. *et al., Z. Naturforsch., C*, 1985, **40**, 465-468 (*isol*)

4-(1-Propenyl)-1,2-benzenediol, 9CI P-503

[72898-29-4]

$C_9H_{10}O_2$ 150.177

(*E*)-*form*
2-Me ether: 2-Methoxy-4-(1-propenyl)-phenol, M-272

Di-Me ether: [6379-72-2]

[93-16-3] *1,2-Dimethoxy-4-(1-propenyl)-benzene, 9CI. 4-(1-Propenyl)veratrole.* ***Methylisoeugenol.*** *Isoeugenyl methyl ether. FEMA 2476*
$C_{11}H_{14}O_2$ 178.23
Constit. of essential oils. Flavouring ingredient. Liq. with a delicate, clove-carnation odour and a bitter burning taste. Mp 16-17°. Bp 258-262° Bp_{12} 138-140°. n_D^{20} 1.5616. Normally isol. as a mixt. of *E*- and *Z*- (see below) isomers.

▶ LD_{50} (mus, ipr) 350 mg/kg.

Di-Me ether, 1′R,2′R-epoxide: [124878-07-5]

[40626-39-9] *2-(3,4-Dimethoxyphenyl)-3-methyloxirane, 9CI. 1-(1,2-Epoxypropyl)-3,4-dimethoxybenzene. 1,2-Dimethoxy-4-(3-methyloxiranyl)benzene. 1-(3,4-Dimethoxyphenyl)-1,2-epoxypropane*
$C_{11}H_{14}O_3$ 194.23
Oil. $[\alpha]_D$ +24 ($CHCl_3$).

1-Et, 2-Me ether: [137138-52-4]

[7784-67-0, 149849-39-8] *1-Ethoxy-2-methoxy-4-(1-propenyl)benzene. Isoeugenyl ethyl ether. FEMA 2472*
$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Cryst. (EtOH or Et_2O) with a floral odour. Sol. Et_2O, C_6H_6, EtOH, AcOH. Mp 63-64°. Bp 245°. *Z*-form also known.

1-Et ether: [94-86-0] *2-Ethoxy-5-(1-propenyl)phenol, 9CI. Isosafroeugenole. Propenylguaethole. Vanitrope. FEMA 2922*
$C_{11}H_{14}O_2$ 178.23
Flavouring ingredient. Cryst. with a vanilla-like odour and flavour. Mp 86-88°.

(*Z*)-*form*
Di-Me ether: [6380-24-1]
Oil. Bp_{13} 134-135°. n_D^{20} 1.5726.

▶ LD_{50} (mus, ipr) 535 mg/kg.

[63477-41-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **3**, 1027D (*ir*)
Aldrich Library of NMR Spectra, **1**, 886C (*pmr*)
Briner, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2249 (*ir, Raman*)
Vajda, M. *et al., Org. Magn. Reson.*, 1976, **8**, 324 (*cmr, deriv*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 2655 (*isol*)

Klungsoeyr, J. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 323 (*metab, glc*)
Della Greca, M. *et al., Phytochemistry*, 1989, **28**, 2319-2321 (*di-Me ether epoxide*)
Armstead, D.E.F. *et al., J. Chem. Educ.*, 1991, **68**, 698-699 (*1-Et 2-Me ether*)
Radhakrishna, A.S. *et al., Synth. Commun.*, 1991, **21**, 379 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 687; 808; 818 (*ethers*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1467-1470; 2330 (*ethers*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IRY000

4-(2-Propenyl)-1,2-benzenediol, 9CI P-504

[1126-61-0]
4-Allylpyrocatechol, 8CI. 4-Propenylcatechol. 4-Allylcatechol. 3,4-Dihydroxyallylbenzene. 3-(3,4-Dihydroxyphenyl)propene

$C_9H_{10}O_2$ 150.177
Cryst. (C_6H_6/petrol). Sol. Me_2CO, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 48-48.5°. Bp_2 120-122°.

1-O-β-D-Glucopyranoside:
$C_{15}H_{20}O_7$ 312.319
Constit. of *Mentha spicata* var. *crispa* (spearmint) and rhizomes of *Alpinia officinarum* (lesser galangal). $[\alpha]_D^{25}$ -108 (c, 0.18 in MeOH) (-52.6). λ_{max} 276 (log ϵ 2.89) (MeOH).

1-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [267668-14-4]
$C_{21}H_{30}O_{11}$ 458.461
Constit. of rhizomes of *Alpinia officinarum* (lesser galangal). $[\alpha]_D$ -106 (c, 0.18 in MeOH). λ_{max} 275 (log ϵ 2.96) (MeOH).

2-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:
$C_{21}H_{30}O_{11}$ 458.461
Amorph. powder.

2-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{21}H_{30}O_{11}$ 458.461
Amorph. powder. Mp 180-182°.

Di-Ac: [13620-82-1] *1,2-Diacetoxy-4-allylbenzene*
$C_{13}H_{14}O_4$ 234.251
Sol. Me_2CO, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Bp_3 150-152°.

Dibenzoyl:
Mp 71-72°.

1-Me ether: See 2-Methoxy-5-(2-propenyl)phenol in *The Combined Chemical Dictionary.*

2-Me ether: 2-Methoxy-4-(2-propenyl)-phenol, M-273

Di-Me ether: [93-15-2] *1,2-Dimethoxy-4-(2-propenyl)benzene. 4-Allylveratrole.* ***Methyleugenol****. FEMA 2475*
$C_{11}H_{14}O_2$ 178.23
Present in many essential oils, e.g. nutmeg, mace and also many fruits, e.g. apple, banana, orange juice or peel, grapefruit, bilberry. Liq. with clove/carnation odour and bitter, burning taste. Sol. MeOH, Et_2O. Fp -4. Bp 255° Bp_{12} 125-127°. Log P 2.67 (calc).

► Fl. p. 99°. Skin irritant. LD_{50} (rat, orl) 1179 mg/kg. CY2450000

2-Et ether:2-Ethoxy-4-(2-propenyl)phenol. 4-Allyl-2-ethoxyphenol
$C_{11}H_{14}O_2$ 178.23

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 209B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 986A (*ir*)
Perkin, W.H. *et al., J.C.S.*, 1927, 1663-1666 (*synth*)
Schöpf, C. *et al., Annalen*, 1940, **544**, 30-62 (*synth*)
Sethi, S.C. *et al., Indian J. Chem.*, 1963, **1**, 435-437; 1964, **2**, 323-326 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 190 (*occur, deriv*)
Evans, P.H. *et al., J. Agric. Food Chem.*, 1984, **32**, 1254-1256 (*isol, di-Ac*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1056-1058 (*occur, props*)
Yamamura, S. *et al., Phytochemistry*, 1998, **48**, 131-136 (*1-glucoside*)
Zhou, Z. *et al., Zhongcaoyao*, 1999, **30**, 801-804
Deng, S.M. *et al., Chin. Chem. Lett.*, 2000, **11**, 1001-1002 (*2-rhamnosylglucosides*)
De Vincenzi, M. *et al., Fitoterapia*, 2000, **71**, 216-221 (*Methyleugenol, rev*)
Pesticide Manual, 12th edn., 2000, 522 (*Methyleugenol*)
Abdel-Mogib, M. *et al., Pharmazie*, 2000, **55**, 693-695 (*2-Et ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGE250

4-(2-Propenyl)-1,3-benzenediol, 9CI P-505

[1616-52-0]
4-Allylresorcinol, 8CI. 4-Allyl-1,3-dihydroxybenzene. 3-(2,4-Dihydroxyphenyl)-propene

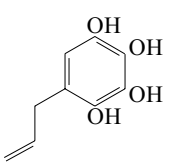
$C_9H_{10}O_2$ 150.177
Cryst. (C_6H_6/petrol). Mp 68-69°.

Di-Me ether: [3698-23-5] *2,4-Dimethoxy-1-(2-propenyl)benzene, 9CI. 1-Allyl-2,4-dimethoxybenzene, 8CI.* ***Osmorhizole***
$C_{11}H_{14}O_2$ 178.23
Constit. of sweet cicely (*Myrrhis odorata*) leaf and root oils. Bp_2 71-72°.

Kaufman, K.D. *et al., J.O.C.*, 1961, **26**, 117; 1965, **30**, 1320 (*synth*)
Nikiforova, I.S. *et al., Zh. Org. Khim.*, 1966, **2**, 1240 (*synth*)
Wenkert, E. *et al., Synthesis*, 1983, 701 (*Osmorhizole*)
Devakumar, C. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 368 (*Osmorhizole*)
Dieter, J.W. *et al., Tet. Lett.*, 1987, **28**, 5415 (*Osmorhizole*)

5-(2-Propenyl)-1,2,3,4-benzenetetrol P-506

5-Allyl-1,2,3,4-benzenetetrol



$C_9H_{10}O_4$ 182.176

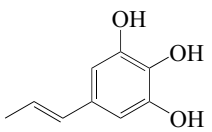
1,2-Methylene, 4-Me ether, 3-O-β-D-glucopyranoside: [149380-62-1] ***Perilloside E***
$C_{17}H_{22}O_9$ 370.355
Constit. of the leaves of *Perilla frutescens* (perilla). Needles. Mp 164-165°. $[\alpha]_D$ -22.8 (c, 0.3 in MeOH). λ_{max} 286 (ϵ 2750) (MeOH).

1,2-Di-Me, 3,4-methylene ether: [23724-27-8] *4,5-Dimethoxy-7-(2-propenyl)-1,3-benzodioxole, 9CI. 1-Allyl-4,5-dimethoxy-2,3-methylenedioxybenzene, 8CI.* ***Pseudodillapiole***
$C_{12}H_{14}O_4$ 222.24
Oil. Bp_2 124-126°. λ_{max} 208 (ϵ 3340); 285 (ϵ 290) (EtOH).

Dallacker, F. *et al., Chem. Ber.*, 1969, **102**, 2663-2676 (*synth*)
Burke, B. *et al., Phytochemistry*, 1986, **25**, 1427-1430 (*isol, uv, pmr, cmr*)
Nair, M.G. *et al., J. Agric. Food Chem.*, 1990, **38**, 1093-1096 (*isol, synth*)
Fujita, T. *et al., Phytochemistry*, 1994, **37**, 543 (*isol, uv, ir, pmr, cmr, ms*)

5-(1-Propenyl)-1,2,3-benzenetriol, 9CI P-507

5-(1-Propenyl)pyrogallol. 1-(3,4,5-Trihydroxyphenyl)-2-propene



(E)-form

$C_9H_{10}O_3$ 166.176

(E)-form
Bp_{10} 153-156°.

1,3-Di-Me ether: [6635-22-9] *2,6-Dimethoxy-4-(1-propenyl)phenol. FEMA 3728*
$C_{11}H_{14}O_3$ 194.23
Flavouring ingredient. Viscous liq. $Bp_{0.13}$ 135°.

1,3-Di-Me ether, 2-O-angeloyl:
$C_{16}H_{20}O_4$ 276.332
Oil.

Tri-Me ether: [5273-85-8] *1,2,3-Trimethoxy-5-(1-propenyl)benzene.* ***Isoelemicin***
$C_{12}H_{16}O_3$ 208.257
Constit. of oil of nutmeg. Bp_{10} 153-156°.

1,2-Methylene, 3-Me ether: [487-62-7] *4-Methoxy-6-(1-propenyl)-1,3-benzodioxole, 9CI. 1-Methoxy-2,3-methylenedioxy-5-(1-propenyl)benzene.* ***Isomyristicin***
$C_{11}H_{12}O_3$ 192.214
Found in dill, parsley and nutmeg oils. Needles or prisms (EtOH). Mp 44-45°. Bp_{18} 166°. $n_D^{45.5}$ 1.5655.

(Z)-form

1,2-Methylene, 3-Me ether:
Present in nutmeg (*Myristica fragrans*).

Thoms, H. *et al., Ber.*, 1903, **36**, 3446 (*Isomyristicin, synth*)
Shulgin, A.T. *et al., Nature (London)*, 1963, **197**, 379 (*Isomyristicin, isol*)

Shulgin, A.T. *et al., Naturwissenschaften*, 1964, **51**, 360 (*isol*)
Sammy, G.M. *et al., Chem. Ind. (London)*, 1968, 1279 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 2655 (*isol, di-Me angelate*)
Achenbach, H. *et al., Phytochemistry*, 1992, **31**, 4263 (*isol, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 686 (*1,3-di-Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2329 (*1,3-di-Me ether*)

5-(2-Propenyl)-1,2,3-benzenetriol P-508

5-Allyl-1,2,3-benzenetriol. 5-Allylpyrogallol

$C_9H_{10}O_3$ 166.176

▶CY2801000

*1-Me ether, 3-*O*-[3,4,5-trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:* [141913-95-3] ***Pimentol***
$C_{23}H_{26}O_{12}$ 494.451
Constit. of allspice (*Pimenta officinalis*). $[\alpha]_D^{24}$ -22.8 (c, 0.08 in MeOH).

*2-Me ether, 1-*O*-β-D-glucopyranoside:* [192324-34-8] ***Sphalleroside A***
$C_{16}H_{22}O_8$ 342.345
Constit. of *Foeniculum vulgare* (fennel). Cryst. Mp 185-186° (145-147°). $[\alpha]_D^{21}$ -48 (c, 0.8 in MeOH). Data of two isolates is at variance.

1,3-Di-Me ether: [6627-88-9] *2,6-Dimethoxy-4-(2-propenyl)phenol, 9CI. 4-Allyl-2,6-dimethoxyphenol, 8CI.* ***Methoxyeugenol****. 4-Allylsyringol*
$C_{11}H_{14}O_3$ 194.23
Found in oil of sassafras (*Sassafras albidum*) root, nutmeg (*Myristica fragrans*) and *Cinnamomum glanduiferum*. Oil. Bp_{10} 166-168° Bp_2 123-125°.

Tri-Me ether: [487-11-6] *1,2,3-Trimethoxy-5-(2-propenyl)benzene, 9CI. 5-Allyl-1,2,3-trimethoxybenzene.* ***Elemicin***
$C_{12}H_{16}O_3$ 208.257
Constit. of Elemi oil and *Myristica fragrans* (nutmeg). Oil. Bp_{10} 144-147°.

*1,2-Methylene ether, 3-*O*-β-D-glucopyranoside:* ***Oenanthoside A***
$C_{16}H_{20}O_8$ 340.329
Constit. of *Oenanthe javanica* (water dropwort). Powder. Mp 155-156°. $[\alpha]_D^{24}$ -55.2 (c, 0.03 in MeOH). λ_{max} 279 (ε 1820) (MeOH).

Semmler, F.W. *et al., Ber.*, 1908, **41**, 1918 (*isol, Elemicin*)
Mauthner, F. *et al., Annalen*, 1917, **44**, 252 (*isol, Elemicin*)
Giesbrecht, A.M. *et al., Phytochemistry*, 1974, **13**, 2285 (*isol, Elemicin*)
Shibuya, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2671 (*1,3-di-Me derivs, isol, ir, ms, pmr*)
Achenbach, H. *et al., Phytochemistry*, 1992, **31**, 4263 (*isol, cmr, Elemicin*)
Fujita, T. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 526 (*Oenanthoside A*)
Oya, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 263-266 (*Pimentol*)
Chen, N.Y. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 107-109 (*Sphalleroside A*)
Sy, L.K. *et al., Phytochemistry*, 1997, **44**, 1099 (*Methoxyeugenol, pmr, cmr*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1587-1590 (*2-Me 1-glucoside*)

5-(2-Propenyl)-1,2,4-benzenetriol P-509

5-Allyl-1,2,4-benzenetriol. 3-(2,4,5-Trihydroxyphenyl)-1-propene

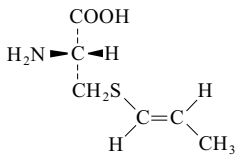
$C_9H_{10}O_3$ 166.176

1,4-Di-Me ether: [90377-06-3] *2,5-Dimethoxy-4-(2-propenyl)phenol, 9CI. 4-Allyl-2,5-dimethoxyphenol*
$C_{11}H_{14}O_3$ 194.23
Constit. of *Sassafras albidum* (sassafras).

Avella, E. *et al., Planta Med.*, 1994, **60**, 195 (*isol, 1,4-di-Me*)

S-(1-Propenyl)cysteine, 9CI P-510

[52438-09-2]
Deoxyalliin



(*R*)-(*E*)-*form*

$C_6H_{11}NO_2S$ 161.224

(R)-(E)-form
L-trans-*form*
Constit. of garlic. Needles (EtOH aq.). Mp 195° dec. $[\alpha]_D^{10}$ -15 (c, 0.4 in 2*N* HCl).

S-*Oxide:* [23315-20-0] *3-(1-Propenylsulfinyl)alanine, 9CI.* S-*(1-Propenyl)cysteine sulfoxide.* ***Isoalliin***
$C_6H_{11}NO_3S$ 177.224
Present in onion (*Allium cepa*). Cryst. (Me_2CO aq.). Mp 153° dec. $[\alpha]_D^{26}$ +74.9 (c, 6.2 in H_2O). Mixt. of diastereoisomers at S.

(R)-(Z)-form [7683-75-2]
L-cis-*form*
Blades (H_2O). Mp 179-180° dec. $[\alpha]_D^{25}$ +59.4 (c, 1.3 in 0.25*N* NaOH).

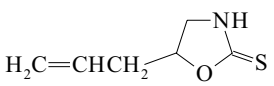
S-*Oxide:* [38570-17-1]
Mp 140° dec. Mixt. of diastereoisomers at S.

[3836-24-6]

Carson, J.F. *et al., Chem. Ind. (London)*, 1963, 1764 (*synth*)
Sugii, M. *et al., Chem. Pharm. Bull.*, 1963, **11**, 548 (*isol*)
Nishimura, H. *et al., Tetrahedron*, 1972, **28**, 4503 (*ms, synth*)
Nishikura, H. *et al., Tet. Lett.*, 1975, 3201 (*synth*)
Freeman, G.C. *et al., Phytochemistry*, 1976, **15**, 521 (*synth*)
Edwards, S.J. *et al., Phytochem. Anal.*, 1994, **5**, 4 (*anal*)
Kubec, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 428-433 (*occur, Isoalliin*)

5-(2-Propenyl)-2-oxazolidinethione, 9CI P-511

[68831-68-5]
5-Allyl-2-oxazolidinethione. ***Napoleiferin***



C_6H_9NOS 143.209

(+)-form [83247-67-0]
Cryst. (Et_2O/pentane/hexane). Mp 60-61°. $[\alpha]_D^{22}$ +10.

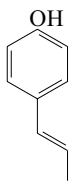
(-)-form [15216-29-2]
Isol. from rape (*Brassica napus*) leaves and stems. Prisms (Et_2O/hexane). Mp 60-61°.

(±)-form
Cryst. Mp 54°.

Tapper, B.A. *et al., Phytochemistry*, 1967, **6**, 749 (*isol*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1982, **30**, 1248 (*isol*)
Latxague, L. *et al., Synth. Commun.*, 1999, **29**, 1627-1637 (*synth, pmr, cmr, ms*)

4-(1-Propenyl)phenol, 9CI P-512

[539-12-8]
1-(4-Hydroxyphenyl)-2-propene. p-*Hydroxy-β-methylstyrene. Anol*



(*E*)-*form*

$C_9H_{10}O$ 134.177

(E)-form [20649-39-2]
Leaflets (H_2O). Mp 93°. Bp_{14} 140°. pK_{a1} 9.82 (25°). Dec. on standing in air.

2-Methylbutanoyl: [205245-83-6] ***Thellungianin F***
$C_{14}H_{18}O_2$ 218.295

3-Methylbutanoyl: [83327-47-3] *Anol isovalerate*
$C_{14}H_{18}O_2$ 218.295
Oil. $Bp_{0.01}$ 60-65° (bath).

Me ether: [4180-23-8] *1-Methoxy-4-(1-propenyl)benzene, 9CI.* p-*Propenylanisole, 8CI.* ***Anethole, USAN****. Anistearoptene. Anise camphor. FEMA 2086*
$C_{10}H_{12}O$ 148.204
Present in anise, fennel and other plant oils. Extensively used in flavour industry. Leaflets (EtOH) with anise odour and sweet taste. Sol. Me_2CO, C_6H_6. Mp 22.5°. Bp 235°. Log P 3.31 (calc). Undergoes cationic polym. λ_{max} 259 (ε 22300) (MeOH) (Berdy).

▶LD_{50} (rat, orl) 2090 mg/kg. Exp. neoplastic agent. Fl. p. 90° ; LD_{50} (mus, ipr) 1450 mg/kg. BZ9275000

O-*(3-Methyl-2-butenyl):* [78259-41-3] ***Foeniculin***†. *Feniculin*
$C_{14}H_{18}O$ 202.296
Isol. from fennel and Chinese star anise oils. Mp 23.5-24.5°.

1′,2′-Epoxide, Me ether:2-(4-Methoxyphenyl)-3-methyloxirane. ***Epoxyanethole***
$C_{10}H_{12}O_2$ 164.204
Constit. of fennel *Foeniculum vulgare*. Needles. Mp 182-184°. Possesses *threo*-config. Racemic.

(Z)-form [85960-81-2]
Me ether: [25679-28-1] ***cis-Anethole***
Liq. d_4^{20} 0.99. $Bp_{2.5}$ 63-65°. n_D^{20} 1.5550. (93% pure). Low level only permitted in flavours. Undergoes cationic polym..

▶Skin irritant. LD_{50} (rat, orl) 150 mg/kg.

BZ9100000

[104-46-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1052D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 208A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 985C (*ir*)
Späth, E. *et al., Ber.*, 1938, **71**, 2708 (*Foeniculin*)
Naves, Y.R. *et al., Helv. Chim. Acta*, 1960, **53**, 230 (*cis-Anethole*)
Briner, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2249 (*ir*)
Klamann, D. *et al., Chem. Ber.*, 1964, **97**, 2534 (*synth*)
Sørensen, J.S. *et al., Acta Chem. Scand.*, 1966, **20**, 992 (*ir*)
Higashimura, T. *et al., J. Polym. Sci., Part A-1*, 1972, **10**, 85 (*polym, Me ether*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Benassi, R. *et al., Org. Magn. Reson.*, 1973, **5**, 391 (*pmr*)
Hamacher, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 309 (*synth*)
Manitto, P. *et al., Tet. Lett.*, 1974, 1567 (*biosynth*)
Higashimura, T. *et al., Polym. J. (Tokyo)*, 1979, **11**, 855-862; *CA*, **92**, 59307h (*polym, Me ether*)
Okely, H.M. *et al., J.C.S. Perkin 1*, 1981, 897 (*Foeniculin*)
Wenkert, E. *et al., Synthesis*, 1983, 701 (*synth*)
Buss, A.D. *et al., Tet. Lett.*, 1983, **24**, 5293 (*synth, Foeniculin*)
Lampman, R.L. *et al., J. Chem. Ecol.*, 1987, **13**, 959
Sangster, S.A. *et al., Xenobiotica*, 1987, **17**, 1223 (*metab*)
Cerrai, P. *et al., Ann. Chim. (Rome)*, 1989, **79**, 33 (*polym, Me ether*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PMQ750
Howes, A.J. *et al., Food Chem. Toxicol.*, 1990, **28**, 537 (*tox*)
Angle, S.R. *et al., J.O.C.*, 1992, **57**, 5937 (*Me ether*)
Mohan, R. *et al., J.O.C.*, 1993, **58**, 2663 (*cis-Anethole, synth, pmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1337
Mi, C. *et al., Zhongcaoyao*, 1998, **29**, 3-5; *CA*, **128**, 261750q (*Thellungianin F*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1448-1450 (*Epoxyanethole*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PMQ750; PMR000; PMR250 (*Y*)

4-(2-Propenyl)phenol, 9CI P-513

[501-92-8]

*3-(*p*-Hydroxyphenyl)-1-propene.* p*-Allylphenol. Chavicol*

$C_9H_{10}O$ 134.177

Found in many essential oils, e.g. anise and Gardenia. Used in perfumery and flavours. Sol. EtOH, hexane; poorly sol. H_2O. Mp 16°. Bp 237° Bp_{17} 120°. pK_{a1} 10.23 (25°).

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* ***Lusitanicoside***
$C_{21}H_{30}O_{10}$ 442.462
Isol. from cherries (*Prunus lusitanica*). Needles (1-propanol). Mp 187-188.5°. $[\alpha]_D^{18}$ -74 (H_2O). λ_{max} 221 (log ϵ 3.42); 273 (log ϵ 2.69) (MeOH).

Me ether: [140-67-0] *1-Methoxy-4-(2-propenyl)benzene, 9CI. 1-Allyl-4-methoxybenzene.* p*-Allylanisole. Methylchavicol. Estragole. Esdragol. Isoanthethole. FEMA 2411*
$C_{10}H_{12}O$ 148.204
Constit. of many essential oils. Found in apple, bilberry and orange fruits and juices. Flavouring agent. Liq. d^{15} 0.98. Bp 216° Bp_{16} 102°. n_D^{27} 1.5230.
▶ Skin irritant. LD_{50} (mus, orl) 1250 mg/kg. Exp. neoplastic agent. BZ8225000

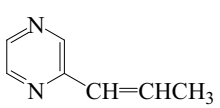
O-*(3-Methyl-2-butenyl):* [56045-79-5] *1-[(3-Methyl-2-butenyl)oxy]-4-(2-propenyl)benzene, 9CI. 1-Allyl-4-prenyloxybenzene.* ***Dictagymnin***
$C_{14}H_{18}O$ 202.296
Isol. from star anise oil. Oil.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1053B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 208B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 985D (*ir*)
Palkin, S. *et al., J.A.C.S.*, 1933, **55**, 1556 (*isol*)
Van der Zanden, J.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1938, **57**, 233 (*synth*)
Suga, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2058 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 165; 166 (*occur*)
Fueno, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 1418 (*pmr*)
Waespe, H.R. *et al., Helv. Chim. Acta*, 1978, **61**, 401 (*synth*)
Okely, H.M. *et al., J.C.S. Perkin 1*, 1981, 897 (*Dictagymnin*)
Wenkert, E. *et al., Synthesis*, 1983, 701 (*synth*)
Sangster, S.A. *et al., Xenobiotica*, 1987, **17**, 1223 (*metab*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AFW750
Howes, A.J. *et al., Food Chem. Toxicol.*, 1990, **28**, 537 (*cytotoxicity, genotoxicity*)
Agharahimi, M.R. *et al., J.O.C.*, 1995, **60**, 1856 (*synth, pmr, cmr, ir, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 934-935 (*Me ether, use, occur*)
Sy, L.K. *et al., Phytochemistry*, 1997, **44**, 1099 (*Dictagymin, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFW750

1-Propenylpyrazine, 9CI P-514

[34413-32-6]

[18217-80-6, 51460-70-9]



$C_7H_8N_2$ 120.154
Maillard product. Volatile constit. of yeast extract, roasted peanut, roasted coconut, roasted sesame, coffee, bread aroma, cocoa and extrusion cooked wheat or maize flour. Characterised spectroscopically.

[110608-57-6]

Bondarovich, H.A. *et al., J. Agric. Food Chem.*, 1967, **15**, 1093-1099 (*isol, ir, ms, uv*)
Wada, F. *et al., Agric. Biol. Chem.*, 1987, **51**, 1753-1760 (*occur, coffee*)
Bredie, W.L.P. *et al., J. Agric. Food Chem.*, 1998, **46**, 1479-1487 (*occur, maize*)

1-(1-Propenylthio)propyl propyl disulfide P-515

[143193-11-7]

6-Ethyl-4,5,7-trithia-8-decene

$H_3CCH{=}CH{-}^{7}S{-}CH(CH_2CH_3){-}S{-}S{-}CH_2CH_2CH_3$

$C_9H_{18}S_3$ 222.439
Constit. of *Allium fistulosum* (Welsh onion).

(E)-form

7-Oxide:

[125017-84-7, 125017-85-8] *1-(1-Propenylsulfinyl)propyl propyl disulfide*
$C_9H_{18}OS_3$ 238.439
Constit. of *Allium cepa* (onion) and *Allium tricoccum* (wood leek).

Bayer, T. *et al., Phytochemistry*, 1989, **28**, 2373-2377 (*deriv, isol*)
Kuo, M.C. *et al., J. Agric. Food Chem.*, 1992, **40**, 1906-1910 (*isol*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol, ms*)

1-(2-Propenylthio)propyl propyl disulfide P-516

6-Ethyl-4,5,7-trithia-9-decene

$H_2C{=}CHCH_2{-}^{7}S{-}CH(CH_2CH_3){-}S{-}S{-}CH_2CH_2CH_3$

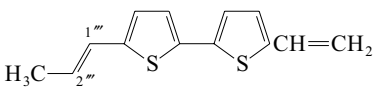
$C_9H_{18}S_3$ 222.439

7-Oxide:1-(2-Propenylsulfinyl)propyl propyl disulfide
$C_9H_{18}OS_3$ 238.439
Constit. of *Allium* sp..

Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422

5-(1-Propenyl)-5′-vinyl-2,2′-bithiophene P-517

5-Ethenyl-5′-(1-propenyl)-2,2′-bithienyl



$C_{13}H_{12}S_2$ 232.37
Light-yellow cryst. (petrol). Mp 46.5-47°.

1‴,2‴-Didehydro: [17257-06-6] *5-(1-Propynyl)-5′-vinyl-2,2′-bithiophene. 5-Ethenyl-5′-(1-propynyl)-2,2′-bithiophene*
$C_{13}H_{10}S_2$ 230.354
Isol. from *Tagetes erecta* (African marigold).

Bohlmann, F. *et al., Chem. Ber.*, 1965, **98**, 1228; 1966, **99**, 984; 1967, **100**, 2518 (*isol, uv, ir, pmr, struct, biosynth*)
Hogstad, S. *et al., Acta Chem. Scand., Ser. B*, 1984, **38**, 902 (*isol*)
D'Auria, M. *et al., Gazz. Chim. Ital.*, 1986, **116**, 747 (*synth*)
Kagan, J. *et al., Prog. Chem. Org. Nat. Prod.*, 1991, **56**, 87 (*rev*)
Rossi, R. *et al., Synth. Commun.*, 1991, **21**, 1875 (*synth*)

Prophenin 1 P-518

[162629-47-2]

A proline-rich peptide comprising 79 amino acid residues including 42 prolines and 15 phenylalanines; the *N*-terminal 60 residues consist of 3 perfect and 3 nearly-perfect repeats of the decamer FPPPNFPGPR. Food preservative.

Harwig, S.S.L. *et al., FEBS Lett.*, 1995, **362**, 65-69 (*isol*)

Prophospholipase A_2 P-519

[9001-84-7]

E.C. 3.1.1.4. Phosphatidylcholine 2-acylhydrolase. Lecithinase A. Phosphatidase. Phosphatidolipase

Enzyme; pancreatic phospholipase A_2 comprises 123 amino acids. Used in food processing for the hydrol. of lecithins, etc..

Hanahan, D.J. *et al., The Enzymes*, (Boyer, P., Ed.), 3rd ed., Academic Press, N.Y., 1971, **5**, 71-85

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2211

Propionicin PLG 1 P-520

[133404-88-3]

PLG 1

Protein comprising 99 aminoacid residues. Isol. from *Propionibacterium thoenii*. Bacteriocin.

Lyon, W.J. *et al., Appl. Environ. Microbiol.*, 1993, **59**, 83-88 (*isol*)
Paik, H.D. *et al., Lait*, 1995, **75**, 367-377 (*struct*)
Hsieh, H.Y. *et al., J. Food Prot.*, 1996, **79**, 734-738 (*isol*)

Propyl 1-(propylthio)propyl disulfide, 9CI P-521

[126876-27-5]

6-Ethyl-4,5,7-trithiadecane

$H_3CCH_2CH_2^7SCH(CH_2CH_3)-S-S-CH_2CH_2CH_3$

$C_9H_{20}S_3$ 224.455

Constit. of *Allium cepa* (onion) and *Allium fistulosum* (Welsh onion).

7-Oxide:Propyl 1-(propylsulfinyl)propyl disulfide
$C_9H_{20}OS_3$ 240.454
Constit. of *Allium tricoccum* (wood leek).

Kuo, M.C. *et al., J. Agric. Food Chem.*, 1990, **38**, 1378-1381; 1992, **40**, 111-117 (*isol*)
Block, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 4414-4422 (*synth*)
Calvey, E.M. *et al., Phytochemistry*, 1998, **49**, 359-364 (*deriv, isol, ms*)

S-Propyl thiosulfate P-522

$H_3CCH_2CH_2-S-SO_3H$

$C_3H_8O_3S_2$ 156.226

Constit. of *Allium cepa* (onion).

[6363-00-4]

Spring, W. *et al., Ber.*, 1882, **15**, 1938 (*synth*)
Schmidt, M. *et al., Angew. Chem.*, 1961, **73**, 394 (*synth*)
Chae, D.K. *et al., CA*, 1974, **80**, 116081 (*synth*)
Asano, Y. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 221 (*isol, synth, pmr, cmr*)

1-Propylamine, 8CI P-523

[107-10-8]

Propanamine, 9CI. 1-Aminopropane

$H_3CCH_2CH_2NH_2$

C_3H_9N 59.111

Isol. from vegetable sources. Liq. d_4^{20} 0.72. Fp -83. Bp 49°. n_D^{20} 1.3910. pK_a 10.4 (30°).

▶ Highly flammable, fl. p. -37°, autoignition temp. 318°. Respiratory tract irritant. Corrosive and irritating to skin and eyes. LD_{50} (rbt, skn) 560 mg/kg. UH9100000

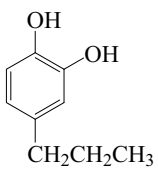
[17033-39-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 280C; 280D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 450A; 450B; 473C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 364C; 379C (*ir*)
Aldrich Library of NMR Spectra, **2**, 2A
Hofmann, A.W. *et al., Ber.*, 1882, **15**, 762 (*synth*)
Iffland, D.C. *et al., J.A.C.S.*, 1952, **74**, 6284 (*synth*)
Nagasawa, A. *et al., CA*, 1966, **65**, 15213 (*synth*)
Faure, R. *et al., Org. Magn. Reson.*, 1980, **14**, 20 (*cmr*)
Colosimo, M. *et al., Org. Mass Spectrom.*, 1982, **17**, 286 (*ms*)
Durig, J.R. *et al., J. Raman Spectrosc.*, 1989, **20**, 311 (*ir, Raman*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 369 (*rev*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 120

4-Propyl-1,2-benzenediol, 9CI P-524

[2525-02-2]

4-Propylpyrocatechol, 8CI. 4-Propylcatechol



$C_9H_{12}O_2$ 152.193

Prisms (C_6H_6). Mp 60°. Bp_{30} 175-180°.

2-Me ether: [2785-87-7] *2-Methoxy-4-propylphenol, 9CI. Cerulignol. Dihydroeugenol. Propylguaiacol. Coerulignol. FEMA 3598*
$C_{10}H_{14}O_2$ 166.219
Flavouring ingredient. Liq. Bp 240-241° $Bp_{0.7}$ 80-82°. n_D^{25} 1.5200.

▶ Skin irritant. LD_{50} (rat, orl) 2600 mg/kg. LD_{50} (rbt, skn) 310 mg/kg. SL8050000

Di-Me ether: [5888-52-8] *1,2-Dimethoxy-4-propylbenzene. 4-Propylveratrole*
$C_{11}H_{16}O_2$ 180.246
Oil. Bp 247° Bp_4 112-114°.

▶ CZ7178000

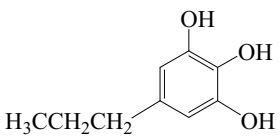
[58539-27-8, 89266-70-6]

Claisen, L. *et al., Annalen*, 1926, **449**, 81-101 (*2-Me ether*)
Tsukervarik, I.P. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1947, **17**, 1009 (*synth*)
Zbiral, E. *et al., Monatsh. Chem.*, 1961, **92**, 654-666 (*synth*)
Katritzky, A.R. *et al., Synthesis*, 1994, 499-504 (*di-Me ether, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 463 (*2-Me ether*)
Hu, T.Q. *et al., Can. J. Chem.*, 1997, **75**, 1234-1239 (*Me ethers, synth, ir, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1703-1704 (*2-Me ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFM750

5-Propyl-1,2,3-benzenetriol, 9CI P-525

[198203-80-4]

5-Propylpyrogallol. Hydroxydivarin



$C_9H_{12}O_3$ 168.192

Mp 78°.

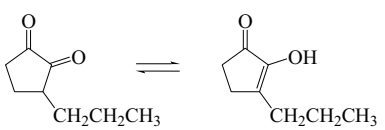
1,3-Di-Me ether: [6766-82-1] *2,6-Dimethoxy-4-propylphenol. FEMA 3729*
$C_{11}H_{16}O_3$ 196.246
Component of smoked food flavourings. Present in Japanese smoked, dried fish products esp. Katsuobushi and smoked bacon. $Bp_{0.38}$ 115°.

Mauthner, F. *et al., J. Prakt. Chem.*, 1926, **112**, 268-272 (*synth*)
Knowles, M.E. *et al., J. Sci. Food Agric.*, 1975, **26**, 189-196 (*1,3-di-Me ether, occur*)
Sakakibara, H. *et al., Agric. Biol. Chem.*, 1990, **54**, 9-16 (*1,3-di-Me ether, occur, fish*)
Angle, S.R. *et al., J.O.C.*, 1992, **57**, 5937-5947 (*1,3-di-Me ether, synth*)
Guillen, M.D. *et al., J. Agric. Food Chem.*, 1995, **43**, 463-468 (*1,3-di-Me ether, occur, smoke flavouring*)

3-Propyl-1,2-cyclopentanedione P-526

[25684-04-2]

2-Hydroxy-3-propyl-2-cyclopenten-1-one, 9CI



$C_8H_{12}O_2$ 140.182

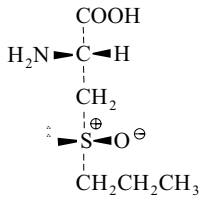
Aroma constit. of Arabica coffee. Cryst. (EtOAc/petrol) with sweet-burnt odour. Mp 56-57°. $Bp_{0.1}$ 75-80°.

Stetter, H. *et al., Tet. Lett.*, 1980, **21**, 3479-3482 (*synth*)
Arnarp, J. *et al., Acta Chem. Scand., Ser. B*, 1986, 839-854 (*occur, synth, ms, pmr*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*occur, ms*)

S-Propylcysteine sulfoxide P-527

[17795-24-3]

3-(Propylsulfinyl)alanine, 9CI. Dihydroalliin. β-Propylsulfenylalanine. ***Propiin***



$(R)_C,(R)_S$ *-form*

$C_6H_{13}NO_3S$ 179.24

$(R)_C(R)_S$-*form* [17935-27-2]
Occurs free in onion bulbs (*Allium cepa*). Mp 161-162°. $[\alpha]_D$ -11 (H_2O). $[\alpha]_D$ -30.9 (c, 1.25 in H_2O).

N-*(2,4-Dinitrophenyl):*
Mp 152-153°. $[\alpha]_D$ -223 (AcOH).

$(R)_C(S)_S$-*form* [17935-26-1]
Constit. of onions (*Allium cepa*) and other *Allium* spp.. Mp 164-168° dec. $[\alpha]_D$ +25 (c, 1.25 in H_2O) (+31.7, +33).

N-*(2,4-Dinitrophenyl):*
Mp 155°. $[\alpha]_D$ -133 (c, 0.247 in AcOH).

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1959, **13**, 1898
Carson, J.F. *et al., J.O.C.*, 1961, **26**, 4997 (*synth*)
Barnsley, E.A. *et al., Tetrahedron*, 1968, **24**, 3747 (*synth, abs config*)
Nishimura, H. *et al., Tetrahedron*, 1972, **28**, 4503 (*ms*)
Freeman, G.C. *et al., Phytochemistry*, 1976, **15**, 521 (*synth*)
Kubec, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 428-433 (*occur*)

2-Propylfuran P-528

[4229-91-8]



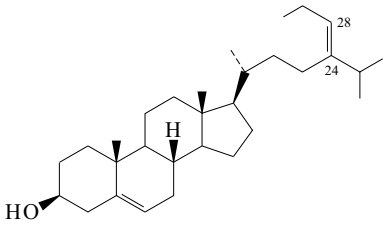
$C_7H_{10}O$ 110.155

Constit. of volatile components of heated peanut oil, apricot, plum and carob bean (*Ceratonia siliqua*). Liq. Bp 114-115°.

Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223-2235 (*ms*)
Gouesnard, J.P. *et al., Bull. Soc. Chim. Fr.*, 1969, 4452-4456 (*synth*)
Ibragimov, I.I. *et al., Khim. Geterotsikl. Soedin.*, 1973, **9**, 1434-1435; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1973, **9**, 1300 (*synth*)
Akimoto, I. *et al., Synthesis*, 1979, 146-147 (*synth*)
Lissi, E.A. *et al., J. Phys. Chem.*, 1980, **84**, 251-255 (*synth*)
Camus, F. *et al., Synth. Commun.*, 1982, **12**, 647-650 (*synth*)
MacLeod, G. *et al., Phytochemistry*, 1992, **31**, 3113-3119 (*occur*)
Chung, T.Y. *et al., J. Agric. Food Chem.*, 1993, **41**, 1467-1470 (*occur*)
Gomez, E. *et al., J. Agric. Food Chem.*, 1993, **41**, 1669-1676 (*occur*)

24-Propylidenecholest-5-en-3-ol P-529

28-Ethylergosta-5,24(28)-dien-3-ol



(3β,24(28)*E*)*-form*

$C_{30}H_{50}O$ 426.724

(3β,24(28)*E*)-*form* [59168-99-9]
24-Propylidenecholesterol
Cryst. (MeOH). Mp 108-110°. $[\alpha]_D^{20}$ -40 (c, 0.29 in $CHCl_3$).

5α,6-Dihydro: [75373-62-5] ***24-Propylidenecholestan-3-ol***
$C_{30}H_{52}O$ 428.74

*24*R*,28-Dihydro:* [64997-52-0] *24-Propylcholest-5-en-3-ol.* ***24-Propylcholesterol***
$C_{30}H_{52}O$ 428.74

5α,6,24ξ,28-Tetrahydro: [117675-19-1] ***24-Propylcholestan-3-ol***
$C_{30}H_{54}O$ 430.756
Constit. of the edible scallop *Trochostoma orientale*.

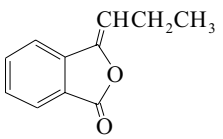
(3β,24(28)*Z*)-*form* [35339-71-0]
29-Methylisofucosterol
Constit. of the edible scallop *Trochostoma orientale*. Cryst. (EtOH). Mp 111-112°. $[\alpha]_D^{20}$ -27 ($CHCl_3$).

Idler, D.R. *et al., Steroids*, 1971, **18**, 545 (*isol*)
Rohmer, M. *et al., Steroids*, 1980, **35**, 219 (*isol*)
Giner, J.-L. *et al., J.A.C.S.*, 1991, **113**, 1386 (*biosynth*)
Stonik, V.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1998, **120**, 337-347 (*isol, ms*)
Giner, J.-L. *et al., Tetrahedron*, 2000, **56**, 9575-9580 (*synth, abs config*)

3-Propylidene-1(3*H*)-isobenzofuranone, 9CI P-530

[17369-59-4]

3-Propylidenephthalide. FEMA 2952



$C_{11}H_{10}O_2$ 174.199

Flavouring ingredient. Liq. with spicy herbaceous flavour. Bp_{15} 173-175° Bp_4 146-149°.

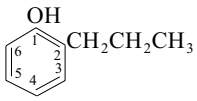
▶ Skin irritant. LD_{50} (rat, orl) 1650 mg/kg. NP7235000

Mowry, D.T. *et al., J.A.C.S.*, 1949, **71**, 120-122 (*synth*)
Tatsuo, K. *et al., Yakugaku Zasshi*, 1953, **73**, 336-338; *CA*, **48**, 2661g (*synth*)
Arcus, C.L. *et al., J.C.S.*, 1956, 1627-1633 (*synth*)
Knight, D.W. *et al., J.C.S. Perkin 1*, 1975, 635-640 (*synth, ir, pmr, ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 865; *CA*, **91**, 216638s (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PNO500

2-Propylphenol, 9CI P-531

[644-35-9]

1-Hydroxy-2-propylbenzene. 1-(2-Hydroxyphenyl)propane. FEMA 3522



$C_9H_{12}O$ 136.193

Flavouring ingredient. Oil. d_{15}^{15} 1. Bp 220-220.5°. pK_{a1} 10.47 (25°).

▶ LD_{50} (rat, orl) 500 mg/kg. SM8600000

Phenylurethane:
Needles (formic acid). Mp 111°.

Me ether: [13629-73-7] *1-Methoxy-2-propylbenzene.* o-*Propylanisole*
$C_{10}H_{14}O$ 150.22
$Bp_{757.700012}$ 207-209°.

Et ether:1-Ethoxy-2-propylbenzene. o-*Propylphenetole*
$C_{11}H_{16}O$ 164.247
Bp_{754} 213° Bp_{16} 99-100°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1069D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 244A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1001D (*ir*)
Farinholt, L.H. *et al., J.A.C.S.*, 1933, **55**, 3386 (*synth*)
Adv. Chem. Ser., 1955, **15**, 286 (***props***)
Yamamoto, O. *et al., Anal. Chem.*, 1972, **44**, 1794 (*nmr*)
Japan. Pat., 1972, 72 48 311; *CA*, **80**, 60966f (*use*)
Cabiddu, S. *et al., J. Organomet. Chem.*, 1975, **88**, 129 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 703
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2371-2372
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PNS250

4-Propylphenol, 9CI P-532

[645-56-7]

1-Hydroxy-4-propylbenzene. 1-(4-Hydroxyphenyl)propane. FEMA 3649

$C_9H_{12}O$ 136.193

Flavouring ingredient. Cryst. d_4^0 1.09. Mp 21-22°. Bp 230-232° Bp_{19} 120°. pK_{a1} 10.34 (20°).

▶ LD_{50} (rat, orl) 500 mg/kg. SM8610000

Phenylurethane:
Cryst. (EtOH). Mp 128.5-129°.

Ac: [61824-46-2]
$C_{11}H_{14}O_2$ 178.23
Bp_{745} 245-246°.

Benzoyl:
$C_{16}H_{16}O_2$ 240.301
Mp 37-38°.

Me ether: [104-45-0] *1-Methoxy-4-propylbenzene, 9CI. 4-Propylanisole, 8CI.*

FEMA 2930
$C_{10}H_{14}O$ 150.22
Flavouring ingredient. Present in dried bonito (Katsuobishi), capers (*Caparis spinosa*), aniseed (*Pimpinella anisum*), leaf oil of apple mint (*Mentha rotundifolia*) and flower honeys. Liq. with anise odour. Bp 215-216° Bp_{10} 86.5°.

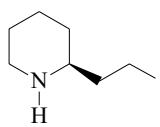
▶ BZ9450000

Et ether:1-Ethoxy-4-propylbenzene. 4-Propylphenetole
$C_{11}H_{16}O$ 164.247
Bp 223-230° Bp_{13} 108-110°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1076B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 251B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1008C (*ir*)
Baranger, P.M. *et al., Bull. Soc. Chim. Fr.*, 1931, **49**, 1213
Farinholt, L.H. *et al., J.A.C.S.*, 1933, **55**, 3386 (*synth*)
Adv. Chem. Ser., 1955, **15**, 288 (***props***)
Yamamoto, O. *et al., Anal. Chem.*, 1972, **44**, 1794 (*nmr*)
Hastbacka, K. *et al., CA*, 1973, **79**, 7013 (*synth*)
Matas, M. *et al., CA*, 1976, **85**, 94052 (*synth*)
Sangster, S.A. *et al., Food Chem. Toxicol.*, 1983, **21**, 263-271 (*Me ether, metab, tox*)
Lau, C.K. *et al., J.O.C.*, 1986, **51**, 3038-3043 (*Me ether, synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 691; 704
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2339; 2372
Pino, J.A. *et al., J. Essent. Oil Res.*, 1999, **11**, 241-242 (*Me ether, occur*)
Kollmannsberger, H. *et al., Adv. Food Sci.*, 2000, **22**, 47-61 (*Me ether, occur*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1534-1535 (*Me ether*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PNE250; PNS500

2-Propylpiperidine P-533

Coniine. *Cicutine. Conicine*



(*R*)-form

$C_8H_{17}N$ 127.229
The first alkaloid to be synthesised.The alkaloid (and its *N*-Me deriv.) from *Conium maculatum* are largely racemic but opt. active forms can be obt. from residues.

(*R*)-*form* [5985-99-9]
Bp 166.5°. $[\alpha]_D$ -15.6.

Hydrochloride: [88057-03-8]
Mp 220-221° (214-215°). $[\alpha]_D^{20}$ -6.8 (c,3.5 in EtOH).

Hydrobromide:
Mp 205°.

N-*Me:***N-*Methyl-(-)-coniine***
Oil. Mp 175-176°. $[\alpha]_D^{20}$ -81.9.

N-*Me; hydrochloride:*
Mp 189-190°.

(*S*)-*form* [458-88-8]
Alkaloid of *Amorphophalus rivieri* (devil's tongue). d_4^{23} 0.84. Mp -2°. Bp 166-167°. $[\alpha]_D$ +15.7 (neat). $[\alpha]_D$ +8 (c, 4 in $CHCl_3$). n_D^{23} 1.4537.

▶ Exp. teratogen. LD_{50} (mus, orl) 100 mg/kg. TN3730000

Hydrochloride:
Rhomboids. Mp 220°.

Hydrobromide:
Mp 207°.

Picrate:
Mp 75°.

N-*Me:* [35305-13-6] **N-*Methyl-(+)-coniine***
$C_9H_{19}N$ 141.256
Bp_{757} 173-174°. $[\alpha]_D^{23}$ +82.4.

N-*Me; hydrochloride:*
Mp 192-193° (188-189°). $[\alpha]_D$ +27.8.

N-*Di-Me:***N,N-*Dimethyl-(+)-coniine***
$C_{10}H_{22}N^{\oplus}$ 156.291
$[\alpha]_D^{24}$ +7.5 (c, 0.1 in MeOH).

(±)-*form* [3238-60-6]
Bp 166° Bp_{70} 93°. pK_a 16 (25°,NH, aq. KOH).

Hydrochloride: [15991-59-0]
Mp 216-217° (211°).

N-*Me:*
Bp 175.5° Bp_{13} 61-63°.

N-*Me; hydrochloride:*
Needles (Me_2CO). Mp 168-168.5°.

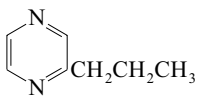
N-*Me; picrate:*
Mp 112-114°.

[553-75-3]

Giesecke, *et al., Arch. Pharm. (Weinheim, Ger.)*, 1827, **20**, 97 (*isol*)
Hofmann, A.W. *et al., Ber.*, 1884, **17**, 825 (*struct*)
Ladenburg, A. *et al., Ber.*, 1886, **19**, 2578; 1894, **27**, 3062 (*synth, resoln*)
Wolffenstein, R. *et al., Ber.*, 1894, **27**, 2611 (*isol, deriv*)
Ahrens, F.B. *et al., Ber.*, 1902, **35**, 1330 (*isol, deriv*)
Chemnitius, F. *et al., J. Prakt. Chem.*, 1928, **118**, 25 (*isol*)
Fairbairn, J.W. *et al., Phytochemistry*, 1961, **1**, 38
Weitkamp, H. *et al., Chem. Ber.*, 1962, **95**, 2896 (*pmr*)
Leete, E. *et al., J.A.C.S.*, 1970, **92**, 3835 (*biosynth*)
Craig, J.C. *et al., J.O.C.*, 1971, **36**, 3648 (*resoln*)
Roberts, M.F. *et al., Phytochemistry*, 1974, **13**, 1841 (*biosynth*)
Aketa, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 621 (*synth*)
Kondrat, R.W. *et al., Science (Washington, D.C.)*, 1978, **199**, 978 (*ms*)
Astier, A. *et al., Tet. Lett.*, 1978, 2051 (*synth*)
Craig, J.C. *et al., Tetrahedron*, 1978, **34**, 501 (*abs config*)
Guerrier, L. *et al., J.A.C.S.*, 1983, **105**, 7754 (*synth*)
Husson, H.P. *et al., Youji Huaxue*, 1987, 314; *CA*, **109**, 73693g (*synth*)
Nagasaka, T. *et al., Heterocycles*, 1988, **27**, 1685 (*synth, ir, pmr*)
Teng, T.-F. *et al., Heterocycles*, 1990, **31**, 1201 (*synth*)
Kiguchi, T. *et al., Heterocycles*, 1990, **31**, 1525 (*synth*)
Higashiyama, K. *et al., Heterocycles*, 1992, **33**, 17 (*synth*)
Ito, M. *et al., Tet. Lett.*, 1992, **33**, 3765 (*synth*)
Enders, D. *et al., Annalen*, 1993, 173 (*synth*)
Al-awar, R.S. *et al., J.O.C.*, 1993, **58**, 7732 (*synth*)
Hattori, K. *et al., Tetrahedron*, 1993, **49**, 1749 (*synth*)
Hirai, Y. *et al., Chem. Lett.*, 1994, 21 (*synth*)
Amat, M. *et al., Tet. Lett.*, 1994, **35**, 2223 (*synth*)
Kim, Y.H. *et al., Tet. Lett.*, 1996, **37**, 5543 (*synth*)
Weymann, M. *et al., Synthesis*, 1997, 1151-1160 (*synth*)
Reding, M.T. *et al., J.O.C.*, 1998, **63**, 6344-6347 (*synth*)
Jo, E. *et al., Tet. Lett.*, 1999, **40**, 5581-5582 (*synth, N-Boc-coniine*)
Wilkinson, T.J. *et al., Org. Lett.*, 2000, **2**, 155-158 (*synth*)
Blitzke, T. *et al., Phytochemistry*, 2000, **55**, 979-982 (*N-Dimethylconiine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PNT000

Propylpyrazine P-534

[18138-03-9]
FEMA 3961



$C_7H_{10}N_2$ 122.169
Found in roasted coffee. Used in food flavouring. Bp_{12} 65°. n_D^{20} 1.4934.

N^1-*Oxide:* [85093-86-3]
$C_7H_{10}N_2O$ 138.169
Bp_{37} 150-160°.

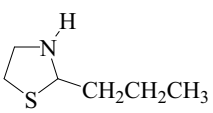
N^4-*Oxide:* [85093-87-4]
$C_7H_{10}N_2O$ 138.169
Bp_{36} 160-165°.

N^1,N^4-*Dioxide:* [85093-88-5]
$C_7H_{10}N_2O_2$ 154.168
Prisms (C_6H_6). Mp 195.5-196.5°.

Behun, J.D. *et al., J.O.C.*, 1961, **26**, 3379
Konakahara, T. *et al., Heterocycles*, 1979, **12**, 373
Ohta, A. *et al., J. Het. Chem.*, 1982, **19**, 1061 (*uv, pmr, ms*)

2-Propylthiazolidine, 9CI P-535

[24050-10-0]
Tetrahydro-2-propylthiazole



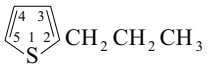
$C_6H_{13}NS$ 131.241

(±)-*form*
Flavouring ingredient. Liq. d^{20} 0.98. Bp_{20} 92-93°. n_D^{20} 1.5047.

Bergmann, E.D. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1959, **78**, 289-314 (*synth*)
Jondeur, R. *et al., Bull. Soc. Chim. Fr.*, 1964, 2493-2499 (*synth*)
Ger. Pat., 1974, 2 333 581; *CA*, **80**, 95930s (*use*)
U.S. Pat., 1977, 4 011 233; *CA*, **87**, 23264z (*use*)
Yasuhara, A. *et al., Agric. Biol. Chem.*, 1989, **53**, 2273-2274 (*synth, pmr, ms*)

2-Propylthiophene P-536

[1551-27-5]



$C_7H_{10}S$ 126.222
Present in roast beef aroma. Liq. d_{20}^{20} 0.97. Bp 158.5° Bp_{50} 70°. n_D^{20} 1.5048.

Steinkopf, W. *et al., Annalen*, 1921, **424**, 21
Scheibler, H. *et al., Ber.*, 1921, **54**, 149
Adv. Chem. Ser., 1955, **15**, 192 (***props***)
Treshkova, E.G. *et al., Zh. Fiz. Khim.*, 1964, **38**, 295 (*ir, uv, Raman*)
Sotoyama, T. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 1865 (*synth, ir, pmr*)
Högberg, H.-E. *et al., J.O.C.*, 1992, **57**, 2052 (*synth*)

1-(Propylthio)-1-propanethiol, 9CI P-537

[53897-64-6]
2-Mercaptodipropyl sulfide
$H_3CCH_2CH(SH)SCH_2CH_2CH_3$
$C_6H_{14}S_2$ 150.309

(±)-*form*
Liq. with allium-blackcurrant odour. Bp_3 42°. n_D^{20} 1.5033.

(ξ)-*form*
Constit. of onion volatiles. Formed by reaction of propanol, H_2S and 1-propanethiol.

Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*isol, ms*)
Farkas, P. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 459-462 (*occur, onion*)

5-Propyltridecane P-538

[55045-11-9]
$H_3C(CH_2)_7CH(CH_2CH_2CH_3)(CH_2)_3CH_3$
$C_{16}H_{34}$ 226.445
Constit. of the essential oils of hops (*Humulus lupulus*).

Liu, G. *et al., CA*, 1987, **107**, 64624s (*isol*)
Tan, L. *et al., CA*, 1993, **118**, 77081q (*isol*)

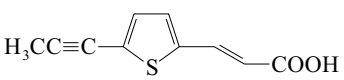
6-Propyltridecane P-539

[55045-10-8]
$H_3C(CH_2)_6CH(CH_2CH_2CH_3)(CH_2)_4CH_3$
$C_{16}H_{34}$ 226.445
Constit. of the esential oil of the peel of *Juglans nigra* (black walnut).

Buchbauer, G. *et al., J. Essent. Oil Res.*, 1992, **4**, 539 (*occur*)

3-[5-(1-Propynyl)-2-thienyl]-2-propenoic acid P-540

5-(1-Propynyl)-2-thienylacrylic acid



(*E*)-*form*

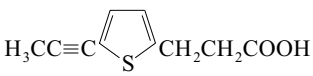
$C_{10}H_8O_2S$ 192.238

(*E*)-*form*
Me ester:
Needles. Mp 77°.

(*Z*)-*form*
Me ester:
$C_{11}H_{10}O_2S$ 206.265
Isol. from *Tanacetum vulgare* (tansy). Prisms (hexane). Mp 101°.

Guddal, E. *et al., Acta Chem. Scand.*, 1959, **13**, 1185 (*isol, struct*)
Skatteböl, L. *et al., Acta Chem. Scand.*, 1959, **13**, 1460 (*synth*)
Bohlmann, F. *et al., Chem. Ber.*, 1960, **93**, 1937; 1965, **98**, 1616 (*isol, uv*)
Schulte, K.E. *et al., Tet. Lett.*, 1965, 659 (*biosynth*)

5-(1-Propynyl)-2-thiophenepropanoic acid, 9CI P-541



$C_{10}H_{10}O_2S$ 194.254

Me ester: [67901-30-8]
$C_{11}H_{12}O_2S$ 208.281
Isol. from *Artemisia absinthium* (wormwood) root.

Greger, H. *et al., Phytochemistry*, 1978, **17**, 806 (*isol, pmr, struct*)

Protein R P-542

Protein. MW approx. 23 kDa. Isol. from barley grain (*Hordeum vulgare*). Shows antifungal activity.

Hejgaard, J. *et al., FEBS Lett.*, 1991, **291**, 127-131 (*isol*)

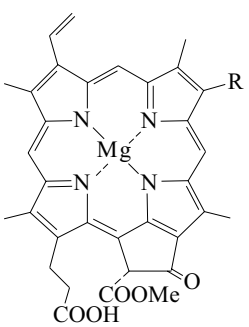
Brassica oleracea Proteinase inhibitors P-543

Six proteins, Mw 9000-25000. Proteinase inhibitors isol. from cabbage foliage (*Brassica oleracea*).

Broadway, R.M. *et al., Phytochemistry*, 1993, **33**, 21-27 (*isol*)

Protochlorophyllide P-544

[14751-08-7]
Magnesium 2,4-divinylphaeoporphyrin a_5 monomethyl ester. Divinyl protochlorophyllide. Monovinyl protochlorophyllide



R = CH=CH_2 or CH_2CH_3

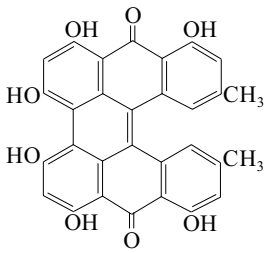
$C_{35}H_{30}MgN_4O_5$ 610.951
Mol. formula given is for divinyl compd., R = CH =CH_2. Isol. from the seed husks of *Cucurbita pepo*. Violet-red solid.

Phytyl ester:Protochlorophyll a. Trichosanthin†
$C_{55}H_{68}MgN_4O_5$ 889.471
Dark green substance.

Fischer, F.G. *et al., Annalen*, 1959, **627**, 35
Jones, O.T.G. *et al., Biochem. J.*, 1963, **88**, 335; **89**, 182; 1966, **101**, 153
Ricketts, T.R. *et al., Phytochemistry*, 1966, **5**, 223 (*isol*)
Shioi, Y. *et al., Arch. Biochem. Biophys.*, 1983, **220**, 286
Shioi, Y. *et al., Biochim. Biophys. Acta*, 1983, **722**, 72
Wu, S.M. *et al., Tetrahedron*, 1984, **40**, 659 (*nmr, ms*)
Wong, Y.S. *et al., Plant Physiol.*, 1985, **79**, 725; 730 (*biosynth*)

Protohypericin P-545

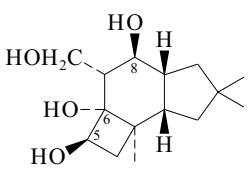
[548-03-8]



$C_{30}H_{18}O_8$ 506.467
Isol. from *Hypericum perforatum* (St. John's Wort). Deep violet solid. Mp 300°. λ_{max} 290 (ε 34000); 340 (ε 26000); 465 (ε 11500); 600 (ε 18500); 640 (ε 22500) (DMSO as potassium salt) (Derep). λ_{max} 384 (ε 12100); 446 (ε 12900); 472 (ε 13800); 509 (ε 10000); 546 (ε 24700); 589 (ε 43600) (MeOH as potassium salt) (Derep). λ_{max} 292 (ε 34000); 340 (ε 26500); 377 (ε 12000); 475 (ε 13500); 509 (ε 10000); 560 (ε 24000); 607 (ε 44000) (DMSO) (Derep).

Brockmann, H. *et al., Chem. Ber.*, 1958, **91**, 547 (*isol*)
Banks, H.J. *et al., Aust. J. Chem.*, 1976, **29**, 1509 (*isol, pmr, synth*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1976, **29**, 1535 (*synth*)
Spitzner, D. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 46 (*synth*)
Pizzolatti, M.G. *et al., Phytochemistry*, 2000, **55**, 819-822 (*isol, cmr*)

5,6,8,14-Protoilludanetetrol P-546



$C_{15}H_{26}O_4$ 270.368

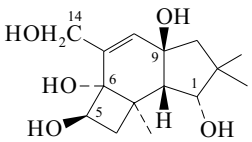
(5β,6α,7α,8β)-*form*
5-(2,4-Dihydroxy-6-methylbenzoyl):
[126006-69-7] ***Armillane***. *Armillarizin*
$C_{23}H_{32}O_7$ 420.502
Metab. of *Armillaria mellea* (honey mushroom). Cryst. (EtOAc/hexane). Sol. MeOH, hexane; poorly sol. H_2O. Mp 195-197° Mp 241-244°. $[\alpha]_D^{20}$ -59 (c,

0.2 in MeOH). $[\alpha]_D^{28}$ -93.5 (c, 0.023 in $CHCl_3$). λ_{max} 229 (ϵ 26610); 267 (ϵ 11313); 298 (ϵ 5157) (MeOH) (Berdy).

Yang, J.S. *et al., Chin. Chem. Lett.*, 1990, **1**, 173; *CA*, **115**, 110168m (*isol, pmr, cmr*)

Donnelly, D.M.X. *et al., Phytochemistry*, 1990, **29**, 179 (*isol, pmr, cmr*)

7-Protoilludene-1,5,6,9,14-pentol P-547



$C_{15}H_{24}O_5$ 284.352

(1α,5β)-*form*

5-(2,4-Dihydroxy-6-methylbenzoyl): [103847-14-9] ***Melledonol***
$C_{23}H_{30}O_8$ 434.485
Prod. by *Armillaria mellea* (honey mushroom). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 216-218°. $[\alpha]_D^{21}$ +44.6 (c, 1 in MeOH).

5-(2-Hydroxy-4-methoxy-6-methylbenzoyl): [101901-56-8] ***Melleolide C***
$C_{24}H_{32}O_8$ 448.512
Prod. by *Armillaria mellea* (honey mushroom). Cryst. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 78-80°. $[\alpha]_D$ +27.9 (c, 0.5 in $CHCl_3$). 9-Config. undefined but prob. as shown λ_{max} 264 (ϵ 14500); 303 (ϵ 6150) (EtOH) (Berdy).

5-(3-Chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [101922-80-9] ***Melleolide D***
$C_{24}H_{31}ClO_8$ 482.957
From *Armillaria mellea* (honey mushroom). Cryst. (CH_2Cl_2/hexane). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 96-98°. λ_{max} 266 ; 305 (MeOH) (Berdy). λ_{max} 303 (ϵ 6150) (EtOH) (Berdy).

14-Aldehyde, 5-(3-chloro-4,6-dihydroxy-2-methylbenzoyl): [117458-36-3] ***Melledonal B***
$C_{23}H_{27}ClO_8$ 466.914
From *Armillaria mellea* (honey mushroom). Cryst (EtOAc/hexane). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 228-232°. $[\alpha]_D$ +101 (c, 0.1 in MeOH). λ_{max} 213 (ϵ 32600); 257 (ϵ 11300); 306 (ϵ 6000) (EtOH) (Berdy).

14-Aldehyde, 5-(2-hydroxy-4-methoxy-6-methylbenzoyl):5′-O-Methylmelledonal
$C_{24}H_{30}O_8$ 446.496
Metab. of *Armillaria mellea* (honey mushroom). Cryst. Mp 170-171°. $[\alpha]_D^{25}$ +64.7 (c, 0.34 in MeOH).

14-Aldehyde, 5-(2,4-dihydroxy-6-methylbenzoyl): [103847-15-0] ***Melledonal***. *Melledonal A*
$C_{23}H_{28}O_8$ 432.469
Prod. by *Armillaria mellea* (honey mushroom). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 136-137°. $[\alpha]_D^{21}$ +195.3 (c, 0.1 in MeOH). λ_{max} 214 (ϵ 27500); 260 (ϵ 13800); 268 (ϵ 5700) (EtOH) (Berdy). λ_{max} 238 (E1%/1cm 625); 280 (E1%/1cm 161); 561 (E1%/1cm 202); 600 (E1%/1cm 169) (MeOH-NaOH) (Berdy).

14-Aldehyde, 5-(3-chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [117458-35-2] ***Melledonal C***
$C_{24}H_{29}ClO_8$ 480.941
Metab. of *Armillaria mellea* (honey mushroom). Cryst. (EtOAc/hexane). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 200-205°. $[\alpha]_D$ +121 (c, 0.1 in MeOH). λ_{max} 214 (ϵ 29300); 257 (ϵ 9300); 304 (ϵ 4000) (EtOH) (Berdy).

14-(2-Hydroxy-4-methoxy-6-methylbenzoyl): [117458-32-9] ***Armellide A***
$C_{24}H_{32}O_8$ 448.512
Glass. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 80-82°. $[\alpha]_D$ -18.4 (c, 0.1 in $CHCl_3$). λ_{max} 212 (ϵ 20000); 252 (ϵ 7000); 300 (ϵ 3600) (MeOH) (Berdy).

14-(3-Chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [117458-31-8] ***Armellide B***
$C_{24}H_{31}ClO_8$ 482.957
Oil. Sol. MeOH, EtOAc; poorly sol. H_2O. $[\alpha]_D$ +66 (c, 0.05 in $CHCl_3$). λ_{max} 300 (MeOH) (Berdy).

Donnelly, D.M.X. *et al., Tet. Lett.*, 1985, **26**, 5343 (*isol, struct, derivs*)

Arnone, A. *et al., Phytochemistry*, 1986, **25**, 471 (*Melleolides*)

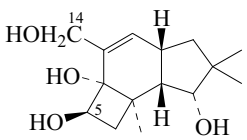
Donnelly, D.M.X. *et al., Phytochemistry*, 1987, **26**, 3075 (*deriv*)

Arnone, A. *et al., Gazz. Chim. Ital.*, 1988, **118**, 517 (*bibl*)

Arnone, A. *et al., Gazz. Chim. Ital.*, 1988, **118**, 523 (*Amellides*)

Arnone, A. *et al., J.C.S. Perkin 1*, 1988, 301; 503 (*isol, pmr, cmr, cryst struct, Melledonals*)

7-Protoilludene-1,5,6,14-tetrol P-548



$C_{15}H_{24}O_4$ 268.352

(1α,5β,6α)-*form*

5-(2,4-Dihydroxy-6-methylbenzoyl): [117258-73-8] ***Melleolide E***
$C_{23}H_{30}O_7$ 418.486
Metab. of *Armillaria mellea* (honey mushroom). Oil. $[\alpha]_D$ +17.9 (c, 0.05 in $CHCl_3$).

5-(2-Hydroxy-4-methoxy-6-methylbenzoyl): [101901-55-7] ***Melleolide B***
$C_{24}H_{32}O_7$ 432.513
Metab. of *Armillaria mellea* (honey mushroom). Glass. Sol. MeOH, EtOAc. Mp 42-45°. $[\alpha]_D$ +19.6 (c, 0.6 in MeOH). λ_{max} 264 (ϵ 14500); 303 (ϵ 6150) (EtOH) (Berdy).

5-(3-Chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [117458-34-1] ***Melleolide I***
$C_{24}H_{31}ClO_7$ 466.957
Cryst. (CH_2Cl_2/hexane). Sol. MeOH, Et_2O, EtOAc; poorly sol. H_2O. Mp 187-189°. $[\alpha]_D$ +24.9 (c, 0.2 in $CHCl_3$). λ_{max} 208 (ϵ 25400); 258 (ϵ 9000); 305 (ϵ 4200) (MeOH) (Berdy).

5-(3-Chloro-4,6-dihydroxy-2-methylbenzoyl): ***Melleolide M***
$C_{23}H_{29}ClO_7$ 452.931
Metab. of *Armillariella mellea* (honey mushroom). Powder. Mp 89-92°. $[\alpha]_D^{24}$ +12 (c, 1 in MeOH). λ_{max} 212 (log ϵ 4.35); 264 (log ϵ 3.88); 310 (log ϵ 3.61) (MeOH).

14-(2,4-Dihydroxy-6-methylbenzoyl): [189342-41-4]
$C_{23}H_{30}O_7$ 418.486
Metab. of *Armillariella mellea* (honey mushroom). Cryst. Mp 205-207°. $[\alpha]_D^{20}$ -16.2 (c, 0.4 in MeOH).

14-Aldehyde, 5-(2,4-dihydroxy-6-methylbenzoyl): [130396-93-9] ***10-Hydroxymelleolide***
$C_{23}H_{28}O_7$ 416.47
Metab. of *Armillariella mellea* (honey mushroom). The different 6-config. (4-config. in the paper) is not commented on and is poss. a drawing error.

14-Aldehyde, 5-(2-hydroxy-4-methoxy-6-methylbenzoyl): [117240-47-8] ***Melleolide H***. *Armillarigin*
$C_{24}H_{30}O_7$ 430.497
Metab. of *Armillariella mellea* (honey mushroom). Cryst. Mp 114-116°. $[\alpha]_D$ +65.4 (c, 0.05 in $CHCl_3$). $[\alpha]_D^{26}$ +186 (c, 0.2 in $CHCl_3$). Armillarigin assigned incorrect struct. in CA.

14-Aldehyde, 5-(3-chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [117458-33-0] ***Melleolide J***. *Armillarikin*
$C_{24}H_{29}ClO_7$ 464.942
Glass. Sol. MeOH, EtOAc, Et_2O; poorly sol. H_2O. Mp 195-197° (176-178°). $[\alpha]_D$ +62.6 (c, 0.2 in $CHCl_3$). $[\alpha]_D^{14}$ +174 (c, 0.04 in $CHCl_3$). λ_{max} 212 (ϵ 31000); 255 (ϵ 11000); 305 (ϵ 4700) (MeOH) (Berdy).

14-Aldehyde, 5-(3-chloro-4,6-dihydroxy-2-methylbenzoyl): [298702-67-7] ***Melleolide L***. *6′-Chloro-10α-hydroxymelleolide*
$C_{23}H_{27}ClO_7$ 450.915
Metab. of *Armillariella mellea* (honey mushroom). Cryst. Mp 123-125° (94-95°). $[\alpha]_D^{24}$ +98.7 (c, 1 in MeOH). λ_{max} 219 (log ϵ 4.38); 261 (log ϵ 3.93); 311 (log ϵ 3.63) (MeOH). λ_{max} 213 (log ϵ 4.43); 265 (log ϵ 4.13); 306 (log ϵ 3.7) (MeOH).

[125185-65-1]

Arnone, A. *et al., Phytochemistry*, 1986, **25**, 471-474 (*Melliolides B-D*)

Arnone, A. *et al., Gazz. Chim. Ital.*, 1988, **118**, 517-521; 523-527 (*Melliolides E-J*)

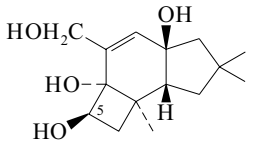
Yang, J.S. *et al., Planta Med.*, 1989, **55**, 479-481 (*Armillarikin, Armillarigin*)

Donnelly, D.M.X. *et al., Phytochemistry*, 1990, **29**, 179-182; 2569-2572; 1997, **44**, 1473-1478 (*isol, pmr, cmr, derivs*)

Momose, I. *et al., J. Antibiot.*, 2000, **53**, 137-143 (*Melleolide L, Melleolide M*)

Cremin, P. *et al., J.C.S. Perkin 1*, 2000, 2325-2329 (*6′-Chloro-10α-hydroxymelleolide*)

7-Protoilludene-5,6,9,14-tetrol P-549



$C_{15}H_{24}O_4$ 268.352

5β-*form*

5-(2,4-Dihydroxy-6-methylbenzoyl): [130396-92-8] ***13-Hydroxydihydromelleolide***
$C_{23}H_{30}O_7$ 418.486
Metab. of *Armillaria mellea* (honey mushroom). Cryst. Mp 112-114°. $[\alpha]_D^{21}$ +29 (c, 0.1 in MeOH).

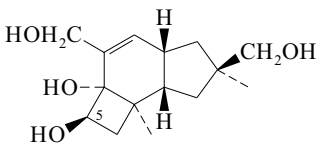
14-Aldehyde, 5-(2-hydroxy-4-methoxy-6-methylbenzoyl): [127500-59-8] ***Armillarilin***
$C_{24}H_{30}O_7$ 430.497
Metab. of *Armillaria mellea* (honey mushroom). Mp 179-180°. $[\alpha]_D^{14}$ +162 (c, 0.1 in $CHCl_3$).

14-Aldehyde, 5-(3-chloro-6-hydroxy-4-methoxy-2-methylbenzoyl): [127486-63-9] ***Armillarinin***
$C_{24}H_{29}ClO_7$ 464.942
Metab. of *Armillaria mellea* (honey mushroom). Mp 152-155°. $[\alpha]_D^{17}$ +153.6 (c, 0.1 in $CHCl_3$).

14-Aldehyde, 6-Me ether, 5-(2,4-dihydroxy-6-methylbenzoyl): [189342-39-0] *13-Hydroxy-4-*O*-methoxymelleolide (incorr.)*
$C_{24}H_{30}O_7$ 430.497
Cryst. Mp 205-206°. $[\alpha]_D^{20}$ +51.2 (c, 1.2 in MeOH).

Donnelly, D.M.X. *et al., Phytochemistry*, 1990, **29**, 2569; 1997, **44**, 1473-1478 (*isol, pmr, cmr, derivs*)
Yang, J.S. *et al., Yaoxue Xuebao*, 1990, **25**, 24 (*Armillarilin, Armillarinin*)

7-Protoilludene-5,6,13,14-tetrol P-550



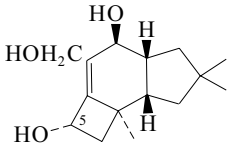
$C_{15}H_{24}O_4$ 268.352

(5β,6α)-*form*

5-(2-Hydroxy-4-methoxy-6-methylbenzoyl): [117258-75-0] ***Melleolide G***
$C_{24}H_{32}O_7$ 432.513
Metab. of *Armillaria mellea* (honey mushroom). Oil. $[\alpha]_D$ +19.6 (c, 0.05 in $CHCl_3$).

Arnone, A. *et al., Gazz. Chim. Ital.*, 1988, **118**, 517 (*isol, pmr, cmr*)

6-Protoilludene-5,8,14-triol P-551



(5α,8β)-*form*

$C_{15}H_{24}O_3$ 252.353

(5α,8β)-*form*

5-Epiarmillol
Oil. $[\alpha]_D^{20}$ -34.8 (c, 0.1 in MeOH). λ_{max} 200 (ϵ 4900); 228 (sh) (ϵ 2570); 265 (ϵ 1650); 273 (ϵ 1660) (no solvent reported) (Derep). λ_{max} 205 (ϵ 9370); 270 (sh) (ϵ 2960) (EtOH) (Derep). λ_{max} 235 (ϵ 4900); 270 (ϵ 3100) (EtOH) (Berdy).

(5β,8β)-*form* [82120-02-3]
Armillol
Oil. $[\alpha]_D^{20}$ -65.9 (c, 0.2 in MeOH). λ_{max} 200 (ϵ 4900); 228 (sh) (ϵ 2570); 265 (ϵ 1650); 273 (ϵ 1660) (no solvent reported) (Derep). λ_{max} 205 (ϵ 9370); 270 (sh) (ϵ 2960) (EtOH) (Derep). λ_{max} 205 (ϵ 9370); 270 (ϵ 2960) (EtOH) (Berdy).

*5-*O*-(2,4-Dihydroxy-6-methylbenzoyl):* [82105-51-9] ***Armillyl orsellinate***
$C_{23}H_{30}O_6$ 402.486
Metab. of *Armillaria mellea* (honey mushroom). Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 91-93°. $[\alpha]_D^{20}$ -126.9 (c, 1.1 in MeOH). λ_{max} 263 (ϵ 14400); 300 (ϵ 5820) (MeOH) (Derep).

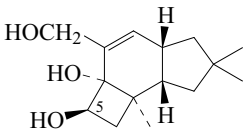
*5-*O*-(2-Hydroxy-4-methoxy-6-methylbenzoyl):* [102092-44-4] ***Armillyl everninate***
$C_{24}H_{32}O_6$ 416.513
Prod. by *Armillaria mellea* (honey mushroom). Cryst. (EtOAc/hexane). Mp 86-87°. $[\alpha]_D^{25}$ -66 (c, 0.79 in MeOH). λ_{max} 211 (ϵ 21250); 261 (ϵ 10990); 298 (ϵ 6000) (MeOH) (Berdy).

*5-*O*-(3-Chloro-6-hydroxy-4-methoxy-2-methylbenzoyl):* [102092-23-9] ***Arnamiol***
$C_{24}H_{31}ClO_6$ 450.958
From *Armillaria mellea* (honey mushroom). Cryst. (EtOAc/hexane). Mp 132-134°. $[\alpha]_D$ -91 (c, 0.79 in MeOH). λ_{max} 217 (ϵ 23000); 259 (ϵ 14450); 298 (ϵ 8500) (MeOH) (Berdy).

*5-*O*-(2,3,4- or 2,3,5-Trihydroxy-6-methylbenzoyl):* ***Judeol***
$C_{23}H_{30}O_7$ 418.486
Metab. of *Armillaria mellea* (honey mushroom). Amorph. solid. Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. λ_{max} 215 ; 263 ; 300 (MeOH) (Berdy).

Donnelly, D.M.X. *et al., Chem. Comm.*, 1982, 135-137; 1984, 222-223 (*Armillyl orsellinate, isol, struct, abs config*)
Donnelly, D.M.X. *et al., J. Nat. Prod.*, 1985, **48**, 10-16; 1986, **49**, 111-116 (*Armillyl everninate, Arnamiol*)
Arnone, A. *et al., Phytochemistry*, 1992, **31**, 2047-2050 (*5-Epiarmillol*)
Cremin, P. *et al., J.C.S. Perkin 1*, 2000, 2325-2329 (*Armillyl orsellinate, isol, activity*)

7-Protoilludene-5,6,14-triol P-552



$C_{15}H_{24}O_3$ 252.353

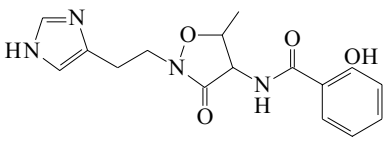
5β-*form*

5-(2,4-Dihydroxy-6-methylbenzoyl): [117258-74-9] ***Melleolide F***
$C_{23}H_{30}O_6$ 402.486
Metab. of *Armillaria mellea* (honey mushroom).

Momose, I. *et al., J. Antibiot.*, 2000, **53**, 137-143

Pseudomonine P-553

[172923-94-3]



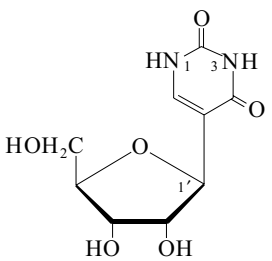
$C_{16}H_{18}N_4O_4$ 330.343
Alkaloid from cultures of *Pseudomonas fluorescens* AH2 isol. from spoiled Nile perch from Lake Victoria. Amorph. brownish solid. Sol. H_2O. $[\alpha]_D$ -80 (c, 0.041 in H_2O). λ_{max} 203 (ϵ 25118); 237 (ϵ 8912); 298 (ϵ 2291) (H_2O) (Berdy).

Anthoni, U. *et al., J. Nat. Prod.*, 1995, **58**, 1786 (*isol, uv, pmr, cmr, struct*)

Pseudouridine C P-554

[1445-07-4]

*5-β-D-Ribofuranosyl-2,4(1*H*,3*H*)-pyrimidinedione, 9CI. 5-β-D-Ribofuranosyluracil, 8CI. Pseudouridine. ψ-Uridine*



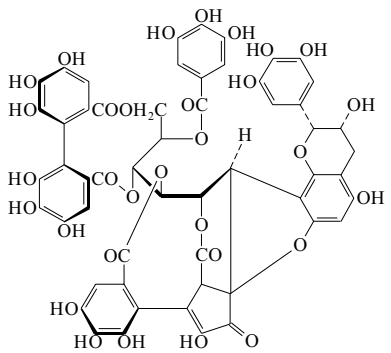
$C_9H_{12}N_2O_6$ 244.204
Isol. from seeds of *Cicer arietinum* (chickpea). Cryst. (EtOH). Mp 222-223°. $[\alpha]_D$ -3 (H_2O). λ_{max} 262 (ϵ 7900); 287 (ϵ 7800 pH 12) (H_2O).

Cohn, W. *et al., J. Biol. Chem.*, 1960, **235**, 1488-1498 (*isol, struct*)
Hruska, F.E. *et al., J.A.C.S.*, 1971, **93**, 4334-4336 (*pmr*)
Lerch, U. *et al., J.O.C.*, 1971, **36**, 1507-1513 (*synth, uv, pmr, ord*)
Wenkert, E. *et al., Biochem. Biophys. Res. Commun.*, 1973, **51**, 318-322 (*cmr*)
Komoroski, R.A. *et al., Biochemistry*, 1974, **13**, 369-372 (*cmr*)
Hruska, F.E. *et al., Can. J. Chem.*, 1974, **52**, 497-508 (*pmr*)

Habermehl, G. *et al., Annalen*, 1978, 427-430 (*synth*)
Brown, D.M. *et al., J.C.S. Perkin 1*, 1981, 723-725 (*synth*)
Smith, D.L. *et al., Biomed. Mass Spectrom.*, 1983, **10**, 269-275 (*ms*)
Handa, G. *et al., Phytochemistry*, 1984, **23**, 1779-1780 (*isol*)
Hempel, A. *et al., Acta Cryst. C*, 1997, **53**, 1707-1709 (*cryst struct*)
Luyten, I. *et al., J.O.C.*, 1998, **63**, 1033-1044 (*tautom*)

Psidinin C P-555

[145826-28-4]

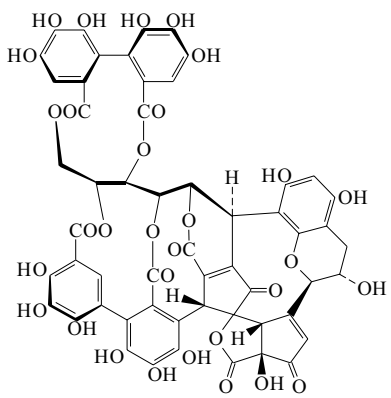


$C_{55}H_{38}O_{31}$ 1194.887
Isol. from the bark of *Psidium guajava* (guava). Pale brown amorph. powder + $6H_2O$. $[\alpha]_D^{31}$ -47.4 (c, 1.0 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2092 (*cd, pmr, cmr*)

Psiguavin P-556

[145826-29-5]

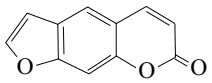


$C_{55}H_{34}O_{31}$ 1190.855
Tannin derived from the bark of *Psidium guajava* (guava). Pale brown amorph. powder + $9\frac{1}{2}H_2O$. $[\alpha]_D^{27}$ -62.9 (c, 0.5 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2092 (*pmr, cmr*)

Psoralen P-557

[66-97-7]
*7*H-*Furo[3,2-g][1]benzopyran-7-one, 9CI. 2*H-*Furo[3,2-g]chromen-2-one. Ficusin. Furo[4′,5′:6,7]coumarin*

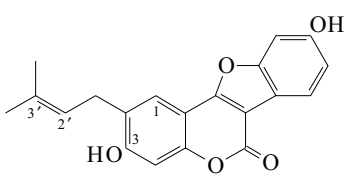


$C_{11}H_6O_3$ 186.167
Found in common vegetables, e.g. parsnip, celery esp. if diseased or 'spoiled'. Needles (H_2O or MeOH or EtOH). Sol. MeOH; fairly sol. H_2O. Mp 171° (161-162°, 165°). λ_{max} 246 (ϵ 22600); 291 (ϵ 10400); 327 (ϵ 6400) (MeOH). λ_{max} 247 (ϵ 28180); 286 (ϵ 19000); 310 (ϵ 8000) (EtOH) (Berdy).
▶ Photocarcinogen. Causes photosensitised skin effects. LV0944000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 173A (*nmr*)
Worden, L.R. *et al., J.O.C.*, 1969, **34**, 2311 (*synth*)
Pardanani, N.H. *et al., Aust. J. Chem.*, 1972, **25**, 1537 (*synth*)
Austin, D.H. *et al., Phytochemistry*, 1973, **12**, 1657 (*biosynth*)
Chatterjee, A. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 212 (*synth, uv, pmr*)
Bergenthal, D. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1978, **311**, 1026 (*cmr*)
Matsumoto, H. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3433 (*uv*)
Reisch, J. *et al., Chem. Ber.*, 1979, **112**, 1491 (*synth*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, (*rev*)
Beier, R.C. *et al., Xenobiotics in Foods and Feeds*, Amer. Chem. Soc., 1983, 295 (*occur*)
Hayakawa, K. *et al., J.A.C.S.*, 1984, **106**, 6735 (*synth*)
Ceska, O. *et al., Experientia*, 1986, **42**, 1302 (*occur, tox*)
Zubia, E. *et al., Tetrahedron*, 1992, **48**, 4239 (*synth*)
Masuda, T. *et al., Phytochemistry*, 1998, **47**, 13-16 (*isol, uv, pmr, cmr*)
Chimichi, S. *et al., Tetrahedron*, 2002, **58**, 4859-4863 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FQD000

Psoralidin P-558

[18642-23-4]
3,9-Dihydroxy-2-prenylcoumestan



$C_{20}H_{16}O_5$ 336.343
Constit. of papadi (*Dolichos biflorus*) and the butter bean (*Phaseolus lunatus*). Cryst. (Me_2CO). Mp 290-292° dec. λ_{max} 208 (ϵ 40800); 244 (ϵ 20300); 305 (ϵ 7000); 347 (ϵ 25300) (EtOH) (Derep).

Di-Ac:
Mp 221-223°.

Di-Me ether:
Mp 190-191°.

2′,3′-Epoxide: ***Psoralidin oxide***
$C_{20}H_{16}O_6$ 352.343
Needles (EtOH) (as di-Ac). Mp 232-234° (di-Ac).

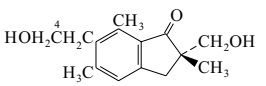
1-Methoxy: [23013-84-5] *3,9-Dihydroxy-1-methoxy-2-prenylcoumestan.* ***Glycyrol.*** *Neoglycyrol*
$C_{21}H_{18}O_6$ 366.37
Isol. from *Glycyrrhiza* sp. root (licorice). Needles (EtOH). Mp 243.5-245°. Formerly assigned 1-hydroxy-3-*O*-methylpsoralidin struct..

1-Methoxy, 3-Me ether: [23013-85-6] ***3-O-Methylglycyrol***
$C_{22}H_{20}O_6$ 380.396
Isol. from *Glycyrrhiza* spp. roots. Needles (Me_2CO). Mp 259-260.5°.

Chakravarti, K.K. *et al., CA*, 1948, **42**, 7492 (*isol*)
Khastgir, H.N. *et al., Tetrahedron*, 1961, **14**, 275 (*struct, uv, ir*)
Abdel-Hay, F.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **86**, 920 (*ms*)
Gupta, B.K. *et al., Phytochemistry*, 1980, **19**, 2232 (*Psoralidin oxide*)
Keen, N.T. *et al., Z. Naturforsch., C*, 1980, **35**, 923 (*isol*)
Shiozawa, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2239 (*Glycyrol*)
Wang, C.L. *et al., Yaoxue Xuebao*, 1991, **26**, 147; *CA*, **115**, 68400 (*Neoglycyrol*)
Yang, Y.M. *et al., Planta Med.*, 1996, **62**, 353 (*isol, pmr, cmr, props*)

Pterosin A P-559

[35910-16-8]
*2,3-Dihydro-6-(2-hydroxyethyl)-2-(hydroxymethyl)-2,5,7-trimethyl-1*H-*inden-1-one, 9CI. 6-(2-Hydroxyethyl)-2-hydroxymethyl-2,5,7-trimethyl-1-indanone*



$C_{15}H_{20}O_3$ 248.321
▶ NK8932000

(S)-form
Constit. of *Pteridium aquilinum* (bracken fern). Cryst. (C_6H_6). Mp 125-127°. $[\alpha]_D$ -21.8 ($CHCl_3$). $[\alpha]_D$ -45.3.

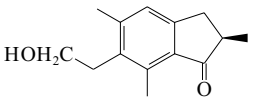
4-O-*β*-D-*Glucopyranoside:* [35910-15-7] ***Pteroside A***
$C_{21}H_{30}O_8$ 410.463
Constit. of *Pteris aquilinum* (bracken fern). Mp 116-118°. $[\alpha]_D$ -49.6.

4-O-*Hexadecanoyl:* ***Palmitoylpterosin A***
$C_{31}H_{50}O_4$ 486.734
Mp 50-51°. $[\alpha]_D$ -37.8.

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1491; 1972, **20**, 426; 1974, **22**, 723; 1979, **27**, 731 (*isol, struct, abs config*)
Hikino, H. *et al., Chem. Pharm. Bull.*, 1972, **20**, 210 (*Pteroside A*)
Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2282 (*Palmitoylpterosin A*)
Banerji, A. *et al., Tet. Lett.*, 1974, 1369 (*deriv*)
Chen, C.-M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2241 (*isol*)
Castillo, U.F. *et al., Phytochemistry*, 1997, **44**, 901 (*isol, pmr, cmr*)

Pterosin B P-560

*2,3-Dihydro-6-(2-hydroxyethyl)-2,5,7-trimethyl-1*H*-inden-1-one, 9CI. 6-(2-Hydroxyethyl)-2,5,7-trimethyl-1-indanone*



(*R*)-*form*

$C_{14}H_{18}O_2$ 218.295

(*R*)-*form* [34175-96-7]
Constit. of *Pteridium aquilinum* (bracken fern) (aerial parts). Cryst. ($CHCl_3$/hexane). Sol. MeOH, C_6H_6; fairly sol. H_2O. Mp 109-110°. $[\alpha]_D$ -31.9 (-11.4). λ_{max} 217 (ϵ 30000); 260 (ϵ 13100); 304 (ϵ 2000) (EtOH) (Berdy).

▶NK7537730

O-*β-D-Glucopyranoside:* [29774-74-1]
Pteroside B
$C_{20}H_{28}O_7$ 380.437
Constit. of *Pteridium aquilinum* (bracken fern). Cryst. + H_2O. Mp 119-121°. $[\alpha]_D$ -48.8.

▶NK8928000

Me ether: [54854-89-6] ***Pterosin O***
$C_{15}H_{20}O_2$ 232.322
Isol. from *Pteridium aquilinum* (bracken fern). Cryst. (hexane). Sol. MeOH, EtOAc. Mp 45-46°. Also descr. as an oil having $[\alpha]_D$ -14.1 ($CHCl_3$) λ_{max} 218 (ϵ 31000); 260 (ϵ 13700); 304 (ϵ 1900) (EtOH) (Berdy).

O-*Benzoyl:* [39815-61-7] ***Benzoylpterosin B***
$C_{21}H_{22}O_3$ 322.403
Mp 68-70°. $[\alpha]_D$ -20 ($CHCl_3$).

O-*(Z-2-Butenoyl):* ***Isocrotonoylpterosin B***
$C_{18}H_{22}O_3$ 286.37
Oil. $[\alpha]_D$ -3.5 ($CHCl_3$).

O-*Hexadecanoyl:Palmitoylpterosin B*
$C_{30}H_{48}O_3$ 456.707
Mp 51-52°. $[\alpha]_D$ -3.3 (cyclohexane).

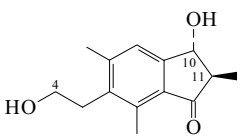
(*S*)-*form* [70561-32-9]
Found as glycosides in the rhizomes of *Pteridium aquilinum* (bracken fern). Mp 106-108°. $[\alpha]_D$ +30.3.

O-*β-D-Glucopyranoside:*
Mp 164-166°. $[\alpha]_D$ -13.6.

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1491; 1972, **20**, 426; 2282; 1974, **22**, 723; 2762; 1978, **26**, 2365; 1979, **27**, 592; 731
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*occur*)
Castillo, U.F. *et al., Phytochemistry*, 1997, **44**, 901 (*isol, pmr, cmr*)

Pterosin C P-561

*2,3-Dihydro-3-hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1*H*-inden-1-one, 9CI. 3-Hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone*



(10*R*,11*R*)-*form*

$C_{14}H_{18}O_3$ 234.294

The nat. prod. is stated to be a diastereoisomeric mixt. in which the (10*S*,11*S*)-isomer is the major constit. The epimers interconvert in alkaline soln. Terpenoid (norilludalane) numbering shown.

(10*S*,11*R*)-*form*
Mp 163-166°. $[\alpha]_D$ -37.1.

4-O-*β-D-Glucopyranoside:*
$C_{20}H_{28}O_8$ 396.436
Isol. from *Pteridium aquilinum* (bracken fern). Mp 174-176°. $[\alpha]_D$ -46.6.

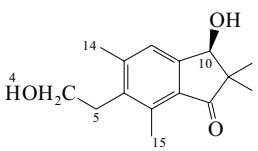
(10*S*,11*S*)-*form* [35938-43-3]
Constit. of *Pteridium aquilinum* (bracken fern). Cryst. (Me_2CO). Mp 153-156°. $[\alpha]_D$ +93.4 (c, 0.2 in MeOH).

Ac: ***Acetylpterosin C***
$C_{16}H_{20}O_4$ 276.332
From *Pteridium aquilinum* (bracken fern). Mp 115-118°. $[\alpha]_D$ +86.1.

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 210; 426; 1974, **22**, 723; 1978, **26**, 2365; 1979, **27**, 731 (*isol, struct, abs config, cd, conformn*)
Chem, C.-M. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1890 (*deriv*)
Ali, E. *et al., Phytochemistry*, 1976, **15**, 995 (*deriv*)
Tanaka, N. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3640
Ng, K.-M.E. *et al., Can. J. Chem.*, 1984, **62**, 1945 (*synth*)
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*occur*)

Pterosin D P-562

*2,3-Dihydro-3-hydroxy-6-(2-hydroxyethyl)-2,2,5,7-tetramethyl-1*H*-inden-1-one, 9CI. 3-Hydroxy-6-(2-hydroxyethyl)-2,2,5,7-tetramethyl-1-indanone*



(*R*)-*form*

$C_{15}H_{20}O_3$ 248.321

Terpenoid (illudalane) numbering shown.

(*R*)-*form* [61138-81-6]
Isol. from *Pteridium aquilinum* (bracken fern). Cryst. (MeOH/CCl_4). Mp 190-192°. $[\alpha]_D^{23}$ +6.3 (c, 0.255 in MeOH).

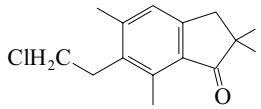
(*S*)-*form* [34169-70-5]
Constit. of *Pteridium aquilinum* (bracken fern). Mp 180-183°. $[\alpha]_D$ -15.4.

4-O-*β-D-Glucopyranoside:* [35943-38-5]
Pteroside D
$C_{21}H_{30}O_8$ 410.463
Constit. of *Pteridium aquilinum* (bracken fern). Amorph. $[\alpha]_D$ -52.4.

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1491; 1972, **20**, 426; 1974, **22**, 723; 1979, **27**, 731 (*isol, struct, abs config*)
Hayashi, Y. *et al., Chem. Lett.*, 1974, 945 (*synth*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2241 (*Pteroside D*)
Chen, C.-M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2241 (*isol*)
Tanaka, N. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3640 (*isol*)
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*rev*)

Pterosin H P-563

[39004-41-6]
*6-(2-Chloroethyl)-2,3-dihydro-2,2,5,7-tetramethyl-1*H*-inden-1-one, 9CI. 6-(2-Chloroethyl)-2,2,5,7-tetramethyl-1-indanone. Hypolepin A*

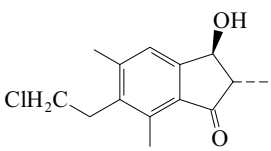


$C_{15}H_{19}ClO$ 250.767
Isol. from *Pteridium aquilinum* (bracken fern). Mp 87.5-88°. λ_{max} 218 (ϵ 32000); 260 (ϵ 14000); 300 (ϵ 2000) (EtOH) (Berdy).

Hayashi, Y. *et al., Chem. Lett.*, 1972, 375 (*isol, struct, synth*)
Yoshihira, K. *et al., Chem. Pharm. Bull.*, 1972, **20**, 426 (*isol, struct*)
McMorris, T.C. *et al., J. Nat. Prod.*, 1977, **40**, 221 (*synth*)
Padwa, A. *et al., J.O.C.*, 1996, **61**, 73 (*synth*)

Pterosin J P-564

[41411-02-3]
*6-(2-Chloroethyl)-2,3-dihydro-3-hydroxy-2,5,7-trimethyl-1*H*-inden-1-one. 6-(2-Chloroethyl)-3-hydroxy-2,5,7-trimethyl-1-indanone*

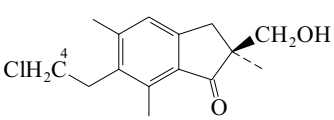


$C_{14}H_{17}ClO_2$ 252.74
Isol. from *Pteridium aquilinum* (bracken fern). Cryst. (C_6H_6/hexane). Mp 136-137°. $[\alpha]_D$ +83.5 (c, 0.17 in $CHCl_3$).

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2282 (*isol, struct*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 723 (*abs config*)
Tanaka, N. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1339 (*isol*)
Yoshihira, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2346 (*isol*)
Fukuoka, *et al., Chem. Pharm. Bull.*, 1978, **26**, 2365 (*struct*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1979, **27**, 731 (*stereochem*)

Pterosin K P-565

*6-(2-Chloroethyl)-2,3-dihydro-2-(hydroxymethyl)-2,5,7-trimethyl-1*H*-inden-1-one, 9CI. 6-(2-Chloroethyl)-2-hydroxymethyl-2,5,7-trimethyl-1-indanone*



$C_{15}H_{19}ClO_2$ 266.767

(*S*)-*form* [41411-03-4]
Constit. of the leaves of *Pteridium aquilinum* (bracken fern). Cryst. (hexane). Mp 85-87°. $[\alpha]_D$ -20 ($CHCl_3$). $[\alpha]_D$ -37.5 (c, 0.14 in MeOH).

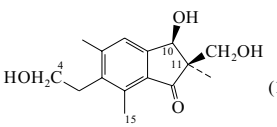
12-O-β-D-Glucopyranoside: [69753-96-4] ***Pteroside K***
$C_{21}H_{29}ClO_7$ 428.909
Mp 94-96°. $[\alpha]_D$ -26.4.

Dechloro, 4-methoxy: [56670-45-2] ***Pterosin V***
$C_{16}H_{22}O_3$ 262.348
Oil. $[\alpha]_D^{22}$ -4 (c, 0.69 in MeOH). λ_{max} 217 (ϵ 29000); 261 (ϵ 12500); 304 (ϵ 1800) (EtOH) (Berdy).

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2282; 1978, **26**, 2365 (*isol, struct, synth*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 723; 1978, **26**, 2365; 1979, **27**, 592; 731 (*struct, abs config*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1630 (*Pterosin V*)
Yoshihira, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2346 (*isol*)
Castillo, U.F. *et al., Phytochemistry*, 1997, **44**, 901 (*isol, pmr, cmr*)

Pterosin L P-566

2,3-Dihydro-3-hydroxy-6-(2-hydroxyethyl)-2-(hydroxymethyl)-2,5,7-trimethyl-1H-inden-1-one, 9CI. 3-Hydroxy-6-(2-hydroxyethyl)-2-hydroxymethyl-2,5,7-trimethyl-1-indanone



(10*R*,11*R*)-*form*

$C_{15}H_{20}O_4$ 264.321

(10*R*,11*R*)-*form* [41411-04-5]
Constit. of *Pteridium aquilinum* (bracken fern). Needles (C_6H_6). Mp 134-135°. $[\alpha]_D^{23}$ +22.2 (c, 0.36 in MeOH).

4-O-β-D-Glucopyranoside:
$C_{21}H_{30}O_9$ 426.463
Syrup. $[\alpha]_D^{23}$ -19 (c, 1.21 in MeOH).

10-O-α-L-Arabinopyranoside:
$C_{20}H_{28}O_8$ 396.436
Needles ($CHCl_3$/MeOH). Mp 209-211°. $[\alpha]_D^{20}$ -21.7 (c, 0.46 in MeOH).

15-Hydroxy: [95377-46-1] ***Jamesonin***
$C_{15}H_{20}O_5$ 280.32
Amorph. $[\alpha]_D^{24}$ +9.6 (c, 0.35 in MeOH).

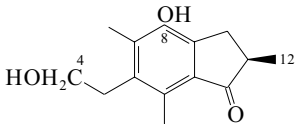
(10*R*,11*S*)-*form* [69753-99-7]
Needles (C_6H_6). Mp 85-87°. $[\alpha]_D^{23}$ +78 (c, 0.28 in MeOH).

4-O-β-D-Glucopyranoside:
Oil. $[\alpha]_D$ +18.4.

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2282; 1974, **22**, 723; 1979, **27**, 731 (*isol, struct, abs config*)
Chen, C.-M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 2241 (*deriv*)
Satake, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4620 (*Jamesonin*)
Kuraishi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2305

Pterosin M P-567

2,3-Dihydro-4-hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1H-inden-1-one, 9CI. 4-Hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone



$C_{14}H_{18}O_3$ 234.294

(*R*)-*form* [52744-25-9]
Cryst. (H_2O or EtOAc). Mp 187°.

Di-Ac:
Cryst. (EtOH). Mp 77-79°.

4-O-β-D-Glucopyranoside: [52715-92-1] ***Pteroside M***
$C_{20}H_{28}O_8$ 396.436
Cryst. (EtOH). Mp 192°. $[\alpha]_D^{18}$ +129 (c, 1.2 in Me_2CO aq.).

4-Carboxylic acid, 8-deoxy: [52528-78-6] ***Pterosin E****. 2,3-Dihydro-2,4,6-trimethyl-3-oxo-1H-indene-5-acetic acid, 9CI. 2,4,6-Trimethyl-3-oxo-5-indanacetic acid, 8CI. BH4*
$C_{14}H_{16}O_3$ 232.279
Constit. of *Pteridium aquilinum* (bracken fern) leaves. Cryst. (CCl_4). Mp 160-162°. λ_{max} 217 ; 260 ; 303 (EtOH) (Berdy).

4,8-Dideoxy, 4-chloro: [34175-98-9] ***Pterosin F****. 6-(2-Chloroethyl)-2,3-dihydro-2,5,7-trimethyl-1H-inden-1-one, 9CI*
$C_{14}H_{17}ClO$ 236.74
Constit. of *Pteridium aquilinum* (bracken fern). Cryst. (hexane). Mp 66-67°. $[\alpha]_D$ -9.2 (C_6H_6). λ_{max} 219 ; 259 ; 303 (EtOH) (Berdy).

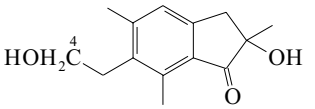
▶ NK7536200

12-Hydroxy, 8-deoxy: [35964-50-2] ***Pterosin G***
$C_{14}H_{18}O_3$ 234.294
Mp 152-153°. $[\alpha]_D$ -14.6. Has (*S*)-config..

Yoshihira, K. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1491; 1972, **20**, 426; 1974, **22**, 723; 1978, **26**, 2346 (*isol, uv, ir, pmr*)
Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 426; 1974, **22**, 723; 1978, **26**, 2365; 1979, **27**, 731 (*isol, uv, ms, ir, pmr, struct, abs config*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 723; 1979, **27**, 592; 731 (*abs config*)
Nambudiry, M.E.N. *et al., J.C.S. Perkin 1*, 1974, 317 (*synth, pmr*)
Hasegawa, M. *et al., Phytochemistry*, 1974, **13**, 509 (*isol*)
McMorris, T.C. *et al., J. Nat. Prod.*, 1977, **40**, 221 (*isol, synth*)
Raju, B. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 914 (*synth*)
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*occur*)
Finkielsztein, L.M. *et al., J. Chem. Res., Synop.*, 1999, 406 (*Pterosin F, synth*)

Pterosin N P-568

[54797-11-4]
2,3-Dihydro-2-hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1H-inden-1-one, 9CI. 2-Hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone



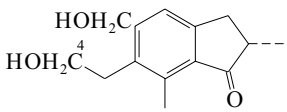
$C_{14}H_{18}O_3$ 234.294
Isol. from *Pteridium aquilinum* (bracken fern). Cryst. (Me_2CO). Mp 165-167°. $[\alpha]_D$ -18.8 (MeOH).

4-Deoxy, 4-chloro: ***Histiopterosin B***
$C_{14}H_{17}ClO_2$ 252.74
Mp 125-126°. Stereochem. not detd..

Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2762; 1976, **24**, 173
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*Histiopterosin B*)

Pterosin P P-569

2,3-Dihydro-6-(2-hydroxyethyl)-5-(hydroxymethyl)-2,7-dimethyl-1H-inden-1-one, 9CI. 6-(2-Hydroxyethyl)-5-hydroxymethyl-2,7-dimethyl-1-indanone



$C_{14}H_{18}O_3$ 234.294

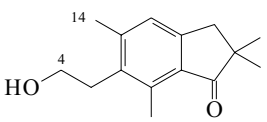
(*S*)-*form* [56374-22-2]
Isol. from *Pteridium aquilinum* (bracken fern). Cryst. ($CHCl_3$/C_6H_6). Mp 115-117°. $[\alpha]_D$ +4.6 (MeOH).

4-O-β-D-Glucopyranoside: [54854-88-5] ***Pteroside P***
$C_{20}H_{28}O_8$ 396.436
Constit. of *Pteridium aquilinum* (bracken fern). Cryst. (MeOH/$CHCl_3$). Mp 191-193°. $[\alpha]_D$ -14.9 (MeOH).

Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2762; 1979, **27**, 592 (*isol*)
Saito, M. *et al., Experientia*, 1975, **31**, 829

Pterosin Z P-570

[34169-69-2]
2,3-Dihydro-6-(2-hydroxyethyl)-2,2,5,7-tetramethyl-1H-inden-1-one, 9CI. 6-(2-Hydroxyethyl)-2,2,5,7-tetramethyl-1-indanone, 8CI. Hypolepin B



$C_{15}H_{20}O_2$ 232.322
Cryst. (hexane). Mp 90-91°. λ_{max} 216 (ϵ 57544); 263 (ϵ 33113); 301 (ϵ 6026) (MeOH) (Berdy). λ_{max} 218 ; 260 ; 305 (EtOH) (Berdy).

O-*β-D-Glucopyranoside:* [35943-37-4] ***Pteroside Z***
$C_{21}H_{30}O_7$ 394.464
Constit. of *Pteridium aquilinum* (bracken fern). Cryst. Mp 86-89°.

Ac: ***Acetylpterosin Z***
$C_{17}H_{22}O_3$ 274.359
Oil.

14-Hydroxy, 4-O-D-glucopyranoside: ***Cryptogrammin***

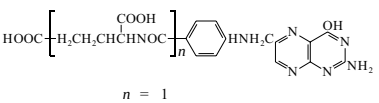
$C_{21}H_{30}O_8$ 410.463
$[\alpha]_D$ -22.

4-Me ether: [35944-01-5] ***Pterosin I***. *Hypolepin C*
$C_{16}H_{22}O_2$ 246.349
Mp 61-62°. λ_{max} 218 (ϵ 33000); 260 (ϵ 13500); 303 (ϵ 1700) (EtOH) (Berdy).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2425 (*isol*)
Hayashi, Y. *et al., Chem. Lett.*, 1972, 373 (*Pterosin I*)
Yoshihara, K. *et al., Chem. Pharm. Bull.*, 1972, **20**, 426 (*Pterosin I*)
Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2365
Bardouille, V. *et al., Phytochemistry*, 1978, **17**, 275
Murakami, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **54**, 1 (*rev, occur*)
Farrell, R. *et al., J. Nat. Prod.*, 1996, **59**, 446 (*synth, pmr, cmr*)
Padwa, A. *et al., J.O.C.*, 1996, **61**, 73 (*synth*)
Castillo, U.F. *et al., Phytochemistry*, 1997, **44**, 901-906 (*isol, pmr, cmr*)

Pteroylglutamic acid P-571

[59-30-3]
N-*[4-[[(2-Amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]glutamic acid, 9CI*. ***Folic acid, BAN, INN***. *Vitamin B_c. Vitamin M. Coenzyme F. Leucal. CoF. Citrovorin. Folacin. Folvite. Foliamin. NSC 3073*



$C_{19}H_{19}N_7O_6$ 441.402

Natural isolates normally contain homologues having n > 1. Dietary supplement. Pale lemon-yellow to light-orange needles (H_2O at pH 3). Almost insol. H_2O; sl. sol. MeOH; mod. sol. AcOH; insol. Et_2O. $[\alpha]_D^{25}$ +23 (c, 0.5 in 1*M* NaOH). pK_{a1} 4.65; pK_{a2} 6.75; pK_{a3} 9 (30°, 0.01*M* KNO_3). Log P -1.02 (calc). Chars above 250°. Component of numerous preparations. Also used as calcium salt (Calcium folinate, BAN, INN).

▶ LD_{50} (mus, orl) 10,000 mg/kg. Exp. teratogen. LP5425000

7,8-Dihydro: See *T*-Kinin in *The Combined Chemical Dictionary.*

*Homologue (*n = *2):* [6807-82-5] ***Pteroyldiglutamic acid***. *Pteroylglutamylglutamic acid. Diopterin*
$C_{24}H_{26}N_8O_9$ 570.518

*Homologue (*n = *3):* [89-38-3] ***Pteroyltriglutamic acid***. *Pteroylglutamylglutamylglutamic acid. Dripterin. Pteropterin. Terapterin*. Lactobacillus casei *Factor. Teropterin*
$C_{29}H_{33}N_9O_{12}$ 699.633
Amorph. Log P -3.65 (calc).

*Homologue (*n = *5):* [33611-85-7] *Pteroylpentaglutamic acid*
$C_{39}H_{47}N_{11}O_{18}$ 957.863

*Homologue (*n = *7):* [6484-74-8] *Pteroylheptaglutamic acid. Pteroylhexaglutamylglutamic acid. Folic acid conjugate. Vitamin B_c conjugate*
$C_{49}H_{61}N_{13}O_{24}$ 1216.094
Microcryst. (H_2O).

[1492-18-8, 6484-89-5, 6713-32-2, 75708-92-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 898A (*ir*)
Pfiffner, J.J. *et al., J.A.C.S.*, 1946, **68**, 1392 (*Pteroylheptaglutamic acid*)
Boothe, J.H. *et al., J.A.C.S.*, 1948, **70**, 1099; 1949, **71**, 2304
Weisblat, D.I. *et al., J.A.C.S.*, 1953, **75**, 3625 (*synth*)
Jaenicke, L. *et al., Prog. Chem. Org. Nat. Prod.*, 1963, **21**, 183 (*rev*)
Pastore, E.J. *et al., Ann. N.Y. Acad. Sci.*, 1971, **186**, 43 (*pmr*)
Godwin, H.A. *et al., J. Biol. Chem.*, 1972, **247**, 2266 (*Pteroyltriglutamic acid*)
Bieri, J. *et al., Helv. Chim. Acta*, 1973, **56**, 2905 (*synth*)
Frick, W. *et al., Helv. Chim. Acta*, 1974, **57**, 2658 (*cmr*)
Drey, C.N.C. *et al., Chem. Comm.*, 1977, 144 (*Pteroyltriglutamic acid*)
Pont, L.O. *et al., Anal. Profiles Drug Subst.*, 1979, **8**, 315 (*rev*)
Murphy, M. *et al., Biochim. Biophys. Acta*, 1979, **583**, 535 (*metab*)
Nixon, P.F. *et al., Clin. Exp. Pharmacol. Physiol.*, Suppl. 1, 1979, **5**, 35 (*rev, pharmacol*)
Poe, M. *et al., Methods Enzymol.*, 1980, **66**, 483 (*pmr*)
Mastropaolo, D. *et al., Science (Washington, D.C.)*, 1980, **210**, 334 (*cryst struct*)
Straw, J.E. *et al., Cancer Res.*, 1984, **44**, 3114 (*metab*)
Cooper, B.A. *et al., Clin. Biochem.*, 1984, **17**, 95 (*metab*)
Blakeley, R.L. *et al., Folates Pterins*, (Eds.), J. Wiley & Sons, NY, 1984, **1**, (*chem, biochem*)
Brody, T. *et al., Food Sci. Technol.*, 1984, **13**, 459 (*biol studies*)
D'Ari, L. *et al., Methods Enzymol.*, 1985, **113**, 169 (*Pteroyltriglutamic acid*)
Shane, B. *et al., Methods Enzymol.*, 1986, **122**, 269; 323 (*detn, synth*)
Moran, R.G. *et al., Methods Enzymol.*, 1986, **122**, 309 (*synth*)
Young, D.W. *et al., Nat. Prod. Rep.*, 1986, **3**, 395 (*biosynth*)
Rees, L. *et al., Chem. Comm.*, 1987, 470 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 5190
Al-Shammary, F.J. *et al., Anal. Profiles Drug Subst.*, 1990, **19**, 221 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1039
Rossi, C. *et al., Spectrosc. Lett.*, 1993, **26**, 1603 (*pmr, conform*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1122-1123
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FMT000

Pterygospermine P-572

$C_{22}H_{18}N_2O_2S_2$ 406.528

A mustard oil precursor. Struct. unknown. Isol. from roots of *Moringa pterygosperma* (horseradish tree). Cryst. (EtOH). Mp 15°. Readily dec. to $PhCH_2NCS$. On acid treatment gives $PhCH_2NH_2$, CO_2, H_2O, benzoquinone and hydroquinone λ_{max} 248 (MeOH) (Berdy).

▶ LD_{50} (mus, scu) 350 - 400 mg/kg.

Rao, P.L.N. *et al., Indian J. Pharm.*, 1953, **15**, 315; *CA*, **48**, 8489 (*isol*)
Rao, P.L.N. *et al., Naturwissenschaften*, 1954, **41**, 66
Rao, P.L.N. *et al., CA*, 1955, **49**, 6870

Ptr Toxin P-573

Protein. Struct. unknown. Prod. by *Pyrenophora tritici-repentens*, the causal agent of tan spot on wheat.

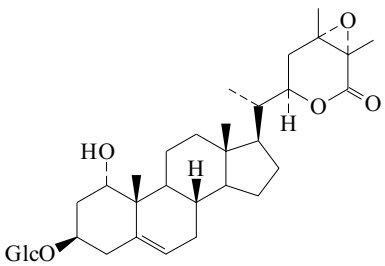
Ptr Toxin A A 13.2 kDa heat-stable protein.

Ptr Toxin B Contains 64 amino acid residues.

Tomas, A. *et al., Mol. Plant-Microbe Interact.*, 1990, **3**, 221-224 (*isol*)
Tuori, R.P. *et al., Mol. Plant-Microbe Interact.*, 1995, **8**, 41-48; 2000, **13**, 456-464 (*PTR Toxin A, isol, struct*)
Martinez, J.P. *et al., Mol. Plant-Microbe Interact.*, 2001, **14**, 675-677 (*Ptr Toxin B, isol, struct*)

Pubescenin P-574

*24,25-Epoxy-3-(*O*-β-*D*-glucopyranosyloxy)-1-hydroxywith-5-enolide*



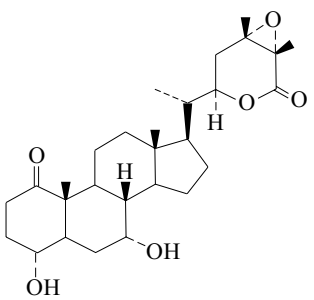
$C_{34}H_{52}O_{10}$ 620.779

(1α,3β,20S,22R,24S,25S)-form [100217-93-4]
Constit. of *Physalis pubescens* (ground cherry). Cryst. (MeOH). Mp 188-189°. $[\alpha]_D$ -38.6 (c, 0.12 in $CHCl_3$).

Glotter, E. *et al., J.C.S. Perkin 1*, 1985, 2241

Pubescenol P-575

[90685-93-1]
*4α,7α-Dihydroxy-1-oxo-24α,25α-epoxywithanolide. 24*S*,25*S*-Epoxy-4α,7α-dihydroxy-1-oxowithanolide*

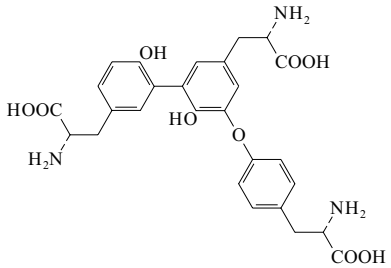


$C_{28}H_{42}O_6$ 474.636
Constit. of *Physalis pubescens* (ground cherry). Cryst. (Me_2CO). Mp 180-182°.

Row, L.R. *et al., Phytochemistry*, 1984, **23**, 427
Reddy, K.S. *et al., J.C.S. Perkin 1*, 1985, 419

Pulcherosine P-576

[126723-16-8]
5-[4-(2-Amino-2-carboxyethyl)phenoxy]-3,3′-dityrosine



$C_{27}H_{29}N_3O_9$ 539.541

Tyrosine trimer. Found in the primary cell walls of tomato cell cultures. No phys. props. reported.

Nomura, K. *et al., Biochemistry*, 1990, **29**, 4525 (*isol, pmr, cmr, uv, struct*)
Brady, J.D. *et al., Phytochemistry*, 1998, **47**, 349-353 (*isol, uv, pmr*)

Pullulan P-577

[9057-02-7]

M = 60000-240000. Consists mainly of Maltotriose, M-45 joined through α(1 → 6)glucosidic linkages plus 5-7% of randomly distributed maltotetraose units.

Poly-O-sulfate:

Bender, H. *et al., Biochem. Z.*, 1961, **334**, 79
Wallenfels, K. *et al., Biochem. Z.*, 1965, **341**, 433
Taguchi, R. *et al., Agric. Biol. Chem.*, 1973, **37**, 1583
Catley, B.J. *et al., Carbohydr. Res.*, 1986, **153**, 79 (*struct*)
Tezuka, Y. *et al., Carbohydr. Res.*, 1998, **305**, 155-161 (*pmr, cmr, nona-Ac*)
Mähner, C. *et al., Carbohydr. Res.*, 2001, **331**, 203-208 (*sulfate*)

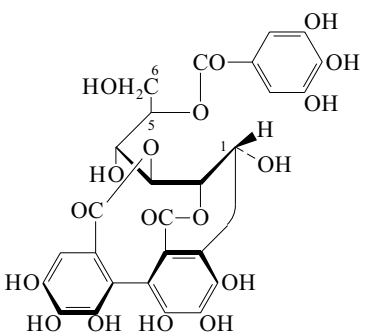
Pumpkin basic peptide P-578

Peptide with approx. 36 amino acid residues. Isol. from pumpkin seeds. λ_{max} 280 (H_2O) (Berdy).

Naisbitt, G.H. *et al., Plant Physiol.*, 1988, **88**, 770-773 (*isol*)

Punicacortein A P-579

[103488-35-3]



$C_{27}H_{22}O_{18}$ 634.46
Isol. from the bark of *Punica granatum* (pomegranate). Tan amorph. powder + ½H_2O. $[\alpha]_D^{28}$ -73.8 (c, 0.6 in MeOH).

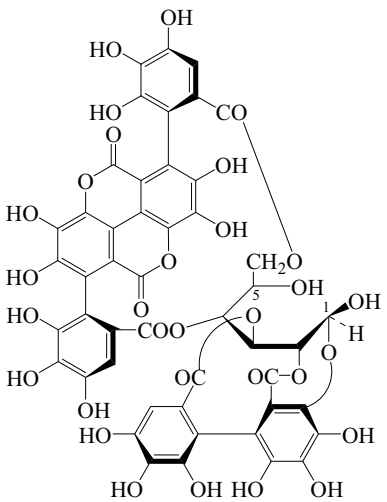
1-Epimer: [136112-45-3] ***Epipunicacortein A***
$C_{27}H_{22}O_{18}$ 634.46
Pale brown amorph. powder + 3½ H_2O. $[\alpha]_D^{13}$ -71.2 (c, 1.0 in MeOH).

5-O-Degalloyl, 6-O-galloyl: [103488-36-4] ***Punicacortein B***
$C_{27}H_{22}O_{18}$ 634.46
Isol. from bark of *Punica granatum* (pomegranate). Tan amorph. powder + ½H_2O. $[\alpha]_D^{28}$ +11.9 (c, 0.5 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 656 (*struct, pmr, cmr*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2151; 1991, **39**, 884 (*struct, pmr, cmr, abs config*)

Punicacortein D P-580

[103616-63-3]



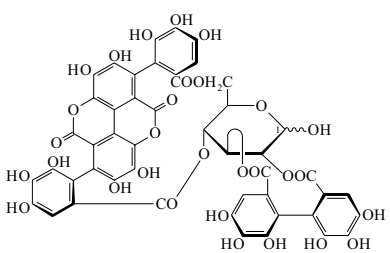
$C_{48}H_{28}O_{30}$ 1084.731
A major tannin constit. from the bark of *Punica granatum* (pomegranate). Yellow amorph. powder + 5H_2O. $[\alpha]_D^{24}$ -96.1 (c, 0.6 in H_2O).

1-Epimer: [103488-37-5] ***Punicacortein C***
$C_{48}H_{28}O_{30}$ 1084.731
Constit. of *Punica granatum* (pomegranate). Yellow amorph. powder + 1H_2O. $[\alpha]_D^{28}$ -37.7 (c, 1.2 in H_2O). Log P -0.1 (uncertain value) (calc).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 656 (*struct, pmr, cmr*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1990, **38**, 215 (*abs config*)
Nonaka, G.-I. *et al., J. Nat. Prod.*, 1990, **53**, 587 (*anti-HIV activity*)

Punicalagin P-581

[65995-63-3]
2,3-(S)-Hexahydroxydiphenoyl-4,6-(S,S)-gallagylglucose



$C_{48}H_{28}O_{30}$ 1084.731
Equilibrated mixt. of anomers. Constit. of *Punica granatum* (pomegranate). Yellow amorph. powder + 1H_2O. $[\alpha]_D^{20}$ -181 (c, 1.0 in H_2O). $[\alpha]_D^{28}$ +3.8 (c, 0.9 in MeOH). λ_{max} 217 (ε 60000); 261 (ε 55000); 375 (ε 12200) (MeOH) (Berdy).

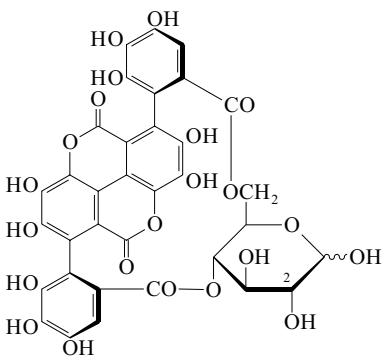
Heptadeca-Me ether:
Prisms (MeOH). Mp 289-191°. $[\alpha]_D^{20}$ -174 (c, 1 in Me_2CO).

1-O-(3,4,5-Trihydroxybenzoyl)(1α-): [108906-54-3] *1α-O-Galloylpunicalagin*. ***Teroblongin***. *Combreglutinin*
$C_{55}H_{32}O_{34}$ 1236.837
Amorph. brown powder. $[\alpha]_D^{20}$ -60 (c, 0.3 in MeOH). λ_{max} 217 (ε 77624); 260 (ε 66070); 379 (ε 10232) (MeOH) (Berdy).

Mayer, W. *et al., Annalen*, 1977, 1976 (*isol*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 650 (*isol*)
Liu, T. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3004 (*isol*)
Nonaka, G.-I. *et al., J. Nat. Prod.*, 1990, **53**, 587 (*anti-HIV activity*)
Doig, A.J. *et al., J.C.S. Perkin 1*, 1990, 2317 (*isol, pmr, cmr, ms*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 60 (*Teroblongin*)
Jossang, A. *et al., J. Nat. Prod.*, 1994, **57**, 732 (*isol, pmr, cmr*)

Punicalin P-582

[65995-64-4]
4,6-Gallagylglucose



$C_{34}H_{22}O_{22}$ 782.535
Anomeric mixt.. Constit. of pomegranate (*Punica granatum*) peel. Yellow amorph. powder + 1H_2O. $[\alpha]_D^{28}$ -81.1 (c, 0.6 in H_2O). λ_{max} 216 (ε 74131); 258 (ε 67610); 329 (ε 14125) (MeOH) (Berdy).

2-O-(3,4,5-Trihydroxybenzoyl): [103488-45-5] ***2-O-Galloylpunicalin***
$C_{41}H_{26}O_{26}$ 934.641
Isol. from bark of pomegranate (*Punica granatum*). Yellow cryst. powder (H_2O). Mp 255° dec. $[\alpha]_D^{28}$ +3.8 (c, 0.9 in MeOH).

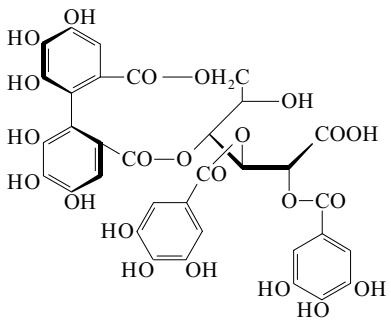
3-O-(3,4,5-Trihydroxybenzoyl):3-O-Galloylpunicalin. ***Arjunin***
$C_{41}H_{26}O_{26}$ 934.641
λ_{max} 279 (MeOH).

Mayer, W. *et al., Annalen*, 1977, 1976-1986 (*isol, struct*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 650 (*struct*)
Nonaka, G.I. *et al., J. Nat. Prod.*, 1990, **53**, 587 (*anti-HIV activity*)

Jossang, A. *et al., J. Nat. Prod.*, 1994, **57**, 732 (*isol, pmr, cmr*)
Shing, T.K.M. *et al., J.O.C.*, 1995, **60**, 3121 (*synth, ir, pmr, cmr*)
Mukai, C. *et al., Tetrahedron*, 1996, **52**, 6547 (*synth*)
Kandil, F.E. *et al., Phytochemistry*, 1998, **47**, 1567-1568 (*Arjunin*)

Punigluconin P-583

[103488-38-6]
2,3-Di-O-galloyl-4,6-(S)-hexahydroxydiphenoylgluconic acid

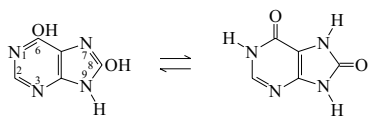


$C_{34}H_{26}O_{23}$ 802.566
A major tannin isol. from the bark of *Punica granatum* (pomegranate). Tan amorph. powder + $2H_2O$. $[\alpha]_D^{25}$ +45.5 (c, 0.7 in MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 656 (*struct, pmr, cmr*)

6,8-Purinediol P-584

6,8-Dihydroxypurine. 7,9-Dihydro-1H-purine-6,8-dione



9H-form *7,9-Dihydro-1H-form*

$C_5H_4N_4O_2$ 152.112
Complex tautom. 7,9-Dihydro-1*H*-form appears to predominate for parent compd.. Component of hen egg yolk. Needles (H_2O). Mp 350°. pK_{a1} 7.65; pK_{a2} 9.87 (20°, H_2O).

Albert, A. *et al., J.C.S.*, 1954, 2060 (*synth*)
Mason, S.F. *et al., J.C.S.*, 1954, 2071 (*uv*)
Robins, R.K. *et al., J.A.C.S.*, 1958, **80**, 6671 (*synth, uv*)
Rahat, M. *et al., J.C.S. Perkin 1*, 1974, 2229 (*synth, pmr, uv*)
Ogawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 612 (*synth, uv, pmr*)

Purothionin AII P-585

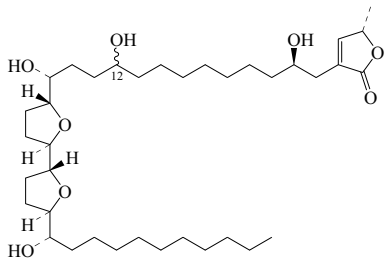
[58239-09-1]
Peptide SP_2. α_1-Purothionin
Peptide. Struct. comprises 45 aminoacid residues. Isol. from wheat (*Triticum monococcum*). Toxic to brewers' yeast.

Jones, B.L. *et al., Cereal Chem.*, 1977, **54**, 511 (*isol, struct*)
Ohtoni, S. *et al., J. Biochem. (Tokyo)*, 1977, **82**, 753 (*struct*)
Oschkinat, H. *et al., Nature (London)*, 1988, **332**, 374 (*conformn, pmr*)

Purpureacin 2 P-586

[149990-60-3]

[187464-96-6, 187464-97-7]
12-Hydroxybullatacin

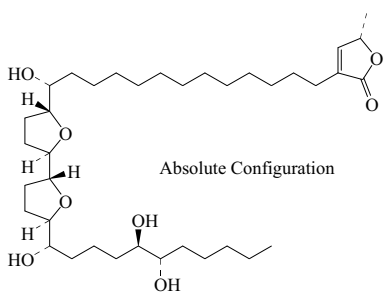


$C_{37}H_{66}O_8$ 638.924
Both epimers of 12-hydroxybullatacin have been characterised. Purpureacin, of undetermined 12-config., appears to be identical with one of them. Props. refer to Purpureacin 2. Isol. from *Rollinia mucosa* (biriba) and *Annona purpurea*. Amorph. powder. $[\alpha]_D$ +6.5 (c, 0.17 in MeOH). λ_{max} 207 (ϵ 7943) (MeOH) (Berdy).

24-Epimer (?): [177932-94-4] ***Araticulin***
$C_{37}H_{66}O_8$ 638.924
Wax. Mp 65-67°. $[\alpha]_D$ +9.6 (c, 0.3 in MeOH). 4- and 12-configs. uncertain.

Cepleanu, F. *et al., Helv. Chim. Acta*, 1993, **76**, 1379-1388 (*Purpureacin 2*)
Santos, L.P. *et al., Phytochemistry*, 1996, **42**, 705-707 (*Araticulin*)
Gu, Z. *et al., J. Nat. Prod.*, 1997, **60**, 242-248 (*12-Hydroxybullatacin*)

Purpurediolin P-587



$C_{37}H_{66}O_8$ 638.924
Constit. of the seeds of *Annona purpurea* (soncoya). Wax. Mp 35-39°. $[\alpha]_D$ +20 (c, 1.3 in MeOH). λ_{max} 205 (log ϵ 3.86) (EtOH).

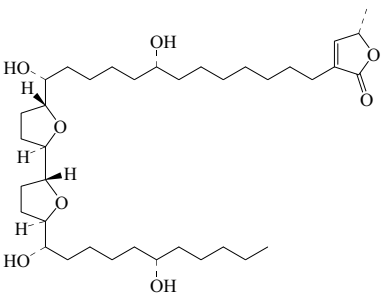
Stereoisomer: ***Spinencin***
$C_{37}H_{66}O_8$ 638.924
Oil. $[\alpha]_D^{20}$ +24 (c, 0.1 in $CHCl_3$). Rel. config. only known. Appears to be the 15,23,29-triepimer of Purpurediolin, or its enantiomer λ_{max} 207 (log ϵ 3.89) (MeOH).

Stereoisomer: [187523-67-7] ***Rollitacin***
$C_{37}H_{66}O_8$ 638.924
Constit. of *Rollinia mucosa* (biriba). Waxy solid. $[\alpha]_D^{23}$ +15.7 (c, 0.6 in $CHCl_3$). λ_{max} 222 (log ϵ 3.54) (MeOH).

Stereoisomer: ***Atemotetrolin***
$C_{37}H_{66}O_8$ 638.924
Constit. of the seeds of *Annona atemoya* (custard apple). Oil. $[\alpha]_D^{20}$ +23 (c, 0.2 in MeOH). *threo*-Config. at C-28, C-29 λ_{max} 219 (log ϵ 3.54) (MeOH).

Queiroz, E.F. *et al., J. Nat. Prod.*, 1997, **60**, 761 (*Spinencin*)
Shi, G. *et al., Phytochemistry*, 1997, **45**, 719-723 (*Rollitacin*)
Chavez, D. *et al., J. Nat. Prod.*, 1998, **61**, 580 (*Purpurediolin*)
Duret, P. *et al., Phytochemistry*, 1998, **48**, 499-506 (*Atemotetrolin*)

Purpurenin P-588

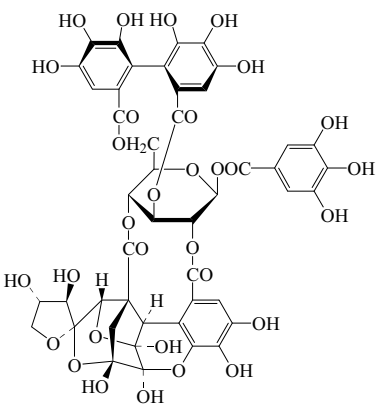


$C_{37}H_{66}O_8$ 638.924
Constit. of the seeds of *Annona muricata* (soursop). Pale yellow wax. Mp 36-38°. $[\alpha]_D$ +27 (c, 1 in MeOH). λ_{max} 208 (log ϵ 4.09) (MeOH).

Chavez, D. *et al., J. Nat. Prod.*, 1998, **61**, 580

Putranjivain A P-589

[131959-62-1]

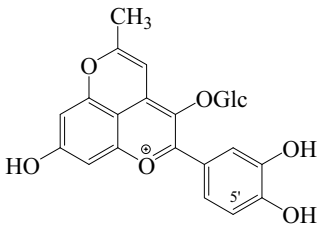


$C_{46}H_{36}O_{31}$ 1084.772
Constit. of *Phyllanthus emblica* (emblic). Amorph. powder. $[\alpha]_D$ -89 (c, 0.1 in MeOH).

El-Mekkawy, S. *et al., Chem. Pharm. Bull.*, 1995, **43**, 641-648 (*isol, pmr, cmr*)

Pyranocyanin B P-590

2-(3,4-Dihydroxyphenyl)-3-glucosyloxy-8-hydroxy-5-methylpyrano[4,3,2-de]-1-benzopyrylium(1+)



$C_{24}H_{23}O_{11}^{\oplus}$ 487.439
Constit. of the seeds of *Ribes nigrum* (blackcurrant). Orange powder. Artifact. Counterion not specified.

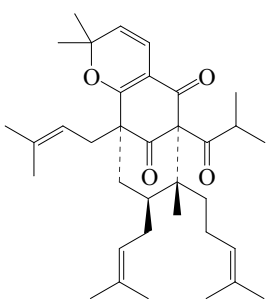
5′-Hydroxy:Pyranodelphinin B
$C_{24}H_{23}O_{12}^{\oplus}$ 503.439
Constit. of the seeds of *Ribes nigrum* (blackcurrant). Orange powder. Artifact.

6″-O-α-L-Rhamnopyranosyl:Pyranocyanin A
$C_{30}H_{33}O_{15}^{\oplus}$ 633.582
Constit. of the seeds of *Ribes nigrum* (blackcurrant). Orange powder. Artifact.

5′-Hydroxy, 6″-O-α-L-rhamnopyranosyl:-Pyranodelphinin A
$C_{30}H_{33}O_{16}^{\oplus}$ 649.581
Constit. of the seeds of *Ribes nigrum* (blackcurrant). Orange powder. Artifact.

Lu, Y. *et al., Tet. Lett.*, 2000, **41**, 5975-5978; 2001, **42**, 1371-1373 (*isol, struct*)

Pyrano[7,28-*b*]hyperforin P-591



$C_{35}H_{50}O_4$ 534.778
Constit. of *Hypericum perforatum* (St. John's Wort). Viscous oil. $[\alpha]_D^{27}$ +83.5 (c, 0.3 in $CHCl_3$). λ_{max} 254 (log ϵ 3.77); 315 (log ϵ 3.53) ($CHCl_3$).

Shan, M.D. *et al., J. Nat. Prod.*, 2001, **64**, 127-130

Pyrazine, 9CI P-592

[290-37-9]
1,4-Diazine. Paradiazine. 1,4-Diazabenzene. Piazine (obsol.)



$C_4H_4N_2$ 80.089
Maillard product. Prisms (H_2O). Sol. H_2O, EtOH, Et_2O. Mp 54-56° (47°). Bp_{768} 115.5-115.8°. pK_{a1} -5.51; pK_{a2} 0.57 (25°, H_2O). Steam-volatile.

▶ LD_{50} (mus, ipr) 2730 mg/kg. UQ2015000

Sulfate:
Mp 136-137°.

Picrate: [65816-19-5]
Yellow needles (EtOH). Mp 157°.

1-Oxide: [2423-65-6]
$C_4H_4N_2O$ 96.088
Needles (C_6H_6). Mp 113-114°.

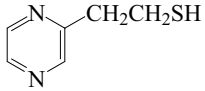
1,4-Dioxide: [2423-84-9]
$C_4H_4N_2O_2$ 112.088
Needles (MeOH). Mp 285-295°.

N-*Me:* [6277-35-6] *1-Methylpyrazinium(1+)*
$C_5H_7N_2^{\oplus}$ 95.124
Cryst. (as iodide). Sol. H_2O, EtOH, Et_2O. CAS no. refers to iodide.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 397A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 839D (*ir*)
Aston, J.G. *et al., J.A.C.S.*, 1934, **56**, 153 (*synth*)
Koelsch, C.F. *et al., J.O.C.*, 1958, **23**, 1603 (*oxides*)
Cheeseman, G.W.H. *et al., Adv. Heterocycl. Chem.*, 1972, **14**, 99 (*rev*)
Kobayashi, Y. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2097 (*oxides*)
Rao, G.V. *et al., Indian J. Chem.*, 1975, **13**, 1090 (*pmr*)
Wadt, W.R. *et al., J.A.C.S.*, 1975, **97**, 2034 (*struct*)
DeWith, G. *et al., Acta Cryst. B*, 1976, 3178 (*cryst struct*)
Toma, H.E. *et al., CA*, 1977, **87**, 77908f (*methiodide, detn, CO, $CN^{\ominus}$, sulfoxides*)
Matsuo, M. *et al., Org. Magn. Reson.*, 1980, **13**, 172 (*cmr*)
Bolovinos, A. *et al., J. Mol. Spectrosc.*, 1984, **103**, 240 (*uv*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
Arenas, J.F. *et al., J.C.S. Faraday 2*, 1985, **81**, 405 (*ir, Raman*)
Cradock, S. *et al., J.A.C.S.*, 1988, **110**, 2758 (*struct*)

Pyrazineethanethiol, 9CI P-593

[35250-53-4]
2-(2-Mercaptoethyl)pyrazine. FEMA 3230

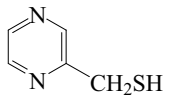


$C_6H_8N_2S$ 140.209
Flavouring ingredient. Bp 220° $Bp_{0.05}$ 57-59°.

U.S. Pat., 1975, 3 924 015; *CA*, **84**, 164364g (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 707 (*use*)
Hérent, M.-F. *et al., J. Agric. Food Chem.*, 1998, **46**, 1975-1980 (*hplc, props*)

Pyrazinemethanethiol, 9CI P-594

[59021-02-2]
2-(Mercaptomethyl)pyrazine

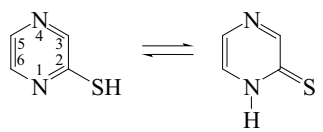


$C_5H_6N_2S$ 126.182
Liq. with roasted, meat-like flavour. Liq. with roasted, meat-like flavour. $Bp_{0.07}$ 44-45°.

U.S. Pat., 1965, 3 924 015; *CA*, **84**, 164364g (*synth, use*)
Barnes, J.H. *et al., Eur. J. Med. Chem. (Chim. Ther.)*, 1983, **18**, 515-519 (*synth*)
Burdock, G.A. *et al., Acute Toxic. Data*, 1990, **1**, 4 (*tox*)

2-Pyrazinethiol, 9CI P-595

[38521-06-1]
2(1H)-Pyrazinethione, 9CI. 2-Mercaptopyrazine



$C_4H_4N_2S$ 112.155
Exists mainly in the thione form in aq. soln..Orange solid or yellow plates. Mp 229° (215-218°) dec. pK_a 6.72 (50% EtOH aq., anion). Mp is not a reliable criterion of purity.

SH-form

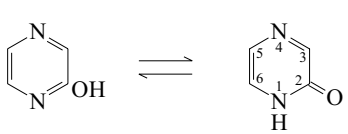
S-*Me:* [21948-70-9] *2-(Methylthio)pyrazine. Pyrazinyl methyl sulfide. FEMA 3231*
$C_5H_6N_2S$ 126.182
Flavouring ingredient. Pale cream solid. Mp 44-47°.

Disulfide: [98437-14-0] *Di(2-pyrazinyl)disulfide*
$C_8H_6N_4S_2$ 222.294
Mp 107-109°.

Roblin, R.O. *et al., J.A.C.S.*, 1950, **72**, 4890 (*synth*)
Cheeseman, G.W.H. *et al., J.C.S.*, 1960, 242 (*synth, uv, tautom*)
Albert, A. *et al., J.C.S.*, 1962, 3129 (*synth*)
Barlin, E.B. *et al., Aust. J. Chem.*, 1986, **39**, 69 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 708
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2386-2387

Pyrazinol, 8CI P-596

2-Hydroxypyrazine. 2(1H)-Pyrazinone



$C_4H_4N_2O$ 96.088
NH-form predominates.Cryst. (C_6H_6).

Mp 185-186°. pK_{a1} -0.1; pK_{a2} 8.25 (20°, H_2SO_4 aq.).

OH-form

Me ether: [3149-28-8] *Methoxypyrazine. FEMA 3302*

$C_5H_6N_2O$ 110.115

Flavouring agent. Present in cooked beef and cocoa. Bp_{29} 60-61° (Bp_{28} 68°). pK_a 0.75. Odour threshold 700 ppb in H_2O.

▶ Skin and eye irritant.

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, MFN285

Plé, N. *et al., Synthesis*, 1996, 838 (*Me ether*)

Pyridine, 9CI, 8CI P-597

[110-86-1]

Azabenzene. Azine. FEMA 2966



C_5H_5N 79.101

Flavouring ingredient. Liq. with characteristic unpleasant odour and sharp taste. Misc. H_2O, petrol, Et_2O, etc. d_4^{25} 0.98. Fp -42. Bp 115.5°. n_D^{21} 1.5092. pK_a 5.58 (25°). pK_a 5.23 (25°). Forms azeotropic mixt. with 3 mols. H_2O, Bp 92-3°. Hygroscopic. Steam-volatile.

▶ Flammable, fl. p. 17°, autoignition temp. 482°. Eye and skin irritant. May cause dermatitis. CNS depressant by inhalation; symptoms include headache, vertigo, insomnia, nausea. Prolonged or repeated exposure injures kidney and liver. LD_{50} (rat, orl) 891 mg/kg. LD_{50} (rbt, skn) 1121 mg/kg. OES: long-term 5 ppm; short-term 10 ppm. UR8400000

[7291-22-7, 16969-45-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 729A; 729B; 730B; 730D (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 233A; 233B; 233C; 237A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1513A (*ir*)

Barnes, R.A. *et al., Chem. Heterocycl. Compd.*, (Part 1), 1960, **14**, (*rev, bibl*)

Luckner, M. *et al., Pharmazie*, 1964, **19**, 1 (*biosynth*)

Cumper, C.W.N. *et al., J.C.S.(B)*, 1968, 649 (*uv*)

Dickinson, R. *et al., J.C.S. Perkin 2*, 1972, 1363 (*ms*)

Boodman, N.S. *et al., Chem. Heterocycl. Compd.*, Suppl. 1, 1974, **14**, 183 (*synth*)

Talukdar, A.N. *et al., Acta Cryst. B*, 1976, **32**, 803 (*cryst struct*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 454 (*rev*)

Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 705

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2387-2388

Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 2nd edn., Butterworths*, 1979, 525; 527

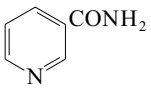
Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 465; 466

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MOZ000; PPC100; POP250; POR750

3-Pyridinecarboxamide, 9CI P-598

[98-92-0]

Nicotinamide, 8CI, INN. *Niacinamide. Nicotinic acid amide. Antipellagra factor. PP-Factor. Vitamin B_3. Many other names*



$C_6H_6N_2O$ 122.126

Widespread in plants, e.g. rice, yeast and fungi. Dietary supplement, may be used in infant formulas. Needles (C_6H_6). Mp 129-130°. $Bp_{0.0005}$ 150-160°. pK_a 3.33 (20°). Log P -0.21 (calc).

▶ QS3675000

[6485-44-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 796B; 917A (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 338B; 342B (*nmr*)

La Forge, F.B. *et al., J.A.C.S.*, 1928, **50**, 2477 (*synth*)

Georg, A. *et al., Helv. Chim. Acta*, 1943, **26**, 358 (*synth*)

Rohrlich, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1950, **283**, 122 (*synth*)

Hackley, B.B. *et al., J.A.C.S.*, 1955, **77**, 3651 (*synth, deriv*)

Birdsall, B. *et al., J.C.S. Perkin 2*, 1972, 1643; 1973, 2145 (*cmr, pmr*)

Auerbach, J. *et al., J.O.C.*, 1976, **41**, 725 (*synth*)

Chen, P.H. *et al., J.O.C.*, 1976, **41**, 2973 (*ms*)

Busha, A. *et al., Synth. Commun.*, 1977, **7**, 549 (*synth, deriv*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **24**, 59 (*rev*)

Oppenheimer, N.J. *et al., Org. Magn. Reson.*, 1980, **13**, 14 (*N-15 nmr*)

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 410

El-Shahawy, A.S. *et al., Spectrochim. Acta A*, 1987, **43A**, 1371 (*uv*)

Abdel Moety, E.M. *et al., Anal. Profiles Drug Subst.*, 1991, **20**, 475 (*rev*)

Bender, D.A. *et al., Nutritional Biochemistry of the Vitamins*, Cambridge University Press, Cambridge, 1992, 184 (*rev*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1045

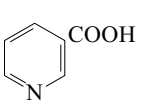
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1953-1955 (*use, props*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NCR000

3-Pyridinecarboxylic acid P-599

[59-67-6]

Nicotinic acid, INN. *Niacin, USAN. Nicamin. Nicobid. Wampocap. Many other names*



$C_6H_5NO_2$ 123.111

Present in fruits and other plant materials. Nutrient supplement. Vitamin, enzyme cofactor. Approved for clinical use in the UK (1999)Needles (H_2O or EtOH). Sol. hot H_2O; spar. sol. Et_2O. Mp 236° (225-227°). pK_{a1} 2; pK_{a2} 4.82 (25°). Log P 0.8 (calc). Sublimes.

▶ Can cause dermal and gastrointestinal reactions and hepatic effects at high therapeutic doses. Low acute mammalian toxicity. QT0525000

Me ester: [93-60-7] *FEMA 3709*

$C_7H_7NO_2$ 137.138

Flavouring ingredient. Present in guava fruit, papaya, strawberry, soursop (*Annona muricata*), beer, grape brandy, coffee, roasted filbert, roasted peanut and Bourbon vanilla. Cryst. Mp 38°. Bp 204° Bp_{25} 118.5°. Log P 0.77 (calc).

▶ QT1925000

[1976-28-9]

Org. Synth., Coll. Vol., 1, 1932, 385 (*synth*)

Oliveto, E.P. *et al., Chem. Heterocycl. Compd.*, (Part 3), 1962, **14**, 179 (*bibl*)

Bild, N. *et al., Helv. Chim. Acta*, 1967, **50**, 1885 (*ms*)

Poluektov, N.S. *et al., Zh. Anal. Khim.*, 1971, **26**, 541 (*detn, U*)

Pollak, P.I. *et al., Chem. Heterocycl. Compd.*, Suppl. 3, 1974, **14**, (*bibl*)

Paraskewas, S. *et al., Synthesis*, 1974, 819 (*synth*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **24**, 59 (*rev*)

Dommisse, R. *et al., Heterocycles*, 1981, **16**, 1893 (*cmr*)

Staedeli, W. *et al., Org. Magn. Reson.*, 1981, **15**, 106 (*N-15 nmr*)

Kutoglu, A. *et al., Acta Cryst. C*, 1983, **39**, 232 (*cryst struct*)

Hotz, W. *et al., Adv. Lipid Res.*, 1983, **20**, 195 (*rev, pharmacol*)

Weiner, M. *et al., Clin. Pharmacol. Vol. 1: Nicotinic Acid Nutrient-Cofactor-Drug*, Dekker, N.Y., 1983, (*book*)

Sauberlich, H.E. *et al., Coenzymes Cofactors*, 1987, **2**, 599; 627 (*revs*)

Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 394 (*synonyms*)

El-Shahawy, A.S. *et al., Spectrochim. Acta A*, 1987, **43**, 1371 (*uv*)

Cossio, F.P. *et al., Tetrahedron*, 1987, **43**, 3963 (*synth*)

de Oliveira, S.M. *et al., Org. Mass Spectrom.*, 1991, **26**, 855 (*ms*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1045

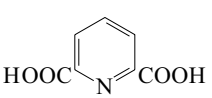
Chattopadhyay, S. *et al., Spectrochim. Acta A*, 1993, **49**, 589 (*ir, Raman*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1806-1807; 1951-1973 (*props, use, Me ester*)

2,6-Pyridinedicarboxylic acid, 9CI, 8CI P-600

[499-83-2]

Dipicolinic acid



$C_7H_5NO_4$ 167.121

Used in sterilising solns. to control the growth of microorganisms in food pro-

ducts. Cryst. + 1½H_2O (H_2O). Mp 252° dec. (anhyd.). pK_{a1} 2.24; pK_{a2} 4.67 (25°). λ_{max} 270 ; 278 (MeOH) (Berdy).

N-*Oxide:* [15905-16-5]
$C_7H_5NO_5$ 183.12
Cryst. (H_2O). Mp 162° (160° dec.).

Mono-Me ester: [7170-36-7]
$C_8H_7NO_4$ 181.148
Cryst. (C_6H_6). Mp 149-150°. pK_a 2.65 (25°).

Di-Me ester: [5453-67-8]
$C_9H_9NO_4$ 195.174
Prisms. Mp 121°. $Bp_{0.5}$ 155-160°.

Mono-Et ester: [21855-16-3]
$C_9H_9NO_4$ 195.174
Mp 121.5°.

Di-Et ester: [15658-60-3]
$C_{11}H_{13}NO_4$ 223.228
Cryst. Mp 44-46° (41-42°). Bp_1 158°.

Bis(2-hydroxyethyl) ester:
$C_{11}H_{13}NO_6$ 255.227
Solid ($CHCl_3$). Mp 116-118°.

Dibutyl ester: [41727-17-7]
$C_{15}H_{21}NO_4$ 279.335
Mp 63-64°.

Di-Ph ester: [10448-12-1]
$C_{19}H_{13}NO_4$ 319.316
Cryst. ($CHCl_3$/petrol). Mp 175°.

Dichloride: [3739-94-4]
$C_7H_3Cl_2NO_2$ 204.012
Cryst. (C_6H_6). Mp 56-58°. Bp 284°.

Diamide: [4663-97-2]
$C_7H_7N_3O_2$ 165.151
Solid.

Diamide, dioxime: See 2,6-Pyridinediamidoxime in *The Combined Chemical Dictionary.*

Bis(diethylamide): [36763-33-4]
$C_{15}H_{23}N_3O_2$ 277.366
Cryst. (hexane). Mp 75°.

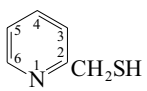
Dihydrazide: [5112-36-7]
$C_7H_9N_5O_2$ 195.18
Needles (H_2O). Mp 290-292° dec. (285°).

Dinitrile: [2893-33-6] *2,6-Dicyanopyridine*
$C_7H_3N_3$ 129.121
Mp 123°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 791D; 795D
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 327B; 334A; 337B (*nmr*)
Black, G. *et al., J.O.C.*, 1949, **14**, 14-21 (*synth*)
Biemann, K. *et al., J.A.C.S.*, 1957, **79**, 5558-5564 (*synth, ir*)
Hartkamp, H. *et al., Fresenius' Z. Anal. Chem.*, 1961, **184**, 98-107; 1962, **187**, 16-29; 1964, **199**, 183-196 (*detn, Ag, Mn, Cr*)
Pearse, G.A. *et al., Anal. Chem.*, 1962, **34**, 536-537 (*detn, V*)
Oliveto, E.P. *et al., Chem. Heterocycl. Compd.*, (Part 3), 1962, **14**, 179-346 (*bibl*)
Hasegawa, M. *et al., Kogyo Kagaku Zasshi*, 1962, **65**, 661-664; *CA*, **57**, 16909h (*polyamides*)
Terent'ev, A.P. *et al., Vysokomol. Soedin.*, 1963, **5**, 837-841; *CA*, **59**, 8882c (*polyamides*)
Den Boef, G. *et al., Fresenius' Z. Anal. Chem.*, 1964, **199**, 348-352 (*detn, Cr*)
Bodalski, R. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1964, **38**, 1337; *CA*, **62**, 1627 (*synth*)
Brown, E.V. *et al., J. Het. Chem.*, 1971, **8**, 189-192 (*ms*)
Takusagawa, F. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2020-2027 (*cryst struct*)
Marangoni, G. *et al., Talanta*, 1973, **20**, 1217-1220 (*detn, U*)
Pollak, P.I. *et al., Chem. Heterocycl. Compd.*, Suppl. 3, 1974, **14**, 257-330 (*bibl*)
Mišič-Vuković, M. *et al., J.C.S. Perkin 2*, 1978, 34-38 (*Me ester, synth*)
Rasshofer, W. *et al., Chem. Ber.*, 1979, **112**, 2095-2119 (*esters*)
Carmona, P. *et al., Spectrochim. Acta A*, 1980, **36**, 705-712 (*ir, Raman*)
Baker, A.T. *et al., Aust. J. Chem.*, 1991, **44**, 1041-1048 (*diamide*)
Iovel, I. *et al., Synth. Commun.*, 1992, **22**, 2691-2696 (*synth, biol*)
Thummel, R.P. *et al., J.O.C.*, 1993, **58**, 1666-1671 (*oxide, synth, pmr, cmr, ir*)
Chênevert, R. *et al., J.O.C.*, 1996, **61**, 3332-3341 (*di-Me ester, pmr, cmr*)
Renault, F. *et al., Chem. Eur. J.*, 1997, **3**, 1646-1659; 1660-1667 (*diethylamide, di-Et ester, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2388
El-ghayouri, A. *et al., J.O.C.*, 2000, **65**, 7757-7763 (*dibutyl ester*)
Habata, Y. *et al., J. Het. Chem.*, 2001, **38**, 1323-1327 (*bishydroxyethyl ester*)
Carranza Téllez, V. *et al., Acta Cryst. C*, 2002, **58**, o228-o230 (*cryst struct*)

2-Pyridinemethanethiol, 9CI P-601

[2044-73-7]
2-(Thiomethyl)pyridine. 2-(Mercaptomethyl)pyridine. FEMA 3232



C_6H_7NS 125.194
Flavouring ingredient. Oil. d^{25} 1.15. Bp_{10} 87-89°. n_D^{20} 1.5758.

Picrate:
Yellow prisms (MeOH). Mp 171-172°.

S-*Me:* [3145-77-5] *2-[(Methylthio)-methyl]pyridine, 9CI*
C_7H_9NS 139.221
Liq. Bp_{17} 100-105°.

S-*Ph:* [71897-63-7]
$C_{12}H_{11}NS$ 201.292
d_{25} 1.15. Mp 124-125° (as picrate). $Bp_{0.1}$ 97-98°. n_D^{25} 1.6238.

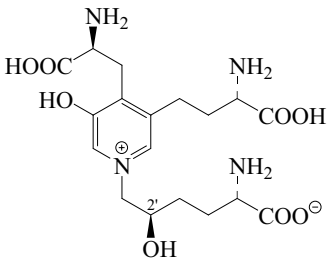
U.S. Pat., 1960, 2 951 848; *CA*, **55**, 4542b (*synth*)
Clechet, P. *et al., Bull. Soc. Chim. Fr.*, 1964, 2644-2658 (*synth*)
Sutton, G.J. *et al., Aust. J. Chem.*, 1966, **19**, 733-739 (*synth*)
Brembilla, A. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1986, **83**, 577-588 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 709
Remuzon, P. *et al., Tetrahedron*, 1995, **51**, 9657-9670 (*synth, pmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2389
Holland, H.L. *et al., Can. J. Chem.*, 1999, **77**, 463-471 (*S-Me*)

Pyridinoline P-602

[77464-35-8]

[63800-01-1, 79646-35-8, 125659-26-9, 128112-67-4, 220243-86-7]

4-(2-Amino-2-carboxyethyl)-1-(5-amino-5-carboxy-2-hydroxypentyl)-3-(3-amino-3-carboxypropyl)-5-hydroxypyridinium(1+), 9CI. Hydroxylysylpyridinoline



$C_{18}H_{28}N_4O_8^{\oplus}$ 428.441
Several diastereomers possible. -ve charge also shown on the phenolic O. Derived from collagen cross-links formed between adjacent hydroxylysine residues in type I and type II collagen of bone and cartilage respectively. Released into serum during bone resorption. Solid. $[\alpha]_D^{20}$ +39.17 (c, 0.24 in MeOH) (as trifluoroacetate salt). CAS no refers to hydroxide inner salt.

2′-Deoxy: [82637-02-3]

[83462-55-9, 90032-33-0, 119241-22-4, 200405-37-4, 220243-98-1] ***Deoxypyridinoline**. Lysylpyridinoline*
$C_{18}H_{28}N_4O_7^{\oplus}$ 412.442
Derived from collagen cross-links formed between adjacent lysine residues in type I collagen of bone and dentine. Released into serum during bone resorption. Pale yellow solid (as trifluoroacetate salt). $[\alpha]_D^{20}$ +31.6 (c, 0.25 in MeOH) (as trifluoroacetate).

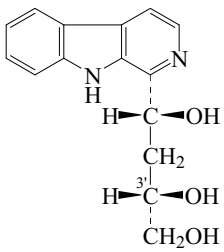
2′-Epimer: [220348-30-1]
$C_{18}H_{28}N_4O_8^{\oplus}$ 428.441
$[\alpha]_D^{20}$ +43.23 (c, 0.26 in MeOH) (as trifluoroacetate salt). CAS no. refers to trifluoroacetate.

Fujimoto, D. *et al., Biochem. Biophys. Res. Commun.*, 1977, **76**, 1124-1129; 1978, **84**, 52-57 (*isol, uv, pmr, cmr, nmr, ms, fluorescence*)
Ogawa, T. *et al., Biochem. Biophys. Res. Commun.*, 1982, **107**, 1252-1257 (*Deoxypyridinoline, isol, pmr*)
Barber, M. *et al., Biochem. Biophys. Res. Commun.*, 1982, **109**, 1041-1046 (*struct, ms, uv*)
Black, D. *et al., Anal. Biochem.*, 1988, **169**, 197-203 (*deoxypyridinoline, isol, chromatog*)
Acil, Y. *et al., J. Chromatogr., A*, 1994, **664**, 183-188 (*isol*)
Arbault, P. *et al., J. Liq. Chromatogr.*, 1994, **17**, 1981-1993 (*isol, chromatog*)
McGuinness, B.J. *et al., Biochem. Soc. Trans.*, 1995, **23**, 3865 (*deoxypyridinoline, pmr*)
Waelchli, R. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 2831-2836 (*synth*)
Lamprecht, G. *et al., J. Chromatogr., B: Biomed. Appl.*, 1997, **691**, 297-304 (*deoxypyridinoline, isol, chromotog*)
Knott, L. *et al., Bone*, 1998, **22**, 181-187 (*rev*)
St Clair, E.W. *et al., J. Rheumatol.*, 1998, **25**, 1472-1479 (*detn, clinical*)
U.S. Pat., 1998, 5 723 619; *CA*, **128**, 205137s (*synth*)
Yilmaz, N. *et al., Clin. Chem. Lab. Med.*, 1999, **37**, 137-143 (*detn, Deoxypyridinoline*)

Adamczyk, M. *et al., Tetrahedron*, 1999, **55**, 63-88; 2000, **56**, 2379-2390 (*synth, pyridinoline, deoxypyridinoline, pmr, cmr, bibl*)
Adamczyk, M. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 2289-2298 (***synth, pyridinoline, 2′-deoxy, pmr***)

4-(9*H*-Pyrido[3,4-*b*]indol-1-yl)-1,2,4-butanetriol, 9CI P-603

*1-(1,3,4-Trihydroxybutyl)-9*H*-pyrido[3,4-*b*]indole*



$C_{15}H_{16}N_2O_3$ 272.303

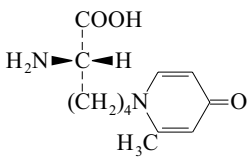
(2*S*,4*R*)-*form* [220345-69-7]
Maillard reaction product from xylose and tryptophan. Pale yellow powder.

3′-Deoxy: [220345-68-6] *1-(9*H*-Pyrido[3,4-*b*]indol-1-yl)-1,4-butanediol, 9CI. 1-(1,4-Dihydroxybutyl)-9*H*-pyrido[3,4-*b*]indole*
$C_{15}H_{16}N_2O_2$ 256.304
Maillard prod. from xylose and tryptophan. Pale yellow powder.

Wang, M. *et al., J. Agric. Food Chem.*, 1999, **47**, 48-50 (*formn, pmr, cmr, uv*)

Pyridosine P-604

α-Amino-5-hydroxy-2-methyl-4-oxo-1(4H)-pyridinehexanoic acid, 9CI. ϵ-(1,4-Dihydro-3-hydroxy-6-methyl-4-oxo-1-pyridyl)lysine



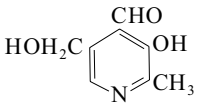
$C_{12}H_{18}N_2O_4$ 254.285

(*S*)-*form* [31489-08-4]
L-form
Acid hydrolysis product of heated milk. Marker for heat treatment of milk and other foodstuffs.

Bricout, J. *et al., Experientia*, 1969, **25**, 134 (*isol, synth*)
Sulser, H. *et al., Lebensm.-Wiss. Technol.*, 1973, **6**, 66-69 (*occur*)
Steinig, J. *et al., Z. Lebensm.-Unters. -Forsch.*, 1982, **174**, 453-457 (*occur, anal*)

Pyridoxal P-605

[66-72-8]
3-Hydroxy-5-hydroxymethyl-2-methyl-4-pyridinecarboxaldehyde, 9CI. 3-Hydroxy-5-hydroxymethyl-2-methylisonicotinic aldehyde

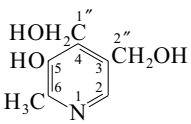


$C_8H_9NO_3$ 167.164
Exhibits vitamin B_6 activity. pK_{a1} 4.2; pK_{a2} 8.66; pK_{a3} 13 (25°).
▶ UV1200600

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 309C (*nmr*)
Harris, S.A. *et al., J.A.C.S.*, 1944, **66**, 2088 (*synth*)
Ahrens, H. *et al., J. Het. Chem.*, 1967, **4**, 625 (*synth*)
de Jongh, D.C. *et al., Org. Mass Spectrom.*, 1968, **1**, 151 (*ms*)
Gansow, O.A. *et al., Tetrahedron*, 1968, **24**, 4477 (*pmr*)
Lapper, R.D. *et al., Can. J. Chem.*, 1975, **53**, 2406 (*cmr*)
Gregory, J.F. *et al., J. Nutr.*, 1983, **113**, 722 (*uv*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSU000

Pyridoxine, BAN, INN P-606

[65-23-6]
5-Hydroxy-6-methyl-3,4-pyridinedimethanol, 9CI. Vitamin B_6, 8CI. 3-Hydroxy-4,5-bis(hydroxymethyl)-2-methylpyridine. Adermin. Pyridoxol. Many other names



$C_8H_{11}NO_3$ 169.18
Found in rice husks, cane molasses, yeast, wheat germ and cod liver oils. Vitamin, dietary supplement, nutrient. Needles (Me_2CO). Mp 160°. pK_{a1} 5; pK_{a2} 8.96 (25°, 0.15*M* NaCl). Log P -0.7 (calc). Readily sublimes.
▶ LD_{50} (rat, orl) 4000 mg/kg. UV1300000

Hydrochloride: [58-56-0] ***Pyridoxine hydrochloride, USAN***. *Aderoxin. Becilan. Gravidox*
Rhombic cryst. (EtOH/Me_2CO). Mp 206-208°. Component of Bendectin and Debendox.
▶ Long-term treatment with large doses associated with development of peripheral neuropathies. Human and exp. reprod. effects. LD_{50} (rat, orl) 4000 mg/kg. UV1350000

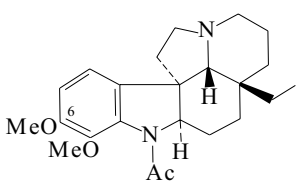
$O^{1''}$-*Me:* [1464-33-1] *5-Hydroxy-4-(methoxymethyl)-6-methyl-3-pyridinemethanol, 9CI. 3-Hydroxy-5-hydroxymethyl-4-methoxymethyl-2-methylpyridine. 4′-Methoxypyridoxine.* ***Ginkgotoxin***
$C_9H_{13}NO_3$ 183.207
Isol. from seeds of maidenhair tree *Ginkgo biloba*. Mp 181° (as hydrochloride).
▶ LD_{50} (mus, orl) 32 mg/kg. UT5009000

[3131-27-9, 8064-77-5, 62154-08-9, 62602-94-2, 63797-00-2, 70829-29-7, 74536-44-0, 79636-52-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 759D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 282B; 283A (*nmr*)
Harris, S.A. *et al., J.A.C.S.*, 1939, **61**, 1245; 3307 (*synth*)
Mowatt, J.H. *et al., J.A.C.S.*, 1943, **65**, 954 (*synth*)
De Jongh, D.C. *et al., J.A.C.S.*, 1966, **88**, 1233 (*ms*)
Firestone, R.A. *et al., Tetrahedron*, 1967, **23**, 943 (*synth, ir, uv*)
Fourneau, J.P. *et al., Boll. Chim. Farm.*, 1970, **109**, 702 (*rev*)
Witherup, T.H. *et al., J.O.C.*, 1975, **40**, 2229 (*cmr*)
Hill, R.E. *et al., J.A.C.S.*, 1977, **99**, 4179 (*biosynth, cmr*)
Coffen, D.L. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **24**, 94 (*rev*)
Longo, J. *et al., Acta Cryst. B*, 1982, **38**, 2721 (*cryst struct*)
Aboul-Enein, H.Y. *et al., Anal. Profiles Drug Subst.*, 1984, **13**, 447 (*rev, synth, anal, pharmacol*)
Shimada, S. *et al., Chem. Pharm. Bull.*, 1984, **32**, 38 (*synth*)
Wada, K. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3555; 1988, **36**, 1779 (*Ginkgotoxin*)
Parnell, C.A. *et al., Tetrahedron*, 1985, **41**, 5791 (*synth*)
Likos, J.J. *et al., Vitamin B_6 Pyridoxal Phosphate: Chemical, Biochemical and Medical Aspects, Part A*, (ed. Dolphin, D. *et al*), Wiley-Interscience, 1986, 13 (*rev*)
Korpela, T. *et al., Biochemistry of Vitamin B_6*, Birkhäuser Verlag, 1987, (*book*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 951
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PPK500
Dakshinamurti, K. *et al., Ann. N.Y. Acad. Sci.*, 1990, **585**, 1 (*revs*)
Lycka, A. *et al., Pharmazie*, 1990, **45**, 371 (*N-15 nmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1054; 1318; 1403
Spenser, I.D. *et al., Nat. Prod. Rep.*, 1995, **12**, 555 (*rev, biosynth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2389; 2391 (*rev*)
Fiehe, K. *et al., J. Nat. Prod.*, 2000, **63**, 185-189 (*Ginkgotoxin, biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MEY000; PPK250; PPK500; MFN600

Pyrifolidine P-607

[639-26-9]
1-Acetyl-16,17-dimethoxyaspidospermidine, 9CI



(−)-*forn*

$C_{23}H_{32}N_2O_3$ 384.517

(+)-*form*
Cryst. (MeOH aq.). Mp 147.5-150°. $[\alpha]_D^{26}$ +90 (c, 1.04 in $CHCl_3$).

Perchlorate:
Cryst. (MeOH aq.). Mp 255-260.5°.

N-*De-Ac:* [25139-33-7] ***Deacetylpyrifolidine***. O-*Methyl*-N-*depropionylaspidoli-*

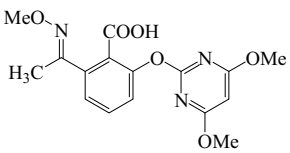
mine
$C_{21}H_{30}N_2O_2$ 342.48
Mp 147-149°. $[\alpha]_D^{25}$ +6.7 (c, 0.89 in $CHCl_3$).

(-)-*form*
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 148-150°. $[\alpha]_D^{28}$ -93 (c, 0.9 in $CHCl_3$).

Gilbert, B. *et al., Experientia*, 1960, **16**, 61 (*isol, uv, ir*)
Djerassi, C. *et al., Experientia*, 1961, **17**, 162 (*Deacetylpyrifolidine*)
Djerassi, C. *et al., Tetrahedron*, 1961, **16**, 212 (*isol, uv, ord*)
Biemann, K. *et al., J.A.C.S.*, 1963, **85**, 631 (*isol, uv, ms*)
Burnell, R.H. *et al., Phytochemistry*, 1968, **7**, 2045 (*synth, uv, ir, pmr*)
Lyon, R.L. *et al., J. Pharm. Sci.*, 1973, **62**, 218 (*isol, uv, ir, pmr*)

Pyriminobac P-608

[136191-56-5]
2-[(4,6-Dimethoxy-2-pyrimidinyl)oxy]-6-[1-(methoxyimino)ethyl]benzoic acid, 9CI



(*E*)-*form*

$C_{16}H_{17}N_3O_6$ 347.327

(*E*)-*form*
Me ester: [136191-64-5]

[136023-17-1] ***Pyriminobac-methyl, BSI***. *Prosper. KIH 6127. KUH 920*
$C_{17}H_{19}N_3O_6$ 361.354
Herbicide used on rice. Cryst. (diisopropyl ether). Mp 105-106°. Mp given for one undefined geom. isomer, prob. *E*-form. Mixt. of (*E*)- and (*Z*)-isomers 4:1 used commercially; (*E*)-isomer (75-78%) is major component.

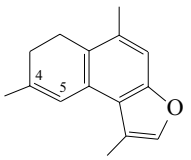
► LD_{50} (rat, orl) >5000 mg/kg.

(*Z*)-*form*
Me ester: [147411-70-9]
Mp 70° (59-60°).

Eur. Pat., 1991, 435 170; *CA*, **115**, 159183b (*synth, Me ester, activity*)
Japan. Pat., 1992, 04 368 361; *CA*, **118**, 234086q (*Me ester, E-form, Z-form*)
Hanai, R. *et al., Brighton Crop Prot. Conf. - Weeds*, 1993, 47-52 (*Me ester, activity*)
Nathan, S. *et al., Chem. Ind. (London)*, 1993, 931 (*Me ester, rev*)
Tamaru, M. *et al., Pestic. Sci.*, 1996, **47**, 125-130; 1997, **49**, 76-84 (*Me ester, synth, SAR*)
Tamaru, M. *et al., J. Agric. Food Chem.*, 1997, **45**, 2777-2783 (*Me ester, cryst struct*)
Pesticide Manual, 12th edn., 2000, No. 676

Pyrocurzerenone P-609

[20013-75-6]
6,7-Dihydro-1,5,8-trimethylnaphtho[2,1-b]-furan, 9CI



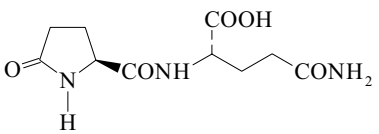
$C_{15}H_{16}O$ 212.291
Constit. of the rhizomes of *Curcuma zedoaria* (zedoary). Cryst. (petrol). Mp 76.5-77.5°. λ_{max} 233 (log ε 4.75); 239 (log ε 4.72); 249 (log ε 4.62); 283 (log ε 4.4); 293 (log ε 4.4) (EtOH).

4,5-Dihydro: [59462-26-9] ***Dihydropyrocurzerenone***
$C_{15}H_{18}O$ 214.307
Cryst. (petrol). Mp 65-66°. $[\alpha]_D^{17}$ -28 (c, 0.84 in $CHCl_3$).

Viswanatha, V. *et al., J.C.S. Perkin 1*, 1974, 450 (*synth*)
Hikino, H. *et al., J.C.S. Perkin 1*, 1975, 478-484 (*isol, struct*)
Takemoto, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 531 (*deriv*)
Miyashita, M. *et al., J.O.C.*, 1984, **49**, 3728 (*synth*)

Pyroglutaminylglutamine P-610

N^2-*(5-Oxoprolyl)glutamine, 9CI*



$C_{10}H_{15}N_3O_5$ 257.246

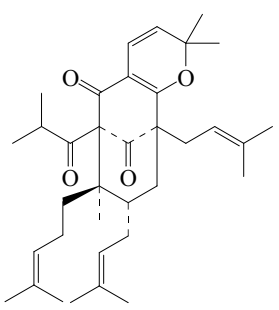
(2*S*,2′*S*)-*form* [109481-23-4]
L,L-form
Constit. of the seeds of *Dolichos biflorus* (papadi). Cryst. Mp 235-237° dec. $[\alpha]_D^{25}$ +36 (c, 0.2 in H_2O).

Me ester: [132210-14-1]
Mp 90-92°.

Handa, G. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 1156 (*isol, synth*)

Pyrohyperforin P-611

[303115-46-0]



$C_{35}H_{50}O_4$ 534.778
Constit. of *Hypericum perforatum* (St. John's Wort). Oil. $[\alpha]_D$ +83.5 (c, 0.28 in $CHCl_3$). λ_{max} 254 (log ε 3.77); 315 (log ε 3.53) ($CHCl_3$).

Shan, M.D. *et al., Chin. Chem. Lett.*, 2000, **11**, 701-704

Pyroligneous acid P-612

[8030-97-5]

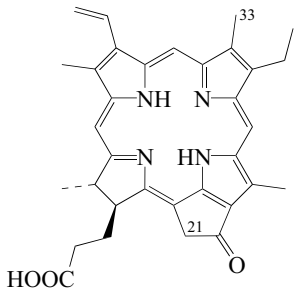
[8028-47-5]
Wood vinegar. Pyroligneous vinegar. Liquid smoke. Wood tar. FEMA 2967

Aq. distillate containing approx. 10% AcOH. Used for smoking meats and fish. Dark brown liq. Misc. H_2O, EtOH. A water-free extract is FEMA 2968.

Merck Index, 12th edn., 1996, 8187
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2393-2397 (*rev, use, props*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1564 (*use, props*)

Pyrophaeophorbide a P-613

[24533-72-0]
9-Ethenyl-14-ethyl-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoic acid, 9CI. Pyropheophorbide a



$C_{33}H_{34}N_4O_3$ 534.657
Isol. from tea. Cryst. (Et_2O). Mp 210°. $[\alpha]_D^{20}$ -342 (c, 1.12 in Me_2CO) (white light). λ_{max} 410 ; 509 ; 538 ; 608 ; 667 (MeOH). λ_{max} 273 ; 324 ; 410 ; 508 ; 539 ; 609 ; 666 (MeOH) (Berdy). λ_{max} 410 ; 509 ; 538 ; 608 ; 667 (EtOH) (Berdy).

Me ester: [6453-67-4]
$C_{34}H_{36}N_4O_3$ 548.683
Dark blue needles (Et_2O). Mp 220-225° (217-219°). $[\alpha]_D^{20}$ -388 (c, 1.39 in Me_2CO) (white light). λ_{max} 409 ; 507 ; 538 ; 608 ; 665 (MeOH).

*3,7*R,*5,11*R-*Tetramethyl-2*E-*hexadecenyl ester:* [14409-87-1] ***Pyropheophytin a***
$C_{53}H_{72}N_4O_3$ 813.177
Dark green oil. λ_{max} 415 ; 510 ; 540 ; 611 ; 668 ($CHCl_3$).

33-Oxo: [82040-65-1] *Pyrophaeophorbide b. Pyropheophorbide b*
$C_{33}H_{32}N_4O_4$ 548.64
Cryst. (CH_2Cl_2) (as Me ester). Mp 245-246° (Me ester).

*33-Oxo, 3,7*R,*5,11*R-*tetramethyl-2*E-*hexadecenyl ester:* [77331-75-0] ***Pyropheophytin b***
$C_{53}H_{70}N_4O_4$ 827.16
Constit. of various plants incl. spinach.

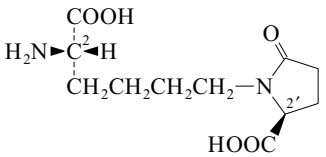
[25145-41-9]

Fischer, H. *et al., Die Chemie des Pyrrols*, Akademische Verlag, Leipzig, Vol. II, (ii), 1940, 73-75 (*rev*)
Pennington, F.C. *et al., J.A.C.S.*, 1964, **86**, 1418-1426 (*synth*)

Smith, K.M. *et al., Tetrahedron*, 1975, **31**, 367-375 (*cmr*)
Kenner, G.W. *et al., J.C.S. Perkin 1*, 1978, 845-852 (*synth*)
Wasielewski, M.R. *et al., J.O.C.*, 1980, **45**, 1969-1974 (*synth, uv, pmr*)
Smith, K.M. *et al., J.A.C.S.*, 1985, **107**, 4946-4954; 1988, **110**, 2854-2861 (*synth, uv, pmr*)
Risch, N. *et al., Annalen*, 1988, 343-347 (*synth, uv*)
Cahyana, A.H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1533-1535 (*Pyropheophytin A*)
Watanabe, N. *et al., J. Nat. Prod.*, 1993, **56**, 305-317 (*isol*)
Chansakaow, S. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1415-1417 (*isol, uv, ir, pmr, cmr, cd*)

Pyrosaccharopine P-614

[100568-98-7]
α-Amino-2-carboxy-5-oxo-1-pyrrolidine-hexanoic acid, 11CI. 1-(5-Amino-5-carboxypentyl)-5-oxoproline, 9CI



$C_{11}H_{18}N_2O_5$ 258.274

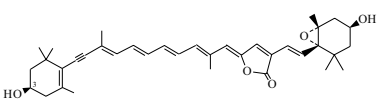
(2*S*,2′*S*)-*form* [38495-84-0]
Isol. from edible dried shiitake mushroom (*Lentinus edodes*) and buckwheat seeds (*Fagopyrum esculentum*). Cryst. (Me_2CO aq.); needles (EtOH aq.). Mp 245-248° dec. (225-227°). $[\alpha]_D$ +9.3 (c, 0.5 in H_2O). $[\alpha]_D$ +18.2 (c, 0.9 in 1*M* HCl). Possibly an artifact, in some cases arising from lactonisation of Saccharopine, S-3.

[100484-55-7]

Larsen, P.O. *et al., Acta Chem. Scand.*, 1972, **26**, 2562 (*synth*)
Nabeta, K. *et al., Agric. Biol. Chem.*, 1973, **37**, 1401-1406 (*isol*)
Soerensen, H. *et al., Phytochemistry*, 1976, **15**, 1527 (*isol*)
Aoyagi, Y. *et al., Agric. Biol. Chem.*, 1982, **46**, 987 (*isol*)
Burkard, U. *et al., Annalen*, 1986, 1030 (*synth, cmr, pmr*)

Pyrrhoxanthinol P-615

[54369-11-8]



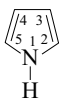
$C_{37}H_{46}O_5$ 570.767
Constit. of *Mytilus edulis* (blue mussel). Oil.

3-Ac: [54369-13-0] ***Pyrrhoxanthin***
$C_{39}H_{48}O_6$ 612.805
Oil. λ_{max} 466 (EtOH). λ_{max} 487 (hexane).

Johansen, J.E. *et al., Phytochemistry*, 1974, **13**, 2261 (*isol*)
Fiksdahl, A. *et al., Biochem. Syst. Ecol.*, 1979, **7**, 173 (*isol*)
Skjenstad, T. *et al., Biochem. Syst. Ecol.*, 1984, **12**, 149 (*Pyrrhoxanthin, isol, pmr, cmr*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*isol, pmr, uv, ms*)
Ito, M. *et al., J.C.S. Perkin 1*, 1990, 197 (*Pyrrhoxanthin, synth*)
Aakermann, T. *et al., Phytochemistry*, 1992, **31**, 1779 (*isol, synth, abs config*)
Yamano, Y. *et al., J.C.S. Perkin 1*, 1993, 1599 (*Pyrrhoxanthin, synth*)

Pyrrole, 8CI P-616

[109-97-7]
Azole. FEMA 3386



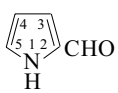
C_4H_5N 67.09
Flavouring ingredient. Liq. with characteristic odour. Sol. EtOH, Et_2O, C_6H_6; insol. H_2O. d_4^{20} 0.97. Mp -24°. Bp_{761} 130-131°. n_D^{20} 1.5085. pK_{a1} -3.8; pK_{a2} 17.51 (25°, KOH aq.). pK_a 23.05 (DMSO). Turns brown in air. Forms metallic salts. Trimerises with HCl. Nitroprussiates in alkali → red col. which turns blue on addn. of acids.
▶ Flammable, fl. p. 39°. Irritant. CNS depressant. LD_{50} (mus, scu) 61mg/kg. UX9275000

[287-95-6, 287-97-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 565A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 1A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1445A (*ir*)
Menczel, S. *et al., Z. Phys. Chem.*, 1927, **125**, 161 (*uv*)
Org. Synth., Coll. Vol., 1, 1932, 473-474 (*synth*)
Jennings, A.L. *et al., J.O.C.*, 1964, **29**, 2065 (*ms*)
Katekar, G.F. *et al., Aust. J. Chem.*, 1969, **22**, 1199 (*pmr, cmr, N-15 nmr*)
Catalotti, R. *et al., Can. J. Chem.*, 1976, **54**, 2451 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 499 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 710
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2397-2398
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2700
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 268

1*H*-Pyrrole-2-carboxaldehyde, 9CI P-617

[1003-29-8]
Pyrrole-2-aldehyde. 2-Formylpyrrole



C_5H_5NO 95.101
Constit. of numerous plant spp. incl. tea, coffee and various legumes. Prisms (petrol). Mp 50-51°. Bp 217-219° Bp_2 78°.

N-*Me:* [1192-58-1] *1-Methyl-2-pyrrolecarboxaldehyde*
C_6H_7NO 109.127
Maillard product. Oil with odour resembling benzaldehyde. Bp_{32} 94-96° Bp_{11} 75-76°. On boiling rapidly turns yellow, then purple, finally deep red. Stable in alkali resinifies with acids.
▶ UX9350000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 568B; 568C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 6C; 7A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1448A; 1448B (*ir*)
Smith, G.F. *et al., J.C.S.*, 1954, 3842 (*synth*)
Silverstein, R.M. *et al., J.O.C.*, 1955, **20**, 668 (*synth*)
Fournari, P. *et al., Bull. Soc. Chim. Fr.*, 1963, 488 (*1-Me*)
Org. Synth., Coll. Vol., 4, 1963, 831 (*synth*)
Khan, M.K.A. *et al., J.C.S.*, 1964, 2579 (*ir*)
Jones, R.F. *et al., J.C.S.(C)*, 1970, 2563 (*synth*)
Matsuo, T. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1349 (*uv*)
Chadwick, D.J. *et al., Tet. Lett.*, 1974, 3183 (*nmr*)
Cushley, R.J. *et al., Can. J. Chem.*, 1975, **53**, 148 (*cmr*)
Severin, T. *et al., Chem. Ber.*, 1975, **108**, 1768 (*1-Me*)
Limage, M.H. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1975, **72**, 914 (*ir, Raman*)
Nikisch, K. *et al., Chem. Ber.*, 1980, **113**, 2036 (*synth, ir, pmr*)
Boykin, D.W. *et al., J. Het. Chem.*, 1988, **25**, 643 (*O-17 nmr*)
Katritzky, A.R. *et al., Org. Prep. Proced. Int.*, 1988, **20**, 585 (*synth*)
Pindur, U. *et al., J. Het. Chem.*, 1989, **26**, 1563 (*synth, ir, ms, pmr*)
Wallace, D.M. *et al., J.O.C.*, 1993, **58**, 7245 (*synth, deriv, pmr*)

Pyrrolidine, 9CI, 8CI P-618

[123-75-1]
Tetrahydropyrrole. Tetramethyleneimine. Azacyclopentane. FEMA 3523



C_4H_9N 71.122
More complex acyl derivatives not given here may be listed as pyrrolidides under the parent carboxylic acids. Widely distributed in foodstuffs in trace amts., presumably as bacterial decarboxylation prod. of proline. Present in bread, milk, cheese, carrots, celery stalks, beer, spirits, coffee, caviar and fatty fish. Flavouring agent. Liq. with odour resembling Piperidine, P-389. Misc. H_2O. d_4^{20} 0.86. Fp -63. Bp 88.5-89°. pK_a 11.31 (25°). Fumes in air. Strongly alkaline.
▶ Highly flammable, fl. p. 3°. Skin, eye and respiratory tract irritant. LD_{50} (rat, orl) 300 mg/kg. UX9650000

N-*Hexadecanoyl:* [70974-48-0] **N-*Hexadecanoylpyrrolidine***. *Hexadecanoic acid pyrrolidide*. N-*Palmitoylpyrrolidine*. *Alkaloid MQ-B_2*
$C_{20}H_{39}NO$ 309.534
Alkaloid from *Ipomoea aquatica* (water spinach).

N-*(14S-Methylhexadecanoyl):* [260058-83-1] **N-*(14-Methylhexadecanoyl)pyrrolidine*.** *14-Methylhexadecanoic pyrrolidide. Alkaloid MQ-A$_3$*
$C_{21}H_{41}NO$ 323.561
Alkaloid from *Ipomoea aquatica* (water spinach). $[\alpha]_D^{20}$ +5 (c, 0.4 in $CHCl_3$).

N-*Nitroso:* [930-55-2]
$C_4H_8N_2O$ 100.12
Found in fried bacon. Oil. Bp 214°. n_D^{20} 1.4900.

▶ Exp. hepatocarcinogen. UY1575000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 353C; 355A; 398B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 557C; 623B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 442A; 443B; 481B (*ir*)
Aldrich Library of NMR Spectra, **2**, 58D (*pmr*)
De Jong, M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1930, **49**, 237 (*synth*)
Ochiai, E. *et al., Ber.*, 1934, **67**, 1017 (*derivs*)
Duffield, A.M. *et al., J.A.C.S.*, 1965, **87**, 2920 (*ms*)
Wilshire, J.F.K. *et al., Aust. J. Chem.*, 1966, **19**, 1935 (*deriv*)
Andersson, B.A. *et al., Lipids*, 1974, **9**, 185; 443; 1975, **10**, 215; 716 (*use*)
Hawthorne, D.G. *et al., Aust. J. Chem.*, 1976, **29**, 315 (*cmr*)
Ahmed, M.G. *et al., J.C.S. Perkin 2*, 1978, 372 (*cmr, derivs*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1985, **A2**, 13 (*rev*)
Barbry, D. *et al., Magn. Reson. Chem.*, 1990, **28**, 560 (*cmr, N-15 nmr*)
Hunt, E.J. *et al., Carcinogenesis (London)*, 1991, **12**, 571 (*N-nitroso, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2398-2399 (*occur*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1090
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BSK250; NLP500; PPS500

2-Pyrrolidineacetic acid, 9CI P-619

β-Homoproline†



(*R*)-*form*

$C_6H_{11}NO_2$ 129.158
Occurs in *Tussilago farfara* (coltsfoot).

(*R*)-*form* [61350-65-0]
Mp 188-190°. $[\alpha]_D$ -44.8 (c, 1 in 3.41*M* HCl).

(*S*)-*form* [56633-75-1]
Needles (propanol). Mp 189-191° (185°) (dec.). $[\alpha]_D^{25}$ +4 (c, 1 in H_2O). $[\alpha]_D$ +45 (c, 1 in 3.41*M* HCl).

Me ester: [53912-83-7]
$C_7H_{13}NO_2$ 143.185
Oil. Bp_1 135-145°. $[\alpha]_D^{20}$ +7 (c, 2.6 in $CHCl_3$).

N-tert-*Butyloxycarbonyl:* [56502-01-3]
$C_{11}H_{19}NO_4$ 229.275
Cryst. (hexane). Mp 99-101°. $[\alpha]_D$ -39.5 (c, 1.9 in DMF) (-41.6).

N-*Benzyloxycarbonyl:* [56633-73-9]
$C_{14}H_{17}NO_4$ 263.293
Cryst. (diisopropyl ether). Mp 74.5-75.5°. $[\alpha]_D$ -35.3 (c, 1 in AcOH).

N-*Benzyloxycarbonyl, Me ester:* [56633-72-8]
$C_{15}H_{19}NO_4$ 277.319
Oil. $[\alpha]_D$ -35.1 (c, 1 in $CHCl_3$).

N-*[(9H-Fluoren-9-ylmethoxy)carbonyl]:* [193693-60-6]
$C_{21}H_{21}NO_4$ 351.401
Cryst. (MeOH). Mp 191-192°. $[\alpha]_D^{20}$ -33.6 (c, 0.9 in DMF).

N-*Me:* [137693-28-8] *1-Methyl-2-pyrrolidineacetic acid. Homohygrinic acid*
$C_7H_{13}NO_2$ 143.185
Plates (C_6H_6). Mp 120-122°. $[\alpha]_D$ -31.3 (c, 1.0 in EtOH).

N-*Me, Me ester:* [51856-76-9]
$C_8H_{15}NO_2$ 157.212
Oil. Bp_7 80-85°.

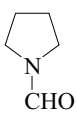
N-*Me, nitrile:* [67824-39-9] *2-Cyanomethyl-1-methylpyrrolidine*
$C_7H_{12}N_2$ 124.185
Oil. $Bp_{0.5}$ 45-46°. $[\alpha]_D$ -36.6 (c, 3 in MeOH).

[52484-80-7]

Bremner, J.B. *et al., Aust. J. Chem.*, 1973, **26**, 2559-2561 (*N-Me Me ester, isol, synth*)
Cassal, J.-M. *et al., Helv. Chim. Acta*, 1976, **59**, 1917-1924 (*synth*)
Wakabayashi, T. *et al., Synth. Commun.*, 1977, **7**, 239-244 (*synth*)
Leete, E. *et al., J.A.C.S.*, 1991, **113**, 9286-9292 (*1-Me, nitrile*)
Passreiter, C.M. *et al., Phytochemistry*, 1992, **31**, 4135-4137 (*isol*)
Ellmerer-Müller, E.P. *et al., Helv. Chim. Acta*, 1998, **81**, 59-65 (*Fmoc deriv, synth, ir, pmr, cmr, ms*)
Harrison, J.R. *et al., J.C.S. Perkin 1*, 1999, 3623-3631 (*Me ester, synth, ir, pmr, cmr*)

1-Pyrrolidinecarboxaldehyde, 9CI P-620

[3760-54-1]
1-Formylpyrrolidine



C_5H_9NO 99.132
Maillard product. Liq. Bp_3 69-70°. n_D^{25} 1.9792.

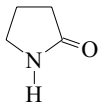
Hydrochloride: [88477-72-9]
Cryst.

Di-Me acetal: [5564-73-8] *1-(Dimethoxymethyl)pyrrolidine, 9CI*
$C_7H_{15}NO_2$ 145.201
Bp_{740} 160-161°. n_D^{20} 1.4320.

Coburn, M.D. *et al., J. Het. Chem.*, 1965, **2**, 308-309 (*synth*)
Bredereck, H. *et al., Chem. Ber.*, 1968, **101**, 41-50 (*di-Me acetal*)
Pews, R.G. *et al., Synth. Commun.*, 1985, **15**, 977-984 (*synth*)

2-Pyrrolidinone, 9CI, 8CI P-621

[616-45-5]
2-Oxopyrrolidine. Butyrolactam. 2-Pyrrolidone. Piperidinic lactam. 4-Aminobutanoic acid lactam



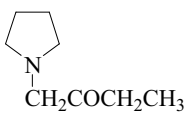
C_4H_7NO 85.105
Present in red ginseng. Cryst. (petrol). V. sol. H_2O, most org. solvs.; spar. sol. petrol. Mp 24.6°. Bp 245° Bp_{12} 133°. pK_a -0.94 (25°). Spar. steam-volatile. Forms a monohydrate in moist air, Mp 35° (30°). Ceiling temp. for polym., T_c 76°.

▶ Eye, skin and mucous membrane irritant. UY5715000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 788D; 789A; 790A; 790C; **2**, 391A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1285B; 1287A; 1287B; 1287C; 1288B; **2**, 1432B; 1432C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 788B; 789A; 1396D (*ir*)
Gabriel, S. *et al., Ber.*, 1889, **22**, 3335 (*synth*)
Metzger, H. *et al., Angew. Chem., Int. Ed.*, 1963, **2**, 624 (*synth*)
Zeifman, V.I. *et al., CA*, 1963, **59**, 5110 (*synth*)
Nielsen, E.B. *et al., J. Phys. Chem.*, 1967, **71**, 2297 (*uv*)
Chen, C.Y.S. *et al., J. Phys. Chem.*, 1969, **73**, 2999 (*ir*)
Fronza, G. *et al., J.C.S. Perkin 2*, 1977, 1746 (*N-15 nmr, cmr*)
Pellegata, R. *et al., Synthesis*, 1978, 614 (*synth*)
Cerioni, G. *et al., Spectrochim. Acta A*, 1983, **39**, 929 (*pmr, cmr*)
Ermakov, A.I. *et al., Zh. Org. Khim.*, 1985, **21**, 1986 (*ms*)
Ansell, J.M. *et al., Food Chem. Toxicol.*, 1988, **26**, 475
Suarez, M. *et al., Flavour Fragrance J.*, 1993, **8**, 215-220 (*isol*)
Pirila, P. *et al., Z. Naturforsch., B*, 1999, **54**, 1599-1601 (*cryst struct*)
Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 2, 1990, 278 (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CPQ275; PPT500

1-(1-Pyrrolidinyl)-2-butanone, 9CI P-622

[97073-14-8]



$C_8H_{15}NO$ 141.213
Maillard product derived from proline and reducing sugars such as glucose. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*occur, ms, glc*)

3-(1-Pyrrolidinyl)-2-butanone, 9CI P-623

[97073-15-9]

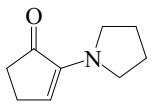
$C_8H_{15}NO$ 141.213
Maillard product. d_4^{25} 0.93. Bp_{14} 73°. n_D^{25} 1.4522.

Moffett, R.B. *et al., J.O.C.*, 1949, **14**, 862-867 (*synth*)

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*occur, glc, ms*)
Debrauwer, L. *et al., Bull. Soc. Chim. Fr.*, 1991, 244-254 (*occur, glc, ms*)

2-(1-Pyrrolidinyl)-2-cyclopenten-1-one P-624

[36287-24-8]

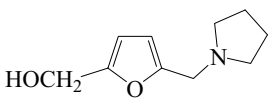


$C_9H_{13}NO$ 151.208
Proline-derived Maillard product. $Bp_{0.23}$ 81-84°. n_D^{20} 1.5401.

Sato, S. *et al., J.O.C.*, 1973, **38**, 551-554 (*synth, ir, pmr, uv*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*synth, ms, pmr, ir*)

5-(1-Pyrrolidinylmethyl)-2-furanmethanol, 9CI P-625

[61481-02-5]
1-[5′-(Hydroxymethyl)furfuryl]pyrrolidine

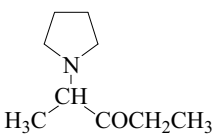


$C_{10}H_{15}NO_2$ 181.234
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928; 1993, **41**, 547-553 (*occur, ms*)
Huyghues-Despoites, A. *et al., J. Agric. Food Chem.*, 1994, **42**, 2519-2524 (*occur, ms*)

2-(1-Pyrrolidinyl)-3-pentanone P-626

[97073-16-0]



$C_9H_{17}NO$ 155.239
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*isol, ms*)

3-(1-Pyrrolidinyl)-2-pentanone P-627

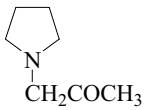
[97073-17-1]

$C_9H_{17}NO$ 155.239
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928 (*isol, ms*)

1-(1-Pyrrolidinyl)-2-propanone, 9CI P-628

[54151-38-1]
1-Acetonylpyrrolidine

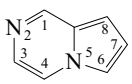


$C_7H_{13}NO$ 127.186
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 924-928; 1993, **41**, 547-553 (*occur, ms*)
Huyghues-Despointes, A. *et al., J. Agric. Food Chem.*, 1994, **42**, 2519-2524 (*occur, ms*)

Pyrrolo[1,2-*a*]pyrazine P-629

[274-45-3]
3a,6-Diazaindene. 7-Azaindolizine



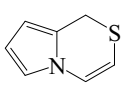
$C_7H_6N_2$ 118.138
Component of roast beef aroma. Oil. Bp_2 71°. n_D^{20} 1.6176. Rapidly darkens in air.

Picrate:
Mp 212°.

Herz, W. *et al., J.A.C.S.*, 1955, **77**, 6355 (*synth, uv*)
Paudler, W.W. *et al., J. Het. Chem.*, 1965, **2**, 410 (*synth, pmr*)
Kuhla, D.E. *et al., Adv. Heterocycl. Chem.*, 1977, **21**, 1 (*rev*)
Corbet, J.P. *et al., Tet. Lett.*, 1982, **23**, 3565 (*synth*)
Cobb, J. *et al., Magn. Reson. Chem.*, 1986, **24**, 231 (*pmr, cmr*)
Mínguez, J.M. *et al., J.O.C.*, 1996, **61**, 4655 (*synth, ir, pmr, cmr, ms*)

1*H*-Pyrrolo[2,1-*c*][1,4]thiazine, 9CI P-630

[51568-37-7]

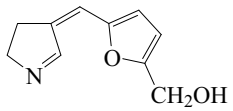


C_7H_7NS 137.205
Cysteine-derived Maillard product with a meaty, roasty aroma. Mp 47-48°. Bp_2 130° Kugelrohr.

Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, ms, pmr*)
Bertram, H.J. *et al., J. Prakt. Chem./Chem.-Ztg.*, 1993, **335**, 101-102 (*synth, pmr, ms*)

5-[2*H*-Pyrrol-4-(3*H*)-ylidenemethyl]-2-furanmethanol, 9CI P-631

[118248-32-1, 118248-33-2]
3-[5-(Hydroxymethyl)furfurylidene]-1-pyrroline



$C_{10}H_{11}NO_2$ 177.202
Putative proline-derived Maillard product formed in model reactions with proline and ascorbic acid. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*occur, ms, ir, pmr*)

Pyruvic acid, 8CI P-632

[127-17-3]
2-Oxopropanoic acid, 9CI. Pyroracemic acid. Acetylformic acid. FEMA 2970

$H_3CCOCOOH$

$C_3H_4O_3$ 88.063
Isol. from cane sugar fermentation broth, *Cicer arietinum* (chickpea), *Pisum sativum* (pea), *Trigonella cerulea* (sweet trefoil) and peppermint. Flavouring ingredient. Cryst. or liq. with odour resembling acetic acid. Misc. H_2O, EtOH, Et_2O. d^{15} 1.27. Mp *ca.* 13.6. Bp 165° part. dec. Bp_{10} 65°. n_D^{20} 1.4138. pK_{a1} 2.39 (25°). Impure samples dec. on standing.

▶ Fl. p. >74°. UZ0829800

Et ester: [617-35-6] *FEMA 2457*
$C_5H_8O_3$ 116.116
Flavouring ingredient. Sl. sol. H_2O, misc. EtOH, Et_2O. d^{14} 1.08. Mp -50°. Bp 155° Bp_{17} 55°. $n_D^{15.4}$ 1.4080.

3-Methylbutyl ester: [7779-72-8] *3-Methylbutyl 2-oxopropanoate. Isoamyl pyruvate. FEMA 2083*
$C_8H_{14}O_3$ 158.197
Flavouring ingredient. d^{17} 0.98. Bp 185°.

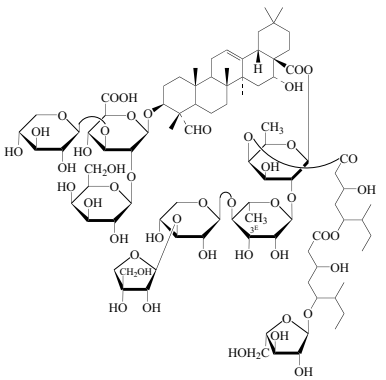
[57-60-3, 113-24-6, 2922-61-4, 4151-33-1, 19728-98-4, 19729-01-2, 63892-24-0, 64291-68-5, 74949-64-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 530C; 684A; 684B; 862A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1095A; 1095B; 1385B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 597C; 740D; 816C (*ir*)
Tschelinzeff, W. *et al., Ber.*, 1929, **62**, 2211 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 475 (*synth*)
Virtanen, A.I. *et al., Nature (London)*, 1939, **144**, 597 (*isol*)
Allen, E.H. *et al., J.A.C.S.*, 1950, **52**, 2955 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 467 (*synth*)
Arnett, J.F. *et al., J.A.C.S.*, 1973, **95**, 7599 (*uv*)
Mukherjee, D. *et al., Curr. Sci.*, 1974, **43**, 118 (*isol*)
Mukherjee, D. *et al., Phytochemistry*, 1975, **14**, 1915 (*isol*)
Harata, K. *et al., Acta Cryst. B*, 1977, **33**, 210 (*cryst struct*)
Mukherjee, D. *et al., Experientia*, 1977, **33**, 304 (*isol*)
Garegg, P.J. *et al., Carbohydr. Res.*, 1979, **77**, 71 (*occur*)
Cooper, A.J.L. *et al., Chem. Rev.*, 1983, **83**, 321 (*rev*)
Neh, K.H. *et al., Gordian*, 1986, **86**, 9; *CA*, **105**, 5347q (*isol*)
Sugiyama, S. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 1542 (*manuf*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 383; **2**, 266; 712
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1039; 1433-1434; 2401-2402
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PQC100

QS 21 Q-1

[141256-04-4]



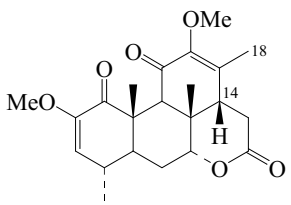
$C_{92}H_{148}O_{46}$ 1990.154
Constit. of the bark of *Quillaja saponaria* (soap-bark tree). Powder.

3^E-O-β-D-Glucopyranoside: [175295-49-5] ***QS 18***
$C_{98}H_{158}O_{51}$ 2152.296
Constit. of the bark of *Quillaja saponaria* (soap-bark tree).

Wu, J.Y. *et al., J. Immunol.*, 1992, **148**, 1519-1525 (*pharmacol*)
Pat. Coop. Treaty (WIPO), 1993, 93 05 789, (*Cambridge Biotech. Corp*); *CA*, **119**, 115325c (*synth, pharmacol, use*)
Kensil, C.R. *et al., Pharm. Biotechnol.*, 1995, **6**, 525-541 (*rev*)
Jacobsen, N.E. *et al., Carbohydr. Res.*, 1996, **280**, 1-14 (*struct*)
Kensil, C.R. *et al., Expert Opin. Invest. Drugs*, 1998, **7**, 1475-1482 (*rev*)

Quassin Q-2

[76-78-8]
Nigakilactone D



$C_{22}H_{28}O_6$ 388.46
Bitter constit. of *Quassia amara* (Surinam quassia) and *Picrasma excelsa* (Jamaican quassiawood). Cryst. (MeOH aq.). Mp 221-222°. $[\alpha]_D^{20}$ +34.5 (c, 5.09 in $CHCl_3$). Log P 0.5 (uncertain value) (calc). λ_{max} 255 (ε 11650) (MeOH) (Derep).

18-Hydroxy: ***18-Hydroxyquassin***
$C_{22}H_{28}O_7$ 404.459
Cryst. (EtOAc). Mp 232-233°. $[\alpha]_D^{20}$ +24 (c, 1 in $CHCl_3$).

14-Epimer: ***Isoquassin***. *Picrasmin*
$C_{22}H_{28}O_6$ 388.46
Plates and rods (MeOH aq.). Mp 222-225°. $[\alpha]_D^{20}$ +46.6 ($CHCl_3$). Log P 0.5 (uncertain value) (calc).

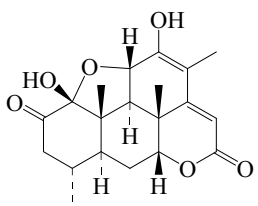
1α-Alcohol, Me ether: ***1α-O-Methylquassin***
$C_{23}H_{32}O_6$ 404.502
Constit. of *Quassia amara* (Surinam quassia). Powder (MeOH). Mp 168-172°.

Clark, E.P. *et al., J.A.C.S.*, 1938, **60**, 1146 (*isol, deriv*)
Adams, W. *et al., J.A.C.S.*, 1950, **72**, 375 (*synth*)
Valente, A. *et al., Tetrahedron*, 1961, **15**, 100; 1962, **18**, 1433 (*isol, struct, uv, ir, pmr*)
Casinovi, C. *et al., CA*, 1966, **66**, 75879 (*18-Hydroxyquassin*)
Vitagliano, J.C. *et al., Phytochemistry*, 1972, **11**, 807 (*synth*)
Stojanac, N. *et al., Can. J. Chem.*, 1975, **53**, 619 (*synth*)
Vidari, G. *et al., J.A.C.S.*, 1984, **106**, 3539 (*synth*)
Kim, M. *et al., J.O.C.*, 1990, **55**, 504 (*synth*)
Barbetti, P. *et al., Phytochemistry*, 1993, **32**, 1007 (*1α-O-Methylquassin*)
Shing, T.K.M. *et al., J.O.C.*, 1998, **63**, 2056-2057; 2000, 7059-7069 (*synth*)

Quassinol Q-3

[21018-87-1]

[23460-60-8]
Bisnorquassin

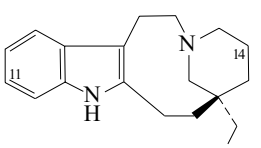


$C_{20}H_{24}O_6$ 360.406
Constit. of *Quassia amara* (Surinam quassia). Prisms (EtOH). Mp 258-260° dec. λ_{max} 313 (log ε 4.27) (EtOH).

Findlay, J.A. *et al., Can. J. Chem.*, 1968, **46**, 3765-3767; 1970, **48**, 313-316
Casinovi, C.G. *et al., Ann. Chim. (Rome)*, 1969, **59**, 230-239 (*isol, struct*)

Quebrachamine Q-4

*7-Ethyl-1,4,5,6,7,8,9,10-octahydro-2*H*-3,7-methanoazacycloundecino[5,4-*b*]indole, 9CI. Kamassine*



(+)-*form*

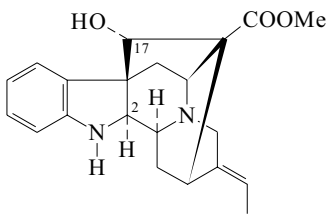
$C_{19}H_{26}N_2$ 282.428

(-)-*form* [4850-21-9]
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Cryst. (C_6H_6, hexane or EtOH). Mp 147-149°. $[\alpha]_D$ -100 ($CHCl_3$). $[\alpha]_D$ -110 (c, 0.496 in Me_2CO).

Hesse, O. *et al., Annalen*, 1882, **211**, 249 (*isol*)
Schlittler, E. *et al., Helv. Chim. Acta*, 1951, **34**, 920 (*isol, uv*)
Gellért, E. *et al., Helv. Chim. Acta*, 1952, **35**, 114 (*struct*)
Orazi, O.O. *et al., J.O.C.*, 1956, **21**, 978 (*isol, ord*)
Witkop, B. *et al., J.A.C.S.*, 1957, **79**, 3193 (*ir, degradn*)
Walls, F. *et al., Tetrahedron*, 1958, **2**, 173 (*isol, uv*)
Cohen, L.A. *et al., J.A.C.S.*, 1960, **82**, 2184 (*pmr*)
Biemann, K. *et al., J.A.C.S.*, 1962, **84**, 4578 (*ms*)
Stork, G. *et al., J.A.C.S.*, 1963, **85**, 2872 (*synth*)
Bycroft, B.W. *et al., Helv. Chim. Acta*, 1964, **47**, 1147 (*isol*)
Kutney, J.P. *et al., J.A.C.S.*, 1966, **88**, 3656; 1968, **90**, 3891 (*synth*)
Dugan, J.J. *et al., Helv. Chim. Acta*, 1967, **50**, 60 (*synth*)
Gorman, A.A. *et al., Helv. Chim. Acta*, 1969, **52**, 33 (*isol, uv*)
Puglisi, C. *et al., Acta Cryst. B*, 1976, **32**, 1900 (*cryst struct*)
Wenkert, E. *et al., Helv. Chim. Acta*, 1976, **59**, 2711 (*cmr*)
Takano, S. *et al., J.A.C.S.*, 1979, **101**, 6414 (*synth*)
Takano, S. *et al., Chem. Comm.*, 1980, 616; 1981, 1153 (*synth*)
Giri, V.S. *et al., J. Het. Chem.*, 1980, **17**, 1133 (*synth, uv, ir, pmr, ms*)
Wenkert, E. *et al., Tetrahedron*, 1981, **37**, 4017 (*synth*)
Ban, Y. *et al., Tetrahedron*, 1983, **39**, 3657 (*synth*)
Mandal, S.B. *et al., J.O.C.*, 1988, **53**, 4236 (*synth*)
Asaoka, M. *et al., Heterocycles*, 1989, **29**, 243 (*synth*)
Node, M. *et al., J.O.C.*, 1990, **55**, 517 (*synth*)
Deutsch, H.F. *et al., J. Pharm. Biomed. Anal.*, 1994, **12**, 1253-1287 (*isol, activity*)
Temme, O. *et al., J.O.C.*, 1998, **63**, 6007-6015 (*synth*)
Wee, A.G.H. *et al., Tetrahedron*, 1998, **54**, 13435-13448 (*synth*)
Meier, A. *et al., J. Antibiot.*, 1999, **52**, 957-959 (*activity*)
Kozmin, S.A. *et al., J.A.C.S.*, 2002, **124**, 4628-4641 (*synth*)
Fujimura, T. *et al., Tet. Lett.*, 2002, **43**, 97-99 (*synth*)

Quebrachidine Q-5

[4835-69-2]
Methyl 19,20-didehydro-1-demethyl-17-hydroxyajmalan-16-carboxylate, 9CI



$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 276-278° (264-265°). $[\alpha]_D^{26}$ +54 ($CHCl_3$). pK_a 6.7.

N-*Me:* See Vincamajine in *The Combined Chemical Dictionary.*

O-*3,4,5-Trimethoxybenzoyl:* [31148-63-7] ***(3,4,5-Trimethoxybenzoyl)quebrachidine***
$C_{31}H_{34}N_2O_7$ 546.619
Needles (MeOH). Mp 231-232°. $[\alpha]_D$ -36 (c, 1.3 in $CHCl_3$).

Stereoisomer: [21641-60-1] ***Vincarine***
$C_{21}H_{24}N_2O_3$ 352.432
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 263-264°. $[\alpha]_D$ +14 (MeOH). Of unknown stereochem..
▶ LD_{50} (mus, ipr) 330 mg/kg. YY8600000

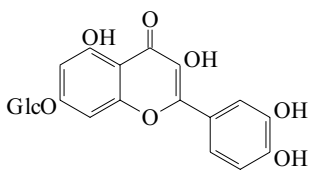
17-Ketone, 2-epimer: [135649-95-5] ***Leepacine***

$C_{21}H_{22}N_2O_3$ 350.416
$[\alpha]_D$ -91 (MeOH). Air- and light-sensitive.

Gorman, M. *et al., Tet. Lett.*, 1963, 39 (*isol, uv, ir, pmr, ms, struct*)
Yuldashev, P.K. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **154**, 1412; 1965, **163**, 123 (*Vincarine*)
Taylor, W.I. *et al., Alkaloids (N.Y.)*, 1968, **11**, 47; 116 (*Vincarine*)
Crow, W.D. *et al., Aust. J. Chem.*, 1970, **23**, 2489 (*3,4,5-Trimethoxybenzoyl*)
Taylor, W.I. *et al., The Vinca Alkaloids*, Marcel Dekker, 1973, (*rev*)
Aynilian, G.H. *et al., J. Nat. Prod.*, 1974, **37**, 299 (*isol, ir, pmr, ms*)
Vercauteren, J. *et al., Phytochemistry*, 1979, **18**, 1729 (*isol*)
Stöckigt, J. *et al., Tet. Lett.*, 1979, 2615 (*biosynth*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1991, **30**, 1285 (*Leepacine*)

Quercimeritrin Q-6

[491-50-9]
7-O-β-D-Glucopyranosyloxy-3,3′,4′,5-tetrahydroxyflavone. Quercetin 7-glucoside. Quercimeritroside



$C_{21}H_{20}O_{12}$ 464.382
Yellow needles + $3H_2O$. Mp 249-250°. λ_{max} 256 ; 374 (MeOH) (Berdy). λ_{max} 328 (MeOH/NaOH) (Berdy). λ_{max} 257 (ϵ 23988); 372 (ϵ 21380) (EtOH) (Berdy).

3-O-α-L-Arabinopyranoside: [28452-84-8]
$C_{26}H_{28}O_{16}$ 596.498
Isol. from *Phytolacca americana* (pokeberry).

4′-O-β-D-Glucopyranoside: [42900-82-3] *Quercetin 4′,7-diglucoside*
$C_{27}H_{30}O_{17}$ 626.524
Isol. from *Allium cepa* (yellow onion). Yellow plates + $1\frac{1}{2}H_2O$ (EtOH/EtOAc). Mp 195-197°. $[\alpha]_D^{25}$ -78 (c, 0.27 in Py).

O″-Rhamnosyl: [73432-00-5] *Quercetin 7-(rhamnosylglucoside)*
$C_{27}H_{30}O_{16}$ 610.524
Constit. of *Gossypium hirsutum* (cotton).

*3-O-[4-Hydroxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:* ***Pisumflavonoside II***
$C_{48}H_{56}O_{29}$ 1096.953
Constit. of *Pisum sativum* (pea). Yellow powder. $[\alpha]_D$ -59 (c, 0.3 in MeOH). λ_{max} 207 (log ϵ 5); 258 (log ϵ 4.3); 314 (log ϵ 4.4) (MeOH).

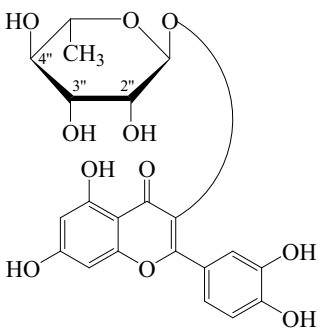
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside]:
$C_{33}H_{40}O_{22}$ 788.666
Constit. of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 199-202°. $[\alpha]_D^{26}$ -37 (c, 0.09 in H_2O). λ_{max} 257 (log ϵ 4.35); 267 (sh) (log ϵ 4.3); 358 (log ϵ 4.21) (MeOH).

6″-O-(3,4,5-Trihydroxybenzoyl):6″-O-Galloylquercimeritrin
$C_{28}H_{24}O_{16}$ 616.488
Constit. of the pods of *Acacia farnesiana* (sweet acacia). Yellow cryst. Mp 215°.

Chumbalev, T.K. *et al., Khim. Prir. Soedin.*, 1969, **5**, 594 (*3-arabinopyranoside*)
Markham, K.R. *et al., Phytochemistry*, 1970, **9**, 2359 (*rhamnosylglucoside*)
Farkas, L. *et al., Chem. Ber.*, 1974, **107**, 1518 (*4′-glucoside*)
Barakat, H.H. *et al., Phytochemistry*, 1999, **51**, 139-142 (*6-Galloylquercimeritrin*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1003-1008 (*Pisumflavonoside II*)
Han, Y. *et al., Phytochemistry*, 2001, **58**, 577-580 (*3-2-glucosylgalactoside*)

Quercitrin Q-7

[522-12-3]
3-O-α-L-Rhamnopyranosyloxy-3′,4′,5,7-tetrahydroxyflavone. Quercetin 3-rhamnoside. Quercitroside. Quercitronic acid. Thujin†



$C_{21}H_{20}O_{11}$ 448.382
Pale yellow cryst. + $2H_2O$. Mp 182-185° Mp 250-252° (anhyd.). $[\alpha]_D^{15}$ -158 (c, 0.61 in MeOH). Log P -1.73 (calc).

▶ UZ5950000

2″-O-β-D-Glucopyranosyl: [143016-74-4] *Quercetin 3-(2-glucosylrhamnoside)*
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Ginkgo biloba* (ginkgo).

2″-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl]: [113447-39-5]
$C_{36}H_{36}O_{18}$ 756.67
Isol. from *Ginkgo biloba* (ginkgo). Yellow-green solid. Mp 231°.

2″-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl], 7-O-β-D-glucopyranoside: [143016-73-3]
$C_{42}H_{46}O_{23}$ 918.812
Isol. from *Ginkgo biloba* (ginkgo).

4″-O-β-D-Glucopyranosyl: [59262-54-3] *Quercetin 3-(4-glucosylrhamnoside).* ***Multinoside A***
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Prunus persica*.

4″-O-Glucopyranosyl, 7-O-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [187410-77-1]
$C_{39}H_{50}O_{25}$ 918.809
Constit. of *Myrsine africana* (cape myrtle). Yellow powder. λ_{max} 256 ; 302 ; 356 (MeOH).

7-O-β-D-Glucuronopyranoside:Quercetin 7-glucuronide 3-rhamnoside
$C_{27}H_{28}O_{17}$ 624.508
Constit. of *Carthamus tinctorius* (safflower).

2″-O-[β-D-Glucopyranosyl-(1→4)-4-hydroxycinnamoyl-(→6)-β-D-glucopyranosyl]: [142997-33-9]
$C_{42}H_{46}O_{23}$ 918.812
Isol. from *Ginkgo biloba* (ginkgo).

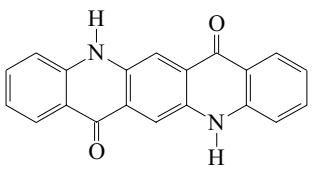
4″-Ac, 7-O-α-L-rhamnopyranoside: [104594-65-2]
$C_{29}H_{32}O_{16}$ 636.562
Isol. from *Mespilus germanica* (European medlar).

[22324-77-2]

Razadkowska-Bodalska, H. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1970, **44**, 283 (*3,7-dirhamnoside*)
Takagi, S. *et al., Yakugaku Zasshi*, 1977, **97**, 109 (*Multinoside A*)
Tanaka, N. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3580 (*acetates*)
Bohm, B.A. *et al., Phytochemistry*, 1983, **22**, 2743 (*3,7-dirhamnoside*)
Nasr, C. *et al., Phytochemistry*, 1987, **26**, 2869 (*2″-4-hydroxycinnamoylglucoside*)
Seto, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2080 (*Multinoside A*)
Hasler, A. *et al., Phytochemistry*, 1992, **31**, 1391 (*2″-glucosyls*)
Sticher, O. *et al., Planta Med.*, 1993, **59**, 2 (*derivs*)
Manguro, L.O.A. *et al., Nat. Prod. Lett.*, 1996, **9**, 121-126 (*4″-glucosyl 7-rhamnosylglucoside*)
Marzouk, M.S. *et al., Phytochemistry*, 1999, **52**, 943-946 (*Quercetin 3,4′-dirhamnoside*)
Kazuma, K. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1588-1599 (*7-glucuronide*)

Quinacridone Q-8

[1047-16-1]
*5,12-Dihydroquino[2,3-*b*]acridine-7,14-dione.* lin-trans-*Quinacridone. C.I. Pigment Violet 19. Quinacridone violet*



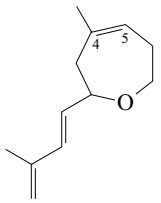
$C_{20}H_{12}N_2O_2$ 312.327
FDA approved colourant for food-contact paper and board packaging. Red-violet cryst., yellow in vapour phase. Insol. most solvents. Mp 390°.

Labana, S.S. *et al., Chem. Rev.*, 1967, **67**, 1 (*rev, uv*)
Kimura, S. *et al., Makromol. Chem.*, 1968, **117**, 203 (*synth, ir*)
Chung, F.H. *et al., J. Appl. Crystallogr.*, 1971, **4**, 506 (*cryst struct*)
Altiparmakian, R.H. *et al., Helv. Chim. Acta*, 1972, **55**, 85 (*pmr*)
Yokoyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 1775 (*pmr, uv*)
Potts, G.D. *et al., Chem. Comm.*, 1994, 2565 (*cryst struct*)
Food Chem. News, 2002, **43(47)**, 21 (*use*)

Quinceoxepine Q-9

[132925-10-1]
2,3,6,7-Tetrahydro-4-methyl-2-(3-methyl-

1,3-butadienyl)oxepin



$C_{12}H_{18}O$ 178.274
Constit. of quince fruit (*Cydonia oblonga*). Oil. Bp_{11} 110-120°.

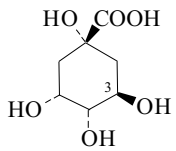
*4,5-Dihydro(*cis-*):* [133005-51-3] *4-Methyl-2-(3-methyl-1,3-butadienyl)oxepane, 9CI*. **cis-*Quinceoxepane***
$C_{12}H_{20}O$ 180.289
Constit. of quince fruit. Oil.

*4,5-Dihydro(*trans-*):* [133005-52-4] **trans-*Quinceoxepane***
$C_{12}H_{20}O$ 180.289
Constit. of quince fruit. Oil.

Escher, S. *et al., Helv. Chim. Acta*, 1991, **74**, 179 (*isol, pmr, cmr, synth*)

Quinic acid Q-10

[36413-60-2]
1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid, 9CI. Hexahydro-1,3,4,5-tetrahydroxybenzoic acid. Chinic acid



(−)-*form*

$C_7H_{12}O_6$ 192.168
Note that the C atom carrying the OH which is *cis* to the COOH is normally numbered 3. Care is needed; see Eliel (1997).

(-)-*form* [77-95-2]
Occurs in coffee beans and many other plant sources. Food acidulant with good taste characteristics, use limited by cost. Sol. H_2O. Mp 162-163°. $[\alpha]_D^{26}$ -42.1 (H_2O). pK_a 3.58 (25°).

▶ LD_{50} (mus, scu) 10000 mg/kg. GU8650000

Lactone: [27783-00-2] *1,3,4-Trihydroxy-6-oxabicyclo[3.2.1]octan-7-one, 9CI*. ***Quinide***
$C_7H_{10}O_5$ 174.153
Mp 187°. $[\alpha]_D^{23}$ -16.75 (c, 8.3 in H_2O). Lactonised onto the C-3 OH group.

*3-*O*-(3,4,5-Trihydroxybenzoyl):* [53584-43-3] *3-*O*-Galloylquinic acid*. ***Theogallin***
$C_{14}H_{16}O_{10}$ 344.274
Isol. from tea. Off-white amorph. powder. $[\alpha]_D^{18}$ -36.4 (c, 0.37 in H_2O).

1,3,4,5-Tetrakis(3,4,5-trihydroxybenzoyl): [123166-70-1] ***1,3,4,5-Tetra-*O*-galloylquinic acid***
$C_{35}H_{28}O_{22}$ 800.593
Tannin constit. isol. from commercial tannic acid. Amorph. powder + $2H_2O$. $[\alpha]_D^{20}$ -72 (c, 0.20 in Me_2CO). Log P 1.51 (calc). λ_{max} 277 (ϵ 34700) (MeOH) (Derep).

*3-*O*-(Galloylgalloyl), 4,5-bis(3,4,5-trihydroxybenzoyl):* [123166-69-8] ***3-Digalloyl-4,5-di-*O*-galloylquinic acid***
$C_{35}H_{28}O_{22}$ 800.593
Isol. from commercial tannic acid. Amorph. powder + H_2O. $[\alpha]_D^{20}$ -106 (c, 0.48 in Me_2CO). λ_{max} 277 (ϵ 23000) (MeOH) (Berdy).

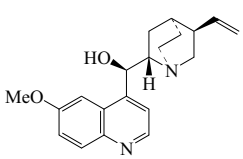
*5-*O*-(Galloylgalloyl), 3,4-bis(3,4,5-trihydroxybenzoyl):* [123134-20-3] *5-*O*-Digalloyl-3,4-di-*O*-galloylquinic acid*
$C_{35}H_{28}O_{22}$ 800.593
Constit. of commercial tannic acid. Amorph. powder + H_2O. $[\alpha]_D^{20}$ -92 (c, 0.60 in Me_2CO). λ_{max} 277 (ϵ 35000) (MeOH) (Berdy).

*4-*O*-(Galloylgalloyl), 3,5-bis(3,4,5-trihydroxybenzoyl):* [123134-19-0] ***4-*O*-Digalloyl-3,5-di-*O*-galloylquinic acid***
$C_{35}H_{28}O_{22}$ 800.593
Isol. from commercial tannic acid. Amorph. powder + H_2O. $[\alpha]_D^{20}$ -91 (c, 0.53 in Me_2CO). λ_{max} 277 (ϵ 34400) (MeOH) (Berdy).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 525A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 814C (*nmr*)
v. Lippmann, E. *et al., Ber.*, 1901, **34**, 1159
Gorter, K. *et al., Annalen*, 1908, **359**, 217
Fischer, H.O.L. *et al., Ber.*, 1932, **65**, 1009 (*struct*)
Grewe, R. *et al., Chem. Ber.*, 1954, **87**, 793 (*synth*)
Wolinsky, J. *et al., J.O.C.*, 1964, **29**, 3596 (*synth, bibl*)
Haslam, E. *et al., J.C.S.(C)*, 1971, 1496 (*pmr*)
Stagg, G.V. *et al., Phytochemistry*, 1971, **10**, 1671 (*Theogallin*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 989 (*occur*)
Kelley, C.J. *et al., J.O.C.*, 1976, **41**, 449 (*cmr*)
Abell, C. *et al., Acta Cryst. C*, 1988, **44**, 1287 (*cryst struct, bibl, abs config*)
Scholz-Böttcher, B.M. *et al., Annalen*, 1991, 1029 (*bibl, stereoisomers*)
Meier, R.M. *et al., Helv. Chim. Acta*, 1991, **74**, 807 (*synth*)
Mahmood, N. *et al., Antiviral Chem. Chemother.*, 1993, **4**, 235 (*3,4,5-trigalloyl, anti-HIV activity*)
Neszmelyi, A. *et al., Planta Med.*, 1993, **59**, 164 (*Tetragalloylquinic acid*)
Manthey, M.K. *et al., J.C.S. Perkin 1*, 1997, 625-628 (*lactone, synth, ir, pmr, cmr*)
Eliel, E.L. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 3551-3554 (*stereochem*)

Quinine, BAN Q-11

[130-95-0]
6′-Methoxycinchonan-9-ol, 9CI



Absolute Configuration

$C_{20}H_{24}N_2O_2$ 324.422
Used in tonics and bitter drinks. Cryst. with v. bitter taste. Sol. H_2O, EtOH, C_6H_6, $CHCl_3$. Mp 177° (anhyd.). $[\alpha]_D^{15}$ -158.7 (Et_2O). $[\alpha]_D$ -158 (-145) (EtOH). pK_{a1} 8.34; pK_{a2} 4.21 (20°). Log P 2.93 (calc). Forms a dihydrate and a trihydrate, Mp 57°(efflorescent). Triboluminescent. Blue fluor. in soln..

▶ Adverse effects from therapeutic or larger doses of quinine or its salts (cinchonism). Irritant to mucous membranes. Human and exp. teratogenic effects. LD_{50} (mus, ipr) 115 mg/kg. VA6020000

Hydrochloride (1:1): [130-89-2]

[7549-43-1] ***Quinine hydrochloride, JAN***. *FEMA 2976*
Needles + $2H_2O$, dehydrating at 100°. Mp 158-160° (anhyd.). $[\alpha]_D^{15}$ -145.5 (EtOH).

▶ VA7700000

Sulfate salt (1:1): [549-56-4] *Quinine bisulfate. FEMA 2975*
Bitter flavouring.

Sulfate salt (2:1): [804-63-7]

[549-56-4, 6119-70-6] ***Quinine sulfate, JAN, USAN***. *Quinanium. Quine. Quinite. FEMA 2977*
Bitter flavouring. Mp 205°. $[\alpha]_D^{15}$ -235 (H_2SO_4 aq.). Forms a dihydrate and an octahydrate. Component of Quinamin.

▶ VA8440000

Gluconate salt (1:1): [4325-25-1]
Mp 159-161° (anhyd.).

9-Epimer: [572-60-1] ***Epiquinine***. epi-*Quinine*
$C_{20}H_{24}N_2O_2$ 324.422
Oil. $[\alpha]_D^{20}$ +43.3 (EtOH).

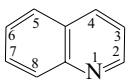
[6119-47-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 864D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 440B; 441C (*nmr*)
Woodward, R.B. *et al., J.A.C.S.*, 1945, **67**, 860 (*synth*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, NY, 1948, **4**, 251 (*use*)
Willemot, J. *et al., Ann. Pharm. Fr.*, 1965, **23**, 203 (*gluconate*)
Lyle, G.G. *et al., Tetrahedron*, 1967, **23**, 51; 3253 (*config, uv, ord, pmr*)
Fales, H.M. *et al., J.A.C.S.*, 1970, **92**, 1590 (*ms*)
Battersby, A.R. *et al., Chem. Comm.*, 1971, 30; 31 (*biosynth*)
Chao, J.M. *et al., Anal. Chem.*, 1974, **46**, 296 (*ms*)
Moreland, C.G. *et al., J.O.C.*, 1974, **39**, 2413 (*cmr*)
Haznagy, H. *et al., Pharmazie*, 1976, **31**, 713 (*ir*)
Grethe, G. *et al., J.A.C.S.*, 1978, **100**, 589 (*synth*)
Hahn, F.E. *et al., Antibiotics (N.Y.)*, 1979, **5**, 353 (*rev, pharmacol, tox*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 430
Muhtadi, F.J. *et al., Anal. Profiles Drug Subst.*, 1983, **12**, 547 (*rev, uv, ir, pmr, cmr, ms, anal*)
Imanishi, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1551 (*synth*)
Hofheinz, W. *et al., Handb. Exp. Pharmacol.*, 1984, **68**, 61 (*rev*)
Smith, E. *et al., J. Chromatogr.*, 1984, **299**, 233 (*hplc*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 5747 (*synonyms*)
Prakash, O. *et al., Indian J. Chem., Sect. B*, 1988, **27**, 950 (*pmr*)
Lander, V. *et al., Z. Lebensm.-Unters. -Forsch.*, 1990, **190**, 410-413 (*hplc*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 408
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2407 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1574-1577 (*use, salts*)
Stork, G. *et al., J.A.C.S.*, 2001, **123**, 3239-3242 (*synth, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QHJ000; QIJ000; QJS000; QMA000; QJJ100

Quinoline Q-12

[91-22-5]
1-Benzazine. 1-Azanaphthalene. FEMA 3470



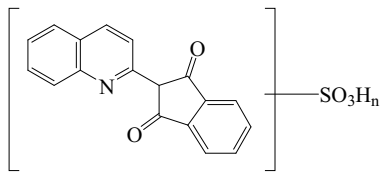
C_9H_7N 129.161
Alkaloid from various plant spp. incl. *Mentha* spp.. Also present in cocoa, black tea and Scotch whisky. Flavouring ingredient. Liq. Mod. sol. H_2O. d_4^{20} 1.09. Fp -15.6. Bp 238.05° Bp_{17} 114°. n_D^{20} 1.6268. pK_a 4.9 (20°). Hygroscopic, steam-volatile.
▶ Fl. p. 99°, autoignition temp. 480°. Often violent synth. (Skraup reaction). Skin and severe eye irritant. Contact with liquid can damage eyes. LD_{50} (rat, orl) 331 mg/kg. LD_{50} (rbt, skn) 540 mg/kg. Reported to be mutagenic and carcinogenic. VA9275000

[1701-63-9, 5436-28-2, 26323-01-3, 27926-80-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 853A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 421A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1565A (*ir*)
Cole, W.G. *et al., J.C.S.(B)*, 1968, 1284 (*ms*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 356
Lienhard, G.E. *et al., Biochemistry*, 1970, **9**, 3011 (*uv*)
Zharekeev, B.K. *et al., Khim. Prir. Soedin.*, 1974, **10**, 264-265; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 282-283 (*isol*)
Johns, S.R. *et al., Aust. J. Chem.*, 1976, **29**, 1617 (*cmr*)
Hirano, K. *et al., Cancer Res.*, 1976, **36**, 329-335 (*tox*)
Jones, G. *et al., Chem. Heterocycl. Compd.*, 1977, **32**, 1 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **19**, 532 (*rev*)
Attimonelli, M. *et al., Org. Magn. Reson.*, 1979, **12**, 17 (*pmr*)
Horino, H. *et al., Tet. Lett.*, 1979, 2403 (*synth*)
Boyd, D.R. *et al., Tet. Lett.*, 1991, **32**, 2963-2966 (*bibl, tox, metab*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2923
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1091
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QMJ000

Quinoline yellow Q-13

[8004-92-0]
C.I. Acid yellow 3, 9CI. E104. CI 47005. FD and C Yellow No. 10



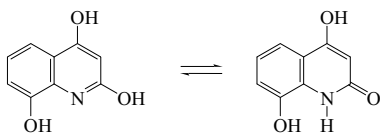
n = 1 or 2

A mixt. of mono- and disulfonic acids. Food dye. Use prohibited in USA, Norway, Australia and Japan. Bright greenish-yellow solid.

Colour Index, 3rd edn., 1971, **4**, 4435 (*synth, bibl*)
Gelbecke, M. *et al., Bull. Soc. Chim. Belg.*, 1982, **91**, 237-242 (*cmr, struct*)
Compagnon, P.A. *et al., Analusis*, 1988, **16**, 428-433 (*pmr, struct*)
Merck Index, 12th edn., 1996, 8256
Frazier, R.A. *et al., J. Chromatogr., A*, 2000, **876**, 213-220 (*hplc*)

2,4,8-Quinolinetriol Q-14

2,4,8-Trihydroxyquinoline. 4,8-Dihydroxy-2(1H)-quinolinone



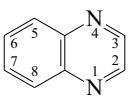
$C_9H_7NO_3$ 177.159
Other tautomers possible.

4,8-Di-Me ether: [15272-24-9] *4,8-Dimethoxy-2(1H)-quinolinone.* ***Edulitine.*** *Robustinine*
$C_{11}H_{11}NO_3$ 205.213
Alkaloid from bark of *Casimiroa edulis* (Mexican apple). Needles (EtOAc). Mp 235-236°.

Iriarte, J. *et al., J.C.S.*, 1956, 4170 (*Edulitine, isol, uv, ir*)
Toube, T.P. *et al., Tetrahedron*, 1967, **23**, 2061 (*Edulitine, pmr, ms*)

Quinoxaline Q-15

[91-19-0]
1,4-Diazanaphthalene. Benzoparadiazine. Phenopiazine. Phenpiazine. 1,4-Naphthyridine. 1,4-Benzodiazine



$C_8H_6N_2$ 130.149
Cryst. (petrol); hydrate by addn. of H_2O to petrol soln. V. sol. H_2O, org. solvs. Mp 28° (anhyd.). Bp_{760} 229° Bp_{40} 140°. pK_{a1} 2.08; pK_{a2} 0.56 (20°, H_2SO_4 aq.). With Na/EtOH → 1,2,3,4-tetrahydro deriv..
▶ LD_{50} (mus, ipr) 250 mg/kg. VD1225000

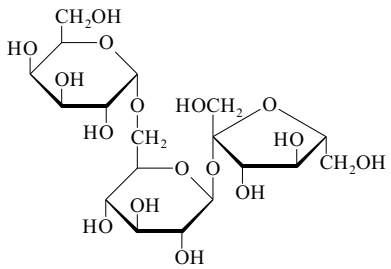
N,N′-*Dioxide:* [2423-66-7] *Quinoxaline 1,4-dioxide.* ***Quindoxin, BAN, INN.*** *Grofas. ICI 8173. RD 2579*
$C_8H_6N_2O_2$ 162.148
Growth promoter for pigs and poultry. Golden yellow needles (EtOH). Mp 241-243°.
▶ LD_{50} (mus, ipr) 500 mg/kg. Exp. carcinogen. VD2275000

Landqvist, J.K. *et al., J.C.S.*, 1953, 2816 (*Quindoxin*)
Tori, K. *et al., Chem. Pharm. Bull.*, 1963, **11**, 681 (*pmr, dioxide*)
Guenther, H. *et al., Heterocycles*, 1978, **11**, 337 (*cmr, dioxide*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13200
Boykin, D.W. *et al., J. Het. Chem.*, 1985, **22**, 981 (*O-17 nmr, Quindoxin*)
Kurasawa, Y. *et al., J. Het. Chem.*, 1995, **32**, 1085 (*rev, oxides*)
Monge, A. *et al., J. Med. Chem.*, 1995, **38**, 4488 (*dioxide, synth, ir, pmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QRJ000; QSA000

Raffinose, 8CI R-1

[512-69-6]

β-D-Fructofuranosyl α-D-galactopyranosyl-(1→6)-α-D-glucopyranoside, 9CI. Melitriose. Gossypose. Melitose



$C_{18}H_{32}O_{16}$ 504.441

Occurs in cotton seeds, sugar beet and manna. Widely distributed in plants, esp. in the seeds. Sweet taste. Sweetness 0.48 x sucrose. Mp 118° (anhyd.). $[\alpha]_D$ +123 (c, 2 in H_2O) (anhyd.). Sweet taste. Sweetness 0.48 x sucrose. Does not reduce Fehling's soln. Invertase or raffinase gives 6-*O*-α-D-Galactopyranosyl-D-glucose, G-22 and Fructose.

▶ LZ5851200

Pentahydrate: [17629-30-0]
Prisms. Mp 78°.

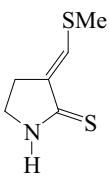
Undeca-Ac:
$C_{40}H_{54}O_{27}$ 966.85
Mp 101°. $[\alpha]_D$ +100 (c, 8 in EtOH).

Undeca-Me:
$C_{29}H_{54}O_{16}$ 658.736
Bp_2 238-240°. $[\alpha]_D^{17}$ +128.4 (c, 1 in H_2O).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 310B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **1**, 197B (*ir*)
Tanret, G. *et al., Bull. Soc. Chim. Fr.* , 1895, 261
Haworth, N.W. *et al., J.C.S.* , 1923, 3125
French, D. *et al., Adv. Carbohydr. Chem. Biochem.* , 1954, **9**, 149 (*rev*)
Duperon, R. *et al., C. R. Hebd. Seances Acad. Sci.* , 1955, **241**, 1817 (*occur*)
Bourne, E.J. *et al., Biochem. J.* , 1965, **97**, 802 (*biosynth*)
Kamerling, J.P. *et al., Tetrahedron* , 1972, **28**, 4375 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe* , 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 671 (*occur*)
Bock, K. *et al., Tet. Lett.* , 1973, 1037 (*cmr*)
Anteunis, M. *et al., Carbohydr. Res.* , 1975, **44**, 101 (*pmr*)
Hough, L. *et al., Carbohydr. Res.* , 1980, **80**, 117; 123 (*derivs*)
Jeffrey, G.A. *et al., Carbohydr. Res.* , 1990, **206**, 173 (*cryst struct*)

Raphanusanin R-2

3-[(Methylthio)methylene]-2-pyrrolidinethione, 9CI. Raphantin



(*E*) - form

$C_6H_9NS_2$ 159.276

There have been various struct. revisions,. The most recent incorrect struct. proposed was a MeOH covalent solvate of the struct. shown. The names Raphanusanin A and Raphanusanin B were erroneously applied to stereoisomers of this solvate.

(*E*)-*form* [128463-44-5]

[104760-73-8]
Isol. from *Raphanus sativus* var. *hortensis* f. *gigantissimus*. Needles (MeOH).

(*Z*)-*form* [148225-27-8]

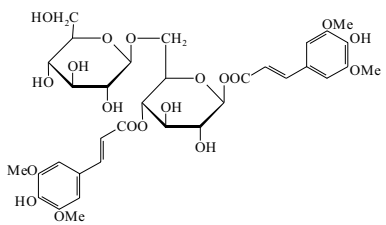
[104760-72-7]
Isol. from *Raphanus sativus* var. *hortensis* f. *gigantissimus*. Amorph. pale yellow powder.

Sakoda, M. *et al., Phytochemistry*, 1990, **29**, 1031 (*isol*)
Harada, N. *et al., Tet. Lett.* , 1991, **32**, 6757 (*uv, ir, pmr, cmr, ms, bibl*)
Kosemura, S. *et al., Tet. Lett.* , 1993, **34**, 481-484 (*struct*)
Matsuoka, H. *et al., Phytochemistry*, 1998, **47**, 975-977 (*isol*)
Hasegawa, T. *et al., Phytochemistry*, 2000, **54**, 275-279 (*biosynth*)

Raphanusol A R-3

[74565-72-3]

6-O-β-D-Glucopyranosyl-β-D-glucopyranose-1,4-bis[3-(4-hydroxy-3,5-dimethoxyphenyl)-2-propenoate], 9CI. 1,4-Di-O-sinapoylgentiobiose



$C_{34}H_{42}O_{19}$ 754.694

Isol. from *Raphanus sativus* (Sakura jima radish) seedling. Powder (Me_2CO/C_6H_6). Sol. MeOH; poorly sol. hexane. Mp 137-138°. $[\alpha]_D^{22}$ +79.4 (c, 0.23 in MeOH). λ_{max} 204 (ε 27400); 241 (ε 23300); 333 (ε 27300) (EtOH) (Berdy).

Hase, T. *et al., Phytochemistry*, 1982, **21**, 1021 (*isol, struct*)
Hase, T. *et al., CA* , 1985, **103**, 138518b

RBF PM R-4

Protein with MW distributed in both of the ranges 30000-50000 and 70000-120000. Present in rice bran (*Oryza sativa*). Sol. bases, AcOH; poorly sol. H_2O, hexane, MeOH. λ_{max} 280 (H_2O) (Berdy).

Eur. Pat. , 1981, 27 514; *CA* , **95**, 12755z (*isol*)

Relaxins R-5

[9002-69-1]

Peptide hormones. All relaxins have a two chain, disulfide-linked insulin-like struct. and two arginine residues in the midregion of the B chain. The primary structs. of relaxins from apparently closely related species can differ significantly in their AA compositions. Present in mammals and other species, e.g. sharks and chickens.

▶ VG0720000

[64339-45-3, 75627-11-1, 75639-98-4, 75639-99-5, 77467-85-7, 77614-15-4, 77640-64-3, 79005-81-5, 82120-04-5, 82611-45-8, 82658-27-3, 82658-28-4, 105231-40-1, 105231-41-2, 105286-99-5, 107628-11-5, 107712-70-9, 107720-74-1, 117697-87-7, 117697-88-8, 119370-85-3, 119397-12-5, 127664-25-9, 135644-72-3, 135644-80-3, 140683-99-4]

Anderson, R.R. *et al., Adv. Exp. Med. Biol.* , 1982, **143**, 1 (*rev*)
Steinetz, B.G. *et al., Ann. N.Y. Acad. Sci.* , 1982, **380**, 1 (*rev*)
Schwabe, C. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.* , 1990, **96**, 15 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1408
Sherwood, O.D. *et al., Oxford Rev. Reprod. Biol.* , 1993, **15**, 143 (*rev*)
Bryant-Greenwood, G.D. *et al., Endocr. Rev.* , 1994, **15**, 5 (*rev*)
Wade, J.D. *et al., J. Protein Chem.* , 1994, **13**, 315 (*synth*)

Rennin R-6

[9001-98-3]

Chymosin. Rennase. Lab ferment. Aniren. Chymogen. E.C. 3.4.23.4

Struct. consists. of a single polypeptide chain containing intramol. disulfide bridges. MW *ca.* 31,000. Component of Rennet which is used commercially in manuf. of cheese. The predominant milk-clotting enzyme from the abomasum of the suckling calf. Derived from the proenzyme renninogen. Slightly hygroscopic yellow powder. Prac. insol. H_2O.

pro-*form* [9059-50-1]

Renninogen. Chymosinogen. Prerennin. Prorennin. Prochymosin

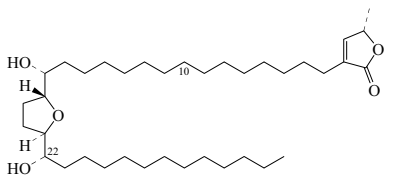
Inactive precursor of rennin. Converted to rennin in the acid environment of the stomach.

Hofmann, T. *et al., Adv. Chem. Ser.* , 1974, **136**, 146 (*rev*)
Sponcet, M. *et al., Dairy Ind. Int.* , 1985, **50**, 27 (*rev, use*)
Merck Index, 11th edn. , 1989, No. 8139
Sjoelin, L. *et al., Acta Cryst. A* , 1991, **47**, 216 (*struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2414-2416 (*use*)
Richter, C. *et al., Biochem. J.* , 1998, **335**, 481-490 (*rev*)
Chen, H. *et al., Biochemistry*, 2000, **39**, 12140-12148 (*conformn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RCZ100

Reticulatain 1 R-7

[166022-35-1]

[170080-02-1]
Neoreticulatacin A



$C_{37}H_{68}O_5$ 592.941
Constit. of *Annona reticulata* (custard apple) and *Annona squamosa* (sugar apple). Amorph. solid. $[\alpha]_D$ +22 (c, 1 in $CHCl_3$). λ_{max} 207 (MeOH).

21-Epimer: [205439-40-3] **cis-*Reticulatacin***. cis-*Uvariamicin II*
$C_{37}H_{68}O_5$ 592.941
Constit. of *Annona muricata* (soursop). Only relative config. known. Not isol. pure.

21-Epimer, 10-oxo: [205439-33-4] **cis-*Reticulatacin-10-one***
$C_{37}H_{66}O_6$ 606.925
Constit. of *Annona muricata* (soursop). Powder. Mp 62-64°. $[\alpha]_D$ +23 (c, 0.18 in MeOH). λ_{max} 220 (log ϵ 3.59) (MeOH).

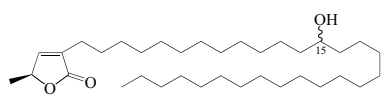
22-Epimer: [132309-10-5]

[134876-18-9, 158705-60-3] ***Reticulatacin***. *Uvariamicin II*
$C_{37}H_{68}O_5$ 592.941
Constit. of *Annona reticulata* (custard apple). Fine needles. Mp 80-80.5°. $[\alpha]_D$ +26 (c, 0.005 in $CHCl_3$).

Hisham, A. *et al., Tet. Lett.*, 1990, **31**, 4649-4652 (*isol*)
Saad, J.M. *et al., Tetrahedron*, 1991, **47**, 2751-2756 (*Reticulatacin, Uvariamicin II*)
Sinha, S.C. *et al., J.A.C.S.*, 1993, **115**, 4891-4892 (*synth*)
Makabe, H. *et al., J.C.S. Perkin 1*, 1994, 1975-1981 (*synth*)
Tam, V.T. *et al., Bull. Soc. Chim. Fr.*, 1995, **132**, 324-329 (*isol, uv, ir, pmr, cmr, ms*)
Zheng, X.-C. *et al., Zhiwu Xuebao*, 1995, **37**, 238-243 (*isol*)
Gleye, C. *et al., J. Nat. Prod.*, 1998, **61**, 576-579 (*cis-Reticulatacin, cis-Reticulatacin-10-one*)

Reticulatamol R-8

[159117-35-8, 159117-40-5]
*3-(13-Hydroxytriacontyl)-5-methyl-2(5*H*)-furanone, 9CI*



$C_{35}H_{66}O_3$ 534.905
Acetogenin precursor. Constit. of the seeds of *Annona reticulata* (custard apple). Amorph. solid (heptane). Mp 92-94°. $[\alpha]_D$ +2 (c, 1 in $CHCl_3$).

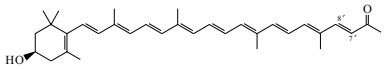
15-Ketone: [165905-07-7]

[159117-34-7] *Reticulatamone. 5-Methyl-3(13-oxotriacontyl)-2(5*H*)-furanone*
$C_{35}H_{64}O_3$ 532.889
Constit. of *Annona reticulata* (custard apple). Solid. Mp 83-85°. $[\alpha]_D$ +12 (c, 1 in $CHCl_3$). CA name is incorrect. Abs. config. uncertain. Struct. shown in ref. has *R*-config. but text states it is the *S-form* λ_{max} 208 (MeOH).

Figadere, B. *et al., J.O.C.*, 1994, **59**, 7138-7141 (*synth*)
Tam, V.T. *et al., Tet. Lett.*, 1994, **35**, 883-886 (*isol, pmr, cmr, ms*)
Tam, V.T. *et al., Bull. Soc. Chim. Fr.*, 1995, **132**, 324-329 (*Reticulatamone*)

Reticulataxanthin R-9

[28368-09-4]
3-Hydroxy-6′-methyl-6′-apo-β-caroten-6′-one. Reticulaxanthin. 3-Hydroxycitraniaxanthin



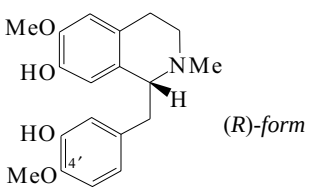
$C_{33}H_{44}O_2$ 472.709
Peel constit. of tangerine (*Citrus reticulata*) and the tangerine hybrid (*Minneola tangor*). Orange-red cryst. (Et_2O/petrol). Mp 171-172°. Poss. artifact.

7′,8′-Dihydro, 8′-hydroxy:7′,8′-Dihydro-8′-hydroxyreticulataxanthin
$C_{33}H_{46}O_3$ 490.725
Isol. from Sinton citrangequat (hybrid of *Citrus sinensis*, *Poncirus trifoliata* and *Fortunella margarita*) peel. λ_{max} 401 ; 422 ; 448 (hexane).

Yokoyama, H. *et al., J.O.C.*, 1965, **30**, 2482 (*isol, struct, pmr*)
Yokoyama, H. *et al., Phytochemistry*, 1966, **5**, 1159 (*8′-hydroxy-7′,8′-dihydroreticulataxanthin*)
Francis, G.W. *et al., Acta Chem. Scand.*, 1969, **23**, 2916 (*ms*)
de Ville, T.E. *et al., Chem. Comm.*, 1969, 1311 (*abs config*)
Stewart, I. *et al., Phytochemistry*, 1973, **12**, 2947 (*synth*)

Reticuline R-10

Laudanosoline 4′,6-dimethyl ether. Coclanoline



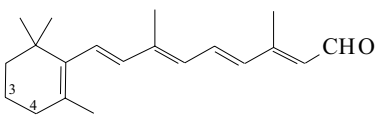
(*R*)-*form*

$C_{19}H_{23}NO_4$ 329.395
(*R*)-*form* Noncryst. $[\alpha]_D^{28}$ -55 (c, 0.44 in EtOH).
(*S*)-*form* [485-19-8]
Alkaloid from *Papaver somniferum* (opium poppy) and *Annona reticulata* (custard apple). Noncryst. $[\alpha]_D$ +132 (MeOH).
▶ LD_{50} (mus, ipr) 56 mg/kg. NX5993000
Perchlorate:
Mp 203-204° (211°). $[\alpha]_D^{31}$ +88 (EtOH).
N-*Oxide:* [71657-63-1] ***Reticuline* N-*oxide***
$C_{19}H_{23}NO_5$ 345.394
N-*Me:* [18446-73-6] ***Tembetarine***
$C_{20}H_{26}NO_4^{\oplus}$ 344.43
Mp 236-237° (as chloride). $[\alpha]_D^{29}$ +123 (c, 0.9 in EtOH).
▶ Toxic, LD_{50} 63mg/kg (rat).
Di-Me ether: Laudanosine, L-53
(±)-*form* [1699-46-3]
Noncryst. Mp 190-192° (as picrate).

Billek, G. *et al., Monatsh. Chem.*, 1956, **87**, 106-112 (*synth, deriv*)
Gopinath, K.W. *et al., Chem. Ber.*, 1959, **92**, 1657-1661 (*synth*)
Arndt, R.R. *et al., J.C.S.*, 1964, 2244-2248 (*isol, uv*)
Albonico, S.M. *et al., Annalen*, 1965, **685**, 200-206 (*isol, uv, pmr, Tembetarine*)
Battersby, A.R. *et al., J.C.S.*, 1965, 3323-3332 (*synth*)
Albonico, S.M. *et al., J.C.S.(C)*, 1966, 1340-1342 (*uv, ord, abs config, Tembetarine*)
Konda, M. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1063-1076 (*pmr, synth, ms*)
Bhakuni, D.S. *et al., J.C.S. Perkin 1*, 1977, 1662-1666 (*biosynth*)
Dasgupta, S. *et al., J. Nat. Prod.*, 1979, **42**, 399-406 (*oxide*)
Hirsenkorn, R. *et al., Tet. Lett.*, 1990, **31**, 7591-7594 (*synth*)
Chen, J. *et al., Planta Med.*, 2000, **66**, 251-256 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SLX500

Retinal, 9CI R-11

Vitamin A_1 aldehyde. Retinene$_1$. Retinaldehyde



$C_{20}H_{28}O$ 284.441
(*all-E*)-*form* [116-31-4]
Cryst. Sol. EtOH, hexane; poorly sol. H_2O. Mp 64-65°. λ_{max} 373 (E1%/1cm 1548) (cyclohexane).
▶ VH6407000
Semicarbazone:
Yellow cryst. ($CHCl_3$/Et_2O). Mp 199-201°.
3,4-Didehydro: [472-87-7] ***Vitamin A_2 aldehyde***. *Retinene$_2$. Dehydroretinal. Didehydroretinal*
$C_{20}H_{26}O$ 282.425
Constit. fish of liver oils. Orange-red cryst. Mp 77-78°.
(7*E*,9*E*,11*E*,13*Z*)-*form* [472-86-6]
13-cis-*Retinal*
Cryst. (petrol); orange oil. Mp 77°.
(7*E*,9*E*,11*Z*,13*E*)-*form* [564-87-4]
11-cis-*Retinal*
Cryst. (petrol). Mp 63.5-64.4°.
*4*R-*Hydroxy:* [140387-20-8]
[117305-82-5] *4-Hydroxy-11*-cis-*retinal*
$C_{20}H_{28}O_2$ 300.44
Oil. $[\alpha]_D$ -76.
(7*E*,9*Z*,11*E*,13*E*)-*form* [514-85-2] *9*-cis-*Retinal*
Mp 56-58°.
▶ VH6406500

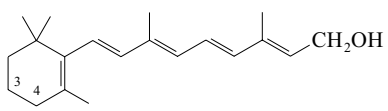
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 746B (*nmr*)
Ball, S. *et al., Biochem. J.*, 1948, **42**, 516-523 (*synth*)
Arens, J.F. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1949, **68**, 604-608 (*synth*)
Robeson, C.D. *et al., J.A.C.S.*, 1955, **77**, 4120-4125 (*isomers, synth*)
Brown, P.K. *et al., J. Biol. Chem.*, 1956, **222**, 865-877 (*11Z-form, 13Z-form, synth, uv*)

Von Plouta, C. *et al., Helv. Chim. Acta*, 1962, **45**, 548-561 (*isomers, synth*)
Sebrell, W.H. *et al., The Vitamins*, Academic Press, Vol. 1, 1967, (*rev*)
Patel, D.J. *et al., Nature (London)*, 1969, **221**, 825-828 (*pmr*)
Hamanaka, T. *et al., Acta Cryst. B*, 1972, **28**, 214-222 (*all-E form, cryst struct*)
Gilardi, R.G. *et al., Acta Cryst. B*, 1972, **28**, 2605-2612 (*11Z-form, cryst struct*)
Yasaka, W.J. *et al., J. Nutr. Sci. Vitaminol.*, 1973, **19**, 369-373 (*isol*)
Honig, B. *et al., Annu. Rev. Biophys. Bioeng.*, 1974, **3**, 151-177 (*rev*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367-2390 (*cmr*)
Shriver, J. *et al., J.A.C.S.*, 1976, **98**, 2407-2409 (*cmr*)
Simmons, C.J. *et al., Acta Cryst. B*, 1981, **37**, 2197-2205 (*13Z-form, synth, cryst struct*)
Asato, A.E. *et al., J.A.C.S.*, 1983, **105**, 2923-2924 (*synth*)
Liu, R.S.H. *et al., Tetrahedron*, 1984, **40**, 1931-1969 (*rev*)
Matsui, S. *et al., Biochim. Biophys. Acta*, 1988, **966**, 370-374 (*4-Hydroxy-11-cis-retinal*)
Zhu, Y. *et al., Tetrahedron*, 1992, **48**, 10061-10078 (*ir, uv, pmr*)
Duhamel, L. *et al., Tet. Lett.*, 1993, **34**, 319-322; 1994, **35**, 1209-1210 (*synth*)
Katsuta, Y. *et al., J.O.C.*, 1994, **59**, 6917-6921 (*4-Hydroxyretinal, synth*)
Bienayme, H. *et al., Tetrahedron*, 1994, **50**, 3389-3396 (*synth*)
Taylor, R.J.K. *et al., J.C.S. Perkin 1*, 1995, 2385-2392 (*13Z-form, synth, ir, pmr, cmr, ms*)
Uenishi, J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 320-322 (*11Z-form, synth*)
Wada, A. *et al., J.O.C.*, 2000, **65**, 2438-2443 (*synth*)
Leuenberger, M.G. *et al., Angew. Chem., Int. Ed.*, 2001, **40**, 2614-2617 (*biosynth*)
van Wijk, A.A.C. *et al., Eur. J. Org. Chem.*, 2003, 863-868 (*4-Hydroxyretinal, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSK975

Retinol, 9CI, BAN, INN R-12

[68-26-8]

3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraen-1-ol. 15-Apo-β-caroten-15-ol. Afaxin. Axerol. Axerophthol. Gadol. Prepalin. Testavol. Vitamin A. Vitamin A alcohol. Vitamin A_1 alcohol



$C_{20}H_{30}O$ 286.456

Constit. of many fish-liver oils, milk, egg-yolk, etc. Nutrient, dietary supplement. Yellow cryst. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 63-64°. $Bp_{0.000001}$ 137-138°. Log P 6.2 (calc). λ_{max} 328 (E1%/1cm 1780) (EtOH) (Berdy).

► Acute and chronic toxic effects in humans (large doses). Exp. and human teratogen. Exp. reprod. effects. LD_{50} (rat, orl) 2000 mg/kg. VH6750000

Ac: [127-47-9] *Retinol acetate. Vitamin A acetate. Many other names*
$C_{22}H_{32}O_2$ 328.494
Dietary supplement, permitted in infant formulas. Cryst. (MeOH). Mp 57-58°.

► LD_{50} (mus, orl) 4100 mg/kg. Exp. reprod. and teratogenic effects. VH6825000

Propanoyl: [7069-42-3] *Retinol propanoate. Axerofluid. Axerophthol propionate. Vitamin A propionate*
$C_{23}H_{34}O_2$ 342.52
n_D^{25} 1.6042. Fluid to -10°.

Hexadecanoyl: [79-81-2] *Retinol palmitate. Vitamin A palmitate. Arovit. Many other names*
$C_{36}H_{60}O_2$ 524.869
Nutrient, appearance control agent for colours and colour modifiers. Found in fish liver oils. Dietary supplement, permitted in infant formulas. Mp 28-29°.

► LD_{50} (mus, orl) 4760 mg/kg. Exp. reprod. and teratogenic effects. VH6860000

3,4-Didehydro: [79-80-1] ***3,4-Didehydroretinol***. *Dehydroretinol. 3-Dehydroretinol. Vitamin A_2*
$C_{20}H_{28}O$ 284.441
Constit. of fresh-water fish oils. Golden-yellow oil. Mixt. of stereoisomers. Has 40% biological activity of Vit. A_1.

15-Aldehyde: Retinal, R-11

15-Carboxylic acid: See Retinoic acid in *The Combined Chemical Dictionary.*

(11*Z*)-*form* [22737-96-8]
Shows about 25% of the biological potency of vitamin A in the rat growth test.Viscous yellow oil.

4-Nitrobenzoyl:
Mp 67°.

(13*Z*)-*form* [2052-63-3] *Neovitamin A*
Shows about 75% of the biological potency of vitamin A in the rat growth test. Constit. of cod liver oil. Mp 58-59°.

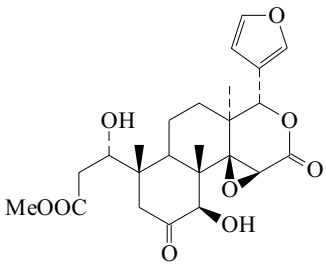
4-Nitrobenzoyl:
Mp 94-95°.

[631-87-8, 631-88-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 149C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 262C (*nmr*)
Robeson, C.D. *et al., J.A.C.S.*, 1955, **77**, 4111-4119 (*13Z-form, synth, uv, ir*)
Oroshnik, W. *et al., J.A.C.S.*, 1956, **78**, 2651-2652 (*11Z-form, synth, uv, props*)
Isler, O. *et al., Adv. Org. Chem.*, 1963, **4**, 115 (*synth, rev*)
Fr. Pat., 1966, 1 452 791; *CA*, **66**, 105072r (*synth, propanoate*)
Isler, O. *et al., Chim. Ind. (Milan)*, 1967, **49**, 1317 (*rev*)
Sebrell, W.H. *et al., The Vitamins*, Academic Press, Vol. 1, 1967, (*rev*)
Westermann, F.H. *et al., Int. J. Vitam. Nutr. Res.*, 1972, **42**, 104 (*metab, palmitate*)
Oberhänsli, W.E. *et al., Acta Cryst. B*, 1974, **30**, 161 (*cryst struct*)
Mukaiyama, T. *et al., Chem. Lett.*, 1975, 1201 (*synth*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367 (*cmr*)
Baumann, C. *et al., Method. Chim.*, 1978, **11**, 200 (*rev, Vitamin A_2*)
Cardillo, G. *et al., J.C.S. Perkin 1*, 1979, 1729 (*synth*)
Mehta, R.R. *et al., J.C.S. Perkin 1*, 1982, **12**, 2921 (*synth, acetate*)
Pitt, G.A. *et al., Proc. Nutr. Soc.*, 1983, **42**, 43 (*struct, activity, rev*)
Pure Appl. Chem., 1983, **55**, 722 (*nomencl*)
Williams, J.B. *et al., J. Lipid Res.*, 1984, **25**, 638 (*metab, acetate*)
Goodman, D.S. *et al., Retinoids*, 1984, **2**, 1; 177 (*metab, biosynth, rev*)
Liu, R.S.H. *et al., Tetrahedron*, 1984, **40**, 1931 (*rev*)
Otera, J. *et al., Chem. Lett.*, 1985, 1883-1886 (*13Z-form*)
Harbison, G.S. *et al., J.A.C.S.*, 1985, **107**, 4809 (*cmr, acetate*)
Ajima, A. *et al., Biotechnol. Lett.*, 1986, **8**, 547 (*synth, hexadecanoate*)
Otera, J. *et al., J.O.C.*, 1986, **51**, 3834 (*synth*)
Sundaresan, P. *et al., J. Sci. Ind. Res.*, 1987, **46**, 105 (*rev, metab*)
Vaezi, H.F. *et al., Org. Prep. Proced. Int.*, 1987, **19**, 187 (*synth, Vitamin A_2*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 5941; 6719; 8103
Hosoda, A. *et al., Tet. Lett.*, 1987, **28**, 65 (*synth*)
Solladie, G. *et al., Tet. Lett.*, 1988, **29**, 209-212 (*13Z-form*)
Vogt, P. *et al., Tet. Lett.*, 1991, **32**, 4115 (*synth*)
Soukup, M. *et al., Tet. Lett.*, 1991, **32**, 4117 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1051
Vitamin A in Health and Disease, (ed. Blomhoff, R.), M. Dekker, 1994, (*book*)
Biesalski, H.-K. *et al., Annalen*, 1995, 717 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2920-2926 (*use, esters*)
Rauchschwalbe, G. *et al., Eur. J. Org. Chem.*, 2001, 3903-3909 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSK600; VSP000; VSK900

Retrocalamin R-13

[74729-98-9]

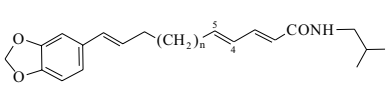


$C_{24}H_{30}O_9$ 462.496

Constit. of calamondin seeds (*Citrus reticulata*). Cryst. (C_6H_6). Mp 197-199°.

Bennett, R.D. *et al., Tetrahedron*, 1981, **37**, 17

Retrofractamides R-14



Retrofractamide A : n = 1
B : n = 3
D : n = 2

Historically, Pipercide was the first alkaloid characterised but they are described here as retrofractamides for ease of presentation..

Retrofractamide A [94079-67-1]

$C_{20}H_{25}NO_3$ 327.422

Alkaloid from the above-ground parts of *Piper retrofractum* (Javanese long pepper) and the fruits of *Piper nigrum* (pepper).

Cryst. (MeOH). Mp 129° (125°).

4,5-Dihydro: [96386-33-3] ***Retrofractamide C***
$C_{20}H_{27}NO_3$ 329.438
Alkaloid from *Piper retrofractum* (Javanese long pepper). Mp 120°.

Hexahydro:
Cryst. (MeOH). Mp 65°. Obt. from either Retrofractamide A or C.

Retrofractamide B [54794-74-0]
Pipercide
$C_{22}H_{29}NO_3$ 355.476
Alkaloid from the aerial parts of *Piper retrofractum* (Javanese long pepper) and the fruits of *Piper nigrum* (pepper). Cryst. (EtOAc). Mp 114-115°.

10,11-Dihydro: [75022-26-3]

[85383-60-4] ***10,11-Dihydropipercide***. *Dihydroretrofractamide B*
$C_{22}H_{31}NO_3$ 357.492
Alkaloid from the fruit of *Piper nigrum* (pepper). Needles (petrol/EtOAc/hexane). Mp 94-95° (89.5-91.5°).

Retrofractamide D [96386-34-4]
$C_{21}H_{27}NO_3$ 341.449
Alkaloid from *Piper retrofractum* (Javanese long pepper). Amorph. solid. Mp 118-120°. λ_{max} 211 (log ε 4.42); 262 (log ε 4.5) (EtOH).

Miyakado, M. *et al., Agric. Biol. Chem.*, 1979, **43**, 1609; 1980, **44**, 1701 (*Pipercide, Dihydropipercide*)
Crombie, L. *et al., Tet. Lett.*, 1984, **25**, 4267-4270 (*Pipercide, synth*)
Banerji, A. *et al., Phytochemistry*, 1985, **24**, 279; 1987, **26**, 3345 (*isol, uv, ir, pmr, cmr, ms, struct, synth*)
Sabharwal, A. *et al., J. Indian Chem. Soc.*, 1990, **67**, 318-320 (*Pipercide, synth*)
Strunz, G.M. *et al., Can. J. Chem.*, 1996, **74**, 419 (*synth, Retrofractamide A*)
Rotherham, L.W. *et al., J.O.C.*, 1998, **63**, 6667-6672 (*Pipercide, Dihydropipercide, synth*)
Park, I.-K. *et al., J. Agric. Food Chem.*, 2002, **50**, 1866-1870 (*isol, pmr, cmr*)
Banerji, A. *et al., Phytochemistry*, 2002, **59**, 897-901 (*Retrofractamide D*)

Reutericin 6 R-15

[141490-27-9]
Protein. Prod. by *Lactobacillus reuteri* LA6. Bacteriocin.

Kabuti, T. *et al., Int. J. Food Microbiol.*, 1997, **34**, 145-156 (*isol*)

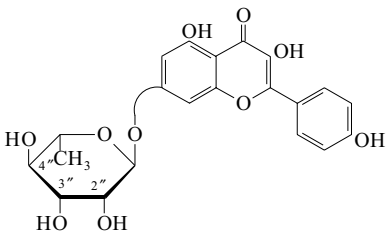
Rhamnogalacturonan II R-16

Small complex polysaccharide containing apiose, 2-*O*-methyl-L-fucose, 2-*O*-methyl-D-xylose, aceric acid, 3-deoxy-D-*lyxo*-heptulosaric acid and other sugars depending on source. Obt. by the action of liquefying enzymes on apple, tomato and carrot juice pectin. The main nondegraded soluble polysaccharide component of the juice. Also present in various other plant products, e.g. leaves of *Panax ginseng* (ginseng).

Doco, T. *et al., Carbohydr. Res.*, 1997, **297**, 181-186 (*isol, bibl*)
Shin, K.S. *et al., Carbohydr. Res.*, 1997, **300**, 239-249 (*isol, struct*)
Vidal, S. *et al., Carbohydr. Res.*, 2000, **326**, 277-294 (*struct*)

α-Rhamnoisorobin R-17

[20196-89-8]
7-O-α-L-Rhamnopyranosyloxy-3,4′,5-trihydroxyflavone. Kaempferol 7-rhamnoside



$C_{21}H_{20}O_{10}$ 432.383
Light yellow needles + $1H_2O$. Mp 221-223°.

3-O-β-D-Galactopyranoside: [38784-79-1]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Vicia faba and Solanum* spp..

3-O-(6-O-Acetyl-β-D-galactopyranoside): [124097-45-6]
$C_{29}H_{32}O_{16}$ 636.562
Isol. from *Vicia faba*.

4′-O-β-D-Glucopyranoside: [205876-37-5] *Kaempferol 4′-glucoside 7-rhamnoside*
$C_{27}H_{30}O_{15}$ 594.525
Constit. of the bracken fern *Pteridium aquilinum*.

3-O-[β-D-Xylopyranosyl-(1→4)-α-L-rhamnopyranoside]: [262852-69-7]
$C_{32}H_{38}O_{18}$ 710.641
Pale yellow cryst. Mp 232°. $[\alpha]_D^{25}$ -154 (c, 0.11 in MeOH). λ_{max} 209 ; 265 ; 326 (MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranoside]: [124027-49-2]
$C_{33}H_{40}O_{19}$ 740.668
Isol. from *Vicia faba*.

3-O-[α-L-Rhamnopyranosyl-(1→2)-6-O-acetyl-β-D-galactopyranoside]: [124027-50-5]
$C_{35}H_{42}O_{20}$ 782.705
Isol. from *Vicia faba*.

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [93098-79-4]
$C_{33}H_{40}O_{20}$ 756.667
Isol. from *Solanum tuberosum* (potato).

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [173740-43-7] *Kaempferol 3-gentiobioside 7-rhamnoside*
$C_{33}H_{40}O_{20}$ 756.667
Constit. of *Sauropus androgynus* (katuk). Amorph. yellow solid. Mp 218-219°. $[\alpha]_D^{17}$ -22 (c, 0.5 in MeOH). λ_{max} 267 (log ε 4.34); 349 (log ε 4.24) (MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]: [50906-48-4]
$C_{39}H_{50}O_{25}$ 918.809
Isol. from *Solanum tuberosum* (potato). Needles. Mp 196-198°.

2′′-O-(2-Methoxybenzoyl): ***Gladiatoside C2***
$C_{29}H_{26}O_{12}$ 566.517
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -32.6 (c, 0.2 in MeOH). λ_{max} 206 (log ε 4.5); 266 (log ε 4.3) (MeOH).

2′′-O-(2-Methoxybenzoyl), 3-O-[α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-galactopyranoside]: ***Gladiatoside B3***
$C_{47}H_{56}O_{25}$ 1020.944
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -107.9 (c, 0.2 in MeOH). λ_{max} 205 (log ε 4.8); 267 (log ε 4.3); 349 (log ε 4.2) (MeOH).

2′′-O-(2-Methoxybenzoyl), 3-O-[β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-galactopyranoside]: ***Gladiatoside A3***
$C_{47}H_{56}O_{26}$ 1036.944
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -76.3 (c, 0.2 in MeOH). λ_{max} 204 (log ε 4.7); 267 (log ε 4.2); 349 (log ε 4.1) (MeOH).

3′′-O-(2-Methoxybenzoyl): ***Gladiatoside C1***
$C_{29}H_{26}O_{12}$ 566.517
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -127 (c, 0.2 in MeOH). λ_{max} 206 (log ε 4.8); 267 (log ε 4.3) (MeOH).

3′′-O-(2-Methoxybenzoyl), 3-O-[α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-galactopyranoside]: ***Gladiatoside B2***
$C_{47}H_{56}O_{25}$ 1020.944
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -152.8 (c, 0.2 in MeOH). λ_{max} 206 (log ε 4.7); 234 (log ε 4.3); 267 (log ε 4.2); 349 (log ε 4.2) (MeOH).

3′′-O-(2-Methoxybenzoyl), 3-O-[β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-galactopyranoside]: ***Gladiatoside A2***
$C_{47}H_{56}O_{26}$ 1036.944
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -91.2 (c, 0.2 in MeOH). λ_{max} 206 (log ε 4.7); 233 (log ε 4.3); 268 (log ε 4.3); 352 (log ε 4.2) (MeOH).

4′′-O-(2-Methoxybenzoyl), 3-O-[α-L-rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-galactopyranoside]: ***Gladiatoside B1***
$C_{47}H_{56}O_{25}$ 1020.944
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -79.6 (c, 0.2 in MeOH). λ_{max} 204 (log ε 4.7); 267 (log ε 4.2) (MeOH).

4′′-O-(2-Methoxybenzoyl), 3-O-[β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-galactopyranoside]: ***Gladiatoside A1***
$C_{47}H_{56}O_{26}$ 1036.944
Constit. of the seeds of *Canavalia gladiata* (sword bean). Yellow powder. $[\alpha]_D^{25}$ -63.8 (c, 0.2 in MeOH). λ_{max} 204 (log ε 4.6); 267 (log ε 4.2); 350 (log ε 4.1) (MeOH).

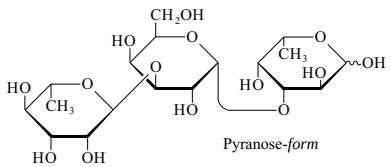
[66767-76-8, 81992-85-0]

Vierstra, R.D. *et al., Plant Physiol.*, 1982, **69**, 522 (*3-galactoside*)
Asen, S. *et al., Phytochemistry*, 1986, **25**, 2509-2513 (*derivs*)

Wang, P.-H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1997, **44**, 145-149 (*3-gentiobioside 7-rhamnoside*)
Imperato, F. *et al., Phytochemistry*, 1998, **47**, 911-913 (*Kaempferol 4′-glucoside 7-rhamnoside*)
Veit, M. *et al., J. Nat. Prod.*, 1999, **62**, 1301-1303 (*Kaempferol 3-gentiobioside 7-rhamnoside*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1673-1680 (*Gladiatosides*)

α-L-Rhamnopyranosyl-(1 → 3)-α-D-galactopyranosyl-(1 → 3)-L-fucose R-18

[71144-75-7]
6-Deoxy-α-L-mannopyranosyl-(1 → 3)-α-D-galactopyranosyl-(1 → 3)-6-deoxy-L-galactose, 9CI

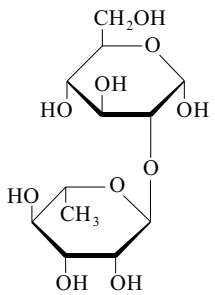


$C_{18}H_{32}O_{14}$ 472.442
Isol. from the partial acid hydrolysate of mucilage from the edible water plant junsai (*Brasenia schreberi*). $[\alpha]_D^{25}$ +21.6 (c, 2.0 in H_2O).

Kakuta, M. *et al., Agric. Biol. Chem.*, 1979, **43**, 1269 (*isol*)

2-*O*-α-L-Rhamnopyranosyl-D-glucose R-19

[17074-02-1]
*2-O-(6-Deoxy-α-L-mannopyranosyl)-D-glucose, 9CI. **Neohesperidose**. Sophorabiose*



α-Pyranose-*form*

$C_{12}H_{22}O_{10}$ 326.3
Occurs in plants as disaccharide component of Naringin and other glycosides. Prisms +1H_2O (EtOH aq.). Mp 191-192°. $[\alpha]_D^{22}$ -53.3 (7 min) → -3.9 (c, 3.0 in H_2O).

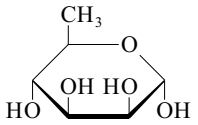
β-Pyranose-*form*

Hepta-Ac: [19949-47-4]
$C_{26}H_{36}O_{17}$ 620.56
Needles (EtOH aq.). Mp 152-153°. $[\alpha]_D^{25}$ +3.4 (c, 4.2 in Me_2CO).

Zemplén, G. *et al., Ber.*, 1938, **71**, 2511 (*isol*)
Horowitz, R.M. *et al., Tetrahedron*, 1963, **19**, 773 (*isol, struct*)
Kamiya, S. *et al., Agric. Biol. Chem.*, 1967, **31**, 261 (*synth*)

Rhamnose R-20

6-Deoxymannose. Mannomethylose



α-D-*form*

$C_6H_{12}O_5$ 164.158
An aq. soln. at 44° contains 60% α-pyr, 40% β-pyr and 0.01% aldehyde.

D-*form* [634-74-2]
Mp 90-91° (monohydrate). $[\alpha]_D$ -8.2 (H_2O).

4-Bromophenylhydrazone:
Mp 167°.

Phenylosazone:
Mp 191°. $[\alpha]_D^{20}$ -95.2 (Py).

*1-O-(3,4-Dihydroxycinnamoyl):**1-O-Caffeoylrhamnose***
$C_{15}H_{18}O_8$ 326.302

2-Me: 2-O-Methyl-D-rhamnose
$C_7H_{14}O_5$ 178.185
Syrup. $[\alpha]_D$ -28 (c, 1.12 in H_2O).

α-D-Pyranose-*form*

Me glycoside: See Methyl rhamnopyranoside in *The Combined Chemical Dictionary.*

D-Furanose-*form*

Me glycoside: See Methyl rhamnofuranoside in *The Combined Chemical Dictionary.*

L-*form* [3615-41-6] *Isodulcitol. Lokaose*
Constit. of many glycosides in plants. Quercetin (main constit. of lemon flavin) and Naringin (from grapefruit-canning wastes) have been used as sources. Crystallises as α- and β-forms which equilibrate in soln. Mp 93-95° (hydrate). $[\alpha]_D$ +8.9 (H_2O, at equilibrium).

Phenylhydrazone:
Mp 159°. $[\alpha]_D$ +54.2 → +27 (H_2O).

2,4-Dinitrophenylhydrazone:
Mp 164-165°.

Phenylosazone:
Mp 190°.

Tetranitrate:
$C_6H_8N_4O_{13}$ 344.148
Mp 135°. $[\alpha]_D$ -68.4 (MeOH).

Di-Me acetal:
$C_8H_{18}O_6$ 210.227
Mp 123-124°. $[\alpha]_D^{20}$ +10 (c, 0.4 in H_2O).

Di-Et dithioacetal:
$C_{10}H_{22}O_4S_2$ 270.413
Mp 135-137°.

Dibenzyl dithioacetal:
$C_{20}H_{26}O_4S_2$ 394.555
Mp 125°. $[\alpha]_D$ +35.3 (Py).

2-Me: [29839-06-3] *6-Deoxy-2-O-methyl-L-mannose, 8CI. 2-O-Methyl-L-rhamnose*
$C_7H_{14}O_5$ 178.185
Cryst. (prev. reported as syrup). Mp 113-114°. $[\alpha]_D$ +31 (+24) (H_2O).

3-Me: [4060-08-6]

[4598-54-3] *6-Deoxy-3-O-methyl-L-mannose, 9CI. 3-O-Methyl-L-rhamnose. **Acofriose***
Mp 118-119° (109-111°). $[\alpha]_D^{22}$ +39.1 (H_2O) (+30).

3-Me, phenylosazone:
Yellow needles (Et_2O/pentane). Mp 138-142°. $[\alpha]_D^{15}$ +128.2 → +53.2 (EtOH/Py).

4-Me: 6-Deoxy-4-O-methyl-L-mannose. 4-O-Methyl-L-rhamnose
$C_7H_{14}O_5$ 178.185
Mp 125-126°. $[\alpha]_D$ +13 (MeOH).

5-Me: 6-Deoxy-5-O-methyl-L-mannose. 5-O-Methyl-L-rhamnose
$C_7H_{14}O_5$ 178.185
Mp 102-103°. $[\alpha]_D$ -4.3 (H_2O).

2,3-Di-Me: [39687-52-0] *6-Deoxy-2,3-di-O-methyl-L-mannose, 9CI. 2,3-Di-O-methyl-L-rhamnose*
$C_8H_{16}O_5$ 192.211
Syrup. $[\alpha]_D$ +47.6 (H_2O).

2,4-Di-Me: 6-Deoxy-2,4-di-O-methyl-L-mannose. 2,4-Di-O-methyl-L-rhamnose
$C_8H_{16}O_5$ 192.211
Mp 91-93°. $[\alpha]_D$ +10.6 (H_2O).

3,4-Di-Me: [4060-11-1] *6-Deoxy-3,4-di-O-methyl-L-mannose, 9CI, 8CI. 3,4-Di-O-methyl-L-rhamnose*
$C_8H_{16}O_5$ 192.211
Mp 98-99°. $[\alpha]_D$ +24 → +18.5 (H_2O).

2,3,4-Tri-Me: [7439-05-6] *6-Deoxy-2,3,4-tri-O-methyl-L-mannose, 9CI. 2,3,4-Tri-O-methyl-L-rhamnose*
$C_9H_{18}O_5$ 206.238
Syrup. $[\alpha]_D$ +26 (H_2O).

α-L-*form*
Rods + 1H_2O (H_2O or EtOH). Mp 93-94°. On heating loses H_2O of cryst. and partly changes to the β-form. V. sweet taste.

α-L-Pyranose-*form* [6014-42-2]

1,2,4-Tri-Ac: 1,2,4-Tri-O-acetyl-6-deoxy-α-L-mannopyranose. 1,2,4-Tri-O-acetyl-α-L-rhamnopyranose
$C_{12}H_{18}O_8$ 290.269
Fine needles. Mp 145-149°. $[\alpha]_D$ -41 (c, 1.1 in $CHCl_3$).

1,2,3,4-Tetra-Ac: [27821-11-0] *1,2,3,4-Tetra-O-acetyl-6-deoxy-α-L-mannopyranose. 1,2,3,4-Tetra-O-acetyl-α-L-rhamnopyranose*
$C_{14}H_{20}O_9$ 332.307
$[\alpha]_D^{23}$ -63 (c, 2.3 in $CHCl_3$).

2-O-(4-Hydroxycinnamoyl)(E-), 3-Ac: ***Ningposide C***
$C_{17}H_{20}O_8$ 352.34
Oil. $[\alpha]_D^{20}$ +79.6 (c, 0.38 in Me_2CO).

3-O-(4-Methoxycinnamoyl)(E-), 2-Ac: ***Buergeriside B_1***
$C_{18}H_{22}O_8$ 366.367
Amorph. powder. λ_{max} 231 (log ε 2.52); 279 (log ε 2.35); 311 (log ε 1.06) (MeOH).

3-O-(4-Methoxycinnamoyl)(Z-), 2-Ac: ***Buergeriside B_2***
Amorph. powder. λ_{max} 231 (log ε 2.52); 278 (log ε 2.34); 311 (log ε 1.04) (MeOH).

4-O-(4-Methoxycinnamoyl)(E-):
[163358-97-2] *Buergeriside C_1*
$C_{16}H_{20}O_7$ 324.33
Pale yellow powder. λ_{max} 232 (log ε 2.54); 311 (log ε 1.22) (MeOH).

3,4-Bis-O-(4-methoxycinnamoyl)(E,E-), 2-Ac: ***Buergeriside A_1***

$C_{28}H_{30}O_{10}$ 526.539
Yellowish needles. λ_{max} 232 (log ϵ 2.54); 289 (log ϵ 1.82); 311 (log ϵ 1.22) (MeOH).

2-O-(4-Hydroxy-3-methoxycinnamoyl)(E-), 3-Ac: ***Ningposide A***
$C_{18}H_{22}O_9$ 382.366
Oil. $[\alpha]_D^{20}$ +116.3 (c, 0.63 in Me_2CO).

2-O-(4-Hydroxy-3-methoxycinnamoyl)(E-), 4-Ac: 4-O-Acetyl-2-O-feruloyl-α-L-rhamnopyranose. ***Ningposide B***
$C_{18}H_{22}O_9$ 382.366
Oil. $[\alpha]_D^{20}$ +87.2 (c, 0.24 in Me_2CO).

Me glycoside: See Methyl rhamnopyranoside in *The Combined Chemical Dictionary.*

Benzyl glycoside: See Benzyl rhamnoside in *The Combined Chemical Dictionary.*

Ph glycoside: Phenyl 6-deoxy-α-L-mannopyranoside. Phenyl α-L-rhamnopyranoside
$C_{12}H_{16}O_5$ 240.255
Mp 75-77°. $[\alpha]_D^{18}$ -106 (H_2O).

Ph glycoside, tri-Ac: Phenyl 2,3,4-tri-O-acetyl-6-deoxy-α-L-mannopyranoside. Phenyl 2,3,4-tri-O-acetyl-α-L-rhamnopyranoside
$C_{18}H_{22}O_8$ 366.367
Mp 130-131°. $[\alpha]_D^{18}$ -80 ($CHCl_3$).

β-L-*form*
Needles (anhyd. Me_2CO/EtOH). Mp 123.5-124.5°. Hygroscopic, converts to the α-form on exp. to moist air.

β-L-Pyranose-*form*

1,2,3-Tri-Ac: 1,2,3-Tri-O-acetyl-6-deoxy-β-L-mannopyranose. 1,2,3-Tri-O-acetyl-β-L-rhamnopyranose
$C_{12}H_{18}O_8$ 290.269
Mp 164-167°. $[\alpha]_D$ +34 (c, 0.9 in $CHCl_3$).

1,2,3,4-Tetra-Ac: 1,2,3,4-Tetra-O-acetyl-6-deoxy-β-L-mannopyranose. 1,2,3,4-Tetra-O-acetyl-β-L-rhamnopyranose
$C_{14}H_{20}O_9$ 332.307
Mp 98-99°. $[\alpha]_D^{19}$ +14.1 ($C_2H_2Cl_4$).

Me glycoside: See Methyl rhamnopyranoside in *The Combined Chemical Dictionary.*

Benzyl glycoside: See Benzyl rhamnoside in *The Combined Chemical Dictionary.*

Ph glycoside: Phenyl 6-deoxy-β-L-mannopyranoside. Phenyl β-L-rhamnopyranoside
$C_{12}H_{16}O_5$ 240.255
Mp 159-161°. $[\alpha]_D^{18}$ +87.5 (H_2O).

Ph glycoside, tri-Ac: Phenyl 2,3,4-tri-O-acetyl-6-deoxy-β-L-mannopyranoside. Phenyl 2,3,4-tri-O-acetyl-β-L-rhamnopyranoside
$C_{18}H_{22}O_8$ 366.367
Mp 147-148°. $[\alpha]_D^{18}$ +52.5 ($CHCl_3$).

L-Furanose-*form*

Me glycoside: See Methyl rhamnofuranoside in *The Combined Chemical Dictionary.*

Et glycoside: See Ethyl rhamnoside in *The Combined Chemical Dictionary.*

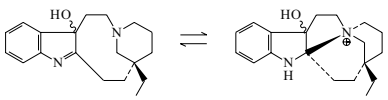
Benzyl glycoside: See Benzyl rhamnoside in *The Combined Chemical Dictionary.*

[10030-85-0]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 908B (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 191A (*ir*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 169 (*β-L-pyr tetra-Ac, L-tetranitrate, β-L-Ph pyr, α-L-Ph pyr, α-L-Ph pyr tri-Ac, β-L-Ph pyr tri-Ac*)
Maher, G.G. *et al., Adv. Carbohydr. Chem.*, 1955, **10**, 266 (*L-Me ethers, rev*)
Muhr, H. *et al., Helv. Chim. Acta*, 1955, **38**, 499 (*synth, 3-Me*)
Wolfrom, M.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 202 (*α-L-form, isol*)
Pacsu, E. *et al., Methods Carbohydr. Chem.*, 1963, **2**, 354 (*α-L-Me pyr tri-Ac*)
Stanek, J. *et al., The Monosaccharides*, Academic Press, N.Y. and London, 1963, 544; 600 (*L-form phenylhydrazones, L-form thioacetals, rev*)
Killean, A.C.G. *et al., Acta Cryst. B*, 1971, **27**, 1707 (*cryst struct*)
Butterworth, R.F. *et al., Adv. Carbohydr. Chem. Biochem.*, 1971, **26**, 279 (*deoxy sugars, props, rev*)
Brimacombe, J.S. *et al., J.C.S.(C)*, 1971, 613 (*synth, pmr, 3-Me*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 589 (*occur*)
Schaffer, R. *et al., The Carbohydrates*, (Pigman, W. *et al*, Ed.), Academic Press,N.Y. and London, 2nd Ed., 1972, 98 (*rev, isol*)
Bebault, G.M. *et al., Carbohydr. Res.*, 1974, **34**, 174 (*α-L-pyr tetra-Ac*)
Gorin, P.J. *et al., Can. J. Chem.*, 1975, **53**, 1212 (*cmr*)
Imperato, F. *et al., Phytochemistry*, 1975, **14**, 2725 (*1-O-Caffeoylrhamnose*)
de Bruyn, A. *et al., Carbohydr. Res.*, 1976, **47**, 158 (*pmr*)
Pozsgay, V. *et al., Carbohydr. Res.*, 1980, **80**, 196 (*cmr, acetates*)
Pozsgay, V. *et al., Carbohydr. Res.*, 1980, **81**, 184 (*synth, 2-Me, 3-Me*)
Kennedy, L.D. *et al., Carbohydr. Res.*, 1980, **87**, 156; 158 (*occur, 2-Me, 3-Me*)
Lipták, A. *et al., Carbohydr. Res.*, 1982, **107**, 300 (*D-2-Me*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)
Joroncic, L.D. *et al., Carbohydr. Res.*, 1989, **191**, 130 (*L-Me*)
Lee, E. *et al., Carbohydr. Res.*, 1990, **197**, 270 (*synth, cryst struct, β-L-pyr 1,2,3-tri-Ac; synth, pmr, α-L-pyr 1,2,4-tri-Ac*)
Merck Index, 12th edn., 1996, 8338
Ogawa, K. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 539 (*isol, pmr, 3-Me*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2421
Kim, S.R. *et al., Phytochemistry*, 2000, **54**, 503-509 (*Buergerisides*)
Li, Y.M. *et al., Phytochemistry*, 2000, **54**, 923-925 (*Ningposides*)

Rhazidigenine R-21

[3384-38-1]
*7-Ethyl-1,2,4,5,6,7,8,9-octahydro-14*bH-*3,7-methanoazacycloundecino[5,4-*b*]indol-14*b*-ol, 9CI. Rhazidine base*



Absolute configuration

$C_{19}H_{26}N_2O$ 298.427
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 187°. $[\alpha]_D$ -612 (EtOH/NaOH).

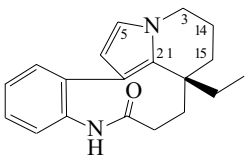
Hydrochloride: [15381-61-0] *Rhazidine. Rhazidine salt*
Mp 285° dec. $[\alpha]_D$ -40 (neutral or acidic EtOH). Quaternary pentacyclic structure.

N^b*-Oxide:* [26066-43-3] ***Rhazidigenine*** **N^b-*oxide***
$C_{19}H_{26}N_2O_2$ 314.427
Alkaloid from the bark of *Aspidosperma quebracho-blanco* (quebracho). Noncryst.

N^b*-Oxide; hydrochloride:*
Mp 325-327°.

Spiteller-Friedmann, M. *et al., Monatsh. Chem.*, 1964, **95**, 1228 (*uv, ir, ms, struct*)
Markey, S. *et al., Tet. Lett.*, 1967, 157 (*uv, struct*)
Tunmann, P. *et al., Z. Naturforsch., B*, 1969, **24**, 1665 (*isol, uv, ir, ms, struct, oxide*)
Miana, G.A. *et al., J. Chem. Soc. Pak.*, 1982, **4**, 119; *CA*, **97**, 159507v (*isol*)

Rhazinilam R-22



$C_{19}H_{22}N_2O$ 294.396

(*R*)-*form* [36193-36-9]
Alkaloidal artifact from *Aspidosperma quebracho-blanco* (quebracho). Mp 176° Mp 214-216°.

5,21-Dihydro: [109305-80-8] ***5,21-Dihydrorhazinilam***
$C_{19}H_{24}N_2O$ 296.411Converted to Rhazinilam on prolonged exp. to air.

3-Oxo: [197141-93-8] *3-Oxorhazinilam.* ***Rhazinicine***
$C_{19}H_{20}N_2O_2$ 308.379
Powder. Mp 201-204°. $[\alpha]_D^{25}$ -247.2 (c, 0.3 in $CHCl_3$).

3-Oxo, 14,15-didehydro: [139955-87-6] ***3-Oxo-14,15-dehydrorhazinilam****. 14,15-Didehydro-3-oxorhazinilam. AQC-3*
$C_{19}H_{18}N_2O_2$ 306.363
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Amorph.

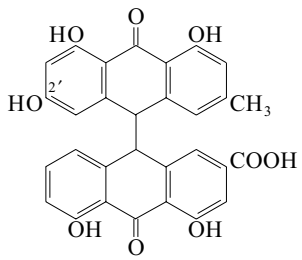
(±)-*form* [52745-52-5]
Mp 222-223°.

Banerji, A. *et al., Phytochemistry*, 1970, **9**, 1491-1493 (*isol, uv, ir, pmr, ms*)
Abraham, D.J. *et al., Tet. Lett.*, 1972, 909-912 (*cryst struct*)
De Silva, K.T. *et al., Tet. Lett.*, 1972, 913-916 (*pmr, struct*)
Ratcliffe, A.H. *et al., Tet. Lett.*, 1973, 5179-5184 (*synth*)
Goh, S.H. *et al., Tet. Lett.*, 1986, **27**, 2501-2504 (*5,21-Dihydrorhazinilam*)
Aimi, N. *et al., Tet. Lett.*, 1991, **32**, 4949-4952 (*3-Oxo-14,15-dehydrorhazinilam*)
Kam, T.-S. *et al., Nat. Prod. Lett.*, 1998, **11**, 131-136 (*Rhazinicine*)
Gerasimenko, I. *et al., J. Nat. Prod.*, 2001, **64**, 114-116 (*Rhazinicine*)

Magnus, P. *et al., Tetrahedron*, 2001, **57**, 8647-8651 (*synth*)
Johnson, J.A. *et al., J.A.C.S.*, 2002, **124**, 6900-6903 (*synth*)

Rheidin A R-23

9,9′,10,10′-Tetrahydro-2′,4,4′,5,5′-pentahydroxy-7′-methyl-10,10′-dioxo-[9,9′-bianthracene]-2-carboxylic acid. Reidin A



$C_{30}H_{20}O_9$ 524.483
Isol. from Turkey rhubarb. No phys. props. reported.

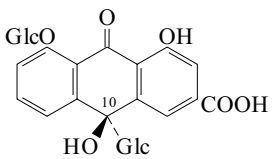
2′-Me ether: ***Rheidin C****. Reidin C*
$C_{31}H_{22}O_9$ 538.509
Isol. from rhubarb roots.

2′-Deoxy: ***Rheidin B****. Reidin B*
$C_{30}H_{20}O_8$ 508.483
Isol. from rhubarb roots.

Lemli, J. *et al., Pharm. Weekbl.*, 1963, **98**, 655; 1964, **99**, 589; 613 (*isol, struct, synth*)

Rheinoside A R-24

[111545-28-9]



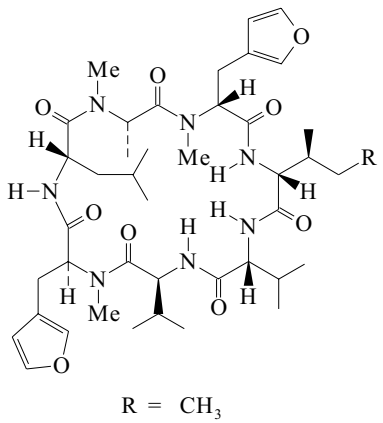
$C_{27}H_{30}O_{16}$ 610.524
Constit. of rhubarb (*Rheum* sp.). Pale yellow powder + $2H_2O$. $[\alpha]_D^{25}$ -53 (c, 0.5 in MeOH). Possesses 10*S*-config. Similar to Aloin, A-190.

10-Epimer: [111614-10-9] ***Rheinoside B***
$C_{27}H_{30}O_{16}$ 610.524
Constit. of rhubarb. Pale yellow powder + $1H_2O$. $[\alpha]_D^{25}$ -43 (c, 0.5 in MeOH).

Yamagishi, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3132 (*isol*)
Manitto, P. *et al., J.C.S. Perkin 1*, 1990, 1297 (*abs config*)

Rhizonin A, 9CI R-25

[85803-92-5]



R = CH_3

$C_{42}H_{65}N_7O_9$ 812.017
Cyclic peptide antibiotic. Mycotoxin prod. by *Rhizopus microsporus*. Isol. from infected peanuts. Cryst. (EtOAc/hexane). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 243°. $[\alpha]_D^{24}$ -25 (c, 1.15 in $CHCl_3$). λ_{max} 206 (ϵ 33000) (MeOH) (Derep).

Steyn, P.S. *et al., Chem. Comm.*, 1983, 47 (*isol, struct*)
Wilson, T. *et al., Food Chem. Toxicol.*, 1984, **22**, 275 (*props*)
Potgieter, M. *et al., Tetrahedron*, 1989, **45**, 2337 (*pmr, cmr, cryst struct*)

Rhizonin B R-26

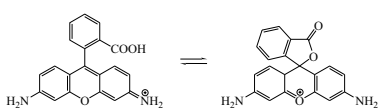
[85875-25-8]
As Rhizonin A, R-25 with
R = H
$C_{41}H_{63}N_7O_9$ 797.99
Cyclic peptide antibiotic. Mycotoxin prod. by *Rhizopus microsporus*. Isol. from infected peanuts. No phys. props. reported. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 206 (ϵ 33000) (MeOH) (Derep).

Steyn, P.S. *et al., Chem. Comm.*, 1983, 47 (*isol, struct*)
Weson, T. *et al., Food Chem. Toxicol.*, 1984, **22**, 275 (*props*)

Rhodamine 110 R-27

[13558-31-1]

[509-72-8, 30378-58-6]
3,6-Diamino-9-(2-carboxyphenyl)xanthylium(1+), 9CI. Rhodamine 560



$C_{20}H_{15}N_2O_3^{\oplus}$ 331.35
The dyestuff is usually the hydrochloride (i.e. chloride of the conjugate base illus.). In general, available samples of rhodamine dyes are notorious for their impurity and misidentification.pK_a 5.53. Mp >300° (as chloride). CAS no. refers to chloride λ_{max} 570 (no solvent reported).

N,N′-*Di-Et:* [2768-89-0] *9-(2-Carboxyphenyl)-3,6-bis(ethylamino)xanthylium(1+), 9CI. Rhodamine G. C.I. Basic Red 8. C.I. 45150*
$C_{24}H_{23}N_2O_3^{\oplus}$ 387.457
Dark red cryst. (MeOH) (as chloride). Sol. H_2O, sl. sol. EtOH. CAS no. refers to chloride.

N,N′-*Di-Et, Et ester:* [7325-85-1]

[14899-07-1] *9-[2-(Ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)xanthylium(1+), 9CI. Rhodamine 6G†. Rhodamine 6Zh. C.I. 752*
$C_{26}H_{27}N_2O_3^{\oplus}$ 415.511
Violet cryst. powder or bronze cryst. (as chloride). Sol. H_2O, EtOH. Scarlet-red with green-yellow fluor. in soln. Often confused with the parent Rhodamine 110.

N,N,N′-*Tri-Et, Et ester:* [6359-21-3] *3-(Diethylamino)-9-[2-(ethoxycarbonyl)phenyl]-6-(ethylamino)xanthylium(1+), 9CI. Rhodamine 4G*
$C_{28}H_{31}N_2O_3^{\oplus}$ 443.565
Violet cryst. powder (as chloride). Sol. H_2O, EtOH. CAS no. refers to chloride.

N,N,N′,N′-*Tetra-Et:* [14899-08-2]

[81-88-9, 509-34-2, 48381-98-2] *9-(2-Carboxyphenyl)-3,6-bis(diethylamino)xanthylium(1+), 9CI.* N-*[9-(2-Carboxyphenyl)-6-(diethylamino)-3*H-*xanthen-3-ylidene]*-N-*ethylethanaminium(1+), 9CI. Pilot 578. Rhodamine B. Rhodamine 610. Tetraethylrhodamine. C.I. Basic Violet 10. C.I. Food Red 15. C.I. Solvent Red 49. C.I. 45170*
$C_{28}H_{31}N_2O_3^{\oplus}$ 443.565
Food dye. Violet cryst. powder (as chloride). Sol. H_2O, EtOH; sl. sol. Me_2CO. Forms red aq. soln. with strong orange-yellow fluorescence.

▶ LD_{50} (mus, orl) 887 mg/kg. Weak mutagen. BP3675000

N,N,N′,N′-*Tetra-Et, Et ester:* [14899-09-3]

[2390-63-8] *3,6-Bis(diethylamino)-9-(2-ethoxyphenyl)xanthylium(1+), 9CI.* N-*[6-(Diethylamino)-9-[2-(ethoxycarbonyl)-phenyl]-3*H-*xanthen-3-ylidene]*-N-*ethylethanaminium(1+), 9CI. Ethylrhodamine B. C.I. 45175*
$C_{30}H_{35}N_2O_3^{\oplus}$ 471.618
Red-violet cryst. (H_2O) (as chloride).

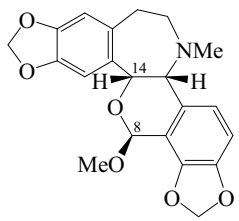
N,N,N′,N′-*Tetra-Et, butyl ester:* [3571-37-7] *9-(2-Butoxycarbonylphenyl)-3,6-bis(-diethylamino)xanthylium(1+), 9CI.* N-*[9-[2-(Butoxycarbonyl)phenyl]-6-(diethylamino)-3*H-*xanthen-3-ylidene]*-N-*ethylethanaminium(1+), 9CI. Butylrhodamine B*
$C_{32}H_{39}N_2O_3$ 499.672
Dark red-brown cryst. (as chloride). Sol. H_2O; insol. C_6H_6. CAS no. refers to chloride.

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1475F (*ir*)
Meyer, R. *et al., Ber.*, 1899, **32**, 2112-2124 (*synth*)
Kuznetsov, V.I. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1946, **52**, 231 (*synth, Butylrhodamine B*)

Onishi, H. *et al., Anal. Chim. Acta*, 1954, **11**, 44 (*detn, Sb*)
Ramette, R.W. *et al., J.A.C.S.*, 1956, **78**, 4872
Kuznetsov, V.I. *et al., Zh. Anal. Khim.*, 1960, **15**, 523 (*synth, Butylrhodamine B*)
Webb, J.M. *et al., Toxicol. Appl. Pharmacol.*, 1961, **3**, 86-95; 696-706; *CA*, **55**, 11671h; **56**, 11961a (*metab*)
Makarova, S.V. *et al., Zh. Anal. Khim.*, 1964, **19**, 564; 847 (*Ethylrhodamine B*)
Ioffe, I.S. *et al., Zh. Org. Khim.*, 1965, **1**, 336-339; 340-343; 343-346; *J. Org. Chem. USSR (Engl. Transl.)*, 1965, **1**, 326-329; 330-332; 333-336 (*uv*)
Golovina, A.P. *et al., Zh. Anal. Khim.*, 1970, **25**, 2242 (*detn, Ga*)
Kish, P.P. *et al., Zh. Anal. Khim.*, 1971, **26**, 514; 1977, **32**, 1942 (*detn, Sb, Hg*)
Khvatkova, Z.M. *et al., Vestn. Mosk. Univ., Ser. 2: Khim.*, 1972, **13**, 355; *CA*, **77**, 134673v (*detn, Te*)
Mitssel, Y.A. *et al., Zh. Anal. Khim.*, 1974, **29**, 596 (*Ethylrhodamine B*)
Shestidesatnya, N.L. *et al., Ukr. Khim. Zh. (Russ. edn.)*, 1975, **41**, 84 (*detn, Bi*)
Lebedeva, S.P. *et al., Zh. Anal. Khim.*, 1975, **30**, 1403 (*detn, Re*)
Rochat, J. *et al., Analusis*, 1976, **4**, 267 (*props*)
Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, 141; 284; 301; 566 (*use*)
IARC Monog., 1978, **16**, 221; *Suppl.* 7, 71 (*rev, tox, Rhodamine B*)
Kauffman, J.M. *et al., Appl. Opt.*, 1980, **19**, 3431 (*bibl, use*)
Alimarin, I.P. *et al., Zh. Anal. Khim.*, 1982, **37**, 855 (*Butylrhodamine B, detn U*)
Nazarenko, V.A. *et al., Zh. Anal. Khim.*, 1982, **37**, 1652 (*Butylrhodamine B, detn As*)
Skripchuk, V.G. *et al., Zavod. Lab.*, 1983, **49**, 1 (*Butylrhodamine B, detn Te*)
Sjoberg, A.M. *et al., J. Chromatogr.*, 1985, **318**, 149 (*hplc, chromatog*)
Takayanagi, M. *et al., Appl. Spectrosc.*, 1986, **40**, 1132 (*Raman*)
Ballard, J.M. *et al., Org. Mass Spectrom.*, 1986, **21**, 575 (*ms*)
Onishi, H. *et al., Photometric Determination of Traces of Metals, Part IIa: Individual Metals. Aluminium to Lithium*, John Wiley, New York, 4th Ed., 1986, 93; 578; 637; *Part IIb: Individual Metals. Magnesium to Zinc*, John Wiley, New York, 4th Ed., 1989, 424
Marczenko, Z. *et al., Separation and Spectrophotometric Determination of Elements*, Horwood, Chichester, 1986, 141; 284; 301; 566 (*use*)
Hinckley, D.A. *et al., Spectrochim. Acta A*, 1986, **42**, 747 (*uv*)
Wegener, J.W. *et al., Chromatographia*, 1987, **24**, 865 (*hplc, uv*)
Chalmers, J.H. *et al., J. Chem. Educ.*, 1987, **64**, 969 (*props*)
Ernsting, N.P. *et al., Chem. Phys.*, 1988, **122**, 431 (*spectra*)
Elliott, G.S. *et al., J. Toxicol. Clin. Exp.*, 1990, **28**, 45 (*tox*)
Wang, X.-Q. *et al., Huaxue Xuebao*, 2000, **58**, 1173-1175 (*cryst struct*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 628
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG070

Rhoeadine R-28

8-Methoxy-16-methyl-2,3:10,11-bis[-methylenebis(oxy)]rheadan, 9CI. Rheadine. O-*Methylrhoeagenine.* N-*Methylpapaverrubine E*



(+)-*form*

$C_{21}H_{21}NO_6$ 383.4

Various numbering schemes in use.

(+)-*form* [2718-25-4]
Needles (MeOH or $CHCl_3$/MeOH). Mp 253-254°. $[\alpha]_D^{22}$ +228.5 (c, 1.008 in $CHCl_3$).

► Toxic, LD_{50} 530 mg/kg (i.p., rat). VI0650000

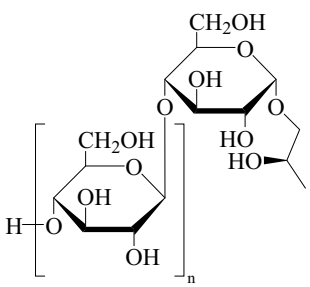
O-*De-Me:* [5574-77-6] ***Rhoeagenine.*** *Rheagenine*
$C_{20}H_{19}NO_6$ 369.373
In some solvents the alkaloid exists as a mixt. of C14 epimers (hemiacetal equilibrium). Alkaloid from *Papaver rhoeas* (corn poppy). Mp 236-238°. $[\alpha]_D^{22}$ +134 (c, 0.96 in Py).

8,14-Diepimer, O-*de-Me:* [17948-35-5] ***Isorhoeagenine.*** *Isorheagenine*
$C_{20}H_{19}NO_6$ 369.373
Alkaloid from *Papaver rhoeas* (corn poppy). Needles (MeOH/Me_2CO). Mp 210-215°. $[\alpha]_D^{22}$ +153 (c, 0.65 in 1:1 $CHCl_3$/MeOH).

8,14-Diepimer, O-*de-Me,* O-α-D-*glucopyranoside:* [17948-36-6] ***Alkaloid RC***
$C_{26}H_{29}NO_{11}$ 531.515
Alkaloid from *Papaver rhoeas* (corn poppy). Mp 240-242°. $[\alpha]_D^{22}$ +250 (c, 0.40 in $CHCl_3$/MeOH 1:1).

Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 3479; 1967, **32**, 461 (*Rhoeadine, Isorhoeagenine, uv, pmr, struct, synth*)
Němečková, A. *et al., Naturwissenschaften*, 1967, **54**, 45 (*Alkaloid RC*)
Huber, C.S. *et al., Acta Cryst. B*, 1970, **26**, 373 (*Rhoeagenine, cryst struct, abs config*)

Rhynchosporosides R-29

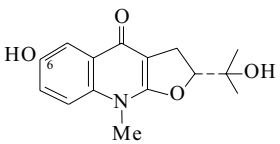


Polysaccharide antibiotics. A family of fungal toxins prod. by *Rhyncosporium secalis*. Causal agent of scald disease in barley. Isol. and struct. elucidation of these compds. has not been fully completed.

Beier, R.C. *et al., Carbohydr. Res.*, 1983, **121**, 79 (*synth, struct*)
Nicolaou, K.C. *et al., J.A.C.S.*, 1985, **107**, 5556 (*synth, bibl*)

Ribaline R-30

[50894-68-3]
*3,9-Dihydro-6-hydroxy-2-(1-hydroxy-1-methylethyl)-9-methylfuro[2,3-*b*]quinolin-4(2*H*)-one, 9CI. Rutalinidine*



(*R*)-*form*

$C_{15}H_{17}NO_4$ 275.304

(*R*)-*form* [6872-52-2]
Cryst. (MeOH). Mp 210-211° (indefinite). $[\alpha]_D^{25}$ +86 (c, 0.44 in MeOH) (+72.1).

O^6-*Ac:*
Glistening plates (Me_2CO). Mp 222-223°. $[\alpha]_D^{25}$ +82.1 (c, 0.6 in MeOH).

(±)-*form* [41234-32-6]
Minor alkaloid from *Ruta graveolens* (rue). Needles (MeOH). Mp 268-269° (259-260° dec.).

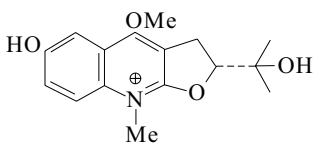
Picrate:
Mp 223-224° dec.

O^6-*Ac:*
Needles (MeOH). Mp 240°.

Szendrei, K. *et al., Herba Hung.*, 1971, **10**, 131-139 (*isol*)
Corral, R.A. *et al., Tetrahedron*, 1973, **29**, 205 (*isol, uv, ir, struct, synth*)
Hammerum, S. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 31 (*ms*)
Jurd, L. *et al., Aust. J. Chem.*, 1983, **36**, 1615 (*isol, ir, pmr, cmr, ms*)
Corral, R.A. *et al., Tet. Lett.*, 1983, **24**, 2359 (*synth*)

Ribalinium R-31

[6883-22-3]
*2,3-Dihydro-6-hydroxy-2-(1-hydroxy-1-methylethyl)-4-methoxy-9-methylfuro[2,3-*b*]quinolinium, 9CI*



$C_{16}H_{20}NO_4^{\oplus}$ 290.338

Alkaloid from the leaves of *Ruta graveolens* (rue).

Chloride:
Cryst. (MeOH/EtOAc or MeOH). Mp 188-190° (gas evoln). $[\alpha]_D^{24}$ +40 (c, 1.25 in MeOH).

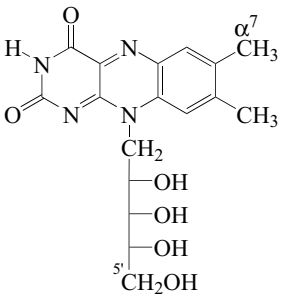
Perchlorate:
Mp 205° (218-220° dec.). $[\alpha]_D^{20}$ +23.6 (c, 0.006 in MeOH).

Picrate:
Cryst. (Me_2CO/EtOH). Mp 192-193° (darkening, gas evoln.).

Corral, R.A. *et al., Tetrahedron*, 1965, **21**, 909 (*isol, uv, ir, pmr, struct*)
Rideau, M. *et al., Phytochemistry*, 1979, **18**, 155 (*isol, pmr, ms, struct*)

Riboflavine, 9CI, BAN, INN R-32

[83-88-5]
1-Deoxy-1-(3,4-dihydro-7,8-dimethyl-2,4-dioxobenzo[g]pteridin-10(2H)-yl)-D-ribitol, 9CI. Flavaxin. Lactoflavine. Ovoflavine. Vitamin B_2. Vitamin G. Russupteridine yellow III. E101. Many other names



$C_{17}H_{20}N_4O_6$ 376.368
Colour additive in food, nutrient supplement. Vitamin cofactor.. Orange needles. Sol. EtOH; spar. sol. H_2O. Mp 280° dec. $[\alpha]_D$ -9.8 (H_2O). $[\alpha]_D$ -125 (20*N* NaOH). pK_{a1} 1.9; pK_{a2} 10.2 (25°). Green fluor. in soln. λ_{max} 220 ; 265 ; 365 ; 455 (H_2O).
▶ LD_{50} (rat, ipr) 560 mg/kg. VJ1400000

5′-Phosphate: [146-17-8]

[130-40-5] *Riboflavine 5′-(dihydrogen phosphate), 9CI. Flavin mononucleotide. Lactoflavin phosphate. Monophosphoriboflavin. Riboflavin monophosphate. Vitamin B_2 phosphate. FMN. Bisulase*
$C_{17}H_{20}N_4O_9P$ 455.34
Vitamin. Sodium salt used as dietary and nutrient supplement. Yellow cryst. ($2H_2O$). Tends to isomerise to isomeric phosphates.
▶ LD_{50} (mus, ivn) 365 mg/kg. VJ1350000

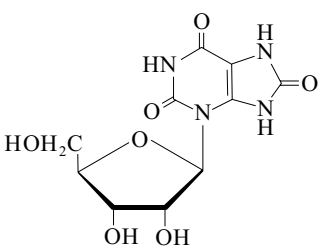
2′,3′,4′,5′-Tetrabutanoyl: [752-56-7] *Riboflavine 2′,3′,4′,5′-tetrabutanoate, 9CI. Riboflavine butyrate. Riboflavine tetrabutyrate. Vitamin B_2 tetrabutyrate. Many other names*
$C_{33}H_{44}N_4O_{10}$ 656.731
Widely used food additive. Transparent red plates (MeOH). Mp 149° (142-146°).
▶ VJ1755000

[6184-17-4, 129569-92-2, 129569-93-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 895B (*ir*)
Viscontini, M. *et al., Helv. Chim. Acta*, 1952, **35**, 457 (*synth, phosphate*)
Tanaka, N. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 1546 (*cryst struct*)
Paterson, T. *et al., Chem. Comm.*, 1969, 290 (*biosynth*)
Beach, R. *et al., Tet. Lett.*, 1969, 3489 (*synth*)
Mayhew, S.S. *et al., Biochim. Biophys. Acta*, 1971, **235**, 289-302 (*synth, uv, 1,5-dihydro 5′-phosphate*)
Kainosho, M. *et al., Biochemistry*, 1972, **11**, 741 (*P-31 nmr, phosphate*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, (*use*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2610 (*occur*)
Tachibana, S. *et al., J. Nutr. Sci. Vitaminol.*, 1975, **21**, 347; 1979, **25**, 361; 1980, **66**, 333 (*Schizoflavins*)
Yagi, K. *et al., Biochemistry*, 1976, **15**, 2877 (*N-15 nmr*)
Yoneda, F. *et al., J.A.C.S.*, 1976, **98**, 830 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **24**, 108 (*rev, synth*)
Walt, D.R. *et al., J.A.C.S.*, 1980, **102**, 7805 (*synth, 5′-phosphate*)
Merrill, A.H. *et al., Methods Enzymol.*, 1980, **66**, 287 (*phosphate, synth*)
Van Schagen, C.G *et al., Eur. J. Biochem.*, 1981, **120**, 33-39 (*synth, cmr, 1,5-dihydro 5′-phosphate*)
Brown, G.M. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1982, **53**, 345 (*rev, biosynth*)
Bacher, A. *et al., J.A.C.S.*, 1982, **104**, 3754 (*biosynth*)
Ulrich, E.L. *et al., Tet. Lett.*, 1983, **24**, 473 (*pmr*)
Keller, P.J. *et al., Tetrahedron*, 1983, **39**, 3471 (*biosynth*)
Moonem, C.T.W. *et al., Biochemistry*, 1984, **23**, 4859-4867 (*pmr, cmr, conformn, tetra-Ac, 5′-phosphate, 1,5-dihydro 5′-phosphate*)
Cooperman, J.M. *et al., Food Sci. Technol.*, 1984, **13**, 299 (*rev, metab, props*)
Nielsen, P. *et al., Methods Enzymol.*, 1986, **122**, 209 (*synth, phosphates*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 4425; 4473; 7551
Ebitani, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2273 (*cryst struct, tetrabutyrate*)
Al-Shammary, F.J. *et al., Anal. Profiles Drug Subst.*, 1990, **19**, 429 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1054
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2431-2435 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RIF500; RIK000

3-Ribofuranosyluric acid, 8CI R-33

7,9-Dihydro-3-ribofuranosyl-1H-purine-2,6,8(3H)-trione, 9CI. Uric acid riboside



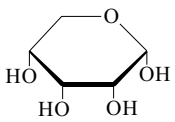
$C_{10}H_{12}N_4O_7$ 300.227
β-D-*form* [2124-54-1]
Isol. from beef blood. Cryst. (MeOH). Mp 220° dec. $[\alpha]_D^{24}$ -19 (0.1N NaOH).

2,3,5-Tribenzoyl:
$C_{31}H_{24}N_4O_{10}$ 612.551
Mp 200°. $[\alpha]_D^{22}$ +38 (c, 6.4 in Me_2CO).

Forrest, H.S. *et al., J.C.S.*, 1961, 963 (*isol, uv, struct*)
Hatfield, D. *et al., J.C.S.*, 1963, 899 (*isol, deriv*)
Lohrmann, R. *et al., J.C.S.*, 1964, 451 (*synth*)
Nishimura, T. *et al., Methods Carbohydr. Chem.*, 1972, **6**, 441 (*β-D-form, synth*)

Ribose R-34

Carnose



α-D-Pyranose-*form*

$C_5H_{10}O_5$ 150.131
An aq. soln at 31° contains 21.5% α-pyr, 58.5% β-pyr, 6.5% α-fur, 13.5% β-fur, and 0.05% aldehyde.
D-*form* [50-69-1]
A constit. of nucleic acids, several coenzymes and bacterial polysaccharides from *Salmonella*. Also occurs in plant glycosides and free in plants. Food additive listed in the EAFUS Food Additive Database (Jan 2001). Hygroscopic. Mp 95° (87°). $[\alpha]_D$ -21.5 → -19.5 (H_2O). pK_{a1} 12.22 (25°). Sweet taste, sweetness = 0.33 x sucrose.
▶ VJ2275000

[7296-61-9, 7296-62-0, 41546-19-4, 41546-20-7]

Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 115; 118
Whistler, R.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 81 (*purifn*)
Humoller, F.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 83 (*synth, L-form*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 580 (*occur*)
Schaffer, R. *et al., The Carbohydrates*, Academic Press, 1972, **1A**, 69
Bock, K. *et al., Annu. Rep. NMR Spectrosc.*, (Webb, G.A. Ed.), Acad. Press, London and New York, 1982, **13**, 38; 41 (*cmr, pmr*)
Horton, D. *et al., Carbohydr. Res.*, 1982, **105**, 145 (*cmr*)
Mathlouthi, M. *et al., Carbohydr. Res.*, 1983, **122**, 31 (*ir, Raman*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)
Lacourt-Gadras, B. *et al., Carbohydr. Res.*, 1992, **235**, 281 (*synth, D-form*)
Benesi, A.J. *et al., Carbohydr. Res.*, 1994, **258**, 27 (*pmr, cmr*)

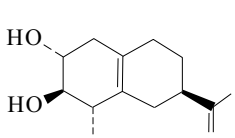
Rice antifungal protein I R-35

RAFPI
Protein, MW approx. 16.59 kDa. Isol. from germinating rice grains. Shows antifungal activity.

Liu, H. *et al., Curr. Plant Sci. Biotech. Agric.*, 1993, **15**, 11-17 (*isol*)

Rishitin R-36

[18178-54-6]



$C_{14}H_{22}O_2$ 222.327
Constit. of the tubers of white potatoes (*Solanum* spp.) infected by *Phytophthora*

infestans. Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 65-67°. $[\alpha]_D^{20}$ -8.7 ($CHCl_3$).

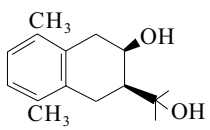
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [88848-61-7] *Rishitin 3-sophoroside*
$C_{26}H_{42}O_{12}$ 546.611

3-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside]: [99499-89-5]
$C_{32}H_{52}O_{16}$ 692.753
Cryst. Mp 208-212.5°. $[\alpha]_D$ -44.6 (c, 0.33 in EtOH).

Bukhari, S.T.K. *et al., J.C.S.(C)*, 1969, 1073 (*struct*)
Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 1206 (*synth*)
Stoessl, A. *et al., Can. J. Chem.*, 1983, **61**, 1766 (*biosynth*)
Kodama, H. *et al., Phytochemistry*, 1984, **23**, 690-692 (*sophoroside*)
Kodama, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 2537 (*rhamnosylglucosylglucoside*)
Brindle, P.A. *et al., Phytochemistry*, 1985, **24**, 1219 (*biosynth*)
Banerjee, A.K. *et al., Tetrahedron*, 1993, **49**, 4761 (*synth, rev*)
Chen, J. *et al., Tet. Lett.*, 1997, **38**, 1889 (*synth*)
Engstrom, K. *et al., Potato Res.*, 1999, **42**, 43-50; *CA*, **131**, 348943 (*activity*)

Rishitinol R-37

[31316-42-4]



$C_{15}H_{22}O_2$ 234.338
Phytoalexin of tubers of white potatoes (*Solanum tuberosum* and *Solanum demissum*) infected by *Phytophthora infestans*. Cryst. (hexane). Mp 127-129°. $[\alpha]_D$ +47 ($CHCl_3$).

Schwochau, M. *et al., Arch. Biochem. Biophys.*, 1969, **134**, 34
Katsui, N. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2871

Rizolipase, INN R-38

[9001-62-1]
Pancrelipase, USAN. *Accelerase. Alipase. Butyrase. Cotazym†. Creon. Entolase. Ilozyme. Lipancreatin. Lipase. Pancrease†. Prolipase. RoBile. Triacylglycerol lipase. Triglyceride lipase. Zymase. E.C. 3.1.1.3*

A concentrate of pancreatic enzymes standardised for lipase content. Food additive and processing agent. Prod. by controlled fermentation of *Aspergillus niger*. Found in milk and milk products. Used in food processing for flavour improvement, e.g. in cheese. Off-white to tan amorph. powder.

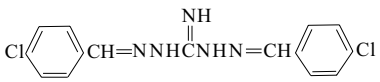
► OJ0400700

[53608-75-6]

Desnuelle, P. *et al., Methods Enzymol.*, 1961, **23**, 129 (*isol*)
Wills, E.D. *et al., Adv. Lipid Res.*, 1965, **3**, 197-240 (*synth*)
Laboureur, P. *et al., Bull. Soc. Chim. Biol.*, 1966, **48**, 747; 1967, **49**, 71; 1968, **50**, 2179 (*isol, props*)
Desnuelle, P. *et al., The Enzymes*, (Boyer, P., Ed.), 3rd Ed., Academic Press, N.Y.,, 1972, **7**, 575-616 (*rev*)
Leger, C. *et al., World Rev. Nutr. Diet.*, 1980, **35**, 96 (*rev*)
Cho, Y.W. *et al., J. Clin. Pharmacol.*, 1981, **21**, 224 (*rev*)
Lorentz, K. *et al., Med. Lab.*, 1981, **34**, 272 (*rev*)
Borgstroem, B. *et al., Lipases*, (Eds.), Elsevier, Amsterdam, 1984, (*book*)
Macrae, A.R. *et al., Biotechnol. Genet. Eng. Rev.*, 1985, **3**, 193 (*rev, use*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1398
Merck Index, 12th edn., 1996, 5336
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1604-1607 (*rev*)
Gotor, V. *et al., J. Biotechnol.*, 2002, **13**, 35-42 (*use in org synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GGA800

Robenidine, BAN, INN R-39

[25875-51-8]
*Bis[(4-chlorophenyl)methylene]carbonimidic dihydrazide, 9CI. 1,3-Bis[(*p*-chlorobenzylidene)amino]guanidine, 8CI*



$C_{15}H_{13}Cl_2N_5$ 334.207
Antiprotozoal, coccidiostat for poultry and rabbits.

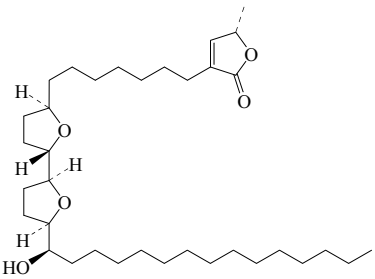
► LD_{50} (rat, orl) 1350 mg/kg. ME8650000

Hydrochloride: [25875-50-7] ***Robenidine hydrochloride, INN, USAN***. *Chemococcid. Chymcoccyd. Cycostat. Khimkoktsid. Robenz. Robenzidene*
Mp 289-290°.

► LD_{50} (rat, orl) 390 mg/kg. ME8651000

Kantor, S. *et al., Science (Washington, D.C.)*, 1970, **168**, 373 (*pharmacol*)
Zulalian, J. *et al., J. Agric. Food Chem.*, 1973, **21**, 794; 1975, **23**, 724 (*metab*)
U.S. Pat., 1976, 3 941 825, (*American Cyanamid*); *CA*, **85**, 5401w (*synth, pharmacol*)
Sorribas, V. *et al., Eur. J. Pharmacol.*, 1993, **248**, 137 (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 629
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RLK890

Robustocin R-40



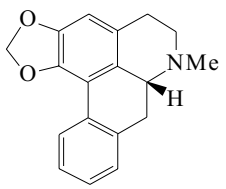
Absolute Configuration

$C_{35}H_{62}O_5$ 562.872
Constit. of the seeds of *Annona muricata* (soursop). Oil. $[\alpha]_D$ +15 (c, 0.55 in $CHCl_3$). λ_{max} 211 (log ε 3.65) (MeOH).

Gleye, C. *et al., Nat. Prod. Lett.*, 2000, **14**, 239-245

Roemerine R-41

*1,2-Methylenedioxyaporphine. Remerine†. N-Methylanonaine. 6,7,7*a*,8-Tetrahydro-7-methyl-5*H*-benzo[*g*]-1,3-benzodioxolo[6,5,4-*de*]quinoline*



(*R*)-*form*

$C_{18}H_{17}NO_2$ 279.338

(R)-form [548-08-3]
Alkaloid from *Nelumbo nucifera* (East India lotus). Mp 102-103° (85-86°). $[\alpha]_D^{25}$ -97 (c, 0.20 in EtOH).

► CE0908000

N-*De-Me:* [1862-41-5] *1,2-Methylenedioxynoraporphine.* ***Anonaine***
$C_{17}H_{15}NO_2$ 265.311
Alkaloid from *Annona muricata* (soursop) and *Nelumbo nucifera* (East India lotus). Mp 122-123°. $[\alpha]_D^{31}$ -68 (c, 0.77 in EtOH).

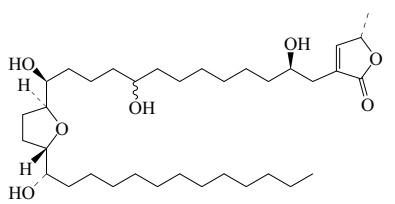
N-*De-Me,* N-*Ac:* [5894-74-6] **N-*Acetylanonaine***
$C_{19}H_{17}NO_3$ 307.348
Alkaloid from the root bark of *Zanthoxylum simulans* (Szechuan pepper). Cryst. (EtOH). Mp 229-230°. $[\alpha]_D^{25}$ -356 (c, 0.49 in $CHCl_3$).

N-*De-Me,* N-*methoxycarbonyl:* [181718-71-8] ***Romucosine***. N-*Methoxycarbonylanonaine*
$C_{19}H_{17}NO_4$ 323.348
Alkaloid from fresh unripe fruits of *Rollinia mucosa* (biriba). Needles ($CHCl_3$). Mp 152-153°. $[\alpha]_D^{25}$ -106.5 (c, 0.04 in $CHCl_3$).

Yunoussoff, S. *et al., Bull. Soc. Chim. Fr.*, 1939, **6**, 811 (*isol*)
Marion, L. *et al., J.A.C.S.*, 1944, **66**, 1290 (*Anonaine, synth*)
Gopinath, K.W. *et al., Chem. Ber.*, 1959, **92**, 776 (*Anonaine, isol*)

Barton, D.H.R. *et al., Chem. Comm.*, 1966, 259 (*biosynth*)
Johns, S.R. *et al., Aust. J. Chem.*, 1968, **21**, 1383 (*Anonaine, pmr, isol*)
Kunitomo, J. *et al., Yakugaku Zasshi*, 1969, **89**, 1691 (*uv, ir, isol*)
Bhakuni, D.S. *et al., Phytochemistry*, 1972, **11**, 1819 (*Anonaine, ms, pmr, uv, isol*)
Ziyaev, R. *et al., Khim. Prir. Soedin.*, 1974, **10**, 685; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 714 (*isol, ir, uv, ms, pmr*)
Hufford, C.D. *et al., Phytochemistry*, 1976, **15**, 1169 (*N-Acetylanonaine*)
Sashida, Y. *et al., Yakugaku Zasshi*, 1976, **96**, 659; *CA*, **88**, 3043u (*N-Acetylanonaine*)
Gray, A.I. *et al., Planta Med.*, 1980, **39**, 209 (*N-Acetylanonaine*)
Ren, L. *et al., Yaoxue Xuebao*, 1981, **16**, 672; *CA*, **96**, 48974e (*N-Acetylanonaine*)

Rolliacocin R-42

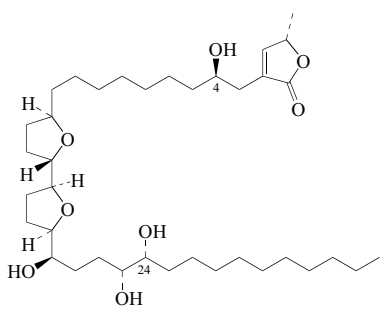


$C_{35}H_{64}O_7$ 596.886
Constit. of the unripe fruit of *Rollinia mucosa* (biriba). Waxy solid. $[\alpha]_D^{25}$ +11.8 (c, 0.33 in $CHCl_3$). λ_{max} 210 (log ϵ 3.84) (MeOH).

Liaw, C.-C. *et al., J. Nat. Prod.*, 1999, **62**, 1613-1617

Rollidecin A R-43

[182074-35-7]



Absolute Configuration

$C_{37}H_{66}O_8$ 638.924
Constit. of *Rollinia mucosa* (biriba). Waxy solid. Mp 60-61°. $[\alpha]_D$ +13 (CH_2Cl_2). λ_{max} 222 (ϵ 3300) (EtOH).

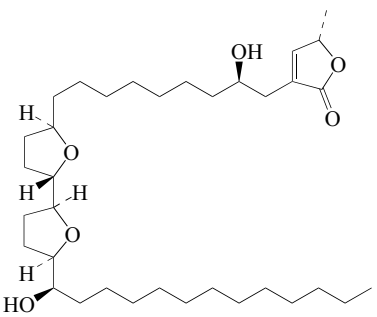
24-Epimer: [181819-77-2] ***Rollidecin B***
$C_{37}H_{66}O_8$ 638.924
Constit. of *Rollinia mucosa* (biriba). Waxy solid. Mp 57-58°. $[\alpha]_D$ +8.8 (CH_2Cl_2). λ_{max} 224 (ϵ 2800) (EtOH). λ_{max} 224 (ϵ 2800) (MeOH) (Berdy).

4-Deoxy, stereoisomer: [164177-57-5] ***Annonsilin A***
$C_{37}H_{66}O_7$ 622.924
Constit. of the seeds of *Annona squamosa* (sugar apple). Mp 107-109°. $[\alpha]_D$ +18.6 (c, 1.7 in $CHCl_3$). No stereochem. assigned.

Yang, R.Z. *et al., Zhiwu Xuebao*, 1995, **37**, 492-495; *CA*, **124**, 170607z (*Annonsilin A*)
Shi, G. *et al., Bioorg. Med. Chem.*, 1996, **4**, 1281 (*isol, uv, ir, pmr, cmr*)

Rollidecin C R-44

[200703-16-8]

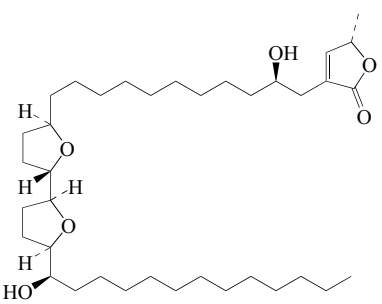


$C_{35}H_{62}O_6$ 578.871
Constit. of *Rollinia mucosa* (biriba). Waxy solid. Mp 42-43°. λ_{max} 222 (log ϵ 3.5) (MeOH).

Gu, Z. *et al., Bioorg. Med. Chem.*, 1997, **5**, 1911-1916 (*isol, uv, pmr, cmr*)

Rollidecin D R-45

[200703-17-9]

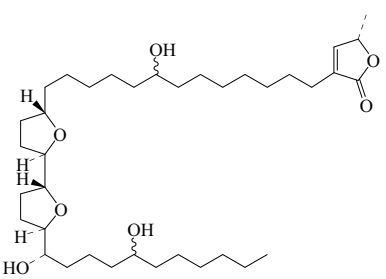


$C_{37}H_{66}O_6$ 606.925
Constit. of *Rollinia mucosa* (biriba). Waxy solid. Mp 41-42°. λ_{max} 222 (log ϵ 3.5) (MeOH).

Gu, Z. *et al., Bioorg. Med. Chem.*, 1997, **5**, 1911-1916 (*isol, uv, pmr, cmr*)

Rollimusin R-46

[252210-57-4]

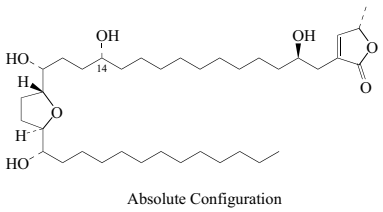


$C_{37}H_{66}O_8$ 638.924
Constit. of the unripe fruit of *Rollinia mucosa* (biriba). Waxy solid. $[\alpha]_D^{25}$ -7.8 (c, 0.55 in $CHCl_3$). λ_{max} 208 (log ϵ 3.84) (MeOH).

Liaw, C.C. *et al., J. Nat. Prod.*, 1999, **62**, 1613-1617 (*isol, pmr, cmr*)

Rollinecin A R-47

[177861-02-8]



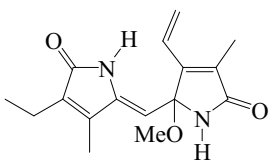
Absolute Configuration

$C_{37}H_{68}O_7$ 624.94
Constit. of *Rollinia mucosa* (biriba). Waxy solid. Mp 61-62°. $[\alpha]_D$ +10 (CH_2Cl_2). λ_{max} 227 (log ϵ 3.8) (MeOH).

14-Epimer: [178034-07-6] ***Rollinecin B***
$C_{37}H_{68}O_7$ 624.94
Constit. of *Rollinia mucosa* (biriba). Waxy solid. Mp 61-62°. $[\alpha]_D^{25}$ +12.7 (CH_2Cl_2). λ_{max} 227 (log ϵ 3.8) (MeOH).

Shi, G. *et al., J. Nat. Prod.*, 1996, **59**, 548-551 (*isol, uv, ir, pmr, cmr, ms*)

Rollipyrrole R-48

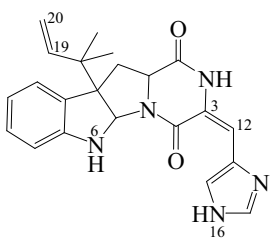


$C_{16}H_{20}N_2O_3$ 288.346
(±)-form
Constit. of the leaves of *Rollinia mucosa* (biriba). Amorph. yellow powder. Possible artifact λ_{max} 266 (no solvent reported).

Kuo, R.-Y. *et al., Tet. Lett.*, 2001, **42**, 7907-7909

Roquefortine R-49

[58735-64-1]
Roquefortine C



$C_{22}H_{23}N_5O_2$ 389.456
CA numbering shown. Metab. of *Penicillium roquefortii, Penicillium commune, Penicillium cyclopium, Penicillium farinosum* and many other *Penicillium* spp. Common constit. of blue cheese. Needles + 1MeOH (MeOH aq.). Mp 195-200° dec. $[\alpha]_D^{22}$ -703 (c, 1 in $CHCl_3$). λ_{max} 210 (ϵ 31200); 243 (ϵ 18200); 325 (ϵ

28800) (MeOH) (Berdy). λ_{max} 209 (ϵ 25500); 240 (ϵ 16200); 328 (ϵ 27000) (EtOH) (Berdy).

▶ LD_{50} (mus, ipr) 169 mg/kg ; LD_{50} (mus, ipr) 15 mg/kg. UQ4730500

N^6-*Formyl:* [158200-10-3] ***N^6-Formylroquefortine C***

$C_{23}H_{23}N_5O_3$ 417.466

Solid (MeOH aq.). Mp 216-219° dec. λ_{max} 207 ; 242 ; 326 (MeOH) (Berdy).

N^{16}-*Et:* [174792-02-0] ***N^{16}-Ethylroquefortine***

$C_{24}H_{27}N_5O_2$ 417.51

3,12-Dihydro: [58735-66-3] ***Roquefortine D. Alkaloid Z***

$C_{22}H_{25}N_5O_2$ 391.472

Prisms (MeCN). Mp 153-154°. $[\alpha]_D^{15}$ -370 (c, 0.23 in Py). λ_{max} 208 (ϵ 195000); 244 (ϵ 35480); 298 (ϵ 15130) (EtOH) (Berdy).

▶ Toxic.

19,20-Dihydro:

Mp 185-187°. $[\alpha]_D^{22}$ -740 (c, 0.15 in $CHCl_3$).

Ohmomo, S. *et al., Agric. Biol. Chem.*, 1975, **39**, 1333; 1977, **41**, 2097; 1978, **42**, 2387; 1979, **43**, 2035; 1980, **44**, 1929 (*isol, uv, ir, pmr, ms, struct, deriv*)

Scott, P.M. *et al., Experientia*, 1976, **32**, 140 (*isol, uv, ir, pmr, cmr, struct*)

Barrow, K.D. *et al., Chem. Comm.*, 1979, 225 (*biosynth*)

Scott, P.M. *et al., J. Agric. Food Chem.*, 1979, **27**, 201 (*config*)

Engel, G. *et al., J. Chromatogr.*, 1979, **170**, 288 (*tlc, uv*)

Wagener, R.E. *et al., Appl. Environ. Microbiol.*, 1980, **39**, 882 (*isol, uv, ir, ms*)

Vesonder, R.F. *et al., Experientia*, 1980, **36**, 1308 (*isol, uv, ir*)

Kozlovskii, A.G. *et al., Experientia*, 1981, **37**, 472 (*isol, biosynth*)

Gorst-Allman, C.P. *et al., Chem. Comm.*, 1982, 652 (*biosynth, cmr*)

Scott, P.M. *et al., Dev. Food Sci.*, 1984, **8**, 463 (*rev*)

Musuku, A. *et al., J. Nat. Prod.*, 1994, **57**, 983 (*N^6-Formylroquefortine C*)

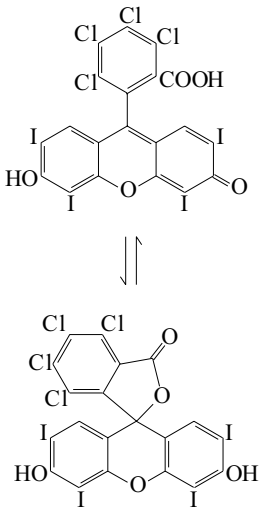
Kozlovskii, A.G. *et al., Prikl. Biokhim. Mikrobiol.*, 1997, **33**, 70-74 (*N-Ethylroquefortine*)

Chen, W.-C. *et al., Tet. Lett.*, 1998, **39**, 8401-8404 (*Roquefortine D, synth*)

Rose bengal, 8CI R-50

[4159-77-7]

4,5,6,7-Tetrachloro-3′,6′-dihydroxy-2′,4′,5′,7′-tetraiodospiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 9CI. 3,4,5,6-Tetrachloro-2′,4′,5′,7′-tetraiodofluorescein, 8CI. C.I. Solvent red 141. C.I. 45440



$C_{20}H_4Cl_4I_4O_5$ 973.677

Food colourant; no longer FDA permitted. Insol. H_2O. Normally used as di-Na salt.

Di-Na salt: [42352-53-4] *Rose bengal sodium, INN. Food red colour 105*

Food dye. Red powder.

▶ Stains clothing, skin, soft contact lenses. Exp. reprod. and teratogenic effects. Exp. goitrogen.

Di-K salt: [632-68-8] *Rose Bengal B. C.I. Acid red 94*

Bright bluish pink solid. Sol. H_2O (blue-red soln., no fluor.).

▶ Binds to and inhibits RNA polymerase.

Bis-Et_3NH salt: [91491-51-9]

Purple red powder.

Lactone-*form*

Colourless or v. pale pink solid.

[152-74-9, 632-69-9, 11121-48-5, 15251-14-6, 24916-55-0, 42352-89-6, 50291-21-9]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 556A (*nmr*)

Sigma-Aldrich Library of Stains, Dyes and Indicators, 639

Sigma-Aldrich Library of Chemical Safety Data, **2**, 3054D

Sanders, H.J. *et al., Chem. Eng. News*, 1966, **44**, (42)100; (43)108 (*rev, use*)

Bellin, J.S. *et al., J. Chromatogr.*, 1966, **24**, 131 (*chromatog*)

Bayley, B.W. *et al., Talanta*, 1966, **13**, 753 (*detn, Cu*)

Dagnall, R.M. *et al., Talanta*, 1968, **15**, 1353 (*detn, Pd*)

Peeples, W.A. *et al., J. Liq. Chromatogr.*, 1981, **4**, 51 (*hplc, purifn*)

Gandin, E. *et al., J. Chromatogr.*, 1982, **249**, 393 (*glc, purifn*)

Lamberts, J.J.M. *et al., Z. Naturforsch., B*, 1984, **39**, 474 (*uv, use, deriv*)

Lamberts, J.J.M. *et al., Tetrahedron*, 1985, **41**, 2183 (*ir, pmr, uv, props, use*)

Ghiggino, K.P. *et al., Aust. J. Chem.*, 1988, **41**, 9 (*purifn, uv, props*)

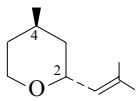
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 778; 1163

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RMP175

Rose oxide R-51

[16409-43-1]

Tetrahydro-4-methyl-2-(2-methyl-1-propenyl)pyran, 9CI. 2-Isobutenyl-4-methyltetrahydropyran. FEMA 3236



(2*R*,4*R*)-*form*

$C_{10}H_{18}O$ 154.252

Constit. of essential oil of *Pelargonium* spp., secretions of *Aromia moschata* and *Geranium bourbon*. Flavouring ingredient.

▶ UQ1470000

(2*R*,4*R*)-*form* [5258-11-7]

(-)-trans-*form*

Oil. $Bp_{1.3}$ 41-47°. $[\alpha]_D$ -18.

(2*R*,4*S*)-*form* [4610-11-1]

(+)-cis-*form*

Oil. Bp_{11} 70-71°. $[\alpha]_D^{21}$ +31.9 (neat) (opt. purity unknown). n_D^{20} 1.4545.

(2*S*,4*R*)-*form* [3033-23-6]

(-)-cis-*form*

Oil. $Bp_{1.3}$ 41-47°. $[\alpha]_D$ -58.1.

(2*RS*,4*RS*)-*form* [5542-69-8]

(±)-trans-*form*

Oil. Bp_{20} 88-89°. n_D^{20} 1.4580.

(2*RS*,4*SR*)-*form* [4610-13-3]

(±)-cis-*form*

Oil. Bp_{20} 86°. n_D^{20} 1.4535.

[876-17-5, 876-18-6, 5258-10-6]

Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1961, 645-647 (*isol, ir*)

Seidel, C.F. *et al., Helv. Chim. Acta*, 1961, **66**, 598 (*isol*)

Eschimasi, E.H. *et al., J.O.C.*, 1970, **35**, 1097-1100 (*synth, pmr*)

Vidari, G. *et al., Tet. Lett.*, 1973, 4065-4067 (*isol*)

Ogawa, T. *et al., Carbohydr. Res.*, 1978, **60**, C4-C6 (*synth*)

Lagrange, A. *et al., Carbohydr. Res.*, 1982, **110**, 165-169 (*synth, cis-form*)

Snowden, R.L. *et al., Helv. Chim. Acta*, 1987, **70**, 1879-1885 (*synth*)

Fronza, G. *et al., Tetrahedron*, 1992, **48**, 7363-7372 (*synth*)

Wuest, M. *et al., Enantiomer*, 1996, **1**, 167 (*biosynth*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2764 (*use*)

Gravel, D. *et al., Tet. Lett.*, 1998, **39**, 8035-8038 (*synth*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RNU000

Rosecin R-52

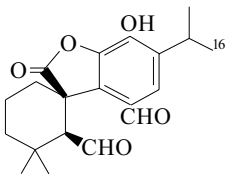
[90015-72-8]

Bacteriocin prod. by *Micrococcus roseus*.

Kato, F. *et al., Agric. Biol. Chem.*, 1984, **48**, 193-200

Rosmadial R-53

[85514-31-4]



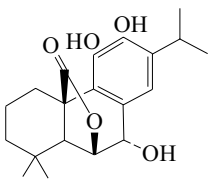
$C_{20}H_{24}O_5$ 344.407
Constit. of *Rosmarinus officinalis* (rosemary). Cryst. (C_6H_6). Mp 225°. $[\alpha]_D^{24}$ -216.8 (c, 0.54 in EtOH).

16-Hydroxy: ***16-Hydroxyrosmadial***
$C_{20}H_{24}O_6$ 360.406
Amorph. solid.

Nakatani, N. *et al., Agric. Biol. Chem.*, 1983, **47**, 353
Luis, J.G. *et al., Phytochemistry*, 1993, **33**, 635 (*isol, pmr, cmr*)

Rosmanol R-54

[80225-53-2]
7,11,12-Trihydroxy-8,11,13-abietatrien-20,6-olide



$C_{20}H_{26}O_5$ 346.422
Isol. from rosemary leaves (*Rosmarinus officinalis*). Cryst. (Me_2CO). Mp 241°. $[\alpha]_D^{18}$ -34.3 (c, 0.7 in EtOH).

7-Me ether: [113085-62-4] ***7-Methylrosmanol***. *7-Methoxyrosmanol*
$C_{21}H_{28}O_5$ 360.449
From aerial parts of rosemary (*Rosmarinus officinalis*). Pale brown powder. $[\alpha]_D^{23}$ -99.2 (c, 0.5 in EtOH).

11,12-Di-Me ether:
$C_{22}H_{30}O_5$ 374.476
Constit. of *Salvia columbariae* (California chia). Light yellow cryst. (MeOH). Mp 225-228°.

14-Hydroxy, 7-Me ether: [197649-67-5] *11,12,14-Trihydroxy-7-methoxy-8,11,13-abietatrien-20,6-olide.* ***14-Hydroxy-7-O-methylrosmanol***
$C_{21}H_{28}O_6$ 376.449
Constit. of leaves of rosemary (*Rosmarinus officinalis*). Yellow solid. $[\alpha]_D^{23}$ -128 (c, 0.17 in $CHCl_3$).

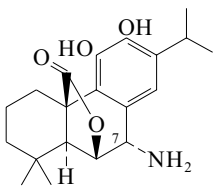
14-Methoxy, 7-Me ether: [197649-68-6] *11,12-Dihydroxy-7,14-dimethoxy-8,11,13-abietatrien-20,6-olide.* ***14-Methoxy-7-O-methylrosmanol***
$C_{22}H_{30}O_6$ 390.475
Constit. of leaves of rosemary (*Rosmarinus officinalis*). Yellow solid. $[\alpha]_D^{23}$ -43 (c, 0.2 in $CHCl_3$).

7-Epimer: [93380-12-2] ***Epirosmanol***
$C_{20}H_{26}O_5$ 346.422
From rosemary leaves (*Rosmarinus officinalis*). Cryst. (Me_2CO). Mp 221-225°.

Nakatani, N. *et al., Agric. Biol. Chem.*, 1981, **45**, 2385-2386; 1984, **48**, 2081-2085 (*Rosmanol, Epirosmanol*)
Fraga, B.N. *et al., Phytochemistry*, 1985, **24**, 1853-1854 (*Rosmanol, cryst struct*)
Arisawa, M. *et al., J. Nat. Prod.*, 1987, **50**, 1164-1166 (*Methoxyrosmanol*)
González, A.G. *et al., Can. J. Chem.*, 1989, **67**, 208-212 (*Rosmanol, 7-Ethoxyrosmanol, 7-Methoxyrosmanol, isol, pmr, cmr*)
Luis, J.G. *et al., Phytochemistry*, 1994, **35**, 1373-1374 (*di-Me ether*)
Takenaka, M. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1440-1444 (*14-Hydroxy-7-O-methylrosmanol, 14-Methoxy-7-O-methylrosmanol*)

Rosmaricine R-55

[3650-11-1]



$C_{20}H_{27}NO_4$ 345.438
Isol. from rosemary (*Rosmarinus officinalis*) using NH_3 during extraction. Mp 199-200° dec. $[\alpha]_D^{19}$ +137 (c, 1.02 in dioxan). Artifact.

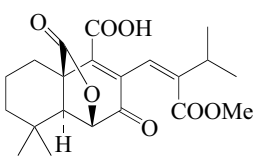
7-Epimer: [33947-58-9] *Isorosmaricine*
$C_{20}H_{27}NO_4$ 345.438
Cryst. (toluene). Mp 197-198° dec.

7-Epimer, hydrochloride:
Cryst. (H_2O). Mp 214-216° dec.

Yakhontova, L.D. *et al., Zh. Obshch. Khim.*, 1962, **32**, 1337; *J. Gen. Chem. USSR (Engl. Transl.)*, 1962, **32**, 1313 (*Rosmaricine*)
Yakhontova, L.D. *et al., Khim. Prir. Soedin.*, 1971, **7**, 416; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 396 (*Isorosmaricine*)

Rosmic acid R-56

[197799-63-6]

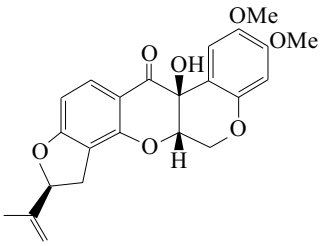


$C_{21}H_{26}O_7$ 390.432
Constit. of *Rosmarinus officinalis* (rosemary). Yellow needles. Mp 191°. $[\alpha]_D^{28}$ +37.5 (c, 0.5 in EtOH).

Takenaka, M. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1440-1444 (*isol, pmr, cmr*)

Rotenolone R-57

*1,2,12,12*a-*Tetrahydro-6*a-*hydroxy-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano[3,4-*b*]furo[2,3-*h*]benzopyran-6(6*a*H)-one, 9CI. 12*a-*Hydroxyrotenone*



$C_{23}H_{22}O_7$ 410.423
(6*aS*,12*aS*)-*form* [509-96-6]
(-)-cis-*form*
Isol. from *Pachyrrhizus erosus* (yam bean). Needles (MeOH), also descr. as oil. Mp 91-92° (88°). $[\alpha]_D^{20}$ -190.1 ($CHCl_3$) (-145). The other 3 stereoisomers obt. from natural Rotenone have all been characterised.
▶ DJ2625000

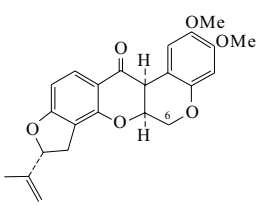
Me ether: [54534-95-1] ***12a-Methoxyrotenone***
$C_{24}H_{24}O_7$ 424.449
Pale-yellow oil. $[\alpha]_D$ -211.

[545-76-6, 16431-42-8, 110508-97-9, 110508-98-0]

Unai, T. *et al., Agric. Biol. Chem.*, 1973, **38**, 387 (*synth, spectra*)
Chubachi, M. *et al., Chem. Lett.*, 1974, 397 (*synth*)
Oberholzer, M.E. *et al., Tet. Lett.*, 1974, 2211 (*isol, config*)
Filho, R.B. *et al., Phytochemistry*, 1975, **14**, 1454 (*isol*)
Kalra, A.J. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 1084 (*isol*)
Crombie, L. *et al., Chem. Comm.*, 1979, 1142
Singhal, A.K. *et al., Chem. Ind. (London)*, 1982, 549 (*synth*)
Abidi, S.L. *et al., J. Het. Chem.*, 1983, **20**, 1687 (*cmr*)
Krishnamurti, M. *et al., J. Indian Chem. Soc.*, 1985, **62**, 629 (*pmr, ms*)
Kostova, I. *et al., Monatsh. Chem.*, 1986, **117**, 689 (*pmr, conformn*)
Van Puyvelde, L. *et al., J. Nat. Prod.*, 1987, **50**, 349 (*isol, pmr, cmr, ms*)
Van Puyvelde, L. *et al., Planta Med.*, 1990, **56**, 643 (*activity*)

Rotenone, BSI, ISO R-58

[83-79-4]
*1,2,12,12*a-*Tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6*a*H)-one, 9CI. Dactinol. Derrin. Derris, JMAF. Drikil. Nicouline. Noxfish. Paraderil. Tubotoxin*



Absolute configuration

$C_{23}H_{22}O_6$ 394.423
Widely distrib. in the Leguminosae (Papilionoideae) e.g. *Pachyrrhizus erosus* (yam bean). Cryst. (Me_2CO aq.). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 163°. $[\alpha]_D$ -225 (C_6H_6). Log P 3.25 (uncertain value) (calc). λ_{max} 212 (ϵ 29510); 237 (ϵ 14400); 295 (ϵ 16980) (EtOH) (Berdy).

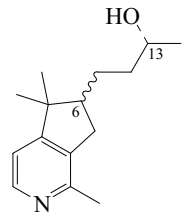
▶ Skin and eye irritant. Acute and chronic toxic effects in humans reported incl. hepatotoxic and nephrotoxic effects. LD_{50} (rat, orl) 60 mg/kg. Exp. neoplastic, reprod. and teratogenic effects. OES: long-term 5 mg m^{-3}; short-term 10 mg m^{-3} ; LD_{50} (mus, ipr) 2.8 mg/kg. DJ2800000

6ξ-Hydroxy: ***6-Hydroxyrotenone***
$C_{23}H_{22}O_7$ 410.423
Amorph. Mp 112-115°.

[24946-59-6, 42344-76-3, 54141-69-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 99A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 923A (*nmr*)
Büchi, G. *et al., J.C.S.*, 1961, 2843 (*abs config*)
Reed, R.I. *et al., J.C.S.*, 1963, 5949 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1424 (*occur*)
Unai, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 387; 897 (*synth*)
Crombie, L. *et al., J.C.S. Perkin 1*, 1973, 1277; 1285; 1975, 1497 (*synth, biosynth, cmr*)
Carlson, D.G. *et al., Tetrahedron*, 1973, **29**, 2731 (*pmr*)
Begley, M.J. *et al., Chem. Comm.*, 1975, 850 (*cryst struct*)
Haley, T.J. *et al., J. Environ. Pathol. Toxicol.*, 1978, **1**, 315 (*rev*)
Sasaki, I. *et al., Agric. Biol. Chem.*, 1979, **43**, 137 (*synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Abidi, S.L. *et al., J. Het. Chem.*, 1987, **24**, 845 (*hplc, resoln*)
Rossi, M. *et al., Bioorg. Chem.*, 1988, **16**, 376 (*cryst struct, conformn*)
Nunlist, R. *et al., J. Het. Chem.*, 1988, **25**, 351 (*pmr, cmr*)
Dangerous Prop. Ind. Mater. Rep., 1989, **9**, 74 (*rev, tox*)
Blaskó, G. *et al., J. Nat. Prod.*, 1989, **52**, 1363 (*cmr*)
Dagne, E. *et al., Phytochemistry*, 1989, **28**, 3207 (*6-Hydroxyrotenone*)
Pesticide Manual, 9th edn., 1991, No. 10610
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A363
Bhandari, P. *et al., J.C.S. Perkin 1*, 1992, 839; 851 (*biosynth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1131
Hayashi, H. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 914-916 (*activity*)
Crombie, L. *et al., Phytochemistry*, 1998, **49**, 1479-1507 (*rev, biosynth*)
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 599 (*tox, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RNZ000

Rotundine B R-59



$C_{15}H_{23}NO$ 233.353
Alkaloid from the rhizomes of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{25}$ -14.7 (c, 0.15 in $CHCl_3$). λ_{max} 264 (log ϵ 3.4) (MeOH).

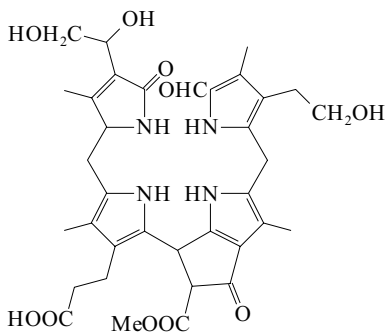
13-Ketone: ***Rotundine A***
$C_{15}H_{21}NO$ 231.337
Alkaloid from the rhizomes of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{27}$ -12.3 (c, 0.31 in $CHCl_3$). λ_{max} 260 (log ϵ 3.15) (MeOH).

6-Epimer: ***Rotundine C***
$C_{15}H_{23}NO$ 233.353
Alkaloid from the rhizomes of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{25}$ -10.2 (c, 0.11 in $CHCl_3$). λ_{max} 262 (log ϵ 3.48) (MeOH).

Jeong, S.-J. *et al., J. Nat. Prod.*, 2000, **63**, 673-675

RP 14 R-60

[135972-64-4]
Hv-*NCC-1*



$C_{35}H_{42}N_4O_{10}$ 678.738
Isol. from barley leaves. Pale yellow powder (as K salt).

Stereoisomer: **So-*NCC-2***
$C_{35}H_{42}N_4O_{10}$ 678.738
Isol. from spinach.

[136144-63-3]

Krautler, B. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 1315 (*isol, pmr, struct*)
Oberhuber, M. *et al., Helv. Chim. Acta*, 2001, **84**, 2615-2627 (*isol, uv, pmr, cmr*)

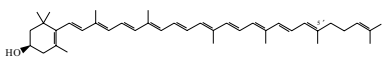
RS thionin R-61

Peptide, MW 5 kDa; a six-cysteine-type thionin. Isol. from the basic protein fraction of radish (*Raphanus sativus*). Shows antifungal activity.

Terras, F.R.G. *et al., Plant Physiol. Biochem. (Paris)*, 1996, **34**, 599-603 (*isol*)

Rubixanthin R-62

[3763-55-1]
β,ψ-Caroten-3-ol. γ-Caroten-3-ol. 3-Hydroxy-γ-carotene



$C_{40}H_{56}O$ 552.882

(all-*E*)-*form*
Constit. of ripe fruit of *Rubus chamaemorus* (cloudberry). Dark red cryst. (C_6H_6/MeOH). Mp 160°.

O-*Hexadecanoyl:* [11001-80-2] ***Rubixanthin palmitate***
$C_{56}H_{86}O_2$ 791.294

5,6-Epoxide: [29706-95-4] *5,6-Epoxy-5,6-dihydro-β,ψ-caroten-3-ol.* ***Rubixanthin 5,6-epoxide***
$C_{40}H_{56}O_2$ 568.881
Orange-red needles (Et_2O/Me_2CO). Mp 170-171°. Not definitely known to occur naturally.

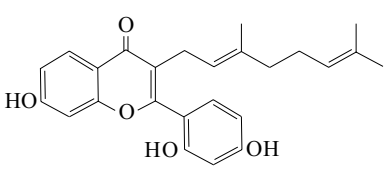
7′,8′-Dihydro: [62667-76-9] *7′,8′-Dihydro-β,ψ-caroten-3-ol. 3-Hydroxy-β-zeacarotene. β-Zeacaroten-3-ol*
$C_{40}H_{58}O$ 554.898
λ_{max} 405 ; 428 ; 453 (EtOH).

(5*Z*)-*form* [19603-65-7] ***Gazaniaxanthin***
Red platelets (C_6H_6/MeOH). Mp 133-137°. $[\alpha]_D^{25}$ +65 (c, 0.09 in $CHCl_3$) (cd).

Zechmeister, L. *et al., J.A.C.S.*, 1943, **65**, 1535-1540 (*Gazaniaxanthin*)
Karrer, P. *et al., Helv. Chim. Acta*, 1947, **30**, 531-535 (*epoxide*)
Neamtu, G. *et al., Stud. Cercet. Biochim.*, 1965, **8**, 67; *CA*, **63**, 10317c (*palmitate*)
Brown, B.O. *et al., Chem. Comm.*, 1968, 382-384 (*Gazaniaxanthin*)
de Ville, T.E. *et al., Chem. Comm.*, 1969, 1311-1312 (*struct*)
Bartlett, L. *et al., J.C.S.(C)*, 1969, 2527-2544 (*ord, abs config*)
Arpin, N. *et al., Phytochemistry*, 1969, **8**, 185-193 (*ir*)
Arpin, N. *et al., Acta Chem. Scand.*, 1973, **27**, 2321-2334 (*pmr, ms, uv*)
McDermott, J.C.B. *et al., Biochem. J.*, 1973, **134**, 1115-1117 (*biosynth*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1983, **66**, 494-513 (*isol, synth*)

Rubraflavone A R-63

[54510-13-3]
*2-(2,4-Dihydroxyphenyl)-3-(3,7-dimethyl-2,6-octadienyl)-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI. 3-Geranyl-2′,4′,7-trihydroxyflavone*



$C_{25}H_{26}O_5$ 406.477
Constit. of *Morus rubra* (red mulberry). Yellow solid.

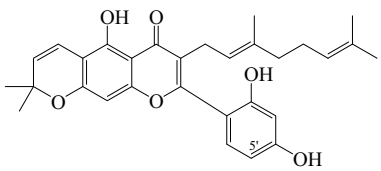
8-(3-Methyl-2-butenyl): [54835-68-6] ***Rubraflavone B***
$C_{30}H_{34}O_5$ 474.596
Constit. of *Morus rubra* (red mulberry).

Yellow solid.

Deshpande, V.H. *et al., Indian J. Chem.*, 1974, **12**, 431 (*isol*)
Wenkert, E. *et al., Phytochemistry*, 1977, **16**, 1811 (*nmr*)
Banerji, A. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 304 (*synth*)

Rubraflavone D R-64

[54835-66-4]
*8-(2,4-Dihydroxyphenyl)-7-(3,7-dimethyl-2,6-octadienyl)-5-hydroxy-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, 9CI*



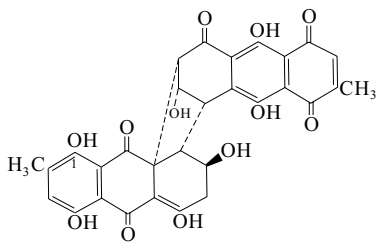
$C_{30}H_{32}O_6$ 488.579
Constit. of *Morus rubra* (red mulberry). Yellow solid.

5′-Hydroxy: ***Artoindonesianin L***
$C_{30}H_{32}O_7$ 504.579
Yellow powder. Mp 226-228°. λ_{max} 206 (log ϵ 4.83); 224 (sh) (log ϵ 4.66); 278 (log ϵ 4.85); 334 (log ϵ 4.3) (MeOH).

Deshpande, V.H. *et al., Indian J. Chem.*, 1974, **12**, 431
Suhartati, T. *et al., Fitoterapia*, 2001, **72**, 912-918 (*Artoindonesianin L*)

Rubroskyrin R-65

[21884-47-9]



$C_{30}H_{22}O_{12}$ 574.497
Mycotoxin from the common food storage mould *Penicillium islandicum*. Red cryst. (EtOH). Mp 289-290° dec. λ_{max} 275 ; 415 ; 435 ; 530 ; 540 ($CHCl_3$) (Berdy).
▶ Shows mutagenic props.. PC4930000

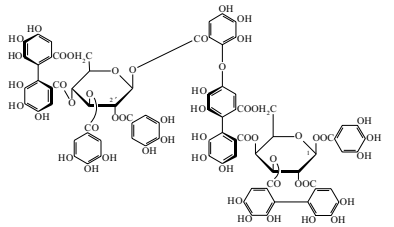
Tri-Ac:
Cryst. Mp 262-263° dec. $[\alpha]_D^{31}$ -333 (dioxan).

1-Deoxy: [52680-04-3] ***Deoxyrubroskyrin***
$C_{30}H_{22}O_{11}$ 558.497
From *Penicillium islandicum*. Red cryst. (Me_2CO). Mp 255°.

Takeda, N. *et al., Tetrahedron*, 1973, **29**, 3703 (*struct*)
Sankawa, U. *et al., Tet. Lett.*, 1973, 2125 (*biosynth*)
Ghosh, A.C. *et al., Appl. Environ. Microbiol.*, 1978, **35**, 563 (*isol*)
Stark, A.A. *et al., J. Environ. Pathol. Toxicol.*, 1978, **2**, 313 (*props*)

Rugosin F R-66

[84744-52-5]



$C_{82}H_{56}O_{52}$ 1873.313
Light-tan amorph. powder + $12H_2O$. $[\alpha]_D$ +88 (c, 1 in Me_2CO).

1-Epimer: [135413-65-9] ***Calamanin B***
$C_{82}H_{56}O_{52}$ 1873.313
Tan amorph. powder + $\frac{1}{2}H_2O$. $[\alpha]_D^{25}$ +132 (c, 1.0 in MeOH).

1-O-*Degalloyl:* ***Degalloylrugosin F***
$C_{75}H_{52}O_{48}$ 1721.207
Isol. from leaves of *Corylus heterophylla* (Siberian filbert). Pale brown amorph. powder. $[\alpha]_D^{20}$ +96 (c, 1.0 in MeOH). Equilibrated mixt. of anomers.

2′,3′-Bis-O-*degalloyl:* ***Davuriciin D_1***
$C_{68}H_{48}O_{44}$ 1569.101
Light brown amorph. powder. $[\alpha]_D^{20}$ -64 (c, 1.0 in MeOH).

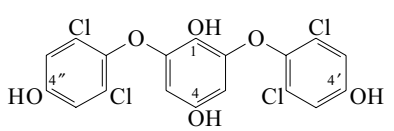
1,2′,3′-Tris-O-*degalloyl:* [145274-70-0] ***Alnusjaponin A***
$C_{61}H_{44}O_{40}$ 1416.995
Light brown amorph. powder. $[\alpha]_D^{25}$ +38.1 (c, 0.8 in MeOH). Equilibrated mixt. of anomers.

2,3-De-O-*(hexahydroxydiphenoyl):* ***Heterophylliin F***
$C_{68}H_{50}O_{44}$ 1571.117
Isol. from leaves of *Corylus heterophylla* (Siberian filbert). Amorph. off-white powder. $[\alpha]_D$ +75.3 (c, 1 in MeOH). λ_{max} 210 (log ϵ 5.34); 285 (log ϵ 4.98) (MeOH).

Okuda, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4234
Hatano, T. *et al., Chem. Pharm. Bull.*, 1990, **30**, 3341 (*pmr, cmr, cd*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 49 (*Degalloylrugosin F*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 60 (*Calamanin B*)
Yoshida, T. *et al., Phytochemistry*, 1991, **30**, 2747 (*Davuricin D_1*)
Lee, M.W. *et al., Phytochemistry*, 1992, **31**, 2835 (*Alnusjaponin A*)
Jin, Z.X. *et al., Phytochemistry*, 1998, **48**, 333-338 (*Heterophylliin F*)

Russuphelin C R-67

[141794-51-6]



$C_{18}H_{10}Cl_4O_6$ 464.084
Pale brown solid. Mp 300° dec.

1-Me ether: [141794-50-5] ***Russuphelin B***
$C_{19}H_{12}Cl_4O_6$ 478.111
Needles. Mp 295-296°. λ_{max} 228 (ϵ 42657); 235 (ϵ 29312); 283 (ϵ 11485); 294 (ϵ 9772) (MeOH) (Berdy).

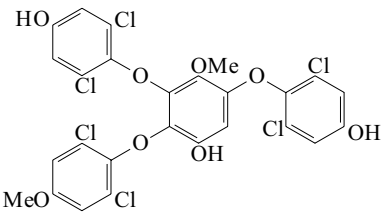
1,4-Di-Me ether: [141794-49-2] ***Russuphelin A***
$C_{20}H_{14}Cl_4O_6$ 492.138
Needles ($CHCl_3$/MeOH). Mp 293-294°. λ_{max} 228 (ϵ 51600); 237 (ϵ 45900); 283 (ϵ 12600); 293 (ϵ 11300) (MeOH) (Berdy).

1,4-Di-Me ether, di-Ac:
Needles ($CHCl_3$/hexane). Mp 172-174°.

Takahashi, A. *et al., Chem. Pharm. Bull.*, 1992, **40**, 3185; 1993, **41**, 1726 (*isol, pmr, cmr, synth, struct, deriv*)
Reddy, K.L. *et al., Synth. Commun.*, 1997, **27**, 107-118 (*synth, pmr, ir, ms*)

Russuphelol R-68

[167172-71-6]

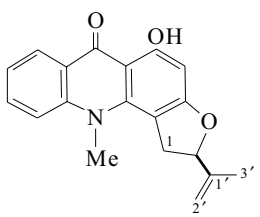


$C_{26}H_{16}Cl_6O_8$ 669.124
Pale brown powder. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 233-234°. $[\alpha]_D^{23}$ -3.2 (c, 1.8 in MeOH). Opt. activity prob. due to bulkiness of the vicinal 2,3-bisphenoxy groups λ_{max} 280 (ϵ 12590) (MeOH) (Berdy).

Ohta, T. *et al., Tet. Lett.*, 1995, **36**, 5223 (*isol, uv, ir, pmr, cmr, ms*)

Rutacridone R-69

[17948-33-3]
*1,11-Dihydro-5-hydroxy-11-methyl-2-(1-methylethenyl)furo[2,3-*c*]acridin-6(2*H*)-one*



$C_{19}H_{17}NO_3$ 307.348
Alkaloid from *Ruta graveolens* (rue). Mp 161-162°. $[\alpha]_D^{21}$ -43.
▶ VM2050000

1′,2′-Epoxide: [77996-03-3] ***Rutacridone epoxide***
$C_{19}H_{17}NO_4$ 323.348
Alkaloid from roots and callus tissue cultures of *Ruta graveolens* (rue). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 226 (ϵ 3710); 263 (ϵ 6760); 300 (ϵ 3710); 390 (ϵ 1200) (MeOH) (Berdy).
▶ LV0850000

3′-Chloro: [142741-38-6] ***Alkaloid A6***
$C_{19}H_{16}ClNO_3$ 341.793
Alkaloid from callus cultures of several

Ruta spp.. Appears not to be an artifact of the isol. procedure.

1-Hydroxy, 1′,2′-epoxide: [101330-59-0] ***1-Hydroxyrutacridone epoxide***
$C_{19}H_{17}NO_5$ 339.347
Alkaloid from the callus tissue of *Ruta graveolens* (rue).

3′-Hydroxy: [81545-69-9] ***Gravacridonol***
$C_{19}H_{17}NO_4$ 323.348
Alkaloid from *Ruta graveolens* (rue). Mp 155-156° (153°). C-2 config. not detd..

3′-Hydroxy, O-*β*-D-*glucopyranoside:* ***Gravacridonol monoglucoside***
$C_{25}H_{27}NO_9$ 485.49

3′-Hydroxy, 1′,2′-epoxide: [80565-10-2] ***20-Hydroxyrutacridone epoxide***
$C_{19}H_{17}NO_5$ 339.347
Alkaloid from the roots and callus tissue cultures of *Ruta graveolens* (rue). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. 20-Posn. in the authors' numbering scheme called here 3′. λ_{max} 227 (ϵ 8910); 250 (ϵ 9770); 264 (ϵ 10470); 274 (ϵ 13800); 301 (ϵ 5370); 330 (ϵ 2450); 392 (ϵ 1740) (MeOH) (Berdy).

1′,2′-Dihydro, 1′-chloro, 2′-hydroxy: [38494-84-7] *2-(1-Chloro-2-hydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one.* ***Gravacridonechlorine***
$C_{19}H_{18}ClNO_4$ 359.808
Alkaloid from *Ruta graveolens* (rue). Mp 254-257°.

1′,2′-Dihydro, 2′-chloro, 1′-hydroxy: [62512-94-1] *2-(2-Chloro-1-hydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one.* ***Isogravacridonechlorine***
$C_{19}H_{18}ClNO_4$ 359.808
Alkaloid from *Ruta graveolens* (rue). Yellow powder (Me_2CO). Mp 224-226° dec Mp 247-250°. $[\alpha]_D^{21}$ -9.2 (c, 0.08 in $CHCl_3$).

▶ Mutagen.

1′,2′-Dihydro, 1′,2′-dihydroxy: [37551-75-0] *2-(1,2-Dihydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one.* ***Gravacridonediol***
$C_{19}H_{19}NO_5$ 341.363
Alkaloid from the root tissue cultures of *Ruta graveolens* (rue). Cryst. (Me_2CO or Me_2CO/C_6H_6). Mp 224-227° dec Mp 227-233° Mp 246-250°. λ_{max} 214 (ϵ 14517); 227 (ϵ 14517); 249 (ϵ 26127); 273 (ϵ 3731); 300 (ϵ 15690); 331 (ϵ 7310); 400 (ϵ 4845) (MeOH).

*1′,2′-Dihydro, 1′,2′-dihydroxy, 2′-*O-*β*-D-*glucopyranoside:* [59086-97-4] ***Gravacridonediol glucoside***
$C_{25}H_{29}NO_{10}$ 503.505
Alkaloid from *Ruta graveolens* (rue). Isol. as a mixt. with Gravacridonetriol glucoside.

1′,2′-Dihydro, 1′,2′-dihydroxy, 2′-Ac: [136591-55-4] ***Gravacridonediolacetate***
$C_{21}H_{21}NO_6$ 383.4
Alkaloid from *Ruta graveolens* (rue). Yellow needles ($CHCl_3$). Mp 221-223°. $[\alpha]_D^{21}$ +59.8 (c, 0.4 in $CHCl_3$).

1′,2′-Dihydro, 1′-hydroxy, 2′-methoxy: [37551-76-1] ***Gravacridonediol methyl ether***
$C_{20}H_{21}NO_5$ 355.39
Alkaloid from the root of *Ruta graveolens* (rue). Cryst. (EtOAc). Mp 219-221°.

1′,2′-Dihydro, 1′,3′-dihydroxy, 2′-chloro: [38494-85-8] *2-[1-Chloro-2-hydroxy-1-(hydroxymethyl)ethyl]-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one.* ***Gravacridonolchlorine***
$C_{19}H_{18}ClNO_5$ 375.808
Alkaloid from *Ruta graveolens* (rue). Mp 223-227°.

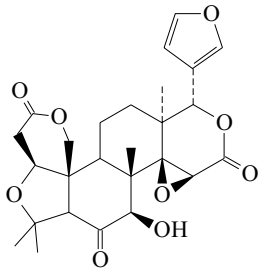
1′,2′-Dihydro, 1′,2′,3′-trihydroxy: [59086-94-1] *2-[1,2-Dihydroxy-1-(hydroxymethyl)ethyl]-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one.* ***Gravacridonetriol***
$C_{19}H_{19}NO_6$ 357.362
Alkaloid from *Ruta graveolens* (rue). Cryst. (MeOH). Mp 230-232°.

*1′,2′-Dihydro, 1′,2′,3′-trihydroxy, 2′-*O-*β*-D-*glucopyranoside:* [59086-96-3] ***Gravacridonetriol glucoside***
$C_{25}H_{29}NO_{11}$ 519.504
Alkaloid from *Ruta graveolens* (rue). Isol. as a mixt. with Gravacridonediol glucoside.

Reisch, J. *et al., Acta Pharm. Suec.*, 1967, **4**, 265; *CA*, **68**, 39861 (*isol, ir, pmr*)
Reisch, J. *et al., Phytochemistry*, 1972, **11**, 2121-2122; 2359; 1976, **15**, 240-241; 1977, **16**, 151 (*Gravacridonediol derivs, Gravacridonechlorine, Gravcridonolchlorine, Gravacridonetriol, Isogravacridonechlorine*)
Rózsa, Zs. *et al., Fitoterapia*, 1976, **47**, 147-149 (*Gravacridonediol, isol*)
Reisch, J. *et al., Z. Naturforsch., B*, 1978, **33**, 957 (*rev, pmr, struct*)
Bergenthal, D. *et al., Phytochemistry*, 1979, **18**, 161-163 (*Gravacridonediol, cmr*)
Wolters, B. *et al., Planta Med.*, 1981, **43**, 166-174 (*activity*)
Nahrstedt, A. *et al., Z. Naturforsch., C*, 1981, **36**, 200 (*Rutacridone epoxide*)
Zschunke, A. *et al., Chem. Comm.*, 1982, 1263 (*biosynth*)
Eilert, U. *et al., Z. Naturforsch., C*, 1982, **37**, 132 (*20-Hydroxyrutacridone epoxide*)
Nahrstedt, A. *et al., Planta Med.*, 1985, 517 (*1-Hydroxyrutacridone epoxide*)
Reisch, J. *et al., Monatsh. Chem.*, 1990, **121**, 829 (*synth*)
Reisch, J. *et al., Annalen*, 1991, 299 (*Gravacridonol*)
Paulini, H. *et al., Planta Med.*, 1991, **57**, 59; 82-83 (*Isogravacridonechlorine, Gravacridonediolacetate*)
Baumert, A. *et al., Plant Cell, Tissue Organ Cult.*, 1992, **28**, 159; *CA*, **117**, 66678t (*Alkaloid A6*)
Reisch, J. *et al., J. Chem. Res., Synop.*, 1994, 157; *J. Chem. Res., Miniprint*, 1994, 911-927 (*Gravacridonediol, synth, ir, pmr, cmr*)
Baumert, A. *et al., Planta Med.*, 1994, **60**, 143 (*Gravacridonol monoglucoside*)

Rutaevin R-70

[33237-37-5]
Evodinone



$C_{26}H_{30}O_9$ 486.518
Cryst. Mp 300°. $[\alpha]_D^{26}$ -130 (Me_2CO). λ_{max} 208 (ϵ 9700) (MeOH) (Berdy). λ_{max} 205 (ϵ 9000); 281 (ϵ 40) (MeCN) (Berdy).

O-*Ac:* [62306-81-4] ***Rutaevin acetate***. O-*Acetylrutaevin*
$C_{28}H_{32}O_{10}$ 528.555
$[\alpha]_D^{20}$ -150 (c, 0.0005 in $CHCl_3$).

O-*(3,4,5-Trihydroxybenzoyl):* [228092-33-9] **O-*Galloylrutaevin***
$C_{33}H_{34}O_{13}$ 638.624
Needles ($CHCl_3/Me_2CO$). Mp 267-268°. $[\alpha]_D^{25}$ -145 (c, 0.005 in $CHCl_3$). λ_{max} 210 ; 265 ($CHCl_3$).

O-*(4-Hydroxycinnamoyl)(*E-*):* [195392-13-3]
$C_{35}H_{36}O_{11}$ 632.663
Powder. Mp 275-276°. $[\alpha]_D^{20}$ -163 (c, 0.0005 in $CHCl_3$). λ_{max} 215 ; 288 ($CHCl_3$).

O-*(4-Hydroxycinnamoyl) (*Z-*):* [195392-12-2]
$C_{35}H_{36}O_{11}$ 632.663
Needles. Mp 272-273°. $[\alpha]_D^{20}$ -165 (c, 0.0005 in $CHCl_3$). λ_{max} 210 ; 285 ($CHCl_3$).

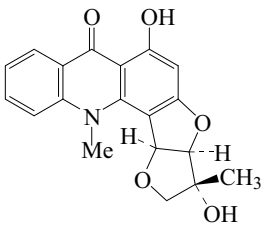
O-*(3,4-Dihydroxycinnamoyl)(*E-*):* [228092-34-0] **O-*Caffeoylrutaevin***
$C_{35}H_{36}O_{12}$ 648.662
Powder ($CHCl_3$/EtOAc). Mp 281-283°. $[\alpha]_D^{25}$ -150 (c, 0.005 in $CHCl_3$). λ_{max} 215 ; 289 ($CHCl_3$).

6β-Alcohol, 7-Ac: [208333-73-7] ***7-Acetoxy-6-hydroxylimonin***
$C_{28}H_{34}O_{10}$ 530.571
Constit. of *Ruta graveolens* (rue). Cryst. Mp 278-280°.

Dreyer, D.L. *et al., Tetrahedron*, 1976, **32**, 2367
Zheng, S. *et al., Planta Med.*, 1997, **63**, 379-380 (*Microula sikkimensis esters*)
Srivastava, S.D. *et al., Fitoterapia*, 1998, **69**, 80-81 (*7-Acetoxy-6-hydroxylimonin*)
Wang, D. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 240-242 (*acyl derivs*)

Rutagravine R-71

[101330-60-3]



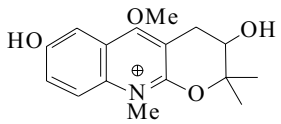
$C_{19}H_{17}NO_5$ 339.347
Alkaloid from the callus tissue of *Ruta*

graveolens (rue). Cryst. (MeOH). Mp 209-212°. $[\alpha]_D^{25}$ -152 ($CHCl_3$). λ_{max} 212 (ϵ 14414); 226 (ϵ 17057); 251 (ϵ 28602); 272 (ϵ 48289); 325 (ϵ 7207); 393 (ϵ 5700) (MeOH).

Nahrstedt, A. *et al., Planta Med.*, 1985, 517-519 (*isol, pmr, cmr, struct*)
Reisch, J. *et al., J. Chem. Res., Synop.*, 1994, 157; *J. Chem. Res., Miniprint*, 1994, 911-927 (*synth, ir, pmr, cmr, struct, abs config*)

Rutalinium R-72

[27539-40-8]

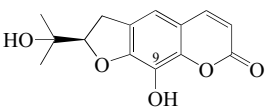


$C_{16}H_{20}NO_4^{\oplus}$ 290.338
Alkaloid from *Ruta graveolens* (rue), *Ruta graveolens* ssp. *hortensis*.

Szendrei, K. *et al., Herba Hung.*, 1971, **10**, 131; *CA*, **79**, 15853k (*isol, pmr, struct*)
Varga, E. *et al., Acta Pharm. Hung.*, 1978, **48**, 193; *CA*, **89**, 176400g (*isol*)

Rutaretin R-73

[13895-92-6]
*2,3-Dihydro-9-hydroxy-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. Campesenitin. Leptophyllin. Racemol. Qianhucoumarin G*



(*R*)-*form*

$C_{14}H_{14}O_5$ 262.262
The *S*-enantiomer is the more common. The *R*-enantiomer (named as Qianhucoumarin G) was isol. only recently.- Poorly sol. hexane. Mp 198°.

9-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [160845-05-6] *Rutaretin 9-rutinoside*
$C_{26}H_{34}O_{14}$ 570.546
Constit. of *Ruta graveolens* (rue). Light yellow cryst. Mp 150-152°. $[\alpha]_D^{25}$ +45 (EtOH). λ_{max} 230 ; 260 ; 310 (no solvent reported).

(*R*)-*form* [68692-61-5]
Mp 206-208°. $[\alpha]_D$ +14 (c, 0.3 in MeOH).

1′-O-*β-D-Glucopyranoside:* [53846-51-8]

[68692-60-4] ***Isorutarin***. *Leptophylloside*
$C_{20}H_{24}O_{10}$ 424.404
From *Ruta graveolens* (rue). Cryst. Mp 275-276° (245-248°). $[\alpha]_D$ -40 (c, 0.4 in MeOH).

1′-O-*[4-Hydroxy-3-methoxycinnamoyl-(→6)-β-D-glucopyranoside]:* [145918-57-6]
$C_{30}H_{32}O_{13}$ 600.575
Cryst. (Me_2CO aq.). Mp 150-153°. $[\alpha]_D^{20}$ +37.9 (c, 0.33 in MeOH).

1′-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(→6)-β-D-glucopyranoside]:*
$C_{31}H_{34}O_{14}$ 630.601
Constit. of *Apium graveolens*. Plates (EtOH). Mp 166-168°. $[\alpha]_D^{25}$ +75 (c, 0.38 in MeOH).

(*S*)-*form*
Isol. from seeds of *Apium graveolens* and *Ruta graveolens* (rue). Pale yellow needles. Mp 198°. $[\alpha]_D^{19}$ -30.4 (c, 0.79 in $CHCl_3$).

9-Ac: [13895-94-8]
Mp 167-168°.

Di-Ac: [65870-41-9]
$C_{18}H_{18}O_7$ 346.336
Mp 162-164°.

9-Me ether: [13895-93-7] ***Rutaretin methyl ether***
$C_{15}H_{16}O_5$ 276.288
Cryst. (MeOH). Mp 147-148°. $[\alpha]_D^{14}$ +10.8 ($CHCl_3$).

9-O-*β-D-Glucopyranoside:* [20320-81-4] ***Rutarin***. *Campesenin*
$C_{20}H_{24}O_{10}$ 424.404
From *Ruta graveolens* (rue). Cryst. Poorly sol. hexane. Mp 145-148°. $[\alpha]_D^{22}$ -47.1 (c, 0.106 in EtOH).

1′-O-*[4-Hydroxy-3-methoxybenzoyl-(→6)-β-D-glucopyranoside]:* [121064-73-1] ***Praeroside I***
$C_{28}H_{30}O_{13}$ 574.537
Cryst. Mp 143-145° dec. $[\alpha]_D^{24}$ +202.3 (H_2O).

1′-O-*[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside]:* [73485-93-5] ***Apiumoside***
$C_{29}H_{30}O_{12}$ 570.549
Constit. of *Apium graveolens*. Cryst. $[\alpha]_D^{25}$ -37.37 (MeOH). Mp > 300°.

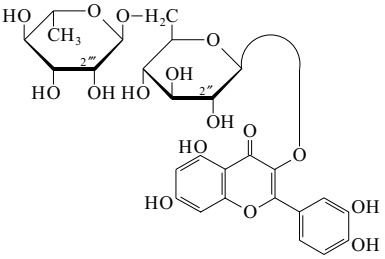
1′-O-*Sulfate:*
$C_{14}H_{14}O_8S$ 342.326
Cryst. (as K salt). Mp 128-130° (K salt). $[\alpha]_D^{23}$ -46.2 (c, 0.4 in MeOH).

[112756-76-0]

Schneider, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1967, **300**, 73; 913 (*isol, ir, uv, pmr, ms*)
Shagova, L.I. *et al., Khim. Prir. Soedin.*, 1973, **9**, 665; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 631 (*isol*)
Varga, E. *et al., Acta Pharm. Hung.*, Suppl. No. 36, 1974, **44**, ; *CA*, **82**, 13996 (*isol*)
Sharma, P. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 563 (*Leptophyllin*)
Garg, S.K. *et al., Phytochemistry*, 1978, **17**, 2135; 1979, **18**, 1769 (*isol, ir, uv, Apiumoside*)
Sharma, B.R. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 647 (*Leptophyllin*)
Sharma, B.R. *et al., Phytochemistry*, 1980, **19**, 1556
Lemmich, J. *et al., Phytochemistry*, 1984, **23**, 863 (*sulfate*)
Ishii, H. *et al., Tetrahedron*, 1986, **37**, 285 (*abs config*)
Thailambal, V.G. *et al., Acta Cryst. C*, 1987, **43**, 2369 (*cryst struct*)
Ahluwalia, V.K. *et al., Phytochemistry*, 1988, **27**, 1181 (*glycoside*)
Okuyama, T. *et al., Planta Med.*, 1989, **55**, 64 (*Praeroside I*)
Reisch, J. *et al., Phytochemistry*, 1992, **31**, 4376 (*acylglycosides*)
Kong, L. *et al., Chin. Chem. Lett.*, 1993, **4**, 37 (*Qianhucoumarin G*)
Srivastava, S.K. *et al., Fitoterapia*, 1994, **65**, 301-303 (*rutinoside*)
Reisch, J. *et al., J.C.S. Perkin 1*, 1994, 3251 (*synth*)

Rutin, JAN R-74

[153-18-4]
Quercetin 3-β-D-rutinoside. ***Rutoside, BAN, INN.*** *Rutinic acid. Sophorin†. Melin. Osyritin. Violaquercitrin. Myrticolorin. Globulariacitrin. Eldrin. Paliuroside. Rutinion. Vitamin P†*



$C_{27}H_{30}O_{16}$ 610.524
The synonym Rutinion refers to the Na salt. The name Vitamin P appears to be loosely applied to various bioflavonoids or mixtures of which Rutin is one component. First isol. from *Ruta graveolens* (rue). Bioflavonoid. Yellow cryst. + $3H_2O$ (H_2O). Mp 214-215° dec. (anhyd.). $[\alpha]_D^{23}$ +13.82 (EtOH). Log P -3.97 (uncertain value) (calc).
▶ LD_{50} (rat, ipr) 2000 mg/kg. VM2975000

4′-O-*β-D-Glucopyranoside:* [89439-59-8]
$C_{33}H_{40}O_{21}$ 772.666

7-O-*β-D-Glucopyranoside:* [30311-61-6]
$C_{33}H_{40}O_{21}$ 772.666

7-O-*[6-O-Benzoyl-β-D-glucopyranoside]:*
$C_{40}H_{44}O_{22}$ 876.774
Light yellow needles ($MeOH/Me_2CO$). Mp 222-223°. $[\alpha]_D^{20}$ -102.1 (c, 0.66 in Py). λ_{max} 257 ; 358 (MeOH).

7-O-*D-Galactopyranoside:* [50867-29-3]
$C_{33}H_{40}O_{21}$ 772.666
Isol. from *Fagopyrum tataricum* (tartary buckwheat).

7-O-*α-L-Rhamnopyranoside:* [57528-70-8]
$C_{33}H_{40}O_{20}$ 756.667
Yellow needles + $9H_2O$ (MeOH aq.). Mp 208-211° (196-198°).

7-O-*β-D-Glucuronopyranoside:*
$C_{33}H_{38}O_{22}$ 786.65

3′,7-Di-O-*β-D-glucopyranoside:* [75213-00-2]
$C_{39}H_{50}O_{26}$ 934.808
Isol. from *Prunus* spp..

7-O-*[Xylosyl-(1→?)-glucoside]:* [132509-94-5] ***Paederinin***†
$C_{38}H_{48}O_{25}$ 904.782
Amorph.

4′-O-*[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:* [75104-66-4]
$C_{39}H_{50}O_{26}$ 934.808
Isol. from *Prunus* spp..

2″-Ac: ***2″-O-Acetylrutin***
$C_{29}H_{32}O_{17}$ 652.562
Constit. of the flowers of *Prunus mume* (Japanese apricot). Yellow powder. $[\alpha]_D^{28}$ -28.9 (c, 0.8 in MeOH). λ_{max} 258 (log ϵ 4.47); 270 (sh) (log ϵ 4.4); 354 (log ϵ 4.36) (MeOH).

O″-*Ac:* [108420-57-1] ***Quercetin 3-(acetylrutinoside)***

$C_{29}H_{32}O_{17}$ 652.562

2‴-O-(3,4,5-Trihydroxybenzoyl): [182753-50-0] ***2‴-O-Galloylrutin***
$C_{34}H_{34}O_{20}$ 762.631
Pale yellow cryst. (H_2O). Mp 228-230°. $[\alpha]_D^{20}$ -96 (c, 0.1 in MeOH). λ_{max} 259 (sh) ; 268 ; 347 (MeOH).

7-O-(2-Hydroxyethyl): [23869-24-1] ***Monoxerutin, INN.*** *Mono 7-HR. Z 12007*
$[C_{29}H_{34}O_{17}]$Log P -4.17 (uncertain value) (calc).

▶LK9275300

4′-(2-Morpholinylethyl) ether: [30851-76-4] ***Ethoxazorutoside, INN.*** *Ethoxazorutin. Solarutine. Solurutine*
$C_{33}H_{41}NO_{17}$ 723.683
Mp 135°. Log P -3.44 (uncertain value) (calc).

2″-O-β-D-Apiofuranosyl: [63947-67-1]
$C_{32}H_{38}O_{20}$ 742.64
Powder.

2″-O-β-D-Xylopyranosyl: [213473-56-4]
$C_{32}H_{38}O_{20}$ 742.64
Mp 190-194°. $[\alpha]_D^{25}$ +10.5 (c, 1 in MeOH). λ_{max} 271 ; 323 ; 370 (no solvent reported).

2″-O-β-D-Glucopyranosyl: [55696-55-4]
$C_{33}H_{40}O_{21}$ 772.666
Isol. from *Solanum tuberosum* (potato) and *Glycine max* (soybean).

2″-O-α-L-Rhamnopyranosyl: [55696-57-6] ***Manghaslin***
$C_{33}H_{40}O_{20}$ 756.667
Isol. from *Glycine max* (soybean) and *Humulus lupulus* (hops). Pale yellow needles + $1\frac{1}{2}H_2O$ (MeOH/EtOH). Mp 194-196°.

2‴-O-α-L-Rhamnopyranosyl: [32453-37-5]
$C_{33}H_{40}O_{20}$ 756.667
Isol. from *Humulus lupulus* (hops).

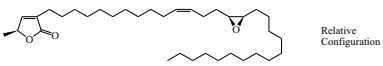
2″-O-β-D-Xylopyranosyl, 2‴-O-α-L-rhamnopyranosyl: [213473-54-2]
$C_{35}H_{48}O_{24}$ 852.75
Mp 232-234°. $[\alpha]_D^{25}$ +16 (c, 1 in MeOH). λ_{max} 269 ; 324 ; 363 (MeOH).

[22519-99-9]

U.S. Pat., 1953, 2 646 428; *CA*, **48**, 8269 (*Ethoxazorutoside*)
Griffith, J.Q. *et al., Rutin and Related Flavonoids*, Mack, Easton, 1955,
Harborne, J.B. *et al., Chem. Ind. (London)*, 1962, 222 (*7-glucuronoside*)
Fr. Pat., 1966, 1 434 376; *CA*, **66**, 29043 (*Ethoxazorutoside*)
Hörhammer, L. *et al., Tet. Lett.*, 1966, 567 (*synth*)
Swiss Pat., 1968, 458 389; *CA*, **70**, 68714m (*Monoxerutin*)
Williams, C.A. *et al., Phytochemistry*, 1971, **10**, 1059; 1973, **12**, 2417 (*7-galactoside*)
Averett, J.E. *et al., Phytochemistry*, 1971, **10**, 2199; 1983, **22**, 2325 (*7-glucoside*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1536 (*bibl*)
Schmid, R.D. *et al., Tetrahedron*, 1972, **28**, 3259 (*ms*)
Buttery, B.R. *et al., Can. J. Bot.*, 1975, **53**, 219 (*glycosylrutinosides*)
Aly, H.F. *et al., Phytochemistry*, 1975, **14**, 1613 (*7-rhamnoside*)
Rappaportt, I. *et al., Phytochemistry*, 1977, **16**, 1115 (*2^G-apioside*)
Wenkert, E. *et al., Phytochemistry*, 1977, **16**, 1811 (*cmr*)
Sakushima, A. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1219 (*Manghaslin*)
Pfendt, L.B. *et al., Mikrochim. Acta*, 1980, **1**, 385
Henning, W. *et al., Phytochemistry*, 1980, **19**, 2727 (*3′,7- and 4′-diglucosides*)
Khandsuren, S. *et al., Khim. Prir. Soedin.*, 1981, **17**, 243 (*7-rhamnoside*)
Voelter, W. *et al., D-(^b-Hydroxyethyl)rutosides: New Results*, Eds,. Springer-Verlag, Berlin, 1983, (*book*)
Khalifa, T.I. *et al., Anal. Profiles Drug Subst.*, 1983, **12**, 623 (*rev*)
Krunz, M.M. *et al., Microchem. J.*, 1983, **28**, 162
Saleh, N.A.M. *et al., Phytochemistry*, 1983, **22**, 2501 (*4′-glucoside*)
Cody, V. *et al., Plant Flavonoids in Biology and Medicine*, A.R., Liss, N.Y., 1986, (*biol, prop*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7530 (*synonyms*)
Cody, V. *et al., Plant Flavonoids in Biology and Medicine II*, A.R., Liss, N.Y., 1988, (*biol, prop*)
Williams, C.A. *et al., Phytochemistry*, 1989, **28**, 1891 (*O″-acetate*)
Ono, K. *et al., Eur. J. Biochem.*, 1990, **190**, 469 (*Rutin, anti-HIV activity*)
Ishikura, N. *et al., Z. Naturforsch., C*, 1990, **45**, 1081 (*Paederinin*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1342
Ahn, B.T. *et al., Planta Med.*, 1996, **62**, 383 (*2"-Galloylrutin*)
De Tommasi, N. *et al., J. Nat. Prod.*, 1998, **61**, 973-977 (*Bidens andicola glycosides*)
Gunasegaran, R. *et al., Fitoterapia*, 2001, **72**, 201-205 (*7-6-benzoylglucoside*)
Yoshikawa, M. *et al., J. Nat. Prod.*, 2002, **65**, 1151-1155 (*2″-Acetylrutin*)
Cody, V. *et al., Plant Flavonoids in Biology and Medicine*, A.R., Liss, N.Y., 1988 (*biol, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RSU000

Sabadelin S-1

3-(15,16-Epoxy-11-triacontenyl)-5-methyl-2(5H)-furanone



$C_{35}H_{62}O_3$ 530.873

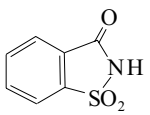
Constit. of the roots of *Annona muricata* (soursop). Waxy solid. $[\alpha]_D$ +12 (c, 0.19 in MeOH). λ_{max} 213 (log ϵ 3.63) (MeOH).

Gleye, C. *et al., Phytochemistry*, 1999, **52**, 1403-1408

Saccharin, USAN S-2

[81-07-2]

1,2-Benzisothiazol-3(2H)-one 1,1-dioxide, 9CI. Benzoic sulfimide. o-*Benzosulfimide. Benzosulfinide.* o-*Benzoylsulfimide.* o-*Sulfobenzoic imide. Garantose. Hermesetas. Sweeta. E954*



$C_7H_5NO_3S$ 183.187

Widely-used sweetening agent. All salts intensely sweet. Permitted in foods at levels of 80-1200 ppm in EU. Cryst. (H_2O). Spar. sol. H_2O, EtOH, Me_2CO; sl. sol. Et_2O, $CHCl_3$. Mp 224°. pK_{a1} 1.31 (25°, 0.2*M* KCl/HCl). Log P 0.52 (uncertain value) (calc). Sweetness approx. 300 × sucrose. No longer considered a possible human carcinogen by the US Department of Health and Human Services (2000).

▶ LD_{50} (mus, orl) 17000 mg/kg. Exp. carcinogenic data. Exp. reprod. and teratogenic effects. DE4200000

Na salt: [128-44-9] *Saccharin sodium, USAN. Sucaryl. FEMA 2997*

Sweetener. Mp 228.8-229.7°.

▶ Possible human carcinogen (IARC classification, 1987). LD_{50} (rat, orl) 14200 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects. DE4550000

Ca salt (2:1): [6485-34-3] *Saccharin calcium, USAN*

Sweetener.

▶ DE4250000

NH_4 salt (1:1):

Sweetener.

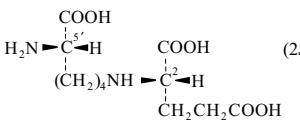
[6155-57-3, 6381-91-5]

Fahlberg, C. *et al., Ber.*, 1879, **12**, 469-473 (*synth*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **3**, 1574 (*detn, Tl*)
Hettler, H. *et al., Adv. Heterocycl. Chem.*, 1973, **15**, 233-276 (*rev*)
Ball, L.M. *et al., Xenobiotica*, 1977, **7**, 189-203 (*metab, Na salt*)
IARC Monog., 1980, **22**, 111; 171; *Suppl.* 7, 334; *Suppl.* 6, 488 (*rev, tox*)
Sweatman, T.W. *et al., Xenobiotica*, 1981, **11**, 531-540 (*pharmacol*)
Stassinopoulou, C.I. *et al., Org. Magn. Reson.*, 1983, **21**, 187-189 (*pmr*)
Byard, J.L. *et al., Adv. Exp. Med. Biol.*, 1984, **177**, 147-151 (*rev, metab, tox*)
Zubair, M.U. *et al., Anal. Profiles Drug Subst.*, 1984, **13**, 487 (*rev*)
Nasser, F.A. *et al., J. Organomet. Chem.*, 1984, **266**, 225-235 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 617
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BCE500
Mitchell, M.L. *et al., Food Sci. Technol.*, 1991, **48**, 127-156 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 415-417; 418-419
Zhang, Y. *et al., Cryst. Res. Technol.*, 1995, **30**, 831-835 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1374
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2469; 2472; 2473; 2475 (*use, salts*)
Ng, S.W. *et al., Acta Cryst. C*, 1998, **54**, 649-951 (*cryst struct*)
Ager, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)
Osvath, R. *et al., Food Chem. News*, 2000, **42(14)**, 12-13 (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCE500; SJN700; CAM750

Saccharopine S-3

[13429-91-9]

N-*(5-Amino-5-carboxypentyl)glutamic acid, 9CI*



(2*S*,5′*S*)-*form*

$C_{11}H_{20}N_2O_6$ 276.289

(2*S*,5′*S*)-*form* [997-68-2]

L-*form*

Amino acid from *Saccharomyces cerevisiae* and *Neurospora crassa*. Also found in mushrooms and seeds. Laths (H_2O). Mp 257-259° dec. $[\alpha]_D^{23}$ +33.6 (c, 1 in 0.5*N* HCl) (c, 2.2 in 0.5*N* NaOH). pK_{a2} 2.6; pK_{a3} 4.1; pK_{a4} 9.2; pK_{a5} 10.3. λ_{max} (MeOH) (Berdy).

(2*R*,5′*S*)-*form*

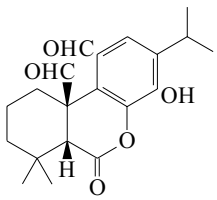
D-*Allo-form*

Cryst. (H_2O). Mp 235-250° dec. $[\alpha]_D^{23}$ -0.8 (c, 0.4 in 0.5*N* HCl).

Larsen, P.O. *et al., Acta Chem. Scand.*, 1961, **15**, 743; 750; 1972, **26**, 2562
Hermann, P. *et al., Pharmazie*, 1976, **31**, 132
Oka, Y. *et al., Agric. Biol. Chem.*, 1979, **43**, 1995 (*isol*)
Griffin, M. *et al., Clin. Chim. Acta*, 1982, **125**, 89 (*hplc*)
Burkard, U. *et al., Annalen*, 1986, 1030 (*synth*)

Sufficinolide S-4

[153660-18-5]



$C_{20}H_{24}O_5$ 344.407

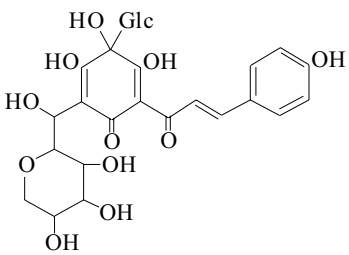
Constit. of *Salvia officinalis* (sage). Cryst. Mp 223-224° dec. $[\alpha]_D^{26}$ -165 (c, 0.41 in EtOH). λ_{max} 235 (ϵ 25118); 290 (ϵ 25703) (EtOH) (Berdy).

Tada, M. *et al., Phytochemistry*, 1994, **35**, 539 (*isol, pmr, cmr*)

Safflomin A S-5

[78281-02-4]

SY-1



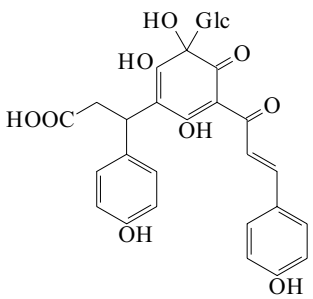
$C_{27}H_{32}O_{16}$ 612.54

Pigment from safflower (*Carthamus tinctorius*). Yellow powder. Mp 300° dec.

Onodera, J. *et al., Chem. Lett.*, 1981, 433; 887
Watanabe, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1179-1183 (*anal*)

Safflomin C S-6

[126093-98-9]



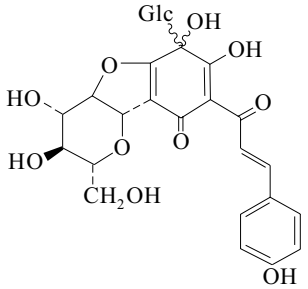
$C_{30}H_{30}O_{14}$ 614.559

Yellow pigment of safflower (*Carthamus tinctorius*). Yellow powder. Mp 300° dec.

Onodera, J. *et al., Chem. Lett.*, 1989, 1571
Sato, S. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 452 (*synth, cmr*)

Safflor Yellow A S-7

[85532-77-0]



$C_{27}H_{30}O_{15}$ 594.525

Yellow pigment of flower petals of *Carthamus tinctorius* (safflower).

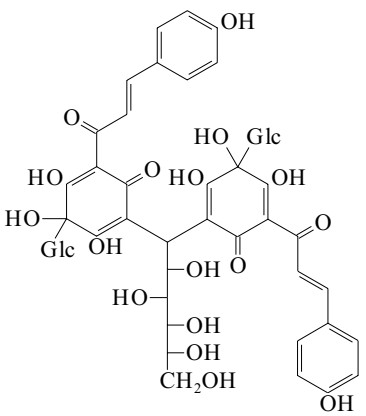
▶ UQ0333750

Takahashi, Y. *et al., Tet. Lett.*, 1982, **23**, 5163 (*struct*)

Safflor Yellow B S-8

[91574-92-4]

1-Deoxy-1,1-bis[3-β-D-glucopyranosyl-2,3,4-trihydroxy-5-[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]-6-oxo-1,4-cyclohexadien-1-yl]-D-glucitol, 9CI



$C_{48}H_{54}O_{27}$ 1062.938

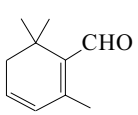
Pigment from the flowers of *Carthamus tinctorius* (safflower). Amorph. yellow powder. λ_{max} 239 (log ε 4.43); 410 (log ε 4.47) (MeOH).

Takahashi, Y. *et al., Tet. Lett.*, 1984, **24**, 2471
Watanabe, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1179-1183 (*anal*)
Kazuma, K. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1588-1599 (*isol, uv, cd, pmr, cmr*)

Safranal S-9

[116-26-7]

2,6,6-Trimethyl-1,3-cyclohexadienecarboxaldehyde, 9CI. 1-Formyl-2,6,6-trimethyl-1,3-cyclohexadiene. Dehydro-β-cyclocitral. FEMA 3389



$C_{10}H_{14}O$ 150.22

Constit. of saffron (*Crocus sativa*). Flavouring ingredient. Liq. with saffron odour and taste. d^{19} 0.97. Bp_{760} 172° Bp_1 70°. n_D^{19} 1.5281. λ_{max} 325 (ε 7500) (H_2O) (Berdy).

Oxime:

$C_{10}H_{15}NO$ 165.235

Cryst. (petrol). Mp 65°.

Semicarbazone:

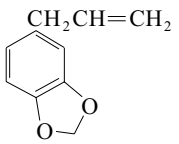
Cryst. (MeOH). Mp 175°.

Kuhn, R. *et al., Ber.*, 1934, **67**, 344-357 (*isol*)
Konst, W.M.B. *et al., Tet. Lett.*, 1974, 3175 (*synth*)
Kametani, T. *et al., Chem. Pharm. Bull.*, 1981, **29**, 105 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 769
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2838-2839
Boulin, B. *et al., Tetrahedron*, 1998, **54**, 2753-2762 (*synth*)

Safrole S-10

[94-59-7]

5-(2-Propenyl)-1,3-benzodioxole, 9CI. 4-Allyl-1,2-(methylenedioxy)benzene, 8CI. 3,4-Methylenedioxyallylbenzene. Allylcatechol methylene ether



$C_{10}H_{10}O_2$ 162.188

Occurs in nutmeg. Banned by FDA for use in food. Formerly used as a food flavour. Prisms. Fp 11.2. Bp 231.5-232° Bp_6 104-105°. n_D^{20} 1.5383. Log P 2.57 (calc).

▶ Possible human carcinogen. Skin irritant. LD_{50} (rat, orl) 1950 mg/kg. Exp. carcinogen. Exp. reprod. effects. Hepatotoxic.

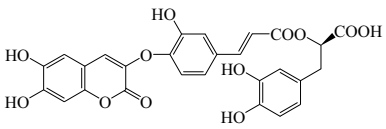
CY2800000

Picrate:

Red cryst. (EtOH). Mp 75°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1054C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 232B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 987A (*ir*)
Perkin, W.J. *et al., J.C.S.*, 1927, 1663 (*synth*)
Bert, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1941, **213**, 873 (*synth*)
Hickey, M.J. *et al., J.O.C.*, 1948, **13**, 448 (*isol*)
Della, E.W. *et al., Aust. J. Chem.*, 1961, **14**, 663 (*isol*)
Willhalm, B. *et al., Tetrahedron*, 1964, **20**, 1185 (*ms*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 983 (*rev, tox*)
IARC Monog., 1976, **10**, 231; *Suppl.*, **7**, 71 (*rev, tox*)
Fiedler, H.P. *et al., Drugs Made Ger.*, 1981, **24**, 163 (*rev*)
Ioannides, C. *et al., Food Cosmet. Toxicol.*, 1981, **19**, 657 (*rev*)
Wilson, S.R. *et al., J.O.C.*, 1982, **47**, 1983 (*synth*)
Howes, A.J. *et al., Food Chem. Toxicol.*, 1990, **28**, 537 (*cytotoxicity, genotoxicity*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1410
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 722
Abel, G. *et al., Adverse Eff. Herb. Drugs*, 1997, **3**, 105-122; 123-127 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SAD000

Sagecoumarin S-11

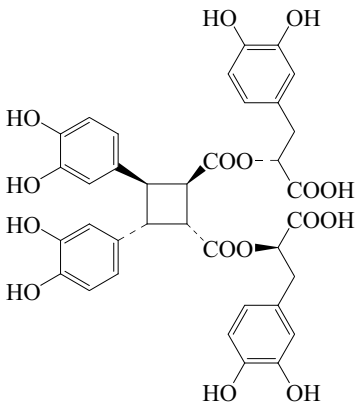


$C_{27}H_{20}O_{12}$ 536.448

Related to Melitric acid A. Constit. of *Salvia officinalis* (sage). Light brown powder. $[\alpha]_D^{20}$ +52 (c, 0.2 in MeOH). λ_{max} 288 (log ε 4.3); 332 (log ε 4.27) (MeOH).

Lu, Y. *et al., Phytochemistry*, 1999, **52**, 1149-1152

Sagerinic acid S-12



$C_{36}H_{32}O_{16}$ 720.639

Derived from Rosmarinic acid, 2-O-(3,4-Dihydroxy-*E*-cinnamoyl). Constit. of *Salvia officinalis* (sage). $[\alpha]_D^{20}$ +4 (c, 0.2 in MeOH). λ_{max} 232 (log ε 4.08); 286 (log ε 4.09) (MeOH).

Lu, Y. *et al., Phytochemistry*, 1999, **51**, 91-94 (*isol, uv, pmr, cmr, ms*)

Sakacin S-13

Peptide bacteriocins. Bacteriocins with possible food uses.

Sakacin A [145266-47-3]
Comprises 41 amino acid residues. Prod. by *Lactobacillus sake* LB706.

Sakacin 674 [154571-33-2]
Comprises 43 amino acid residues. Prod. by *Lactobacillus sake* LB764.

Sakacin B [157243-38-4]
Prod. by *Lactobacillus sake* 251 isol. from a fermented dry sausage.

Sakacin K [223919-88-8]
Prod. by *Lactobacillus sake* CTC 494 isol. from Spanish dry fermented sausage.

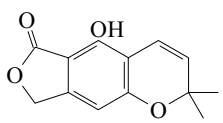
Sakacin M [146104-83-8]
Prod. by *Lactobacillus sake* 148.

Sakacin P [146240-19-9]
Comprises 43 amino acid residues. Prod. by *Lactobacillus sake* LTH 673 isol. from fermented dry sausage.

Subrino, O.J. *et al., Int. J. Food Microbiol.*, 1992, **16**, 215-225 (*Sakacin M*)
Holck, A.L. *et al., J. Gen. Microbiol.*, 1992, **138**, 2715-2720 (*Sakacin A*)
Holck, A.L. *et al., FEMS Microbiol. Lett.*, 1994, **115**, 143-149 (*Sakacin 674*)
Samelis, J. *et al., J. Appl. Bacteriol.*, 1994, **76**, 475-486 (*Sakacin B*)
Tichaczek, P.S. *et al., Microbiology (Reading, U.K.)*, 1994, **140**, 361-367 (*Sakacin P*)
Leroy, F. *et al., Appl. Environ. Microbiol.*, 1999, **65**, 947-981 (*Sakacin K*)

Salfredin B_{11} S-14

[165467-63-0]
*2,8-Dihydro-5-hydroxy-2,2-dimethyl-6*H-*furo[3,4-*g*]-1-benzopyran-6-one, 9CI*



$C_{13}H_{12}O_4$ 232.235
Constit. of the seeds of *Nigella sativa* (black cumin). Prisms. Mp 179-180°. λ_{max} 245 (ϵ 34800); 295 (ϵ 3940); 325 (ϵ 2780) (MeOH/NaOH) (Derep). λ_{max} 250 (ϵ 34800); 295 (ϵ 3940); 325 (ϵ 2780) (MeOH) (Derep).

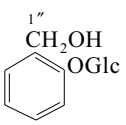
8ξ-Hydroxy: [261521-87-3] *2,8-Dihydro-5,8-dihydroxy-2,2-dimethyl-6*H-*furo[3,4-*g*]-1-benzopyran-6-one*
$C_{13}H_{12}O_5$ 248.235

8ξ-Methoxy: [261521-91-9] *2,8-Dihydro-5-hydroxy-8-methoxy-2,2-dimethyl-6*H-*furo[3,4-*g*]-1-benzopyran-6-one*
$C_{14}H_{14}O_5$ 262.262

Matsumoto, K. *et al., J. Antibiot.*, 1995, **48**, 439 (*isol, pmr, cmr, cryst struct*)
Mali, R.S. *et al., J. Chem. Res., Synop.*, 1998, 292-293 (*synth*)
Neumann, T. *et al., J. Basic Microbiol.*, 1999, **39**, 357-363 (*8-hydroxy, 8-methoxy*)
Joshi, B.S. *et al., Magn. Reson. Chem.*, 2001, **39**, 771-772 (*isol, pmr, cmr*)

Salicin S-15

[138-52-3]
2-(Hydroxymethyl)phenyl β-D-glucopyranoside, 9CI. Saligenin glucoside. Salicoside



$C_{13}H_{18}O_7$ 286.281
Needles (H_2O) with burning taste. Mod. sol. H_2O. Mp 204.7-208.7°. $[\alpha]_D^{20}$ -62.56 (H_2O). Log P -2.38 (calc). Hydrol. by Emulsin → Glucose + Saligenin.

1″-(2-Hydroxybenzoyl): ***ω-Salicoylsalicin***
$C_{20}H_{22}O_9$ 406.388
Isol. from the leaves of *Populus balsamifera* (balsam poplar). Mp 166-169°. $[\alpha]_D$ -43 (80% Me_2CO aq.).

6′-O-(4-Hydroxycinnamoyl): [17063-94-4] ***Trichocarposide***
$C_{22}H_{24}O_9$ 432.426
Constit. of *Populus balsamifera* (balsam poplar). Cryst. (H_2O). Mp 180-182°. $[\alpha]_D^{20}$ -11.4 (c, 2.3 in Me_2CO aq.).

Pearl, I.A. *et al., Arch. Biochem. Biophys.*, 1963, **102**, 33-38 (*Salicoylsalicin benzoates*)
Estes, T.K. *et al., CA*, 1967, **67**, 114359n (*Trichocarposide*)
Pearl, I.A. *et al., Phytochemistry*, 1970, **9**, 1277-1281; 1971, **10**, 2844-2847 (*Salicoylsalicin*)

Salivacin 140 S-16

[179158-00-0]
Prod. by *Lactobacillus salivarius* ssp. *salicinius* T140 isol. from the surface of Japanese pampas grass leaves. Bacteriocin.

Arihara, K. *et al., Lett. Appl. Microbiol.*, 1996, **22**, 420-424 (*isol*)

Salivaricin A S-17

[150952-06-0]
Lantibiotic peptide comprising 22 amino acid residues with one lanthionine and 2 β-methyllanthionine residues. Bacteriocin prod. by *Streptococcus salivarius* 20P3.

Ross, K.F. *et al., Appl. Environ. Microbiol.*, 1993, **59**, 2014-2021 (*isol*)

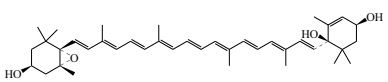
Salivaricin B S-18

[160307-64-2]
Lantibiotic peptide. Prod. by *Lactobacillus salivarius* M7. Bacteriocin.

Ten Brink, B. *et al., J. Appl. Bacteriol.*, 1994, **77**, 140-148 (*isol*)

Salmoxanthin S-19

[75138-59-9]
5,6-Epoxy-5,6-dihydro-β,ϵ-carotene-3,3′,6′-triol

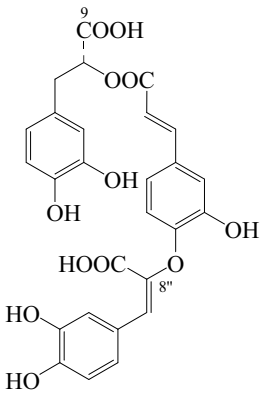


$C_{40}H_{56}O_4$ 600.88
Constit. of *Oncorhynchus keta* and other salmon spp.. Mp 208°. λ_{max} 416 ; 440 ; 470 (Et_2O).

Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1980, **46**, 879; 911 (*occur, struct*)
Matsuno, T. *et al., J. Nat. Prod.*, 2001, **64**, 507-510 (*isol, pmr, uv, cd, abs config*)

Salvianolic acid I S-20

[150072-80-3]



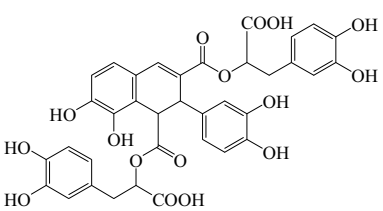
$C_{27}H_{22}O_{12}$ 538.464
Neolignan. Lignan numbering shown.Amorph. powder. $[\alpha]_D^{14}$ +71 (c, 0.1 in EtOH).

8″Z-Isomer: [153765-45-8] ***Melitric acid A***. *Schizotenuin E*
$C_{27}H_{22}O_{12}$ 538.464
Constit. of *Melissa officinalis* (lemon balm) *Salvia officinalis* (sage). Light brown powder + $1/2H_2O$. Mp 135-138°. $[\alpha]_D^{23}$ +45 (c, 0.2 in MeOH). Related to Rosmarinic acid, 2-O-(3,4-Dihydroxy-*E*-cinnamoyl) λ_{max} 290 (log ϵ 4.32); 328 (log ϵ 4.34) (MeOH).

8″Z-Isomer, 8″-Me ester: [127498-36-6] ***Schizotenuin F***. *Methyl melitrate A*
$C_{28}H_{24}O_{12}$ 552.49
Constit. of *Salvia officinalis* (sage). Light brown powder. λ_{max} 292 (log ϵ 4.33); 330 (log ϵ 4.36) (MeOH).

Agata, I. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1608 (*Melitric acid A*)
Li, L. *et al., Youji Huaxue*, 1993, **13**, 303; *CA*, **119**, 156298q (*isol, abs config*)
Zhang, H.-J. *et al., Planta Med.*, 1994, **60**, 70 (*isol, pmr, cmr*)
Matsuta, M. *et al., Nat. Med. (Tokyo)*, 1996, **50**, 204-211 (*Schizotenuins*)
Lu, Y. *et al., Phytochemistry*, 1999, **52**, 1149-1152 (*Melitric acid A*)

Salvianolic acid L S-21

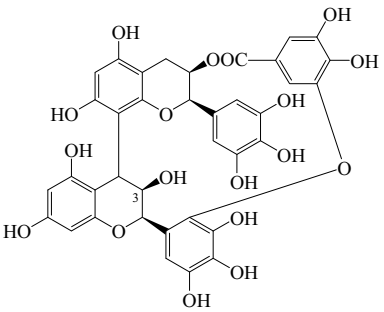


$C_{36}H_{30}O_{16}$ 718.623
Constit. of *Salvia officinalis* (sage). Brownish powder. $[\alpha]_D$ -177.5 (c, 0.2 in MeOH). Related to Rabdosiin λ_{max} 212 (log ϵ 4.48); 288 (log ϵ 4.05); 334 (log ϵ 4.12) (MeOH).

Lu, Y. *et al., Tet. Lett.*, 2001, **42**, 8223-8225

Samarangenin A S-22

[147103-18-2]



$C_{37}H_{28}O_{18}$ 760.617

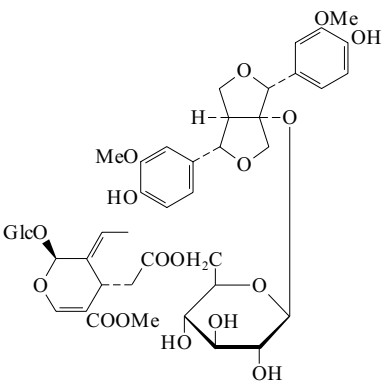
Isol. from the leaf of *Syzygium samarangense* (Java apple) and *Syzygium aqueum* (water apple). Brown amorph. powder + $2H_2O$. $[\alpha]_D^{27}$ -218.4 (c, 0.6 in Me_2CO).

3-O-(3,4,5-Trihydroxybenzoyl): [147103-19-3] ***Samarangenin B***
$C_{44}H_{32}O_{22}$ 912.724
Tannin constit. of *Syzygium samarangense* (Java apple) and *Syzygium aqueum* (water apple). Brown amorph. powder + $3H_2O$. $[\alpha]_D^{27}$ -246.9 (c, 0.7 in Me_2CO).

Nonaka, G. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2671-2673 (*isol, struct, pmr, cmr*)
Lin, L.-C. *et al., Planta Med.*, 2000, **66**, 333-336 (*pmr, cmr, Samarangenin B*)

Sambacolignoside S-23

[114449-12-6]



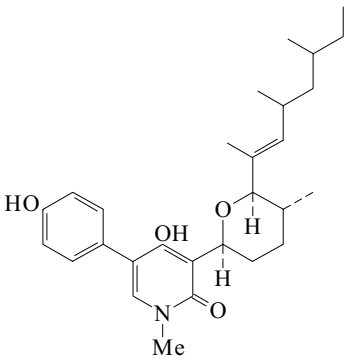
$C_{43}H_{54}O_{22}$ 922.886

Complex glycoside of 8-Hydroxypinoresinol, H-756 and Oleoside, O-149. Isol. from leaves of *Jasminum sambac* (Arabian jasmine). Powder.

Tanahashi, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 5032

Sambutoxin, 9CI S-24

[160047-56-3]

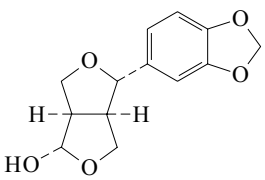


$C_{28}H_{39}NO_4$ 453.62

Isol. from the fungi *Fusarium sambucinum* and *Fusarium oxysporum*. Mycotoxin. Prisms (MeOH). Sol. MeOH, toluene, C_6H_6, EtOH, butanol, EtOAc; poorly sol. H_2O, hexane. Mp 196.5-197.5°. $[\alpha]_D^{25}$ -200 (c, 0.1 in MeOH). λ_{max} 213 (ϵ 38000); 233 (ϵ 17000); 254 (ϵ 29000) (MeOH) (Berdy).

Kim, J.-C. *et al., Tet. Lett.*, 1995, **36**, 1047 (*isol, uv, ir, pmr, cmr, struct*)

Samin S-25



$C_{13}H_{14}O_5$ 250.251

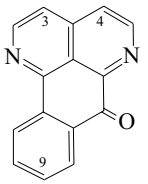
Isol. from sesame seed oil (*Sesamum* sp.). Mp 106°. $[\alpha]_D$ +103. Config. not certain.

O-*(3,4-Methylenedioxyphenyl):* [526-07-8] ***Sesamolin***
$C_{20}H_{18}O_7$ 370.358
Constit. of sesame oil. Plates (EtOH). Mp 94°. $[\alpha]_D$ +220 (c, 1.13 in $CHCl_3$).

Boesken, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1936, **55**, 815
Carnmalm, B. *et al., Acta Chem. Scand.*, 1955, **9**, 1111
Erdtman, H. *et al., Chem. Ind. (London)*, 1955, 567
Beroza, M. *et al., J.A.C.S.*, 1955, **77**, 3332
Haslam, E. *et al., J.C.S.*, 1955, 827
Haslam, E. *et al., J.C.S.(C)*, 1970, 2332 (*abs config, pmr, ms*)
Fukuda, Y. *et al., Heterocycles*, 1986, **24**, 926
Maiti, G. *et al., Tetrahedron*, 1995, **51**, 8389 (*synth*)
Wirth, T. *et al., J.O.C.*, 1996, **61**, 2686 (*synth, pmr, cmr, ms*)
Lutz, G. *et al., Heterocycles*, 1997, **45**, 287 (*Sesamolin, pmr, conformn, cryst struct*)
Hull, H.M. *et al., J.C.S. Perkin 1*, 1997, 857 (*synth*)
Hull, H.M. *et al., J.C.S. Perkin 1*, 1998, 1779-1787 (*synth*)
Kato, M.J. *et al., Phytochemistry*, 1998, **47**, 583-591 (*Sesamolin, biosynth*)

Sampangine S-26

[116664-93-8]
7H-Naphtho[1,2,3,-ij][2,7]naphthyridin-7-one, 9CI



$C_{15}H_8N_2O$ 232.241

Erroneous systematic name and CAS no. in *CA* attributable to a drawing error in the abstract incorrectly depicting Sampangine as the diazafluoranthene alkaloid Indeno[1,2,3-*ij*][2,7]naphthyridine, I-17. Alkaloid from the stem bark of *Cananga odorata* (ylang ylang). Bright yellow needles (C_6H_6). Mp 210° dec. λ_{max} 220 ; 252 ; 312 ; 326 ; 392 (MeOH) (Berdy).

3-Methoxy: [128129-42-0] ***3-Methoxysampangine***
$C_{16}H_{10}N_2O_2$ 262.267
Yellow needles (EtOAc/hexane). Mp 225-227° (213-215°).

4-Methoxy: [139253-60-4] ***Eupomatidine 2***. *4-Methoxysampangine*
$C_{16}H_{10}N_2O_2$ 262.267
Fine lemon needles (MeOH/CH_2Cl_2). Mp 262-265° dec.

8-Hydroxy: [225938-87-4] ***8-Hydroxysampangine***
$C_{15}H_8N_2O_2$ 248.24
Orange powder. Mp 223-226°. λ_{max} 233 ; 315 ; 337 ; 447 (MeOH).

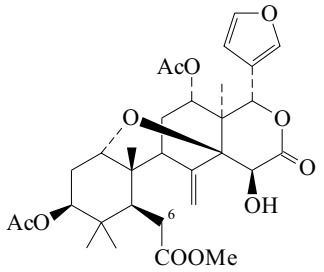
9-Methoxy: [139220-15-8] ***Eupomatidine 1***. *9-Methoxysampangine*
$C_{16}H_{10}N_2O_2$ 262.267
Yellow prisms (MeOH). Mp 195-197° (natural) Mp 228-231° (synthetic).

4,9-Dimethoxy: [139220-16-9] ***Eupomatidine 3***. *4,9-Dimethoxysampangine*
$C_{17}H_{12}N_2O_3$ 292.293
Yellow needles (MeOH/CH_2Cl_2). Mp 245-248° dec. (natural), 278-281 dec. (synthetic).

Rao, J.U.M. *et al., J. Nat. Prod.*, 1986, **49**, 346 (*isol, uv, ir, pmr, ms, struct*)
Bracher, F. *et al., Annalen*, 1989, 87 (*synth, uv, ir, pmr, cmr, ms*)
Liu, S. *et al., Antimicrob. Agents Chemother.*, 1990, **34**, 529 (*3-Methoxysampangine*)
Carroll, A.R. *et al., Aust. J. Chem.*, 1991, **44**, 1615 (*Eupomatidines, isol*)
Zjawiony, J.K. *et al., J. Het. Chem.*, 1997, **34**, 1233-1237 (*3-Methoxysampangine, synth, ir, pmr, cmr*)
Kitahara, Y. *et al., Tetrahedron*, 1997, **53**, 6001 (*Eupomatidines, synth*)
Akendengue, B. *et al., Nat. Prod. Lett.*, 1999, **13**, 147-150 (*8-Hydroxysampangine*)

Sandoricin S-27

[133585-55-4]



$C_{31}H_{40}O_{11}$ 588.65
Constit. of *Sandoricum koetjape* (santol). Cryst. (1-propanol/hexane). Mp 215-217°.

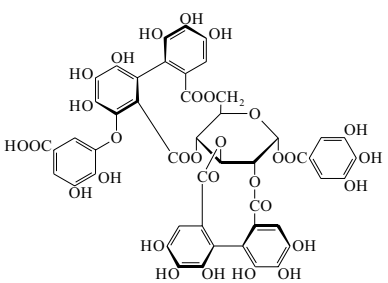
*6*R-*Hydroxy:* [133585-56-5] ***6-Hydroxysandoricin***
$C_{31}H_{40}O_{12}$ 604.65
Constit. of *Sandoricum koetjape* (santol). Cryst. (1-propanol/hexane). Mp 250-255° dec.

15-O-*[α-L-Rhamnopyranosyl(1→6)-β-D-glucopyranoside]:* [182565-73-7] ***Azecin 1***
$C_{43}H_{60}O_{20}$ 896.935
Cryst. Mp 180-182°.

Powell, R.G. *et al., J. Nat. Prod.*, 1991, **54**, 241 (*isol, pmr, cmr, cryst struct*)
Srivastava, S.D. *et al., J. Indian Chem. Soc.*, 1996, **73**, 467 (*Azecin 1*)

Sanguiin H2 S-28

[82200-04-2]
1-O-*Galloyl-2,3-(*S*)-hexahydroxydiphenoyl-4,6-sanguisorboyl-α-D-glucopyranose*

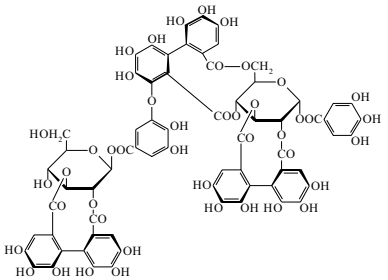


$C_{48}H_{32}O_{31}$ 1104.762
An ellagitannin constit. of *Sanguisorba officinalis* (burnet bloodwort). Tan amorph. powder + $5H_2O$. $[\alpha]_D^{20}$ +7.9 (c, 0.98 in Me_2CO).

Nonaka, G.-I. *et al., J.C.S. Perkin 1*, 1982, 1067 (*pmr, cmr, ms*)
Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)

Sanguiin H3 S-29

[82262-86-0]

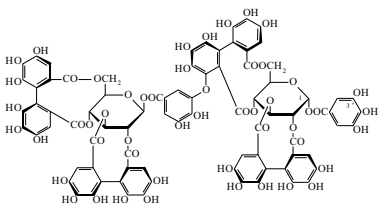


$C_{68}H_{48}O_{44}$ 1569.101
A dimeric tannin from the underground parts of *Sanguisorba officinalis* (burnet bloodwort). Tan amorph. powder + $3H_2O$. $[\alpha]_D^{20}$ +63.2 (c, 0.7 in Me_2CO).

Nonaka, G.-I. *et al., J.C.S. Perkin 1*, 1982, 1067 (*pmr, cmr, ms*)
Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)

Sanguiin H6 S-30

[82978-00-5]



$C_{82}H_{54}O_{52}$ 1871.297
Struct. revised in 1985. Tannin from *Sanguisorba officinalis* (burnet bloodwort), *Rubus fruticosus* (blackberry) and *Rubus idaeus* (raspberry). Brown amorph. powder. $[\alpha]_D$ +72 (Me_2CO).

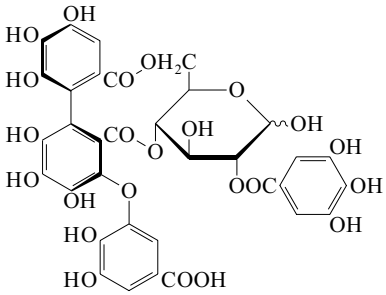
1-Epimer: ***Lambertianin A***
$C_{82}H_{54}O_{52}$ 1871.297
Pale brown powder + $8H_2O$. $[\alpha]_D^{20}$ -6.76 (c, 3 in MeOH). This name originally given to the tannin now named Lambertianin C.

*1-Epimer, 3′-*O*-(5-ellagyl)ether:* [152580-83-1] ***Lambertianin B***
$C_{96}H_{58}O_{60}$ 2171.478
Pale brown powder + $1H_2O$. $[\alpha]_D^{20}$ -4.1 (c, 1.2 in MeOH). See Ellagic acid, E-36 for ether.

Nonaka, G. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2255 (*isol*)
Gupta, R.K. *et al., J.C.S. Perkin 1*, 1982, 2525 (*pmr, cmr*)
Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1214 (*Lambertianin A, Lambertianin B*)

Sanguiin H7 S-31

[98917-86-3]
2-O-*Galloyl-4,6-(*S*)-sanguisorboyl-D-glucopyranose*

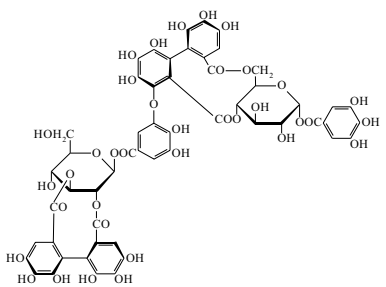


$C_{34}H_{26}O_{23}$ 802.566
Isol. from the underground parts of *Sanguisorba officinalis* (burnet bloodwort). Off-white amorph. powder.

Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)

Sanguiin H8 S-32

[98975-04-3]

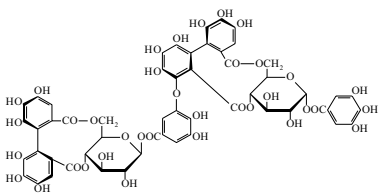


$C_{54}H_{42}O_{36}$ 1266.904
Ellagitannin isol. from *Sanguisorba officinalis* (burnet bloodwort). Off-white amorph. powder.

Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)

Sanguiin H9 S-33

[98917-88-5]

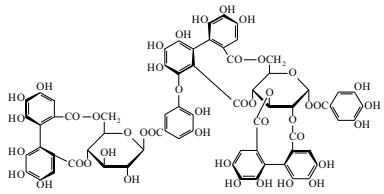


$C_{54}H_{42}O_{36}$ 1266.904
Ellagitannin derived from *Sanguisorba officinalis* (burnet bloodwort). Off-white amorph. powder.

Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)

Sanguiin H10 S-34

[98975-05-4]



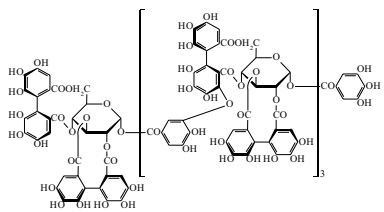
$C_{68}H_{48}O_{44}$ 1569.101

Ellagitannin constit. of *Sanguisorba officinalis* (burnet bloodwort). Off-white amorph. powder.

Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)

Sanguiin H11 S-35

[96292-46-5]



$C_{164}H_{106}O_{104}$ 3740.579

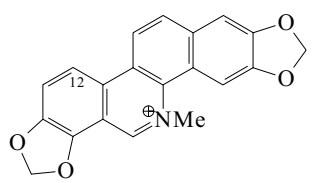
Tetrameric ellagitannin from *Sanguisorba officinalis* (burnet bloodwort). Amorph. powder.

Tanaka, T. *et al., J. Chem. Res., Synop.*, 1985, 176 (*struct*)

Sanguinarine S-36

[2447-54-3]

13-Methyl[1,3]benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridinium(1+), 9CI. 5-Methyl-2,3:7,8-bis(methylenedioxy)benzo[c]phenanthridinium(1+). Pseudochelerythrine. ψ-Chelerythrine



$C_{20}H_{14}NO_4^{\oplus}$ 332.335

Several numbering systems have been used. Consumption of Sanguinarine, present in poppy seeds and in the oil of *Argemone mexicana* which has been used as an adulterant for mustard oil in India, has been linked to development of glaucoma. Banned by FDA. Sol. MeOH, $CHCl_3$. Log P 0.01 (uncertain value) (calc). λ_{max} 234 ; 284 ; 324 (MeOH) (Berdy). λ_{max} 234 (ϵ 31500); 283 (ϵ 33100); 325 (ϵ 14100) (EtOH) (Berdy).

► LD_{50} (mus, ivn) 22 mg/kg , LD_{50} (mus, ipr) 18 mg/kg , LD_{50} (mus, scu) 112 mg/kg , LD_{50} (mus, ivn) 16 mg/kg. VP5200000

Chloride: [5578-73-4] ***Sanguinarium chloride, INN, USAN***

$C_{20}H_{14}ClNO_4$ 367.788

Orange needles (dil. HCl). Mp 277-280° dec. (273-274°, 284-289° dec.).

► VP5220000

Pseudocyanide:

$C_{21}H_{14}N_2O_4$ 358.353

Mp 244-245° (236-237°).

N-*De-Me:* [522-30-5] *[1,3]Benzodioxolo[5,6-c]-1,3-dioxolo[4,5-i]phenanthridine. 2,3;7,8-Bis(methylenedioxy)benzo[c]phenanthridine.* ***Norsanguinarine***

$C_{19}H_{11}NO_4$ 317.3

Alkaloid from *Papaver rhoeas* (corn poppy). Pale-yellow needles (Me_2CO, $CHCl_3$/MeOH or $CHCl_3$/EtOH). Mp 285-287° (278-280° dec.).

12-Methoxy: See Chelirubine in *The Combined Chemical Dictionary.*

8-Methoxy (?): See Pancorine in *The Combined Chemical Dictionary.*

Späth, E. *et al., Ber.*, 1931, **64**, 370 (*struct*)

Slavík, J. *et al., Coll. Czech. Chem. Comm.*, 1968, **33**, 1619 (*ms, pmr*)

Hruban, L. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 3420 (*uv*)

Sainsbury, M. *et al., J.C.S.(C)*, 1970, 1797 (*synth, uv, ir*)

Onda, M. *et al., Chem. Pharm. Bull.*, 1971, **19**, 31 (*synth*)

Furuya, T. *et al., Phytochemistry*, 1972, **11**, 3401 (*Norsanguinarine*)

Haisová, K. *et al., Coll. Czech. Chem. Comm.*, 1973, **38**, 3312; 1975, **40**, 1576 (*Norsanguinarine*)

Ikuta, A. *et al., Phytochemistry*, 1974, **13**, 2175; 1976, **15**, 577 (*Norsanguinarine*)

Battersby, A.R. *et al., J.C.S. Perkin 1*, 1975, 1140; 1147 (*isol, biosynth*)

Ishii, H. *et al., Chem. Pharm. Bull.*, 1978, **26**, 864 (*pmr*)

Lenfeld, J. *et al., Planta Med.*, 1981, **43**, 161; 1983, **48**, 111 (*pharmacol*)

Maiti, M. *et al., FEBS Lett.*, 1982, **142**, 280 (*pharmacol*)

Takao, N. *et al., Helv. Chim. Acta*, 1983, **66**, 473 (*biosynth*)

Šmidrkal, J. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1412 (*synth*)

Šimánek, V. *et al., Alkaloids (N.Y.)*, 1985, **26**, 185 (*rev*)

Nagao, Y. *et al., Nucleic Acids Symp. Ser.*, 1985, **16**, 37 (*pharmacol*)

Hanaoka, M. *et al., Chem. Lett.*, 1986, 739 (*synth*)

Blaskó, G. *et al., Heterocycles*, 1988, **27**, 911 (*cmr*)

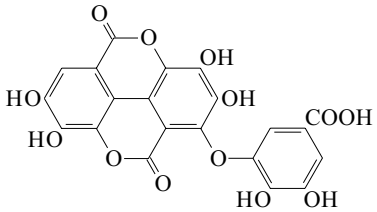
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1410

Vavreckova, C. *et al., Chem. Listy*, 1994, **88**, 238 (*rev*)

Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 964

Sanguisobic acid dilactone S-37

[82203-11-0]

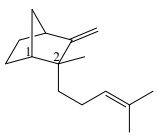


$C_{21}H_{10}O_{13}$ 470.302

Isol. from the underground parts of *Sanguisorba officinalis* (burnet bloodwort). Cryst. + $3H_2O$ ($CHCl_3$/MeOH). Sol. Py only. Mp 300°.

Nonaka, G.-I. *et al., J.C.S. Perkin 1*, 1982, 1067 (*ir, pmr, cmr, struct*)

β-Santala-3(15),10-diene S-38



(1*R*,2*R*)-*form*

$C_{15}H_{24}$ 204.355

(1*R*,2*R*)-*form* [25532-78-9]

Epi-β-santalene

Constit. of the famine food *Santalum album* (sandalwood). Flavouring ingredient. Bp_5 105-107°. $[\alpha]_D^{20}$ -26.6 (c, 1 in $CHCl_3$).

(1*S*,2*R*)-*form* [511-59-1]

β-Santalene

Constit. from oil of the famine food *Santalum album* (sandalwood). Flavouring ingredient. Oil with cedar odour. Bp_9 125-127°. $[\alpha]_D$ -35.

Hodgson, G.L. *et al., J.C.S. Perkin 1*, 1973, 2113 (*synth, abs config*)

Eck, C.R. *et al., J.C.S. Perkin 1*, 1974, 1938 (*synth*)

Christenson, P.A. *et al., J.O.C.*, 1979, **44**, 2012 (*synth*)

Bertrand, M. *et al., Tet. Lett.*, 1979, 15 (*synth*)

Oppolzer, W. *et al., Helv. Chim. Acta*, 1985, **68**, 2100 (*synth*)

Takano, S. *et al., Chem. Comm.*, 1987, 1720 (*synth*)

Arai, Y. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 467 (*synth*)

Sonawane, H.R. *et al., J.O.C.*, 1991, **56**, 1434 (*synth*)

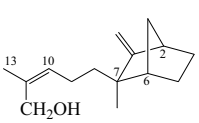
Krotz, A. *et al., Annalen*, 1994, 601 (*synth*)

Zhong, G.F. *et al., Synlett*, 1994, 173-174 (*synth*)

Kamikubo, T. *et al., Chem. Lett.*, 1995, 95 (*synth*)

Saito, M. *et al., Tet. Lett.*, 1995, **36**, 9003 (*synth*)

β-Santala-3(15),10-dien-12-ol S-39



(2*R*,6*S*,7*R*,10*Z*)-*form*

$C_{15}H_{24}O$ 220.354

Terpenoid numbering shown. Inversion of C-10 config. changes numbering C-12 vs C-13.

(2*R*,6*S*,7*R*,10*Z*)-*form* [77-42-9]
β-Santalol. *FEMA 3006*
Flavouring ingredient. Constit. of sandalwood oil (*Santalum album*). Oil. Bp_{17} 177-178°. $[\alpha]_{Hg}$ -87.1. $[\alpha]_D^{20}$ -109.5 (c, 0.86 in MeOH).

Ac: [77-43-0] *β-Santalyl acetate*
$C_{17}H_{26}O_2$ 262.391
Mixt. with α-santalyl acetate (FEMA 3007) is used as flavouring ingredient. $[\alpha]_D^{20}$ -91 (c, 1.00 in 1,4-dioxan).

Phenylacetyl:β-Santalyl phenylacetate
$C_{23}H_{30}O_2$ 338.489
Mixt. with α-santalyl phenylacetate (FEMA 3008) is used as flavouring ingredient.

12-Carboxylic acid: [73590-17-7] *β-Santala-3(15),10-dien-12-oic acid.* ***β-Santalic acid***
$C_{15}H_{22}O_2$ 234.338
Flavouring ingredient. Constit. of *Santalum album* (sandalwood) oil. Oil.

13-Hydroxy: [173615-77-5] *β-Santala-3(15),10-diene-12,13-diol.* ***β-Santaldiol***
$C_{15}H_{24}O_2$ 236.353
Oil. $[\alpha]_D^{25}$ -66 (c, 0.1 in $CHCl_3$). Abs. config. not detd. but opt. rotn. implies same abs. stereochem. as β-Santalol. Shown in the paper having the opposite abs. config..

(2*R*,6*S*,7*R*,10*E*)-*form* [37172-32-0]
β-Santala-3(15),10-dien-13-ol. **trans-*β*-*Santalol***
Flavouring ingredient. Constit. of *Santalum album* (sandalwood). Oil. $[\alpha]_D^{21}$ -113.7 (c, 0.3 in $CHCl_3$) (synthetic).

Aldehyde: [59331-82-7] *β-Santal-3(15),10-dien-13-al.* ***β-Santalal***
$C_{15}H_{22}O$ 218.338
Isol. from *Santalum album* (sandalwood) oil. Flavouring ingredient.

(2*R*,6*S*,7*S*,10*Z*)-*form*
Constit. of *Santalum album* (sandalwood). Flavouring ingredient.

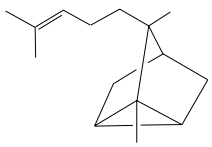
(2*S*,6*R*,7*R*,10*Z*)-*form* [42495-69-2]
epi-*β*-*Santalol*
Flavouring ingredient. Constit. of *Santalum album* (sandalwood). Oil. + ve opt. rotation.

[1323-00-8, 1323-75-7, 130930-05-1, 131726-06-2, 131726-07-3]

Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737-747 (*β-Santalal*)
Baumann, M. *et al., Annalen*, 1979, 743-750 (*(±)-β-Santalol, synth*)
Christenson, P.A. *et al., Phytochemistry*, 1981, **20**, 1139-1141 (*trans-β-Santalol*)
Brunke, E.-J. *et al., Annalen*, 1982, 1105-1110 (*abs config*)
Monti, H. *et al., Tet. Lett.*, 1982, **23**, 5539-5540 (*(±)-β-Santalol, synth*)
Solas, D. *et al., J.O.C.*, 1983, **48**, 1988-1991 (*β-Santalol, synth, bibl*)
Buchbauer, G. *et al., Annalen*, 1990, 119-121 (*β-Santalic acid*)
Krotz, A. *et al., Tetrahedron: Asymmetry*, 1990, **1**, 537-540 (*E-β-Santalol, Z-β-Santalol, synth*)
Krotz, A. *et al., Annalen*, 1994, 601-609 (*E-β-Santalol, Z-β-Santalol, synth, isol*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 723-724 (*Ac, phenylacetyl*)
Alpha, T. *et al., Phytochemistry*, 1996, **41**, 829 (*β-Santaldiol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2491-2493 (*Ac, phenylacetyl*)

α-Santal-10-ene S-40

[512-61-8]
α-Santalene. *Santalene*



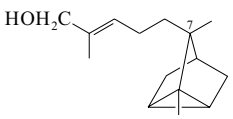
$C_{15}H_{24}$ 204.355
Constit. of sandalwood oil. Flavouring ingredient. Oil. Bp_{753} 252°. $[\alpha]_D$ -15.

*Epoxide:**10,11-Epoxy-α-santalane**. 12,13-Epoxy-α-santalene*
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D^{23}$ +2.4 (c, 5.5 in $CHCl_3$).

Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1973, 3065 (*synth*)
Hodgson, G.L. *et al., J.C.S. Perkin 1*, 1973, 2113 (*synth, abs config*)
Monti, S.A. *et al., J.O.C.*, 1978, **43**, 2282 (*synth*)
Wu, T.-S. *et al., Phytochemistry*, 1984, **23**, 595 (*epoxide*)
Ngo, K.-S. *et al., Phytochemistry*, 1999, **50**, 1213-1218 (*pmr, cmr*)

α-Santal-10-en-12-ol S-41

α-Santalol. 5-(2,3-Dimethyltricyclo[2.2.1.0^{2,6}]hept-3-yl)-2-methyl-2-penten-1-ol, 9CI



(7*R*,10*E*)-*form*

$C_{15}H_{24}O$ 220.354
A coml. mixture of α-santalol and, obtained by fractional distillation of sandalwood oil is used as a flavouring ingredient, FEMA 3006.
► Fl. p. >100°.

(7*R*,10*E*)-*form* [14490-17-6]
Oil. $Bp_{0.5}$ 113-119°. $[\alpha]_D^{25}$ +18.09 ($CHCl_3$).

Aldehyde: [59331-83-8] *α-Santal-10-en-12-al.* ***α-Santalal***
$C_{15}H_{22}O$ 218.338
Constit. of sandalwood oil (*Santalum album*). Oil.

11,12-Dihydro, carboxylic acid:α-Santalan-12-oic acid. ***Dihydro-α-santalic acid***
$C_{15}H_{24}O_2$ 236.353
Constit. of East Indian sandalwood oil. Oil.

(7*R*,10*Z*)-*form* [115-71-9]
Constit. of sandalwood oil. Flavouring agent. Oil. Bp_{14} 166-167°. $[\alpha]_D^{23}$ +17.5 (c, 3.3 in $CHCl_3$).
► LD_{50} (rat, orl) 3800 mg/kg. Skin irritant. SB3400000

Ac: [41414-75-9]
[77-87-2] *α-Santalyl acetate*
$C_{17}H_{26}O_2$ 262.391
Mixts. with β-santalyl acetate are used as flavouring ingredients.

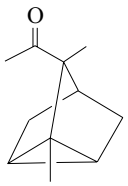
Phenylacetyl:α-Santalyl phenylacetate
$C_{23}H_{30}O_2$ 338.489
Mixts. with β-santalyl phenylacetate are used as flavouring ingredients.

[1323-00-8, 1323-75-7]

Lewis, R.G. *et al., Tet. Lett.*, 1967, 401 (*synth*)
Bohlmann, F. *et al., Tet. Lett.*, 1968, 1533 (*isol, synth*)
Corey, E.J. *et al., J.A.C.S.*, 1970, **92**, 6314 (*synth*)
Julia, M. *et al., Bull. Soc. Chim. Fr.*, 1973, 3065 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 991 (*rev, tox*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3351 (*synth*)
Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*isol, aldehyde*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 723-724 (*Ac, phenylacetyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2490-2493 (*Ac, phenylacetyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, OHG000

Santalone S-42

[59300-51-5]
10,11,12,13-Tetranor-α-santalan-8-one

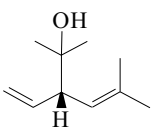


$C_{11}H_{16}O$ 164.247
Flavouring ingredient. Constit. of the oil of *Santalum album* (sandalwood). Oil.

Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737

Santolina alcohol S-43

[35671-15-9]
3-Ethenyl-2,5-dimethyl-4-hexen-2-ol, 9CI. 2,5-Dimethyl-3-vinyl-4-hexen-2-ol



Absolute configuration

$C_{10}H_{18}O$ 154.252

(*S*)-*form* [21149-19-9]
Oil. d_4^{20} 0.86. $[\alpha]_D^{23}$ +13.5.

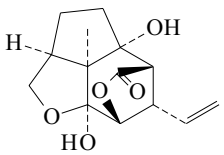
Ac: [79507-88-3]
$C_{12}H_{20}O_2$ 196.289
Constit. of *Artemisia vulgaris* (mugwort).

Chrétien-Bessière, Y. *et al., Bull. Soc. Chim. Fr.*, 1968, 2018 (*isol, struct*)
Poulter, C.D. *et al., Tet. Lett.*, 1972, 71 (*abs config*)

Näf-Müller, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1424 (*Ac*)
Moiseenkov, A.M. *et al., Chem. Comm.*, 1982, 109 (*synth*)

Sapidolide A S-44

[182191-87-3]

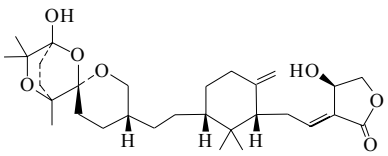


$C_{14}H_{18}O_5$ 266.293
Constit. of *Baccaurea sapida* (Burmese grape). Cryst. Mp 147°. $[\alpha]_D^{31}$ +23.2 (c, 0.4 in $CHCl_3$).

Bordoloi, M. *et al., Tet. Lett.*, 1996, **37**, 6791-6792 (*isol, pmr, cmr, cryst struct*)

Saponaceolide A S-45

[118584-14-8]



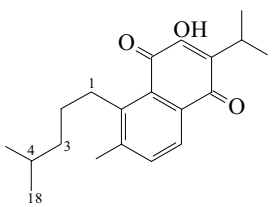
$C_{30}H_{46}O_7$ 518.689
Needles (Me_2CO/hexane). Mp 145-146°. $[\alpha]_D^{20}$ +78.14 (c, 1.1 in $CHCl_3$). λ_{max} 220 (ε 5000) (EtOH) (Derep).

▶ Cytotoxic.

De Bernardi, M. *et al., Tetrahedron*, 1988, **44**, 235; 1991, **47**, 7109 (*cryst struct, abs config*)

Sapriparaquinone S-46

[119139-54-7]
20(10→5)Abeo-12-hydroxy-4,5-seco-5(10),6,8,12-abietatetraene-11,14-dione



$C_{20}H_{26}O_3$ 314.424

4,18-Didehydro, Ac: ***Acetylsalvipisone***
$C_{22}H_{26}O_4$ 354.445
Constit. of *Salvia sclarea* (clary sage). Amorph. orange solid. λ_{max} 245 (log ε 4.2); 280 (log ε 4); 360 (log ε 3.5); 425 (log ε 2.4) (MeOH).

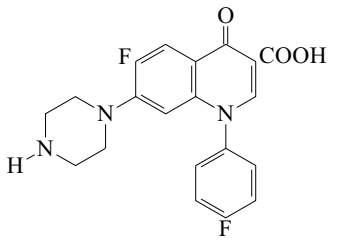
2,3,4,18-Tetradehydro: ***2,3-Dehydrosalvipisone***
$C_{20}H_{22}O_3$ 310.392
Constit. of *Salvia sclarea* (clary sage). Yellow amorph. solid. λ_{max} 248 (ε 7943); 281 (ε 31622); 358 (ε 6310) (MeOH) (Berdy).

Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 971 (*2,3-Dehydrosalvipisone*)

Ulubelen, A. *et al., Phytochemistry*, 1997, **44**, 1297 (*Acetylsalvipisone*)

Sarafloxacin, BAN, INN S-47

[98105-99-8]
6-Fluoro-1-(4-fluorophenyl)-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid, 9CI. Saraflox. A 57135



$C_{20}H_{17}F_2N_3O_3$ 385.369
Used for control of *Campylobacter* infections in poultry. Log P -0.06 (calc).

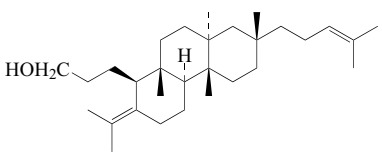
Hydrochloride: [91296-87-6] ***Sarafloxacin hydrochloride, USAN. A 56620***
Solid + $x H_2O$. Mp 275° (hydrate).

[102856-02-0]

Chu, D.T. *et al., J. Med. Chem.*, 1985, **28**, 1558 (*synth*)
Fernandes, P.B. *et al., Antimicrob. Agents Chemother.*, 1986, **29**, 201 (*activity*)
Granneman, G.R. *et al., J. Chromatogr.*, 1987, **413**, 199 (*hplc*)
Fernandes, C.J. *et al., Chemotherapy (Basel)*, 1988, **34**, 216 (*activity*)
Bouzard, D. *et al., J. Med. Chem.*, 1989, **32**, 537 (*activity*)
Xiao, W. *et al., J. Pharm. Sci.*, 1989, **78**, 585 (*synth, pharmacol*)
Bauer, J.F. *et al., Pharm. Res.*, 1990, **7**, 1177 (*hplc*)

Sasanquol S-48

[211183-83-4]



$C_{30}H_{52}O$ 428.74
Constit. of *Camellia sasanqua*. Needles. Mp 89-91°.

Akihisa, T. *et al., Phytochemistry*, 1998, **48**, 301-305 (*isol, pmr, cmr*)

Savoury taste-enhancing peptide S-49

[73984-05-1]
Lysylglycylaspartylglutamylglutamylseryl-leucylalanine. Delicious peptide. Beefy meaty peptide. BMP. STEP

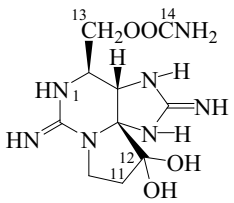
H-Lys-Gly-Asp-Glu-Glu-Ser-Leu-Ala-OH

$C_{34}H_{57}N_9O_{16}$ 847.875
Claimed as isol. from beef extract with a taste variously descr. as delicious tasting or umami/sour tasting. More recent workers concluded that the compd. was not in fact present in beef extract and furthermore had little or no flavour or flavour enhancing props.. Mp 182-184°. $[\alpha]_D^{25}$ -48 (H_2O).

Yamasaki, Y. *et al., Agric. Biol. Chem.*, 1978, **42**, 1761-1765; 1980, **44**, 93-97 (*isol, synth, props*)
Tamura, M. *et al., Agric. Biol. Chem.*, 1989, **53**, 319-325 (*synth*)
Cutts, R.L. *et al., J. Agric. Food Chem.*, 1996, **44**, 1409-1415 (*pmr, conformn*)
Hau, J. *et al., J. Agric. Food Chem.*, 1997, **45**, 1351-1355 (*props, bibl*)

Saxitoxin S-50

[35523-89-8]



$C_{10}H_{17}N_7O_4$ 299.289
Paralytic poison from Alaska butter clams (*Saxidomus giganteus*), toxic mussels (*Mytilus californianus*), the plankton *Gonyaulax cantenella* and *Protogonyaulax tamarensis*. Causal agent of paralytic shellfish poisoning. Noncryst. Sol. H_2O, MeOH; fairly sol. EtOH, AcOH; poorly sol. butanol, hexane. $[\alpha]_D$ +130. See also Gonyautoxin I, G-297 and Gonyautoxin VI, G-298.

▶ Extremely toxic, among the most toxic substances known. LD_{50} (rat, orl) 0.192 mg/kg. LD_{50} (mus, ipr) 0.005 mg/kg. LD_{50} (mus, ivn) 0.008 mg/kg. UY8708500

Decarbamoyl: [58911-04-9] ***Decarbamoylsaxitoxin***
$C_9H_{16}N_6O_3$ 256.264
Isol. from various shellfish.

Decarbamoyl, 13-O-Ac: [133144-32-8]
$C_{11}H_{18}N_6O_4$ 298.301

1-Hydroxy: [64296-20-4] ***Neosaxitoxin***
$C_{10}H_{17}N_7O_5$ 315.288
Prod. by *Protogonyaulax* and found in shellfish.

▶ Potent neurotoxin; LD_{50} (mus, ipr) 5 mg/kg.

1-Hydroxy, decarbamoyl: [68683-58-9] ***Decarbamoylneosaxitoxin***
$C_9H_{16}N_6O_4$ 272.263
Isol. from the crab *Zosimus aeneus*.

N^{14}*-Hydroxy:* [153856-77-0] **N′-*Hydroxysaxitoxin***
$C_{10}H_{17}N_7O_5$ 315.288
Isol. from the crab *Zosimus aeneus*. Contains an *N*-hydroxycarbamoyl group.

N^{14}*,1-Dihydroxy:* [153856-78-1] **N′-*Hydroxyneosaxitoxin***
$C_{10}H_{17}N_7O_6$ 331.288
Isol. from the crab *Zosimus aeneus*.

12-Deoxy(12S-), decarbamoyl: [75352-31-7]

[80844-68-4] ***Dearbamoyl-12-deoxysaxitoxin***
$C_9H_{16}N_6O_2$ 240.264

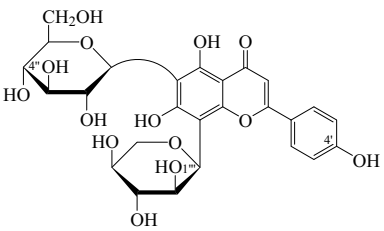
*12-Deoxy, decarbamoyl, 13-*O*-Ac:*
[200816-98-4]
$C_{11}H_{18}N_6O_3$ 282.302

[35554-08-6]

Schantz, E.J. *et al., Biochemistry*, 1966, **5**, 1191
Bordner, J. *et al., J.A.C.S.*, 1975, **97**, 6008 (*cryst struct, pmr, cmr*)
Tanino, H. *et al., J.A.C.S.*, 1977, **99**, 2818 (*synth*)
Koehn, F.E. *et al., Bioorg. Chem.*, 1981, **10**, 412-428 (*synth, derivs*)
Hall, S. *et al., Tet. Lett.*, 1984, **25**, 3537 (*struct, isol, deriv*)
Kodama, M. *et al., Agric. Biol. Chem.*, 1988, **52**, 1075 (*isol*)
Hall, S. *et al., ACS Symp. Ser.*, 1990, **418**, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1410
Arakama, O. *et al., Toxicon*, 1994, **32**, 175-183 (*isol, derivs*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SBA500; SBA600

Schaftoside S-51

[51938-32-0]
8-α-L-Arabinopyranosyl-6-β-D-glucopyranosylapigenin



$C_{26}H_{28}O_{14}$ 564.499
Yellow needles. Mp 226°. $[\alpha]_D^{23}$ +63.7 (Py). Incorrectly descr. as a mono-*O*-glycoside in the English summary of the Chopin paper.

*4′-*O*-β-D-Glucopyranoside:* [151922-20-2] *Schaftoside 4′-glucoside*
$C_{32}H_{38}O_{19}$ 726.641
Constit. of *Ceratonia siliqua* (carob).

*6″-*O*-β-D-Glucopyranosyl:* [94530-41-3] *8-Arabinosyl-6-gentiobiosylapigenin*
$C_{32}H_{38}O_{19}$ 726.641A *C*-gentiobioside.

1‴-Epimer: [61328-41-4] ***Neoschaftoside.*** *Isoschaftoside. 8-β-L-Arabinopyranosyl-6-β-D-glucopyranosylapigenin*
$C_{26}H_{28}O_{14}$ 564.499

4″-Epimer: [83856-66-0]

[65634-13-1] ***Isocorymboside.*** *8-α-L-Arabinopyranosyl-6-β-D-galactopyranosylapigenin*
Yellow needles (H_2O). Mp 219-222°. $[\alpha]_D$ +109 (c, 2 in DMSO aq.).

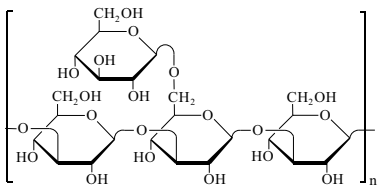
1‴,4‴-Diepimer: [207461-10-7] *6-β-D-Glucopyranosyl-8-β-D-ribopyranosylapigenin*
$C_{26}H_{28}O_{14}$ 564.499
Constit. of *Passiflora incarnata* (maypops).

2‴,3‴,4‴-Triepimer: [59914-91-9] ***Vicenin 3.*** *6-β-D-Glucopyranosyl-8-β-D-xylopyranosylapigenin*
$C_{26}H_{28}O_{14}$ 564.499
Amorph.

Bouillant, M.L. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **273**, 1759 (*Vicenin 3*)
Chopin, M.J. *et al., Phytochemistry*, 1974, **13**, 2583; 1977, **16**, 1999 (*Schaftoside, Isocorymboside*)
Dillon, M.O. *et al., Phytochemistry*, 1976, **15**, 1085 (*Neoschaftoside*)
Osterdahl, B.G. *et al., Acta Chem. Scand., Ser. B*, 1979, **33**, 400 (*isol, cmr, Isoschaftoside*)
Shirane, S. *et al., Agric. Biol. Chem.*, 1982, **46**, 2595 (*isol, Neoschaftoside*)
Dubois, M.A. *et al., Planta Med.*, 1982, **46**, 56 (*Corymboside*)
Besson, E. *et al., Phytochemistry*, 1984, **23**, 159 (*isol, struct, Neoschaftoside*)
Gaffield, W. *et al., Phytochemistry*, 1984, **23**, 1317 (*cd, conformn*)
Bouillant, M.L. *et al., Phytochemistry*, 1984, **23**, 2653 (*8-Arabinosyl-6-gentiobiosylapigenin*)
Batista, M.T. *et al., Phytochemistry*, 1993, **34**, 1191 (*Schaftoside 4′-glucoside*)
Chimichi, S. *et al., Nat. Prod. Lett.*, 1998, **11**, 225-232 (*1‴,4‴-diepimer*)

Schizophyllan S-52

[9050-67-3]
Sizofiran, 9CI, INN, JAN. *Sonfilan. SPG*



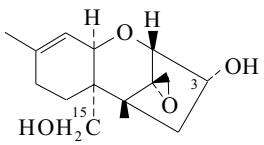
$C_{24}H_{40}O_{20}$ 648.568
Polysaccharide antibiotic. Minimum formula given. A highly (1→6) branched (1→3) β-D-glucan. Polymeric. Launched 1985. Sol. H_2O; poorly sol. MeOH, hexane, EtOH. Possesses triple-helical struct..
▶ VX2600000

Stereoisomer: [39464-87-4] ***Scleroglucan.*** *Sclerosan. Sclerogum*
$C_{24}H_{40}O_{20}$ 648.568
Used in the food industry as a non-caloric, stable, gelling agent. Sol. H_2O, MeOH; poorly sol. EtOH, Me_2CO, hexane. $[\alpha]_D$ -1 (NaOH aq.).

Belg. Pat., 1964, 639 361, (*Pillsbury*); *CA*, **62**, 11119e (*Scleroglucan, isol*)
Komatsu, N. *et al., Gann*, 1969, **60**, 137 (*isol, props*)
Kikumoto, S. *et al., Nippon Nogei Kagaku Kaishi*, 1970, **44**, 337; 1971, **45**, 162 (*isol, struct*)
Singh, P.P. *et al., Carbohydr. Res.*, 1974, **37**, 245 (*Scleroglucan, pharmacol*)
Saito, H. *et al., Carbohydr. Res.*, 1979, **74**, 227 (*cmr, struct*)
Cottrell, I.W. *et al., ACS Symp. Ser.*, 1980, **126**, 251 (*rev*)
Rinaudo, M. *et al., Carbohydr. Res.*, 1980, **100**, 117 (*deriv*)
Tabata, K. *et al., Carbohydr. Res.*, 1981, **89**, 121
Rinaudo, M. *et al., Carbohydr. Polym.*, 1982, **2**, 135 (*deriv, cmr, struct, conformn*)
Bluhm, T.L. *et al., Carbohydr. Res.*, 1982, **100**, 117 (*conformn*)
Van, K. *et al., Polym. J. (Tokyo)*, 1984, **16**, 61 (*ord*)
Takeo, K. *et al., Carbohydr. Res.*, 1986, **145**, 293 (*synth*)
Furue, H. *et al., Drugs of Today (Barcelona)*, 1987, **23**, 335 (*rev*)
Pretus, H.A. *et al., J. Pharmacol. Exp. Ther.*, 1991, **257**, 500 (*Scleroglucan*)
Ikeuchi, K. *et al., Keio J. Med.*, 1991, **40**, 132 (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1412
Teramoto, A. *et al., Biopolymers*, 1995, **36**, 803 (*conformn*)

3,15-Scirpenediol S-53

[38818-51-8]
12,13-Epoxy-9-trichothecene-3,15-diol



$C_{15}H_{22}O_4$ 266.336
▶ YC9950600

3α-form

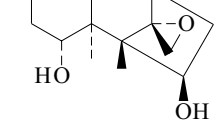
3-Ac: [38818-66-5] ***15-Deacetylcalonectrin***
$C_{17}H_{24}O_5$ 308.374
Metab. of *Calonectria nivalis*. Cryst. (Et_2O/petrol). Mp 184-186°. $[\alpha]_D$ +11.2 (c, 1 in $CHCl_3$).

3,15-Di-Ac: ***Calonectrin***
$C_{19}H_{26}O_6$ 350.411
Mycotoxin. of *Calonectria nivalis*. Cryst. (Et_2O/petrol). Mp 83-85°. $[\alpha]_D^{27}$ +14.6 (c, 1 in $CHCl_3$).

Gardner, D. *et al., J.C.S. Perkin 1*, 1972, 2576 (*isol, struct*)
Hanson, J.R. *et al., J.C.S. Perkin 1*, 1974, 1033 (*cmr*)
Brumley, W.C. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 451 (*ms*)
Kraus, G.A. *et al., J.A.C.S.*, 1982, **104**, 1114 (*synth*)
Jeker, N. *et al., Tet. Lett.*, 1984, **25**, 5637 (*synth*)
Cameron, S. *et al., J.C.S. Perkin 1*, 1989, 887 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 192; 193

4,7-Scirpenediol S-54

12,13-Epoxy-9-trichothecene-4,7-diol



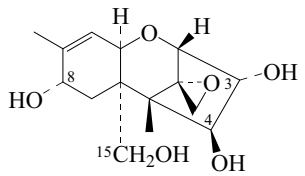
$C_{15}H_{22}O_4$ 266.336

(4β,7α)-*form* [99624-08-5]
7-Hydroxytrichodermol
Mycotoxin from *Myrothecium roridum*. Cryst. (EtOAc/hexane). Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. Mp 214-215°. $[\alpha]_D$ -7.5 (c, 0.15 in MeOH). λ_{max} (MeOH) (Berdy).

Jarvis, B.B. *et al., Appl. Environ. Microbiol.*, 1985, **50**, 1225

3,4,8,15-Scirpenetetrol S-55

12,13-Epoxy-9-trichothecene-3,4,8,15-tetrol, 9CI



$C_{15}H_{22}O_6$ 298.335

(3α,4β,8α)-*form* [34114-99-3]
Toxin T2 tetrol. *T2 tetrol*
Mycotoxin from *Fusarium poae* and *Fusarium sporotrichioides*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

► YC9980000

4-Ac: [76348-84-0] ***NT 2 Toxin***. *Toxin NT 2*
$C_{17}H_{24}O_7$ 340.372
Mycotoxin from *Fusarium sporotrichioides* and *Fusarium tricinctum*. Needles (EtOAc/hexane). Poorly sol. hexane. Mp 172-173°.

8-Ac: ***8-Acetyl-T2 tetrol***
$C_{17}H_{24}O_7$ 340.372
Mycotoxin from *Fusarium sporotrichioides*.

15-Ac: [74833-39-9] ***4-Deacetylneosolaniol***. *TMR 1*
$C_{17}H_{24}O_7$ 340.372
Mycotoxin prod. by *Fusarium heterosporum*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

► LD_{50} (mus, orl) >10mg/kg.

4,8-Di-Ac: [65180-29-2] *NT 1 Toxin*. ***4,8-Diacetyl-T2-tetrol***. *Toxin T1*
$C_{19}H_{26}O_8$ 382.41
Mycotoxin prod. by *Fusarium sporotrichioides, Fusarium tricinctum* and *Haemophilus parainfluenzae*. Cryst. (C_6H_6/hexane). Mp 172.5-173.5°.

4,15-Di-Ac: [36519-25-2] ***Neosolaniol***. *Solaniol*†. *Neozolaniol*
$C_{19}H_{26}O_8$ 382.41
Trichothecene antibiotic.Cryst. (EtOAc/hexane). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 171-172°. $[\alpha]_D$ -35 (MeOH). λ_{max} 208 (ϵ 600) (MeOH) (Berdy).

► Skin irritant. LD_{50} (ckn, orl) *ca*. 25 mg/kg ; LD_{50} (mus, ipr) 14.5 mg/kg. YD0080000

4,8,15-Tri-Ac: ***Acetylneosolaniol***
$C_{21}H_{28}O_9$ 424.447
Needles (C_6H_6/heptane). Mp 190-190.5°.

8-O-*Propanoyl, 4,15-di-Ac:* [111112-47-1] ***8-Propanoylneosolaniol***
$C_{22}H_{30}O_9$ 438.474
Prod. by *Fusarium sporotrichioides*.

8-O-*Butanoyl, 4,15-di-Ac:* [98813-18-4] ***8-Butanoylneosolaniol***
$C_{23}H_{32}O_9$ 452.5
Prod. by *Fusarium sporotrichioides*.

8-O-*(2-Methylpropanoyl), 4,15-di-Ac:* [111112-48-2] ***8-Isobutanoylneosolaniol***
$C_{23}H_{32}O_9$ 452.5
Prod. by *Fusarium sporotrichioides*.

8-O-*Pentanoyl, 4,15-di-Ac:* [116163-74-7] ***8-Pentanoylneosolaniol***
$C_{24}H_{34}O_9$ 466.527
Prod. by *Fusarium sporotrichioides*. Cryst. Mp 152-153°. λ_{max} 198 (ϵ 6600) (MeOH) (Berdy).

8-O-*(3-Methylbutanoyl):* [34114-98-2] ***T2 Triol***
$C_{20}H_{30}O_7$ 382.453
Mycotoxin from *Fusarium sporotrichiella*.

► YD0105000

8-O-*(3-Methylbutanoyl), 15-Ac:* [26934-87-2] ***Toxin HT 2***. *HT2 Toxin*. *Mycotoxin HT2*. *4-Deacetyl T2 Toxin*
$C_{22}H_{32}O_8$ 424.49
Yellow oil. Sol. MeOH, Et_2O; poorly sol. H_2O.

► LD_{50} (mus, ipr) 9.0 mg/kg. YD0050000

8-O-*(3-Methylbutanoyl), 4,15-di-Ac:* [21259-20-1] ***T2 Toxin***. *Neosolaniol 8-(3-methylbutanoate)*. *Fusariotoxin T2*. *Insariotoxin*. *Mycotoxin T2*
$C_{24}H_{34}O_9$ 466.527
Trichothecene antibiotic. Isol. from *Fusarium* spp. and *Trichoderma lignorum*. Important mycotoxin occurring naturally in various agricultural products. Needles. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 151-152°. $[\alpha]_D^{21}$ -15.5 ($CHCl_3$). λ_{max} 187 (ϵ 13900) (MeOH) (Berdy).

► LD_{50} (rat, orl) 4 mg/kg; LD_{50} (mus, ipr) 5.2 mg/kg; LD_{50} (mus, orl) 3.8 mg/kg; LD_{50} (mus, ipr) 3 mg/kg. Exp. effects incl. emesis, anorexia, ataxia. Exp. neoplastigenic data. Pulmonary toxin, haemorrhagic agent. YD0100000

8-O-*(3-Methylbutanoyl), tri-Ac:* [21259-21-2] ***Acetyl-T2 Toxin***
$C_{26}H_{36}O_{10}$ 508.564
Metab. of *Fusarium graminearum, Fusarium poae* and *Fusarium sporotrichioides*. Potential contaminant of cereals. Cryst. (Et_2O/pentane). $[\alpha]_D^{30}$ +27 (c, 0.9 in EtOH aq.).

8-O-*(3-Methylbutanoyl), 4-propanoyl, 15-Ac:* [104903-80-2] ***4-Propanoyl-HT2 toxin***
$C_{25}H_{36}O_9$ 480.554
From *Fusarium sporotrichioides*. Needles. Mp 141-142°.

8-O-*Hexanoyl, 4,15-di-Ac:* [118143-01-4] ***8-Hexanoylneosolaniol***
$C_{25}H_{36}O_9$ 480.554
From *Fusarium sporotrichioides*. Glass. λ_{max} 204 (ϵ 5400) (MeOH) (Berdy).

8-O-*(3-Hydroxy-3-methylbutanoyl):* ***3′-Hydroxy-T2-triol***
$C_{20}H_{30}O_8$ 398.452
Mycotoxin prod. by *Fusarium heterosporum*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

8-O-*(3-Hydroxy-3-methylbutanoyl), 15-Ac:* [78368-54-4] ***3′-Hydroxy-HT2 toxin***. *TC3 toxin*. *Toxin TC 3*
$C_{22}H_{32}O_9$ 440.489
Mycotoxin from *Fusarium heterosporum*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

► LD_{50} (mus, orl) 8.5 mg/kg. YC9990000

8-O-*(3-Hydroxy-3-methylbutanoyl), 4,15-di-Ac:* [84474-35-1] ***3′-Hydroxy-T2 Toxin***
$C_{24}H_{34}O_{10}$ 482.527
Mycotoxin from *Fusarium sporotrichiella poae*. Metab. of T2 Toxin. Potential cereal contaminant.

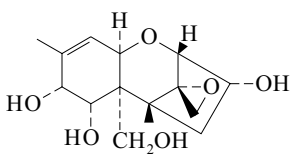
► YD0090000

8-Ketone, 4,15-di-Ac: [77620-47-4] ***8-Oxo-diacetoxyscirpenol***
$C_{19}H_{24}O_8$ 380.394
From *Fusarium sporotrichioides*. Oil. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 226 (ϵ 6100) (MeCN).

Bamburg, J.R. *et al., Tetrahedron*, 1968, **24**, 3329 (*isol, struct*)
Smalley, E.B. *et al., Mycotoxins*, (I.F.H. Purchase Ed.), Elsevier, N.Y., 1974, 199 (*bibl*)
Kotsonis, F.N. *et al., Appl. Microbiol.*, 1975, **30**, 493-495 (*Acetyl-T2 Toxin*)
Ellison, R.A. *et al., J.O.C.*, 1976, **41**, 576 (*cmr*)
Ilus, T. *et al., Phytochemistry*, 1977, **16**, 1839 (*deriv*)
Yoshizawa, T. *et al., Appl. Environ. Microbiol.*, 1980, **39**, 1172; **40**, 901; 1984, **47**, 130
Ishii, K. *et al., Appl. Environ. Microbiol.*, 1981, **42**, 541
Cole, R.J. *et al., J. Nat. Prod.*, 1981, **44**, 324 (*isol, deriv*)
Yoshizawa, T. *et al., Agric. Biol. Chem.*, 1982, **46**, 2613 (*deriv*)
Brumley, W.C. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 451 (*ms*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2219 (*uv, ir, pmr, cmr, ms*)
Tutel'yan, V.A. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1984, **274**, 727; *Dev. Food Sci.*, 1984, **7**, 282 (*isol*)
Berger, W.W.A. *et al., Appl. Environ. Microbiol.*, 1985, **50**, 656 (*deriv*)
Eller, K.I. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1985, **283**, 1481 (*deriv*)
Oltz, E.M. *et al., Tetrahedron*, 1986, **42**, 2615 (*deriv*)
Wani, M.C. *et al., J.O.C.*, 1987, **52**, 3468 (*synth*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, 1989, 206 (*rev*)
Trichothecene Mycotoxicosis: Pathophysiologic Effects, ed. Beasley, V. CRC Press, Boca Raton, 1989, (*book*)
Gilardi, R. *et al., Acta Cryst. C*, 1990, **46**, 645 (*cryst struct*)
Colvin, E.W. *et al., Chem. Comm.*, 1990, 1200 (*synth*)
Van Middlesworth, F. *et al., J.O.C.*, 1990, **55**, 1237 (*biosynth, cmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 162; 185
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAD600; FQS000

3,7,8,15-Scirpenetetrol S-56

[128534-67-8]
12,13-Epoxy-9-trichothecene-3,7,8,15-tetrol



$C_{15}H_{22}O_6$ 298.335
Mycotoxin from *Fusarium graminearum*. Cryst. (Me_2CO/C_6H_6). Mp 185-187°. $[\alpha]_D^{25}$ -60 (c, 1.02 in MeOH).

3,15-Di-Ac: [95673-99-7] ***7α,8α-Dihydrox-***

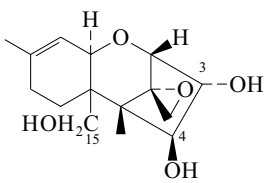
ycalonectrin
$C_{19}H_{26}O_8$ 382.41
Mycotoxin from *Fusarium culmorum* and *Fusarium roseum*. Cryst. (Me_2CO/Et_2O). Mp 190-192°.

8-Ketone, 15-Ac: [88337-96-6] *15-Acetoxy-12,13-epoxy-3,7-dihydroxy-9-trichothecen-8-one.* ***15-Acetyl-4-deoxynivalenol***
$C_{17}H_{22}O_7$ 338.357
Mycotoxin prod. by *Fusarium graminearum* and *Gibberella zeae*. Cryst. Mp 140-141°.

Greenhalgh, R. *et al., J. Agric. Food Chem.*, 1984, **32**, 1261 (*isol, deriv*)
Hanson, A.W. *et al., Acta Cryst. C*, 1986, **42**, 503 (*cryst struct, deriv*)
Savard, M.E. *et al., Can. J. Chem.*, 1987, **65**, 2254 (*pmr, deriv*)
Baldwin, N.C.P. *et al., Z. Naturforsch., C*, 1987, **42**, 1043 (*deriv*)
Grove, J.F. *et al., J.O.C.*, 1988, **53**, 3860-3862 (*15-Acetyldeoxynivalenol*)
Kononenko, G.P. *et al., Khim. Prir. Soedin.*, 1990, **26**, 267; *Chem. Nat. Compd. (Engl. Transl.)*, 219 (*isol, pmr*)

3,4,15-Scirpenetriol S-57

12,13-Epoxy-9-trichothecene-3,4,15-triol, 9CI



$C_{15}H_{22}O_5$ 282.336

(3α,4β)-*form* [2270-41-9]
Anguidol. *Scirpenetriol*
Prod. by *Fusarium roseum, Fusarium equiseti* and *Fusarium sporotrichiella*. Mycotoxin. Cryst. (AcOH). Mp 189-191°. $[\alpha]_D^{24}$ -10 (c, 0.76 in $CHCl_3$).
▶ YD0110500

3-Ac: [70402-13-0]
$C_{17}H_{24}O_6$ 324.373
Metab. of *Fusarium oxysporum*. Mycotoxin. $[\alpha]_D$ -11.7 ($CHCl_3$).

4-Ac:
$C_{17}H_{24}O_6$ 324.373
Mycotoxin from *Fusarium roseum* and *Fusarium sulphureum*. Oil. $[\alpha]_D$ +10.3 (c, 1 in Me_2CO).

15-Ac: [2623-22-5] ***Monoacetoxyscirpenol***
$C_{17}H_{24}O_6$ 324.373
Mycotoxin from *Fusarium roseum* and *Fusarium sulphureum*. Cryst. (EtOAc/2,2,4-trimethylpentane). Sol. MeOH, C_6H_6; fairly sol. H_2O, Et_2O, hexane. Mp 172-173°. $[\alpha]_D$ -25 ($CHCl_3$).
▶ YD0111000

15-Ac, 4-O-α-D-glucopyranoside: [99124-45-5]
$C_{23}H_{34}O_{11}$ 486.515
From *Fusarium sulphureum*. Pale-yellow gum. $[\alpha]_D^{20}$ +79.5 (c, 0.585 in MeOH). Less toxic than other trichothecenes.

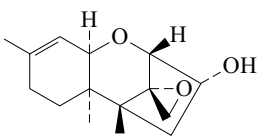
4,15-Di-Ac: [2270-40-8] ***Diacetoxyscirpenol***. *Anguidin. ANG 66. NSC 141537*
$C_{19}H_{26}O_7$ 366.41
Constit. of *Fusarium* spp. Mycotoxin. Cryst. (EtOAc). Mp 161-162°. $[\alpha]_D^{19}$ +20 (c, 1 in Me_2CO). Log P -0.12 (uncertain value) (calc).
▶ Very toxic if swallowed. Skin irritant. LD_{50} (rat, orl) 7 mg/kg. Exp. reprod. and teratogenic effects. Exp. immunotoxicological props. Other exp. effects. Associated with outbreaks of mycotoxicoses in farm animals. YD0112000

Tri-Ac:
Cryst. (EtOH). Mp 124-125°. $[\alpha]_D^{23}$ +44 (c, 1 in Me_2CO).

Sigg, H.P. *et al., Helv. Chim. Acta*, 1965, **48**, 962 (*struct*)
Tidd, B.K. *et al., J.C.S.(C)*, 1967, 218 (*pmr*)
Bamburg, J.R. *et al., Tetrahedron*, 1968, **24**, 3329 (*deriv*)
Cole, M. *et al., Appl. Microbiol.*, 1972, **24**, 660 (*use*)
Ripperger, H. *et al., Phytochemistry*, 1975, **14**, 2298 (*isol*)
Pathre, S.V. *et al., J. Agric. Food Chem.*, 1976, **24**, 97 (*isol*)
Ellison, R.A. *et al., J.O.C.*, 1976, **41**, 576 (*cmr*)
Steyn, P.S. *et al., Phytochemistry*, 1978, **17**, 949 (*isol*)
Hartmann, G.R. *et al., Planta Med.*, 1978, **34**, 231 (*rev, Anguidin*)
Claridge, C.A. *et al., Appl. Environ. Microbiol.*, 1979, **37**, 693-696 (*3-Ac*)
Brumley, W.C. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 451 (*ms*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220 (*uv, ir, pmr, ms, cd*)
Brooks, D.W. *et al., J.A.C.S.*, 1983, **105**, 4472 (*synth, deriv*)
Trichothecenes - Chemical, Biological and Toxicological Aspects, (ed. Ueno, Y.), Elsevier, 1983, (*tox, rev*)
Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1985, 1553 (*deriv*)
Roush, W.R. *et al., J.O.C.*, 1985, **50**, 3224 (*deriv*)
Anderson, D.W. *et al., Tet. Lett.*, 1987, **28**, 2661 (*Anguidin*)
Ziegler, F.E. *et al., J.A.C.S.*, 1990, **112**, 2749 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 160; 168; 171
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AOP250

3-Scirpenol S-58

12,13-Epoxy-9-trichothecen-3-ol, 9CI



$C_{15}H_{22}O_3$ 250.337

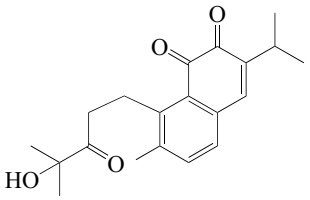
3α-*form* [104155-10-4]
3-Hydroxytrichothecene
Isol. from *Fusarium* sp. Dec. prod. of Trichotriol. No phys. props. reported.

Ac: [91423-90-4] ***Isotrichodermin***
$C_{17}H_{24}O_4$ 292.374
From *Fusarium culmorum* and *Fusarium roseum*.

Greenhalgh, R. *et al., J. Agric. Food Chem.*, 1984, **32**, 1261; 1986, **34**, 98; 1987, **35**, 125; 127 (*isol*)
Corley, D.G. *et al., J.O.C.*, 1987, **52**, 4405 (*isol, struct*)

Sclareapinone S-59

[189155-46-2]

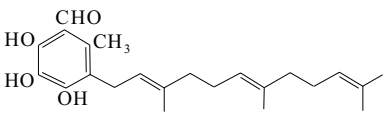


$C_{20}H_{24}O_4$ 328.407
Constit. of *Salvia sclarea* (clary sage). Amorph. orange solid. λ_{max} 230 (log ε 4.2); 332 (log ε 3.1); 390 (log ε 2); 432 (sh) (MeOH).

Ulubelen, A. *et al., Phytochemistry*, 1997, **44**, 1297-1299 (*isol, pmr, cmr*)

Scutigeral S-60

[65195-50-8]
2,3,4-Trihydroxy-6-methyl-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)benzaldehyde. 1-Formyl-3-hydroxyneogrifolin



$C_{23}H_{32}O_4$ 372.503
Constit. of *Albatrellus ovinus*. Yellow cryst. (hexane). Mp 81°.

2-Deoxy:2,4-Dihydroxy-6-methyl-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-benzaldehyde. ***1-Formylneogrifolin***
$C_{23}H_{32}O_3$ 356.504
Constit. of *Albatrellus ovinus*. Plates. Mp 98-102°. λ_{max} 202 (log ε 4.33); 239 (log ε 3.92); 293 (log ε 4.03); 338 (log ε 3.68) (EtOH).

Besl, H. *et al., Chem. Ber.*, 1977, **110**, 3770
Nukata, M. *et al., Phytochemistry*, 2002, **59**, 731-737 (*isol, uv, pmr, cmr*)

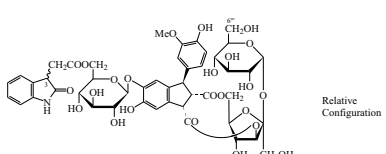
Scyllin S-61

[184378-81-2]
Glycoprotein rich in acidic and neutral amino acids and containing a large amount of mannose; MW 4.8-5 kDa. Isol. from the haemolymph of the crab *Scylla serrata* (Mud crab). Lectin.

Chattopadhyay, T. *et al., Biochem. Mol. Biol. Int.*, 1997, **42**, 183-191 (*isol*)

Secaloside A S-62

[188834-49-3]



$C_{46}H_{51}NO_{24}$ 1001.901
Constit. of the pollen of rye (*Secale cereale*). Amorph. powder. Mp 178-186°

dec. $[\alpha]_D$ +4.6 (c, 0.6 in MeOH). λ_{max} 280 ; 320 (sh) (H_2O).

6‴-O-β-D-Glucopyranoside: [188834-50-6]
Secaloside C
$C_{52}H_{61}NO_{29}$ 1164.043
Constit. of rye pollen. Tentative struct. assigned.

3-Epimer: [188855-24-5] ***Secaloside B***
$C_{46}H_{51}NO_{24}$ 1001.901
Constit. of the pollen of rye. Amorph. powder. Mp 192-201° dec. $[\alpha]_D$ +6.8 (c, 0.4 in MeOH). λ_{max} 280 ; 320 (sh) (H_2O).

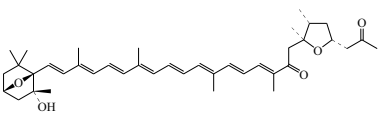
3-Epimer, 6‴-O-β-D-glucopyranoside: [188899-19-6] ***Secaloside D***
$C_{52}H_{61}NO_{29}$ 1164.043
Constit. of rye pollen. Tentative struct. assigned.

[187988-50-7, 187988-51-8]

Jaton, J.-C. *et al., J. Nat. Prod.*, 1997, **60**, 356-360; 361-365

Crassostrea Secocarotenoid S-63

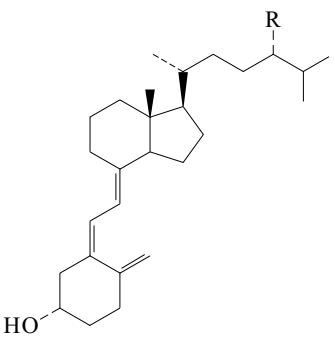
[256505-51-8]



$C_{40}H_{56}O_5$ 616.879
Constit. of the oyster *Crassostrea gigas*. Orange amorph. solid. λ_{max} 443 ; 468 (Et_2O).

Maoka, T. *et al., J. Nat. Prod.*, 2001, **64**, 578-581 (*isol, pmr*)

9,10-Secocholesta-5,7,10(19)-trien-3-ol, 9CI S-64



R = H

$C_{27}H_{44}O$ 384.644

(3*S*,5*Z*,7*E*)-*form* [67-97-0]
Vitamin D₃. *Cholecalciferol, BAN. Colecalciferol, INN. Calciol. Delsterol. Provitina. Ricketon. Vigorsan*
Constit. of fish-liver oil, esp. tuna oil. Antirachitic vitamin with approx. the same potency as vitamin D_2 in humans. Cryst. (Me_2CO). Mp 87-88°. $[\alpha]_D^{20}$ +84.8 (c, 1.6 in Me_2CO). Log P 9.48 (uncertain value) (calc). A lower-melting form, Mp 63-4° (from MeOH) was also reported.
► Excessive intake can cause hypercalcaemia and other effects. LD_{50} (rat, orl) 42 mg/kg. Exp. teratogen. VS2900000

3-O-Sulfate:
$C_{27}H_{44}O_4S$ 464.708
Amorph. solid (as Na salt). Mp 113-120° (Na salt).

Ac: [22350-49-8]
$C_{29}H_{46}O_2$ 426.681
Mp 131-132°. $[\alpha]_D^{18}$ +142 ($CHCl_3$).

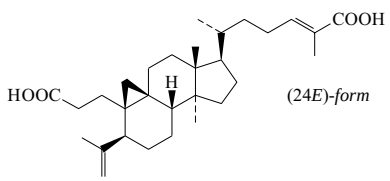
Benzoyl:
$C_{34}H_{48}O_2$ 488.752
Mp 63-64°. $[\alpha]_D$ +39 ($CHCl_3$).

3,5-Dinitrobenzoyl:
Yellow needles. Mp 131°.

[1406-16-2, 2200-64-8, 3844-73-3, 7489-19-2, 10597-47-4, 13083-02-8, 22350-41-0, 57651-82-8, 57651-83-9, 72409-70-2, 72506-00-4, 74512-98-4, 74512-99-5, 77286-64-7, 80666-48-4, 81126-11-6, 81126-44-5, 98744-46-8, 98818-17-8, 118584-54-6, 122958-39-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1049D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 570C (*nmr*)
Inhoffen, M. *et al., Angew. Chem.*, 1960, **72**, 875 (*rev*)
Haussler, M.S. *et al., J. Biol. Chem.*, 1972, **247**, 2328 (*rev*)
Borle, A.B. *et al., Annu. Rev. Physiol.*, 1974, **36**, 361 (*rev, metab*)
Wing, R.M. *et al., J.A.C.S.*, 1975, **97**, 4980 (*pmr, conformn*)
Okamura, W.H. *et al., Tet. Lett.*, 1976, 4807 (*ms*)
Lythgoe, B. *et al., Tet. Lett.*, 1977, 3685 (*synth*)
Fraser, D.R. *et al., Br. Med. Bull.*, 1981, **37**, 37 (*rev, metab*)
Pure Appl. Chem., 1982, **54**, 1511 (*nomencl*)
Koshy, K.T. *et al., Anal. Profiles Drug Subst.*, 1984, **13**, 655 (*rev*)
Wilson, S.R. *et al., Tet. Lett.*, 1984, **25**, 3147 (*synth*)
Nemoto, H. *et al., Heterocycles*, 1985, **23**, 567 (*synth*)
Nemoto, H. *et al., J.O.C.*, 1986, **51**, 5311 (*synth*)
Coldwell, R.D. *et al., Steroids*, 1990, **55**, 418 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1058
Zhu, G.-D. *et al., Chem. Rev.*, 1995, **95**, 1877 (*rev, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2935-2937 (*props, use*)
Jankowski, P. *et al., Tetrahedron*, 1998, **54**, 12071-12150 (*rev, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CMC750; HJV000

3,4-Secocycloarta-4(28),24-diene-3,26-dioic acid S-65



$C_{30}H_{46}O_4$ 470.691

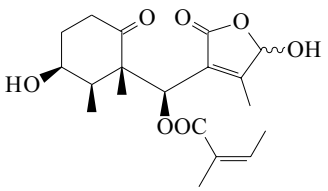
(24*Z*)-*form* [39111-07-4]
Nigranoic acid
Needles. Mp 128-130°. $[\alpha]_D$ +61.5 (c, 1.15 in MeOH).

26-Me ester: [212830-20-1]
$C_{31}H_{48}O_4$ 484.718
Constit. of *Illicium verum* (Chinese star anise). $[\alpha]_D$ +17.9 (c, 1.2 in $CHCl_3$).

Sy, L.-K. *et al., Phytochemistry*, 1998, **48**, 1169-1171 (*26-Me ester*)

Secoeremopetasitolide A S-66

[178402-70-5]

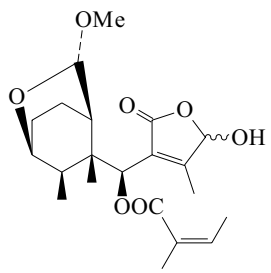


$C_{19}H_{26}O_7$ 366.41
Constit. of *Petasites japonicus* (sweet coltsfoot). Needles ($CHCl_3$/MeOH). Mp 168-169°. $[\alpha]_D^{26}$ -34.7 (c, 0.3 in MeOH). λ_{max} 213 (log ε 4.2) (MeOH).

Yaoita, Y. *et al., Phytochemistry*, 1996, **42**, 751 (*isol, pmr, cmr*)

Secoeremopetasitolide B S-67

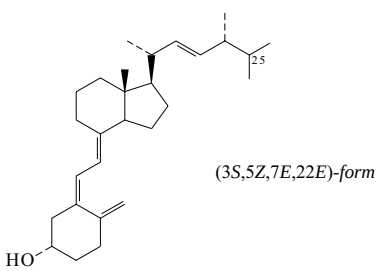
[178402-71-6]



$C_{21}H_{30}O_7$ 394.464
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{26}$ -5.1 (c, 0.4 in MeOH). λ_{max} 210 (log ε 4.1) (MeOH).

Yaoita, Y. *et al., Phytochemistry*, 1996, **42**, 751 (*isol, pmr, cmr*)

9,10-Secoergosta-5,7,10(19),22-tetraen-3-ol, 9CI S-68



(3*S*,5*Z*,7*E*,22*E*)-*form*

$C_{28}H_{44}O$ 396.655
Log P 9.39 (uncertain value) (calc).

(3*R*,5*Z*,7*E*,22*E*)-*form* [116559-84-3]
3-Epivitamin D_2
Cryst. (MeOH). Mp 46-58°.

Benzoyl: [116467-93-7]
Cryst. (MeOH/Et_2O). Mp 92-94°.

(3*S*,5*E*,7*E*,22*E*)-*form* [51744-66-2] *5,6-trans-Vitamin D_2*
Cryst. (diisopropyl ether). Mp 99-101° (87-90°).

(3*S*,5*Z*,7*E*,22*E*)-*form* [50-14-6] ***Ergocalciferol, BAN, INN, USAN.*** *Vitamin D_2. Calciferol. Ercalciol. Ergosterol (activated). Oleovitamin D_2. Viosterol. Many other names*
Antirachitic vitamin. Prisms (Me_2CO). Mp 114.5-117°. $[\alpha]_D^{20}$ +102.5 (EtOH). Log P 9.39 (uncertain value) (calc). Stable in cryst. state but solns. oxid. in air λ_{max} 265 (EtOH).

► Excessive intake can cause hypercalcaemia and other adverse effects. LD_{50} (rat, orl) 56 mg/kg, exp. reprod. and teratogenic effects. KE1050000

O-*Phosphate:* [863-53-6] *Ergocalciferol phosphate. Vitamin D_2 monophosphate. Derol*
$C_{28}H_{45}O_4P$ 476.635

O-*Sulfate:*
$C_{28}H_{44}O_4S$ 476.719
Mp 113-115° (as NH_4 salt).

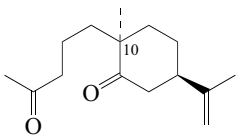
Benzoyl: [65338-41-2]
Cryst. (Me_2CO/Et_2O). Mp 88-90°.

25-Hydroxy:25-Hydroxyvitamin D_2. 25-Hydroxyergocalciferol
$C_{28}H_{44}O_2$ 412.654
Oil. $[\alpha]_D^{25}$ +56.8 (c, 0.2 in EtOH).

[1061-48-9, 1406-16-2, 1784-46-9, 3844-58-4, 34026-98-7, 39662-43-6, 80265-34-5, 84284-84-4, 85704-61-6]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 266C (*nmr*)
Fieser, L.F. *et al., Steroids*, Reinhold, N.Y., 1959, 90 (*rev*)
Dahlqvist, A. *et al., Acta Chem. Scand.*, 1964, **18**, 1607-1615 (*phosphate*)
Sanders, G.M. *et al., Prog. Chem. Org. Nat. Prod.*, 1969, **27**, 131-157 (*rev*)
Hull, S.E. *et al., Acta Cryst. B*, 1976, **32**, 2374-2381 (*cryst struct*)
Lythgoe, B. *et al., J.C.S. Perkin 1*, 1978, 590-595 (*synth*)
Mourino, A. *et al., J.O.C.*, 1978, **43**, 1653-1656 (*synth*)
Bell, P.A. *et al., Vitam. D. 1978*, 1978, 1-50 (*rev*)
Morzycki, J.W. *et al., J.O.C.*, 1984, **49**, 2148-2151 (*25-Hydroxyvitamin D_2*)
Yamada, S. *et al., Tet. Lett.*, 1984, **25**, 3347-3350 (*synth, 25-Hydroxyvitamin D_2*)
Synform, 1985, **3**, 70 (*rev, synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7725
Cota, J.G. *et al., J.O.C.*, 1988, **53**, 6094-6099 (*synth, isomers, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1058
Zhu, G.-D. *et al., Chem. Rev.*, 1995, **95**, 1877-1952 (*rev, synth*)
Jankowski, P. *et al., Tetrahedron*, 1998, **54**, 12071-12150 (*rev, synth*)
Org. Synth., 1999, **76**, 275-286 (*synth, uv, pmr, cmr*)
Blakemore, P.R. *et al., Synthesis*, 1999, 1209-1215 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSZ100

4,5-Seco-11-eudesmene-4,5-dione S-69



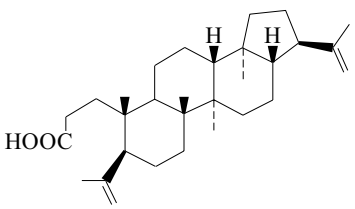
$C_{15}H_{24}O_2$ 236.353

10α-*form* [210106-14-2]
Constit. of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{21}$ +90 (c, 0.21 in $CHCl_3$).

10β-*form* [210106-15-3]
Azoridione
Constit. of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{21}$ +39 (c, 0.33 in $CHCl_3$).

Ohira, S. *et al., Phytochemistry*, 1998, **47**, 1577-1581 (*isol, pmr, cmr*)
Fraga, B.M. *et al., Z. Naturforsch., C*, 2001, **56**, 503-505 (*Azoridione*)

3,4-Seco-4(23),22(29)-hopadien-3-oic acid S-70



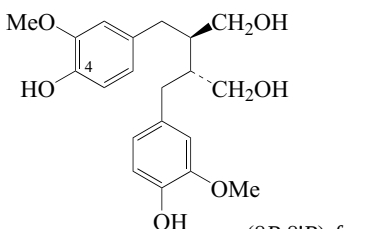
$C_{30}H_{48}O_2$ 440.708

(21α*H*)-*form* [52809-09-3]
Sebiferic acid
Constit. of the bark of *Sapium sebiferum* (Chinese tallowtree). Amorph. solid (MeOH). Mp 178-180°. $[\alpha]_D$ +28.57 ($CHCl_3$).

Pradhan, B.P. *et al., Indian J. Chem.*, 1973, **11**, 1217
Pradhan, B.P. *et al., Phytochemistry*, 1984, **23**, 2593 (*struct*)

Secoisolariciresinol S-71

2,3-Bis[(4-hydroxy-3-methoxyphenyl)-methyl]-1,4-butanediol, 9CI. 4,4′,9,9′-Tetrahydroxy-3,3′-dimethoxylignan. seco-*Isolariciresinol*



(8*R*,8'*R*)-*form*

$C_{20}H_{26}O_6$ 362.422
Lignan numbering shown.

(8*R*,8′*R*)-*form* [29388-59-8]
Cryst. (C_6H_6/Me_2CO). Mp 112-114°. $[\alpha]_D^{25}$ -32 (c, 1 in Me_2CO). λ_{max} 229 ; 282 (MeOH) (Berdy).

9-O-β-D-Glucopyranoside: [63320-67-2]
$C_{26}H_{36}O_{11}$ 524.564
Constit. of *Pinus sylvestris* (Scotch pine), Riesling wine and nettles. Amorph. powder. $[\alpha]_D$ -22.9 (c, 0.5 in EtOH). $[\alpha]_D^{20}$ -20.5 (c, 3.2 in EtOH). λ_{max} 223 (sh) (log ε 4.26); 282 (log ε 3.88) (MeOH). λ_{max} 210 ; 282 (EtOH).

9,9′-Di-O-β-D-glucopyranoside: [158932-33-3] *Secoisolariciresinol 9,9′-diglucoside. SDG*
$C_{32}H_{46}O_{16}$ 686.706
Constit. of the seeds of flax (*Linum usitatissimum*). Powder. $[\alpha]_D$ -4.4 (c, 0.2 in MeOH).

9-O-[4-Carboxy-3-hydroxy-3-methylbutanoyl-(→6)-β-D-glucopyranoside], 9′-O-β-D-glucopyranoside:6′-HMG SDG
$C_{38}H_{54}O_{20}$ 830.833
Constit. of the seeds of flax (*Linum usitatissimum*). Powder. Forms dimers and trimers λ_{max} 280 (log ε 3.59) (no solvent reported).

9,9′-Bis-O-[4-carboxy-3-hydroxy-3-methylbutanoyl-(→6)-β-D-glucopyranoside]:
$C_{44}H_{62}O_{24}$ 974.959
Constit. of the seeds of flax (*Linum usitatissimum*).

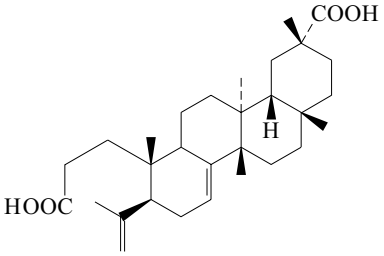
(8*S*,8′*S*)-*form*
9-O-β-D-Xylopyranoside: [145213-58-7]
Constit. of *Laurus nobilis* (bay laurel).

[145265-02-7]

Briggs, L.H. *et al., Tet. Lett.*, 1959, **No. 4**, 14 (*isol, struct*)
Freudenberg, K. *et al., Tet. Lett.*, 1959, **No. 17**, 19 (*isol*)
Traveso, G. *et al., Gazz. Chim. Ital.*, 1962, **90**, 792 (*abs config*)
Majumdar, R.B. *et al., Indian J. Chem.*, 1972, **10**, 677 (*isol, struct*)
Andersson, R. *et al., Acta Chem. Scand., Ser. B*, 1975, **29**, 835 (*isol*)
Fonseca, S.F. *et al., Phytochemistry*, 1978, **17**, 499 (*isol, cmr*)
Agrawal, P.K. *et al., Phytochemistry*, 1982, **21**, 1459 (*isol*)
Mahalanabis, K.K. *et al., Tet. Lett.*, 1982, **23**, 3975 (*synth*)
Lundgren, L.N. *et al., Acta Chem. Scand., Ser. B*, 1985, **35**, 241-248 (*9-xyloside*)
Inoshiri, S. *et al., Phytochemistry*, 1987, **26**, 2811-2814 (*9-glucoside*)
Marinos, V.A. *et al., Phytochemistry*, 1992, **31**, 4307-4312 (*9-glucoside, isol, wine*)
Chimichi, S. *et al., Magn. Reson. Chem.*, 1999, **37**, 860-863 (*9,9′-diglucoside, isol, pmr, cmr*)
Baderschneider, B. *et al., J. Agric. Food Chem.*, 2001, **49**, 2788-2798 (*9-glucoside*)
Ford, J.D. *et al., J. Nat. Prod.*, 2001, **64**, 1388-1397 (*9,9′-diglucoside, isol, pmr, cmr, bibl*)

3,4-Seco-4(23),7-multifloradiene-3,29-dioic acid S-72

[162898-23-9]
Secoisobryonic acid

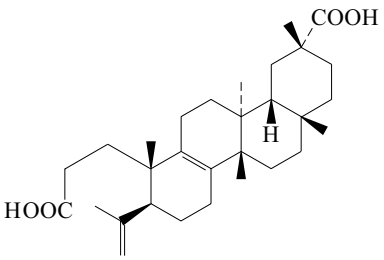


$C_{30}H_{46}O_4$ 470.691
Constit. of *Sandoricum koetjape* (santol). $[\alpha]_D^{22}$ -23.2 (c, 0.92 in $CHCl_3$) (Me ester).

Kosela, S. *et al., Phytochemistry*, 1995, **38**, 691 (*isol, pmr, cmr*)

3,4-Seco-4(23),8-multiflora-diene-3,29-dioic acid S-73

[162898-22-8]
Secobryonanic acid

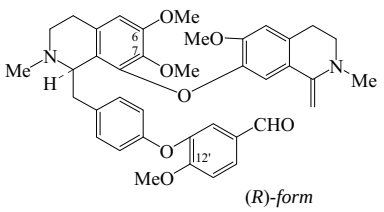


$C_{30}H_{46}O_4$ 470.691
Constit. of *Sandoricum koetjape* (santol). $[\alpha]_D^{22}$ +18.2 (c, 1.65 in $CHCl_3$) (Me ester).

Kosela, S. *et al., Phytochemistry*, 1995, **38**, 691 (*isol, pmr, cmr*)

Secoobaberine S-74

Auroramine



(*R*)-*form*

$C_{38}H_{40}N_2O_8$ 652.743
Secoobaberine as isolated was the *S*-form and Auroramine the *R*-form.

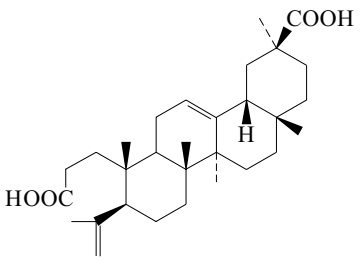
(*R*)-*form* [115653-32-2]
O^6-*De-Me:* [115610-42-9] ***Maroumine***
$C_{37}H_{38}N_2O_8$ 638.716

(*S*)-*form* [55085-45-5]
Amorph. $[\alpha]_D$ -5 (c, 0.2 in $CHCl_3$).
O^7-*De-Me:* [175097-24-2] ***Secohomoaromaline***
$C_{37}H_{38}N_2O_8$ 638.716
Needles. $[\alpha]_D^{20}$ -5.4 (c, 5.3 in $CHCl_3$).
$O^{12'}$-*De-Me:* [55085-44-4] ***Baluchistanamine***
$C_{37}H_{38}N_2O_8$ 638.716
Cryst. (cyclohexane/C_6H_6).
1''-Carboxylic acid, $O^{12'}$-de-Me, Me ester: [221001-23-6] ***Tejedine***
$C_{38}H_{40}N_2O_9$ 668.742
Alkaloid from *Berberis vulgaris* ssp. *australis* (barberry). Amorph. powder. Mp 132-134°. $[\alpha]_D$ -40.6 (c, 0.06 in MeOH). λ_{max} 206 (log ϵ 4.83); 224 (log ϵ 4.79); 260 (log ϵ 4.36); 292 (log ϵ 3.99) (MeOH).

Shamma, M. *et al., J.A.C.S.*, 1974, **96**, 7809 (*isol, ir, uv, ms, pmr, cd, struct, Baluchistanamine*)
Leete, J.E. *et al., Heterocycles*, 1982, **19**, 2355 (*isol, Baluchistanamine*)
Cortes, D. *et al., J. Nat. Prod.*, 1985, **48**, 76 (*Secoobaberine*)
Duté, P. *et al., Phytochemistry*, 1988, **27**, 655 (*Auroramine, Maroumine*)
Kanyinda, B. *et al., J. Nat. Prod.*, 1996, **59**, 498 (*Secohomoaromaline*)
Suau, R. *et al., Phytochemistry*, 1998, **49**, 2545-2549 (*Tejedine*)
Wang, Y.-C. *et al., Org. Lett.*, 2002, **4**, 2675-2678 (*Tejedine, synth*)

3,4-Seco-4(23),12-oleana-diene-3,30-dioic acid S-75

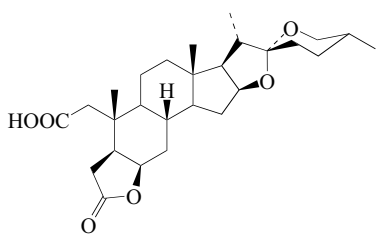
[142905-27-9]
Koetjapic acid



$C_{30}H_{46}O_4$ 470.691
Constit. of *Sandoricum koetjape* (santol). Cryst. (MeOH). Mp 296-298°. $[\alpha]_D^{24}$ +114.2 (c, 0.12 in MeOH).

Kaneda, N. *et al., J. Nat. Prod.*, 1992, **55**, 654-659 (*isol, pmr, cmr*)

2,3-Secospirostan-3,6-olid-2-oic acid S-76



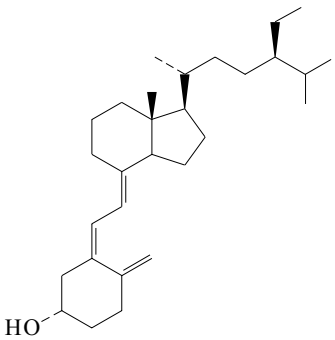
$C_{27}H_{40}O_6$ 460.609

(6β,25*R*)-*form* [189014-46-8]
2,3-Secoporrigenin
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -16 (c, 0.03 in $CHCl_3$).

(6β,25*S*)-*form* [189007-92-9]
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -28 (c, 0.003 in $CHCl_3$).

Carotenuto, A *et al., Tetrahedron*, 1997, **53**, 3401-3406 (*isol, pmr, cmr*)

9,10-Seco-5,7,10(19)-stigmas-tatrien-3-ol S-77



$C_{29}H_{48}O$ 412.698

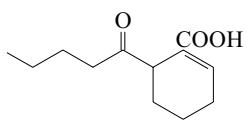
(3*S*,5*Z*,7*E*)-*form* [71761-06-3]

[1406-16-2]
Vitamin D_5
Synthetic vitamin with about 0.4% at the antirachitic potency of, or, in rats.

Napoli, J.L. *et al., Arch. Biochem. Biophys.*, 1979, **197**, 119 (*synth, uv, ms, biol*)
Yakhimovich, R.I. *et al., Khim.-Farm. Zh.*, 1981, **15**, 75 (*synth*)
Pardo, R. *et al., Bull. Soc. Chim. Fr.*, 1985, 98 (*synth*)

Sedanonic acid S-78

[6697-07-0]
6-(1-Oxopentyl)-1-cyclohexene-1-carboxylic acid, 9CI



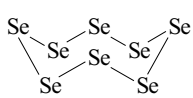
$C_{12}H_{18}O_3$ 210.272
Isol. from celery oil (*Apium graveolens*) after hydrol.. Cryst. (C_6H_6). Mp 113°.

[62006-38-6]

Ciamician, G. *et al., Ber.*, 1897, **30**, 492; 501; 1419 (*isol, struct*)
Barton, D.H.R. *et al., J.C.S.*, 1963, 1916 (*isol*)
Bjeldanes, L.F. *et al., J.O.C.*, 1977, **42**, 2333 (*ir, pmr, ms*)

Selenium, 11CI S-79

[7782-49-2]



Se 78.96

Atomic No. 34. Ground state electron config. [Ar]$3d^{10}4s^24p^4$. There are 20 isotopes of which 6 are stable. ^{77}Se is used in nmr. Discovered in 1817 by J.J. Berzelius. Exists in 6 allotropic forms: α, β, γ, grey "metallic", red amorphous, black vitreous. The α, β, and γ forms are all monoclinic with Se_8 rings. Grey, "metallic" comprises hexagonal helical polymeric chains. Struct. of black vitreous form is complex, irregular struct.

of large polymeric rings. Essential dietary component. Visc. of liq. decreases with temp., unlike S. Grey Se cryst. most stable form, conductor, photoconductor. Grey Se insol. CS_2; black vitreous and red amorphous forms spar. sol. CS_2; sol. conc. H_2SO_4 forming $Se_4^{2\oplus}$ in yellow-green soln. Mp 217° (grey). d 4.82 (grey form), 4.46 (monoclinic form). Recommended Dietary Allowance (RDA) of 55 and 70μg/day for men and women respectively.

► OES: long-term 0.1 mg m^{-3}. LD_{50} (rat, orl) 6700 mg/kg. LD_{50} (rat, ivn) 6 mg/kg. VS8310000

[14701-24-7, 14809-46-2, 22541-55-5, 54603-71-3]

Mellor Compr. Treat. Inorg. Theor. Chem., 1930, **10**, 693 (*rev*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 10, 1942, **A1**, ; 1950, **A2**, ; 1953, **A3**, ; *Suppl. Vol*., 1979, **A1**, ; 1980, **A2**, ; 1981, **A3**, (*element, rev, bibl*)
Bagnall, K.W. *et al., The Chemistry of Se, Te, Po*, Elsevier, 1966, (*rev*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 935 (*rev*)
Inorg. Synth., 1974, **15**, 218 (*synth*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 410 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **20**, 575 (*rev*)
Minamoto, Y. *et al., Jpn. J. Appl. Phys.*, 1980, **19**, 1813 (*synth, cryst struct*)
Grimley, R.T. *et al., J. Phys. Chem.*, 1982, **86**, 976 (*ms*)
Odom, J.D. *et al., Struct. Bonding (Berlin)*, 1983, **54**, 1 (*biochem*)
Steudel, R. *et al., Nova Acta Leopold.*, 1985, **59**, 231 (*rev*)
Steudel, R. *et al., Angew. Chem., Int. Ed.*, 1986, **25**, 99 (*synth*)
Högberg, J. *et al., Handb. Toxicol. Met.*, (Eds. Friberg, L. *et al*), 2nd edn., Elsevier, 1986, **2**, 482 (*tox, rev*)
Recommended Dietary Allowances, 10th. Ed., National Academic Press, Washington, D.C., 1989, 1989, 217-224 (*rev*)
Stadtman, T.C. *et al., Annu. Rev. Biochem.*, 1990, **59**, 111 (*biochem, rev*)
Schrauzer, G.N. *et al., Biol. Trace Elem. Res.*, 1992, **33**, 51 (*rev*)
Selenium Biol. Hum. Health., (Ed. Burk, R.F.), Springer-Verlag, 1994, (*book*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1467
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SBO500; SBP000

Selenocysteine S-80

[3614-08-2]
3-Selenylalanine, 9CI, 8CI. 2-Amino-3-selenylpropanoic acid
$HSeCH_2CH(NH_2)COOH$
$C_3H_7NO_2Se$ 168.054
Formed by seleniferous plants, e.g. onion, cabbage. Unstable compd., phys. props. not well documented. Various *Se*-protected derivs. made.

Se-*Me:* [2574-71-2] *3-(Methylseleno)alanine, 9CI.* Se-*Methylselenocysteine*
$C_4H_9NO_2Se$ 182.081

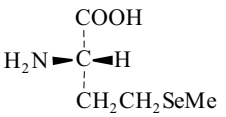
Diselenide: See Selenocystine in *The Combined Chemical Dictionary.*

Painter, E.P. *et al., J.A.C.S.*, 1947, **69**, 229 (*synth*)
Trelease, S.F. *et al., Science (Washington, D.C.)*, 1960, **132**, 618 (*isol*)
Schrift, A. *et al., Biochim. Biophys. Acta*, 1963, **71**, 483; 1965, **100**, 65 (*biosynth*)
Hamilton, J.W. *et al., J. Agric. Food Chem.*, 1975, **23**, 1150 (*isol*)
Stadtman, T.C. *et al., Annu. Rev. Biochem.*, 1996, **65**, 83 (*rev*)
Block, E. *et al., J. Agric. Food Chem.*, 2001, **49**, 458-470 (*synth*)

Selenomethionine S-81

[1464-42-2]

[1187-56-0]
2-Amino-4-(methylseleno)butanoic acid, 9CI. 2-Amino-4-(methylselenyl)butyric acid, 8CI


(*S*)-*form*

$C_5H_{11}NO_2Se$ 196.107
► ES7100000

(*S*)-*form* [3211-76-5]
L-form
Found in onion, cabbage, coco de mono (*Lecythis elliptica*), Brazil nuts (*Bertholletia excelsa*), wheat grains and other plants. Dietary supplement for avoidance of Se deficiency in humans and ruminants. Sol. H_2O. $[\alpha]_D^{25}$ +18.1 (c, 1.22 in 1*M* HCl).
► LD_{50} (rat, ipr) 11 mg/kg. Exp. fetotoxic.

Se-*Me:* [52553-55-6]

[7728-97-4] *2-Amino-4-(dimethylseleno)butanoic acid.* Se-*Methylselenomethionine*
$C_6H_{14}NO_2Se^{\oplus}$ 211.142

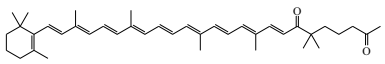
(±)-*form* [2578-28-1]
Hexagonal sheets or plates with metallic lustre (MeOH aq.). Mp 265° dec.

[7246-06-2, 13091-98-0, 97507-74-9, 99028-81-6]

Painter, E.P. *et al., J.A.C.S.*, 1947, **69**, 232-234 (*synth*)
Zdansky, G. *et al., Ark. Kemi*, 1968, **29**, 437; *CA*, **69**, 87433q (*synth, ir*)
Shepherd, L. *et al., Can. J. Biochem.*, 1969, **47**, 876 (*ir, props*)
Johnstone, R.A.W. *et al., J.C.S.(B)*, 1971, 1800 (*ms*)
Pan, W.H. *et al., J.A.C.S.*, 1978, **100**, 5783 (*Se-77 nmr*)
Rajeswaran, M. *et al., Acta Cryst. C*, 1984, **40**, 647 (*cryst struct*)
Willett, W.C. *et al., J. Am. Coll. Toxicol.*, 1986, **5**, 29 (*use*)
Krief, A. *et al., Synth. Commun.*, 1989, **19**, 1203 (*synth*)
Willhite, C.C. *et al., Food Chem. Toxicol.*, 1992, **30**, 903 (*metab*)
Grunau, J.A. *et al., J. Chromatogr.*, 1992, **594**, 165 (*hplc*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1164
Buchardt, O. *et al., Synthesis*, 1993, 1065 (*synth, bibl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SBU725

Semi-β-carotenone S-82

[20126-73-2]

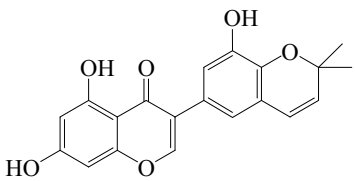


$C_{40}H_{56}O_2$ 568.881
Isol. from *Triphasia trifolia* (limeberry). Purple leaflets (MeOH); cryst. (hexane). Mp 118-119°. λ_{max} 440 ; 467 ; 495 (hexane).

Kuhn, R. *et al., Annalen*, 1935, **516**, 95 (*synth*)
Yokoyama, H. *et al., Phytochemistry*, 1968, **7**, 1031 (*isol*)

Semilicoisoflavone B S-83

[129280-33-7]
5,7-Dihydroxy-3-(8-hydroxy-2,2-dimethyl-2H-1-benzopyran-6-yl)-4H-1-benzopyran-4-one, 9CI



$C_{20}H_{16}O_6$ 352.343
Constit. of licorice (*Glycyrrhiza* sp.). Needles ($CHCl_3$). Mp 131-134°.

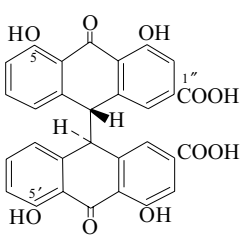
5-Me ether: [197304-07-7] ***Glycyrrhizaisoflavone B***
$C_{21}H_{18}O_6$ 366.37
Constit. of *Glycyrrhiza* sp.. Needles. Mp 197°. λ_{max} 209 (log ε 4.47); 258 (log ε 4.52); 282 (sh) (MeOH).

3′,4′-Dihydro, 3′-hydroxy: [197304-06-6] ***Glycyrrhizaisoflavone A***
$C_{20}H_{18}O_7$ 370.358
Constit. of *Glycyrrhiza* sp.. Needles. Mp 141°. Racemic λ_{max} 209 (log ε 4.6); 264 (log ε 4.32); 286 (sh) (MeOH).

Kiuchi, F. *et al., Heterocycles*, 1990, **31**, 629 (*isol, pmr, cmr*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1485-1492 (*Glycyrrhizaisoflavone A,B*)

Sennidin S-84

9,9′,10,10′-Tetrahydro-4,4′,5,5′-tetrahydroxy-10,10′-dioxo-[9,9′-bianthracene]-2,2′-dicarboxylic acid, 9CI. Dirhein


(*R**,*R**)-*form*

$C_{30}H_{18}O_{10}$ 538.466
Log P 4.4 (calc).

(*R,*R**)-*form*** [641-12-3]
Sennidin A
Yellow green powder. $[\alpha]_D^{24}$ +180 (c, 0.1 in 70% dioxan aq.). Log P 4.4 (calc).

5,5′-Di-O-*β*-D-*glucopyranoside:* [81-27-6] ***Sennoside A***. *Amyran. Exprep. Glaxenna. Moivat. Senan. Tisasen A. Many other names*
$C_{42}H_{38}O_{20}$ 862.75
Cathartic principle from rhubarb. Yellow plates (Me_2CO aq.). Mp 220-243° dec. $[\alpha]_D^{20}$ -164 (c, 0.1 in 60% Me_2CO aq.). Log P -1.38 (uncertain value) (calc).

5,5′-Di-O-*β*-D-*glucopyranoside, di-Me ester:*
Yellow plates (Me_2CO aq.). Mp 206-208°. $[\alpha]_D^{20}$ -90 (c, 0.2 in 70% dioxan).

5,5′-Di-O-*β*-D-*glucopyranoside, oxalyl:* [11137-63-6] ***Sennoside E***
$C_{44}H_{38}O_{23}$ 934.77
Found in rhubarb. Mp 214-215°. A deriv. of Sennoside A having an oxalyl -COCOOH substit. in one glucose residue. Complete struct. unknown.

1′′-Alcohol: [5355-93-1] ***Sennidin C***
$C_{30}H_{20}O_9$ 524.483
Aglycone from Sennoside C. Isol. from Chinese rhubarb (*Rheum palmatum*). Platelets ($CHCl_3/Me_2CO$). Mp 230-240° dec. $[\alpha]_D^{22}$ +80 (c, 0.09 in 70% dioxan aq.). Contains CH_2OH in place of one COOH.

1′′-Alcohol, 5,5′-di-O-*β*-D-*glucopyranoside:* [37271-16-2] ***Sennoside C***
$C_{42}H_{40}O_{19}$ 848.767
Yellow tablets (Me_2CO aq.). Mp 214-216° dec. (204-206°). $[\alpha]_D^{24}$ -123 (c, 0.1 in 70% Me_2CO aq.).

(*S,*S**)-*form*** [67479-20-3] *Sennidin A1. Sennidin G*
$[\alpha]_D^{24}$ -180 (c, 0.1 in 70% dioxan aq.).

5,5′-Di-O-*β*-D-*glucopyranoside:* [66575-30-2] ***Sennoside A1***. *Sennoside G*
$C_{42}H_{38}O_{20}$ 862.75
Yellow plates. Mp 162-176° dec. $[\alpha]_D^{28}$ -110 (c, 0.1 in 70% dioxan aq.).

(*RS*,*SR*)-*form* [517-44-2] meso-*form. Sennidin B*
Yellow powder.

5,5′-Di-O-*β*-D-*glucopyranoside:* [128-57-4] ***Sennoside B***. *Tisasen B*
$C_{42}H_{38}O_{20}$ 862.75
Light-yellow prisms (H_2O). Mp 209-212°. $[\alpha]_D^{20}$ -100 (c, 0.2 in 70% Me_2CO aq.). Log P -1.38 (uncertain value) (calc).

5,5′-Di-O-*β*-D-*glucopyranoside, di-Me ester:*
Prisms (Me_2CO aq.). Mp 196-198°. $[\alpha]_D^{20}$ -48 (c, 0.2 in 70% dioxan).

5,5′-Di-O-*β*-D-*glucopyranoside, oxalyl:* [52842-23-6] ***Sennoside F***
$C_{44}H_{38}O_{23}$ 934.77
From rhubarb. Yellow powder. Mp 171-175° dec. $[\alpha]_D$ -48.7 (c, 0.2 in Me_2CO aq.). A deriv. of Sennoside B having an oxalyl substit. in one glucose residue.

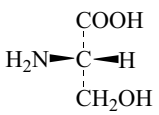
1′′-Alcohol: [62279-78-1] *Sennidin D*
$C_{30}H_{20}O_9$ 524.483

1′′-Alcohol, 5,5′-di-O-*β*-*glucopyranoside:* [37271-17-3] ***Sennoside D***
$C_{42}H_{40}O_{19}$ 848.767

Stoll, A. *et al., Helv. Chim. Acta*, 1949, **32**, 1892; 1950, **33**, 313 (*struct, isol*)
Schmid, W. *et al., Helv. Chim. Acta*, 1965, **48**, 1911
Oshio, H. *et al., Chem. Pharm. Bull.*, 1974, **22**, 823; 1978, **26**, 2458-2456 (*Sennosides, isol, ir, uv*)
Yamasaki, K. *et al., Tet. Lett.*, 1977, 1231 (*cmr*)
Christ, B. *et al., Arzneim.-Forsch.*, 1978, **28**, 225 (*ms, uv*)
Lemmens, L. *et al., Pharm. Weekbl.*, 1979, **1**, 178 (*metab*)
Tanaka, H. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1550 (*isol*)
Pharmacology, *Suppl*. 1, 1988, **36**, (*pharmacol, metab, use, rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 903
Pharmacology, *Suppl*. 1, 1993, **47**, (*pharmacol, metab, use, rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 11693 (*synonyms*)

Serine S-85

[6898-95-9]
2-Amino-3-hydroxypropanoic acid, 9CI. 3-Hydroxy-α-alanine. Ser



(S)-form

$C_3H_7NO_3$ 105.093

(*R*)-*form* [312-84-5]
D-*form*
Prisms (H_2O). Mp 228° dec. $[\alpha]_D^{20}$ +6.87 (H_2O).

Me ester: [5874-57-7]
$C_4H_9NO_3$ 119.12
Cryst. (MeOH) (as hydrochloride). Mp 164-166° (hydrochloride). $[\alpha]_D$ -40 (c, 4.0 in EtOH). CAS no. refers to hydrochloride.

N-*(4-Hydroxycinnamoyl):* [155179-34-3] N-p-*Coumaroyl*-D-*serine*
$C_{12}H_{13}NO_5$ 251.238

(*S*)-*form* [56-45-1]
L-*form*
Dietary supplement. Cryst. (H_2O). Mod. sol. H_2O (5.0 g/100g at 25°). Mp 228° dec. $[\alpha]_D^{20}$ -7.9 (H_2O). $[\alpha]_D$ -69.5 (5*M* HCl). pK_{a2} 9.34 (15°, 0.2*M* KNO_3). Isoelectric point 5.68. Sweet taste.
▶ VT8100000

Me ester: [2788-84-3]

[5680-80-8]
Cryst. (as hydrochloride). Mp 163-167° (hydrochloride).

Et ester: [26348-61-8]
$C_5H_{11}NO_3$ 133.147
Mp 130-132° (as hydrochloride). $[\alpha]_D^{25}$ -5.7 (c, 10.2 in EtOH). CAS no. refers to hydrochloride.

Amide: [65414-74-6]
$C_3H_8N_2O_2$ 104.108
Mp 185-188° (as hydrochloride). $[\alpha]_D^{20}$ +14 (c, 1 in 1*M* HCl) (hydrochloride). CAS no. refers to hydrochloride.

O-*Ac:* [5147-00-2]
$C_5H_9NO_4$ 147.13

N-*Ac:* [16354-58-8] N-*Acetyl*-L-*serine*
$C_5H_9NO_4$ 147.13
Mp 207.6°. $[\alpha]_D^{22}$ -205 (c, 1 in MeOH).

N-*Benzoyl:* [4877-23-0]
$C_{10}H_{11}NO_4$ 209.201
Needles (MeOH). Mp 148-150°.

N-tert-*Butyloxycarbonyl:* See *tert*-Butyloxycarbonylserine in *The Combined Chemical Dictionary.*

N-*Benzyloxycarbonyl:* See Benzyloxycarbonylserine in *The Combined Chemical Dictionary.*

N-*Me:* [2480-26-4]
$C_4H_9NO_3$ 119.12

Me ether: [32620-11-4] *2-Amino-3-methoxypropanoic acid. 3-Methoxyalanine*
$C_4H_9NO_3$ 119.12
$[\alpha]_D^{18}$ +16 (c, 1 in 1*M* HCl).

N,O-*Di-Me:*
$C_5H_{11}NO_3$ 133.147
Platelets (EtOH/Me_2CO). $[\alpha]_D$ +4 (H_2O). $[\alpha]_D$ +8 (dil. HCl).

N-*(2,4-Dinitrophenyl):* [1655-64-7]
$C_9H_9N_3O_7$ 271.186
Cryst. (MeOH). Mp 173-174°.

Benzyl ether: [4726-96-9]
$C_{10}H_{13}NO_3$ 195.218
Mp 219-221° (214-215°). $[\alpha]_D^{25}$ +2.5 (c, 2 in MeOH).

N-*(3*-C-*Glucosyl-5,6-dihydroxybenzoyl), Me ester:*
$C_{17}H_{23}NO_{11}$ 417.369Config. not stated but presumably *S*-. Ref. not accessible.

(±)-*form* [302-84-1]
Cryst. (H_2O). Mp 246° dec. pK_{a2} 9.21 (25°).

Hydrochloride: [51221-50-2]
Cryst. Mp 135° dec.

Me ester: [5619-04-5]
Mp 135-136° (114°) (as hydrochloride). CAS no. refers to hydrochloride.

Et ester: [39978-59-1]
Mp 100-102° (as hydrochloride).

Amide:
Cryst. (EtOH). Mp 96-97°.

O-*Ac:* [4985-36-8]
Cryst. (EtOH aq.). Mp 151-152° dec.

N-*Ac:* [97-14-3]
Cryst. (Me_2CO aq.). Mp 129-131°.

N,O-*Di-Ac:*
$C_7H_{11}NO_5$ 189.168
Mp 0°. $Bp_{0.8}$ 135°.

N-*Me:*
Cryst. (EtOH aq.). Mp 210°.

Me ether: [19794-53-7]
Cryst. (EtOH aq.). Mp 239° (236°) dec.

N,O-*Di-Me:*
Mp 233° (203-205°) dec.

Et ether:2-Amino-3-ethoxypropanoic acid
$C_5H_{11}NO_3$ 133.147
Cryst. (EtOH). Mp 256° dec.

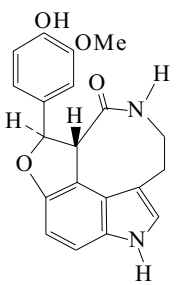
N-*(2,4-Dinitrophenyl):*
Mp 200-202°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 579D; 580A; 580B; 677B; 677D; **2**, 261C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 879C; 880A; 1076B; 1077A; 1269A (*nmr*)
Org. Synth., Coll. Vol., 3, 1955, 774 (*synth*)

Tsurumi, K. *et al., CA*, 1957, **51**, 1847e (*N-Acetyl-L-serine*)
Gundermann, K.D. *et al., Chem. Ber.*, 1959, **92**, 1081 (*synth, Me ether*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, 2202 (*rev*)
Johnson, H. *et al., J.O.C.*, 1962, **27**, 798 (*amide*)
Fujiwara, S. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 344 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Vilkas, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1965, **261**, 4258 (*isol, N,O-di-Me*)
Ogawa, H. *et al., J. Mol. Spectrosc.*, 1967, **23**, 76 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2356 (*occur*)
Bendetti, E. *et al., Gazz. Chim. Ital.*, 1973, **103**, 555 (*cryst struct*)
Kistenmacher, T.J. *et al., Acta Cryst. B*, 1974, **30**, 2573 (*cryst struct*)
L'vov, V.L. *et al., Carbohydr. Res.*, 1983, **112**, 233 (*occur, N-Ac*)
Hashem, K.M.E. *et al., Bull. Soc. Chim. Belg.*, 1985, **94**, 735 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, SCA350; SCA355
Chen, S.-T. *et al., Synthesis*, 1989, 36-37 (*benzyl ether*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 616
Song, K.S. *et al., Arch. Pharmacal Res.*, 1994, **17**, 48 (*N-coumaroyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2502-2503
Hulme, A.N. *et al., J.C.S. Perkin 1*, 2000, 1837-1841 (*R-form, Me ester*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SCA350; SCA355

Serotobenine S-86

[99615-94-8]
Moschamindole



$C_{20}H_{18}N_2O_4$ 350.373
Isol. from safflower meal (*Carthamus tinctorius*). Cryst. (MeOH). Mp 282-284.5° dec.

Ac:
Needles. Mp 211-214°. $[\alpha]_D^{25}$ 0 (c, 0.15 in Me_2CO).

Sato, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 2969 (*isol, ir, pmr, cmr, ms, cryst struct*)
Sarker, S.D. *et al., Nat. Prod. Lett.*, 1997, **9**, 189-199 (*Moschamindole*)

Serylvalylglycylglutamic acid S-87

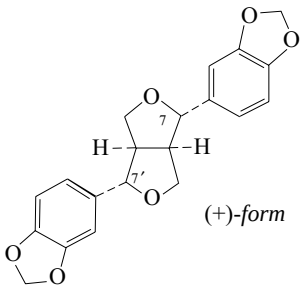
Toxin AS I. *AS I*
H-Ser-Val-Gly-Glu-OH

$C_{15}H_{26}N_4O_8$ 390.392
Prod. by *Alternaria alternata* on *Helianthus annuus* (sunflower). Cryst. (Et_2O). λ_{max} 210 (MeOH) (Berdy).

Liakopoulou-Kyriakides, M. *et al., Phytochemistry*, 1997, **45**, 37 (*isol, synth, ms*)

Sesamin S-88

*5,5′-(Tetrahydro-1*H*,3*H*-furo[3,4-c]furan-1,4-diyl)bis-1,3-benzodioxole,9CI. 2,6-Bis(3,4-methylenedioxyphenyl)-3,7-dioxabicyclo[3.3.0]octane. 3,4:3′,4′-Bis(methylenedioxy)-7,9′:7′,9-diepoxylignan. Pseudocubebin. Fagarol*



(+)-*form*

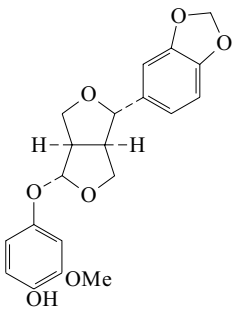
$C_{20}H_{18}O_6$ 354.359
Lignan numbering shown.Log P 1.9 (calc).

(+)-*form* [607-80-7]
Constit. of sesame oil. Needles (EtOH). Mp 123-124°. $[\alpha]_D^{20}$ +78.4 ($CHCl_3$).

Davenport, J.B. *et al., Aust. J. Chem.*, 1954, **1**, 384 (*isol*)
Beroza, M. *et al., J.A.C.S.*, 1956, **78**, 1242; 5082 (*struct, ms, synth*)
Freudenberg, K. *et al., Chem. Ber.*, 1961, **94**, 851 (*config*)
Takahashi, K. *et al., Chem. Pharm. Bull.*, 1966, **14**, 641 (*pmr, config*)
Pelter, A. *et al., J.C.S.(C)*, 1967, 1376 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1154 (*occur*)
Krajniak, R.E. *et al., Aust. J. Chem.*, 1973, **26**, 687 (*isol*)
Abe, F. *et al., Chem. Pharm. Bull.*, 1974, **22**, 2650 (*isol*)
Talapatra, B. *et al., Phytochemistry*, 1975, **14**, 589 (*isol*)
Pelter, A. *et al., Tetrahedron*, 1976, **32**, 2783 (*struct, nmr*)
Pelter, A. *et al., Tet. Lett.*, 1977, 4137; 1978, 1509 (*cmr*)
Anjaneyulu, A.S.R. *et al., Tetrahedron*, 1977, **33**, 133 (*pmr*)
Jaensch, M. *et al., Phytochemistry*, 1989, **28**, 3497 (*isol, pmr*)
Baures, P.W. *et al., Acta Cryst. C*, 1992, **48**, 574 (*cryst struct*)
Stevens, D.R. *et al., J.C.S. Perkin 1*, 1992, 185 (*synth*)
Suginone, H. *et al., J.O.C.*, 1995, **60**, 3052 (*synth, pmr*)
Kato, M.J. *et al., Phytochemistry*, 1998, **47**, 583-591 (*biosynth*)
Christov, R. *et al., Fitoterapia*, 1999, **70**, 89-92 (*cmr*)

Sesamolinol S-89

[100016-94-2]



Relative configuration

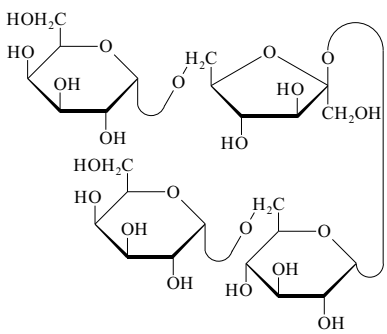
$C_{20}H_{20}O_7$ 372.374
Isol. from sesame seeds (*Sesamum indicum*). Oil. $[\alpha]_D$ +184 (c, 1 in $CHCl_3$).

3,5-Dinitrobenzoyl:
Cryst. Mp 205°. $[\alpha]_D$ +88 (c, 1 in $CHCl_3$).

Osawa, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 3351

Sesamose S-90

α-D-Galactopyranosyl-(1→6)-[α-D-galactopyranosyl-(1→6)-α-D-glucopyranosyl-(1→2)]-β-D-fructofuranoside. α-D-Galactopyranosyl-(1→6)-β-D-fructofuranosyl-(2→1)-[α-D-galactopyranosyl-(1→6)]-α-D-glucopyranoside

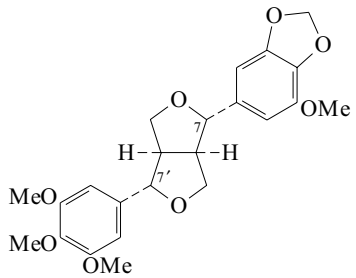


$C_{24}H_{42}O_{21}$ 666.583
Tentative struct.. Isol. from seeds of *Sesamum indicum* (sesame). Not obt. pure.

Hatanaka, S. *et al., Arch. Biochem. Biophys.*, 1959, **82**, 188

Sesartemin S-91

[77394-27-5]
*4-Methoxy-6-[tetrahydro-4-(3,4,5-trimethoxyphenyl)-1*H*,3*H*-furo[3,4-c]furan-1-yl]-1,3-benzodioxole, 9CI. 2-(3-Methoxy-4,5-methylenedioxyphenyl)-6-(3,4,5-trimethoxyphenyl)-3,7-dioxabicyclo[3.3.0]octane. 3,3′,4′,5′-Tetramethoxy-4,5-methylenedioxy-7,9′,7′,9-diepoxylignan. Sesalatin*



$C_{23}H_{26}O_8$ 430.454
Isol. from roots of *Artemisia absinthium* (wormwood). Mp 115-116°. $[\alpha]_D^{25}$ +50 ($CHCl_3$).

7-Epimer: [77449-31-1] ***Episesartemin A***
$C_{23}H_{26}O_8$ 430.454
Isol. from roots of *Artemisia absinthium* (wormwood). Mp 112-114°. $[\alpha]_D$ +115.

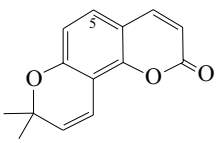
7′-Epimer: [77449-32-2] ***Episesartemin B***. *2-Episesalatin*
$C_{23}H_{26}O_8$ 430.454
Mp 114-115°. $[\alpha]_D$ +127.

7,7′-Diepimer: [77449-33-3] ***Diasesartemin***
$C_{23}H_{26}O_8$ 430.454
Isol. from roots of *Artemisia absinthium* (wormwood). Mp 102-104°. $[\alpha]_D$ +315.

Greger, H. *et al., Tetrahedron*, 1980, **36**, 3551 (*isol, nmr, ms*)
MacRae, W.D. *et al., Phytochemistry*, 1985, **24**, 561 (*isol, nmr*)
Hofer, O. *et al., Monatsh. Chem.*, 1988, **119**, 1143 (*cryst struct*)
Kamal-Eldin, A. *et al., Phytochemistry*, 1992, **31**, 2911 (*Episesalitin*)

Seselin S-92

[523-59-1]
*8,8-Dimethyl-2*H,*8*H-*benzo[1,2-*b:*3,4-*b′*]dipyran-2-one, 9CI. Amyrolin*



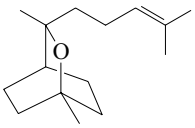
$C_{14}H_{12}O_3$ 228.247
Constit. of *Carum roxburghianum* (Bishop's weed). Cryst. (MeOH/Et_2O). Mp 119-120°. λ_{max} 294 ; 330 (MeOH) (Berdy). λ_{max} 216 (ϵ 11500); 292 (ϵ 5150); 327 (ϵ 5250) (EtOH) (Berdy).

2-Deoxo: [98119-92-7] *8,8-Dimethyl-2*H,*8*H-*benzo[1,2-*b:*3,4-*b′*]dipyran, 9CI*. ***Sesalin***
$C_{14}H_{14}O_2$ 214.263
Pale yellow oil.

Späth, E. *et al., Ber.*, 1939, **72**, 821; 963; 2093 (*isol, synth*)
Barnes, C.S. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
Shanbhag, S.N. *et al., Tetrahedron*, 1964, **20**, 2605 (*synth, pmr*)
Kato, K. *et al., Acta Cryst. B*, 1970, **26**, 2022 (*cryst struct*)
Hlubucek, J. *et al., Aust. J. Chem.*, 1971, **24**, 2347 (*synth*)
Gupta, G.S. *et al., J. Indian Chem. Soc.*, 1974, **51**, 904 (*isol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1975, **28**, 1393 (*isol*)
Gray, A.I. *et al., J.C.S. Perkin 2*, 1978, 391 (*pmr*)
Sattar, A. *et al., Phytochemistry*, 1978, **17**, 559 (*isol*)
Dominguez, X.A. *et al., Rev. Latinoam. Quim.*, 1985, **16**, 52 (*Sesalin*)
Narkhede, D.D. *et al., Tetrahedron*, 1990, **46**, 2031 (*Sesalin*)

Sesquicineol S-93

[90131-02-5]
3,7-Epoxy-10-bisabolene. 3,7-Oxido-10-bisabolene



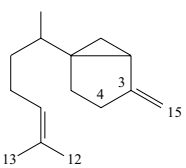
$C_{15}H_{26}O$ 222.37
Constit. of *Boronia megastigma* (brown boronia). Oil. Bp_5 90-94° $Bp_{0.1}$ 120°. $[\alpha]_D^{24}$ -8.4 (c, 4.06 in $CHCl_3$).

1,2-Didehydro:3,7-Epoxy-1,10-bisaboladiene. ***Dehydrosesquicineol***
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D^{20}$ -21.8 (c, 0.1 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1697 (*isol*)
Pascual Teresa, J. de. *et al., Tetrahedron*, 1988, **44**, 5109 (*synth, ir, pmr, cmr, ms*)
Weyerstahl, P. *et al., Tetrahedron*, 1990, **46**, 3503 (*synth*)
Weyerstahl, P. *et al., Annalen*, 1993, 111 (*Dehydrosesquicineol*)

Sesquisabinene S-94

[58319-04-3]
1-(1,5-Dimethyl-4-hexenyl)-4-methylenebicyclo[3.1.0]hexane, 9CI



$C_{15}H_{24}$ 204.355
Constit. of *Piper nigrum* (pepper). Isol. by glc.

$\Delta^{3,4}$-Isomer: [58319-06-5] ***Sesquithujene***
$C_{15}H_{24}$ 204.355
Isol. from *Zingiber officinale* (ginger).

*3,15-Dihydro, 3-hydroxy (*cis-*):****Sesquisabinene hydrate***
$C_{15}H_{26}O$ 222.37
Isol. from essential oil of *Zingiber officinale* (ginger).

*12-Acetoxy:****12-Sesquisabinenol acetate****. 12-Acetoxysesquisabinene*
$C_{17}H_{26}O_2$ 262.391
Oil.

12-Oxo: [83161-51-7] ***12-Sesquisabinenal***. *2-Methyl-6-(4-methylenebicyclo[3.1.0]-hex-1-yl)-2-heptenal, 9CI*
$C_{15}H_{22}O$ 218.338
Oil.

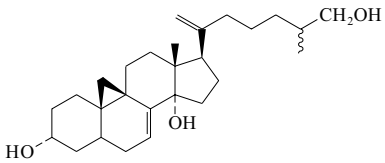
*13-Acetoxy:****13-Sesquisabinenol acetate****. 13-Acetoxysesquisabinene*
$C_{17}H_{26}O_2$ 262.391
Oil. $[\alpha]_D^{24}$ -39.5 (c, 0.2 in $CHCl_3$).

[83212-53-7]

Terhune, S.J. *et al., Can. J. Chem.*, 1975, **53**, 3285 (*isol, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1666-1667 (*isol, pmr*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1157 (*isol, struct*)
Sharma, P.K. *et al., Phytochemistry*, 1988, **27**, 3471 (*biosynth*)

Setariol S-95

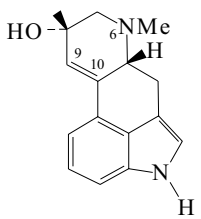
[142942-85-6]
9,19-Cyclocholesta-7,20-diene-3,14,26-triol



$C_{27}H_{42}O_3$ 414.627
Constit. of the leaves of *Setaria italica* (foxtail millet). Cryst. Mp 270-271°.

Kamil, M. *et al., Indian J. Pharm. Sci.*, 1992, **54**, 83-85; *CA*, **117**, 108123r (*isol, pmr, cmr, ms*)

Setoclavine S-96



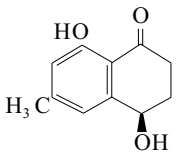
$C_{16}H_{18}N_2O$ 254.331
λ_{max} 242 (ϵ 26300); 317 (ϵ 12600) (EtOH) (Derep).

(+)-form [519-12-0]
Alkaloid from ergot found on *Pennisetum typhoideum* (pearl millet). Prisms (MeOH or Me_2CO). Mp 229-234° dec. $[\alpha]_D^{20}$ +174 (c, 1.1 in Py). $[\alpha]_D^{20}$ +165 (c, 0.3 in EtOH).

Hofmann, A. *et al., Helv. Chim. Acta*, 1957, **40**, 1358 (*isol, uv, ir, struct*)
Mrtek, R.G. *et al., Phytochemistry*, 1968, **7**, 1535 (*pmr*)
Chao, J.-M. *et al., Phytochemistry*, 1973, **12**, 2435 (*occur*)
Rebek, J. *et al., Heterocycles*, 1983, **20**, 583 (*synth*)
Rebek, J. *et al., J.A.C.S.*, 1984, **106**, 1813 (*synth, ir, pmr, ms*)
Liras, S. *et al., J.A.C.S.*, 2001, **123**, 5918-5924 (*synth*)

Shinanolone S-97

[34987-22-9]
*3,4-Dihydro-4,8-dihydroxy-6-methyl-1(2*H*)-naphthalenone, 9CI*



$C_{11}H_{12}O_3$ 192.214

(*R*)-*form*

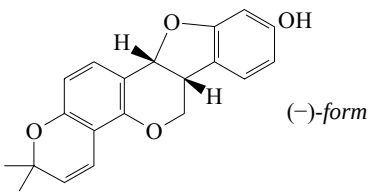
Isol. from *Diospyros kaki* (Japanese persimmon). Cryst. (hexane). Mp 110-111°. $[\alpha]_D^{21}$ -22.8 ($CHCl_3$).

Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2314 (*isol*)

Tezuka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2029 (*isol*)

Shinpterocarpin S-98

6a,11a-Dihydro-2,2-dimethyl-2H,6H-benzofuro[3,2-c]pyrano[2,3-h][1]benzopyran-9-ol, 9CI



(−)-*form*

$C_{20}H_{18}O_4$ 322.36

(-)-*form* [157414-04-5]

Isol. from roots of *Glycyrrhiza glabra* (licorice). Yellowish oil. $[\alpha]_D$ -9.9 (c, 1.02 in MeOH).

(+)-*form*

Me ether: [66446-92-2] *Hemileiocarpin*

$C_{21}H_{20}O_4$ 336.387

Oil.

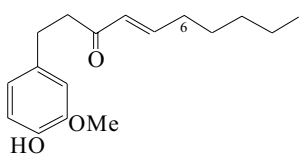
Brandt, E.V. *et al., J.C.S. Perkin 1*, 1978, 137 (*Hemileiocarpin*)

Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1056 (*Shinpterocarpin*)

Shogaol S-99

[555-66-8]

1-(4-Hydroxy-3-methoxyphenyl)-4-decen-3-one, 9CI. [6]Shogaol



$C_{17}H_{24}O_3$ 276.375

Occurs in "Shoga" ginger; isol. also from grains of paradise (*Amomum melegueta*) seed. Pale yellow oil. $Bp_{2.25}$ 201.3° (Lit. gives a pressure range). Other shogaol homologues are also present, prob. formed as artifacts from dehydration of gingerols (see [6]-Gingerol, G-120).

▶ HE2097000

1,2-Didehydro: [212137-55-8] *1-(4-Hydroxy-3-methoxyphenyl)-1,4-decadien-3-one.* ***[6]Dehydroshogaol***

$C_{17}H_{22}O_3$ 274.359

Constit. of ginger (*Zingiber officinale*) rhizomes. Yellow syrup. Possesses (*E*,*E*)-config. λ_{max} 258 (log ε 3.93); 355 (log ε 4.02) (MeOH).

Demethoxy: [153311-54-7] *1-(4-Hydroxyphenyl)-4-decen-3-one.* ***Demethoxyshogaol***

$C_{16}H_{22}O_2$ 246.349

Constit. of ginger (*Zingiber officinale*).

Me ether: [79067-86-0]

$C_{18}H_{26}O_3$ 290.402

Yellow oil. $Bp_{0.06}$ 160-165°.

6-Hydroxy: [143114-93-6] *6-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-4-decen-3-one.* ***6-Hydroxyshogaol***

$C_{17}H_{24}O_4$ 292.374

Constit. of ginger (*Zingiber officinale*). $[\alpha]_D$ -1.7 (c, 1.81 in $CHCl_3$).

[99742-07-1, 99742-10-6, 104264-52-0, 104264-53-1, 162794-32-3]

Connell, D.W. *et al., Aust. J. Chem.*, 1970, **23**, 369 (*isol*)

Tackre, A.N. *et al., Phytochemistry*, 1975, **14**, 853 (*isol*)

Banno, K. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1453 (*synth*)

Chen, C.C. *et al., J. Chromatogr.*, 1986, **360**, 175

Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 284 (*synth*)

Hatanaka, M. *et al., J.O.C.*, 1994, **59**, 111 (*synth*)

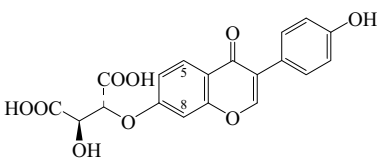
Matsushita, Y. *et al., Tet. Lett.*, 1995, **36**, 1879 (*6-Hydroxyshogaol*)

Wu, T.-S. *et al., Phytochemistry*, 1998, **48**, 889-891 (*Dehydroshogaol*)

Fleming, S.A. *et al., Synth. Commun.*, 1999, **29**, 1933-1939 (*synth, pmr, cmr*)

Shoyuflavone A S-100

[190712-87-9]



$C_{19}H_{14}O_9$ 386.314

Tartaroyl ether of 4′,7-Dihydroxyisoflavone, D-513. Isol. from fermented soy sauce. Prod. by *Aspergillus oryzae*. Amorph. off-white powder. Mp 212-218° dec. λ_{max} 233 (sh) ; 249 ; 259 ; 297 (sh) (MeOH). λ_{max} 248 (log ε 4.5); 302 (log ε 4.15) (H_2O).

5-Hydroxy: [190712-88-0] ***Shoyuflavone B***

$C_{19}H_{14}O_{10}$ 402.314

Isol. from fermented soy sauce. Prod. by *Aspergillus oryzae*. Amorph. pale yellow powder. Mp 138-144° dec. Tartaroyl ether of 4′,5,7-Trihydroxyisoflavone, T-601 λ_{max} 260 (log ε 4.63) (H_2O). λ_{max} 261 ; 324 (sh) (MeOH).

5,8-Dihydroxy: [194664-54-5]

[199852-70-5] ***Shoyuflavone C***

$C_{19}H_{14}O_{11}$ 418.313

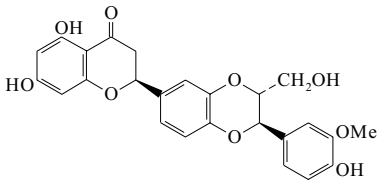
Isol. from fermented soy sauce. Prod. by *Aspergillus oryzae*. Amorph. pale yellow powder. Mp 209-212° dec. Tartaroyl ether of 4′,5,7,8-Tetrahydroxyisoflavone, T-226 λ_{max} 266 (log ε 4.5) (H_2O). λ_{max} 266 ; 307 (sh) ; 356 (MeOH).

Kinoshita, E. *et al., J. Agric. Food Chem.*, 1997, **45**, 3753-3759

Japan. Pat., 1997, 97 110 857; 1998, 98 59 956; *CA*, **127**, 32931m; **128**, 256476a

Silandrin S-101

[70815-32-6]



$C_{25}H_{22}O_9$ 466.443

Constit. of *Silybum marianum* (milk thistle). Cryst. Mp 234-236°. $[\alpha]_D$ -42.7.

Szilágyi, I. *et al., Herba Hung.*, 1978, **17**, 65

Szilagi, I. *et al., Planta Med.*, 1981, **43**, 121 (*isol*)

Antus, S. *et al., Annalen*, 1991, 633; 1993, 105 (*synth, abs config*)

Silica, 9CI S-102

[7631-86-9]

[11126-22-0, 98759-73-0]

Silicon dioxide. Silicic anhydride. Silicon(IV) oxide (SiO_2). E551

SiO_2

O_2Si 60.084

SiO_2 occurs in many forms. There are 3 principal cryst. polymorphs at ordinary pressures which are not readily interconvertible (quartz, tridymite and cristobalite), 3 high-pressure cryst. phases (keatite, coesite and stishovite), various microcryst. materials and several noncryst. forms such as vitreous silica and silica gel.Transparent, tasteless cryst. or amorphous powder. Melts to a glass. At ordinary temps., chemically resistant to most reagents. Insol. H_2O; sol. HF (giving fluorosilicate ions). Mp 1716-1736°. Bp 2230°.

▶ Toxic as an acute irritating dust. The chief cause of pulmonary dust disease. Prolonged inhalation may result in silicosis. VV7310000

Amorphous-*form*

Silica gel

Comprises a coherent, rigid, continuous 3-D network of spherical particles of colloidal silica. Used in foods as a colouring adjunct, a defoaming agent and an anticaking agent. Able to adsorb large volumes of gases on its interior and exterior surface.

Earthy-*form* [61790-53-2]

Kieselguhr. Diatomaceous earth. Infusorial earth. Siliceous earth. Fossil flour. Celite. Super-cel

Formed from marine unicellular algae (diatoms) which accrete silica on their cell walls. Sometimes regarded as a variety of opal. Occurs in food as a substance migrating from paper and paperboard products used in packaging. White or buff-coloured powder; can take up about 4 times its weight of H_2O. Insol.

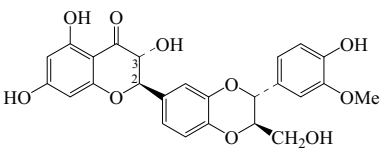
[10279-57-9, 12173-08-9, 14832-85-0, 14832-86-1, 14832-92-9, 16610-72-3, 18587-85-4, 18723-06-3, 19472-03-8, 20243-18-9, 24270-57-3, 29847-98-1]

Gmelin Handbook Inorg. Chem., *Syst. No.* 15, 1959, 269 (*rev*)
Compr. Inorg. Chem., Pergamon, 1973, **1**, 1388 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **20**, 748 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 424-427
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1540
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 805-806; 2507-2511
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SCI000; SCJ000; SCK000; SCJ500; SCK600

Silybin S-103

[22888-70-6]

[87725-91-5, 142797-34-0]
Silibinin, INN. *Silybum substance E6. Silymarin. Many other names*



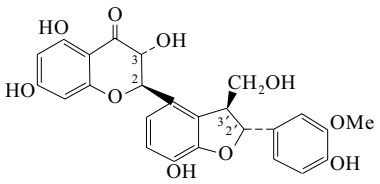
$C_{25}H_{22}O_{10}$ 482.443
Isol. from *Silybum marianum* (milk thistle). Cryst. + $1H_2O$ (Me_2CO/petrol). Mp 167°. $[\alpha]_D^{20}$ +11 (c, 0.25 in Me_2CO). Dec. at 180°.

2,3-Didehydro: [25166-14-7] ***2,3-Dehydrosilybin***
$C_{25}H_{20}O_{10}$ 480.427
Constit. of *Silybum marianum* (milk thistle). Mp 254-255°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 97C (*ir*)
Zoltan, O.T. *et al., Arzneim.-Forsch.*, 1970, **20**, 1248 (*pharmacol*)
Pelter, A. *et al., Chem. Ber.*, 1975, **108**, 790 (*isol, struct*)
Hänsel, R. *et al., Chem. Ber.*, 1975, **108**, 1482 (*isol, struct*)
Cavallini, L. *et al., Gazz. Med. Ital.*, 1976, **135**, 365 (*rev*)
Merlini, L. *et al., J.C.S. Perkin 1*, 1980, 775 (*synth*)
Lotter, H. *et al., Z. Naturforsch., C*, 1983, **38**, 339 (*cryst struct*)
Tanaka, H. *et al., Chem. Pharm. Bull.*, 1984, **33**, 1419 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7244 (*synonyms*)
Mericli, A.H. *et al., Planta Med.*, 1988, **54**, 44 (*Dehydrosilybin*)
Delfini, M. *et al., Spectrosc. Lett.*, 1990, **23**, 1007 (*pmr, conformn*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 693
Morazzoni, P. *et al., Fitoterapia*, 1995, **6**, 3 (*rev*)

Silychristin S-104

[33889-69-9]
Silicristin, INN. *Silymarin II*



$C_{25}H_{22}O_{10}$ 482.443
Two incorrect structs. prev. proposed. Isol. from fruits of *Silybum marianum* (milk thistle). Cryst. (H_2O). Mp 174-176°. $[\alpha]_D^{23}$ +81.4 (Py).

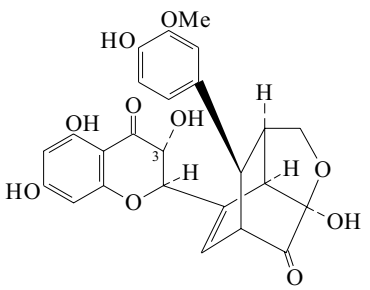
2,3-Didehydro: [57499-41-9] ***2,3-Dehydrosilychristin***
$C_{25}H_{20}O_{10}$ 480.427
Constit. of the fruit of *Silybum marianum anatolicum*. Mp 254-256°.

[119435-01-7, 125762-44-9]

Wagner, H. *et al., Tet. Lett.*, 1971, 1895 (*isol*)
Bandopadhyay, M. *et al., Indian J. Chem.*, 1972, **10**, 808 (*isol*)
Greiml, A. *et al., Experientia*, 1977, **33**, 1417
Wagner, H. *et al., Tet. Lett.*, 1978, 381 (*struct*)
Fiebrich, F. *et al., Experientia*, 1979, **35**, 1548 (*props*)
Zanarotti, A. *et al., Heterocycles*, 1982, **19**, 1585 (*stereochem, cd*)
Mericli, A.H. *et al., Planta Med.*, 1988, **54**, 44 (*Dehydrosilychristin*)
Tanaka, H. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1441 (*synth*)
Delfini, M. *et al., Spectrosc. Lett.*, 1990, **23**, 1007 (*pmr, conformn*)

Silydianin S-105

[29782-68-1]
Silidianin, INN. *Silybum substance E5*



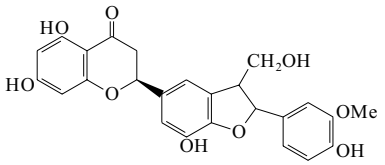
$C_{25}H_{24}O_{10}$ 484.458
Constit. of *Silybum marianum* (milk thistle). Mp 191°. $[\alpha]_D^{24}$ +175 (Me_2CO). $[\alpha]_D$ +218.

3-Deoxy: [70815-31-5] ***Silymonin***
$C_{25}H_{24}O_9$ 468.459
Constit. of *Silybum marianum* (milk thistle). Cryst. Mp 258-260°. $[\alpha]_D$ +127.

Janiak, B. *et al., Planta Med.*, 1960, **8**, 71 (*isol*)
Abraham, D.J. *et al., Tet. Lett.*, 1970, 2675 (*struct*)
Hoelzl, J. *et al., Z. Naturforsch., C*, 1974, **29**, 82 (*biosynth*)
Wagner, H. *et al., Z. Naturforsch., B*, 1976, **31**, 876 (*isol, ms, pmr, cryst struct, abs config*)
Szilágyi, I. *et al., Herba Hung.*, 1978, **17**, 65 (*isol*)

Silyhermin S-106

[96238-88-9]

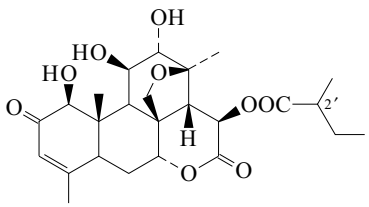


$C_{25}H_{22}O_9$ 466.443
Constit. of *Silybum marianum* (milk thistle). Cryst. (as penta-Ac). Mp 93-95° (penta-Ac). $[\alpha]_D$ +29.9 ($CHCl_3$) (penta-Ac).

Fiebig, M. *et al., Planta Med.*, 1984, **51**, 310
Antus, S. *et al., Annalen*, 1993, 503 (*synth*)

Simalikalactone D S-107

[35321-80-3]



$C_{25}H_{34}O_9$ 478.538
Cryst. Mp 228-230°. $[\alpha]_D$ +53. λ_{max} 239 (EtOH) (Berdy).

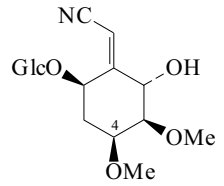
2′-Acetoxy: [59938-97-5] ***Quassimarin***
$C_{27}H_{36}O_{11}$ 536.575
Constit. of *Quassia amara* (Surinam quassia). Cryst. (EtOAc/hexane). Mp 237.5-238.5°. $[\alpha]_D^{26}$ +22.4 (c, 0.29 in $CHCl_3$). Log P -2.06 (uncertain value) (calc). λ_{max} 239 (ϵ 10800) (EtOH) (Berdy).

15-Deacyl, 15-(3-methyl-2-butenoyl): ***Gutolactone***
$C_{25}H_{32}O_9$ 476.522
Cryst. (Me_2CO). Mp 230°.

Teresa, J.-P. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **273**, 601 (*Simalikalactone D*)
Kupchan, S.M. *et al., J.O.C.*, 1976, **41**, 3481 (*Quassimarin*)
Kraus, G.A. *et al., J.O.C.*, 1980, **45**, 1175 (*synth*)
Moher, E.D. *et al., J.A.C.S.*, 1992, **114**, 2764 (*synth*)
Cabral, J.A. *et al., J. Nat. Prod.*, 1993, **56**, 1954 (*Gutolactone*)
Rodriguez Fo, E. *et al., Phytochemistry*, 1993, **34**, 501 (*isol, pmr, cmr*)
Ozeki, A. *et al., J. Nat. Prod.*, 1998, **61**, 776-780 (*activity*)

Simmondsin S-108

[51771-52-9]
[6-(β-D-Glucopyranosyloxy)-2-hydroxy-3,4-dimethoxycyclohexylidene]acetonitrile, 9CI. 2-Cyanomethylene-1-glucosyloxy-3-hydroxy-4,5-dimethoxycyclohexane



$C_{16}H_{25}NO_9$ 375.375
Constit. of *Simmondsia chinensis* (jojoba). Waxy solid. Mp 95-100°. $[\alpha]_D^{25}$ -78 (c, 1 in MeOH).

▶ AM0250000

Penta-Ac:
Mp 165-166°.

*2′-*O*-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* [179466-18-3]

[67411-22-7, 179466-19-4] *Simmondsin 2′-ferulate*
$C_{26}H_{33}NO_{12}$ 551.546
Constit. of the seeds of jojoba.

*3-*O*-De-Me, 2′-(4-hydroxy-3-methoxy-Z-cinnamoyl):* [162290-39-3]

[179466-20-7]
$C_{25}H_{31}NO_{12}$ 537.519
Constit. of jojoba meal.

*4-*O*-De-Me:* [135105-75-8] ***De-O-methylsimmondsin***
$C_{15}H_{23}NO_9$ 361.348
Constit. of jojoba meal.

*4-*O*-De-Me, 2′-(4-hydroxy-3-methoxy-E-cinnamoyl):* [162290-38-2]

[179601-21-9]
$C_{25}H_{31}NO_{12}$ 537.519
Constit. of jojoba meal.

*Di-*O*-de-Me:* [135074-86-1] ***Dide-O-methylsimmondsin***
$C_{14}H_{21}NO_9$ 347.321
Constit. of jojoba meal. Amorph. $[\alpha]_D^{20}$ -50 (c, 0.52 in H_2O). λ_{max} 215 (log ϵ 3.97) (H_2O).

*Di-*O*-de-Me, 4-*O*-α-D-glucopyranoside:* [370068-00-1] ***Dide-O-methyl-4-O-α-D-glucopyranosylsimmondsin***
$C_{20}H_{31}NO_{14}$ 509.463
Constit. of jojoba meal (*Simmonsia chinensis*).

*Di-*O*-de-Me, 2-*O*-(3-methyl-2-butenoyl):* [156368-87-5] ***Ehretioside A₃***
$C_{19}H_{27}NO_{10}$ 429.423
Waxy solid. $[\alpha]_D^{25}$ -53 (c, 1 in MeOH). Has (*E*)-config. (change of Cahn-Ingold-Prelog priorities).

*Di-*O*-de-Me, 3-*O*-(3-methyl-2-butenoyl):* [156368-85-3] ***Ehretioside A₁***
$C_{19}H_{27}NO_{10}$ 429.423
Amorph. $[\alpha]_D^{25}$ +39 (c, 1 in Py).

*Di-*O*-de-Me, 4-*O*-(3-methyl-2-butenoyl):* [156368-86-4] ***Ehretioside A₂***
$C_{19}H_{27}NO_{10}$ 429.423
Waxy solid. $[\alpha]_D^{25}$ -53 (c, 1 in MeOH).

*Di-*O*-de-Me, 2-*O*-benzoyl:* [158022-45-8] ***Lanceolin A***
$C_{21}H_{25}NO_{10}$ 451.429
Amorph. solid. Has (*E*)-config. (change of Cahn-Ingold priorities).

*Di-*O*-de-Me, 3-*O*-benzoyl:* [221149-42-4] ***Lanceolin C***
$C_{21}H_{25}NO_{10}$ 451.429
Amorph. solid.

*Di-*O*-de-Me, 4-*O*-benzoyl:* [151197-19-2] ***Lanceolin B***
$C_{21}H_{25}NO_{10}$ 451.429
Amorph. solid.

*Di-*O*-de-Me, 2,4-di-*O*-benzoyl:* [151171-81-2] ***Lophiroside A₂***
$C_{28}H_{29}NO_{11}$ 555.537
Amorph. $[\alpha]_D^{20}$ -22.6 (c, 0.93 in MeOH). λ_{max} 229 (log ϵ 4.54); 274 (log ϵ 3.26) (MeOH).

*Di-*O*-de-Me, 3,4-di-*O*-benzoyl:* [151171-80-1] ***Lophiroside A₁***
$C_{28}H_{29}NO_{11}$ 555.537
Amorph. $[\alpha]_D^{20}$ +11.5 (c, 0.87 in MeOH). λ_{max} 229 (log ϵ 4.54); 274 (log ϵ 3.26) (MeOH).

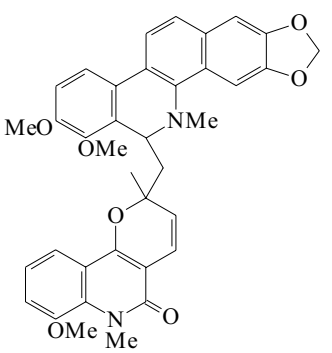
*Di-*O*-de-Me, 2-*O*-E-cinnamoyl, 4-*O*-benzoyl:* [151171-83-4] ***Lophiroside B₂***
$C_{30}H_{31}NO_{11}$ 581.575
Amorph. $[\alpha]_D^{20}$ -22.9 (c, 0.83 in MeOH). Has (*E*)-config. (change of Cahn-Ingold-Prelog priorities) λ_{max} 222 (log ϵ 4.25); 279 (log ϵ 4.14) (MeOH).

*Di-*O*-de-Me, 3-*O*-E-cinnamoyl, 4-*O*-benzoyl:* [151171-82-3] ***Lophiroside B₁***
$C_{30}H_{31}NO_{11}$ 581.575
Amorph. $[\alpha]_D^{20}$ +63 (c, 0.54 in MeOH). λ_{max} 222 (log ϵ 4.25); 279 (log ϵ 4.14) (MeOH).

Elliger, C.A. *et al., J.O.C.*, 1974, **39**, 2930 (*struct*)
Elliger, C.A. *et al., Phytochemistry*, 1974, **13**, 2319 (*isol*)
Verbiscar, A.J. *et al., J. Agric. Food Chem.*, 1978, **26**, 1456-1459 (*2′-ferulate*)
Chida, N. *et al., J.C.S. Perkin 1*, 1992, 1131 (*synth, abs config*)
Van Boven, M. *et al., J. Agric. Food Chem.*, 1993, **41**, 1605; 1994, **42**, 2684; 1996, **44**, 2239-2243 (*isol, cryst struct, derivs*)
Murakami, A. *et al., Phytochemistry*, 1993, **32**, 1461-1466 (*Lophirosides*)
Tih, A.E. *et al., J. Nat. Prod.*, 1994, **57**, 971-974 (*Lanceolin A, Lanceolin B*)
Simpol, L.R. *et al., Phytochemistry*, 1994, **36**, 91-95 (*Ehretiosides*)
Messanga, B.B. *et al., Fitoterapia*, 1998, **79**, 439-442 (*Lanceolin C*)
Van Boven, M. *et al., J. Agric. Food Chem.*, 2001, **49**, 4278-4283 (*Didemethyl-4-glucosylsimmondsin*)

Simulanoquinoline S-109

[155416-22-1]

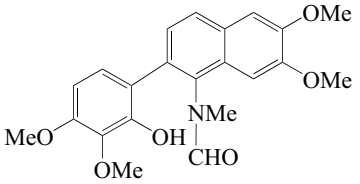


$C_{37}H_{34}N_2O_7$ 618.685
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Prisms ($CHCl_3$/MeOH). Mp 240-243°.

Wu, S.-J. *et al., Phytochemistry*, 1993, **34**, 1659 (*isol, uv, ir, pmr, ms, struct*)

Simulansamide S-110

[176713-29-4]

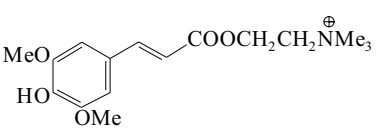


$C_{22}H_{23}NO_6$ 397.427
A secobenzo[*c*]phenanthridine alkaloid. Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Cryst. ($MeOH/CHCl_3$). Mp 257-259°.

Wu, S.-J. *et al., J. Chin. Chem. Soc. (Taipei)*, 1996, **43**, 195-198; *CA*, **124**, 337827k (*synth, uv, ir, pmr, ms*)

Sinapine S-111

[18696-26-9]
*2-[[3-(4-Hydroxy-3,5-dimethoxyphenyl)-1-oxo-2-propenyl]oxy]-*N,N,N*- trimethylethanaminium, 9CI. Choline 4-hydroxy-3,5-dimethoxycinnamate, 8CI*



$C_{16}H_{24}NO_5^{\oplus}$ 310.369
Alkaloid from seeds of black mustard (*Brassica nigra*), white mustard (*Sinapis alba*) and many other spp. in the Cruciferae.

Iodide: [5655-06-1]
$C_{16}H_{24}INO_5$ 437.274
Mp 185-186° (178-179°).

Sulfate: [6509-38-2]
$C_{16}H_{25}NO_8S$ 391.441
Mp 186-188° (anhyd.) Mp 126.5-127.5° dec. (dihydrate).

O-β-D-Glucopyranoside: [21848-40-8]

[87206-57-3, 87206-59-5]
$C_{22}H_{34}NO_{10}^{\oplus}$ 472.511
Semicryst. (as acetate salt). Obt. as a mix. of *E*- and *Z*-isomers λ_{max} 315 (H_2O).

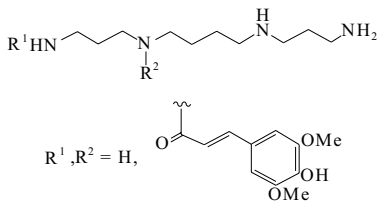
[84123-21-7, 84123-22-8]

Gadamer, J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1897, **235**, 44 (*isol*)
Späth, E. *et al., Monatsh. Chem.*, 1920, **41**, 271 (*synth*)
Kung, H.P. *et al., J.A.C.S.*, 1949, **71**, 1836 (*isol, uv*)
Schwartze, P. *et al., Naturwissenschaften*, 1949, **36**, 88 (*isol*)
Tzagoloff, A. *et al., Plant Physiol.*, 1963, **38**, 202 (*metab*)
Durkee, A.B. *et al., J. Food Sci.*, 1975, **40**, 820 (*occur*)
Sosulski, F.W. *et al., Dev. Food Proteins*, 1983, **2**, 109 (*rev*)

Larsen, L.M. *et al., Phytochemistry*, 1983, **22**, 219-222 (*glucoside*)
Regenbrecht, J. *et al., Phytochemistry*, 1985, **24**, 407

Sinapoylspermine S-112

[70185-65-8]

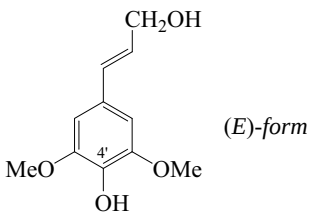


$C_{21}H_{36}N_4O_4$ 408.54
Alkaloid from *Brassica oleracea* var. *botrytis* (cauliflower).

Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*occur*)

Sinapyl alcohol S-113

[537-33-7]
4-(3-Hydroxy-1-propenyl)-2,6-dimethoxyphenol, 9CI. 3-(4-Hydroxy-3,5-dimethoxyphenyl)-2-propen-1-ol, 8CI. Syringenin



$C_{11}H_{14}O_4$ 210.229

(*E*)-*form* [20675-96-1]
Needles (petrol). Mp 63-65°.

*1,4′-Di-*O*-β-D-glucopyranoside:* [152686-85-6] ***Isosyringinoside***
$C_{23}H_{34}O_{14}$ 534.513
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 197-201°. $[\alpha]_D^{28}$ -43 (c, 1 in H_2O).

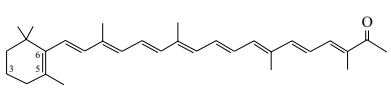
*1-Me ether, 4′-*O*-β-D-glucopyranoside:* [139742-20-4] ***Methylsyringin***. *Syringin methyl ether*
$C_{18}H_{26}O_9$ 386.398
Constit. of *Foeniculum vulgare* (fennel). Needles (MeOH). Mp 193-195°. $[\alpha]_D^{21}$ -33.4 (c, 1.5 in Py).

[132335-93-4]

Sugiyama, M. *et al., Phytochemistry*, 1993, **33**, 1215 (*Isosyringinoside*)
Ono, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 337 (*Isosyringinoside*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1587-1590 (*Methylsyringin*)

Sintaxanthin S-114

[4586-97-4]
7′-Apo-β-caroten-8′-one. 7′,8′-Dihydro-7′-apo-β-caroten-8′-one



$C_{31}H_{42}O$ 430.672
Isol. from the exocarp of Sinton citrangequat (a *Citrus*/*Poncirus*/*Fortunella* hybrid). Cryst. (hexane). Mp 144-145°. λ_{max} 425 (sh) ; 448 ; 475 (hexane).

3ξ-Hydroxy: ***3-Hydroxysintaxanthin***
$C_{31}H_{42}O_2$ 446.672
Isol. from the peel of Sinton citrangequat. λ_{max} 426 (sh) ; 474 (hexane).

3-Hydroxy, 5,6-epoxide:5,6-Epoxy-3-hydroxy-5,6,7′,8′-tetrahydro-7′-apo-β-caroten-8′-one. ***Hydroxysintaxanthin 5,6-epoxide***
$C_{31}H_{42}O_3$ 462.671
Present in juice of *Citrus sinensis*. Struct. assignment considered tentative λ_{max} 445 (EtOH).

Yokayama, H. *et al., J.O.C.*, 1965, **30**, 3994; 1966, **31**, 3452 (*isol, uv, ir, pmr, biosynth*)
Gross, J. *et al., Phytochemistry*, 1972, **11**, 303; 1974, **13**, 1917
Stewart, I. *et al., Phytochemistry*, 1973, **12**, 2947
Haugan, J.A. *et al., Acta Chem. Scand.*, 1994, **48**, 657 (*synth*)

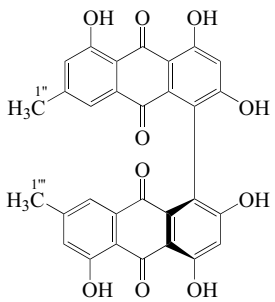
α_3-Sitosterol S-115

Struct. unknown. Prob. occurs in the plant in the form of its glycoside. Constit. of wheatgerm oil. Needles (EtOH). Mp 162-164°.

Bernstein, S. *et al., J.A.C.S.*, 1939, **61**, 1903 (*isol*)
Ginde, B.S. *et al., J.C.S.(C)*, 1970, 1285 (*isol*)
Kudav, N.A. *et al., Indian J. Chem.*, 1974, **12**, 1042 (*isol*)

Skyrin S-116

2,2′,4,4′,5,5′-Hexahydroxy-7,7′-dimethyl[1,1′-bianthracene]-9,9′,10,10′-tetrone. Endothianin. Rhodophyscin



$C_{30}H_{18}O_{10}$ 538.466

(*R*)-*form* [131233-49-3]

*2-*O*-α-Arabinopyranoside:*
$C_{35}H_{26}O_{14}$ 670.582
Constit. of *Hypericum perforatum* (St John's wort). Orange-red powder. λ_{max} 219 (log ε 4.44); 258 (log ε 4.39); 294 (log ε 4.15); 459 (log ε 3.92) (MeOH).

*2-*O*-β-D-Xylopyranoside:*
$C_{35}H_{26}O_{14}$ 670.582
Constit. of *Hypericum perforatum* (St John's wort). Orange-red powder. λ_{max} 219 (log ε 4.41); 258 (log ε 4.37); 294 (log ε 4.1); 456 (log ε 3.87) (MeOH).

*2-*O*-β-D-Glucopyranoside:*
$C_{36}H_{28}O_{15}$ 700.608
Constit. of *Hypericum perforatum* (St John's wort). Orange-red powder. Mp >300° λ_{max} 222 (log ε 4.59); 258 (log ε 4.54); 296 (log ε 4.28); 455 (log ε 4.14) (MeOH).

(*S*)-*form* [602-06-2]
Orange-red cryst. Sol. Et_2O, Py; poorly sol. hexane, H_2O. Mp 380°. λ_{max} 258 (ε 49000); 295 (ε 33100); 450 (ε 25700) (dioxan) (Berdy). λ_{max} 257 (ε 49000); 300 (ε 31600); 462 (ε 23440) (EtOH) (Berdy).

*2-*O*-β-D-Glucopyranoside:*
Constit. of *Hypericum perforatum* (St John's wort). Orange-red powder. Mp >300° λ_{max} 219 (log ε 4.53); 258 (log ε 4.49); 298 (log ε 4.21); 455 (log ε 4.03) (MeOH).

Wirz, A. *et al., Phytochemistry*, 2000, **55**, 941-947 (*Hypericum glycosides*)

Mytilus Small cardioactive peptide S-117

[150213-97-1]

H-Ala-Pro-Asn-Phe-Leu-Ala-Tyr-Pro-Arg-Leu-NH_2

$C_{56}H_{85}N_{15}O_{12}$ 1160.381
Constit. of the anterior byssus retractor muscles of *Mytilus edulis* (blue mussel).

Fujisawa, Y. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1993, **104**, 469; **105**, 471 (*isol, struct, pharmacol*)

Sodalite S-118

[1302-90-5]

[1344-00-9]

$Na_6[Al_6Si_6O_{24}].2NaCl$

$Al_3ClNa_4O_{12}Si_3$ 484.605

Zeolite struct. SOD. Parent of a group of cubic alumino silicates having general formula $(Na,Ca)_{4\text{-}8}Al_6Si_6(O,S)_{24}(SO_4,Cl,OH)$. 'Sodalite cages', comprising stacked 14-hedra (truncated octahedra) with apertures formed by $(Al,Si-O)_6$ rings, are commonly found in other zeolites (Zeolite A, etc.).White cryst. Mineral samples show various colours. n_D 1.483.

Chloride form:
$Al_6Cl_2Na_8O_{24}Si_6$ 969.211
White solid.

Hydroxide form:Basic sodalite
$Al_6H_6Na_8O_{28}Si_6$ 968.35
Dodecahedral white cryst.

Sulfate form:Nosean. Noselite
$Al_6Na_8O_{28}SSi_6$ 994.369

Ultramarine: [1317-97-1]

[1302-83-6]
$Al_6Na_8O_{24}S_4Si_6$ 1026.569
Blue cryst. Related green, violet and red substances cont. different S-cont. spp. also descr. Zeolite struct. SOD cont. $S_2^{\ominus}$ and $S_3^{\ominus}$ radical ions.

Me_4N form:
$C_4H_{12}AlNO_{12}Si_5$ 433.547
White cryst. (aq. melt).

Non-basic form:
$Al_3Na_3O_{12}Si_3$ 426.163
White solid. Sodalite hydrates obt. from hydroxy form at 127°; anhydrous form by subsequent dehydration.

Barrer, R.M. *et al., J.C.S.*, 1951, 195; 1952, 1561 (*synth*)
Barrer, R.M. *et al., Proc. R. Soc. London*, 1956, **236**, 227 (*ion exchange*)
Löns, J. *et al., Acta Cryst. B*, 1967, **23**, 434 (*cryst struct*)
Kroone, B. *et al., Chem. Ind. (London)*, 1968, 287 (*reactions, ultramarine*)
Baerlochev, C. *et al., Helv. Chim. Acta*, 1969, **52**, 1853 (*cryst struct, Me_4N form*)
Holzer, W. *et al., J. Mol. Spectrosc.*, 1969, **32**, 13 (*Raman, ultramarine*)
Hofmann, U. *et al., Z. Anorg. Allg. Chem.*, 1969, **367**, 119 (*synth, props, uv-vis, epr, ultramarine*)
Aiello, R. *et al., J.C.S.(A)*, 1970, 1470 (*synth*)
McLaughlan, S.D. *et al., J. Phys. Chem.*, 1970, **74**, 1359 (*synth, epr, ultramarine*)
Schwarz, K.-H. *et al., Z. Anorg. Allg. Chem.*, 1970, **378**, 52 (*x-ray fluorescence, uv, ir, epr, ultramarine*)
Barrer, R.M. *et al., J. Phys. Chem. Solids*, 1971, **32**, 731 (*absorption*)
Henderson, C.M.B. *et al., Spectrochim. Acta A*, 1977, **33**, 283 (*ir*)
Clark, R.J.H. *et al., Inorg. Chem.*, 1978, **17**, 3169 (*Raman, ultramarine*)
Lippmaa, E. *et al., J.A.C.S.*, 1981, **103**, 4992 (*Si-29 nmr*)
Klinowski, J. *et al., J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Koch, E. *et al., Z. Kristallogr.*, 1981, **154**, 95 (*rev*)
Fyfe, C.A. *et al., J. Phys. Chem.*, 1982, **86**, 1247 (*Al-27 nmr*)
Hassan, I. *et al., Acta Cryst. C*, 1983, **39**, 3 (*cryst struct, OH form*)
Hassan, I. *et al., Acta Cryst. B*, 1984, **40**, 6 (*cryst struct, Cl form, expansion*)
Depmeier, W. *et al., Acta Cryst. B*, 1984, **40**, 185 (*rev*)
Felsche, J. *et al., Zeolites*, 1986, **6**, 367 (*cryst struct, non basic form*)
Meier, W.H. *et al., Atlas of Zeolite Structure Types*, 2nd edn., Butterworth, London, 1987, 128
Weller, M.T. *et al., Chem. Comm.*, 1988, 1103; 1991, 734 (*powder struct, Si-29 nmr, ir*)

Sodium acetate S-119

[127-09-3]
Acetic acid, sodium salt, 8CI. Ethanoic acid, sodium salt. FEMA 3024. E262

NaOAc

$C_2H_3NaO_2$ 82.034

Food additive. Flavouring agent; pH control agent. White powder. V. sol. H_2O (119 g per 100 cm^3 at 0°; 170 g per 100 cm^3 at 100°); spar. sol. EtOH. Mp 324°. ΔH_f° -710 kJ mol^{-1}.

▶ AJ4375000

Trihydrate: [6131-90-4]
$C_2H_9NaO_5$ 136.08
Colourless monoclinic cryst., efflorescent. Dec. on heating by H_2O loss (-$3H_2O$ at 123°). V. sol. H_2O (76 g per 100 cm^3 at 0°; 139 g per 100 cm^3 at 50°); sol. EtOH (2.1 g per 100 cm^3 at 18°), Et_2O. ΔH_f° -1605 kJ mol^{-1}.

▶ AJ4580000

AcOH complex (1:1): [126-96-5] *Acetic acid sodium salt (2:1), 9CI. Sodium hydrogen diacetate. Sodium diacetate. FEMA 3900. E 262*
$C_4H_7NaO_4$ 142.087
Flavouring agent for snack foods. Antibacterial and mold inhibitor esp. for baked goods. pH control agent. Hygroscopic cryst. powder. V. sol. H_2O to weakly acid soln.

[39230-37-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 545D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 849A (*nmr*)
Rossini, F.D. *et al., Natl. Bur. Stand. Circ. (U.S.)*, No. 500, 1952, 470 (*thermochem props*)
Padmanabhan, V.M. *et al., Proc. Indian Natl. Sci. Acad., Part A*, 1953, **37**, 401 (*trihydrate, Raman*)
Jones, L.H. *et al., J. Chem. Phys.*, 1954, **22**, 1796 (*trihydrate, ir*)
Flett, M. *et al., Spectrochim. Acta*, 1962, **18**, 1537 (*ir*)
Spinner, E. *et al., J.C.S.*, 1964, 4217 (*Raman*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1024 (*uses*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1412; 1418 (*rev, bibl*)
Barrow, M.J. *et al., J.C.S. Perkin 2*, 1975, 15-18 (*sodium diacetate, cryst struct*)
Kirichenko, E.A. *et al., Zh. Strukt. Khim.*, 1976, **17**, 379 (*struct*)
Wei, K.T. *et al., Acta Cryst. B*, 1977, **33**, 522 (*trihydrate, struct*)
Aue, W.P. *et al., J. Chem. Phys.*, 1984, **80**, 1729 (*cmr*)
South African Pat., 1985, 85 02 520; *CA*, **105**, 45267v (*sodium diacetate, manuf*)
Tabeta, R. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 15D; 16A (*haz*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 727
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2517-2518
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1637-1638 (*sodium diacetate, use*)
Ash, M. *et al., Handbook of Food Additives*, Gower, 1995, 725 (*sodium diacetate, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SEG500

Sodium aluminium phosphate S-120

[7785-88-8]

[12764-58-1]
E541. SALP

$NaAl_3H_{14}(PO_4)_8$

$Al_3H_{14}NaO_{32}P_8$ 877.816

Emulsifying agent esp. for processed cheese. Slow acting acid for chemical leavening of bakery products. Powder + $4H_2O$.

Ger. Pat., 1970, 1 931 237; *CA*, **72**, 120268b (*manuf*)
Holmes, J.T. *et al., Cereal Chem.*, 1987, **64**, 343-348 (*use*)
Savello, P.A. *et al., J. Dairy Sci.*, 1989, **72**, 1-11 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2523-2524 (*use*)

Sodium borohydride S-121

[16940-66-2]
Tetrahydroborate sodium salt, 8CI. Sodium tetrahydroborate(III)

$NaBH_4$

BH_4Na 37.832

Reducing agent used in the prepn. of modified hop extract. White cubic cryst. Dec. on heating into constituent elements. V. sol H_2O (56 g per 100 cm^3 at 24°); mod. sol. EtOH, MeOH; spar. sol. Py; insol. Et_2O; sol. liq. NH_3. Mp 497°. Dissolves in cold H_2O to cryst. as the dihydrate; at higher temps. hydrolysis occurs. ΔH_f° -191.8 kJ mol^{-1}; ΔG_f° -127.1 kJ mol^{-1}; S° 101.4 J K^{-1} mol^{-1}.

▶ Flammable solid, corrosive. ED3325000

Tetra-deutero deriv.: [15681-89-7] *Sodium borodeuteride. Sodium tetradeuteroborate*
BD_4Na 41.857
White cubic cryst. V. sol. H_2O; mod. sol. EtOH, MeOH; spar. sol. Py; insol. Et_2O; sol. liq. NH_3.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1249B (*ir*)
Ford, P.T. *et al., Acta Cryst.*, 1954, **7**, 604 (*cryst struct*)
Emery, A.R. *et al., J. Chem. Phys.*, 1958, **28**, 1029 (*$NaBD_4$, synth, Raman*)
Taylor, R.C. *et al., J.A.C.S.*, 1958, **80**, 27 (*Raman*)
Onak, T.P. *et al., J. Phys. Chem.*, 1959, **63**, 1533 (*B-11 nmr*)
Davies, R.E. *et al., J.A.C.S.*, 1960, **82**, 5950 (*$NaBD_4$, hydrolysis*)
Schutte, C.J.H. *et al., Spectrochim. Acta*, 1960, **16**, 1054 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 257; 1966, **3**, 1212; 1230 (*rev, bibl*)
Canadian Pat., 1967, 762 843; *CA*, **67**, 110184 (*manuf, $NaBD_4$*)
Pyykko, P. *et al., Turun Yliopiston Julk., Sar. A*, 1967, **103**, 46; *CA*, 1968, **68**, 118370 (*$NaBD_4$, D-2 nmr*)
Smith, B.E. *et al., Inorg. Chem.*, 1977, **16**, 2057 (*$NaBD_4$, B-11 nmr*)
Buechner, W. *et al., Pure Appl. Chem.*, 1977, **49**, 733 (*rev, bibl, uses*)
Bernstein, M.A. *et al., J.A.C.S.*, 1979, **101**, 2744 (*uses, $NaBD_4$*)
Francois, P. *et al., Inf. Chim.*, 1985, **258**, 115 (*rev*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 234 (*thermochem data*)
Davis, R.L. *et al., J. Solid State Chem.*, 1985, **59**, 393 (*$NaBD_4$, cryst struct*)
Tabeta, R. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1996, **7**, 4522-4528 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2533
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFF500

Sodium carbonate (Na_2CO_3) S-122

[497-19-8]

[7542-12-3]
Carbonic acid disodium salt, 8CI. Soda ash. E500

Na_2CO_3

CNa_2O_3 105.989

Used in food processing as an antioxidant, curing and pickling agent, flavouring adjuvant, pH control agent and processing aid. White monoclinic powder, hygroscopic. Dec. on heating by CO_2 loss. Undergoes monoclinic (β) to monoclinic (α) transition at 361° and monoclinic (β)

to hexagonal (α) transition at 489°. V. sol. H_2O (7.1 g per 100 cm^3 at 0°; 46 g per 100 cm^3 at 100°); spar. sol. EtOH; insol. Me_2CO. Mp 850°. ΔH_f° -1130.8 kJ mol^{-1}; ΔG_f° -1048.0 kJ mol^{-1}; S° 138.8 JK^{-1} mol^{-1}. The name E500 is also used for Sodium hydrogen carbonate, S-130 and Trisodium hydrogen carbonate dihydrate, T-818.

▶ Irritant. VZ4050000

Monohydrate: See Sodium carbonate monohydrate in *The Combined Chemical Dictionary.*

Heptahydrate: See Sodium carbonate (Na_2CO_3) heptahydrate in *The Combined Chemical Dictionary.*

Decahydrate: See Sodium carbonate (Na_2CO_3) decahydrate in *The Combined Chemical Dictionary.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 545A; **2**, 1272C (*ir*)
Vratny, F. *et al., Appl. Spectrosc.*, 1960, **14**, 76 (*Raman*)
Jardetzky, O. *et al., J.A.C.S.*, 1960, **82**, 318 (*Na-23 nmr*)
Buijs, K. *et al., Spectrochim. Acta*, 1961, **17**, 927 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 2nd edn., Wiley, 1963, **18**, 458 (*rev, uses*)
Brouns, E. *et al., Acta Cryst.*, 1964, **17**, 614 (*cryst struct*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 267; 1966, **3**, 1317 (*rev, bibl*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th. Ed., 1974, 123 (*rev, uses*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 623 (*thermochem data*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3134D (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2535-2536
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFO000

Sodium chloride (NaCl), 8CI, JAN, USAN S-123

[7647-14-5]

[14762-51-7]

Rock salt. Salt. Halite. Ayr. Hypersal. Brine. Natritope chloride

NaCl

ClNa 58.442

Structural prototype. Preservative, chilling medium, curing agent, flavour enhancer, firming agent, pH control agent, antimicrobial agent, separation/filtration aid, moisture control agent, texturizer, colourant aid, emulsifier, material handling aid, leavening agent and clarifying/flocculating agent. Colourless cubic cryst., hygroscopic. V. sol H_2O (36 g per 100 cm^3 at 0°; 39 g per 100 cm^3 at 100°); spar. sol. EtOH. Mp 801°. Bp 1413°. ^{22}Na labelled compd. used as radioactive agent (Sodium chloride Na 22, USAN). Component of Lytears. ΔH_f° -411.1 kJ mol^{-1}; ΔG_f° -384.0 kJ mol^{-1}; S° 72.1 J K^{-1} mol^{-1}.

▶ Adverse therapeutic effects include hypertension, oedema, and gastrointestinal disturbances. Excessive administration can lead to hypernatraemia with resultant dehydration of internal organs. VZ4725000

[17112-21-9]

Nickels, J.E. *et al., J. Phys., Colloq.*, 1949, **53**, 625
Kaufmann, D.W. *et al., Sodium Chloride*, ACS Monograph Ser. 145, Reinhold, NY, 1960, (*rev*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 126 (*rev, bibl*)
Krishnamurthy, N. *et al., Z. Phys.*, 1965, **183**, 130 (*Raman*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 1974, 123 (*rev, uses*)
Lowenheim, F.A. *et al., Industrial Chemicals*, (Eds.), 4th Ed., Wiley-Interscience, N.Y., 1975, 722 (*manuf*)
Heiss, J.F. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **21**, 205 (*rev*)
Kare, M.R. *et al., Biol. Behav. Aspects Salt Intake, [Int. Conf.], 1979*, Academic Press, New York, 1980, (*book*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 770 (*thermochem data*)
Tabeta, R. *et al., Bull. Chem. Soc. Jpn.*, 1986, 1986, **59**, 1957 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3135d (*haz*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 439-442
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1184
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2539-2544 (*use, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFT000

Sodium chlorite S-124

[7758-19-2]

Chlorous acid, sodium salt, 8CI. Chloric(III) acid, sodium salt

$NaClO_2$

$ClNaO_2$ 90.441

Bleaching agent for starch; slimicide in the manuf. of paper and paperboard that contact food. Used in processing waters for fruit, vegetables and red meats. White monoclinic cryst., hygroscopic. Dec. on heating with evolution of O_2. V. sol. H_2O (39 g per 100 cm^3 at 17°; 55 g per 100 cm^3 at 60°). Mp 257°.

▶ Oxidiser, toxic. Recrystallised/purified samples are explosive; should not be stored for >3 months (technical grade 79-81% more stable). VZ4808000

Taylor, M.C. *et al., Ind. Eng. Chem.*, 1940, **32**, 899; *CA*, **34**, 5253[7] (*props*)
Mathieu, J.-P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1952, **234**, 2272 (*ir*)
Seibert, H. *et al., Z. Anorg. Allg. Chem.*, 1954, **275**, 225 (*Raman*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 161; 1970, **5**, 1741 (*rev, bibl*)
Cvikl, B. *et al., J. Chem. Phys.*, 1968, **49**, 3323 (*Na-23 nmr*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th Ed., 1974, 123 (*rev, uses*)
Nakamura, H. *et al., Kogyo Kayaku*, 1975, **36**, 331; *CA*, 1977, **86**, 64699 (*synth, thermal dec*)
Tarimci, C. *et al., Acta Cryst. B*, 1976, **32**, 610 (*cryst struct*)
Chartier, R.A. *et al., Encycl. Chem. Process. Des.*, 1977, **4**, 430 (*bleaching props*)
U.S. Pat., 1978, 4 087 515; *CA*, **89**, 113406 (*manuf*)
Ger. Pat., 1979, 2 833 038; *CA*, **90**, 177161 (*manuf*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3136A (*haz*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4533-4534 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2544-2545
Food Chem. News, 2000, **41(48)**, 26; 2001, **43(32)**, 11 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFT500; SFU000

Sodium dimethyldithiocarbamate S-125

[128-04-1]

Dimethylcarbamodithioic acid sodium salt, 9CI. Dimethyldithiocarbamic acid sodium salt, 8CI. Sodium dimethylcarbamodithioate

$Na(S_2CNMe_2)$

$C_3H_6NNaS_2$ 143.209

Antimicrobial agent used in cane-sugar and beet-sugar mills. Oxidation with air/Cl_2 mixtures affords $Me_2N(S)SC(S)NMe_2$. Photolysis yields CS_2.

▶ FD3500000

Dihydrate: [72140-17-1]

Colourless cryst. (H_2O). Mp 120-122°.

▶ FA0880000

Yamase, T. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 934 (*photol*)
Maj, J. *et al., Eur. J. Pharmacol.*, 1970, **9**, 183 (*pharmacol*)
Gorton, A.D.T. *et al., NR Technol.*, 1975, **6**, 52; *CA*, 1976, **84**, 32303 (*use, vulcanisation*)
Ger. Pat., 1977, 2 533 989; *CA*, **86**, 189245 (*oxidn*)
Given, K.W. *et al., J. Inorg. Nucl. Chem.*, 1977, **39**, 1309 (*ms*)
Oktavec, D. *et al., Coll. Czech. Chem. Comm.*, 1979, **44**, 2487 (*uv-vis*)
Yasuda, S. *et al., Spectrochim. Acta A*, 1979, **35**, 485 (*x-ray, dihydrate*)
Oktavec, D. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 1495 (*ir*)
Oskarsson, A. *et al., Acta Cryst. C*, 1983, **39**, 66 (*cryst struct, dihydrate*)
Japan. Pat., 1983, 58 224 178; *CA*, 1984, **100**, 179028 (*use, corrosion inhibition*)
Kajdasz, R. *et al., Proc. Int. Water Conf., Eng. Soc. West. Pa.*, 45th, 1984, 85; *CA*, 1985, **102**, 225778 (*use, biocide*)
Mereiter, K. *et al., Inorg. Chim. Acta*, 1985, **98**, 71 (*Raman, dihydrate*)
Japan. Pat., 1985, 60 129 125; *CA*, **103**, 182990 (*use, flue gas purifn*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2552-2553
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SGM500

Sodium diphosphate ($Na_4(P_2O_7)$) S-126

[7722-88-5]

Tetrasodium diphosphate, 9CI. Tetrasodium pyrophosphate, 8CI. Sodium pyrophosphate

$Na_4(P_2O_7)$

$Na_4O_7P_2$ 265.902

The tetrasodium salt of Diphosphoric acid. Orthorhombic cell with anion in eclipsed conformn. Na atoms are coordinated to 5 O or to 6 O. POP 127.5°, P–O(P) 163.1, 164.2, P–O (terminal) 151.3 pm. Used in foods as a buffering

agent, pH control agent, alkalinity source, dispersing agent, protein modifier, coagulant and sequestrant. White orthorhombic cryst. Sol. cold H_2O (3.2 g per 100 cm^3 at 0°; 40 g per 100 cm^3 at 100°). Mp 993° (985°). Forms 1:1, 1:2 and 1:3 complexes with H_2O_2 . Exists in polymorphic forms with transition temps. 400°, 510°, 545° and 560°. ΔH_f° -3183 kJ mol^{-1}.

► UX7350000

Decahydrate: [13472-36-1]
$H_{20}Na_4O_{17}P_2$ 446.055
Colourless efflorescent cryst. V. sol. H_2O (5.4 g per 100 cm^3 at 0°; 93 g per 100 cm^3 at 100°); insol. EtOH. Mp 79.5°. Monoclinic. Molecular dimensions: POP 130.2°, P−$O(P)_{av}$ 161.2, P −O_{av} 152.3 (terminal) pm. ΔH_f° -6143 kJ mol^{-1}. Water of cryst. may be replaced by H_2O_2. Lose H_2O at 93.8°.

H_2O_2 complex (1:2): [15039-07-3] *Sodium pyrophosphate peroxohydrate. Tetrasodium pyrophosphate perhydrate. Diphosphoric acid tetrasodium salt compd. with H_2O_2 (1:2), 12CI. Pyrophosphoric acid tetrasodium salt compd. with H_2O_2 (1:2), 8CI*
$H_4Na_4O_9P_2$ 301.933
Colourless cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1268D (*ir*)
Inorg. Synth., 1950, **3**, 100 (*synth*)
Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301 (*Raman, decahydrate*)
Corbridge, D.E.C. *et al., J.C.S.*, 1954, 493 (*ir, decahydrate*)
Corbridge, D.E.C. *et al., Anal. Chem.*, 1958, **30**, 1101 (*H_2O_2 complex, xrd*)
Simon, A. *et al., Z. Anorg. Allg. Chem.*, 1959, **301**, 154 (*synth, decahydrate*)
Cruickshank, D.W. *et al., Acta Cryst.*, 1964, **17**, 672 (*cryst struct, decahydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 357; 1967, **4**, 1611 (*rev, bibl*)
McDonald, W.S. *et al., Acta Cryst.*, 1967, **22**, 43 (*cryst struct*)
Steger, E. *et al., Z. Anorg. Allg. Chem.*, 1967, **355**, 131 (*ir*)
Shen, C.Y. *et al., J. Am. Oil Chem. Soc.*, 1968, **45**, 510 (*uses*)
Inoue, T. *et al., CA*, 1969, **70**, 53472 (*H_2O_2 complex, prep, ir, props*)
Nakatani, H. *et al., CA*, 1969, **71**, 119082 (*H_2O_2 complex, ir, xrd, tga*)
Nakatani, M. *et al., CA*, 1969, **71**, 119154 (*H_2O_2 complex, polarog, chromatog*)
Derbyshire, W. *et al., Mol. Phys.*, 1969, **17**, 449 (*P-31 nmr*)
Mardirosova, I.V. *et al., Zh. Neorg. Khim.*, 1970, **15**, 2507; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1970, **15**, 1297 (*synth, props*)
Leung, K.Y. *et al., Can. J. Chem.*, 1972, **50**, 2519 (*cryst struct, polymorphs*)
Morgan, W.E. *et al., J.A.C.S.*, 1973, **95**, 751 (*pe*)
Fichter, M. *et al., Spectrochim. Acta B*, 1975, **30**, 417
Mazalov, L.N. *et al., Zh. Strukt. Khim.*, 1981, **22**, 18; *J. Struct. Chem. (Engl. Transl.)*, 1981, **22**, 12 (*struct*)
Tabeta, R. *et al., Chem. Lett.*, 1984, 293 (*Na-23 nmr*)
Griffiths, L. *et al., J.C.S. Dalton*, 1986, 2247 (*P-31 nmr*)
Nefedov, V.I. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1988, **46**, 381 (*pe, Auger*)
Hayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3061 (*P-31 nmr*)
Marshall, W.L. *et al., J.C.S. Faraday 2*, 1989, **85**, 1963 (*Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2603-2605
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEE500

Sodium disulfite S-127

[7681-57-4]

[23134-05-6]
Disulfurous acid disodium salt, 9CI. Pyrosulfurous acid disodium salt, 8CI. Sodium disulfate(IV). Sodium pyrosulfite. Sodium metabisulfite, USAN. Sodium bisulfite. E223

$Na_2(O_3SSO_2)$
$Na_2O_5S_2$ 190.108
Food preservative; sanitising agent for food containers and fermentation equipment. Dec. on heating with ultimate formation of Na_2SO_4. V. sol. H_2O → aq. $NaHSO_3$ (54 g per 100 cm^3 at 20°; 82 g per 100 cm^3 at 100°); mod. sol. EtOH.

► OES: long-term 5 mg m^{-3}. Irritant. Induces bronchoconstriction in asthmatics. UX8225000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1296C (*ir*)
Inorg. Synth., 1946, **2**, 162 (*synth*)
Simon, A. *et al., Z. Anorg. Allg. Chem.*, 1955, **281**, 135 (*Raman*)
Griffiths, T.R. *et al., Anal. Chem.*, 1959, **31**, 1338 (*ir, uv-vis*)
Rocchiccioli, C. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **250**, 2347 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 211; 1966, **3**, 1086 (*rev, bibl*)
Erdey, L. *et al., Talanta*, 1966, **13**, 67 (*dta*)
Cleghorn, H.P. *et al., J.C.S.(A)*, 1970, 137 (*thermal dec, ir*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3146A (*haz*)
Til, H.P. *et al., Food Addit. Contam.*, 1992, **9**, 587 (*tox, rev*)
IARC Monog., 1992, **54**, 131 (*tox, rev*)
Nichol, G.M. *et al., Br. J. Pharmacol.*, 1994, **111**, 918 (*pharmacol, exp*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 451-453
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1146
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2569-2570
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 4476
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SII000

Sodium dithionite ($Na_2S_2O_4$) S-128

[7775-14-6]
Sodium hydrosulfite. Sodium hyposulfite. Sodium sulfoxylate. Dithionous acid, disodium salt, 8CI

$Na_2(O_2SSO_2)$
$Na_2O_4S_2$ 174.109
Bleaching agent which may occur adventitiously in food, occurrence not well documented. Colourless monoclinic cryst. Mp 300°. Dec. on heating to form Na_2SO_4.

► Flammable solid. JP2100000

Dihydrate: [13466-11-0]
Colourless cryst. (aq. $Na_2S_2O_4$). Dec. on heating by H_2O loss. V. sol. H_2O (25 g per 100 cm^3).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1296B (*ir*)
Dunitz, J.D. *et al., Acta Cryst.*, 1956, **9**, 579 (*cryst struct*)
Dunitz, J.D. *et al., J.A.C.S.*, 1956, **78**, 878 (*cryst struct*)
Griffiths, T.R. *et al., Anal. Chem.*, 1959, **31**, 1338 (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 252 (*rev, bibl*)
Cleghorn, H.P. *et al., J.C.S.(A)*, 1970, 137 (*thermal dec*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th Ed., 1974, 123 (*rev, uses*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 374 (*synth*)
Gert, E. *et al., Angew. Chem., Int. Ed.*, 1979, **91**, 333 (*synth*)
Takahashi, K. *et al., Spectrochim. Acta A*, 1982, **38**, 1147 (*ir, Raman*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3143D (*haz*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4554-4557 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SHR500

Sodium fluoride (NaF), 8CI, JAN, USAN S-129

[7681-49-4]

NaF
FNa 41.988
Rock salt struct.. Indirect food contaminant arising from its use in adhesives for aluminium foil. White cubic cryst. Mod. sol. H_2O (4.2 g per 100 cm^3 at 18°); spar. sol. EtOH. Mp 996°. Bp 1695° Bp 1704°. ΔH_f° -575.4 kJ mol^{-1}; ΔG_f° -545.1 kJ mol^{-1}; S° 51.21 J K^{-1} mol^{-1}.Component of Checkmate, Fluoral, Pediaflor, Zendium and Fluorinse.

► OES: long-term 2.5 mg/m^3 (as $F^\ominus$). Lethal dose (70 kg man) estimated to be 5-10 g. Systemic acute effects include tremors, hyperreflexia, paraesthesia, tetany, convulsions, cardiac arrhythmias, and respiratory arrest. Chronic exposure may result in skeletal fluorosis. LD_{50} (rat, orl) 52 mg/kg. Exp. reprod. and teratogenic effects. WB0350000

Mineral-*form*
Villiaumite
Minute cryst. Deep carmine red to lavender pink to light orange.

[15501-87-8, 22554-99-0, 39456-59-2]

Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, 1953, **1**, 63 (*cryst struct*)
Raman, C.V. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1962, **56**, 223; *CA*, 1963, **58**, 10879e (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 119 (*rev, bibl*)
Caruso, F.S. *et al., Handb. Exp. Pharmacol.*, (Part 2), 1970, **20**, 144 (*pharmacol*)
Ashley, F.P. *et al., Br. Dent. J.*, 1977, **143**, 333 (*use*)
Golightly, L.K. *et al., Can. J. Hosp. Pharm.*, 1978, **31**, 85 (*pharmacol, rev*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1037 (*thermochem data*)

Tabeta, R. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Clark, J.H. *et al., Chem. Comm.*, 1986, 657 (*F-19 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3140C (*haz*)
Whitford, G.M. *et al., The Metabolism and Toxicity of Fluoride*, Karger, 1989, (*book*)
Bucher, J.R. *et al., Int. J. Cancer*, 1991, **48**, 733 (*tox, rodent*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1413
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2557 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SHF500; SHG000

Sodium hydrogen carbonate S-130

[144-55-8]

[15752-47-3]

Sodium bicarbonate, JAN, USAN. Carbonic acid monosodium salt, 8CI. Baking soda. E500

$NaHCO_3$

$CHNaO_3$ 84.007

Leavening agent; component of self-raising flour. pH control agent for foods. White monoclinic cryst. or powder. Dec. on heating → CO_2, H_2O and Na_2CO_3. Mod. sol. H_2O (6.9 g per 100 cm^3 at 0°; 16 g per 100 cm^3 at 60°); spar. sol. EtOH. ΔH_f° -951 kJ mol^{-1}; ΔG_f° -851 kJ mol^{-1}; S° 102 J K^{-1} mol^{-1}. The name E500 is also used for Sodium carbonate (Na_2CO_3), S-122 and Trisodium hydrogen carbonate dihydrate, T-818.

▶ Skin and eye irritant. VZ0950000

[71-52-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1273C (*ir*)
Sass, R.L. *et al., Acta Cryst.*, 1962, **15**, 77 (*cryst struct*)
Novak, A. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1385 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 2nd edn., Wiley, 1963, **18**, 458 (*rev, uses*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 267; 1966, **3**, 1349 (*rev, bibl*)
Davies, J. *et al., Trans. Faraday Soc.*, 1971, **67**, 3465 (*pmr*)
Tabeta, R. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1951 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3143A (*haz*)
Washington, N. *et al., Antacids and Anti-Reflux Agents*, CRC Press, 1991, (*book*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 436-438
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1174
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2529-2531 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0372
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFC500

Sodium hydrogen sulfate S-131

[7681-38-1]

Sodium bisulfate. Sulfuric acid monosodium salt, 8CI. Sodium acid sulfate. E514

$NaHSO_4$

$HNaO_4S$ 120.061

Acidity regulator. Colourless triclinic cryst. Dec. on heating with H_2O loss to form $Na_2S_2O_7$ which on further heating dec. to form Na_2SO_4. V. sol. H_2O (29 g per 100 cm^3 at 25°; 100 g per 100 cm^3 at 100°), spar. sol. EtOH. Mp 182°. ΔH_f° -1126 kJ mol^{-1}; ΔG_f° -993 kJ mol^{-1}; S° 113 JK^{-1} mol^{-1}. The name E514 is also used for Sodium sulfate, S-144.

▶ Corrosive. VZ1860000

Monohydrate: [10034-88-5]
H_3NaO_5S 138.076
Colourless monoclinic deliquescent cryst. Dec. on heating by H_2O loss. ΔH_f° -1419.2 kJ mol^{-1}.

▶ Corrosive. VZ1870000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1266A (*ir*)
Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301; 424 (*Raman*)
Rossini, F.D. *et al., Natl. Bur. Stand. Circ. (U.S.)*, No. 500, 1952, 461 (*thermochem data*)
Freeman, D.E. *et al., Aust. J. Chem.*, 1957, **10**, 227 (*ir, Raman*)
Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 246; 1966, **3**, 1149; 1154 (*rev, bibl*)
Pringle, G.E. *et al., Acta Cryst.*, 1965, **19**, 426 (*monohydrate, cryst struct*)
Sonneveld, E.J. *et al., Acta Cryst. B*, 1978, **34**, 643; 1979, **35**, 1975 (*dehydration of monohydrate, cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 205 (*rev, uses*)
Skobeev, I. *et al., CA*, 1979, **91**, 131498 (*ir*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3131B (*haz*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SEG800

Sodium hydrogen sulfite S-132

[7631-90-5]

[10579-83-6]

Sulfurous acid, monosodium salt, 8CI. Sodium bisulfite. Sodium acid sulfite. E222

$NaHSO_3$

$HNaO_3S$ 104.062

Exists in soln. but crystallises as $Na_2S_2O_5$. Used in food processing as sanitising agent for food containers and fermentation equipment, preservative to reduce or prevent microbial spoilage, selective inhibitor of undesirable microorganisms in the fermentation industries, and as an antioxidant and inhibitor of enzyme-catalysed oxidative discoloration and non-enzymic browning. Yellow in soln. V. sol. H_2O; spar. sol. EtOH.

▶ Corrosive. VZ2000000

[15181-46-1]

Ghosh, J.C. *et al., J. Phys. Chem.*, 1932, **36**, 586 (*Raman*)
Inorg. Synth., 1946, **2**, 146 (*synth*)
Valyashko, N.A. *et al., CA*, 1955, **49**, 836 (*uv*)
Evans, J.C. *et al., Can. J. Chem.*, 1955, **33**, 1270 (*Raman*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 211; 1966, **3**, 1086 (*rev, bibl*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th Ed., 1974, 123 (*rev, ind, uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3131C
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2531-2533
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFE000

Sodium hydroxide (NaOH), 8CI S-133

[1310-73-2]

Caustic soda. Soda lye. Sodium hydrate. E524

NaOH

HNaO 39.997

Industry's most important alkali. TlI struct. type. Used in food processing as a pH control agent, washing/surface removal agent, clarifying/flocculating agent, oxidising/reducing agent, flavour and flavour modifier, sanitising/fumigating agent, appearance control agent for colours and colour modifiers. Deliquescent orthorhombic white powder. Undergoes polymorphic transition at 299°. Readily reacts with atm. CO_2 forming Na_2CO_3. V. sol. H_2O (42 g per 100 cm^3 at 0°; 347 g per 100 cm^3 at 100°); EtOH; insol. Et_2O, Me_2CO. Mp 323°. Bp 1390°. ΔH_f° -425.9 kJ mol^{-1}; ΔG_f° -379.7 kJ mol^{-1}; S° 64.4 J K^{-1} mol^{-1}.

▶ Toxic; corrosive. WB4900000

Monohydrate: [12200-64-5]
H_3NaO_2 58.012
Colourless orthorhombic cryst.; dec. on heating by H_2O loss. V. sol. H_2O (114 g per 100 cm^3 at 25°). Mp 65°. ΔH_f° -735 kJ mol^{-1}; ΔG_f° -629 kJ mol^{-1}; S° 100 J K^{-1} mol^{-1}. Many less important hydrates also reported.

Deutero compd.: [14014-06-3] *Deuterated sodium hydroxide. Sodium deuteroxide*
DNaO 41.003
Air-sensitive white powder. Reacts with atm. CO_2 forming Na_2CO_3. Dissolves in H_2O with isotope exchange. V. sol. H_2O, EtOH; insol. Et_2O, Me_2CO. Undergoes orthorhombic to monoclinic transition at =227° and monoclinic to cubic transition at =287°.

▶ Toxic, corrosive.

[8006-28-8]

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1518B (*ir*)
Ernst, T. *et al., Angew. Chem.*, 1948, **60**, 77 (*cryst struct*)
Busing, R.W. *et al., J. Chem. Phys.*, 1955, **23**, 933 (*ir, Raman, hydroxide, deuteroxide*)
Wunderlich, J.A. *et al., Acta Cryst.*, 1957, **10**, 462 (*monohydrate, cryst struct, source*)
Wunderlich, J.A. *et al., Bull. Soc. Fr. Mineral. Cristallogr.*, 1959, **82**, 17 (*monohydrate, synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 18; 1965, **2**, 833; 835 (*rev, bibl*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th Ed., 1974, 123 (*rev, uses*)
Luibrand, R.T. *et al., J.O.C.*, 1980, **45**, 958 (*synth, uses, deuteroxide*)
Bleif, H.J. *et al., Acta Cryst. A*, 1982, **38**, 470 (*cryst struct, polymorphs, deuteroxide*)
Amm, D.T. *et al., J. Chem. Phys.*, 1985, **82**, 2529 (*pmr*)

Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1243 (*thermochem data*)
Amm, D.T. *et al., Thermochim. Acta*, 1985, **95**, 447 (*polymorphs, deuteroxide*)
Amm, D.T. *et al., Z. Naturforsch., A*, 1986, **41**, 305; 311 (*Na-23 nmr, hydroxide, deuteroxide*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3144A (*haz*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4576-4578 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2561-2564
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SHS000; SHS500

Sodium hypochlorite, JAN, USAN S-134

[7681-52-9]

*Sodium chlorate(*I*). Chloric(*I*) acid sodium salt. Hypochlorous acid sodium salt, 8CI*

NaOCl

ClNaO 74.442

Cannot be isolated in anhydrous form. Bleaching agent for starch; also used in washing and lye peeling of fruits and vegetables. Aq. solns. form $NaClO_3$ slowly in air.

► Has formed explosive NCl_3 with aq. $NH_4^{\oplus}$ by contact in drainage system. Explosive products with primary amines, aziridine, acidified benzyl cyanide. Skin and eye irritant. Corrosive to mucous membranes. NH3486300

Dihydrate:

ClH_4NaO_3 110.472

Hygroscopic colourless solid. V. sol. H_2O. Mp 57.5°.

Pentahydrate: [10022-70-5]

$ClH_{10}NaO_6$ 164.518

Orthorhombic cryst. Mp 25.5°.

Kujumzelis, Th.G. *et al., Z. Phys.*, 1938, **39**, 665 (*Raman*)
Feher, F. *et al., Acta Cryst.*, 1962, **15**, 1188 (*cryst struct, pentahydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 152; 1970, **5**, 1740 (*rev, bibl*)
Griffiths, V.S. *et al., J. Mol. Spectrosc.*, 1968, **27**, 358 (*Na-23 nmr*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th Ed., 1974, 123 (*rev, uses*)
Chartier, R.A. *et al., Encycl. Chem. Process. Des.*, 1977, **4**, 430 (*bleaching props*)
Dylewski, R. *et al., Przem. Chem.*, 1978, **57**, 254; *CA*, **89**, 91773 (*synth*)
De Lange, A.M. *et al., Spectrum (Pretoria)*, 1982, **20**, 6; *CA*, **97**, 91150 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3144D (*haz*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 803
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4580-4586 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2564-2565
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 3741
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1142
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SHU500

Sodium magnesium aluminosilicate S-135

[12040-43-6]

A series of synthetic hydrated sodium magnesium aluminosilicates having Na_2O:MgO:Al_2O_3:SiO_2 molar ratios of approximately 2:1:2:24 respectively. Anticaking agent. Amorph. fine powders or beads.

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2579-2580 (*props, use*)

Sodium metaphosphate ($NaPO_3$), 9CI, 8CI S-136

[10361-03-2]

$NaPO_3$

NaO_3P 101.962Monomeric form may be obt. by vaporisation.

► OY3750000

I-form

Maddrell's salt

Two closely related structs. (low temp. form obt. during synth. at 265-275°; high temp. at 300°) consist of chains of corner-sharing phosphate tetrahedra.Insol. H_2O. Poorly sol. AcOH. V. sol. cold dil. H_2SO_4 or HNO_3. Heated at >400° → Trisodium metaphosphate ($P_3O_9^{3\ominus}$).

II-form

Kurrol's salt

Two closely related forms consist of corner sharing phosphate tetrahedra in helical chains, forms A and B differing in relative config. of the tetrahedra in both right-handed and left-handed spirals. In type A, PbO_{term} 147.9 pm, and P $-O_{bridge}$ 161.0 pm.Colourless, fibrous or needle-like cryst. Insol. H_2O, but swells. Forms A and B are interconvertible at 390-420°. Kurrol's salt A at 380-490° yields Maddrell's salt. Kurrol's salt B at 380-630° → Trisodium metaphosphate ($P_3O_9^{3\ominus}$), also obt. from form B at 490-630°. Moisture or pressure converts salt A into salt B.

III-form

Graham's salt

Used in foods as emulsifier, sequestrant and texturiser. V. hygroscopic. Slowly sol. cold H_2O, but much more sol. warm H_2O. Mp 628°.

[35270-09-8, 60620-17-9, 60734-85-2]

Gmelin Handbook Inorg. Chem., Syst. No. 21, 1967, **4**, 1640 (*rev, bibl*)
McAdam, A. *et al., Acta Cryst. B*, 1968, **24**, 1621 (*cryst struct*)
Hisar, R.S. *et al., Bull. Soc. Chim. Fr.*, 1971, 3885 (*synth*)
Mehrotra, R.C. *et al., Indian J. Chem.*, 1972, **10**, 726 (*ir*)
Steblevskii, A.V. *et al., Zh. Neorg. Khim.*, 1974, **19**, 1450; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1974, **19**, 789 (*ms*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 534; 535; 536 (*synth*)
Bowling, R.A. *et al., J. Electron Spectrosc. Relat. Phenom.*, 1979, **17**, 25 (*pe*)
Wagner, C.D. *et al., Anal. Chem.*, 1980, **52**, 1445
Konerding, K. *et al., Chem. Tech. Umsch.*, 1980, **12**, 3; *CA*, **94**, 90005 (*synth, rev, bibl*)
Immirzi, A. *et al., Acta Cryst. B*, 1982, **38**, 2788 (*cryst struct*)
Mustafaev, N.M. *et al., Zh. Neorg. Khim.*, 1983, **28**, 20; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1983, **28**, 11 (*synth*)
Watanabe, M. *et al., J. Mater. Sci.*, 1986, **21**, 2623 (*synth, ir, P-31 nmr*)
Sidorov, L.N. *et al., Zh. Strukt. Khim.*, 1988, **29**, 51; *J. Struct. Chem. (Engl. Transl.)*, 1988, **29**, 866 (*ms*)
Hayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3061 (*P-31 nmr*)
Lebenze, A. *et al., Phys. Rev. B*, 1989, **39**, 11055 (*pe*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2596-2597
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SII500

Sodium methyl sulfate S-137

[512-42-5]

Methyl sulfate sodium salt. Sulfuric acid monomethyl ester sodium salt, 8CI

$MeOSO_3Na$

CH_3NaO_4S 134.088

Secondary direct food additive present in pectin as a result of methylation by H_2SO_4 and MeOH. Hygroscopic. Mp 91-94°. Hydrol. leads to MeOH and $NaHSO_4$.

Monohydrate: [6106-12-3]

Hygroscopic colourless cryst. Sol. H_2O, EtOH.

Ger. Pat., 1954, 907 054; *CA*, 1955, **49**, 3243d (*manuf*)
Kurz, J.L. *et al., J. Phys. Chem.*, 1962, **66**, 2239 (*hydrol*)
Okabayashi, H. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1075 (*Raman*)
U.S.S.R. Pat., 1982, SU 952 802; *CA*, 1983, **98**, 112685 (*uses*)
Koda, S. *et al., J. Solution Chem.*, 1985, **14**, 355 (*Raman, Na-23 nmr*)
Belton, P.S. *et al., J.C.S. Faraday 2*, 1985, **81**, 63 (*S-33 nmr*)
Japan. Pat., 1986, 61 246 145; *CA*, 1987, **106**, 137946 (*esterification*)
Wuensch, G. *et al., Fresenius' Z. Anal. Chem.*, 1989, **334**, 16 (*ir*)
Japan. Pat., 1990, 02 103 298; *CA*, **113**, 61792 (*use, detergent*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2574

Sodium nitrate ($NaNO_3$) S-138

[7631-99-4]

Nitric acid, sodium salt, 8CI. Sodium nitrate. Chile saltpeter. Cubic niter. Chile nitre. E251

$NaNO_3$

$NNaO_3$ 84.995

Isostructural with calcite. Preservative. Added to food as an appearance and colour control agent, flavour/flavour modifier and aerating/foaming agent.. Colourless trigonal (rhombohedral) cryst.; undergoes transition to high temp. rhombohedral polymorph at =278°. Dec. on heating to form $NaNO_2$. V. sol. H_2O (92g per 100 cm^3 at 25°; 180 g per 100 cm^3 at 100°); sol. EtOH, MeOH; prac. insol. Me_2CO. Mp 306°. ΔH_f° -468 kJ mol^{-1}; ΔG_f° -367 kJ mol^{-1}; S° 117 J K^{-1} mol^{-1}.

► Oxidiser; toxic. WC5600000

Mineral-*form*

Sodanitre. *Soda-niter. Nitratine*
White or off-white cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1258D (*ir*)
Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, 1956, **6**, 50 (*cryst struct*)
Vollmar, P.M. *et al., J. Chem. Phys.*, 1963, **39**, 2236 (*uv*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 95; 1966, **3**, 982 (*rev, bibl*)
Nakagawa, I. *et al., J. Chem. Phys.*, 1969, **51**, 1389 (*ir, Raman*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 228 (*rev, uses*)
Fiorucci, L.C. *et al., CA*, 1983, **98**, 163824 (*heat storage*)
Tabeta, R. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3147D (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2576-2577
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SIO900

Sodium nitrite, USAN S-139

[7632-00-0]
Nitrous acid, sodium salt, 8CI. Erinitrit. E250

$NaNO_2$

$NNaO_2$ 68.995

Colour fixative and preservative for fish and meat products. Pale yellow hygroscopic orthorhombic cryst. V. sol. H_2O (82 g per 100 cm^3 at 15°; 163 g per 100 cm^3 at 100°); mod. sol. MeOH (4.4 g per 100 cm^3 at 20°); spar. sol. Et_2O (0.3 g per 100 cm^3 at 20°). Mp 271°. ΔH_f° -359 kJ mol^{-1}; ΔG_f° -285 kJ mol^{-1}; S° 104 J K^{-1} mol^{-1}. Ferroelectric below 158°; undergoes transition to high temp. orthorhombic polymorph at 158°. Dec. on heating at 320° → NO, O_2 and Na_2O.

▶ Causes dose-related methaemoglobinaemia. Vasodilator. Fatal human dose *ca*. 33-250 mg/kg. Mutagenic props. Forms explosive prods. when heated with cyanide salts and complexes. Violent reactions reported with KCNS, phthalic acid, sodium disulfite and other substances. RA1225000

[82010-95-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1295D (*ir*)
Ziegler, G.E. *et al., Phys. Rev.*, 1931, **38**, 1040 (*cryst struct*)
Tramer, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1959, **248**, 3546 (*Raman*)
Kay, W.B. *et al., Acta Cryst.*, 1961, **14**, 56 (*ferroelectric, props*)
Ketelaar, J.A.A. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1961, **80**, 721 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1966, **3**, 960 (*rev, bibl*)
Plekhotkun, V.F. *et al., Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1843
Smyth, H.F. *et al., Am. Ind. Hyg. Assoc. J.*, 1969, **30**, 470 (*tox*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 240 (*rev, uses*)
Choh, S.H. *et al., Ferroelectrics*, 1981, **36**, 297 (*Na-23 nmr*)
Agarwala, V.S. *et al., Mater. Perform.*, 1985, **24**, 9 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3148A (*haz*)
Walker, R. *et al., Food Addit. Contam.*, 1990, **7**, 717 (*occur, tox*)
Antidotes for Poisoning by Cyanide, (Eds. Meredith, T.J. *et al*), Cambridge University Press, 1993, 105 (*use*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 695
Meah, M.N. *et al., Food Addit. Contam.*, 1994, **11**, 519 (*dietary occur*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4604-4609 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2577-2578
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 4392
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1145
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SIQ500

Sodium phosphate ($Na(H_2PO_4)$) S-140

[7558-80-7]
Monosodium phosphate, 9CI, 8CI. Sodium dihydrogen phosphate. Sodium phosphate monobasic, USAN

$Na(H_2PO_4)$

H_2NaO_4P 119.977

Monoclinic unit cell. $Na^\oplus$ ions present in distorted coordination octahedra forming double layers and sharing edges with PO_4 tetrahedra. P–O 154.0 pm OPO 104.0-118.5°. Used in foods as a dry acidulant, buffering agent, emulsifier, leavening agent, protein modifier, sequestrant and nutrient supplement. Colourless monoclinic cryst. V. sol. H_2O (95 g per 100 cm^3 at 25°; 196 g per 100 cm^3 at 70°). Loses structural H_2O at 200-240° → $Na_2H_2P_2O_7$.

▶ Eye irritant (hmn data). LD_{50} (rat, orl) 8290 mg/kg. WA1900000

Monohydrate: [10049-21-5]
H_4NaO_5P 137.992
Colourless prisms (H_2O), stable at r.t. V. sol. H_2O; sl. sol. Et_2O. Exists in two forms, the normal one being orthorhombic, and in which chains of Na coordination octahedra share edges developing channels occupied by PO_4 tetrahedra. Whole system H-bonded. P–O 155.2 pm. Dehydrates at 67-130°.

Dihydrate: [13472-35-0]
H_6NaO_6P 156.007
Colourless cryst. of variable form (H_2O) which lose H_2O at r.t. in dry air → monohydrate. Orthorhombic unit cell. PO_4 tetrahedra are linked by H-bonds to a distorted diamond-shaped framework of pseudo-hexagonal channels, the layer accommodating a chain of Na coordination octahedra. P–O 155.1 pm. P–O(H) 114.6, 119.2 pm.

Tetrahydrate: Claimed to be stable at -20°.

[7632-05-5, 10028-24-7]

Morey, G.W. *et al., J.A.C.S.*, 1953, **75**, 5794 (*thermal dec*)
Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 342; 1967, **4**, 1600 (*rev, bibl*)
Steger, E. *et al., Z. Anorg. Allg. Chem.*, 1964, **331**, 169 (*ir, Raman*)
Rommel, M.A. *et al., Talanta*, 1967, **14**, 1205 (*chromatog*)
Catti, M. *et al., Acta Cryst. B*, 1974, **30**, 1; 1976, **32**, 359 (*cryst struct*)
Fluck, E. *et al., Pure Appl. Chem.*, 1975, **44**, 373 (*pe*)
Bartl, H. *et al., Acta Cryst. B*, 1976, **32**, 987 (*cryst struct*)
Toupry-Krauzman, N. *et al., J. Raman Spectrosc.*, 1979, **8**, 115 (*ir, Raman, struct*)
Pacey, R.A. *et al., Thermochim. Acta*, 1979, **30**, 115 (*props*)
Gerothanassis, I.P. *et al., J. Magn. Reson.*, 1982, **46**, 423 (*O-17 nmr*)
Tabeta, R. *et al., Chem. Lett.*, 1984, 293 (*Na-23 nmr*)
Bohatý, L. *et al., Z. Kristallogr.*, 1984, **167**, 303 (*props*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Griffiths, L. *et al., J.C.S. Dalton*, 1986, 2247 (*P-31 nmr*)
Cerreta, M.K. *et al., J. Cryst. Growth*, 1987, **84**, 577 (*synth, Raman*)
Choi, B.K. *et al., J. Raman Spectrosc.*, 1989, **20**, 11 (*Raman*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 457-458
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1181
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2589-2593
Ichikawa, M. *et al., Acta Cryst. B*, 1998, **54**, 29-34 (*cryst struct, electron density*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJH100

Sodium phosphate (Na_3PO_4) S-141

[7601-54-9]
Trisodium phosphate, 9CI, 8CI. Sodium orthophosphate

Na_3PO_4

Na_3O_4P 163.94

Forms several double salts with cavity-type structs.. Nutrient supplement, pH control agent, sequestrant, stabiliser, protein modifier, emulsifier in production of processed cheeses, indirect food additive arising from use as a boiler water additive. Colourless cryst. Sol. H_2O (14.5 g per 100 cm^3 at 25°; 95 g per 100 cm^3 at 100°). Mp 1583°. Aq. solns. are alkaline. ΔH_f° -1917 kJ mol^{-1}; ΔG_f° -1789 kJ mol^{-1}; S° 174 J K^{-1} mol^{-1}.

▶ TC9490000

Hemihydrate: [60593-58-0]
Stout prisms, cryst. from aq. soln. at Bp. Mp 180°. Monoclinic lattice, possessing 3-D network of distorted NaO_6 octahedra and PO_4 tetrahedra.

Monohydrate: [27176-08-5] Of doubtful existence.

Hexahydrate: [15819-50-8]
Cryst. (H_2O at >86°). Mp 110°.

Octahydrate: [60593-59-1]
Mp 86°. Triclinic lattice. Na ions are hexacoord. PO_4 tetrahedra have OPO 108.2-110.2°, P–O 153.3-154.4 pm.

Dodecahydrate: [10101-89-0]
Colourless cryst. V. sol. H_2O (157 g per 100 cm^3 at 70°). Mp 73.3-76.7° (dec.).

Readily loses $4H_2O$ at 15°, and further $2H_2O$ at 26°, and yields a hemihydrate at 36-37°. The pseudo-dodecahydrate contains structural NaOH and is better represented as $4Na_3PO_4.48H_2O.NaOH$, and loses $4H_2O$ at 26°. ΔH_f° -5477 kJ mol^{-1}. Several further hydrates have been claimed.

►TC9575000

α-form

Low temp. form

Tetragonal lattice.Undergoes reversible phase transition to γ-form at 325°.

β-form Said to be formed, always admixed with α or γ form in their reversible interconversion.

γ-form

High temp.-form

Orthorhombic (pseudocubic) lattice. Possesses fcc struct. with PO_4 groups oriented in two ways.Stabilised at r.t. by traces of Silicoaluminophosphate molecular sieves. A good $Na^{\oplus}$ ion conductor.

[10361-89-4, 15819-50-8]

Clark, G.L. *et al., Z. Kristallogr.*, 1937, **98**, 107 (*cryst struct, dodecahydrate*)
Bell, R.N. *et al., Ind. Eng. Chem.*, 1949, **41**, 2901 (*synth*)
Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 349; 1967, **4**, 1568
Palazzi, M. *et al., Bull. Soc. Chim. Fr.*, 1971, 2795
Morgan, W.E. *et al., J.A.C.S.*, 1973, **95**, 751 (*pe*)
Kizilyalli, M. *et al., J. Inorg. Nucl. Chem.*, 1976, **38**, 1237 (*synth, cryst struct*)
Newsan, J.M. *et al., Solid State Ionics*, 1980, **1**, 377 (*nd, struct*)
Wiench, D.M. *et al., Z. Anorg. Allg. Chem.*, 1980, **461**, 101 (*synth, cryst struct*)
Mazalov, L.N. *et al., Zh. Strukt. Khim.*, 1981, **22**, 18; *J. Struct. Chem. (Engl. Transl.)*, 1981, **22**, 12 (*pe*)
Gerothanassis, I.P. *et al., J. Magn. Reson.*, 1982, **46**, 423 (*O-17 nmr*)
Larbot, A. *et al., Acta Cryst. C*, 1983, **39**, 12 (*cryst struct*)
Averbuch-Pouchot, M.T. *et al., J. Solid State Chem.*, 1983, **46**, 193 (*synth, cryst struct, hemihydrate*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Griffiths, L. *et al., J.C.S. Dalton*, 1986, 2247 (*P-31 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2593-2595
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJH200

Sodium phosphinate, 9CI, 8CI S-142

[7681-53-0]

Sodium hypophosphite

$NaOP(O)H_2$

H_2NaO_2P 87.978

Emulsifier or stabilizer used in foods, e.g. cod-liver oil emulsions. V. sol. H_2O (52 g per 100 cm^3).

►WB5950000

Monohydrate: [10039-56-2]
H_4NaO_3P 105.993
V. hygroscopic colourless cryst. V. sol. H_2O (100 g per 100 cm^3 at 25°, 667 g per 100 cm^3 at 100°), EtOH. Begins to dec. at 310° → PH_3 + H_2O + Sodium phosphonate ($Na_2(HPO_3)$), Sodium metaphosphate ($NaPO_3$), S-136, and Sodium diphosphate ($Na_4(P_2O_7)$), S-126.

►Violent dec. on heating. SZ5640000

Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Ziomek, J.S. *et al., J. Mol. Spectrosc.*, 1962, **8**, 42
Strezhnev, I.V. *et al., Zh. Prikl. Khim. (Leningrad)*, 1963, **36**, 1873 (*synth*)
Zobel, D. *et al., Chem. Tech. (Leipzig)*, 1967, **19**, 762; 1982, **34**, 192; 1990, **42**, 47 (*rev, manuf, props, bibl*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1967, **4**, 1542 (*rev, bibl*)
Morgunova, É.M. *et al., Zh. Prikl. Khim. (Leningrad)*, 1967, **40**, 1660; 1970, **43**, 24; *J. Appl. Chem. USSR (Engl. Transl.)*, 1967, **40**, 1602; 1970, **43**, 21 (*synth*)
Griffiths, V.S. *et al., J. Mol. Spectrosc.*, 1968, **27**, 358 (*Na-23 nmr*)
Takahashi, Y. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 4
Zhagrov, A.S. *et al., Zh. Fiz. Khim.*, 1974, **48**, 504 (*pmr*)
Niderprum, H. *et al., Angew. Chem., Int. Ed.*, 1975, **14**, 814
Fluck, E. *et al., Pure Appl. Chem.*, 1975, **44**, 373 (*pe*)
Boyer, S.K. *et al., J.O.C.*, 1985, **50**, 3408 (*use*)
Monti, D. *et al., Synth. Commun.*, 1986, **16**, 803 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2565-2566
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1197
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SHV000

Sodium silicate (Na_2SiO_3) S-143

[6834-92-0]

Sodium metasilicate (Na_2SiO_3). Waterglass

Na_2SiO_3

Na_2O_3Si 122.063

A synthetic single-chain silicate (2 SiO_4 tetrahedra per chain). Used in food processing as a boiler water additive, in washing and lye peeling of fruits, vegetables and nuts; denuding agent for tripe; hog scald agent for removing hair, corrosion preventative in canned and bottled water. Potential food migration residue from paper/board or cotton fabric packaging. Usually a glass, also cryst. Sol. H_2O; insol. EtOH. Mp 1089°. The composition of the commonly available solid sodium silicates correspond to Na_2SiO_3, $Na_6Si_2O_7$ and Sodium silicate ($Na_2Si_3O_7$) as various hydrates.

►A skin irritant. VV9275000

Pentahydrate: [10213-79-3]
$H_{10}Na_2O_8Si$ 212.139
Cryst.

Octahydrate: [27121-04-6]

Nonahydrate: [13517-24-3]
Efflorescent platelets (2-3% aq. NaOH). V. sol. H_2O. Mp 48°.

[1344-09-8, 15859-24-2]

Schwarz, R. *et al., Ber.*, 1924, **57**, 1477 (*synth*)
Miller, F.A. *et al., Spectrochim. Acta*, 1960, **16**, 135 (*ir*)
Jamieson, P.B. *et al., Acta Cryst.*, 1966, **20**, 373; 688 (*cryst struct, hydrates*)
McDonald, W.S. *et al., Acta Cryst.*, 1967, **22**, 37 (*cryst struct*)
Doremieux-Morin, C. *et al., Bull. Soc. Chim. Fr.*, 1973, 418 (*pmr, hydration*)
Rao, C.S. *et al., Indian J. Chem.*, 1977, **12**, 18 (*synth*)
Harris, R.K. *et al., J.C.S. Faraday 2*, 1977, **73**, 1204 (*Si-29 nmr*)
Waseda, Y. *et al., Trans. Iron Steel Inst. Jpn.*, 1977, **17**, 601 (*cryst struct*)
Krol, D.M. *et al., J. Phys., Colloq.*, *C*, 1982, **9**, 347 (*Raman*)
Magi, M. *et al., J. Phys. Chem.*, 1984, **88**, 1518 (*Si-29 nmr*)
Stebbins, J.F. *et al., Nature (London)*, 1985, **315**, 250 (*Si-29 nmr*)
Merck Index, 12th edn., 1996, No. 8788; No. 8824 (*props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2572-2573; 2606-2607 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJU000

Sodium sulfate, USAN S-144

[7757-82-6]

Disodium sulfate. Sulfuric acid disodium salt, 8CI. Salt cake. Sodium sulfoxylate. E514

Na_2SO_4

Na_2O_4S 142.043

Acidity regulator. Colourless orthorhombic cryst. Undergoes a transition between two orthorhombic polymorphs at 185° and an orthorhombic to hexagonal transition at 241°. A metastable orthorhombic polymorph is formed on cooling the hexagonal polymorph under anhydrous conditions. A fifth polymorph may exist above 713°. Mod. sol. H_2O (4.8 g per 100 cm^3 at 0°; 43 g per 100 cm^3 at 100°). Mp 884°. ΔH_f° -1387.8 kJ mol^{-1}; ΔG_f° -1269.8 kJ mol^{-1}; S° 149.6 J K^{-1} mol^{-1}. The name E514 is also used for Sodium hydrogen sulfate, S-131.

►WE1650000

Mineral-*form* [13759-07-4]

Thenardite

Colourless to grey or yellow translucent cryst.

Heptahydrate: [13472-39-4]
$H_{14}Na_2O_{11}S$ 268.149
White orthorhombic cryst.; dec. on heating by H_2O loss. V. sol. H_2O (20 g per 100 cm^3 at 0°; 44 g per 100 cm^3 at 20°); insol. EtOH.

Decahydrate: Sodium sulfate decahydrate, S-145

Peroxohydrate, hydrate: [29761-94-2] *Sodium sulfate peroxohydrate hydrate*

[14262-80-7, 29381-14-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1261A (*ir*)
Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301; 424 (*Raman*)
Swanson, H.E. *et al., Natl. Bur. Stand. Circ. (U.S.)*, 1953, **2**, 59 (*cryst struct*)
Schumb, W.C. *et al., Hydrogen Peroxide*, Reinhold, 1955, **26**, 641 (*rev*)
Steger, E. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1964, **68**, 102 (*ir*)

Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 213; 1966, **3**, 1091; 1117 (*rev, bibl*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th. Ed., 1974, 123 (*rev, uses*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 205; 245 (*rev, uses*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1587 (*thermochem data, polymorphs*)
Belton, P.S. *et al., Magn. Reson. Chem.*, 1986, **24**, 171 (*S-33 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3154B (*haz*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 904; 1164
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJY000

Sodium sulfate decahydrate S-145

[7727-73-3]
Glauber's salt

$Na_2SO_4.10H_2O$

$H_{20}Na_2O_{14}S$ 322.195

Added to food as a flavour or flavour-modifier, pH control agent or clarifying/flocculating agent. Colourless monoclinic cryst., efflorescent. Dec. on heating with H_2O loss (-$10H_2O$ at 100°) to form Na_2SO_4. V. sol. H_2O (11 g per 100 cm^3 at 0°; 93 g per 100 cm^3 at 30°); insol. EtOH. ΔH_f° -4324 kJ mol^{-1}; ΔG_f° -3644 kJ mol^{-1}; S° 593 JK^{-1} mol^{-1}.

► Irritant. WS8402000

Mineral-*form* [14567-58-9]
Mirabilite
White cryst.

Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301; 424 (*Raman*)
Ruben, H.W. *et al., J.A.C.S.*, 1961, **83**, 820 (*cryst struct*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1966, **3**, 1113 (*rev, bibl*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th. Ed., 1974, 123 (*rev, uses*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 205 (*rev, uses*)
Kimura, H. *et al., Ind. Eng. Chem. Fundam.*, 1985, **24**, 192; *CA*, **102**, 175305 (*ir*)
Tabeta, R. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957 (*Na-23 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3154C (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2611-2612

Sodium sulfide (Na_2S), 8CI S-146

[1313-82-2]
Disodium sulfide. Sodium monosulfide. Sodium sulfuret

Na_2S

Na_2S 78.045

Antifluorite struct.. Reaction control agent in the manuf. of chewing gum. White cubic cryst., deliquescent. V. sol. H_2O (15 g per 100 cm^3 at 10°; 57 g per 100 cm^3 at 90°), spar. sol. EtOH; insol. Et_2O. Mp 1172°. ΔH_f° -366 kJ mol^{-1}; ΔG_f° -355 kJ mol^{-1}; S° 96 JK^{-1} mol^{-1}.

► Reacts with acids to release H_2S. WE1905000

Pentahydrate: [1313-83-3]
$H_{10}Na_2O_5S$ 168.121

Nonahydrate: [1313-84-4]
$H_{18}Na_2O_9S$ 240.182
Colourless tetragonal deliquescent cryst. (H_2O). Dec. on heating with H_2O loss. V. sol. H_2O (48 g per 100 cm^3 at 10°; 97 g per 100 cm^3 at 100°), spar. sol. EtOH. ΔH_f° -3082 kJ mol^{-1}.

► Flammable, corrosive. WE1925000

[27610-45-3]

Ley, H. *et al., Z. Phys. Chem., Abt. B*, 1932, **15**, 311 (*uv*)
Zintl, E. *et al., Z. Elektrochem.*, 1934, **40**, 588 (*cryst struct*)
Jardetzky, O. *et al., J.A.C.S.*, 1960, **82**, 318 (*Na-23 nmr*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 185; 1966, **3**, 1049; 1052 (*rev, bibl*)
Bedlivy, D. *et al., Z. Kristallogr.*, 1965, **121**, 114 (*cryst struct, nonahydrate*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th. Ed., 1974, 123 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 256 (*rev, uses*)
Mereitner, K. *et al., J.C.S. Dalton*, 1984, 1275 (*pentahydrate, cryst struct, ir, Raman*)
Chase, M.W. *et al., J. Phys. Chem. Ref. Data*, 1985, **14**, 1595 (*thermochem data*)
Eckret, H. *et al., J.A.C.S.*, 1986, **108**, 2140 (*S-33 nmr*)
Malghan, S.G. *et al., Miner. Metall. Process.*, 1986, **3**, 158 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3154D (*nonahydrate, haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2612
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJY500

Sodium sulfite (Na_2SO_3) S-147

[7757-83-7]

[10102-15-5, 10579-83-6]
Sulfurous acid disodium salt, 8CI. Disodium sulfite. Sodium sulfite. E221

Na_2SO_3

Na_2O_3S 126.044

Used as a sanitising agent for food containers and fermentation equipment, as a preservative to reduce or prevent microbial spoilage of food, as a selective inhibitor of undesirable microorganisms in the fermentation industries, and as an antioxidant and inhibitor of enzyme-catalysed oxidative discoloration and non-enzymic browning during prepn., storage and distribution of foods. Moisture-sensitive white hexagonal cryst. V. sol. H_2O (13 g per 100 cm^3 at 0°; 28 g per 100 cm^3 at 80°); spar. sol. EtOH. ΔH_f -1090 kJ mol^{-1}; ΔG_f° -1002 kJ mol^{-1}; S° 146 JK^{-1} mol^{-1}.

► Irritant. WE2150000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1296A (*ir*)
Zachariasen, W.H. *et al., Phys. Rev.*, 1931, **37**, 1295 (*cryst struct*)
Inorg. Synth., 1946, **2**, 162 (*synth*)
Seibert, H. *et al., Z. Anorg. Allg. Chem.*, 1954, **275**, 225 (*Raman*)
Evans, J.C. *et al., Can. J. Chem.*, 1955, **33**, 1270 (*ir, Raman*)
Newman, G. *et al., Spectrochim. Acta*, 1963, **19**, 213 (*ir*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 205; 1966, **3**, 1079 (*rev, bibl*)
U.S. Pat., 1983, 4 383 027; *CA*, **99**, 222319 (*uses*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3155A (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2612-2613
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJZ000

Sodium thiosulfate, JAN, USAN S-148

[7772-98-7]
Sodothiol. Thiosulfuric acid disodium salt, 8CI. Sulfothiorine. Antichlor. Ametox. Sulfactol. NSC 45624

$Na_2S_2O_3$

$Na_2O_3S_2$ 158.11

Formulation aid and reducing agent used in alcoholic beverages and table salt. Deliquescent, colourless, monoclinic cryst. Dec. on heating with ultimate formation of Na_2SO_4. V. sol. H_2O (231 g per 100 cm^3 at 100°); insol. EtOH. ΔH_f° -1123 kJ mol^{-1}; ΔG_f° -1028 kJ mol^{-1}; S° 155 JK^{-1} mol^{-1}. Component of Komed and Tinver.

► XN6476000

Pentahydrate: [10102-17-7] *Hypo. Sodium hyposulfite*
$H_{10}Na_2O_8S_2$ 248.186
Colourless monoclinic cryst., efflorescent. Dec. on heating by H_2O loss (-$5H_2O$ at 100°). V. sol. H_2O (79 g per 100 cm^3 at 0°; 291 g per 100 cm^3 at 45°); insol. EtOH. Mp 50°. ΔH_f° -2608 kJ mol^{-1}; ΔG_f° -2230 kJ mol^{-1}; S° 372 JK^{-1} mol^{-1}.

► Low acute human toxicity. LD_{50} (mus, ipr) 5600 mg/kg. LD_{50} (mus, ivn) 2350 mg/kg. WE6660000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1266B (*ir*)
Voegtlin, C. *et al., J. Pharmacol. Exp. Ther.*, 1925, **25**, 297 (*tox*)
Deines, U. *et al., Z. Anorg. Allg. Chem.*, 1934, **220**, 337 (*synth, pentahydrate*)
Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301 (*pentahydrate, Raman*)
Taylor, P.G. *et al., Acta Cryst.*, 1952, **5**, 341 (*pentahydrate, cryst struct*)
Seibert, H. *et al., Z. Anorg. Allg. Chem.*, 1954, **275**, 225 (*Raman*)
Duval, C. *et al., Anal. Chim. Acta*, 1957, **16**, 221 (*ir, pentahydrate*)
Sandor, E. *et al., Acta Cryst.*, 1961, **14**, 237 (*cryst struct*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 21, 1964, **1**, 247; 1966, **3**, 1162 (*rev, bibl*)
Cleghorn, H.P. *et al., J.C.S.(A)*, 1970, 137 (*thermal dec, pentahydrate*)
Clough, R.W. *et al., Handb. Ind. Chem.*, 7th Ed., 1974, 123 (*rev, uses*)
Lowenheim, F.A. *et al., Industrial Chemicals*, (Eds.), 4th Ed., Wiley-Interscience, N.Y., 1975, 769 (*synth*)
Uraz, A.A. *et al., Acta Cryst. B*, 1977, **33**, 1396 (*cryst struct*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3157C; 3157D (*haz*)
Goel, R. *et al., J. Natl. Cancer Inst.*, 1989, **81**, 1552
Baskin, S.I. *et al., J. Clin. Pharmacol.*, 1992, **32**, 368 (*use*)
Meredith, T.J. *et al., Antidotes for Poisoning by Cyanide*, Cambridge University Press, 1993, 43 (*use*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 696
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2615-2616
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKI000; SKI500

Sodium triphosphate ($Na_5(P_3O_{10})$) S-149

[7758-29-4]

[13573-18-7]

Pentasodium triphosphate, 9CI, 8CI. Sodium tripolyphosphate

$Na_5(P_3O_{10})$

$Na_5O_{10}P_3$ 367.864

The penta sodium salt of Triphosphoric acid. In addition to the common hexahydrate and the claimed octahydrate, mono-, tetra-, and pentahydrates have also been claimed. Employed in the food industry as a moisture control agent, sequestrant, texturiser, thickener, emulsifier, stabiliser, antioxidant and pH control agent. Solid. V. sol. H_2O (15 g per 100 cm^3 at 25°; 33 g per 100 cm^3 at 100°). Mp 622° (incongr.). Stabilises H_2O_2.

► YK4570000

Hexahydrate: [15091-98-2]
Colourless plate-like cryst. V. sol. H_2O (27 g per 100 cm^3 at 25°). Triclinic unit cell with P–O(P) 166, 162 pm, $P_{1,3}$–O 145-149 (terminal), P_2–O 152 pm. Dec. without melting at *ca.* 120°, but at 320° regenerates the anhydrous salt. Hydrol. spontaneously on long standing.

Octahydrate: In air readily forms the hexahydrate.

Pentahydrate, mono-H_2O_2 complex:
White powder. Dec. at 125° losing all H_2O_2 and most H_2O.

Hydrate, tetra-H_2O_2 complex:
Visc. white mass which slowly cryst. over P_4O_{10}. Loses H_2O at 80-100° before dec..

Hydrate, hexa-H_2O_2 complex:
Visc. white mass which slowly cryst. over P_4O_{10}. Loses H_2O at 80-100°, before dec..

Phase I-*form*
Monoclinic unit cell with P–O 148, 162, 166 pm. Some $Na^{\oplus}$ ions are coordinated in distorted octahedra, but others are in unusual 4-coordination.With H_2O, cakes and then dissolves slowly. Transforms into phase II at *ca.* 420° depending on physical state. In absence of moisture indefinitely stable at r.t..

Phase II-*form*
Monoclinic unit cell. $Na^{\oplus}$ ions coordinated by oxygens in distorted octahedra with P–O 150, 161, 168 pm.Sol. H_2O. Cryst. at $< 470°$. Converts into Phase I at *ca.* 420° in sealed tube only if H_2O present. In absence of moisture indefinitely stable at r.t..

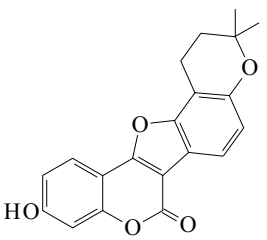
[14127-68-5, 34275-69-9, 35138-68-2, 90906-71-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1268B (*ir*)
Inorg. Synth., 1950, **3**, 101 (*synth*)
Bues, W. *et al., Z. Anorg. Allg. Chem.*, 1956, **288**, 291 (*ir, Raman*)
Davies, D.R. *et al., Acta Cryst.*, 1958, **11**, 315 (*cryst struct, phase II*)
Corbridge, D.E.C. *et al., Acta Cryst.*, 1960, **13**, 263 (*cryst struct, phase I*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1964, **1**, 362; 1967, **4**, 1629 (*rev, bibl*)
U.K. Pat., 1969, 1 161 693; *CA*, **71**, 114777 (*manuf*)
Ionova, L.A. *et al., Zh. Prikl. Khim. (Leningrad)*, 1969, **42**, 1894; *J. Appl. Chem. USSR (Engl. Transl.)*, 1969, **42**, 1782 (*props*)
Pelavin, M. *et al., J. Phys. Chem.*, 1970, **74**, 1116 (*pe*)
Bus, J. *et al., Anal. Chem.*, 1974, **46**, 1824 (*Raman, props*)
Gingerich, K.A. *et al., J. Chem. Phys.*, 1975, **63**, 1211 (*ms*)
Sojka, S.A. *et al., Anal. Chem.*, 1978, **50**, 585 (*P-31 nmr, anal*)
Wiench, D.M. *et al., Z. Anorg. Allg. Chem.*, 1982, **488**, 80 (*cryst struct*)
Sotnikova-Yuzhik, V.A. *et al., Izv. Akad. Nauk SSSR, Neorg. Mater.*, 1984, **20**, 632; *Inorg. Mater. (Engl. Transl.)*, 1984, **20**, 547 (*props, reactions, struct*)
Griffiths, L. *et al., J.C.S. Dalton*, 1986, 2247 (*P-31 nmr*)
Haubenreisser, U. *et al., Z. Anorg. Allg. Chem.*, 1986, **532**, 157 (*P-31 nmr, polymorphs*)
Ivashkevich, I.S. *et al., Zh. Prikl. Spektrosk.*, 1988, **48**, 262; *J. Appl. Spectrosc. (Engl. Transl.)*, 1988, **48**, 180 (*ir*)
Hayashi, S. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 3061 (*P-31 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2616-2617

Sojagol S-150

[18979-00-5]

2,3-Dihydro-10-hydroxy-3,3-dimethyl-1H,7H-furo[2,3-c:5,4-f']bis[1]benzopyran-7-one, 9CI. Soyagol



$C_{20}H_{16}O_5$ 336.343
Isol. from soya (leaves and hypocotyls) and from mung beans (*Phaseolus aureus*). Needles by subl. Mp 284-286°.

Zilg, H. *et al., Phytochemistry*, 1968, **7**, 1765 (*isol, ir, ms, struct*)
Keen, N.T. *et al., Phytochemistry*, 1972, **11**, 1031 (*isol, uv*)

Solacaproine S-151

[35771-90-5]

N,N-Bis[4-(dimethylamino)butyl]hexanamide, 9CI

$H_3C(CH_2)_4CON(CH_2CH_2CH_2CH_2NMe_2)_2$

$C_{18}H_{39}N_3O$ 313.526
Alkaloid from the roots of *Cyphomandra betacea* (tree tomato). Gum.

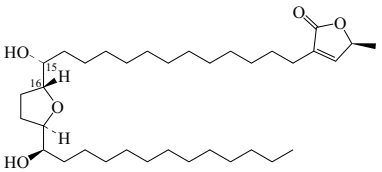
Dipicrate:
Fine needles (EtOH). Mp 149-150°.

Evans, W.C. *et al., J.C.S. Perkin 1*, 1972, 2017 (*isol, ir, ms, synth, struct*)

Solamin S-152

[138682-32-3]

3-[13-Hydroxy-13-[tetrahydro-5-(1-hydroxytridecyl)-2-furanyl]tridecyl]-5-methyl-2(5H)-furanone, 9CI. 4-Desoxyhowiicin



$C_{35}H_{64}O_5$ 564.888
Constit. of *Annona glabra* (pond apple), *Annona muricata* (soursop) and *Annona reticulata* (custard apple). Needles (hexane). Mp 76-77° (64-68°). $[\alpha]_D$ +22 (c, 0.2 in MeOH). λ_{max} 216 (ϵ 3550) (MeOH) (Berdy). λ_{max} 220 (ϵ 3640) (EtOH) (Berdy).

19,20-Diepimer: [158705-59-0] **cis-*Solamin***
$C_{35}H_{64}O_5$ 564.888
Constit. of the roots of *Annona muricata* (soursop). Powder. Mp 63-66°. $[\alpha]_D$ +22 (c, 0.5 in MeOH). λ_{max} 217 (log ϵ 3.61) (MeOH).

15-Hexadecanoyl: [213313-60-1] *15-Hexadecanoylsolamin.* ***15-Palmitoylsolamin***
$C_{51}H_{94}O_6$ 803.3
Constit. of *Annona muricata* (soursop).

15-(9Z-Octadecenoyl): [213313-62-3] *15-(9-Octadecenoyl)solamin.* ***15-Oleoylsolamin***
$C_{53}H_{96}O_6$ 829.338
Constit. of *Annona muricata* (soursop).

Myint, S.H. *et al., Phytochemistry*, 1991, **30**, 3335 (*isol, struct, ir, pmr, ms*)
Sinha, S.C. *et al., J.A.C.S.*, 1993, **115**, 4891 (*synth*)
Hisham, A. *et al., Tetrahedron*, 1993, **49**, 6913 (*isol, struct*)
Trost, B.M. *et al., J.A.C.S.*, 1994, **116**, 7459 (*synth*)
Makabe, H. *et al., J.C.S. Perkin 1*, 1994, 1975 (*synth*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)
Gleye, C. *et al., J. Nat. Prod.*, 1998, **61**, 576-579 (*cis-Solamin*)
Gleye, C. *et al., Rapid Commun. Mass Spectrom.*, 1998, **12**, 1051-1056 (*Palmitoylsolamin, Oleoylsolamin*)
Kuriyama, W. *et al., Heterocycles*, 1999, **50**, 981-988 (*synth*)
Makabe, H. *et al., Org. Lett.*, 2002, **4**, 1083-1085 (*cis-Solamin, synth, abs config*)

Solamine S-153

[17232-87-0]

N'-[4-(Dimethylamino)butyl]-N,N-dimethyl-1,4-butanediamine, 9CI. 4,4'-Bis(dimethylamino)dibutylamine, 8CI

$Me_2N(CH_2)_4NH(CH_2)_4NMe_2$

$C_{12}H_{29}N_3$ 215.381
Constit. of the roots of *Cyphomandra betacea* (tree tomato). Bp_{10} 80-90° (bath).

Hydrochloride (1:3):
Small prisms (EtOH/Et_2O). Mp 262° dec.

Tripicrate:
Shining plates (EtOH aq.). Mp 113-114°.

N-*Ac:*
Oil.

N-*Ac; methiodide (1:2):*

Needles. Mp 241-243°.

N-*Hexanoyl:* Solacaproine, S-151

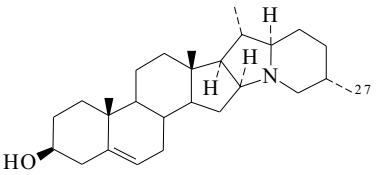
N-*Heptanoyl:***N-*Heptanoylsolamine***
$C_{19}H_{41}N_3O$ 327.552
Tentatively identified as a constit. of *Cyphomandra betacea* (tree tomato).

N-*Hexadecanoyl:* See Solapalmitine in *The Combined Chemical Dictionary.*

Kupchan, S.M. *et al., J.O.C.*, 1969, **34**, 3888 (*synth, ir, pmr, ms*)
Evans, W.C. *et al., J.C.S. Perkin 1*, 1972, 2017 (*isol, ir, pmr*)
Evans, W.C. *et al., Phytochemistry*, 1977, **16**, 1859 (*isol*)

Solanidine S-154

[80-78-4]
Solanid-5-en-3β-ol, 9CI. Solatubine. Solanidine T



$C_{27}H_{43}NO$ 397.643
Alkaloid from potato (*Solanum tuberosum*). Glycosides, (esp. Solanines and chaconine) are trace toxic constits. of potato tubers (esp. greened tubers), and interbreeding of potatoes with wild strains may increase their concn. or introduce other more toxic, solanidine glycosides. Mp 219°. $[\alpha]_D$ -27 ($CHCl_3$) (Py).

▶ WF0500000

Hydrochloride:
Mp 335° dec.

O-*Ac:*
Mp 208°.

O-*β-D-Galactopyranoside:* [511-37-5] ***γ-Solanine***
$C_{33}H_{53}NO_6$ 559.785
Alkaloid from potato spp. (*Solanum tuberosum* and *Solanum chacoense*). Mp *ca.*° 250. $[\alpha]_D$ -26 (MeOH). Log P 4.15 (uncertain value) (calc).

O-*β-D-Glucopyranoside:* [511-36-4] ***γ-Chaconine***
$C_{33}H_{53}NO_6$ 559.785
Alkaloid from potato spp. *Solanum tuberosum* and *Solanum chacoense* (Solanaceae). Mp 243-244°. $[\alpha]_D$ -40 (Py).

O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]:* [61877-94-9] ***β-Solanine***
$C_{39}H_{63}NO_{11}$ 721.927
Alkaloid from potato spp. (*Solanum tuberosum* and *Solanum chacoense*, Solanaceae). Mp 290°. $[\alpha]_D$ -31 (MeOH).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [80248-81-3] ***Stenantidine***
$C_{39}H_{63}NO_{11}$ 721.927
Mp 269-271°. $[\alpha]_D$ -47.5.

O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [472-51-5] ***β$_1$-Chaconine***
$C_{39}H_{63}NO_{10}$ 705.927
Alkaloid from potato spp. (*Solanum chacoense, Solanum commersonii, Solanum crispum, Solanum tuberosum, Solanum ajanhuiri* and *Solanum stenotomum*, Solanaceae). Mp 287-292° dec. $[\alpha]_D$ -52.5 (c, 0.9 in Py).

O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [80248-79-9] ***Stenantine***
$C_{45}H_{73}NO_{15}$ 868.069
Mp 262-264°. $[\alpha]_D$ +46.5. Partial hydrol → β_2 and γ-Chaconines.

O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside]:* [81942-09-8]
$C_{45}H_{73}NO_{15}$ 868.069
Needles + $2H_2O$ (MeOH). Mp 278-283° dec. $[\alpha]_D$ -58.4 (c, 1 in Py).

O-*[α-L-Rhamnopyranosyl-(1→2)*-O-*[β-D-glucopyranosyl-(1→3)]-β-D-galactopyranoside]:* [20562-02-1] ***α-Solanine***
$C_{45}H_{73}NO_{15}$ 868.069
Alkaloid from potato (*Solanum tuberosum*) and very many other *Solanum* spp. (Solanaceae). Responsible for the teratogenicity of sprouting potatoes. Poorly sol. H_2O, Et_2O, $CHCl_3$. Mp 286°. $[\alpha]_D$ -59 (Py). Log P 0.96 (uncertain value) (calc).

▶ Adverse human CNS and gastrointestinal effects by ingestion (associated with consumption of damaged or rotten potatoes). LD_{50} (rat, orl) 590 mg/kg. LD_{50} (mus, ipr) 42 mg/kg. Exp. reprod. and teratogenic effects. WF0250000

O-*[α-L-Rhamnopyranosyl-(1→2)*-O-*[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyanoside]:* [20562-03-2] ***α-Chaconine***
$C_{45}H_{73}NO_{14}$ 852.07
Alkaloid from *Solanum chacoense* and very many other *Solanum* spp. (Solanaceae). Mp 243°. $[\alpha]_D$ -85 (Py).

▶ Adverse human CNS and gastrointestinal effects by ingestion (associated with consumption of damaged or rotten potatoes). LD_{50} (rat, ipr) 84 mg/kg. Exp. reprod. and teratogenic effects. FL6700000

O-*[β-D-Glucopyranosyl-(1→4)-β-D-xylopyranosyl-(1→4)-β-D-xylopyranoside]:* ***Solacauline***
$C_{43}H_{69}NO_{14}$ 824.016
Alkaloid from potato spp. *Solanum acaule, Solanum punae* and *Solanum schreiteri* (Solanaceae). Mp 260-265°. $[\alpha]_D$ -30 (Py).

O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [102728-60-9] ***Hyacinthoside***
$C_{51}H_{83}NO_{20}$ 1030.211

O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [195433-57-9] ***Δ^5-Demissine***. *5,6-Dehydrodemissine*
$C_{50}H_{81}NO_{20}$ 1016.185
Alkaloid from potato (*Solanum commersonii*).

O-*[β-D-Glucopyranosyl-(1→6)-[α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside]:* [115491-59-3] ***Neohyacinthoside***
$C_{57}H_{93}NO_{25}$ 1192.353
Powder. Mp 262-265°. $[\alpha]_D^{20}$ -25.9 (c, 0.29 in Py).

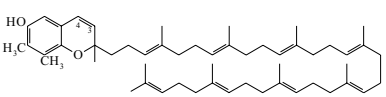
5,6-Dihydro: Demissidine, D-77

27-Hydroxy: [78719-99-0] ***Camtschatcanidine***
$C_{27}H_{43}NO_2$ 413.642
Needles (Me_2CO). Mp 261-265°. $[\alpha]_D$ -19.4 (c, 0.1 in MeOH).

Clemo, G.R. *et al., J.C.S.*, 1936, 1299 (*isol*)
Prelog, V. *et al., Helv. Chim. Acta*, 1942, **25**, 1306; 1944, **27**, 390 (*struct*)
Schreiber, K. *et al., Chem. Ber.*, 1954, **87**, 1007 (*Solacauline*)
Correia Alves, L. *et al., Garcia de Orta*, 1961, **9**, 713; *CA*, **61**, 12326d (*trioside*)
Budzikiewicz, H. *et al., Tetrahedron*, 1964, **20**, 2267 (*ms*)
Höhne, E. *et al., Tetrahedron*, 1966, **22**, 673 (*cryst struct*)
Schreiber, K. *et al., Alkaloids (N.Y.)*, 1968, **10**, 1 (*rev*)
Kessar, S.V. *et al., Tetrahedron*, 1971, **27**, 2153 (*synth*)
Radeglia, R. *et al., Tet. Lett.*, 1977, 903 (*cmr*)
Ripperger, H. *et al., Alkaloids (N.Y.)*, 1981, **19**, 81 (*rev*)
Samikov, K. *et al., Khim. Prir. Soedin.*, 1981, **17**, 349; *Chem. Nat. Compd. (Engl. Transl.)*, 273 (*Stenantine, Stenantidine*)
Kaneko, K. *et al., Phytochemistry*, 1981, **20**, 327 (*Camtschatcanidine*)
Katajima, J. *et al., Phytochemistry*, 1982, **21**, 187 (*glycosides*)
Qiu, F. *et al., CA*, 1983, **98**, 104286n (*glycoside*)
Keeler, R.F. *et al., Alkaloids: Chem. Biol. Perspect.*, 1984, **4**, 389 (*rev, tox*)
Xu, W.H. *et al., Yaoxue Xuebao*, 1986, **21**, 177; *CA*, **105**, 21663 (*Hyacinthoside*)
Xu, W.H. *et al., Yaoxue Xuebao*, 1988, **23**, 61-63 (*Neohyacinthoside*)
Vazquez, A. *et al., Euphytica*, 1997, **95**, 195-201 (*Δ^5-Demissine*)
Lawson, D.R. *et al., J. Agric. Food Chem.*, 1997, **45**, 4122-4126 (*pmr, cmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDG500; SKS000

Solanochromene S-155

[24946-64-3]
Plastochromenol 8



$C_{53}H_{80}O_2$ 749.214
Oil or cryst. Mp 16-19°.

3,4-Dihydro: [4382-43-8] ***Plastochromanol 8***
$C_{53}H_{82}O_2$ 751.23
Isol. from *Medicago sativa* (alfalfa) and other plants. Oil.

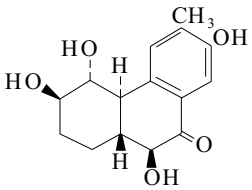
[16772-36-4, 30382-15-1, 56084-94-7]

Rowland, R.L. *et al., J.A.C.S.*, 1958, **80**, 6130 (*isol*)
Kofler, M. *et al., Helv. Chim. Acta*, 1959, **42**, 2252 (*struct*)
Hemming, F.W. *et al., Biochem. J.*, 1961, **80**, 445 (*struct*)
Whittle, K.J. *et al., Biochem. J.*, 1965, **96**, 17C (*Plastochromanol 8*)
Mayer, H. *et al., Helv. Chim. Acta*, 1967, **50**, 1376 (*pmr, ms, config, bibl*)
Thompson, J.N. *et al., J. Liq. Chromatogr.*, 1979, **2**, 327 (*hplc*)

Findlay, J.A. *et al., J. Nat. Prod.*, 1984, **47**, 560 (*isol*)

Solanolone S-156

[105933-57-1]



$C_{15}H_{18}O_5$ 278.304

Constit. of potato tubers infected with *Phoma exigua* var. *foveata*. Amorph. $[\alpha]_D^{22}$ +51.8 (c, 1 in MeOH).

Andersson, R. *et al., Acta Chem. Scand., Ser. B*, 1986, **40**, 370 (*isol, nmr*)

Somatostatin, BAN, INN S-157

[51110-01-1]

Growth hormone release-inhibiting factor, 9CI. Somatotropin release inhibiting factor. Panhibin. GH-RIF. SRIF. Aminopan. CM 9357. Modustatine. Somatofalk. Somiaton. Stilamin. Sumestil

H-Ala-Gly-Cys-Lys-Asn-Phe-Phe-Trp-Lys-Thr-Phe-Thr-Ser-Cys-OH

$C_{76}H_{104}N_{18}O_{19}S_2$ 1637.899

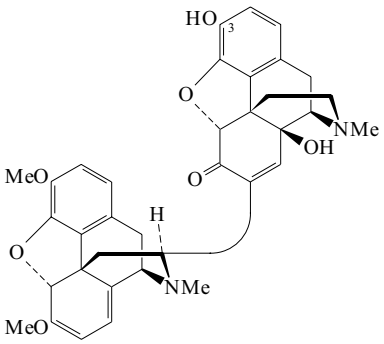
Reduced form shown.Intensive research continues to find analogues of prolonged and/or selective activity.

▶ LD_{50} (rat, ivn) 21 mg/kg. Exp. reprod. effects. WF8751700

Burgus, R. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1973, **70**, 684 (*isol*)
Fujii, N. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1596 (*synth*)
Itakura, K. *et al., Science (Washington, D.C.)*, 1977, **198**, 1056 (*cloning*)
Schally, A.V. *et al., Horm. Proteins Pept.*, (Li, C.H., Ed.), Academic Press, New York, 1979, **4**, 2 (*rev*)
McCann, S.M. *et al., Adv. Biochem. Psychopharmacol.*, 1980, **22**, 131 (*pharmacol, rev*)
Buffington, L. *et al., Biochem. Biophys. Res. Commun.*, 1980, **93**, 376 (*pmr*)
Moroder, L. *et al., Bioorg. Chem.*, 1980, **9**, 27 (*synth*)
Bodanszky, M. *et al., Gastrointest. Horm.*, 1980, 413 (*rev, synth*)
Wünsch, E. *et al., Biopolymers*, 1981, **20**, 1741 (*conformn*)
Veber, D.F. *et al., Nature (London)*, 1981, **292**, 55
Gyr, K. *et al., Trends Pharmacol. Sci.*, 1982, **3**, 367 (*pharmacol*)
Conlon, J.M. *et al., Int. Congr. Ser. Excerpta Med.*, 1983, **600**, 243 (*biosynth, struct*)
Zingg, H.H. *et al., Adv. Exp. Med. Biol.*, 1985, **188**, 49; 71; 229 (*biosynth, formn, activity*)
Lamberts, S.W.J. *et al., Front. Horm. Res.*, 1985, **14**, 137 (*rev*)
Dileepan, K.N. *et al., Life Sci.*, 1985, **37**, 2335 (*physiol, metab*)
Patel, Y. *et al., Prog. Endocr. Res. Ther.*, 1987, **3**, 21 (*rev, biosynth, biol activity*)
Elofsson, A. *et al., Int. J. Pept. Protein Res.*, 1990, **36**, 297 (*conformn*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 964
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKS600

Somniferine S-158

[117611-63-9]



$C_{36}H_{36}N_2O_7$ 608.69

Alkaloid from *Papaver somniferum* (opium poppy). Amorph. $[\alpha]_D^{20}$ -297 (c, 1 in $CHCl_3$). Log P 0.28 (uncertain value) (calc).

3-Me ether: [117611-62-8] **O-*Methylsomniferine***

$C_{37}H_{38}N_2O_7$ 622.716

Alkaloid from *Papaver somniferum* (opium poppy). No phys. props. reported.

Dragar, C. *et al., Tet. Lett.*, 1988, **29**, 3115 (*struct*)

Sorbimacrogol S-159

Poly(oxy-1,2-ethanediyl)sorbitan

Polymer obt. from 1,4-Anhydroglucitol, A-335 and Oxirane, O-193.

Monododecanoyl: [9005-64-5] *Polysorbate 20. Sorbimacrogol laurate 300. POE(20) sorbitan monolaurate. E432*
Emulsifier, stabiliser, flavouring agent, dispersant. Mixt. of sorbitan laurate esters with ca. 20 moles of ethylene oxide.

Monohexadecanoyl: [9005-66-7] *Polysorbate 40. Sorbimacrogol palmitate 300. E434. POE(20) sorbitan monopalmitate*
Emulsifier, dough improver, crystallisation retarder, solubiliser, stabiliser, flavour dispersant, wetting agent, fruit or vegetable coating, defoamer for yeast/sugar. Mixt. of sorbitan palmitate esters with ca. 20 moles of ethylene oxide.

Monooctadecanoyl: [9005-67-8] *Polysorbate 60. Sorbomacrogol stearate 300. POE(20) orbitan monostearate. E435*
Emulsifier, opacifier, protective coating, dough conditioner, dispersant, wetting agent, stabiliser, defoamer, poultry scald agent, flavour.. Mixt. of sorbitan stearate esters with ca. 20 moles of ethylene oxide.

Trioctadecanoyl: [9005-71-4] *Polysorbate 65. Sorbimacrogol tristearate 300. POE(20) sorbitan tristearate. E436*
Emulsifier, stabiliser, defoamer. Mixt. of stearate esters with ca. 20 moles of ethylene oxide.

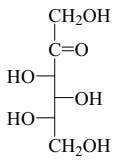
Mono-9-octadecenoyl: [9005-65-6] *Polysorbate 80. Sorbimacrogol oleate 300. POE(20) sorbitan monooleate. E433*
Emulsifier, surfactant in production of coarse cryst. NaCl, stabiliser, wetting agent in poultry scalds, colour diluent, flavour. Mixt. of sorbitan oleate esters with ca. 20 moles of ethylene oxide.

Tri-9-octadecenoyl: [9005-70-3] *Polysorbate 85. Sorbimacrogol trioleate 300. POE(20) sorbitan trioleate*
Emulsifier, wetting agent, dispersant, stabiliser, solubiliser. Mixt. of sorbitan oleate esters with ca. 20 moles of ethylene oxide.

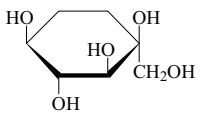
Ash, M. *et al., Handbook of Food Additives*, Gower, 1995, 675-677

Sorbose, 9CI, 8CI S-160

xylo-*Hexulose. Sorbinose*



L-*form*



α-L-Pyranose-*form*

$C_6H_{12}O_6$ 180.157

A 4*M* aq. soln. at 31° contains 93% α-pyr, 2% β-pyr, 4% α-fur, 1% β-fur, and 0.3% ketone.

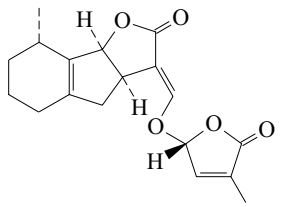
L-*form* [87-79-6]

Indirect food additive arising from its use as a constituent of cotton, cotton fabrics, paper and paperboard in contact with dry food. Mp 165°. $[\alpha]_D^{20}$ -43.2 (H_2O). Sweet taste.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 193C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 297C; 298A (*nmr*)
Karabinos, J.V. *et al., Adv. Carbohydr. Chem.*, 1952, **7**, 99 (*rev*)
Olin, S.M. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 148 (*D-form, L-form*)
Lockwood, L.B. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 151 (*D-form, L-form*)
Nordenson, S. *et al., Acta Cryst. B*, 1979, **35**, 1005 (*cryst struct*)
Bock, K. *et al., Adv. Carbohydr. Chem. Biochem.*, 1983, **41**, 27 (*cmr*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **44**, 15 (*equilib*)
Bock, K. *et al., Carbohydr. Res.*, 1991, **216**, 141 (***synth, D-form***)
Huwig, A. *et al., Carbohydr. Res.*, 1996, **281**, 183 (*synth, bibl, D-form*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2628-2629
Lichtenthaler, F.W. *et al., Carbohydr. Res.*, 1998, **313**, 69-89 (*rev, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKV400

Sorgolactone S-161

[141262-39-7]



$C_{18}H_{20}O_5$ 316.353
Isol. from the roots of *Sorghum bicolor* (sorghum) (genuine host plant for *Striga* spp.). Cryst. Mp 139-142°. $[\alpha]_D$ +271.2 (c, 0.25 in $CDCl_3$). Similar to Strigol, S-251 λ_{max} 230 (ϵ 20) (no solvent reported). λ_{max} 236 (MeCN aq.).

Hauck, C. *et al., J. Plant Physiol.*, 1992, **139**, 474-478 (*isol, pmr, ir, cmr, ms*)
Mori, K. *et al., Tet. Lett.*, 1997, **38**, 7891-7892 (*synth*)
Sugimoto, Y. *et al., J.O.C.*, 1998, **63**, 1259-1267 (*synth*)
Welzel, P. *et al., Chem. Comm.*, 1999, 2017-2022 (*rev*)
Matsui, J. *et al., Eur. J. Org. Chem.*, 1999, 2183-2194 (*synth, ir, pmr, cmr, ms*)

Soyasapogenol F S-162

[97503-03-2]
Constit. of *Trifolium pratense* (red clover). Prob. artifact. Struct. unknown.

Gorski, P.M. *et al., Acta Soc. Bot. Pol.*, 1984, **53**, 515; 527; 1987, **56**, 101; 119 (*isol*)
Oleszek, W. *et al., Acta Soc. Bot. Pol.*, 1986, **55**, 247 (*isol*)

SP_1 S-163

[75977-11-6]
Polypeptide containing 45 amino acid residues. Isol. from wheat flour (*Triticum monococcum*). λ_{max} 278 (H_2O) (Berdy).

Japan. Pat., 1980, 80 20 748; *CA*, **94**, 52916p (*isol*)
Japan. Pat., 1981, 81 77 228; *CA*, **95**, 162316w (*antitumour activity*)

Spermidine S-164

[124-20-9]
N-*(3-Aminopropyl)-1,4-butanediamine, 9CI*
$H_2NCH_2CH_2CH_2N'HCH_2CH_2CH_2CH_2-N''H_2$
$C_7H_{19}N_3$ 145.247
Constit. of meat products. Isol from the edible shaggy ink cap mushroom (*Coprinus comatus*) and from commercial/household prepared sauerkraut. Bp_{14} 128-130°.
▶ LD_{50} (mus, ivn) 78 mg/kg. EJ7000000
N′-*Hexanoyl:* [97141-37-2] **N^5-*Hexanoylspermidine***
$C_{13}H_{29}N_3O$ 243.392
Alkaloid from senescing ovaries of pea (*Pisum sativum*).
N″-*(4-Hydroxy-3-methoxycinnamoyl),* N-*(3,4-dihydroxycinnamoyl):* [101164-74-3] **N^1-*Caffeoyl*-N^{10}-*feruloylspermidine***
$C_{26}H_{33}N_3O_6$ 483.563
Alkaloid from *Corylus avellana* (filbert) pollen.

[49721-50-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 309D; 310A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 501B (*nmr*)
v. Braun, J. *et al., Ber.*, 1937, **70**, 1230 (*synth*)
Danzig, M. *et al., J.A.C.S.*, 1952, **74**, 1836 (*synth*)
Herbst, E.J. *et al., Arch. Biochem. Biophys.*, 1958, **75**, 171 (*isol*)
Raina, A. *et al., Acta Chem. Scand.*, 1970, **24**, 3061 (*biosynth*)
Williams-Ashman, H.G. *et al., CA*, 1974, **81**, 23332w (*rev*)
Tait, G.H. *et al., Biochem. Soc. Trans.*, 1976, **4**, 610 (*biosynth*)
Meurer, B. *et al., Phytochemistry*, 1986, **25**, 433 (*N-Caffeoyl-N″-feruloylspermidine*)
Polyamines in the Gastrointestinal Tract, (eds. Dowling, R.H. *et al*), Kluwer Academic Publishers, Dordrecht, 1992, (*book*)
Perez-Amador, M.A. *et al., Plant Physiol.*, 1996, **110**, 1177 (*Hexanoylspermidine*)
Hernandez-Jover, T. *et al., J. Agric. Food Chem.*, 1997, **45**, 2098-2102 (*occur*)
Kalač, P. *et al., Biologically-active Phytochemicals in Food*, (eds. Pfannhauser, W. *et al*), Royal Society of Chemistry, 2001, 217-220 (*sauerkraut*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SLA000

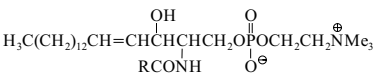
Spermine S-165

[71-44-3]
N,N′-*Bis(3-aminopropyl)-1,4-butanediamine, 9CI. Bis(3-aminopropyl)tetramethylenediamine. Musculamine. Neuridine. Gerontine*
$H_2N(CH_2)_3NH(CH_2)_4NH(CH_2)_3NH_2$
$C_{10}H_{26}N_4$ 202.342
Occurs as phosphate in ox pancreas, yeast and meat products. Deliquescent cryst. $Bp_{0.5}$ 141-142°. Absorbs CO_2 from the air.
▶ LD_{50} (mus, ivn) 56 mg/kg. EJ7175000
Hydrochloride (1:4): [306-67-2]
Cryst. (EtOH). Mp 312-314.5°.
▶ EJ7230000
Phosphate: [3891-79-0]
Sol. hot H_2O, insol. EtOH, Et_2O. Mp 230-234°.
N^1-*Ac:* [25593-72-0] N-*Acetylspermine. Monoacetylspermine*
$C_{12}H_{28}N_4O$ 244.379
No phys. props. reported.
Tetrabenzoyl:
Needles (Me_2CO aq.). Mp 155°.
N^1,N^5,N^{10}-*Tris(4-hydroxy*-E-*cinnamoyl):* **N^1,N^5,N^{10}-*Tris*-trans-p-*coumaroylspermine***
$C_{37}H_{44}N_4O_6$ 640.778
Constit. of *Matricaria chamomilla* (German chamomile). Yellow powder (as trifluoroacetate). Mp 109-111° dec. (trifluoroacetate).
N^1,N^5,N^{10},N^{14}-*Tetrakis(4-hydroxy*-E-*cinnamoyl):* **N^1,N^5,N^{10},N^{14}-*Tetra*-trans-p-*coumaroylspermine***
$C_{46}H_{50}N_4O_8$ 786.923
Constit. of *Matricaria chamomilla* (German chamomile). Cryst. (MeOH aq.). Mp 139-141° dec. λ_{max} 227 (log ϵ 4.7); 299 (log ϵ 4.93); 311 (log ϵ 4.94) (MeOH).
Bis(4-hydroxy-3-methoxycinnamoyl): [70208-06-9] ***Diferuloylspermine***
$C_{30}H_{42}N_4O_6$ 554.685
Alkaloid from *Ananas comosus* (pineapple). Substituted on two of the *N* atoms. Exact struct. unknown.
Bis(4-hydroxy-3,5-dimethoxycinnamoyl): [70185-66-9] ***Disinapoylspermine***
$C_{32}H_{46}N_4O_8$ 614.737Substituted on two of the *N* atoms. Exact struct. unknown.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 312B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 503C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 399A (*ir*)
Dudley, H.W. *et al., Biochem. J.*, 1924, **18**, 1263; 1926, **20**, 1082; 1927, **21**, 97
Dubin, D.T. *et al., J. Biol. Chem.*, 1960, **235**, 776-782 (*Monoacetylspermine*)
Israel, M. *et al., J. Med. Chem.*, 1964, **7**, 710 (*synth*)
Raina, A. *et al., Acta Chem. Scand.*, 1970, **24**, 3061 (*biosynth*)
Williams-Ashman, M.G. *et al., Adv. Enzyme Regul.*, 1972, **10**, 225; *CA*, **81**, 23332w (*rev*)
Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*Diferuloylspermine, Disinapoylspermine*)
Federico, R. *et al., Phytochemistry*, 1989, **28**, 2045-2046; 1990, **29**, 2411-2414 (*Monoacetylspermine, activity*)
Polyamines in the Gastrointestinal Tract, (eds. Dowling, R.H. *et al*), Kluwer Academic Publishers, Dordrecht, 1992, (*book*)
Hernandez-Jover, T. *et al., J. Agric. Food Chem.*, 1997, **45**, 2098-2102 (*occur*)
Yamamoto, A. *et al., Chem. Pharm. Bull.*, 2002, **50**, 47-52 (*Tricoumaroylspermine, Tetracoumaroylspermine*)
Rubio, M. *et al., Synth. Commun.*, 2002, **32**, 2441-2452 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DCC400; GEK000

Sphingomyelins S-166

[85187-10-6]

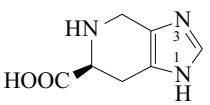


A class of sphingolipids with the general structure indicated. Hydrolysis furnishes sphing-4-enine (or other long-chain amine), a fatty acid, phosphoric acid and choline (or ethanolamine)..

Rodd's Chem. Carbon Compd. (2nd edn.), 1976, **1E**, 425

Spinacine S-167

*4,5,6,7-Tetrahydro-1*H-*imidazo[4,5-*c*]pyridine-6-carboxylic acid, 9CI*



$C_7H_9N_3O_2$ 167.167
(*S*)-*form* [59981-63-4]

Isol. from the crab (*Crango vulgaris*), from the liver of the shark (*Acanthias vulgaris*) and from spinach. Also isol. from the roots of *Panax ginseng*. Mp 265°. $[\alpha]_D^{20}$ -174.6 (H_2O). Forms a sesquihydrate.

Hydrochloride:
Mp 286-287° (279-280°).

1-Me: [133807-71-3]
$C_8H_{11}N_3O_2$ 181.194
Cryst. (MeOH/Et_2O) (as dihydrochloride). Mp 287-290° dec. (dihydrochloride). $[\alpha]_D^{23}$ -9597 (c, 1.11 in H_2O).

3-Me: [114787-98-3]
$C_8H_{11}N_3O_2$ 181.194
Cryst. (MeOH/Et_2O) (as dihydrochloride). Mp 262-265° dec. (dihydrochloride). $[\alpha]_D^{23}$ -93.5 (c, 1.05 in H_2O).

(±)-*form*
Mp 265°.

Ackermann, D. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1949, **284**, 129; 1962, **328**, 275 (*isol, struct, synth*)
Vitali, T. *et al., Gazz. Chim. Ital.*, 1964, **94**, 296 (*synth*)
Nardelli, M. *et al., Ric. Sci., Parte 2: Sez. A*, 1964, **7**, 718; *CA*, **63**, 12440g (*cryst struct*)
Andreetti, G.D. *et al., Gazz. Chim. Ital.*, 1971, **101**, 625 (*cryst struct*)
Eilazyan, O.G. *et al., CA*, 1982, **96**, 85467n (*synth*)
Han, Y.N. *et al., Arch. Pharmacal Res.*, 1987, **10**, 258; *CA*, **108**, 201742r (*isol*)
Klutchko, S. *et al., J. Het. Chem.*, 1991, **28**, 97 (*synth, pmr, derivs*)

δ-Spinasterol S-168

$C_{29}H_{48}O$ 412.698

Struct. unknown. Isol. from alfalfa seed oil. Mp 143-144°. $[\alpha]_D^{19}$ +6.2 ($CHCl_3$).

King, I.C. *et al., J.A.C.S.*, 1942, **64**, 2488

γ-Spinasterol S-169

$C_{29}H_{48}O$ 412.698

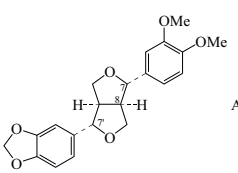
Struct. unknown.Mp 159.5-160°. $[\alpha]_D$ 0.

Glucoside:
$C_{35}H_{58}O_6$ 574.84
Isol. from spinach leaves. Mp 275-280° dec.

Heyl, F.W. *et al., J.A.C.S.*, 1934, **56**, 942

Spinescin S-170

5-[4-(3,4-Dimethoxyphenyl)tetrahydro-1H,3H-furo[3,4-c]furan-1-yl]-1,3-benzodioxole, 9CI. 2-(3,4-Dimethoxyphenyl)-6-(3,4-methylenedioxyphenyl)3,7-dioxabicyclo[3.3.0]octane. 3,4-Dimethoxy-3′,4′-methylenedioxy-7,9′:7′,9-diepoxylignan. Kobusin†. Spinescen. Demethoxyaschantin. O-Methylpiperitol



Absolute Configuration

$C_{21}H_{22}O_6$ 370.401

Identity of Spinescin and Kobusin does not appear confirmed.

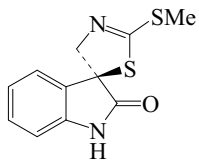
(+)-*form* [36150-23-9]
Constit. of sassafras root. Cryst. or oil. Sol. MeOH, $CHCl_3$. Mp 55° Mp 75°. $[\alpha]_D$ +58.6 (c, 3.33 in $CHCl_3$). $[\alpha]_D^{20}$ +73.6 ($CHCl_3$). $[\alpha]_D$ +272. λ_{max} 232 ; 284 (MeOH) (Berdy). λ_{max} 233 (ϵ 12950); 284 (ϵ 7480) (EtOH) (Berdy).

7-Epimer: [68296-27-5] ***(+)-Fargesin***. *Planinin*
$C_{21}H_{22}O_6$ 370.401
Constit. of *Artemisia absinthium* (wormwood). Cryst. Mp 135-136°. $[\alpha]_D^{20}$ +122 (c, 1 in $CHCl_3$).

Kakisawa, H. *et al., Phytochemistry*, 1972, **11**, 2289 (*Fargesin*)
Rao, E.V. *et al., Curr. Sci.*, 1975, **44**, 228 (*Fargesin*)
Chen, J. *et al., Yaoxue Xuebao*, 1988, **23**, 422-425 (*Planinin*)
Brown, R.C.D. *et al., J.O.C.*, 2001, **66**, 6719-6728 (*Fargesin, synth*)

Spirobrassinin S-171

[113866-40-3]
2′-(Methylthio)spiro[3H-indole-3,5′(4′H)thiazol]-2(1H)-one, 9CI



Absolute Configuration

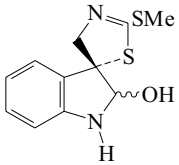
$C_{11}H_{10}N_2OS_2$ 250.345

(*S*)-*form*
Phytoalexin of *Raphanus sativus* var. *hortensis* (Japanese radish Daikon). Cryst. $[\alpha]_D$ -69.5 (c, 1.14 in $CHCl_3$) (natural). $[\alpha]_D$ -143.6 (opt. pure). The nat. prod. is a partial racemate. Undergoes strong enantiomeric enrichment in achiral chromatographic phase λ_{max} 215 (ϵ 23500); 250 (ϵ 8200); 300 (ϵ 1900) (MeOH).

(ξ)-*form*
N*1*-*Methoxy:* [156499-63-7] ***1-Methoxyspirobrassinin***
$C_{12}H_{12}N_2O_2S_2$ 280.371
Phytoalexin from *Brassica oleracea* var. *gongylodes* (kohlrabi).

Takasugi, M. *et al., Chem. Lett.*, 1987, 1631-1632 (*isol, struct*)
Monde, K. *et al., J.A.C.S.*, 1994, **116**, 6650-6657 (*synth*)
Gross, D. *et al., Z. Naturforsch., C*, 1994, **49**, 281-285 (*1-Methoxyspirobrassinin*)
Monde, K. *et al., Chem. Lett.*, 2000, 886-887 (*abs config*)
Monde, K. *et al., J. Nat. Prod.*, 2000, **63**, 1312-1314 (*opt purity*)
Pedras, M.S.C. *et al., Phytochemistry*, 2000, **53**, 161-176 (*rev*)
Suchy, M. *et al., J.O.C.*, 2001, **66**, 3940-3947 (*synth, cd, abs config*)
Kutschy, P. *et al., Tet. Lett.*, 2002, **43**, 9489-9492 (*1-Methoxyspirobrassinin, synth*)

Spirobrassinol S-172



Relative configuration

$C_{11}H_{12}N_2OS_2$ 252.361

N-*Methoxy:*

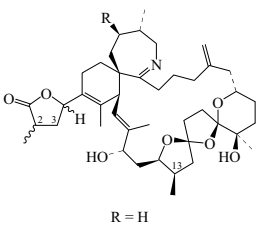
[165746-57-6, 166020-09-3] **N-*Methoxyspirobrassinol***
$C_{12}H_{14}N_2O_2S_2$ 282.387
Stress metab. from the Japanese radish Daikon (*Raphanus sativus* var. *hortensis*) (Cruciferae) inoculated with *Pseudomonas cichorii*. Gum. $[\alpha]_D^{20}$ 0 (c, 0.52 in $CHCl_3$). Unusual hemi-aminal struct. Occurs as a mixt. of diastereoisomers; ratio α-*OH*: β-*OH* estimated as 2.5:1 λ_{max} 211 (ϵ 27300); 246 (ϵ 15500); 292 (ϵ 3630) (EtOH) (Berdy).

Me ether, N-*methoxy:* [113866-41-4] **N-*Methoxyspirobrassinol methyl ether***
$C_{13}H_{16}N_2O_2S_2$ 296.414
Stress metab. from Japanese daikon radish inoculated with *Pseudomonas cichorii*. Gum. $[\alpha]_D^{18}$ -1.9 (c, 1.57 in $CHCl_3$). Has 2β-OMe config. Abs. config. not known λ_{max} 210 (ϵ 26400); 291 (ϵ 2880) (EtOH) (Berdy).

Monde, K. *et al., Phytochemistry*, 1995, **39**, 581-586 (*isol, pmr, cmr, ms*)
Kutschy, P. *et al., Tet. Lett.*, 2002, **43**, 9489-9492 (*synth*)

Spirolide B S-173

[170713-72-1]



Relative Configuration

R = H

$C_{42}H_{63}NO_7$ 693.962
Isol. from *Mytilus edulis* (mussels) and *Placopecten magellanicus* (scallops). Related to Pinnatoxin A.

2,3-Didehydro: ***Spirolide A***
$C_{42}H_{61}NO_7$ 691.946
Isol. from toxic plankton and contaminated shellfish.

Hu, T. *et al., Chem. Comm.*, 1995, 2159-2161 (*isol, pmr, cmr, ms*)
Hu, T. *et al., J. Nat. Prod.*, 2001, **64**, 308-312 (*Spirolide A*)
Falk, M. *et al., Tetrahedron*, 2001, **57**, 8659-8665 (*config*)

Spirolide D S-174

[170713-73-2]
As Spirolide B, S-173 with
R = CH_3
$C_{43}H_{65}NO_7$ 707.989

Isol. from *Mytilus edulis* (blue mussel).

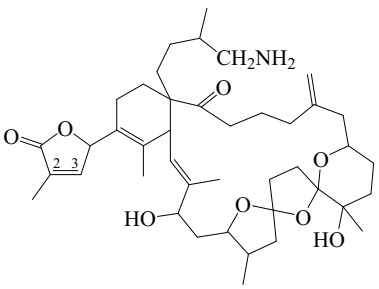
2,3-Didehydro: [318996-49-5] ***Spirolide C***
$C_{43}H_{63}NO_7$ 705.973
Isol. from contaminated shellfish.

13-Demethyl, 2,3-didehydro: [334974-07-1] ***13-Demethylspirolide C***. *13-Desmethylspirolide C*
$C_{42}H_{61}NO_7$ 691.946
Isol. from contaminated shellfish.

Hu, T. *et al., Chem. Comm.*, 1995, 2159-2161 (*isol, pmr, cmr, ms*)
Hu, T. *et al., J. Nat. Prod.*, 2001, **64**, 308-312 (*Spirolide C, Demethylspirolide C*)
Falk, M. *et al., Tetrahedron*, 2001, **57**, 8659-8665 (*config*)

Spirolide E S-175

[183159-71-9]

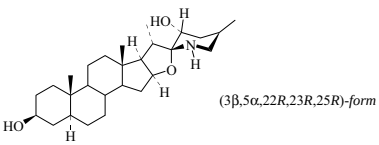


$C_{42}H_{63}NO_8$ 709.962
Isol. from shellfish extracts.

2,3-Dihydro: [183159-73-1] ***Spirolide F***
$C_{42}H_{65}NO_8$ 711.977
Isol. from shellfish extracts.

Hu, T. *et al., Tet. Lett.*, 1996, **37**, 7671-7674 (*isol, pmr, cmr, ms*)

Spirosolane-3,23-diol S-176



$C_{27}H_{45}NO_3$ 431.657
The 23-*OH* group changes the *R,S*-priorities compared with other spirosolanes.

(3β,5α,22*R*,23*R*,25*R*)-*form*
23*R-*Hydroxysoladulcidine
Mp 192-193°. $[\alpha]_D^{22}$ -65.4 (c, 0.44 in MeOH).

(3β,5α,22*R*,23*S*,25*R*)-*form*
23-Ac: [152128-85-3] ***23-Acetoxysoladulcidine***
$C_{29}H_{47}NO_4$ 473.695
Alkaloid from the roots of a *Lycopersicon esculentum-Lycopersicon hirsutum* hybrid. Amorph. $[\alpha]_D^{20}$ -46 (c, 0.37 in $CHCl_3$).

23-Ac, 3-O-*[β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [176300-86-0] ***Lycoperoside B***
$C_{52}H_{85}NO_{23}$ 1092.236
Alkaloid from *Lycopersicon esculentum* (tomato). Amorph. powder. $[\alpha]_D^{27}$ -40.3 (c, 0.56 in MeOH).

(3β,5α,22*R*,23*S*,25*S*)-*form*
23-Ac: [152128-86-4] ***23-Acetoxy-25-epiosoladulcidine***
$C_{29}H_{47}NO_4$ 473.695
Alkaloid from roots of a *Lycopersicon esculentum-Lycopersicon hirsutum* hybrid. Amorph. $[\alpha]_D^{20}$ -36.7 (c, 1.2 in $CHCl_3$).

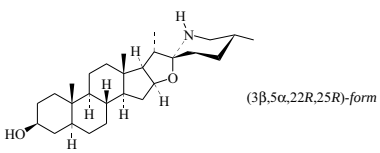
23-Ac, 3-O-*[β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [176300-87-1] ***Lycoperoside C***
$C_{52}H_{85}NO_{23}$ 1092.236
Alkaloid from *Lycopersicon esculentum* (tomato). Amorph. powder. $[\alpha]_D^{27}$ -26.3 (c, 0.63 in MeOH).

(3β,5α,22*S*,23*R*,25*S*)-*form*
23-Ac: [152128-84-2] ***23*R-*Acetoxytomatidine***
$C_{29}H_{47}NO_4$ 473.695
Alkaloid from roots of a *Lycopersicon esculentum/Lycopersicon hirsutum* hybrid. Amorph. $[\alpha]_D^{20}$ -2.8 (c, 0.42 in $CHCl_3$).

23-Ac, 3-O-*[β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [176181-33-2] *23*R-*Acetoxytomatine*. ***Lycoperoside A***
$C_{52}H_{85}NO_{23}$ 1092.236
Alkaloid from *Lycopersicon esculentum* (tomato). Amorph. powder. $[\alpha]_D^{27}$ -31.6 (c, 0.8 in MeOH).

Ripperger, H. *et al., Phytochemistry*, 1993, **32**, 1607 (*23-Hydroxysoladulcidine*)
Nagaoka, T. *et al., Phytochemistry*, 1993, **34**, 1153 (*23-Acetoxysoladulcidines, 23-Acetoxytomatidine*)
Yahara, S. *et al., Phytochemistry*, 1996, **42**, 169-172 (*Lycoperosides*)

Spirosolan-3-ol, 9CI S-177



$C_{27}H_{45}NO_2$ 415.658
Log P 6.08 (uncertain value) (calc).

(3β,5α,22*R*,25*R*)-*form* [511-98-8] ***Soladulcidine***. *5α-Solasodan-3β-ol, 8CI. Megacarpidine. Dihydrosolasodine. Solasodanol*
Said to occur free in *Lycopersicon pimpinellifolium* (currant tomato). Mp 209-211°. $[\alpha]_D$ -53 (c, 0.64 in Py). $[\alpha]_D$ -50 (c, 0.4 in $CHCl_3$).

Hydrochloride:
Mp 298-299°.

Picrate:
Mp 152-154°.

3-O-*[β-D-Xylopyranosyl-(1→4)-β-D-galactopyranoside]:* ***Solalyratine A***
$C_{38}H_{63}NO_{11}$ 709.916
Needles + $3H_2O$. Mp 252-254°. $[\alpha]_D$ -89.2 (c, 0.5 in Py).

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* ***Solalyratine B***
$C_{44}H_{73}NO_{16}$ 872.058
Needles + $2H_2O$. Mp 274-279°. $[\alpha]_D$ -17.9 (c, 0.5 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→2)]-β-D-galactopyranoside]:* ***Dihydrosolasuaveoline***
$C_{51}H_{85}NO_{21}$ 1048.227
Cryst. (MeOH aq.). Mp 275-277° dec. $[\alpha]_D^{24}$ -43.8 (c, 0.5 in Py).

Glycoside(1): ***Megacarpine***
$C_{44}H_{73}NO_{16}$ 872.058
Mp 259-260°. $[\alpha]_D$ -61.6 (Py). Hydrol. gives 1 Glu, 1 Gal and 2 Xyl.

Glycoside(2): ***Soladulcidine tetroside***
$C_{45}H_{75}NO_{17}$ 902.084
Mp 268-270°. $[\alpha]_D$ -53 (Py). Hydrol. gives 2 Glu, 1 Gal and 1-Xyl.

Glycoside(3): [37337-73-8] ***α-Soladulcine***
$C_{50}H_{83}NO_{21}$ 1034.2
Mp 265-269°. $[\alpha]_D$ -56 (MeOH). Hydrol. gives 2 Glu, 1 Gal and 1 D-Xyl.

Glycoside(4): [11093-43-9] ***β-Soladulcine***
$C_{45}H_{75}NO_{16}$ 886.085
Mp 246-248° dec. $[\alpha]_D$ -39 (c, 0.38 in MeOH). Hydrol. gives 1 Glu, 1 Gal and 1 Rha.

Glycoside(5): ***γ-Soladulcine*** Not well characterised. Isol. only (Schreiber) as a mixt. with α- and β-Soladulcines.

(3β,5α,22*S*,25*S*)-*form* [77-59-8] ***Tomatidine***. *5α-Tomatidan-3β-ol, 8CI*
Alkaloid from *Lycopersicon esculentum* (tomato). Mp 210-211°. $[\alpha]_D^{20}$ +5 (MeOH). Log P 6.08 (uncertain value) (calc).

Hydrochloride:
Mp 275-280° dec. $[\alpha]_D^{25}$ -9 (MeOH).

Picrate:
Mp 131-133°.

O-*β-D-Glucopyranoside:* [177354-90-4] ***Tomatidine 3*-O-*β-D-glucopyranoside***
$C_{33}H_{55}NO_7$ 577.8
Cryst. Mp 174-177° (as penta-Ac). $[\alpha]_D^{23}$ -13.6 (c, 0.44 in $CHCl_3$).

O-*β-D-Galactopyranoside:* [99304-79-7] *Tomatidine 3*-O-*β-D-galactopyranoside. δ-Tomatine*
$C_{33}H_{55}NO_7$ 577.8

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [177354-91-5]
$C_{38}H_{63}NO_{11}$ 709.916
Needles. Mp 238-240° (as hepta-Ac). $[\alpha]_D^{23}$ -7.3 (c, 1.64 in $CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [81037-16-3] ***γ-Tomatine***. *Lycoperoside D*
$C_{39}H_{65}NO_{12}$ 739.942
Alkaloid from *Lycopersicon esculentum* (tomato). Amorph. powder. $[\alpha]_D^{27}$ -10.8 (c, 0.6 in MeOH).

O-*[β-D-Xylopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranoside]:* ***Polyanine***
$C_{43}H_{71}NO_{15}$ 842.032
Needles (MeOH aq.). Mp 263-270° dec. $[\alpha]_D^{21}$ -36.3 (c, 1.05 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopya-*

nosyl-(1→4)-β-D-galactopyranoside]: [85547-35-9] ***Sisunine***. *Neotomatine*
$C_{51}H_{85}NO_{22}$ 1064.226

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [17406-46-1] ***β$_1$-Tomatine***
$C_{45}H_{75}NO_{17}$ 902.084
Present in tomatoes. Amorph. solid + $1H_2O$. Mp 240-260° dec. $[\alpha]_D^{22}$ -28 (c, 1 in Py). Not obt. completely pure. Other Tomatines (β_2-, γ- and δ-) are other nonalkaloidal partial hydrol. prods. of Tomatine.

O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [17406-45-0] ***Tomatine***. *α-Tomatine. Lycopersicin*
$C_{50}H_{83}NO_{21}$ 1034.2
High levels found in green tomatoes (up to 500 mg/kg) which decline on ripening. Sol. MeOH, EtOH, dioxan; fairly sol. H_2O, Et_2O, acids, hexane; poorly sol. $CHCl_3$, EtOAc, C_6H_6. Mp 263-267° dec. $[\alpha]_D$ -19 (Py). Log P -3.27 (uncertain value) (calc).

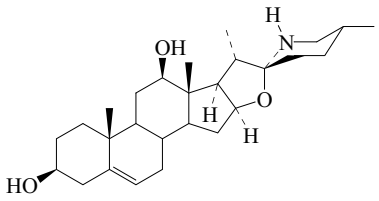
► LD_{50} (rat, orl) 900 mg/kg; LD_{50} (mus, ipr) 25 mg/kg; LD_{50} (mus, scu) 1000 mg/kg; LD_{50} (mus, orl) 500 mg/kg. XW1050000

N-*Nitroso:* [4847-05-6] **N-*Nitrosotomatidine***
$C_{27}H_{44}N_2O_3$ 444.656
Present in tomatoes. Hexagonal cryst. changing to flat rods on heating. Mp 234-237°. Mp. quoted is for synthetic material.

3-Ketone: [6870-84-4] ***5α-Tomatidan-3-one***
$C_{27}H_{43}NO_2$ 413.642
Alkaloid from roots of a *Lycopersicon esculentum/Lycopersicon hirsutum* hybrid. Needles (MeOH). Mp 195-198°. $[\alpha]_D^{20}$ +19 (c, 0.38 in $CHCl_3$).

Brink, N.G. *et al., J.A.C.S.*, 1951, **73**, 4018 (*isol, Tomatidine*)
Kuhn, R. *et al., Chem. Ber.*, 1957, **90**, 203 (*Tomatines*)
Sato, Y. *et al., J.A.C.S.*, 1957, **79**, 6089 (*Tomatidine, struct*)
Schreiber, K. *et al., Planta Med.*, 1958, **6**, 94 (*Soladulcines*)
Uhle, F.C. *et al., J.O.C.*, 1962, **27**, 656 (*synth, Soladulcidine*)
Schreiber, K. *et al., Annalen*, 1964, **674**, 168 (*Polyanine*)
Budzikiewicz, H. *et al., Tetrahedron*, 1964, **20**, 2265 (*Tomatidine, ms*)
Boll, P.M. *et al., Acta Chem. Scand.*, 1965, **19**, 1365 (*pmr, stereochem*)
Schreiber, K. *et al., Annalen*, 1965, **682**, 219 (*config*)
Schreiber, K. *et al., Phytochemistry*, 1966, **5**, 707 (*isol*)
Adam, G. *et al., Tetrahedron*, 1966, **22**, 3591 (*synth*)
Kennard, O. *et al., J.C.S.(C)*, 1967, 956 (*cryst struct, Tomatidine*)
Tukalo, E.A. *et al., Khim. Prir. Soedin.*, 1971, **7**, 207; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 203 (*Soladulcines*)
Roddick, J.G. *et al., Phytochemistry*, 1974, **13**, 1459 (*biosynth*)
Weston, R.J. *et al., Aust. J. Chem.*, 1977, **30**, 917 (*Tomatidine, cmr*)
Garnero, J. *et al., CA*, 1982, **96**, 148962t (*N-Nitrosotomatidine*)
Osman, S.F. *et al., Phytochemistry*, 1986, **25**, 967 (*Sisunine*)
Willker, W. *et al., Magn. Reson. Chem.*, 1992, **30**, 645-650 (*pmr, cmr*)
Nagaoka, T. *et al., Phytochemistry*, 1993, **34**, 1153 (*5α-Tomatidan-3-one*)
Yahara, S. *et al., Phytochemistry*, 1996, **42**, 169-172 (*Lycoperosides*)
Maxwell, A. *et al., Phytochemistry*, 1996, **42**, 543 (*derivs*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, THG250

Spirosol-5-ene-3,12-diol S-178



$C_{27}H_{43}NO_3$ 429.642

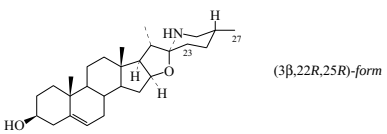
(3β,12β,22*R*,25*R*)-*form* [74131-93-4]
Solanaviol. *Alkaloid SN-b*
Mp 229-232.5°. $[\alpha]_D$ -113 (c, 0.97 in $CHCl_3$).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]:* ***Alkaloid SN-e***. *Solanaviol solanotrioside*
$C_{45}H_{73}NO_{17}$ 900.068
Amorph. powder. $[\alpha]_D$ -53.3 (Py).

3-Ac:
Mp 225-229°.

Kaneko, K. *et al., Phytochemistry*, 1980, **19**, 299 (*Solanaviol*)
Yoshida, X. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1645 (*Alkaloid SN-e*)

Spirosol-5-en-3-ol S-179



(3β,22*R*,25*R*)-*form*

$C_{27}H_{43}NO_2$ 413.642

► WF1300000

(3β,22*R*,25*R*)-*form* [126-17-0]
Solasodine. *Solancarpidine. Purapuridine. Solanidine S. Solancarpine*
Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 200-201°. $[\alpha]_D$ -98 (MeOH). Log P 5.59 (uncertain value) (calc). Dimorph., both forms with same Mp.

► LD_{50} (rat, orl) 4978 mg/kg. Exp. reprod. and teratogenic effects.

Glycoside (1): ***β-Solanigrine***
Alkaloid from *Solanum melanocerasum* (garden huckleberry),. Struct. unknown. Hydrol. gives 2 L-rhamnose, 1 D-glucose and 1 D-galactose.

Glycoside (5): ***α-Solanigrine***
Alkaloid from *Solanum melanocerasum* (garden huckleberry). Sugar residues not identified.

(3β,22*S*,25*S*)-*form* [546-40-7]
Tomatidenol. *Soladulcamaridine. Tomatid-5-en-3-ol*
Mp 235-238° (206°, 226-228°). $[\alpha]_D$ -45 ($CHCl_3$). Soladulcamaridine was shown to be impure Tomatidenol.

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [157604-98-3] ***Dehydrotomatine***. *Tomatidenol 3-lycotetraoside*
$C_{50}H_{81}NO_{21}$ 1032.184
Alkaloid from *Lycopersicon esculentum* (tomato).

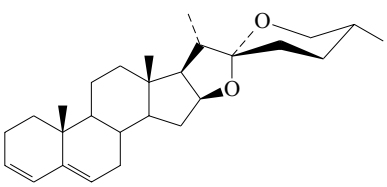
3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-β-D-galactopyranoside]:* [20318-30-3] ***α-Solamarine***
$C_{45}H_{73}NO_{16}$ 884.069
Alkaloid from *Solanum juzepczukii* (bitter potato). Mp 278-281° dec. $[\alpha]_D^{20}$ -45 (c, 0.65 in Py).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* [3671-38-3] ***β-Solamarine***
$C_{45}H_{73}NO_{15}$ 868.069
Alkaloid from *Solanum juzepczukii* (bitter potato). Mp 275-277° dec. $[\alpha]_D^{20}$ -85.6 (c, 0.4 in Py). Log P 1.31 (uncertain value) (calc).

3-O-*[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* [11034-34-7] ***γ$_2$-Solamarine***. *γ-Solamarine*
$C_{39}H_{63}NO_{11}$ 721.927
Alkaloid from *Solanum juzepczukii* (bitter potato). Mp 243-248° dec. $[\alpha]_D^{20}$ -86 (c, 0.36 in Py).

Schreiber, K. *et al., Planta Med.*, 1958, **6**, 435 (*Solanigrines*)
Rönsch, H. *et al., Phytochemistry*, 1966, **5**, 1227 (*Solamarines*)
Friedman, M. *et al., J. Agric. Food Chem.*, 1997, **45**, 1541-1547 (*Dehydrotomatine*)
Weissenberg, M. *et al., Phytochemistry*, 2001, **58**, 501-508 (*β-Solamarine, cmr, ms*)

Spirosta-3,5-diene, 9CI S-180



$C_{27}H_{40}O_2$ 396.612

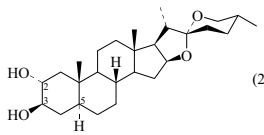
(25*R*)-*form* [1672-65-7]
Δ^{3,5}-Deoxytigogenin
Isol. from *Balanites aegyptiaca* (soapberry tree fruits). Needles ($CHCl_3$/MeOH). Mp 165-167°. $[\alpha]_D^{33}$ -178.8 (c, 1 in $CHCl_3$).

(25*S*)-*form* [37064-21-4]
Δ^{3,5}-Deoxyneotigogenin
Isol. from *Trigonella foenum-graecum* (fenugreek). Cryst. (Me_2CO). Mp 181° (164°). $[\alpha]_D^{25}$ -175 ($CHCl_3$). Prob. artifact.

Wall, M.E. *et al., J.A.C.S.*, 1956, **78**, 1747 (*synth*)
Panizo, F.M. *et al., CA*, 1962, **60**, 853 (*isol*)
Bedour, M.S. *et al., J. Pharm. Sci.*, 1964, **53**, 1276 (*isol*)
Dawidar, A.A.M. *et al., Phytochemistry*, 1969, **8**, 261 (*isol, 25R-form*)

Hardman, R. *et al., Phytochemistry*, 1972, **11**, 2073 (*resoln*)
Dawidar, A.A.M. *et al., J. Pharm. Sci.*, 1974, **63**, 140 (*ms*)
Irismetov, M.P. *et al., Izv. Akad. Nauk Kaz. SSR, Ser. Khim.*, 1981, 47 (*synth, pmr*)
Minghe, Y. *et al., Planta Med.*, 1983, **49**, 38 (*isol*)
Reddy, K.S. *et al., J.C.S. Perkin 1*, 1984, 987 (*synth*)

Spirostane-2,3-diol S-181



(2α,3β,5α,25*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

(2α,3β,5α,25*R*)-*form* [511-96-6]
Gitogenin. *Digine*
Cryst. (Et_2O). Mp 271-272°. $[\alpha]_D^{25}$ -75 ($CHCl_3$). Log P 5.07 (uncertain value) (calc).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:
$C_{45}H_{74}O_{19}$ 919.068
Constit. of *Allium chinense* (rakkyo).

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-galactopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [109575-83-9] ***Capsicoside E1***. *Capsicosin E1*
$C_{56}H_{92}O_{28}$ 1213.326
Constit. of *Capsicum annuum* seeds.
Cryst. Mp 253-254°. $[\alpha]_D^{20}$ -67 (c, 4.8 in MeOH/$CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranosyl-(1→3)-β-D-glucopyranoside]: [54963-35-8] ***Capsicosin***
$C_{57}H_{94}O_{29}$ 1243.352
Constit. of *Capsicum annuum* root.
Cryst. (MeOH). Mp 285-290° dec. $[\alpha]_D^{22}$ -47 (c, 0.1 in MeOH aq.).

(2α,3β,5α,25*S*)-*form* [6811-13-8]
Neogitogenin
Cryst. (Et_2O). Mp 248°.

3-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside]: [234771-06-3] ***Tuberoside D***
$C_{45}H_{74}O_{17}$ 887.069
Constit. of *Allium tuberosum* (Chinese chives). Amorph. solid. $[\alpha]_D^{24}$ -31.2 (c, 0.33 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside]: [234771-07-4] ***Tuberoside E***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of *Allium tuberosum* (Chinese chives). Amorph. solid. $[\alpha]_D^{22}$ -29.5 (c, 0.3 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:
$C_{45}H_{74}O_{19}$ 919.068
Constit. of *Allium chinense* (rakkyo).

3-O-[β-D-Glucopyranosyl-(1→2)-[β--D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [155545-00-9] ***Cistocardin***
$C_{51}H_{84}O_{24}$ 1081.21
Constit. of *Allium chinense* (rakkyo).
Cryst. +8 H_2O (MeOH). Mp 254°. $[\alpha]_D^{20}$ -47 (c, 1.2 in Py).

(2β,3β,5β,25ξ)-*form*

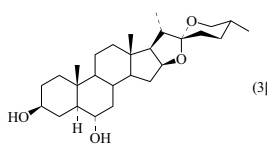
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside]: [267003-05-4] ***Schidigerasaponin F2***
$C_{39}H_{64}O_{14}$ 756.926
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -57.3 (c, 1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-galactopyranoside]: [266998-42-9] ***Schidigerasaponin F1***
$C_{44}H_{72}O_{18}$ 889.042
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -56.2 (c, 1.59 in MeOH).

[469-98-7, 23599-51-1, 61046-17-1, 61046-18-2]

Tschesche, R. *et al., Chem. Ber.*, 1975, **108**, 265 (*Capsicosin*)
Gutsa, E.V. *et al., Khim. Prir. Soedin.*, 1986, **22**, 708; 1987, **23**, 307; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 661; 1987, **23**, 260 (*Capsicosides*)
Achenbach, H. *et al., Phytochemistry*, 1994, **35**, 1527-1543 (*Cistocardin*)
Kuroda, M. *et al., Phytochemistry*, 1995, **40**, 1071 (*Allium chinense saponins*)
Sang, S. *et al., J. Nat. Prod.*, 1999, **62**, 1028-1029 (*Tuberosides D and E*)
Miyakoshi, M. *et al., J. Nat. Prod.*, 2000, **63**, 332-338 (*Schidigerasaponins*)
Plock, A. *et al., Phytochemistry*, 2001, **57**, 489-496 (*Yucca filamentosa saponin*)

Spirostane-3,6-diol, 9CI S-182



(3β,5α,6α,25*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

(3β,5α,6α,25*R*)-*form* [562-34-5]
Chlorogenin
Cryst. (MeOH aq.), needles ($CHCl_3$). Mp 275-276°. $[\alpha]_D^{25}$ -64 ($CHCl_3$). Log P 4.21 (uncertain value) (calc).

3,6-Diketone: [3514-59-8] *Spirostane-3,6-dione*. ***Chlorogenone***
$C_{27}H_{40}O_4$ 428.611
Isol. from fruits of *Solanum torvum* (pea eggplant). Cryst. (Me_2CO). Mp 243.5-244.5° (233-236°).

(3β,5α,6α,25*S*)-*form* [511-91-1]
Neochlorogenin
Aglycone from *Solanum torvum* (pea eggplant). Cryst. (Me_2CO). Mp 262° (252-256°). $[\alpha]_D^{21}$ -61 (c, 3.2 in MeOH).

3-O-[β-L-Rhamnopyranosyl-(1→2)-β-L-rhamnopyranoside]: [99956-65-7] ***Torvonin A***
$C_{39}H_{64}O_{12}$ 724.927
Constit. of *Solanum torvum* (pea eggplant). Powder. Mp 285°. $[\alpha]_D$ -37.3 (c, 0.3 in Py).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [186545-52-8] ***Isoeruboside B***
$C_{51}H_{84}O_{24}$ 1081.21
Constit. of fresh garlic bulbs (*Allium sativum*). Cryst. Mp 310-312°. $[\alpha]_D^{20}$ -32.8 (c, 1 in Py).

(3β,5α,6β,25*R*)-*form* [41743-71-9]
β-Chlorogenin
Cryst. (C_6H_6). Mp 231-233°. $[\alpha]_D^{25}$ -74.2 (c, 1.42 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [145594-56-5]
$C_{50}H_{82}O_{23}$ 1051.184
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -57 (MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [72994-87-7] ***Eruboside B***
$C_{51}H_{84}O_{24}$ 1081.21
From *Allium sativum* (fresh garlic bulbs). Amorph. Sol. MeOH, Py; fairly sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D^{21}$ -61.3 (c, 0.5 in Py).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [244764-96-3]
$C_{56}H_{92}O_{28}$ 1213.326
Constit. of *Allium porrum* (leek). $[\alpha]_D^{25}$ -56 (MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside]: [256642-44-1]
$C_{45}H_{74}O_{17}$ 887.069
Constit. of *Allium ampeloprasum* (great-head garlic).

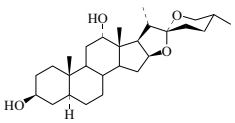
(3β,5β,6α,25*S*)-*form*
25-Epiruizgenin

3-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside]: [265092-99-7]
$C_{39}H_{64}O_{13}$ 740.927
Constit. of *Allium tuberosum* (Chinese chives). Amorph. powder. $[\alpha]_D^{30}$ -60.3 (c, 0.27 in MeOH).

Marker, R.E. *et al., J.A.C.S.*, 1942, **64**, 809-813 (*Chlorogenin, struct*)
Wall, M.E. *et al., J.A.C.S.*, 1955, **77**, 5661-5665 (*3β 5α 6α 25R-form, synth*)
Rippergev, H. *et al., Chem. Ber.*, 1967, **100**, 1741-1752 (*3β 5α 6α 25S-form, synth*)
Chakravarty, A.K. *et al., Tet. Lett.*, 1978, 3875-3878 (*3β 5α 6α 25S-form, isol*)
Chincharadze, D.G. *et al., Khim. Prir. Soedin.*, 1979, **15**, 509-514; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 442-446 (*Eruboside B, β-Chlorogenin*)
Chakravarty, A.K. *et al., Phytochemistry*, 1979, **18**, 902-903 (*3β 5α 6β 25S-form, Hispinin C, synth, pmr*)
Mahmood, U. *et al., Phytochemistry*, 1985, **24**, 2456-2457 (*Torvonin A*)
Usubillaga, A.N. *et al., J. Nat. Prod.*, 1987, **50**, 636-641 (*Chlorogenin, Neochlorogenin, ir, pmr, cmr*)
Cuervo, A.C. *et al., Phytochemistry*, 1991, **30**, 1339-1341 (*diketone, isol*)
Peng, J.P. *et al., Yaoxue Xuebao*, 1996, **31**, 607-612 (*Eruboside B, Isoeruboside B*)

Mimaki, Y. *et al., Nat. Med. (Tokyo)*, 1999, **53**, 134-137; *CA*, **132**, 134748c (*Allium ampeloprasum saponin*)
Carotenuto, A. *et al., Phytochemistry*, 1999, **51**, 1077-1082 (*Allium porrum saponins*)
Ikeda, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 362-365 (*Allium tuberosum saponin*)

Spirostane-3,12-diol S-183



(3β,5α,12α,25*R*)-*form*

$C_{27}H_{44}O_4$ 432.642

(3β,5α,12α,25*R*)-*form* [545-77-7] ***12-Epirockogenin***. *12*-epi-*Rockogenin*
Cryst. (MeOH). Mp 218-220° (214-217°). $[\alpha]_D$ -42.1 ($CHCl_3$).

Di-Ac: [10007-75-7]
Mp 156-159°. $[\alpha]_D^{23}$ -15 (c, 1.0 in Me_2CO).

(3β,5α,12β,25*R*)-*form* [16653-52-4] ***Rockogenin***. *Rocogenin*
Constit. of the famine food *Agave americana*. Cryst. (MeOH), needles (Me_2CO). Mp 218-220° (208-210°).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [354575-45-4]
$C_{63}H_{104}O_{33}$ 1389.495
Amorph. powder. $[\alpha]_D^{25}$ -34 (c, 0.1 in MeOH).

Di-Ac: [10007-76-8]
Mp 204-206°.

(3β,5α,12β,25*S*)-*form* [90457-38-8] ***Dihydrochiapagenin***
Cryst. (MeOH aq.). Mp 194-196° Mp 204-205° (double Mp). $[\alpha]_D$ -79 (c, 1.1 in $CHCl_3$).

12-Ac:
Cryst. (hexane/C_6H_6). Mp 213-214°. $[\alpha]_D$ -84 (c, 0.3 in $CHCl_3$).

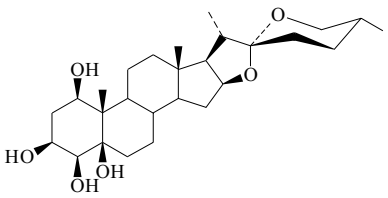
Di-Ac:
Cryst. (MeOH). Mp 204-205°. $[\alpha]_D$ -76 (c, 0.6 in $CHCl_3$).

3,12-Diketone: [32101-23-8] *Spirostane-3,12-dione.* ***Sisalagenone***
$C_{27}H_{40}O_4$ 428.611

(3β,5β,12β,25*R*)-*form* [38673-26-6] ***12β-Hydroxysmilagenin***
Cryst. (Me_2CO). Mp 233-235°. $[\alpha]_D$ -62.3 (c, 0.27 in $CHCl_3$).

Hirschman, R.F. *et al., J.A.C.S.*, 1952, **74**, 2693; 1954, **76**, 4013
Elks, J. *et al., J.C.S.*, 1954, 1739 (*synth, ir*)
Harrison, I.T. *et al., J.O.C.*, 1961, **26**, 155 (*synth, 3β,5α,12β,25S-form*)
Kabasakalian, P. *et al., J.O.C.*, 1961, **26**, 1738 (*synth, 3β,5α,12β,25R-form*)
Nussim, M. *et al., J.O.C.*, 1964, **29**, 1120 (*synth, 3β,5α,12α,25R-form*)
Ricca, G.S. *et al., Gazz. Chim. Ital.*, 1969, **99**, 1284 (*pmr*)
Morales, M. *et al., Rev. Latinoam. Quim.*, 1970, **1**, 1 (*Sisalagenone*)
González, A.G. *et al., An. Quim.*, 1972, **68**, 309 (*isol*)
Garcia, J.A.R. *et al., Magn. Reson. Chem.*, 1987, **25**, 831 (*cmr*)
Arteaga, M.A.I. *et al., Synth. Commun.*, 1999, **29**, 1811-1818 (*di-Ac*)
Kuroda, M. *et al., Chem. Pharm. Bull.*, 2001, **49**, 726-731 (*Camassia leichtlinii saponin*)

Spirostane-1,3,4,5-tetrol S-184



$C_{27}H_{44}O_6$ 464.641

2(1β,3β,4β,5β,25*R*)-*form* [6869-43-8] ***Kitigenin***
Cryst. Mp 298°. $[\alpha]_D^{10}$ -35.

5-O-*β-D-Glucopyranoside:Kitigenin 5-glucopyranoside*
$C_{33}H_{54}O_{11}$ 626.783
Amorph. powder. $[\alpha]_D^{25}$ -38 (c, 0.1 in MeOH).

(1β,3β,4β,5β,25*S*)-*form* [17934-59-7] ***Convallagenin B***
Cryst. (MeOH). Mp 277-278°. $[\alpha]_D$ -42.7 ($CHCl_3$).

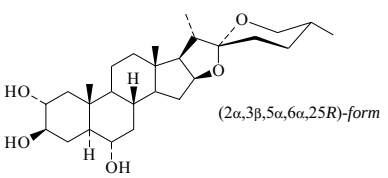
1,3,4-Tri-Ac: [17934-58-6]
Mp 228-230°. $[\alpha]_D$ -46.5.

5-O-*α-L-Arabinopyranoside:* [19317-00-1] ***Convallasaponin B***
$C_{32}H_{52}O_{10}$ 596.757
Needles (MeOH/$CHCl_3$). Mp 273-274°. $[\alpha]_D^{22}$ -55.7 (c, 0.435 in MeOH/$CHCl_3$). V. rare glycosidation of a steroidal sapogenin other than at C-3.

3-O-*β-D-Glucopyranoside, 5*-O-*α-L-arabinopyranoside:* [16939-88-1] ***Glucoconvallasaponin B***
$C_{38}H_{62}O_{15}$ 758.899
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Cryst. (MeOH). Mp 221-222.5°. $[\alpha]_D^{18}$ -35 (Py).

(1β,3β,4α,5β,25*S*)-*form* [110996-55-9] ***Ranmogenin D***
Sasahi, K. *et al., Chem. Pharm. Bull.*, 1961, **9**, 693
Kimura, M. *et al., Chem. Pharm. Bull.*, 1966, **14**, 50; 1967, **15**, 1204; 1968, **16**, 25 (*Convallasaponins*)
Yoshizawa, I. *et al., Chem. Pharm. Bull.*, 1967, **15**, 129 (*isol*)
Agrawal, P.K. *et al., Phytochemistry*, 1985, **24**, 2479 (*cmr*)
Yang, R. *et al., CA*, 1987, **107**, 194913w (*Ranmogenin D*)
Kanmoto, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 926 (*Kitigenin 5-glucopyranoside*)

Spirostane-2,3,6-triol S-185



(2α,3β,5α,6α,25*R*)-*form*

$C_{27}H_{44}O_5$ 448.642

(2α,3β,5α,6α,25*R*)-*form* [58383-94-1] ***Gantogenin***
Cryst. (MeOH). Mp 265-268°. $[\alpha]_D^{20}$ -49.1 (c, 1.01 in $CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [219296-09-0]
$C_{50}H_{82}O_{24}$ 1067.183
Amorph. solid. $[\alpha]_D^{27}$ -42 (c, 0.1 in MeOH).

(2α,3β,5α,6β,25*R*)-*form* [55332-76-8] ***Agigenin***
Mp 265-267°. $[\alpha]_D^{24}$ -74.2 (c, 1.27 in $CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [61478-53-3] ***Aginoside progenin***
$C_{39}H_{64}O_{15}$ 772.926
Constit. of *Allium ampeloprasum* (great-head garlic). Needles (MeOH aq.). Sol. MeOH, Py; fairly sol. H_2O; poorly sol. Me_2CO, hexane. Mp 249-251°. $[\alpha]_D^{17}$ +48.3 (c, 1.1 in Py).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [118524-12-2] ***Ampeloside Bs$_1$***
$C_{45}H_{74}O_{20}$ 935.068
Constit. of *Allium ampeloprasum* (great-head garlic). Needles (MeOH). Sol. MeOH, Py; fairly sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D^{17}$ -52.5 (c, 1.1 in Py). Mp >300°.

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [61478-50-0] ***Aginoside***
$C_{50}H_{82}O_{24}$ 1067.183
Mp 272-276° dec. $[\alpha]_D^{29}$ -66.7 (c, 1.21 in $CHCl_3$/MeOH 10:1).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [218934-75-9] ***Yayoisaponin C***
$C_{51}H_{84}O_{25}$ 1097.21
Constit. of a mutant of *Allium ampeloprasum* (great-head garlic). Amorph. solid. $[\alpha]_D^{23}$ -41.4 (c, 0.21 in Py).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* ***Yayoisaponin A***
$C_{56}H_{92}O_{29}$ 1229.325
Constit. of a mutant of *Allium ampeloprasum* (great-head garlic). Amorph. solid. $[\alpha]_D^{23}$ -44.5 (c, 0.5 in Py). Incorrectly indexed by CA.

2-Ketone, 3-O-*[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [218934-74-8] ***Yayoisaponin B***
$C_{56}H_{90}O_{29}$ 1227.31
Constit. of mutant of *Allium ampeloprasum* (great-head garlic). Amorph. solid. $[\alpha]_D^{23}$ -23 (c, 0.02 in Py).

(2α,3β,5α,6β,25*S*)-*form* [50863-63-3] ***Neoagigenin***
Cryst. (MeOH). Mp 269-270°. $[\alpha]_D^{20}$ -76 (c, 1.45 in $CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-*

xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [68170-51-4] ***Turoside A***
$C_{50}H_{82}O_{24}$ 1067.183
Cryst. (MeOH). Mp 279-284°. $[\alpha]_D^{20}$ -60.9 (c, 0.92 in $CHCl_3$/MeOH).

Tri-Ac:
Cryst. (MeOH). Mp 143-146°. $[\alpha]_D^{20}$ -177.3 (c, 1.76 in $CHCl_3$).

6-Benzoyl: [64791-73-7] *Neoagigenin 6-benzoate*
$C_{34}H_{48}O_6$ 552.75
Cryst. (Et_2O/hexane). Mp 138-140°. $[\alpha]_D^{20}$ -63.7 (c, 1.57 in $CHCl_3$).

(2β,3β,5α,6β,25*R*)-*form* [196607-75-7] ***Porrigenin A***
Constit. of *Allium porrum* (leek). Powder. $[\alpha]_D^{25}$ -20 (c, 0.03 in $CHCl_3$).

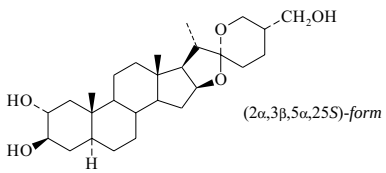
(2β,3β,5α,6β,25*S*)-*form* [196607-76-8] ***Neoporrigenin A***
Constit. of *Allium porrum* (leek). Powder. $[\alpha]_D^{25}$ -37 (c, 0.003 in $CHCl_3$).

(2ξ,3ξ,5α,6ξ,25*R*)-*form* *Magogenin*
Cryst. (petrol). Mp 284°.

Tri-Ac:
Cryst. (MeOH). Mp 214°.

Marker, R.E. *et al., J.A.C.S.*, 1947, **69**, 2399-2401 (*Magogenin*)
Kel'ginbaev, A.N. *et al., Khim. Prir. Soedin.*, 1974, **10**, 801-802; 1975, **11**, 521-522; 1976, **12**, 480-486; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 829-830; 1975, **11**, 546-547; 1976, **12**, 422-426 (*Neoagigenin, Agigenin, Gantogenin, Aginoside*)
Pirtskhalava, G.V. *et al., Khim. Prir. Soedin.*, 1977, **13**, 532-533; 534-537; 1978, **14**, 355-360; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 446-448; 1978, **14**, 294-298; 459-460 (*Neoagigenin 6-benzoate, Turoside A*)
Morita, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3480-3483 (*Ampeloside Bs_1, Aginoside progenin*)
Carotenuto, A. *et al., J. Nat. Prod.*, 1997, **60**, 1003-1007 (*isol, pmr, cmr*)
Sata, N. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1904-1911 (*Yayoisaponins, Aginoside*)
Mimaki, Y. *et al., J. Nat. Prod.*, 1999, **62**, 194-197 (*Allium jesdianum constit*)

Spirostane-2,3,27-triol, 9CI S-186



$C_{27}H_{44}O_5$ 448.642

(2α,3β,5α,25*S*)-*form* [27303-32-8] ***Crestagenin***
Mp 255-260°. $[\alpha]_D$ -44.

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [373647-08-6] ***Tuberoside J***
$C_{39}H_{64}O_{14}$ 756.926
Constit. of Chinese chive seeds (*Allium tuberosum*). Amorph. solid. $[\alpha]_D^{24}$ -35.1 (c, 0.28 in MeOH).

3-O-[α-L-Rhamopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside]: [366464-43-9] ***Tuberoside. Tuberoside K***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of seeds of Chinese chives (*Allium tuberosum*). Amorph. powder. Mp 292-293°. $[\alpha]_D^{25}$ -33 (c, 0.02 in MeOH). $[\alpha]_D^{23}$ -39.8 (c, 0.3 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside], 27-O-β-D-glucopyranoside: [373647-11-1] ***Tuberoside L***
$C_{51}H_{84}O_{23}$ 1065.211
Constit. of Chinese chives seeds (*Allium tuberosum*). Amorph. solid. $[\alpha]_D^{25}$ -46.4 (c, 0.44 in MeOH).

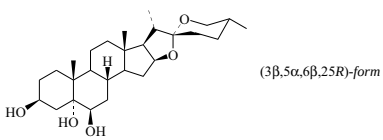
Tri-Ac: [27303-33-9]
Mp 196-201°. $[\alpha]_D$ -94 ($CHCl_3$).

(2β,3α,5β,25*S*)-*form* [21152-89-6] ***Igagenin***
Mp 248-249°. $[\alpha]_D$ -43.6 ($CHCl_3$).

Tri-Ac: [21152-92-1]
Mp 191-192°. $[\alpha]_D$ -15 ($CHCl_3$).

Yasuda, F. *et al., Tetrahedron*, 1968, **24**, 6535 (*Igagenin*)
Delgado, J.M. *et al., An. Quim.*, 1969, **65**, 817 (*Crestagenin*)
Gonzalez, A.G. *et al., An. Quim.*, 1972, **68**, 1021 (*Crestagenin*)
Gonzalez, A.G. *et al., Farmaco, Ed. Sci.*, 1983, **38**, 3 (*props*)
Sang, S. *et al., J. Agric. Food Chem.*, 2001, **49**, 4780-4783 (*Tuberosides J-L*)
Zou, Z.-M. *et al., Phytochemistry*, 2001, **57**, 1219-1222 (*Tuberoside*)

Spirostane-3,5,6-triol S-187



$C_{27}H_{44}O_5$ 448.642

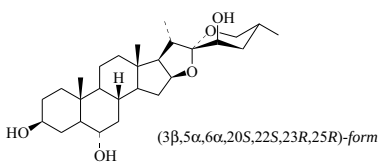
(3β,5α,6β,25*R*)-*form* [56816-69-4] ***Anzurogenin D***
Cryst. (MeOH). Mp 290-292°. $[\alpha]_D^{20}$ -86.4 (c, 1.24 in EtOH).

(3β,5β,6α,25*S*)-*form*

3-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside]: [265092-98-6]
$C_{39}H_{64}O_{14}$ 756.926
Constit. of *Allium tuberosum* (Chinese chives). Amorph. powder. $[\alpha]_D^{29}$ -61.1 (c, 0.14 in MeOH).

Kravets, S.D. *et al., Khim. Prir. Soedin.*, 1994, **30**, 443; *Chem. Nat. Compd. (Engl. Transl.)*, 1994, **30**, 408 (*isol, pmr*)
Ikeda, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 362-365 (*Allium tuberosum saponin*)

Spirostane-3,6,23-triol S-188



$C_{27}H_{44}O_5$ 448.642

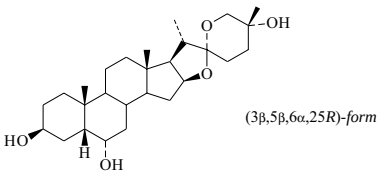
(3β,5α,6α,20*S*,22*S*,23*R*,25*S*)-*form* [76094-30-9] ***Neosolaspigenin***
Mp 236-240°. $[\alpha]_D$ -70.8 ($CHCl_3$/EtOH).

6-O-[α-L-Rhamnopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside]: [185012-38-8] ***Torvoside C***
$C_{39}H_{64}O_{13}$ 740.927
Constit. of *Solanum torvum* (pea eggplant). Amorph. powder. $[\alpha]_D^{27}$ -47.9 (c, 2.9 in MeOH).

6-O-[β-D-Xylopyranosyl-(1→3)-6-deoxy-β-D-glucopyranoside]: ***Torvoside D***
$C_{38}H_{62}O_{13}$ 726.9
Constit. of *Solanum torvum* (pea eggplant). Amorph. powder. $[\alpha]_D^{27}$ -30.7 (c, 2.7 in MeOH). Stereochem. incorr. cited in CAS.

Yahara, S. *et al., Phytochemistry*, 1996, **43**, 1069-1074 (*Torvosides*)

Spirostane-3,6,25-triol S-189



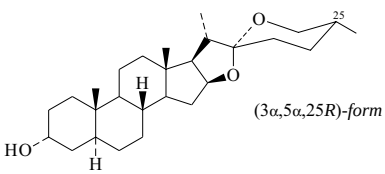
$C_{27}H_{44}O_5$ 448.642

(3β,5β,6α,25*R*)-*form* [17305-15-6] ***Asperagenin***
Isol. from *Smilax aspera* (Sarsaparilla). Mp 265-268°. $[\alpha]_D$ -135.9 ($CHCl_3$).

Tri-Ac:
Mp 185-186°. $[\alpha]_D$ -89 ($CHCl_3$).

Ayengar, K.N.N. *et al., Curr. Sci.*, 1967, **36**, 653 (*isol, ir, nmr*)
Rangaswami, S. *et al., J. Res. Indian Med.*, 1968, **3**, 1 (*isol*)

Spirostan-3-ol S-190



$C_{27}H_{44}O_3$ 416.643

(3β,5α,25*R*)-*form* [77-60-1] ***Tigogenin***. *22-Isoallospirostan-3β-ol*
Cryst. + $1H_2O$ (EtOH aq.). Mp 205-206°. $[\alpha]_D^{18}$ -67.2 ($CHCl_3$).

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3-O-β-D-Glucopyranoside: [35068-81-6] ***Melongoside A***
$C_{33}H_{54}O_8$ 578.785
Constit. of aubergine (*Solanum melongena*). Cryst. (MeOH). Mp 267-270°.

3-O-β-D-Galactopyranoside: [35959-24-1] ***Capsicoside A_2***
$C_{33}H_{54}O_8$ 578.785
Constit. of bell pepper (*Capsicum annuum*) roots.

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-galactopyranoside]: [110124-76-0] ***Capsicoside B_2***
$C_{39}H_{64}O_{13}$ 740.927
Constit. of bell pepper (*Capsicum annuum*).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [94805-84-2] ***Melongoside E***
$C_{39}H_{64}O_{13}$ 740.927
Constit. of aubergine (*Solanum melongena*). Cryst. (MeOH). Mp 265-268°. $[\alpha]_D$ -52.3 (MeOH).

3-O-[β-D-Xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-galactopyranoside]: [125456-09-9] ***Capsicoside C_2***
$C_{44}H_{72}O_{17}$ 873.043
Constit. of bell pepper (*Capsicum annuum*) roots.

3-O-[α-L-Rhamnopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]: [94805-86-4] ***Melongoside G***
$C_{45}H_{74}O_{17}$ 887.069
Constit. of aubergine (*Solanum melongena*).

3-O-[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→3)]-β-D-glucopyranoside]: [95522-98-8] ***Melongoside L***
$C_{57}H_{94}O_{27}$ 1211.353
Constit. of aubergine (*Solanum melongena*). Cryst. Mp 290°. $[\alpha]_D^{20}$ -105 (c, 1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [126643-24-1] ***Sativoside R2***
$C_{56}H_{92}O_{27}$ 1197.327
Constit. of garlic roots (*Allium sativum*). Cryst. + $4H_2O$ (MeOH/$CHCl_3$). Mp 265-270° dec. $[\alpha]_D^{26}$ -51.5 (c, 0.51 in Py).

(3β,5α,25*S*)-*form* [470-01-9]
Neotigogenin
Constit. of currant tomato (*Lycopersicon pimpinellifolium*). Cryst. + EtOH (EtOH). Mp 202-203°. $[\alpha]_D^{26}$ -64.9 ($CHCl_3$).

3-O-[β-D-Fucopyranosyl-(1→6)-β-D-glucopyranoside]: [166736-13-6] ***Smilanippin A***
$C_{39}H_{64}O_{12}$ 724.927
Constit. of Japanese sarsaparilla root (*Smilax nipponica*).

3-O-[β-D-Glucopyranosyl-(1→4)-[α-L-arabinopyranosyl-(1→6)]-β-D-glucopyranoside]: [181492-99-9]
$C_{44}H_{72}O_{17}$ 873.043
Constit. of sarsaparilla rhizome (*Smilax officinalis*). Amorph. powder (MeOH). $[\alpha]_D$ -30.2 (c, 0.3 in EtOH).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [75556-25-1] ***Tomatoside B***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of tomato (*Lycopersicon esculentum*). Cryst. Mp 267-270° dec. $[\alpha]_D^{20}$ -50.5 (c, 0.9 in Py).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-6-O-acetyl-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [226713-77-5] ***Neomacrostemonoside D***
$C_{53}H_{86}O_{24}$ 1107.248
Constit. of *Allium chinense* (rakkyo). Amorph. powder. Mp 272-274°.

(3β,5β,25*R*)-*form* [126-18-1]
Smilagenin. *Isosarsapogenin*
Constit. of Jamaica sarsaparilla (*Smilax ornata*). Cryst. (Me_2CO). Mp 185°. $[\alpha]_D^{25}$ -69 (c, 0.5 in $CHCl_3$).

3-O-[β-D-Glucopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→6)]-β-D-glucopyranoside]: [244762-26-3]
$C_{44}H_{72}O_{17}$ 873.043
Constit. of the wild asparagus (*Asparagus africanus*). Flakes (MeOH). Mp 266-267°. $[\alpha]_D^{20}$ +57 (c, 0.05 in CH_2Cl_2). λ_{max} 230 (MeOH).

3-Ketone: [512-07-2] *Spirostan-3-one.* ***Smilagenone***. *25-Episarsasapogenone*
Constit. of the wild yam *Dioscorea deltoidea*. Mp 188-189°.

(3β,5β,25*S*)-*form* [126-19-2]
Sarsasapogenin. *Parigenin*
Constit. of Radix sarsaparilla (sarsaparilla root). Cryst. (Me_2CO). Mp 200-201.5°. $[\alpha]_D^{25}$ -75 ($CHCl_3$).

3-O-β-D-Glucopyranoside: [14835-43-9] ***Asparagoside A***. *Sarsasaponin monoglucoside*
$C_{33}H_{54}O_8$ 578.785
Isol. from rhizomes of Mexican sarsaparilla (*Smilax aristolochiaefolia*) and from asparagus (*Asparagus officinalis*) root. Needles (MeOH). Mp 245-247°. $[\alpha]_D^{20}$ -65.1 (c, 0.68 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]: [60267-23-4] ***Asparagoside C***
$C_{39}H_{64}O_{13}$ 740.927
Constit. of asparagus (*Asparagus officinalis*) root. Mp 287-290°. $[\alpha]_D^{20}$ -13 (c, 0.4 in H_2O).

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [96351-58-5] ***Desglucodesrhamnoparillin***
$C_{39}H_{64}O_{13}$ 740.927
Isol. from rhizomes of Mexican sarsaparilla (*Smilax aristolochiaefolia*). Needles + $1H_2O$ (MeOH aq.). Mp *ca.*° 250-265. $[\alpha]_D^{20}$ -65.5 (c, 0.80 in $CHCl_3$/EtOH 1:1).

3-O-[α-L-Rhamnopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]: [11025-83-5] ***Desglucoparillin***
$C_{45}H_{74}O_{17}$ 887.069
Isol. from Mexican sarsaparilla root (*Smilax aristolochiaefolia*). Cryst. + $2H_2O$ (EtOH aq.). Mp 250-265°. $[\alpha]_D^{20}$ -67.5 (c, 1.18 in EtOH).

3-O-[α-D-Galactopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside]: [55826-88-5] ***Yuccoside C***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of asparagus (*Asparagus officinalis*). Amorph.

▶ LZ6400000

3-O-[β-D-Glucopyranosyl-(1→4)-[α-L-arabinopyranosyl-(1→6)]-β-D-glucopyranoside]: [181492-98-8]
$C_{44}H_{72}O_{17}$ 873.043
Constit. of sarsaparilla root (*Smilax officinalis*). Amorph. powder (MeOH). $[\alpha]_D^{25}$ -49.3 (c, 0.3 in EtOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→4)]-β-D-glucopyranoside]: [131622-60-1] ***AS 1***
$C_{44}H_{72}O_{17}$ 873.043
Constit. of *Asparagus officinalis* (asparagus). Cryst. Mp 182-184°. $[\alpha]_D^{24}$ -26.8 (c, 0.1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside]: [60267-24-5] ***Asparagoside D***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of asparagus (*Asparagus officinalis*) roots. Mp 246-250°. $[\alpha]_D^{20}$ -166 (c, 0.43 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→2)]-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]: [19057-61-5] ***Parillin***
$C_{51}H_{84}O_{22}$ 1049.211
Constit. of Mexican sarsaparilla root (*Smilax aristolochiaefolia*). Cryst. + $2H_2O$ (MeOH). Mp 220-223°. $[\alpha]_D^{20}$ -64 (c, 1 in EtOH). Log P -1.41 (uncertain value) (calc).

▶ LD_{50} (mus, ipr) 10 mg/kg. RW2000000

3-O-[β-D-Glucopyranosyl-(1→3)-[α-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside]: [60267-26-7] ***Asparagoside F***
$C_{50}H_{82}O_{22}$ 1035.185
Constit. of asparagus (*Asparagus officinalis*) roots. Amorph.

(3β,5β,25ξ)-*form*

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [266998-04-3] ***Schidigerasaponin D5***
$C_{39}H_{64}O_{13}$ 740.927
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -44.4 (c, 0.65 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-galactopyranoside]: [168960-80-3] ***Schidigerasaponin D2***
$C_{44}H_{72}O_{17}$ 873.043
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{28}$ -56.4 (c, 0.93 in Py).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranoside]: [266997-53-9] ***Schidigerasaponin D1***
$C_{44}H_{72}O_{17}$ 873.043
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -42.5 (c, 1.1 in MeOH).

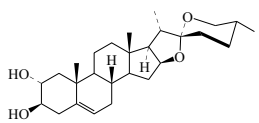
3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-galactopyranoside]: [266998-01-0] ***Schidigerasaponin D4***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{28}$ -35.7 (c, 0.79 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]: [266997-85-7] ***Schidigerasaponin D3***
$C_{45}H_{74}O_{18}$ 903.069
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{28}$ -42.5 (c, 0.88 in MeOH).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 564A (*nmr*)

Wall, M.E. *et al., J.A.C.S.*, 1955, **77**, 5661-5665 (*20α, 20β, synth*)
Mazur, Y. *et al., J.A.C.S.*, 1959, **81**, 3161-3162 (*Tigogenin, Neotigogenin*)
Chakravarti, R.N. *et al., J. Indian Chem. Soc.*, 1961, **38**, 635-641 (*Smilagenone*)
Kutney, J.P. *et al., Steroids*, 1963, **2**, 225-235 (*pmr*)
Callow, R.K. *et al., J.C.S.(C)*, 1966, 288-297 (*struct, pmr, Tigogenin Ac, Neotigogenin Ac*)
Kazuo, T. *et al., Tet. Lett.*, 1981, 2405-2408 (*cmr*)
Benidze, M.M. *et al., Khim. Prir. Soedin.*, 1987, **23**, 537-542; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 448-452 (*Yuccaloisides*)
Shimoyamada, M. *et al., Agric. Biol. Chem.*, 1990, **54**, 2553-2557 (*AS 1*)
Debella, A. *et al., Phytochemistry*, 1999, **51**, 1069-1075 (*glucosylarabinosylglucoside*)
Jiang, Y. *et al., Stud. Plant Sci.*, 1999, **6**, 212-219 (*Neomacrostemonoside D*)
Miyakoshi, M. *et al., J. Nat. Prod.*, 2000, **63**, 332-338 (*Schidigerasaponins*)

Spirost-5-ene-2,3-diol, 9CI S-191



(2α,3β,25*R*)-*form*

$C_{27}H_{42}O_4$ 430.626

(2α,3β,25*R*)-*form* [511-97-7]
Yuccagenin
Cryst. (Et_2O). Mp 252°. $[\alpha]_D^{25}$ -120 ($CHCl_3$).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranoside]: [139606-31-8] ***Fistuloside A***
$C_{39}H_{62}O_{13}$ 738.911
Constit. of *Allium fistulosum* (Welsh onion). Amorph. powder (MeOH). Mp 238-240°. $[\alpha]_D^{21}$ -64 (c, 0.08 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-β-D-galactopyranoside]: [142287-77-2] ***Fistuloside B***
$C_{45}H_{72}O_{18}$ 901.053
Constit. of *Allium fistulosum* (Welsh onion). Amorph. powder (MeOH). $[\alpha]_D^{21}$ -98 (c, 0.16 in Py). Mp >300°.

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [142293-74-1] ***Fistuloside C***
$C_{45}H_{72}O_{19}$ 917.052
Constit. of *Allium fistulosum* (Welsh onion). Needles (MeOH). Mp 230-233°. $[\alpha]_D^{21}$ -48 (c, 0.15 in Py).

3-O-[(3-Hydroxy-3-methylglutaroyl)-(→4)-β-D-xylopyranosyl-(1→3)-[β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [86408-16-4] ***Karatavioside B***
$C_{56}H_{88}O_{27}$ 1193.295

3-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside]: [319481-57-7]
$C_{51}H_{82}O_{21}$ 1031.196
Amorph. powder. $[\alpha]_D^{24}$ -93.3 (c, 0.12 in $CHCl_3$/MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [70880-60-3] ***Karatavioside A***
$C_{50}H_{80}O_{23}$ 1049.168

Di-Ac:
Mp 178°. $[\alpha]_D$ -139.

(2α,3β,25*S*)-*form* [469-99-8] ***Lilagenin***.
Neoyuccagenin. Liligenin
Cryst. (EtOH). Mp 245-246°.

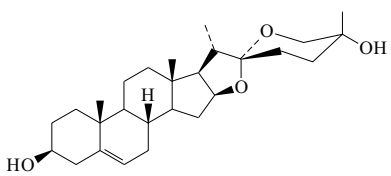
3-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside]: [265092-97-5] ***β-Chacotriosyllilagen***
$C_{45}H_{72}O_{17}$ 885.054
Constit. of *Allium tuberosum* (Chinese chives). Amorph. powder. $[\alpha]_D^{29}$ -94.2 (c, 0.12 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]: [195304-82-6] ***Anemarsaponin G***
$C_{50}H_{80}O_{23}$ 1049.168
Amorph. powder. Mp 258° dec.

Di-Ac:
Mp 155°.

Marker, R.E. *et al., J.A.C.S.*, 1940, **62**, 2620; 1947, **69**, 24; 2167; 2373; 2389 (*isol, struct, Yuccagenin*)
Pataki, J. *et al., J.A.C.S.*, 1951, **73**, 5375 (*Lilagenin*)
Herran, J.F. *et al., J.A.C.S.*, 1954, **76**, 5531 (*struct*)
Gonzalez, A.G. *et al., Phytochemistry*, 1974, **13**, 627 (*isol*)
Pirtskhalava, G.V. *et al., Khim. Prir. Soedin.*, 1977, **13**, 823; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 693 (*isol, struct*)
Vollerner, Y.S. *et al., Khim. Prir. Soedin.*, 1978, 740; 1983, 197 (*Karataviosides*)
Do, J.C. *et al., J. Nat. Prod.*, 1992, **55**, 168-173 (*Fistulosides*)
Ma, B. *et al., Planta Med.*, 1997, **63**, 376-379 (*Anemarsaponin G*)
Ikeda, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 362-365 (*β-Chacrotriosyllilagen*)
Mimaki, Y. *et al., J. Nat. Prod.*, 2001, **64**, 17-22 (*Cestrum nocturnum saponin*)

Spirost-5-ene-3,25-diol S-192



$C_{27}H_{42}O_4$ 430.626

(3β,25*S*)-*form* [7050-41-1]
Isonuatigenin
Cryst. (MeOH). Mp 260-262° (248-251°). $[\alpha]_D^{23}$ -123 (c, 2 in $CHCl_3$).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:
$C_{39}H_{62}O_{13}$ 738.911
Isol. from *Allium vineale* (wild garlic).

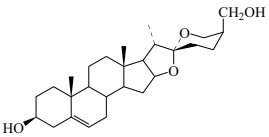
3-O-[α-L-Rhamnopyranosyl-(1→2)[α-L-rhamnopyranosyl-(1→4)]-β-D-glucopyranoside]: [173740-42-6]
$C_{45}H_{72}O_{17}$ 885.054

3-Ac:
Needles (MeOH/petrol). Mp 215.5-218.5°. $[\alpha]_D^{22}$ -140 (c, 2 in $CHCl_3$).

Di-Ac:
Cryst. (petrol). Mp 211.5-215.5°. $[\alpha]_D^{27}$ -109 (c, 2 in $CHCl_3$).

Tschesche, R. *et al., Tetrahedron*, 1964, **20**, 387 (*isol*)
Faini, F. *et al., Phytochemistry*, 1984, **23**, 1301 (*isol*)
Agrawal, P.K. *et al., Phytochemistry*, 1985, **24**, 2479 (*cmr*)
Chen, S. *et al., Tet. Lett.*, 1987, **28**, 5603 (*glycoside*)
Chen, C.X. *et al., CA*, 1996, **124**, 170602 (*3-dirhamnosylglucoside*)

Spirost-5-ene-3,27-diol S-193



(3β,25*R*)-*form*

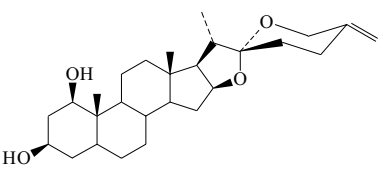
$C_{27}H_{42}O_4$ 430.626

(3β,25*S*)-*form* [7050-40-0]
Isonarthogenin
Prisms (MeOH). Mp 240-242°. $[\alpha]_D^{23}$ -110.2 (c, 0.65 in $CHCl_3$). Note that Isonarthogenin itself has (25*S*)-config. but its 27-esters are (25*R*)-.

3-O-[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside], 27-O-β-D-glucopyranoside: [62751-68-2] ***Deltoside***
$C_{51}H_{82}O_{23}$ 1063.195
Constit. of the wild yam *Dioscorea deltoidea*.

Lukoyanova, M.A. *et al., Dokl. Akad. Nauk SSSR*, 1978, **239**, 736 (*Deltoside*)

Spirost-25(27)-ene-1,3-diol S-194



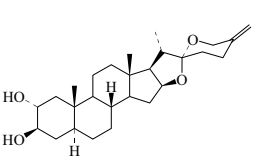
$C_{27}H_{42}O_4$ 430.626

(1β,3β,5α)-*form* [90865-22-8]
Australigenin
Sapogenin from *Cordyline australis* (cabbage tree). Oil.

(1β,3β,5β)-*form* [16683-27-5]
Convallamarogenin
Sapogenin from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Cryst. (MeOH). Mp 258-263°. $[\alpha]_D^{27}$ -78 (c, 0.92 in $CHCl_3$).

Blunden, G. *et al., J. Nat. Prod.*, 1984, **47**, 266 (*Australigenin, Hydroxycrabbogenin*)

Spirost-25(27)-ene-2,3-diol S-195



(2α,3β,5α)-*form*

$C_{27}H_{42}O_4$ 430.626

(2α,3β,5α)-*form* [3514-45-2]
Dehydrogitogenin
Cryst. (MeOH). Mp 266-267° (242-243°). $[\alpha]_D^{25}$ -80.1 (c, 0.507 in $CHCl_3$).

Di-Ac:
Mp 226-228°. $[\alpha]_D$ -97.1 ($CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [164592-98-7]
$C_{56}H_{90}O_{28}$ 1211.31
Amorph. powder. $[\alpha]_D^{26}$ -44 (c, 0.1 in MeOH).

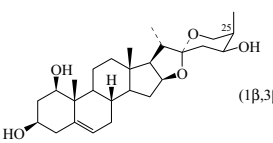
(2β,3β,5β)-*form* [267003-22-5] ***Schidigeragenin C***
Genin from *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{23}$ -85 (c, 0.24 in $CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-galactopyranoside]:* [266997-36-8] ***Schidigerasaponin C2***
$C_{39}H_{62}O_{14}$ 754.91
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -38.2 (c, 0.55 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-galactopyranoside]:* [266997-35-7] ***Schidigerasaponin C1***
$C_{44}H_{70}O_{18}$ 887.026
Constit. of *Yucca schidigera* (Mojave yucca). Amorph. powder. $[\alpha]_D^{24}$ -56.4 (c, 0.11 in MeOH).

Takeda, K. *et al., Tetrahedron*, 1965, **21**, 2089; 2742 (*isol, struct*)
Mimaki, Y. *et al., Phytochemistry*, 1995, **38**, 1279 (*saponin*)
Miyakoshi, M. *et al., J. Nat. Prod.*, 2000, **63**, 332-338 (*Schidigerasaponins*)
Mimaki, Y. *et al., J. Nat. Prod.*, 2001, **68**, 17-27 (*Cestrum nocturnum saponin, isol, activity*)

Spirost-5-ene-1,3,24-triol S-196



(1β,3β,24S,25R)-*form*

$C_{27}H_{42}O_5$ 446.626

(1β,3β,24*S*,25*R*)-*form*

1-O-*β-D-Fucopyranoside, 24*-O-*β-D-glucopyranoside:* [295313-06-3] ***Surculoside B***
$C_{39}H_{62}O_{14}$ 754.91
Amorph. solid. $[\alpha]_D^{25}$ -114 (c, 0.1 in $CHCl_3$/MeOH).

1-O-*β-D-Fucopyranoside, 3*-O-*[β-D-apiofuranosyl-(1→4)-β-D-glucopyranoside]:* [295313-04-1] ***Surculoside A***
$C_{44}H_{70}O_{18}$ 887.026
Amorph. solid. $[\alpha]_D^{25}$ -106 (c, 0.1 in $CHCl_3$/MeOH).

1-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-fucopyranoside], 24*-O-*β-D-glucopyranoside:* [295313-09-6] ***Surculoside C***
$C_{45}H_{72}O_{18}$ 901.053
Amorph. solid. $[\alpha]_D^{25}$ -136 (c, 0.1 in $CHCl_3$/MeOH).

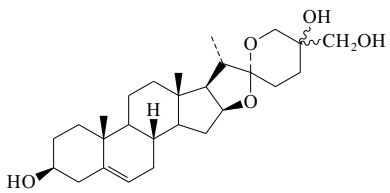
(1β,3β,24*S*,25*S*)-*form* [114317-59-8] ***Cepagenin***
Genin isol from *Allium cepa* (onion). Mp 267-269°.

1-O-*[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranoside]:* [114317-57-6] ***Alliospiroside C***
$C_{38}H_{60}O_{13}$ 724.884
Constit. of *Allium cepa* (onion). Cryst. (MeOH aq.). Mp 223-225°. $[\alpha]_D^{22}$ -105.7 (c, 0.94 in Py).

1-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranoside]:* [114317-58-7] ***Alliospiroside D***
$C_{39}H_{62}O_{14}$ 754.91
Constit. of *Allium cepa* (onion). Cryst. (MeOH). Mp 242-243°. $[\alpha]_D^{22}$ -89.9 (c, 0.75 in Py).

Kravets, S.D. *et al., Khim. Prir. Soedin.*, 1987, **23**, 843-849; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 700-706 (*Cepagenin, Alliospirosides*)
Yokosuka, A. *et al., J. Nat. Prod.*, 2000, **63**, 1239-1243 (*Surculosides*)

Spirost-5-ene-3,25,27-triol S-197

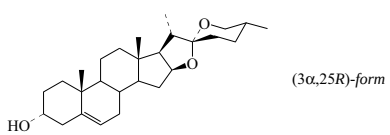


$C_{27}H_{42}O_5$ 446.626

(3β,25ξ)-*form*
Spirotaccagenin
Constit. of *Tacca leontopetaloides* (Polynesian arrowroot). Cryst. Mp 225-227°.

Abdel-Aziz, A. *et al., Phytochemistry*, 1990, **29**, 1643 (*isol, pmr, cmr, ms*)

Spirost-5-en-3-ol S-198



(3α,25R)-*form*

$C_{27}H_{42}O_3$ 414.627

(3β,25*R*)-*form* [512-04-9]
Diosgenin. *Nitogenin. Dioscorea sapogenin*
Cryst. (Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 204-207°. $[\alpha]_D^{25}$ -129 (c, 1.4 in $CHCl_3$). Log P 5.82 (uncertain value) (calc).
▶ LD_{50} (rat, ipr) 4872 mg/kg. LD_{50} (mus, orl) >8000 mg/kg. LD_{50} (mus, ipr) 4000 mg/kg. WH1450000

3-O-*β-D-Galactopyranoside:* [14270-72-5] ***Capsicoside A3***
$C_{33}H_{52}O_8$ 576.769
Constit. of *Capsicum annuum* roots.

3-O-*β-D-Glucopyranoside:* [14144-06-0] ***Trillin***. *Disogluside, INN. Alliumoside A. Collettiside I. Funkioside A. Melongoside B. Polygonatoside A. Polyphyllin A. Prosapogenin D3. WA 185*
$C_{33}H_{52}O_8$ 576.769
Constit. of *Trigonella foenum-graecum* (fenugreek). Cryst. + ½ H_2O (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 275-280° dec. $[\alpha]_D$ -103 (dioxan). Log P 3.54 (uncertain value) (calc).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [19057-67-1] ***Ophiopogonin C′***. *Prosapogenin A*†. *Prosapogenin D′. Progenin III*
$C_{39}H_{62}O_{12}$ 722.912
Constit. of *Allium vineale* (wild garlic). Cryst. (MeOH). Mp 238-240° dec. $[\alpha]_D^{21}$ -99.2 (c, 0.21 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [94805-85-3] ***Melongoside F***
$C_{39}H_{62}O_{13}$ 738.911
Constit. of *Solanum melongena* (aubergine).

3-O-*[β-D-Xylopyranosyl-(1→3)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [125456-10-2] ***Capsicoside C3***
$C_{44}H_{70}O_{17}$ 871.027
Constit. of *Capsicum annuum* roots. Mp 263-265°. $[\alpha]_D^{20}$ -60 (c, 1.0 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside]:* [55659-75-1] ***Deltonin***. *Trilloside A*
$C_{45}H_{72}O_{17}$ 885.054
Constit. of *Allium vineale* (wild garlic). Cryst. Mp 196-200°. $[\alpha]_D^{26}$ -2.2 (c, 1.3 in MeOH). Log P 0.34 (uncertain value) (calc). Deltonin and Trilloside A assumed to be identical but not compared.

3-O-*[α-L-Rhamnopyranosyl-(1→3)-[α-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]:* [89203-43-0] ***Melongoside H***. *Zingiberenin A*
$C_{45}H_{72}O_{17}$ 885.054
Constit. of *Solanum melongena* (aubergine).

3-O-*[α-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)-α-D-glucopyranoside]:* [74350-31-5] ***Graecunin G***
$C_{45}H_{72}O_{17}$ 885.054
Isol. from the leaves of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 123-125°. $[\alpha]_D$ -3 (EtOH).

3-O-*[β-D-Glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-β-D-glucopyranoside]:* [113576-38-8]
$C_{45}H_{72}O_{17}$ 885.054
Constit. of *Allium vineale* (wild garlic).

3-O-*[α-L-Rhamnopyranosyl-(1→3)-[β-D-galactopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside]:* [94696-62-5] ***Melongoside K***
$C_{51}H_{82}O_{22}$ 1047.196
Constit. of *Solanum melongena* (aubergine).

3-O-*[β-D-Glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranoside]:* [113576-37-7]
$C_{51}H_{82}O_{21}$ 1031.196
Constit. of *Allium vineale* (wild garlic). Log P -1.7 (uncertain value) (calc).

3-O-*[α-D-Glucopyranosyl-(1→4)-α-D-glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)-α-D-glucopyranoside]:* [74350-30-4] ***Graecunin E***

$C_{51}H_{82}O_{22}$ 1047.196
Isol. from the leaves of *Trigonella foenum-graecum* (fenugreek). Amorph. powder. Mp 136-138°. $[\alpha]_D$ +24.6 (EtOH).

3-O-[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→3)]-β-D-glucopyranoside]: [95522-99-9] ***Melongoside M***
$C_{57}H_{92}O_{27}$ 1209.338
Constit. of *Solanum melongena* (aubergine). Cryst. Mp 285°. $[\alpha]_D^{20}$ -110 (c, 1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)[α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranoside]: [121372-76-7]
$C_{57}H_{92}O_{26}$ 1193.338
Isol. from *Allium vineale* (wild garlic). Powder.

3-O-[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-galactopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranoside]: [122018-50-2] ***Ceposide D***
$C_{56}H_{90}O_{26}$ 1179.311
Constit. of *Allium cepa* (onion) seed.

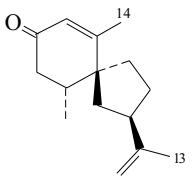
3-O-[β-D-Glucopyranosyl-(1→4)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→2)]-β-D-glucopyranoside]: [121372-77-8]
$C_{63}H_{102}O_{31}$ 1355.48
Isol. from *Allium vineale* (wild garlic). Powder.

[53846-52-9]

Budzikiewicz, H. *et al., Monatsh. Chem.*, 1962, **93**, 1031-1045 (*ms*)
Bite, P. *et al., Acta Chim. Acad. Sci. Hung.*, 1967, **52**, 79-82 (*Trillin, Capsicoside A_3, synth*)
Kessar, S.V. *et al., Tetrahedron*, 1968, **24**, 899-904 (*synth*)
Hardman, R. *et al., Planta Med.*, 1971, **20**, 193 (*biosynth*)
Paseshnichenko, V.A. *et al., Prikl. Biokhim. Mikrobiol.*, 1975, **11**, 94 (*Deltonin*)
Eggert, H. *et al., Tet. Lett.*, 1975, 3635-3638 (*cmr*)
Kintya, P.K. *et al., Khim. Prir. Soedin.*, 1978, **14**, 350-354; 1984, **20**, 610-614; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 290-294; 1984, **20**, 575-578 (*Polygonatoside E', Melongosides, Zingiberenin A*)
Kazuo, T. *et al., Tet. Lett.*, 1981, 2405-2408 (*cmr*)
Watanabe, Y. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3486-3495 (*Deltonin, Ophiopogonin C'*)
Tang, S. *et al., CA*, 1984, **100**, 117829b (*Zingiberenins*)
Varshney, I.P. *et al., J. Nat. Prod.*, 1984, **47**, 44-46 (*Graecunins*)
Ger. Pat., 1985, 3 416 112; *CA*, **104**, 161977 (*Trillin*)
Kintya, P.K. *et al., Phytochemistry*, 1985, **24**, 197-198 (*Melongoside M*)
Agrawal, P.R. *et al., Phytochemistry*, 1985, **24**, 2479-2496 (*cmr*)
Gutsa, E.V. *et al., Khim. Prir. Soedin.*, 1987, **23**, 242-246; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 202-205 (*Capsicoside A_3*)
Tang, S. *et al., CA*, 1988, **108**, 3403 (*Zingiberosides*)
Chen, S. *et al., J.O.C.*, 1989, **54**, 3679-3689 (*Allium vineale saponins*)
Kintya, P.K. *et al., Khim. Prir. Soedin.*, 1989, 139-140; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 124-125 (*Ceposide D*)
Gutsa, E.V. *et al., Khim. Prir. Soedin.*, 1989, **25**, 582-584; *Chem. Nat. Compd. (Engl. Transl.)*, 1989, **25**, 500-501 (*Capsicoside C_3*)
Puri, R. *et al., Magn. Reson. Chem.*, 1993, **31**, 278-282 (*pmr, cmr*)
Deng, S. *et al., J.O.C.*, 1999, **64**, 7265-7266 (*Trillin, synth*)

1(10),11-Spirovetivadien-2-one S-199

[54878-25-0]
Solavetivone. *Katahdinone*



$C_{15}H_{22}O$ 218.338
Stress metab. from potato tubers (*Solanum tuberosum*). Oil. $[\alpha]_D$ -119 (EtOH). λ_{max} 243 (ϵ 12900) (EtOH) (Berdy).

14-Hydroxy: [103573-06-4] *14-Hydroxy-1(10),11-spirovetivadien-2-one.* ***Oxysolavetivone***. *15-Hydroxysolavetivone*
$C_{15}H_{22}O_2$ 234.338
Intermediate metabolite in the pathway to the phytoalexins of potato. Oil. $[\alpha]_D^{21}$ -91.6 (c, 1.00 in EtOH).

13-Hydroxy: [62574-28-1] *13-Hydroxy-1(10),11-spirovetivadien-2-one.* ***Aglycone A_3***
$C_{15}H_{22}O_2$ 234.338

Coxon, D.T. *et al., Tet. Lett.*, 1974, 2921 (*isol, struct*)
Anderson, R.C. *et al., Chem. Comm.*, 1977, 27 (*isol, abs config*)
Yamada, K. *et al., Chem. Comm.*, 1977, 554 (*synth*)
Murai, A. *et al., Chem. Comm.*, 1982, 32 (*biosynth*)
Murai, A. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 2276; 2282 (*synth*)
Murai, A. *et al., Chem. Lett.*, 1986, 771-772 (*Oxysalavetivone*)
Iwata, C. *et al., Chem. Pharm. Bull.*, 1987, **35**, 544 (*synth*)
Hwu, J.R. *et al., J.O.C.*, 1992, **57**, 922 (*Solavetivone, bibl*)
Takemoto, Y. *et al., Tetrahedron*, 1997, **53**, 603-616 (*synth*)
Engstrom, K. *et al., Potato Res.*, 1999, **42**, 43-50; *CA*, **131**, 348943 (*Solavetivone, activity*)

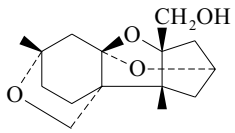
Sporamin S-200

Ipomoein
Protein. MW 25Kd for the monomeric form. Exists in two forms A and B in ca. 2:1 ratio which differ in amino acid sequence.. The major storage protein of sweet potato tubers *Ipomoea batatas* accounting for ca. 80% of total soluble protein. Possesses Trypsin inhibiting activity which may have a defence role against tuber damage.

Maeshima, M. *et al., Phytochemistry*, 1985, **24**, 1899-1902 (*isol, props*)
Hattori, T. *et al., Plant Mol. Biol.*, 1985, **5**, 313-320; 1986, **7**, 343-355 (*struct*)
Yeh, K.W. *et al., Plant Mol. Biol.*, 1997, **33**, 565-570 (*props*)

Sporol S-201

[101401-88-1]

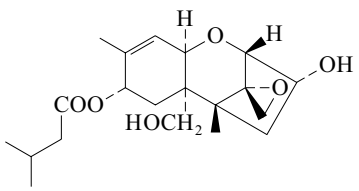


$C_{15}H_{22}O_4$ 266.336
Mycotoxin from *Fusarium sporotrichioides* MC-72083. Oil. Sol. $CHCl_3$, MeOH, C_6H_6, Me_2CO; poorly sol. H_2O, hexane. Related to Sambucinol.

Corley, D.G. *et al., Tet. Lett.*, 1986, **27**, 427 (*isol*)
Ziegler, F.E. *et al., Tet. Lett.*, 1988, **29**, 1665 (*struct*)
Ziegler, F.E. *et al., J.A.C.S.*, 1993, **115**, 2581 (*synth*)

Sporotrichiol S-202

[101401-89-2]
12,13-Epoxy-9-trichothecene-3,8,15-triol 8-(3-methylbutenoate), 9CI

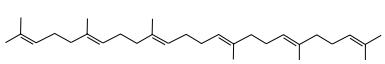


$C_{20}H_{30}O_6$ 366.453
Trichothecene antibiotic. Prod. by *Fusarium sporotrichioides*. Oil. Sol. $CHCl_3$, Me_2CO, MeOH, C_6H_6; poorly sol. H_2O, hexane.

Corley, D.G. *et al., Tet. Lett.*, 1986, **27**, 427 (*isol, struct, nmr*)
Wani, M.C. *et al., J.O.C.*, 1987, **52**, 3468 (*synth*)

Squalene S-203

[7683-64-9]
2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene, 9CI. Spinacene



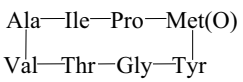
$C_{30}H_{50}$ 410.725
▶ XB6010000
(All-E)-form [111-02-4]
Found in fish liver oils, yeast lipids and many vegetable oils, e.g. palm oil, cottonseed oil, rapeseed oil. Oil. Insol. H_2O; sl. sol. EtOH. Mp -4.8°. Bp_{25} 284-285°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 46A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 33B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 48A (*ir*)
Johnson, W.S. *et al., J.A.C.S.*, 1970, **92**, 741 (*synth*)

Bhalerao, U.T. *et al., J.A.C.S.*, 1971, **93**, 531 (*synth*)
Biellmann, J.F. *et al., Tetrahedron*, 1971, **27**, 5861 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 34 (*occur*)
Grieco, P.A. *et al., J.O.C.*, 1974, **39**, 2135 (*synth*)
Suga, T. *et al., Phytochemistry*, 1975, **14**, 2411 (*biosynth*)
v. Dommelen, M.E. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1975, **94**, 182 (*cmr*)
Johnson, W.S. *et al., Angew. Chem., Int. Ed.*, 1976, **15**, 9 (*rev*)
Ernst, J. *et al., Angew. Chem., Int. Ed.*, 1976, **15**, 778 (*cryst struct*)
Ernst, J. *et al., Annalen*, 1979, 1635 (*cryst struct*)
Belcher, A. *et al., J. Chem. Ecol.*, 1988, **14**, 1367
Nes, W.D. *et al., Phytochemistry*, 1988, **27**, 628 (*biosynth*)
Nordstrom, K.M. *et al., J. Chem. Ecol.*, 1989, **15**, 629

Squamin A S-204

[241486-93-1]

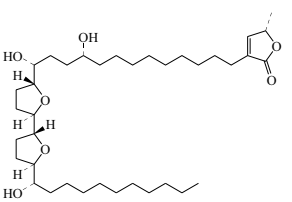


$C_{39}H_{60}N_8O_{11}S$ 849.016
Constit. of *Annona squamosa* (sugar apple). Cryst. $[\alpha]_D^{18}$ -48.4 (MeOH). Mp >300°.

Shi, J.X. *et al., Chin. Chem. Lett.*, 1999, **10**, 299-302

Squamocin F S-205

[159957-81-0]



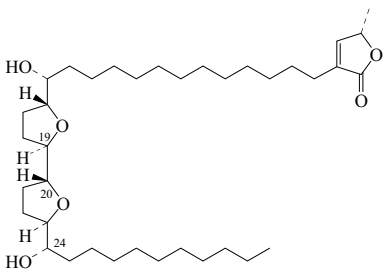
Absolute Configuration

$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona squamosa* (sugar apple). Wax. $[\alpha]_D^{25}$ +21 (c, 0.6 in MeOH).

Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*isol*)
Araya, H. *et al., Phytochemistry*, 2002, **61**, 999-1004 (*abs config*)

Squamocin L S-206

[98767-45-4]
Desacetyluvaricin. Neodesacetyluvaricin



Absolute Configuration

$C_{37}H_{66}O_6$ 606.925
Isol. from *Annona squamosa* (sugar apple). Mp *ca.* ° 25. $[\alpha]_D$ +21.1 (c, 0.5 in $CHCl_3$). λ_{max} 207 (ϵ 12700) (EtOH) (Derep).

24-Ac: [82064-83-3] ***Uvaricin***. *Squamocin L*
$C_{39}H_{68}O_7$ 648.962
Waxy solid. Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 25° approx. $[\alpha]_D^{25}$ +11.3 (MeOH). The first Annonaceous acetogenin to be characterized λ_{max} 210 (ϵ 10000) (no solvent reported) (Derep).

24-Epimer: [136033-39-1] ***Isodesacetyluvaricin***. *4-Deoxyasimicin. Squamocin M*
$C_{37}H_{66}O_6$ 606.925
Isol. from *Annona* spp.. $[\alpha]_D$ +26 (c, 0.5 in MeOH). $[\alpha]_D$ +17.8 (c, 0.006 in $CHCl_3$). Mp < 30°.

19,20-Diepimer: [148152-15-2] ***Membranacin***
$C_{37}H_{66}O_6$ 606.925
$[\alpha]_D$ +22.5 (c, 0.2 in MeOH).

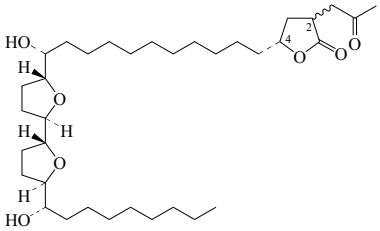
19,20,24-Triepimer: [159993-40-5] ***Squamocin N***
$C_{37}H_{66}O_6$ 606.925
Constit. of the seeds of *Annona squamosa* (sugar apple). Oil. $[\alpha]_D^{25}$ +40.6 (c, 0.4 in MeOH).

[145165-08-8]

Jolad, S.D. *et al., J.O.C.*, 1982, **47**, 3151
Jolad, S.D. *et al., J. Nat. Prod.*, 1985, **48**, 644 (*deriv*)
Hoye, T.R. *et al., J.A.C.S.*, 1987, **109**, 4402; 1991, **113**, 9369 (*synth*)
Hisham, A. *et al., Phytochemistry*, 1991, **30**, 2373 (*Isodesacetyluvaricin*)
Hui, Y.-H. *et al., Nat. Toxins*, 1992, **1**, 4-14 (*4-Deoxyasimicin*)
Saez, J. *et al., J. Nat. Prod.*, 1993, **56**, 351 (*Membranacin*)
Gu, Z. *et al., Tetrahedron*, 1993, **49**, 747 (*Desacetyluvaricin*)
Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*Squamocins*)
Yazbak, A. *et al., J.O.C.*, 1998, **63**, 5863-5868 (*synth*)
Chavez, D. *et al., J. Nat. Prod.*, 1999, **62**, 119-1122 (*Membranacin, abs config*)

Squamolinone S-207

[210230-72-1, 210230-73-2]

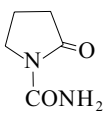


$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona squamosa* (sugar apple). Amorph. powder. $[\alpha]_D$ +21.4 (c, 0.07 in CH_2Cl_2). Isol. as a mixt. of 2,4-*cis*- and *trans*- isomers λ_{max} 203 (log ϵ 2.85) (MeOH).

Hopp, D.C. *et al., Bioorg. Med. Chem.*, 1998, **6**, 569-575

Squamolone S-208

[40451-67-0]
2-Oxo-1-pyrrolidinecarboxamide, 9CI. 1-Carbamoyl-2-pyrrolidone

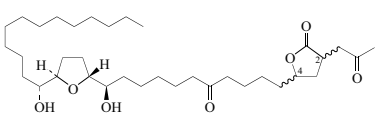


$C_5H_8N_2O_2$ 128.13
An incorrect diazepinedione struct. was originally assigned. Constit. of *Annona squamosa* (sugar apple) and *Asimina triloba* (pawpaw). Prisms (C_6H_6). Mp 148°.

Yang, T.H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1972, **19**, 149; *CA*, **78**, 16151w (*isol, uv, pmr, ms*)
Marquez, V.E. *et al., J.O.C.*, 1980, **45**, 5308 (*struct, synth, ir, pmr, ms*)
Achenbach, H. *et al., Annalen*, 1982, 1623 (*isol, cmr*)
Zhao, G.-X. *et al., Phytochemistry*, 1993, **33**, 1065 (*isol, synth*)
Sahai, M. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 510 (*isol, synth, ir, pmr, cmr, ms*)

Squamone S-209

[126655-24-1]

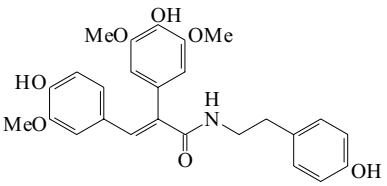


$C_{35}H_{62}O_7$ 594.871
Constit. of *Annona squamosa* (sugar apple) and *Annona reticulata* (custard apple). Waxy solid. Sol. MeOH, hexane; poorly sol. H_2O. Mp 89°. $[\alpha]_D$ +7 (c, 0.1 in $CHCL_3$). Isol. as a mixture of 2,4-*cis*- and *trans*-isomers λ_{max} 204 (ϵ 10800) (MeOH) (Berdy).

Li, X.-H. *et al., J. Nat. Prod.*, 1990, **53**, 81 (*isol, pmr, cmr, ms*)
Chang, F.-R. *et al., J. Nat. Prod.*, 1993, **56**, 1688-1694 (*isol*)

Squamosamide S-210

*4-Hydroxy-α-[(4-hydroxy-3-methoxyphenyl)methylene]-*N*-[2-(4-hydroxyphenyl)ethyl]-3,5-dimethoxybenzeneacetamide, 9CI*



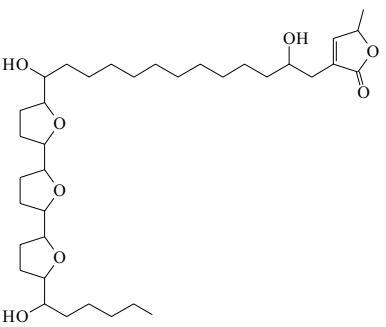
$C_{26}H_{27}NO_7$ 465.502

(*E*)-*form* [142750-35-4]
Isol. from branches of *Annona squamosa* (sugar apple). Mp 206-207°.

Yang, X.J. *et al., Yaoxue Xuebao*, 1992, **27**, 185-190; *CA*, **117**, 86699d (*isol, struct*)
Ji, X. *et al., Chin. Chem. Lett.*, 1993, **4**, 297-298 (*synth, pmr, cmr*)

Squamosinin A S-211

[163597-71-5]

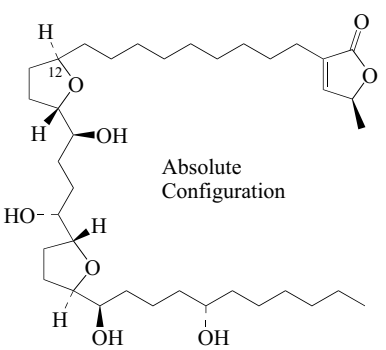


$C_{36}H_{62}O_8$ 622.881
Struct. doubtful due to biogenetic improbability of C-36 chain. Constit. of *Annona squamosa* (sugar apple). $[\alpha]_D$ +24.7 (c, 1.4 in $CHCl_3$).

Yang, R. *et al., Zhiwu Xuebao*, 1994, **36**, 809-812; *CA*, **123**, 5595r (*isol, struct*)

Squamostatin A S-212

[129138-53-0]
Almunequin. Annonin XVI



$C_{37}H_{66}O_8$ 638.924
Constit. of *Annona squamosa* (sugar apple) and *Annona cherimola* (cherimoya). Amorph. wax. Mp 105-126° (87-89°). $[\alpha]_D$ +13.5 (c, 0.1 in $CHCl_3$). $[\alpha]_D$ +25 (c, 0.38 in MeOH).

12-Epimer: ***12,15*-cis-*Squamostatin A***
$C_{37}H_{66}O_8$ 638.924
Constit. of the seeds of *Annona atemoya* (custard apple). Cytotoxic. Oil. Isol. as a mixt. with Squamostatin A.

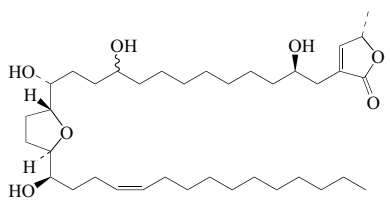
Stereoisomer: ***Squamostatin B***†
$C_{37}H_{66}O_8$ 638.924
Constit. of *Annona squamosa* (sugar apple). Not to be confused with, 24-Epimer. Possible identity with Squamostatin A λ_{max} 219 (ε 3090) (MeOH) (Berdy).

[128232-75-7]

Kawazu, K. *et al., Agric. Biol. Chem.*, 1989, **53**, 2719-2722 (*isol, Annonin*)
Nonfon, M. *et al., Phytochemistry*, 1990, **29**, 1951 (*isol, pmr, cmr, ms*)
Fujimoto, Y. *et al., Tet. Lett.*, 1990, **31**, 535 (*Squamostatin A*)
Yu, J. *et al., Chin. Chem. Lett.*, 1993, **4**, 423 (*Squamostatin B*)
Fang, X.-P. *et al., J. Nat. Prod.*, 1993, **56**, 1095 (*pmr, struct*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1175 (*cmr, pmr*)
Shimada, H. *et al., Tet. Lett.*, 1994, **35**, 3961-3964 (*abs config*)
Laprevote, O. *et al., Tetrahedron*, 1994, **50**, 8479 (*ms, struct*)
Zafra-Polo, M.C. *et al., Phytochemistry*, 1996, **42**, 253-271 (*rev*)
Cave, A. *et al., Prog. Chem. Org. Nat. Prod.*, 1997, **70**, 81-288 (*rev*)
Chang, F.-R. *et al., Phytochemistry*, 1999, **51**, 883-889 (*12,15-cis-Squamostatin A*)

Squamosten A S-213

[155834-22-3]



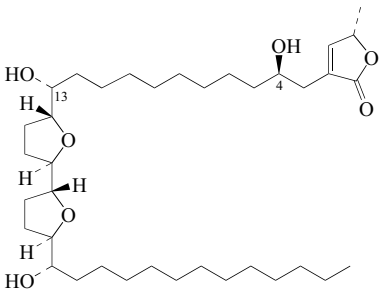
$C_{37}H_{66}O_7$ 622.924
Isol. from the seeds of *Annona squamosa* (sugar apple). Solid. Mp 64-67°. $[\alpha]_D^{24}$ +9 (c, 0.1 in MeOH). λ_{max} 210 (ε 7000) (MeOH) (Berdy).

Araya, H. *et al., Chem. Pharm. Bull.*, 1994, **42**, 388-391 (*isol, pmr, cmr, ms*)

Squamotacin S-214

[174158-66-8]

[181657-10-3]
Glaucanisin



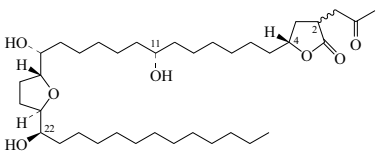
$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona squamosa* (sugar apple). $[\alpha]_D$ +13 (c, 0.6 in MeOH). Config. of Glaucanisin not fully elucidated. Identity with Squamotacin not certain.

*4-Deoxy, 6*S*-hydroxy:* ***4-Deoxy-6-hydroxysquamotacin***
$C_{37}H_{66}O_7$ 622.924
Constit. of *Annona glabra* (pond apple). Waxy solid. $[\alpha]_D^{25}$ +5.3 ($CHCl_3$). λ_{max} 218 (log ε 3.68) (MeOH).

Waechter, A.-I. *et al., Nat. Prod. Lett.*, 1995, **6**, 133-138 (*isol, struct*)
Hopp, D.C. *et al., J. Nat. Prod.*, 1996, **59**, 96 (*isol, pmr, cmr*)
Sinha, S.C. *et al., J.O.C.*, 1999, **64**, 7067-7073 (*synth*)
Liu, X. *et al., Nat. Prod. Lett.*, 2000, **14**, 255-263 (*4-Deoxy-6-hydroxysquamotacin*)

Squamoxinone S-215

[206192-81-6]



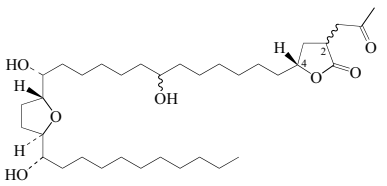
$C_{37}H_{68}O_7$ 624.94
Constit. of *Annona squamosa* (sugar apple). Amorph. powder. $[\alpha]_D^{23}$ +13.3 (c, 0.02 in CH_2Cl_2). Obt. as a mixt. of 2,4-*cis*- and *trans*-isomers λ_{max} 203 (log ε 3.2) (MeOH).

22-Epimer: [255901-21-4] ***Squamoxinone B***
$C_{37}H_{68}O_7$ 624.94
Constit. of *Annona squamosa* (sugar apple). Amorph. powder. $[\alpha]_D$ +23.6 (c, 0.2 in CH_2Cl_2). Obt. as a mixt. of 2,4-*cis*- and *trans*-isomers. C-11 config. not determined λ_{max} 203 (log ε 2.85) (MeOH).

Hopp, D.C. *et al., Phytochemistry*, 1998, **47**, 803-809 (*isol, uv, ir, pmr, cmr, ms*)
Hopp, D.C. *et al., Phytochem. Anal.*, 1999, **10**, 339-347 (*Squamoxinone B*)

Squamoxinone C S-216

[255901-22-5]



$C_{35}H_{64}O_7$ 596.886

Constit. of *Annona squamosa* (sugar apple). Wax. $[\alpha]_D$ -13.3 (c, 0.02 in CH_2Cl_2). Isol. as a mixt. of 2,4-*cis*- and *trans*-isomers λ_{max} 207 (log ϵ 3.35) (MeOH).

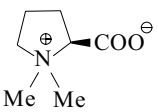
Hopp, D.C. *et al., Phytochem. Anal.*, 1999, **10**, 339-347

Stachydrine S-217

[32039-73-9]

[167936-48-3]

2-Carboxy-1,1-dimethylpyrrolidinium hydroxide inner salt, 9CI. Hygric acid methylbetaine, 8CI. N-*Methylproline methylbetaine. Cadabine. Chrysanthemine*



$C_7H_{13}NO_2$ 143.185

Chrysanthemine was a mixt. of stachydrine with Choline, C-239.

(*S*)-*form* [471-87-4]

L-form

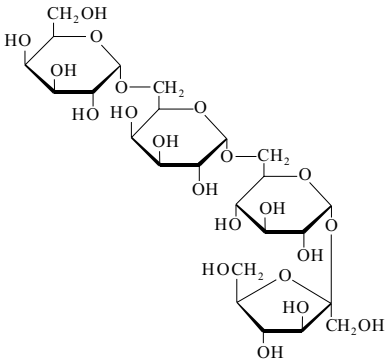
Alkaloid from *Citrus* spp *Medicago sativa* and *Stachys* spp.(alfalfa). Mp 116-118° (monohydrate) Mp 235° dec. (anhyd.). $[\alpha]_D$ -40.25 (c, 4 in H_2O). Fairly readily racemised, (±)-form often obt..

King, H. *et al., J.C.S.*, 1950, 2866, (*isol, struct*)
Cornforth, J.W. *et al., J.C.S.*, 1952, 597; 601 (*isol, props*)
Marian, L. *et al., Phytochemistry*, 1962, **1**, 209 (*biosynth*)
Paudler, W.W. *et al., Chem. Ind. (London)*, 1963, 1693 (*pmr*)
Mandava, N. *et al., Annalen*, 1970, **741**, 167 (*pmr*)
Musich, J.A. *et al., J.O.C.*, 1977, **42**, 139 (*synth*)
Massiot, G. *et al., Alkaloids (N.Y.)*, 1986, **27**, 310 (*bibl, pharmacol*)
Jones, G.P. *et al., Acta Cryst. C*, 1988, **44**, 1669 (*cryst struct*)

Stachyose S-218

[470-55-3]

β-D-Fructofuranosyl O-α-*D-galactopyranosyl-(1→6)-*O-α-*D-galactopyranosyl-(1→6)-*α-*D-glucopyranoside, 9CI, 8CI. Manneotetrose. β-Galactan. Cicerose. Lupeose*



$C_{24}H_{42}O_{21}$ 666.583

Isol. from soybean meal (*Glycine max*), tubers of Japanese artichoke (*Stachys tubifera*) and lentils. Cryst. + 4 or $5H_2O$. Mp 101-105° (sealed tube) Mp 167-170° (anhyd.). $[\alpha]_D^{23}$ +131.3 (c, 4.5 in H_2O).

Tetradeca-Ac:
Mp 95-96°. $[\alpha]_D^{20}$ +120 (c, 3.8 in EtOH).

Tetradecakis-4-nitrobenzoyl:
Mp 166°.

Tetradeca-Me:
Syrup. $[\alpha]_D^{24.5}$ +139.2 ($CHCl_3$).

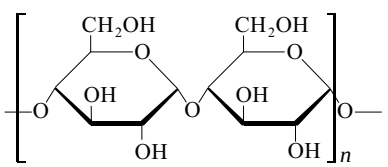
[10094-58-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 197C (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 913D (*nmr*)
Wolfrom, M.L. *et al., J.A.C.S.*, 1952, **74**, 6299 (*synth*)
Wolfrom, M.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 368 (*isol*)
Pazur, J.H. *et al., The Carbohydrates*, Academic Press, 2nd Ed., 1970, 69 (*rev*)
Allerhand, A. *et al., J.A.C.S.*, 1971, **93**, 2777 (*cmr*)
Kamerling, J.P. *et al., Tetrahedron*, 1972, **28**, 3037 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 672 (*occur, bibl*)
Gilardi, R.D. *et al., J.A.C.S.*, 1975, **97**, 6264 (*cryst struct*)
Gilardi, G. *et al., Acta Cryst. C*, 1987, **43**, 806 (*cryst struct*)
McIntyre, D.D. *et al., J. Nat. Prod.*, 1989, **52**, 1008 (*pmr*)
Jeffrey, G.A. *et al., Carbohydr. Res.*, 1991, **210**, 89 (*cryst struct*)

Starch, 9CI, 8CI S-219

[9005-25-8]

Amylum. Polyamylose



Starch is composed of Amylose and Amylopectin. Amylose is preponderantly a linear polymer of several thousand D-glucose units mainly α-(1→4) linked. Amylopectin is a branched polymer composed largely of α-D-(1→4)-linked glucose units. The branch is α-(1→6) and occurs at the 6 position every 20-25 glucose units. Pullulanase, *R*-enzyme and Isoamylase hydrol. the α-D-(1→6) linkages. Polymeric. Minimum formula given.

▶ Starch dust is a respiratory tract irritant OES (8-hr TWA) total inhalable dust 10 mg m^{-3}, respirable dust 5 mg m^{-3}. Mod. explosive when exposed to flame.

Phosphate: [11120-02-8]

[39373-98-3]

Stabiliser, thickener, moisture control agent., flavour modifier, release agent and firming agent for processed foods. Many different structs. are present at different phosphorylation levels.

Carboxymethyl ether: [9057-06-1]
Modified starch used as thickening agent in food industry. Powder.

2-Hydroxypropyl ether: [9049-76-7]
Used in food processing including stabiliser, thickener, moisture control agent, flavour modifier, release agent, handling and firming agent.

Unbranched-*form* [9005-82-7]

Amylose

Stored in all parts of plants as insol. granules. Coml. starches come mainly from corn (maize), sorghum grains, tapioca root and potato tuber. Most starch samples contain 20 ± 5% Amylose which can be pptd. from aq. starch soln. with, e.g., Thymol. Various uses in food processing including thickener, stabilizer, flavour modifier, filler for baking powder, flour additive, firming agent and release/antisticking agent. Many modified forms also used. $[\alpha]_D$ +200 (H_2O). $[\alpha]_D$ +162 (1*M* NaOH). $[\alpha]_D$ +175 (DMSO). Hydrol. by acid, α-Amylase and β-Amylase. Forms inclusion complexes, gives a deep-blue colour with I_2. Four polymorphs (A,B,C and V amyloses) have been studied structurally and differ in helical conformation and packing.

Per-Ac:

[9045-28-7]

Many uses in processed foods including stabilizer, thickener, moisture control, flavour modifier, release/antisticking agent and firming agent. $[\alpha]_D$ +175 ($CHCl_3$).

Branched-*form* [9037-22-3]

Amylopectin

$[\alpha]_D$ +200 (H_2O). $[\alpha]_D$ +163 (1*M* NaOH).

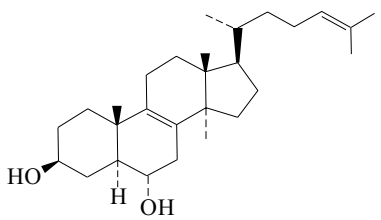
[9063-38-1, 11116-64-6, 56780-58-6]

Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, NY, 1948, **4**, 283 (*use*)
Whistler, R.L. *et al., Methods Carbohydr. Chem.*, 1964, **4**, 3
Paschall, E.F. *et al., Methods Carbohydr. Chem.*, 1964, **4**, 294-296 (*rev, phosphate*)
Whistler, R.L. *et al., Arch. Biochem. Biophys.*, 1969, **135**, 396-401 (***synth, phosphate***)
Greenwood, C.T. *et al., The Carbohydrates*, Academic Press, 1970, **2B**, 471
U.K. Pat., 1973, 1 309 473; *CA*, **79**, 116473s (***synth, props, phosphate***)
U.S. Pat., 1974, 3 842 071; *CA*, **82**, 74775w (*synth, props, phosphate*)
St. Jacques, M. *et al., J.A.C.S.*, 1976, **98**, 4386 (*pmr*)

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 492 (*rev*)
Rappenecker, G. *et al., Carbohydr. Res.*, 1981, **89**, 11 (*cryst struct, V-amylose*)
Dais, P. *et al., Carbohydr. Res.*, 1982, **100**, 103 (*cmr, Amylopectin*)
Whistler, R.L. *et al., Starch: Chem. Technol.*, 2nd Ed., Academic Press, 1984,
Takeda, Y. *et al., Carbohydr. Res.*, 1986, **148**, 299 (*purifn, amylose*)
Marczenko, Z. *et al., Separation and Spectrophotometric Determination of Elements*, Ellis Horwood, Chichester, 1986, 316
Modif. Starches: Prop. Uses. 1987, (ed. Wurzburg, O.B.), CRC Press, 1987, 79-96 (*rev*)
Starch: Properties and Potential, (Ed., Gulliard, T.), Wiley, 1987, (*book*)
Saito, H. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 3528 (*cmr, bibl, struct, amyloses*)
Zhang, J. *et al., J. Appl. Polym. Sci.*, 1992, **46**, 369-374 (*carboxymethyl ether*)
Takeda, Y. *et al., Carbohydr. Res.*, 1993, **240**, 265 (*bibl, struct*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 483-488
Tomasik, P. *et al., Adv. Carbohydr. Chem. Biochem.*, 1995, **51**, 243 (*rev, modification*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1377
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2643-2675 (*use, props, modification*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SLJ500

Stenocereol S-220

[84780-12-1]
14α-Methyl-5α-cholesta-8,24-diene-3β,6α-diol

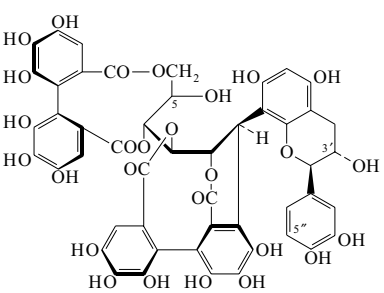


$C_{28}H_{46}O_2$ 414.67
Constit. of *Stenocereus thurberi* (organ pipe cactus). Cryst. Mp 150.5-151.5°. $[\alpha]_D$ +72 (c, 3 in $CHCl_3$).

Kircher, H.W. *et al., Phytochemistry*, 1982, **21**, 1705

Stenophyllanin C S-221

[97775-90-1]



$C_{49}H_{36}O_{27}$ 1056.807
Off-white amorph. powder + 2½ H_2O. $[\alpha]_D^{21}$ +80.7 (c, 1.3 in MeOH).

5-O-(3,4,5-Trihydroxybenzoyl): [97775-88-7] ***Stenophyllanin A***
$C_{56}H_{40}O_{31}$ 1208.913
Amorph. powder. $[\alpha]_D^{28}$ +48.1 (c, 1.2 in MeOH).

3′-Epimer: [138256-93-6] ***Camelliatannin A***
$C_{49}H_{36}O_{27}$ 1056.807
Isol. from leaves of *Camellia japonica*. Off-white powder + 7H_2O. $[\alpha]_D^{20}$ +68 (c, 1.2 in MeOH).

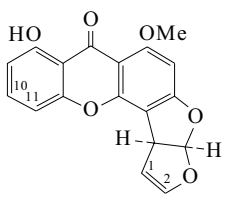
5-(3,4,5-Trihydroxybenzoyl), 5″-hydroxy: [145826-24-0] ***Guajavin A***
$C_{56}H_{40}O_{32}$ 1224.913
Constit. of the bark of *Psidium guajava* (guava). Pale brown powder + 6H_2O. $[\alpha]_D^{19}$ +73 (c, 1 in MeOH). Conformational isomerisation observed.

5″-Hydroxy: [154971-07-0] ***Strobilanin***
$C_{49}H_{36}O_{28}$ 1072.807
Tan powder + 2H_2O. $[\alpha]_D^{22}$ +39.4 (c, 0.8 in Me_2CO).

Nonaka, G.-I. *et al., J.C.S. Perkin 1*, 1985, 163 (*struct, pmr, cmr*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2151 (*abs config*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2092 (*Guajavin A*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1708 (*Strobilanin*)

Sterigmatocystin S-222

[10048-13-2]
3a,12c-Dihydro-8-hydroxy-6-methoxy-7H-furo[3′,2′:4,5]furo[2,3-c]xanthen-7-one, 9CI



Absolute configuration

$C_{18}H_{12}O_6$ 324.289
Numbering systems vary. Mycotoxin of *Aspergillus versicolor* and *Chaetomium* spp.. Pale yellow needles. Mp 246° dec. $[\alpha]_D^{21}$ -387 (c, 0.424 in $CHCl_3$). λ_{max} 205 (ε 25100); 233 (ε 30900); 246 (ε 33900); 325 (ε 16000) (EtOH) (Derep).
▶ Carcinogenic. LV1750000

Me ether: [17878-69-2] **O-*Methylsterigmatocystin***
$C_{19}H_{14}O_6$ 338.316
Mycotoxin of *Aspergillus flavus*. Mp 265° dec.
▶ LV1742000

O-*De-Me:* [30461-65-5] ***De*-O-*methylsterigmatocystin***
$C_{17}H_{10}O_6$ 310.262
Mycotoxin of *Aspergillus versicolor*. Mp 253-255°. $[\alpha]_D^{24}$ -483 (c, 0.2 in $CHCl_3$).

1,2-Dihydro: [6795-16-0] ***Dihydrosterigmatocystin***
$C_{18}H_{14}O_6$ 326.305
Mycotoxin of *Aspergillus versicolor*. Pale yellow needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 230° dec. $[\alpha]_D^{20}$ -311.7 (c, 0.85 in $CHCl_3$). λ_{max} 233 (ε 27600); 247 (ε 32200); 325 (ε 16600) (MeOH) (Berdy).
▶ LV1761000

1,2-Dihydro, Me ether: [21793-91-9] ***Dihydro*-O-*methylsterigmatocystin***
$C_{19}H_{16}O_6$ 340.332
Mycotoxin from *Aspergillus flavus*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 282-283°. λ_{max} 238 ; 313 (MeOH) (Berdy).

1,2-Dihydro, O-*de-Me:* [30517-66-9] ***De*-O-*methyldihydrosterigmatocystin***. *Dihydrodemethylsterigmatocystin*
$C_{17}H_{12}O_6$ 312.278
Mycotoxin prod. by *Aspergillus versicolor*. Pale yellow needles (Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 202° dec. $[\alpha]_D^{25}$ -376.6 (c, 0.9 in $CHCl_3$). λ_{max} 233 (ε 26800); 250 (ε 33100); 259 (ε 30300); 335 (ε 19400) (EtOH). λ_{max} 233 (ε 26800); 250 (ε 33100); 259 (ε 30300); 335 (ε 19400) (MeOH) (Berdy).

1,2-Dihydro, 2-hydroxy, 8-Me ether: [30099-66-2] ***Dihydrohydroxy*-O-*methylsterigmatocystin***
$C_{19}H_{16}O_7$ 356.331
Mycotoxin prod. by *Aspergillus parasiticus*. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 209 (ε 21770); 238 (ε 25710); 317 (ε 11370) (MeOH).

8-Deoxy: [149792-60-9] ***8-Deoxysterigmatocystin***. *PF 1093. Antibiotic PF 1093*
$C_{18}H_{12}O_5$ 308.29
Pale yellow solid. Sol. $CHCl_3$, Me_2CO, EtOAc, MeOH; poorly sol. H_2O. Mp 216-218°. $[\alpha]_D^{24}$ -382 (c, 0.25 in $CHCl_3$). $[\alpha]_D$ -184 (c, 0.1 in Me_2CO). The Mp. and higher opt. rotn. refer to PF 1093 λ_{max} 248 (ε 10000); 304 (ε 6400); 336 (ε 3500) (MeOH).

10,11-Dimethoxy: [65176-75-2] ***10,11-Dimethoxysterigmatocystin***. *5,6-Dimethoxysterigmatocystin*
$C_{20}H_{16}O_8$ 384.342
Mycotoxin prod. by *Aspergillus multicolor*. Pale yellow needles. Mp 253-254°. Bp 321°. $[\alpha]_D^{20}$ -363 (c, 1 in $CHCl_3$). λ_{max} 233 (ε 27200); 248 (ε 34000); 275 (ε 7700); 330 (ε 19200) (EtOH) (Derep). λ_{max} 233 (ε 27200); 248 (ε 34000); 330 (ε 19200) (EtOH) (Berdy).
▶ LV1750500

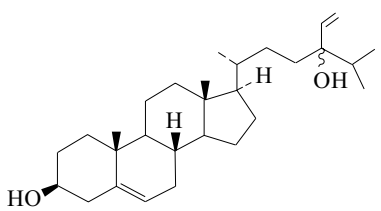
9-Chloro: [222855-39-2] ***Antibiotic N 0532A***. *N 0532A*
$C_{18}H_{11}ClO_6$ 358.734Stereochem. not determined.

9-Chloro, 8-Me ether: [222855-40-5] ***Antibiotic N 0532B***. *N 0532B*
$C_{19}H_{13}ClO_6$ 372.761Stereochem. not determined.

Davies, J.E. *et al., J.C.S.*, 1962, 4179-4183 (*isol*)
Elsworthy, G.C. *et al., Chem. Comm.*, 1970, 1069-1070 (*De-O-methylsterigmatocystin*)
Hatsuda, Y. *et al., Agric. Biol. Chem.*, 1972, **36**, 521-522 (*De-O-methyldihydrosterigmatocystin*)
Ishida, M. *et al., Agric. Biol. Chem.*, 1975, **39**, 2181-2184 (*isol*)
Fukuyama, K. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 1980-1983; 1976, **49**, 1153-1154 (*cryst struct*)

Pachler, K.G.R. *et al., J.C.S. Perkin 1*, 1976, 1182-1189 (*cmr, biosynth*)
Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1977, 1360-1364 (*conformn*)
Cox, R.H. *et al., J.O.C.*, 1977, **42**, 112-114 (*cmr, O-Methylsterigmatocystin*)
Hamasaki, T. *et al., Tet. Lett.*, 1977, 2765-2766 (*10,11-dimethoxy*)
Hamasaki, T. *et al., CA*, 1978, **88**, 146819 (*tox*)
Udagawa, S. *et al., Can. J. Microbiol.*, 1979, **25**, 170-177 (*isol*)
Nakashima, T.T. *et al., Chem. Comm.*, 1982, 206-208 (*biosynth*)
Simpson, T.J. *et al., Chem. Comm.*, 1982, 890-892 (*biosynth*)
Sankawa, U. *et al., Heterocycles*, 1982, **19**, 1053-1058 (*biosynth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220-2284 (*uv, ir, pmr, ms, cd*)
Cleveland, T.E. *et al., Appl. Environ. Microbiol.*, 1987, **53**, 2804-2807 (*Dihydrohydroxy-O-methylsterigmatocystin*)
Barnes, S.E. *et al., Mycopathologia*, 1994, **125**, 173-178 (*synth*)
Casillas, L.K. *et al., J.O.C.*, 1999, **64**, 4050-4059 (*synth*)
Japan. Pat., 1999, 99 80 162; *CA*, **130**, 280918h (*N 0532*)
Joshi, B.K. *et al., J. Nat. Prod.*, 2002, **65**, 1734-1737 (*8-Deoxysterigmatocystin*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 68; 73; 77; 81
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SLP000

Stigmasta-5,28-diene-3,24-diol, 9CI S-223



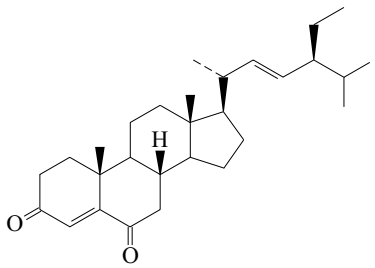
$C_{29}H_{48}O_2$ 428.697

3β-*form* [6901-60-6]
Saringosterol. *24-Hydroxy-24-vinylcholesterol. Saningosterol*
Cryst. (C_6H_6/hexane). Mp 160-161°. $[\alpha]_D$ -31 ($CHCl_3$). Saningosterol is presumably a misprint.

3-O-β-D-Glucopyranoside:
$C_{35}H_{58}O_7$ 590.839
Constit. of immature French bean seeds (*Phaseolus vulgaris*).

Ikekawa, N. *et al., Chem. Ind. (London)*, 1966, 1179
Kim, S.-K. *et al., J. Plant Biol.*, 1994, **37**, 441; *CA*, **123**, 79492b (*glucoside*)

Stigmasta-4,22-diene-3,6-dione S-224



$C_{29}H_{44}O_2$ 424.665

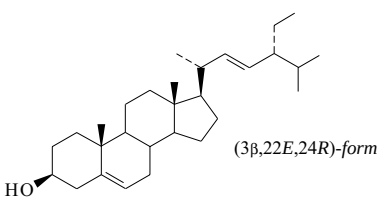
(22*E*,24*R*)-*form* [50868-51-4]
Isol. from *Glycine max* (soybean) and *Pistia stratiotes* (date). Pale yellow cryst. (MeOH). Mp 154-156°.

Phenylhydrazone:
Yellow cryst. Mp 250° dec.

Fernholz, E. *et al., Annalen*, 1934, **508**, 215 (*synth*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1386 (*isol*)
Weber, N. *et al., Phytochemistry*, 1977, **16**, 1849 (*isol*)
Fernandez, M.I. *et al., Phytochemistry*, 1983, **22**, 2087 (*isol*)
D'Auria, M. *et al., Synthesis*, 1985, 988 (*synth*)
Galagovsky, L.R. *et al., J. Chem. Res., Synop.*, 1990, 366 (*synth, pmr*)
Ayyad, S.N. *et al., Pharmazie*, 2001, **56**, 212-214 (*isol, pmr, cmr*)

Stigmasta-5,22-dien-3-ol S-225

24-Ethylcholesta-5,22-dien-3-ol



(3β,22*E*,24*R*)-*form*

$C_{29}H_{48}O$ 412.698

(3β,22*E*,24*S*)-*form* [83-48-7]

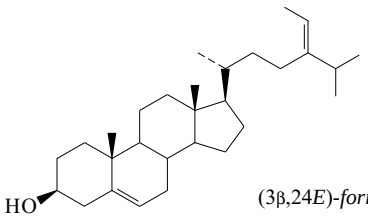
[32345-19-0]
Stigmasterol. *Serposterol*
Cryst. (EtOH). Mp 170°. $[\alpha]_D^{22}$ -57 ($CHCl_3$).

3-O-β-D-Glucopyranoside: [19716-26-8]
$C_{35}H_{58}O_6$ 574.84
Isol. from soya bean oil (*Glycine max*). Cryst. (EtOH/Py). Mp 299°.

Hexadecanoyl: [2308-84-1] ***Palmitoylstigmasterol***
$C_{45}H_{78}O_2$ 651.11
Isol. from fennel (*Foeniculum vulgare*) roots and seeds. Mp 94-96°.

Wright, H.E. *et al., J.O.C.*, 1962, **27**, 918 (*glucopyranoside*)
Kartnig, T. *et al., Fette, Seifen, Anstrichm.*, 1965, **67**, 10 (*Palmitoylstigmasterol*)
Alam, M.S. *et al., Phytochemistry*, 1996, **41**, 1197-1200 (*glucoside, pmr, cmr*)

Stigmasta-5,24(28)-dien-3-ol, 9CI S-226



(3β,24*E*)-*form*

$C_{29}H_{48}O$ 412.698

(3β,24*E*)-*form* [17605-67-3]
Fucosterol
Characteristic sterol of seaweeds; isol. from bladderwrack *Fucus vesiculosus*. Needles (MeOH). Mp 124°. $[\alpha]_D^{20}$ -38.4 ($CHCl_3$).

(3β,20*R*,24*Z*)-*form* [481-14-1]
Isofucosterol
Present in oats (*Avena sativa*). Plates (MeOH). Mp 137° (130-131°). $[\alpha]_D^{26}$ -37.6 (MeOH).

3-O-β-D-Glucopyranoside: [87678-84-0]
Isofucosterol glucoside
$C_{35}H_{58}O_6$ 574.84
Constit. of *Lycopersicon esculentum* (tomato). Cryst. Mp 266-268°. $[\alpha]_D$ -40.8 (c, 0.05 in $CHCl_3$).

3-O-[6-O-Hexadecanoyl-β-D-glucopyranoside]: [209903-43-5]
$C_{51}H_{88}O_7$ 813.252
Constit. of *Lycopersicon esculentum* (tomato).

3-O-[6-O-Octadecanoyl-β-D-glucopyranoside]: [209903-44-6]
$C_{53}H_{92}O_7$ 841.306
Constit. of *Lycopersicon esculentum* (tomato).

3-O-[6-O-(9-Octadecenoyl)-β-D-glucopyranoside]: [209903-45-7]
$C_{53}H_{90}O_7$ 839.29
Constit. of *Lycopersicon esculentum* (tomato).

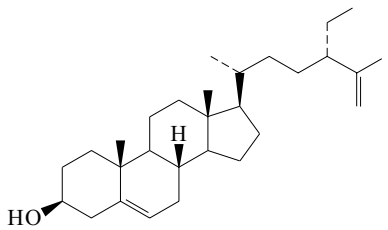
3-O-[6-O-(9,12-Octadecadienoyl)-β-D-glucopyranoside]: [209903-47-9]
$C_{53}H_{88}O_7$ 837.274
Constit. of *Lycopersicon esculentum* (tomato).

[6793-19-7, 20584-62-7, 55870-01-4, 83997-22-2]

Heilbron, I. *et al., J.C.S.*, 1934, 1572 (*isol*)
Idler, D.R. *et al., J.A.C.S.*, 1953, **75**, 1712 (*Isofucosterol, isol*)
Hayazu, R. *et al., Pharm. Bull.*, 1957, **5**, 452 (*synth*)
Dusza, J.P. *et al., J.O.C.*, 1960, **25**, 93 (*synth, Isofucosterol*)
Nes, W.R. *et al., Steroids*, 1966, **8**, 655 (*pmr*)
Bates, R.B. *et al., Tet. Lett.*, 1968, 6163 (*struct*)
Brooks, C.J.W. *et al., Steroids*, 1972, **20**, 487 (*ms, struct*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*pmr*)
Massey, I.J. *et al., J.O.C.*, 1979, **44**, 2448 (*ms, synth*)
Nicotra, F. *et al., Gazz. Chim. Ital.*, 1980, **110**, 579
McInnes, A.G. *et al., Org. Magn. Reson.*, 1980, **13**, 302 (*cmr*)
Srivastava, S.K. *et al., Phytochemistry*, 1980, **19**, 2510 (*isol*)

Seo, S. *et al., J.C.S. Perkin 1*, 1990, 105-108 (*biosynth*)
De Rosa, S. *et al., Phytochemistry*, 1997, **44**, 861-864; 1998, **48**, 103-105 (*Isofucosterol glucoside, acylglucosylisofucosterols*)
Okuzumi, T. *et al., Tet. Lett.*, 2000, **41**, 3623-3626 (*biosynth*)

Stigmasta-5,25-dien-3-ol S-227



$C_{29}H_{48}O$ 412.698

(3β,24*S*)-*form* [2364-23-0]
Clerosterol. *Poriferasta-5,25-dien-3-ol*
Constit. of *Clerodendrum infortunatum*. Also from *Momordica charantia* (bitter melon). Cryst. (petrol). Mp 147° (120-121°). $[\alpha]_D^{23}$ -50.5 (c, 1.2 in $CHCl_3$).

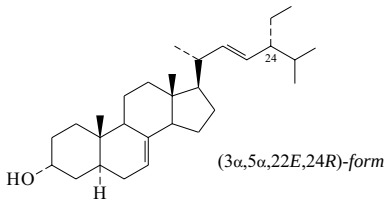
3-O-*β-D-Glucopyranoside:* [123621-00-1]
$C_{35}H_{58}O_6$ 574.84
Isol. from fruits of bitter melon (*Momordica charantia*). Cryst. Mp 258-262° dec. Obt. as mixt. with β-sitosterol glucoside.

3-O-*(6*-O-*Acyl-β-D-glucopyranoside):* $[\alpha]_D^{18}$ -51.5 (c, 0.163 in $CHCl_3$). Mixt. of fatty acid esters (palmitic, stearic, oleic, linoleic, linolenic, tetradecanoic, pentadecanoic, heptadecanoic, eicosanoic, docosanoic).

3-Butanoyl: [256512-61-5] ***Mighavide***
$C_{33}H_{54}O_2$ 482.788

Sucrow, W. *et al., Chem. Ber.*, 1966, **99**, 2765 (*glucoside*)
Manzoor-i-Khuda, M. *et al., Tetrahedron*, 1966, **22**, 2377
Wilkomirski, B. *et al., Phytochemistry*, 1983, **22**, 929 (*biosynth*)
Stoilov, I.L. *et al., Tetrahedron*, 1987, **43**, 2213 (*biosynth*)
Ahmad, V.U. *et al., Phytochemistry*, 1993, **33**, 1189 (*cmr*)
Goswami, P. *et al., Phytochemistry*, 1996, **41**, 279 (*isol, pmr, cmr, glucoside*)
Yagi, T. *et al., Phytochemistry*, 1996, **41**, 1057 (*biosynth*)
Gaspar, H. *et al., Phytochemistry*, 1996, **43**, 613 (*isol, pmr, cmr*)
Chaari, A. *et al., J. Soc. Chim. Tunis.*, 1998, **4**, 257-265; *CA*, **132**, 134733u (*3-butanoyl*)
Fontana, G. *et al., Phytochemistry*, 1999, **50**, 283-285 (*6′-Acylglucopyranoside*)
Jannet, H.B. *et al., Industrial Crops and Products*, 2001, **14**, 213-222 (*Mighavide*)
Koami, T. *et al., Tet. Lett.*, 2002, **43**, 5479-5781 (*biosynth*)

Stigmasta-7,22-dien-3-ol S-228



$C_{29}H_{48}O$ 412.698

(3β,5α,22*E*,24*R*)-*form* [481-17-4]
Chondrillasterol. *Poriferasta-7,22-dien-3-ol*
Cryst. (Me_2CO/MeOH). Mp 174.5-175.5°. $[\alpha]_D^{20}$ -2 ($CHCl_3$).

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranoside]:*
$C_{41}H_{68}O_{11}$ 736.982
Constit. of *Amaranthus spinosus* (spiny amaranth). Cryst. (MeOH/$CHCl_3$). Mp 290°. $[\alpha]_D^{28}$ -40.1 (c, 1 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{47}H_{78}O_{16}$ 899.124
Constit. of *Amaranthus spinosus* (spiny amaranth). Cryst. (MeOH/$CHCl_3$). Mp 340° dec. $[\alpha]_D^{28}$ -51.1 (c, 1. in Py).

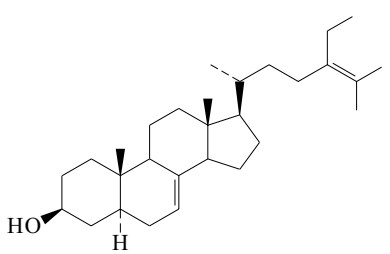
(3β,5α,22*E*,24*S*)-*form* [481-18-5]
α-Spinasterol. *Bessisterol*
Constit. of spinach (*Spinacia oleracea*) leaves, cucumber (*Cucumis sativus*), alfalfa meal, pumpkin seeds and senega root. Cryst. (EtOH/C_6H_6). Mp 171-173°. $[\alpha]_D^{22}$ -2.5 ($CHCl_3$).

▶ WJ2480000

O-*β-D-Glucopyranoside:* [1745-36-4]
Constit. of *Pithecellobium dulce* (manila tamarind). Cryst. Mp 292-294° Mp 340°. $[\alpha]_D$ -29 (c, 1 in Py).

Nigam, S.K. *et al., Indian J. Chem.*, 1967, **5**, 395 (*isol, glucoside*)
Thompson, M.J. *et al., Phytochemistry*, 1972, **11**, 1781 (*pmr*)
Kircher, H.W. *et al., J.O.C.*, 1973, **38**, 2259 (*α-Spinasterol, synth*)
Armarego, W.L.F. *et al., Phytochemistry*, 1973, **12**, 2181 (*biosynth*)
Sucrow, W. *et al., Phytochemistry*, 1976, **15**, 1533 (*config*)
Banerji, N. *et al., J. Indian Chem. Soc.*, 1980, **57**, 417; 1043 (*isol*)
Anastasia, M. *et al., J.C.S. Perkin 1*, 1981, 2561 (*α-Spinasterol, synth*)
Jahan, N. *et al., J. Nat. Prod.*, 1995, **58**, 1244 (*glycosides*)

Stigmasta-7,24-dien-3-ol S-229



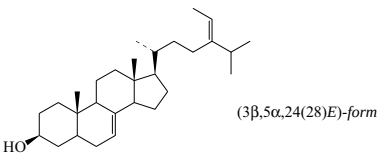
$C_{29}H_{48}O$ 412.698

(3β,5α)-*form* [50632-69-4]
Peposterol
Constit. of sunflower seed oil (*Helianthus annuus*) and marrow leaves (*Cucurbita pepo*). Cryst. (MeOH). Mp 130-131°. $[\alpha]_D^{21}$ +5 (c, 0.8 in $CHCl_3$).

Hamberg, E.E. *et al., Phytochemistry*, 1973, **12**, 1767 (*isol*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 754 (*synth*)
Nes, W.D. *et al., Lipids*, 1977, **12**, 511; 521; 522 (*Peposterol*)
Akihisa, T. *et al., Lipids*, 1986, **21**, 39 (*isol, pmr, cmr*)

Stigmasta-7,24(28)-dien-3-ol S-230

24-Ethylidenecholest-7-en-3-ol



$C_{29}H_{48}O$ 412.698

(3β,5α,24(28)*E*)-*form*

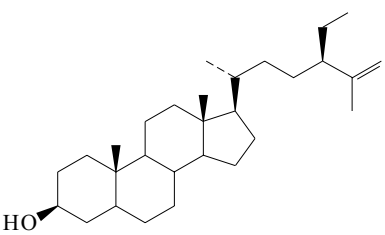
*24*R,*28*R-*Epoxide:* [260390-78-1] *24,28-Epoxystigmast-7-en-3-ol*. ***24,28-Epoxyisoavenasterol***
$C_{29}H_{48}O_2$ 428.697

*24*S,*28*S-*Epoxide:* [260390-79-2]

(3β,5α,24(28)*Z*)-*form* [23290-26-8]
Δ⁷-Avenasterol
Constit. of oats and pumpkin seeds. Cryst. (MeOH). Mp 148-151°. $[\alpha]_D^{22}$ +12.7 (c, 1.28 in $CHCl_3$). Originally considered to be the 7,11-diene.

Idler, D.R. *et al., J.A.C.S.*, 1953, **75**, 1712 (*isol*)
Frost, D.J. *et al., Tet. Lett.*, 1968, 3779 (*struct*)
Sucrow, W. *et al., Chem. Ber.*, 1970, **103**, 2711 (*synth*)
Lin, H.-K. *et al., Phytochemistry*, 1972, **11**, 2319 (*isol*)
Akihisa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1202 (*isol, pmr, ms*)
Akihisa, T. *et al., Phytochemistry*, 1999, **52**, 1601-1605 (*epoxides*)

Stigmasta-7,25-dien-3-ol S-231



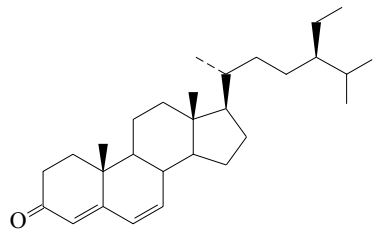
$C_{29}H_{48}O$ 412.698

(3β,5α,24*S*)-*form* [6785-58-6]
Constit. of *Momordica charantia* (bitter melon) and *Cucurbita pepo*. Cryst. (MeOH). Mp 135-142°. $[\alpha]_D^{20}$ +1.2 (c, 1.25 in $CHCl_3$).

Sucrow, W. *et al., Chem. Ber.*, 1966, **99**, 3559; 1970, **103**, 745 (*isol, synth*)
Sucrow, W. *et al., Phytochemistry*, 1976, **15**, 1533 (*abs config*)
Uomori, A. *et al., Phytochemistry*, 1992, **31**, 3861 (*biosynth*)

Stigmasta-4,6-dien-3-one S-232

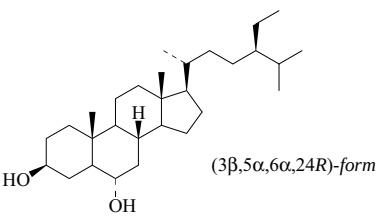
[29374-98-9]
24-Ethylcholesta-4,6-dien-3-one



$C_{29}H_{46}O$ 410.682
Constit. of a stress metab. of *Manihot esculenta* (cassava). Mp 66-70°. $Bp_{0.002}$ 210°. $[\alpha]_D^{25}$ +43 ($CHCl_3$).

Jaworska, R. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1970, **44**, 1409 (*synth*)
Polish Pat., 1978, 95 726; *CA*, **90**, 168833f (*synth*)
Conner, A.H. *et al., Phytochemistry*, 1980, **19**, 1121 (*isol, synth*)
Sakai, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 2905 (*isol*)
Iribarren, A.M. *et al., An. Asoc. Quim. Argent.*, 1989, **77**, 461 (*isol*)

Stigmastane-3,6-diol S-233



(3β,5α,6α,24*R*)-*form*

$C_{29}H_{52}O_2$ 432.729
(3β,5α,6β,24*R*)-*form* [112244-29-8]
Prisms. Mp 207-209°. $[\alpha]_D^{20}$ +41.8 (c, 0.74 in EtOH).

Diketone: ***Stigmastane-3,6-dione***
$C_{29}H_{48}O_2$ 428.697
Constit. of mature wheat straw (*Triticum aestivum*). Cryst. Mp 195-198°.

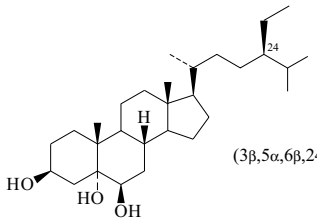
(3β,5α,6α,24*S*)-*form*
Cryst. (MeOH). Mp 214-215°. $[\alpha]_D^{25}$ +46.2 (c, 0.25 in $CHCl_3$).

(3β,5α,6β,24*S*)-*form*
Poriferastane-3,6-diol
Cryst. Mp 211-212°. $[\alpha]_D$ +29.5 (c, 0.2 in MeOH).

Fukuyama, Y. *et al., Planta Med.*, 1988, **54**, 34
Das, B. *et al., Phytochemistry*, 1992, **31**, 4371 (*isol, pmr*)
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523 (*diketone*)
Das, B. *et al., Planta Med.*, 1993, **59**, 572 (*isol, pmr, cmr*)
Kimura, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1813 (*isol, pmr, cmr*)

Stigmastane-3,5,6-triol S-234

24-Ethylcholestane-3,5,6-triol



(3β,5α,6β,24*R*)-*form*

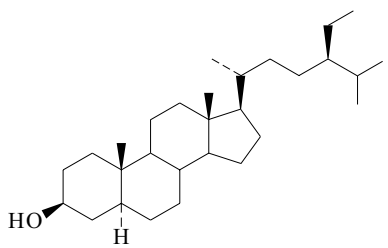
$C_{29}H_{52}O_3$ 448.728
(3β,5α,6β,24*R*)-*form* [20835-91-0]
Constit. of cane sugar (*Saccharum officinarum*). Cryst. (EtOH). Mp 250-252°. $[\alpha]_D$ 0 ($CHCl_3$). $[\alpha]_D$ -2.9 (Py).

(3β,5α,6β,24*S*)-*form*
Cryst. (MeOH). Mp 242-243°. $[\alpha]_D^{25}$ +35.63 (c, 0.25 in MeOH).

Deshmane, S.S. *et al., Tetrahedron*, 1971, **27**, 1109 (*isol, struct*)
Atabekyan, V.G. *et al., Zh. Org. Khim.*, 1976, **12**, 1231 (*synth*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3137 (*isol*)
Dawidar, A.M. *et al., Z. Naturforsch., B*, 1980, **35**, 102 (*synth*)
Notaro, G. *et al., J. Nat. Prod.*, 1991, **54**, 1570 (*isol, pmr*)
Das, B. *et al., J. Nat. Prod.*, 1993, **56**, 2210 (*isol, pmr, cmr*)

Stigmastan-3-ol S-235

24-Ethylcholestan-3-ol



$C_{29}H_{52}O$ 416.729
(3β,5α,24*R*)-*form* [83-45-4]

[19466-47-8]
Fucostanol. *β-Sitostanol. Stigmastanol. Spinastanol. Dihydro-β-sitosterol*
Constit. of pot marigold (*Calendula officinalis*), sweet corn (*Zea mays*) and Carolina allspice (*Calycanthus floridus*). Cryst. (EtOH). Mp 136-137°. $[\alpha]_D^{20}$ +24.8 ($CHCl_3$).

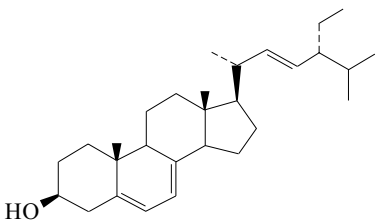
3-O-*Sulfate:*
$C_{29}H_{52}O_4S$ 496.793
Mp 188-190° (as Py salt).

O-*(4-Hydroxy-3-methoxycinnamoyl):* ***Feruloyldihydro-β-sitosterol***
$C_{39}H_{60}O_4$ 592.901
Isol. from maize bran oil. Mp 156-157°. $[\alpha]_D$ +131.

[19044-02-1]

Larsen, C.D. *et al., J.A.C.S.*, 1938, **60**, 2431
Coleman, D.L. *et al., Arch. Biochem. Biophys.*, 1957, **72**, 219 (*synth*)
Tamura, T. *et al., Nippon Kagaku Zasshi*, 1958, **79**, 1011; *CA*, **54**, 24857 (*Feruloyldihydro-β-sitosterol*)
Khaletskii, A.M. *et al., Zh. Obshch. Khim.*, 1961, **31**, 2996 (*sulfate*)
Sucrow, W. *et al., Chem. Ber.*, 1975, **108**, 1101 (*synth*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*pmr*)

Stigmasta-5,7,22-trien-3-ol S-236



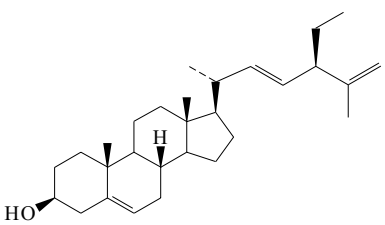
$C_{29}H_{46}O$ 410.682
(3β,24*R*)-*form* [481-19-6]
Corbisterol. *7-Dehydroporiferasterol. Δ^7-Stigmasterol*
Constit. of boiled chicken and seed oils. Mp 151-152°. $[\alpha]_D$ -105.5 (EtOH).

Ac: [39533-73-8]
Mp 152-153° (172-173°). $[\alpha]_D$ -72.8.

[19432-13-4, 21674-20-4]

Toyama, Y. *et al., Bull. Chem. Soc. Jpn.*, 1952, **25**, 355 (*isol*)
Hori, T. *et al., Nippon Kagaku Zasshi*, 1954, **75**, 1144; *CA*, **52**, 10443 (*isol*)
Matsumoto, T. *et al., Nippon Kagaku Zasshi*, 1956, **77**, 1596; *CA*, **53**, 22071 (*isol*)
Nishioki, I. *et al., Yakugaku Zasshi*, 1958, **78**, 1432
Smith, F.R. *et al., J. Lipid Res.*, 1968, **9**, 405
Itoh, T. *et al., Lipids*, 1974, **9**, 173 (*isol*)
Knights, B.A. *et al., Biochim. Biophys. Acta*, 1976, **44**, 341 (*metab*)
Eichenberger, W. *et al., Chimia*, 1976, **30**, 75 (*isol*)

Stigmasta-5,22,25-trien-3-ol S-237



$C_{29}H_{46}O$ 410.682
(3β,22*E*,24*R*)-*form*
Cryst. (MeOH aq.). Mp 151-152°. $[\alpha]_D$ -44 (c, 0.5 in $CHCl_3$).

3-O-*β-D-Galactopyranoside:* [194783-26-1]
$C_{35}H_{56}O_6$ 572.824

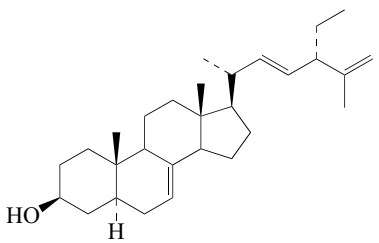
(3β,22*E*,24*S*)-*form* [26315-07-1]
*Poriferasta-5,22*E*,25-trien-3β-ol*. ***22-Dehydroclerosterol***
Constit. of pumpkin (leaves). Cryst. Mp 146°. $[\alpha]_D^{22}$ -37.8 ($CHCl_3$).

(3β,22*Z*,24*S*)-*form*
Bolger, L.M. *et al., Tet. Lett.*, 1970, 3043 (*isol, struct*)
Pakrashi, S.C. *et al., Tet. Lett.*, 1971, 365 (*isol, struct*)

Sucrow, W. *et al., Tet. Lett.*, 1971, 1883; *Chem. Ber.*, 1973, **106**, 2236 (*synth*)
Akihisa, T. *et al., J.C.S. Perkin 1*, 1990, 2213 (*isol, bibl, pmr, ms, cmr*)
Yagi, T. *et al., Phytochemistry*, 1996, **41**, 1057 (*biosynth*)
Atta-ur Rahman, *et al., Phytochemistry*, 1997, **45**, 1721-1722 (*galactoside*)

Stigmasta-7,22,25-trien-3-ol S-238

24-Ethylcholesta-7,22,25-trien-3-ol



$C_{29}H_{46}O$ 410.682

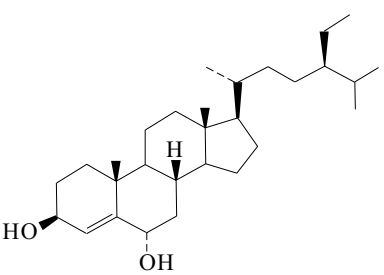
(3β,5α,22*E*,24*S*)-*form* [34991-42-9]
Constit. of *Momordica charantia* (bitter melon). Cryst. (MeOH). Mp 157-161°. $[\alpha]_D^{21}$ +11.2 (c, 0.69 in $CHCl_3$).

O-*β*-D-*Glucopyranoside:* [99782-87-3]
$C_{35}H_{56}O_6$ 572.824
Constit. of *Cucurbita pepo* and *Momordica charantia* (bitter melon).

[14485-48-4, 18070-05-8, 54352-26-0, 86594-37-8]

Sucrow, W. *et al., Chem. Ber.*, 1966, **99**, 3559; 1970, **103**, 750 (*isol, synth*)
Sucrow, W. *et al., Phytochemistry*, 1976, **15**, 1533 (*struct*)
Homberg, E.E. *et al., Phytochemistry*, 1977, **16**, 288 (*isol*)
Hylands, P.J. *et al., Phytochemistry*, 1979, **18**, 1543 (*isol*)
Cattel, L. *et al., Planta Med.*, 1980, **38**, 112 (*isol*)
Itoh, T. *et al., Phytochemistry*, 1981, **20**, 761 (*cmr*)
Rauwald, H.-W. *et al., Phytochemistry*, 1985, **24**, 2746-2748 (*glucoside*)
Akihisa, T. *et al., Lipids*, 1986, **21**, 39,48 (*isol, config*)

Stigmast-4-ene-3,6-diol S-239



$C_{29}H_{50}O_2$ 430.713

(3β,6α,24*R*)-*form*
Cryst. (MeOH). Mp 220°. $[\alpha]_D$ +21.5 (c, 0.5 in $CHCl_3$).

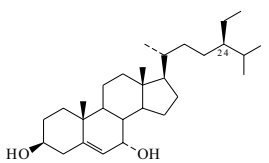
3,6-Diketone: [57458-57-8]

[23670-94-2] ***Stigmast-4-ene-3,6-dione***. *24-Ethylcholest-4-ene-3,6-dione*
$C_{29}H_{46}O_2$ 426.681
Constit. of mature wheat straw (*Triticum aestivum*). Cryst. Mp 170-172°. $[\alpha]_D$ -60.5 (c, 0.99 in $CHCl_3$).

3,6-Diketone, 6-oxime: ***6-Hydroxyiminostigmast-4-en-3-one***
$C_{29}H_{47}NO_2$ 441.696
Amorph. solid. $[\alpha]_D$ +99. λ_{max} 271 (no solvent reported).

Tumann, P. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1974, **307**, 891 (*diketone*)
Chaudhuri, P.K. *et al., Phytochemistry*, 1987, **26**, 3361
Aiello, A. *et al., J. Nat. Prod.*, 1991, **54**, 281 (*diketone*)
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523-527 (*isol, pmr, cmr*)
Rodriguez, J. *et al., Tet. Lett.*, 1997, **38**, 1833 (*oxime, isol*)
Shen, C.-C. *et al., J. Nat. Prod.*, 2002, **65**, 1857-1862 (*diketone, pmr, cmr*)

Stigmast-5-ene-3,7-diol S-240



(3β,7α,24*R*)-*form*

$C_{29}H_{50}O_2$ 430.713

(3β,7α,24*R*)-*form* [34427-61-7]
Ikshusterol. *7α-Hydroxysitosterol*
Constit. of cane sugar (*Saccharum officinarum*) and pineapple leaves (*Ananas comosus*). Cryst. (MeOH). Mp 129-133° (202-204°). $[\alpha]_D$ -27 ($CHCl_3$).

7-Me ether: [256445-68-8] ***Schleichol 2***
$C_{30}H_{52}O_2$ 444.74
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 92-95°. $[\alpha]_D$ -93 (c, 1.7 in $CHCl_3$).

(3β,7β,24*R*)-*form* [15140-59-7]
7-Epiikshusterol. *7*-epi-*Ikshusterol. 7β-Hydroxysitosterol*
Constit. of cane sugar wax. Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 211-214°. $[\alpha]_D$ -22.5 ($CHCl_3$).

7-Me ether: [256445-66-6] *7-Methoxystigmast-5-en-3-ol*. ***Schleichol 1***
$C_{30}H_{52}O_2$ 444.74
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 82-88°. $[\alpha]_D$ +34 (c, 0.7 in $CHCl_3$).

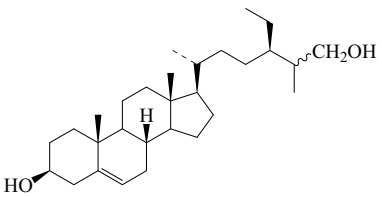
7-Ketone: [2034-74-4] *3-Hydroxystigmast-5-en-7-one*. ***7-Oxo-β-sitosterol***
$C_{29}H_{48}O_2$ 428.697
Isol. after saponification from *Brassica napus* (rapeseed) and *Glycine max* (soyabean) oils. Prisms (MeOH) or needles (hexane). Mp 165-167° Mp 129° (synthetic).

[80666-94-0]

Rowe, J.W. *et al., Phytochemistry*, 1965, **4**, 1 (*isol*)
Bishara, R.H. *et al., J. Nat. Prod.*, 1970, **33**, 477 (*isol, props*)
Deshmane, S.S. *et al., Tetrahedron*, 1971, **27**, 1109 (*isol, struct*)
Mondon, A. *et al., Chem. Ber.*, 1975, **108**, 1989 (*pmr*)
Pakrashi, S.C. *et al., Indian J. Chem.*, 1975, **13**, 755 (*isol*)
Fukuyama, Y. *et al., Planta Med.*, 1988, **54**, 34 (*isol, pmr, cmr*)
Notaro, G. *et al., J. Nat. Prod.*, 1992, **55**, 1588 (*7-ketone, isol, pmr, ms*)
Achenbach, H. *et al., Phytochemistry*, 1992, **31**, 4263
Guerriero, A. *et al., J. Nat. Prod.*, 1993, **56**, 1962 (*7-Hydroxysitosterols, 7-ketone, pmr, cmr*)
Kovganko, N.V. *et al., Khim. Prir. Soedin.*, 1999, **35**, 484-487; *Chem. Nat. Compd. (Engl. Transl.)*, 1999, **35**, 433-436 (*synth*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 72-78 (*Schleicheols*)

Stigmast-5-ene-3,26-diol S-241

24-Ethylcholest-5-ene-3,26-diol



$C_{29}H_{50}O_2$ 430.713

(3β,24*R*,25ξ)-*form* [234429-50-6]
Cryst. Mp 135-136°.

26-Benzoyl: [234429-47-1]
$C_{36}H_{54}O_3$ 534.821
Constit. of *Lepidium sativum* (garden cress). Cryst. ($CHCl_3$/MeOH). Mp 140-141°. λ_{max} 205 (log ϵ 1.7); 240 (log ϵ 1) (no solvent reported).

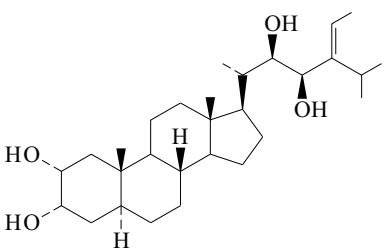
(3β,24ξ,25ξ)-*form* [66760-37-0]
Plates (Me_2CO). Mp 148-150°. $[\alpha]_D^{18}$ -23.5 (c, 2 in $CHCl_3$/MeOH).

Di-Ac:
Plates (Me_2CO). Mp 60°. $[\alpha]_D^{17}$ -50.9 (c, 1.08 in $CHCl_3$).

Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1894
Saba, *et al., Phytochemistry*, 1999, **50**, 1375-1377 (*26-benzoyl*)

Stigmast-24(28)-ene-2,3,22,23-tetrol, 9CI S-242

24-Ethylidenecholestane-2,3,22,23-tetrol

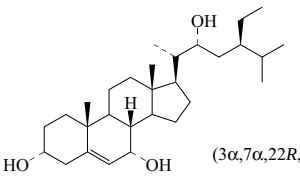


$C_{29}H_{50}O_4$ 462.712

(2α,3α,5α,22*R*,23*R*,24(28)*E*)-*form* [110345-06-7]
6-Deoxohomodolichosterone
Constit. of *Phaseolus vulgaris* (kidney bean) seed. Cryst. (MeOH). Mp 225-227°.

Takatsuti, S. *et al., J.C.S. Perkin 1*, 1986, 2269
Yokota, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 1625

Stigmast-5-ene-3,7,22-triol S-243



(3α,7α,22*R*,24*R*)-*form*

$C_{29}H_{50}O_3$ 446.712

(3α,7α,22*R*,24*R*)-*form*
Stigmastentriol
Isol. from *Corylus avellana* (filbert). Needles(Me$_2$CO/MeOH). Mp 130-140° , 176-178° (double Mp). $[\alpha]_D^{20}$ -61.5 ($CHCl_3$).

(3β,7α,22*R*,24*R*)-*form*
7-Me ether: [256445-50-8] ***Schleicherastatin 2***
$C_{30}H_{52}O_3$ 460.739
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 185-187°. $[\alpha]_D$ -97 (c, 0.2 in $CHCl_3$).

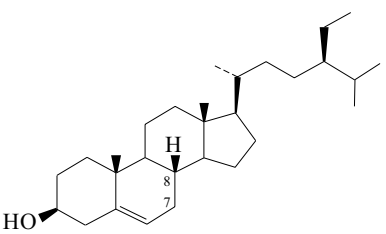
7-Ketone: [256445-58-6] *3,22-Dihydroxystigmast-5-en-7-one.* ***Schleicherastatin 5***
$C_{29}H_{48}O_3$ 444.696
Constit. of the famine food *Schleichera oleosa*. Cryst. Mp 162-166°. $[\alpha]_D$ -49 (c, 1 in $CHCl_3$). λ_{max} 237 (log ε 4.14) (EtOH).

(3β,7β,22*R*,24*R*)-*form*
7-Me ether: [256445-47-3] ***Schleicherastatin 1***
$C_{30}H_{52}O_3$ 460.739
Constit. of the famine food *Schleichera oleosa*. Cryst. (MeOH). Mp 185-187°. $[\alpha]_D$ +57 (c, 0.4 in $CHCl_3$).

Fischer, F.G. *et al., Annalen*, 1960, **636**, 88 (*isol. struct*)
Seiler, N. *et al., Z. Naturforsch., B*, 1966, **21**, 78 (*isol*)
Pettit, G.R. *et al., J. Nat. Prod.*, 2000, **63**, 72-78 (*Schleicherastatins, cryst struct*)

Stigmast-5-en-3-ol S-244

24-Ethylcholest-5-en-3-ol



$C_{29}H_{50}O$ 414.713
Log P 10.45 (uncertain value) (calc).

(3β,24*R*)-*form* [83-46-5]
β-Sitosterol. *Nimbosterol. Cupreol. Quebrachol. Rhamnol. Cinchol. Verosterol. Slanutosterol. Raphanisterol. Papaveristerol. Sitosterol. Angelicin*†. *22,23-Dihydrostigmasterol*
Cryst. (MeOH). Mp 136-137°. $[\alpha]_D^{22}$ -35 ($CHCl_3$). Log P 10.45 (uncertain value) (calc). Pharmacol. active isomer. Early isolates usually contd. *ca*. 5-30% campesterol.

► Exp. reprod. effects. WJ2600000

O-*β-D-Galactopyranoside:* [55057-29-9]
[51704-25-7]
$C_{35}H_{60}O_6$ 576.855
Constit. of *Hibiscus sabdariffa* (roselle) leaves. Cryst. ($CHCl_3$). Mp 275-277°. $[\alpha]_D$ -63 (c, 0.52 in Py).

O-*(6-O-Hexadecanoyl-β-D-glucopyranoside):* [18749-71-8] ***Sitoindoside I***
$C_{51}H_{90}O_7$ 815.268
Constit. of fruits of banana (*Musa paradisiaca*). Amorph. powder. Mp 163-165°. $[\alpha]_D$ -18.8 ($CHCl_3$).

O-*[9Z-Octadecenoyl-(→6)-β-D-glucopyranoside]:* [53657-29-7] ***Sitoindoside II***. *β-Sitosterol 6-oleoylglucoside*
$C_{53}H_{92}O_7$ 841.306
Constit. of banana fruits (*Musa paradisiaca*). Amorph. powder. $[\alpha]_D$ -10.2 ($CHCl_3$).

Ac: [915-05-9] *β-Sitosterol acetate*
$C_{31}H_{52}O_2$ 456.751
Constit. of pods of kiker (*Acacia leucophloea*). Cryst. (MeOH). Mp 134°. $[\alpha]_D^{22}$ -38.5.

Hexadecanoyl: [2308-85-2] *β-Sitosterol palmitate*
$C_{45}H_{80}O_2$ 653.126
Constit. of many plants. Cryst. Mp 89°. $[\alpha]_D$ -16.5 (c, 1.8 in $CHCl_3$).

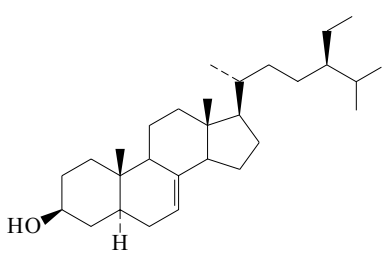
Docosanoyl: [22554-56-9] *β-Sitosterol behenate*
$C_{51}H_{92}O_2$ 737.287
Constit. of wild Himalayan cherry (*Prunus cerasoides*).

O-*(4-Hydroxy-3-methoxycinnamoyl):* [4952-28-7] ***Feruloyl-β-sitosterol***
$C_{39}H_{58}O_4$ 590.885
Isol. from rice bran oil (*Oryza sativa*). Mp 131°. $[\alpha]_D$ +11 ($CHCl_3$).

[19044-06-5]

Neilsen, B.E. *et al., Acta Chem. Scand.*, 1963, **17**, 1161 (*arachidate, palmitate*)
Tanaka, A. *et al., Yukagaku*, 1964, **13**, 260 (*Feruloyl-β-sitosterol*)
Osman, A.M. *et al., Aust. J. Chem.*, 1975, **28**, 217 (*galactoside*)
Ghosal, S. *et al., J. Chem. Res., Miniprint*, 1984, 965-975 (*Sitoindosides, isol*)
Chaudhuri, K. *et al., J. Nat. Prod.*, 1987, **50**, 1183 (*docosanate*)
Khan, M.S.Y. *et al., Indian Drugs Pharm. Ind.*, 1990, **28**, 97; *CA*, **114**, 118494q (*acetate*)

Stigmast-7-en-3-ol S-245



$C_{29}H_{50}O$ 414.713

(3β,5α,24*R*)-*form* [521-03-9]
Schottenol. *22-Dihydrochondrillasterol. 22,23-Dihydro-α-spinasterol*
Constit. of cucumber leaves (*Cucumis sativus*). Cryst. (MeOH). Mp 151-151.5°. $[\alpha]_D^{30}$ +9.1 (c, 0.95 in $CHCl_3$).
Prob. identical with β-Spinasterol.

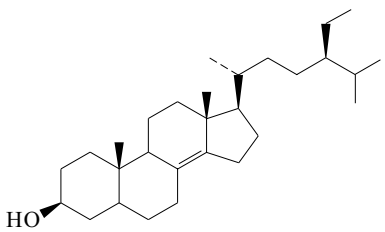
3-O-β-D-Glucopyranoside: [61376-86-1]
$C_{35}H_{60}O_6$ 576.855
Constit. of citron-melon fruits (*Citrullus lanatus* var. *citroides*). Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

[6869-99-4]

Takeda, K. *et al., CA*, 1959, **53**, 9284
Terauchi, H. *et al., Chem. Pharm. Bull.*, 1970, **18**, 213 (*isol, struct*)
Lin, H.-K. *et al., Phytochemistry*, 1972, **11**, 2319 (*isol*)
Kircher, H.W. *et al., J.O.C.*, 1973, **38**, 2259 (*synth*)
Rubinstein, I. *et al., Phytochemistry*, 1976, **15**, 195 (*pmr*)
Ulubelen, A. *et al., Planta Med.*, 1976, **30**, 221 (*isol*)
Siefert, K. *et al., Pharmazie*, 1977, **32**, 125 (*isol*)
Seo, S. *et al., Chem. Comm.*, 1987, 1876 (*biosynth*)
Uomori, A. *et al., Phytochemistry*, 1992, **31**, 3861 (*biosynth*)

Stigmast-8(14)-en-3-ol, 9CI S-246

24-Ethylcholest-8(14)-en-3-ol



$C_{29}H_{50}O$ 414.713

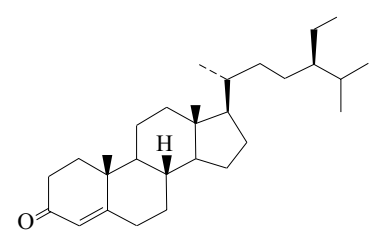
(3β,5α,24*R*)-*form* [14291-38-4]
Constit. of *Dioscorea batatas* (Chinese yam). Cryst. (MeOH). Mp 113.5-114° (108-111°). $[\alpha]_D^{20}$ +23.6 ($CHCl_3$).

Ac:
Cryst. (MeOH). Mp 112-115°. $[\alpha]_D^{21}$ +9.5 (c, 1.3 in $CHCl_3$).

Barton, D.H.R. *et al., J.C.S.*, 1948, 1354
Sucrow, W. *et al., Chem. Ber.*, 1966, **99**, 3559 (*synth*)
Gonzalez, B.R. *et al., CA*, 1968, **68**, 78485k
Akihisa, T. *et al., Phytochemistry*, 1991, **30**, 2369 (*isol, pmr, ms*)

Stigmast-4-en-3-one S-247

[1058-61-3]
Sitost-4-en-3-one. ***β-Sitostenone***



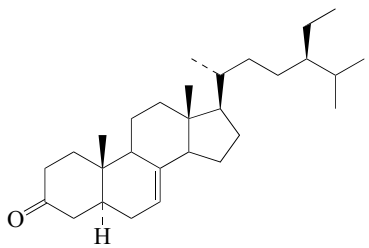
$C_{29}H_{48}O$ 412.698
Constit. of the wood of *Quassia amara* (Surinam quassia). Needles (Et_2O/MeOH). Mp 95-96.5°. $[\alpha]_D$ +81.3.

Oxime:
Cryst. (EtOAc). Mp 175-176°.

Jones, E.R.H. *et al., J.C.S.*, 1942, 391 (*synth*)
Barton, D.H.R. *et al., J.C.S.*, 1943, 599 (*synth*)
Lavie, D. *et al., J.C.S.*, 1963, 5001 (*isol*)
Joshi, K.C. *et al., Indian J. Chem.*, 1974, **12**, 903 (*ms, pmr*)
Smith, A.G. *et al., Biomed. Mass Spectrom.*, 1976, **3**, 64 (*ms, synth*)
Gaspar, E.M.M. *et al., Phytochemistry*, 1993, **34**, 523 (*isol, pmr, cmr*)

Stigmast-7-en-3-one S-248

[18069-96-0]
24-Ethylcholest-7-en-3-one



$C_{29}H_{48}O$ 412.698

(5α,24*R*)-*form* [77790-54-6]
22,23-Dihydro-α-spinasterone
Constit. of *Thea sinensis* (tea). Needles (EtOAc/hexane). Mp 159-160°. $[\alpha]_D^{26}$ +26.1 (c, 0.6 in $CHCl_3$).

(5α,24ξ)-*form* [107739-89-9]

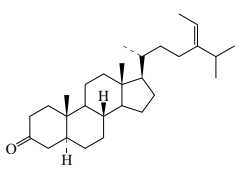
(5β,24*R*)-*form* [137567-08-9]

[158251-01-5]

Sucrow, W. *et al., Z. Naturforsch., B*, 1968, **23**, 42 (*isol*)
Itoh, T. *et al., Phytochemistry*, 1981, **20**, 175-176 (*isol, ms*)
Khuroo, M.A. *et al., Phytochemistry*, 1988, **27**, 3541-3544 (*isol, ms*)
Wu, F. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2281-2282 (*isol, ir, pmr, ms*)
Ding, L. *et al., CA*, 1991, **115**, 275715a (*isol*)

Stigmast-24(28)-en-3-one S-249

[84711-17-1]
24-Ethylidenecholestan-3-one



(5α,24(28)*E*)-*form*

$C_{29}H_{48}O$ 412.698

(5α,24(28)*E*)-*form* [53755-10-5]
Constit. of the seeds of *Setaria italica* (foxtail millet). Mp 137-138.5°.

(5α,24(28)*Z*)-*form* [126576-88-3]
Constit. of *Setaria italica* (foxtail millet).

Sheikh, Y.M. *et al., J.C.S. Perkin 1*, 1974, 909-914 (*synth*)
Seldes, A.M. *et al., Z. Naturforsch., B*, 1990, **45**, 83-86 (*isol, pmr*)
Narumi, Y. *et al., Nihon Yukagakkaishi*, 1999, **48**, 1307-1313; *CA*, **132**, 194547w (*isol, pmr, cmr, synth*)

Streptococcin Sal P S-250

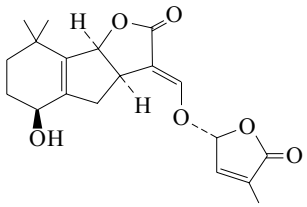
[79956-86-8]

Protein. Bacteriocin prod. by *Streptococcus salivarius* strain P. Poorly sol. hexane.

Taggs, J.R. *et al., Can. J. Microbiol.*, 1981, **27**, 918-923 (*isol*)

Strigol S-251

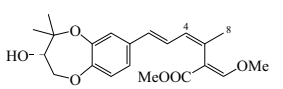
[11017-56-4]



$C_{19}H_{22}O_6$ 346.379
Constit. of the root of *Gossypium hirsutum* (cotton). Cryst. (C_6H_6/hexane). Mp 200-202° dec.(191-193°). $[\alpha]_D^{23}$ +260 (c, 0.25 in $CHCl_3$).

Cook, C.E. *et al., J.A.C.S.*, 1972, **94**, 6198-6199 (*isol*)
Coggon, P. *et al., J.C.S. Perkin 2*, 1973, 465-469 (*cryst struct*)
Heather, J.B. *et al., J.A.C.S.*, 1976, **98**, 3661-3669 (*synth*)
MacAlpine, G.A. *et al., J.C.S. Perkin 1*, 1976, 410-416 (*(±)-form, synth*)
Johnson, A.W. *et al., J.C.S. Perkin 1*, 1981, 1734-1743 (*bibl*)
Brooks, D.W. *et al., J.O.C.*, 1985, **50**, 628-632; 3779-3781 (*synth, cryst struct*)
Dailey, O.D. *et al., J.O.C.*, 1987, **52**, 1984-1989 (*(±)-form, synth*)
Berlage, U. *et al., Tet. Lett.*, 1987, **28**, 3091-3094; 3095-3098 (*synth*)
Samson, E. *et al., Tetrahedron*, 1991, **47**, 1411-1416 (*synth*)
Schröer, J. *et al., Tetrahedron*, 1994, **50**, 6839-6858 (*synth*)
Yokota, T. *et al., Phytochemistry*, 1998, **49**, 1967-1973 (*isol, ms*)
Boulin, B. *et al., Tetrahedron*, 1998, **54**, 2753-2762 (*synth*)
Welzel, P. *et al., Chem. Comm.*, 1999, 2017-2022 (*rev*)
Hirayama, K. *et al., Eur. J. Org. Chem.*, 1999, 2211-2217 (*synth*)
Reizelman, A. *et al., Synthesis*, 2000, 1944-1951; 1952-1955 (*synth, cd, abs config, pmr, cmr*)

Strobilurin I S-252



Absolute Configuration

$C_{21}H_{26}O_6$ 374.433
Pale yellow oil. $[\alpha]_D^{20}$ +20 (c, 0.14 in MeOH). λ_{max} 230 (log ϵ 4.74); 290 (sh) (log ϵ 4.74); 302 (sh) (log ϵ 4.78); 314 (log ϵ 4.74) (MeOH).

2″-O-*(3-Methyl-2-butenoyl):* [267402-20-0] ***Strobilurin P***
$C_{26}H_{32}O_7$ 456.535
Oil. $[\alpha]_D$ -36 (c, 0.23 in MeOH). λ_{max} 225 (log ϵ 4.36); 290 (sh) (log ϵ 4.19); 300 (log ϵ 4.23); 320 (sh) (log ϵ 4.21) (MeOH).

2″-O-*(2,3-Epoxy-3-methylbutanyl):* [267401-98-9] ***Strobilurin O***
$C_{26}H_{34}O_7$ 458.55
Oil. $[\alpha]_D^{22}$ -55 (c, 0.18 in MeOH). λ_{max} 230 (log ϵ 4.36); 235 (sh) (log ϵ 4.36); 290 (sh) (log ϵ 5.64); 300 (log ϵ 4.46); 320 (sh) (log ϵ 4.69) (MeOH).

2″-O-*(3-Methyl-2-butenyl):* [129145-64-8] ***Strobilurin D***. *Strobilurin G*
$C_{26}H_{34}O_6$ 442.551
Yellowish oil. $[\alpha]_D^{20}$ +26.8 (c, 0.75 in EtOH) (+23.8). The struct. of Strobilurin D was revised (1997) to that of the previously reported Strobilurin G λ_{max} 222 (ϵ 26300); 235 (ϵ 22900); 289 (sh) (ϵ 19050); 300 (ϵ 19950); 316 (sh) (ϵ 17380) (MeOH).

2″-O-*(1,1-Dimethyl-2-propenyl):* ***Strobilurin K***
$C_{26}H_{34}O_6$ 442.551
Oil. $[\alpha]_D^{25}$ +1.6 (c, 0.22 in MeOH). λ_{max} 206 (log ϵ 3.34); 279 (log ϵ 3.36); 292 (sh) (log ϵ 3.32) (MeOH).

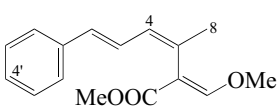
8-Hydroxy, 2″-O-*(3-methyl-2-butenyl):* [113489-65-9] ***Hydroxystrobilurin D***
$C_{26}H_{34}O_7$ 458.55
Isol. from *Mycena sanguinolenta* (blood mycena). Yellow oil. Sol. MeOH, EtOAc, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{22}$ +22 (c, 0.29 in $CHCl_3$). Struct. revised in 1997 λ_{max} 228 (ϵ 15850); 234 (ϵ 12300); 302 (ϵ 18620); 311 (sh) (ϵ 17780) (MeOH).

4-Methoxy, 2″-O-*(1,1-dimethyl-2-propenyl):* [162341-10-8] ***9-Methoxystrobilurin K***
$C_{27}H_{36}O_7$ 472.577
Yellowish oil. $[\alpha]_D$ -8.8. Struct. revised in 1997. Numbering systems vary λ_{max} 230 (ϵ 23440); 306 (ϵ 24550) (MeOH).

Backens, S. *et al., Annalen*, 1988, 405-409 (*Hydroxystrobilurin D*)
Fredenhagen, A. *et al., J. Antibiot.*, 1990, **43**, 655; 661 (*Strobilurin G*)
Weber, W. *et al., Planta Med.*, 1990, **56**, 446-450 (*Strobilurin D*)
Nicholas, G.M. *et al., Tet. Lett.*, 1997, **38**, 7465-7468 (*struct*)
Hellwig, V. *et al., Tetrahedron*, 1999, **55**, 10101-10118 (*isol, struct, abs config*)
Hosokawa, N. *et al., J. Antibiot.*, 2000, **53**, 297-300 (*Strobilurin O, Strobilurin P*)
Uchiro, H. *et al., Tet. Lett.*, 2001, **42**, 4531-4534 (*9-Methoxystrobilurin K, synth*)

Strobilurin A S-253

[52110-55-1]
Methyl 2-(methoxymethylene)-3-methyl-6-phenyl-3,5-hexadienoate, 9CI. Mucidin. Mucidermin. Mucidin B



$C_{16}H_{18}O_3$ 258.316
Prod. by *Oudemansiella mucida*, (porcelain fungus) and many other fungi. Oil. λ_{max} 224 (sh) (ϵ 15800); 229 (ϵ 17800); 237 (ϵ 15500); 285 (sh) (ϵ 20000); 293 (ϵ 21900); 301 (sh) (ϵ 21400) (EtOH) (Derep).

▶ LD_{50} (mus, orl) 500 mg/kg. QG1120000

8-Hydroxy: [167388-39-8] ***Hydroxystrobilurin A***
$C_{16}H_{18}O_4$ 274.316
Brown-yellow oil. Sol. MeOH, Me_2CO. λ_{max} 229 (ϵ 14454); 236 (ϵ 13490); 260 (ϵ 11750); 294 (ϵ 16600) (MeOH) (Berdy).

4-Methoxy: [161270-47-9] ***9-Methoxystrobilurin A***
$C_{17}H_{20}O_4$ 288.343
Oil. Numbering systems vary λ_{max} 230 (ϵ 21880); 301 (ϵ 24550) (MeOH).

3′-Methoxy: [129145-65-9] *3′-Methoxymucidin*. ***Strobilurin H***
$C_{17}H_{20}O_4$ 288.343
Yellowish oil. λ_{max} 232 (ϵ 23200); 298 (ϵ 23400) (EtOH) (Derep).

3′-Methoxy, 4′-chloro: [65105-52-4] ***Strobilurin B, 9CI***
$C_{17}H_{19}ClO_4$ 322.787
Sol. MeOH, $CHCl_3$, CCl_4; poorly sol. H_2O. λ_{max} 227 (ϵ 53700); 279 (ϵ 28200); 287 (ϵ 30900); 304 (ϵ 30200); 315 (sh) (ϵ 26900) (MeOH) (Derep). λ_{max} 225 (ϵ 53700); 279 (ϵ 28180); 287 (ϵ 30900); 303 (ϵ 30200) (MeOH) (Berdy). λ_{max} 229 (ϵ 26800); 304 (ϵ 28400) (EtOH) (Berdy).

4′-Methoxy: [86421-33-2] ***4′-Methoxymucidin***
$C_{17}H_{20}O_4$ 288.343
Isol. from *Oudemansiella mucida* (porcelain fungus). Cryst. (petrol). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 70-71°. λ_{max} 222 (ϵ 21400); 227 (ϵ 4200); 299 (ϵ 29400) (MeOH) (Berdy).

▶ LD_{50} (mus, per os) 422.5 mg/kg. MM2590000

3′-(3-Methyl-2-butenyloxy): [87081-57-0] ***Strobilurin C***
$C_{21}H_{26}O_4$ 342.434
Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 226 (ϵ 83200); 231 (sh) (ϵ 79400); 240 (sh) (ϵ 72400); 262 (sh) (ϵ 44700); 297 (ϵ 83200) (MeOH) (Derep).

3′-Hydroxy, 4′-(3-methyl-2-butenyloxy): [129145-63-7] ***Strobilurin F***
$C_{21}H_{26}O_5$ 358.433
Cubes (Et_2O/hexane). Mp 77.5-78°. λ_{max} 230 (ϵ 26100); 299 (ϵ 24700); 322 (ϵ 25200) (EtOH) (Derep).

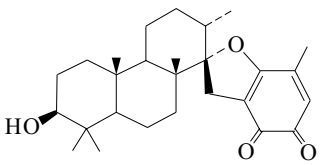
(E,E,E)-isomer: [81436-40-0]
Mp 75-77°.

[65105-51-3]

Anke, T. *et al., J. Antibiot.*, 1977, **30**, 806 (*isol, props*)
Schramm, G. *et al., Chem. Ber.*, 1978, **111**, 2779 (*struct, uv, ir, ms, pmr*)
Sedmara, P. *et al., J. Antibiot.*, 1981, **34**, 1069
Nerud, F. *et al., Coll. Czech. Chem. Comm.*, 1982, **47**, 1020 (*biosynth*)
Vondráček, M. *et al., Coll. Czech. Chem. Comm.*, 1983, **48**, 1508 (*deriv*)
Anke, T. *et al., J. Antibiot.*, 1983, **36**, 661 (*isol, config, synth*)
Anke, T. *et al., Annalen*, 1984, 1616 (*isol, config, synth*)
Beautement, K. *et al., Tet. Lett.*, 1987, **28**, 475 (*synth*)
Sutter, M. *et al., Tet. Lett.*, 1989, **30**, 5417 (*synth*)
Fredenhagen, A. *et al., J. Antibiot.*, 1990, **43**, 655; 661 (*isol, pmr, cmr*)
Zapf, S. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 196 (*9-Methoxystrobilurin A*)
Engler, M. *et al., J. Antibiot.*, 1995, **48**, 884 (*Hydroxystrobilurin A*)
Sauter, H. *et al., Angew. Chem., Int. Ed.*, 1999, **38**, 1329-1349 (*rev*)
Uchiro, H. *et al., Tet. Lett.*, 2000, **41**, 4165-4168 (*9-Methoxystrobilurin A, synth*)

Stypoldione S-254

[71103-05-4]



$C_{27}H_{38}O_4$ 426.595
Red cryst. (Et_2O). Mp 170° dec. $[\alpha]_D$ -65.1 (c, 0.46 in $CHCl_3$). λ_{max} 270 (ϵ 2470); 475 (ϵ 882) (MeOH) (Derep). λ_{max} 270 (ϵ 2470); 475 (ϵ 882) (MeOH) (Berdy).

Gerwick, W.H. *et al., J.O.C.*, 1981, **46**, 22
Jacobs, R.S. *et al., Tetrahedron*, 1985, **41**, 981 (*rev*)
Mori, K. *et al., Bioorg. Med. Chem. Lett.*, 1992, **2**, 391 (*synth*)
Falck, J.R. *et al., J.A.C.S.*, 1993, **115**, 11606 (*synth*)
Rovirosa, J. *et al., Bol. Soc. Chil. Quim.*, 1994, **39**, 219 (*isol, pmr, cmr*)
Mori, K. *et al., Annalen*, 1995, 1755 (*synth*)

Styrene S-255

[100-42-5]
Ethenylbenzene, 9CI. Cinnamene. Cinnamol. Phenethylene. Phenylethene. Phenylethylene. Styrol. Styrolene. Vinylbenzene
$PhCH{=}CH_2$
C_8H_8 104.151
Present in cranberry, bilberry, currants, grapes, vinegar, parsley, milk and dairy products, whisky, cocoa, coffee, tea, roasted filberts and peanuts. Flavouring ingredient. Polymers are used in ion-exchange resins in food processing. Indirect food additive arising from adhesives, oatings and packaging materials. Liq. with penetrating odour. Insol. H_2O; sol. EtOH, Et_2O, Me_2CO, CS_2. d^{20} 0.91. Mp -33°. Bp 145-146° Bp_{20} 48°. n_D^{20} 1.5463. Vp 6 mmHg (25°). Polym. in light or on heating. Coml. samples contain 4-*tert*-butylcatechol or a similar inhibitor. Can be polym. by radical, cationic, anionic, or coordinative polym. Polystyrene is usually manuf. by bulk or suspension radical-initiated polym. Arbitrarily assigned Q/e values for copolym. of Q = 1.00, e = -0.80. Rate for radical polym., k_p 44 L mol^{-1} s^{-1}, k_t 4.75 × 10^{-5} L mol^{-1} s^{-1} (25°). Copolym. with vinylidene chloride: r_{VOC} 0.14, r_{ST} 2.0 (typical values). Copolym. with vinyl chloride: r_{ST} 17; r_{VC} 0.02 (typical values, 60°): Q 1.0; e -0.80.

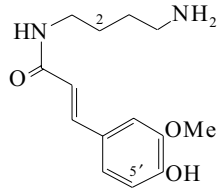
▶ Flammable, fl. p. 30°, autoignition temp. 490°. Irritant. MEL: long-term 100 ppm; short-term 250 ppm. Autocatalytic exothermic polymerisation is self-sustaining above 95°. Forms explosive peroxide on exposure to O_2 at 40-60°. Skin, eye and mucous membrane irritant. Lachrymator, which can cause severe human eye injury on contact with liq. CNS depressant. Symptoms of exposure include headache, nausea, decreased dexterity, coordination and other transient neurological effects. WL3675000

[19361-62-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 945B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 23A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 866C (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 440
Lewis, F.M. *et al., J.A.C.S.*, 1945, **67**, 1701 (*copolym, reactivity ratios*)
Matheson, M.S. *et al., J.A.C.S.*, 1951, **73**, 1700 (*polym, kinetics*)
Adv. Chem. Ser., 1955, **15**, 159 (***props***)
Wilen, S.H. *et al., J. Chem. Educ.*, 1961, **38**, 304 (*synth*)
Mitchell, R.H. *et al., Chem. Comm.*, 1974, 990 (*synth*)
Palmer, M.H. *et al., J.C.S. Perkin 2*, 1974, 1893 (*struct*)
Jones, G. *et al., J.O.C.*, 1978, **43**, 2184 (*ms*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 770; 801; **23**, 910 (*rev*)
Echte, A. *et al., Angew. Chem., Int. Ed.*, 1981, **20**, 344 (*rev, polystyrene*)
Watson, W.D. *et al., ACS Symp. Ser.*, 1985, **285**, 363 (*rev, polymers*)
Van der Veen, R.H. *et al., Tetrahedron*, 1985, **41**, 585 (*uv*)
Schaefer, T. *et al., Can. J. Chem.*, 1988, **66**, 584 (*pmr*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Bond, J.A. *et al., Crit. Rev. Toxicol.*, 1989, **19**, 227 (*rev*)
Encyclopaedia of Polymer Science and Engineering, Wiley-Interscience, New York, 2nd edn., 1989, **15**, 763; **16**, 1 (*rev*)
van Schaik, H.P. *et al., Angew. Chem., Int. Ed.*, 1994, **33**, 1611 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 731
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2687-2690
Vainio, H. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 199 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2755
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 519
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1161
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SMQ000

Subaphylline S-256

[501-13-3]
N-*(4-Hydroxy-3-methoxycinnamoyl)-1,4-butanediamine. Feruloylputrescine*



$C_{14}H_{20}N_2O_3$ 264.324
Alkaloid from *Ananas comosus* (pineapple). Cryst. (C_6H_6 or MeOH). Mp 171.5-172°.

▶ GD6981000

Hydrochloride:
Cryst. + $1H_2O$. Mp 151-152°.

Picrate:
Mp 225-226° dec.

5′-Methoxy: [70185-57-8] ***Sinapoylputrescine***. N-*(3,4-Dihydroxy-5-methoxycinnamoyl)-1,4-butanediamine*
$C_{15}H_{22}N_2O_4$ 294.35
Alkaloid from *Ananas comosus* (pineapple).

2S-Hydroxy:

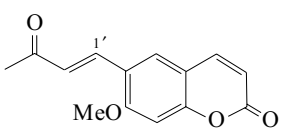
[24177-48-8, 24177-49-9] ***Feruloyl-2-hydroxyputrescine***
$C_{14}H_{20}N_2O_4$ 280.323
Alkaloid from *Triticum aestivum* (wheat). Mixt. of *E*- and *Z*-forms.

2S-Hydroxy, N,O,O-*Tri-Ac:*
$[\alpha]_D^{24}$ -20 (c, 0.7 in $CHCl_3$).

Ryabinin, A.A. *et al., Dokl. Akad. Nauk SSSR*, 1949, **67**, 513; 1951, **76**, 689; *CA*, **44**, 1455h; **45**, 8479d (*isol, struct*)
Wheaton, T.A. *et al., Nature (London)*, 1965, **206**, 620 (*isol, uv, ir, ms, struct*)
Stoessl, A. *et al., Tet. Lett.*, 1969, 2807 (*Feruloyl-2-hydroxyputrescine*)
Mizusaki, S. *et al., Phytochemistry*, 1971, **10**, 1347 (*isol, synth*)
Martin-Tanguy, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1973, **276**, 1433 (*uv, synth*)
Martin-Tanguy, J. *et al., Phytochemistry*, 1978, **17**, 1927 (*occur, Subaphylline, Sinapoylputresine*)
Keller, H. *et al., Phytochemistry*, 1996, **42**, 389-396 (*isol, pmr*)

Suberenone S-257

[35897-95-1]
*7-Methoxy-6-(3-oxo-1-butenyl)-2*H*-1-benzopyran-2-one, 9CI. 7-Methoxy-6-(3-oxo-1-butenyl)coumarin*



$C_{14}H_{12}O_4$ 244.246
Constit. of *Ruta graveolens* (rue). Yellow needles (MeOH/petrol). Mp 225°.

1′,2′-Dihydro, 2′-hydroxy: [117597-78-1] ***Funadonin***
$C_{14}H_{14}O_5$ 262.262
Oil. $[\alpha]_D$ +9.43 (c, 0.003 in $CHCl_3$).

Minker, E. *et al., Magy. Kem. Foly.*, 1972, **78**, 6 (*isol, struct*)
Talapatra, S.K. *et al., Phytochemistry*, 1975, **14**, 836 (*isol, struct*)
Ju-ichi, M. *et al., Heterocycles*, 1988, **27**, 1451 (*Funadonin*)

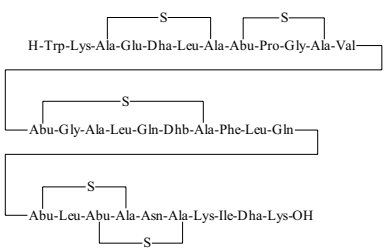
Substance P, 9CI S-258

[33507-63-0]
SP
Arg-Pro-Lys-^{4}Pro-Gln-Gln-Phe-Phe-Gly-Leu-^{11}Met-NH_2
$C_{63}H_{98}N_{18}O_{13}S$ 1347.646
Cryst. + 3AcOH + $4H_2O$. $[\alpha]_D^{27}$ -76 (5% AcOH aq.). Fragment 4-11 is reported to be as active as Substance P itself.

Zuber, H. *et al., Angew. Chem., Int. Ed.*, 1962, **1**, 160 (*isol*)
Chang, M.M. *et al., J. Biol. Chem.*, 1970, **245**, 4748 (*isol*)
Chang, M.M. *et al., Nature (London), New Biol.*, 1971, **232**, 86 (*struct, synth*)
Yajima, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 682 (*synth*)
Studer, R.O. *et al., Helv. Chim. Acta*, 1973, **56**, 860 (*isol, struct*)
Bayer, E. *et al., Chem. Ber.*, 1974, **107**, 1344 (*synth*)
Leeman, S. *et al., Pept. Neurobiol.*, (Gainer, H., Ed.), Plenum, N.Y., 1977, 99 (*rev*)
Kitagawa, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 1604 (*synth*)
Iversen, L.L. *et al., Br. Med. Bull.*, 1982, **38**, 277 (*rev*)
Chassaing, G. *et al., J.O.C.*, 1983, **48**, 1757 (*synth*)
Subst. P Metab. Biol. Actions, [Proc. Symp.], 1984, (Eds. Jordan, C.C. *et al*), Taylor and Francis, London, 1985, (*book*)
Schwyzer, R. *et al., Helv. Chim. Acta*, 1986, **69**, 1789; 1798; 1807 (*cd, struct, props*)
Sivanandaiah, K.M. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 1045 (*synth*)
Payan, D.G. *et al., Ann. N.Y. Acad. Sci.*, 1987, **512**, 465 (*rev*)
Williams, R.W. *et al., J. Biol. Chem.*, 1990, **265**, 2505 (*Raman, cd, conformn*)
Snider, R.M. *et al., Chem. Ind. (London)*, 1991, 792 (*rev*)
Saulitis, J. *et al., J.A.C.S.*, 1992, **114**, 4818 (*pmr, cmr, conformn*)
Regul. Pept., 1993, **46**, 1 (*tachykinins, pharmacol, rev*)
Dockray, G.J. *et al., Gut Pept. 1994*, (Eds. Walsh, J.H. *et al*), Raven Press, 1994, 401 (*rev*)
Regoli, D. *et al., Pharmacol. Rev.*, 1994, **46**, 551 (*pharmacol, rev*)
Rissler, K. *et al., J. Chromatogr., B: Biomed. Appl.*, 1995, **665**, 233 (*hplc, rev*)

Subtilin, 9CI S-259

[1393-38-0]



$C_{148}H_{227}N_{39}O_{38}S_5$ 3320.99
Lantibiotic. Modified polypeptide with 5 sulfur bridges. Used as a food preservative. Amorph. $[\alpha]_D^{23}$ -29.

▶ WM2975000

4-L-Isoleucine analogue: [158183-23-4] $C_{149}H_{231}N_{39}O_{36}S_5$ 3305.034A mutant subtilin with dramatically improved chem. and antimicrobial props..

Jansen, E.F. *et al., Arch. Biochem. Biophys.*, 1944, **4**, 297 (*isol*)
Salle, A.J. *et al., Proc. Soc. Exp. Biol. Med.*, 1945, **60**, 60 (*isol*)
Steenken, W. *et al., J. Bacteriol.*, 1949, **57**, 453 (*props*)
Alderton, G. *et al., J.A.C.S.*, 1953, **75**, 2391 (*struct*)
Reshetov, P.D. *et al., Khim. Prir. Soedin.*, 1971, **6**, 101; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **6**, 89 (*isol*)
Jay, J.M. *et al., Econ. Microbiol.*, 1983, **8**, 117 (*rev*)
Kurahashi, K. *et al., CA*, 1985, **103**, 138113 (*rev*)
Jung, G. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 1051 (*rev*)
Chan, W.C. *et al., FEBS Lett.*, 1992, **300**, 56 (*pmr, struct*)
Liu, W. *et al., J. Biol. Chem.*, 1992, **267**, 25678-25685 (*Isl analogue*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SMW500

Subtilisins S-260

[9014-01-1]
E.C. 3.4.21.62

A group of alkaline serine proteases with a particularly reactive serine at the active site. Used in food processing as a meat tenderiser, as a cheese flavour developer, to improve dough texture and in flour treatment.

Subtilisin BPN[1] Contains 275 amino acids.
Subtilisin (Bacillus subtilis amylosaccharitics) A protein containing 275 amino acid residues.
Subtilisin A50 Contains 264 amino acid residues.
Subtilisin Pfizer Protease of 274 amino acid residues.
Subtilisin ISP An intracellular serine protease of 296 amino acid residues.
Subtilisin Carlsberg Contains 274 residues with 85 different residues from Subtilisin BPN[1].

Wright, C.S. *et al., Nature (London)*, 1969, **221**, 235 (*struct*)
Ottesen, M. *et al., Methods Enzymol.*, 1970, **19**, 199-215 (*rev*)
Markland, F.S. *et al., The Enzymes*, (Boyer, P.D., Ed.), Vol. 3, Academic Press, 1971, 561-608
Smith, E.L. *et al., J. Biol. Chem.*, 1972, **247**, 5619
Strongin, A.La. *et al., Bioorg. Khim.*, 1975, **1**, 1441
Munnelly, K.P. *et al., Int. J. Pept. Protein Res.*, 1976, **8**, 141
Stepanov, V.M. *et al., Biochem. Biophys. Res. Commun.*, 1977, **77**, 298
Wells, J.A. *et al., Nucleic Acids Res.*, 1983, **11**, 7911 (*cloning*)
Nedkov, P. *et al., Biol. Chem. Hoppe-Seyler*, 1985, **366**, 421 (*struct*)
Bayley, P.M. *et al., FEBS Lett.*, 1989, **250**, 389 (*conformn*)

Succinic acid, 8CI S-261

[110-15-6]
Butanedioic acid, 9CI. Ethane-1,2-dicarboxylic acid. Amber acid. Wormwood acid. E363

$HOOCCH_2CH_2COOH$

$C_4H_6O_4$ 118.089

Widely distributed in higher plants and prod. by microorganisms. Present in cheeses and fresh meats. Flavour enhancer, pH control agent. Prisms (H_2O). Sol. H_2O, EtOH, Me_2CO, Et_2O; prac. insol. C_6H_6, CS_2, CCl_4, petrol. Mp 184-185°. Bp 235° dec.. pK_{a1} 4.22; pK_{a2} 5.7 (25°, H_2O).

▶ Severe eye irritant. LD_{50} (rat, orl) 2260 mg/kg. WM4900000

Di-Na salt: [150-90-3]

[6106-21-4] *FEMA 3277*

Flavour enhancer. Cryst. + $6H_2O$. Loses water of cryst. at 120°.

Di-Me ester: [106-65-0] *Dimethyl succinate. Methyl succinate. FEMA 2396*

$C_6H_{10}O_4$ 146.143

Present in roasted filberts. Flavouring ingredient. Liq. Sl. sol. H_2O; sol. EtOH, Et_2O, Me_2CO. d_4^{18} 1.12. Mp 19°. Bp 200° Bp_{11} 80°. n_D^{20} 1.4197.

▶ Fl. p. 85°. WM7675000

Di-Et ester: [123-25-1] *Diethyl succinate. Ethyl succinate*

$C_8H_{14}O_4$ 174.196

Flavour ingredient. Insol. H_2O; sol. EtOH, Et_2O, Me_2CO. d_4^{20} 1.04. Mp -21°. Bp 217.7° Bp_{15} 105°. n_D^{20} 1.4201.

▶ Fl. p. 90°. Skin and eye irritant. LD_{50} (rat, orl) 8530 mg/kg. WM7400000

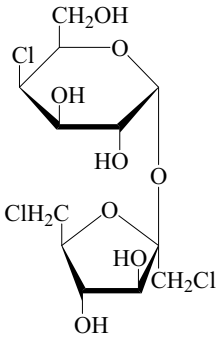
[56-14-4, 2226-88-2, 2922-54-5, 14047-56-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 492A; 547A; 617A; 617B; 695B; 740C; 767C; 767D; 770B; 840D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 766B; 940A; 940B; 1118C; 1211C; 1253A; 1256B; 1356B (*nmr*)
Weintraub, L. *et al., Chem. Ind. (London)*, 1965, 185 (*synth*)
Homes, J.L. *et al., Org. Mass Spectrom.*, 1970, **3**, 1505 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 837 (*occur*)
Williamson, K.L. *et al., J. Magn. Reson.*, 1978, **30**, 367 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 848 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, SMY000; SNB000
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 615
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 278; 896-897; 2692 (*di-Na salt, di-Me ester, occur, use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, **18**, 677 (*di-Me ester, rev, tox*)

Sucralose, BAN S-262

[56038-13-2]

1,6-Dichloro-1,6-dideoxy-β-D-fructofuranosyl 4-chloro-4-deoxy-α-D-galactopyranoside, 9CI. 4,1′,6′-Trichloro-4,1′,6′-trideoxygalactosucrose. Trichlorogalactosucrose. Splenda



$C_{12}H_{19}Cl_3O_8$ 397.635

Noncalorific sweetener with good taste props.. Mp 130° (114.5°). $[\alpha]_D$ +85.6 (c, 1.0 in H_2O). Sweetness approx. 650 x sucrose. Use currently (1999) permitted in Canada, Australia, Russia, Romania, Mexico and USA.

Penta-Ac: [55832-20-7]

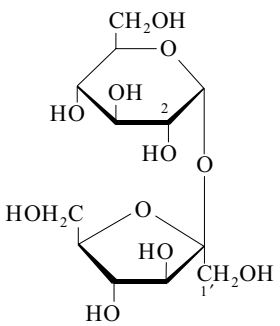
Mp 92-94°. $[\alpha]_D$ +66.8 ($CHCl_3$).

Fairclough, P.H. *et al., Carbohydr. Res.*, 1975, **40**, 285-298 (*synth*)
Eur. Pat., 1981, 31 651, (*Tate and Lyle*); *CA*, **95**, 169700a (*synth*)
Kanters, J.A. *et al., Carbohydr. Res.*, 1988, **180**, 175-182 (*cryst struct*)
Jenner, M.R. *et al., J. Food Sci.*, 1989, **54**, 1646-1649 (*props*)
Jenner, M.R. *et al., ACS Symp. Ser.*, 1991, **450**, 68-87 (*rev*)
Miller, G.A. *et al., Food Sci. Technol.*, 1991, **48**, 173-195 (*rev, props, synth, anal, use, tox*)
Knight, I. *et al., Can. J. Physiol. Pharmacol.*, 1994, **72**, 435-439 (*rev*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1995, **15**, 249-261 (*rev, degradn*)
Bouchemal-Chibani, N. *et al., Int. J. Biol. Macromol.*, 1995, **17**, 177-182 (*conformn*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1378
U.S. Pat., 1996, 5 498 709, (*McNeil-PPC*); *CA*, **124**, 343978 (*synth*)
Auger, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)

Sucrose, 9CI, 8CI S-263

[57-50-1]

β-D-Fructofuranosyl α-D-glucopyranoside, 9CI. Saccharose. Cane sugar. Beet sugar



$C_{12}H_{22}O_{11}$ 342.299

Sweetening agent and food source assimilated by most organisms. Also used in food products as a preservative, antioxidant, moisture control agent, stabiliser and thickening agent. Widespread in seeds, leaves, fruits, flowers and roots of plants, where it functions as an energy store for metabolism and as a carbon source for biosynth. Annual world production is in excess of 90 × 10^6 tons mainly from the juice of sugar cane and sugar beet which contain respectively *ca.* 20% and *ca.* 17% of the sugar. Cryst. (H_2O or EtOH). Mp 185-187°. $[\alpha]_D$ +66.5 (H_2O). Log P -5.72 (uncertain value) (calc). Does not reduce Fehling's soln., form an osazone or mutarotate. Hydrol. with invertase or acid gives D-glucose and D-fructose.

▶ OES long-term 10 mg m^{-3}; short-term 20 mg m^{-3}. LD_{50} (rat, orl) 29700 mg/kg. Exp. teratogen (very large doses). WN6500000

Octa-Ac: [126-14-7] *FEMA 3038*

$C_{28}H_{38}O_{19}$ 678.597

Flavouring ingredient, alcohol denaturant. Cryst. with intensely bitter flavour. Mp 84° (69°). $[\alpha]_D$ +59.6 ($CHCl_3$).

▶ WN6620000

Monohexadecanoyl: [26446-38-8] *β-D-Fructofuranosyl α-D-glucopyranoside monohexadecanoate, 9CI. Sucrose monopalmitate, 8CI. Sucrapan P. Sucrodet. Ryoto Sugar Ester P-170*

$C_{28}H_{52}O_{12}$ 580.712

Inhibits deterioration of starch in wheat flour, and growth of microorganisms in soft drinks. Emulsifier, smooth texture agent, antifreeze and dispersing agent for foods. Component of protective coatings for fruit. Mp 60-62°. $[\alpha]_D^{20}$ +36 (c, 1 in EtOH).

Monooctadecanoyl: [25168-73-4] *β-D-Fructofuranosyl α-D-glucopyranoside monooctadecanoate, 9CI. Sucrose monostearate, 8CI. Sucrapan S. Ryoto sugar Ester S-1170*

$C_{30}H_{56}O_{12}$ 608.765

Dispersant, solubiliser, dough strengthener, emulsifier for coffee whitening, shortening and ice cream. Used for similar purposes to Sucrapan P above. Mp 56-60°. $[\alpha]_D^{20}$ +36.2 (c, 1 in EtOH).

Octakis(alkanoyl): [121854-29-3] *Olestra*

Nondigestible fat substitute for low-calorie food. Olestra stated to contain C-6, C-7 and C-8 alkanoyl residues.

1′-O-(3,4,5-Trihydroxybenzoyl): [115713-45-6] ***1′-O-Galloylsucrose***

$C_{19}H_{26}O_{15}$ 494.405

A tannin isol. from commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ +47 (c, 0.84 in MeOH).

2-O-(3,4,5-Trihydroxybenzoyl): [115713-46-7] ***2-O-Galloylsucrose***

$C_{19}H_{26}O_{15}$ 494.405

Isol. from the commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $2H_2O$. $[\alpha]_D^{27}$ +67.1 (c, 0.79 in MeOH).

4′-O-(3,4,5-Trihydroxybenzoyl): [115713-44-5] ***4′-O-Galloylsucrose***

$C_{19}H_{26}O_{15}$ 494.405

Tannin constit. of commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ +14.9 (c, 0.72 in MeOH).

6-O-(3,4,5-Trihydroxybenzoyl): [115731-

15-2] ***6-O-Galloylsucrose***
$C_{19}H_{26}O_{15}$ 494.405
Isol. from commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ +48 (c, 0.65 in MeOH).

6′-O-(3,4,5-Trihydroxybenzoyl): [115713-43-4] ***6′-O-Galloylsucrose***
$C_{19}H_{26}O_{15}$ 494.405
Isol. from commercial Chinese rhubarb (*Rheum* spp.). Needles + $2H_2O$ (H_2O). Mp 149-151°. $[\alpha]_D^{28}$ +88.6 (c, 0.74 in MeOH).

6-O-(3,4-Dihydroxycinnamoyl)(E-):6-Caffeoylsucrose
$C_{21}H_{28}O_{14}$ 504.444
Constit. of *Salvia officinalis* (sage). Cryst. (MeOH). Mp 210-212°. $[\alpha]_D^{23}$ +27.2 (c, 0.13 in MeOH).

3′,6-Bis-O-(4-hydroxy-3,5-dimethoxycinnamoyl): [139891-98-8] *3′,6-Disinapoylsucrose*
$C_{34}H_{42}O_{19}$ 754.694
Constit. of radish (*Raphanus sativus*). Yellow powder. Mp 138-141°. $[\alpha]_D$ -94 (c, 0.2 in MeOH).

[12738-64-6, 31835-06-0, 35867-41-5, 73264-44-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 196B; 625D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 305C; 1060A (*nmr*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 477 (*rev*)
Lemieux, R.U. *et al., J.A.C.S.*, 1953, **75**, 4118 (*synth*)
Van der Veen, J.M. *et al., J.O.C.*, 1963, **28**, 564 (*pmr*)
Kollonitsch, V. *et al., Sucrose Chemicals*, Kline, The International Sugar Research Foundation, Washington, D.C., 1970, (*rev*)
Allerhand, A. *et al., J.A.C.S.*, 1971, **93**, 2777 (*cmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 654 (*occur*)
Hanson, J.C. *et al., Acta Cryst. B*, 1973, **29**, 797 (*cryst struct*)
Khan, R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1976, **33**, 235 (*rev*)
Sucrochemistry, (Ed. Hickson, J.L.), ACS Symp. Series, 1977, **41**, (*rev*)
Pfeffer, P.E. *et al., J.A.C.S.*, 1979, **107**, 1265 (*cmr*)
Mathlouthi, M. *et al., Carbohydr. Res.*, 1980, **81**, 203; 213 (*Raman*)
Eur. Pat., 1980, 20 122; *CA*, **95**, 7697c (*Sucrapans*)
Block, K. *et al., Carbohydr. Res.*, 1982, **100**, 63 (*conformn*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 827 (*rev, tox, octa-Ac*)
Hull, W.E. *et al., Two-Dimensional NMR Brochure*, Brüker Analytische Messtechnik, Karlsruhe, 1982, (*pmr*)
Machida, H. *et al., CA*, 1988, **109**, 229005x (*Sucrapans*)
Eur. Pat., 1988, 275 939; *CA*, 1989, **110**, 173692v (*Sucrapans*)
Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1469 (*gallates*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, SNH000
James, C.E. *et al., Prog. Chem. Org. Nat. Prod.*, 1989, **55**, 117 (*rev*)
Mathlouthi, M. *et al., Sucrose*, Blackie, 1995, (*book*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1347; 1378; 1756
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2045; 2697; 2701; 2702 (*Olestra, Sucrapans*)
Wang, M. *et al., J. Nat. Prod.*, 1999, **62**, 454-456 (*6-Caffeoylsucrose*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SNH000

Sucrose acetate isobutyrate S-264

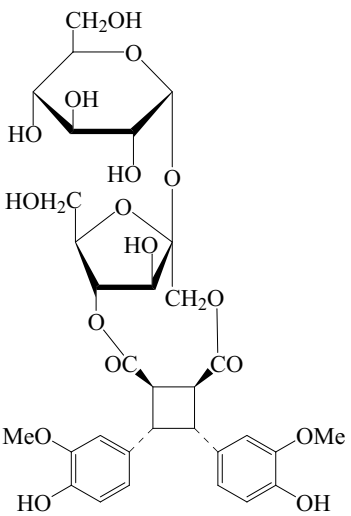
[126-13-6]
Sucrose diacetate hexaisobutyrate, 8CI. Sucrose acetate 2-methylpropanoate. SAIB

$C_{40}H_{62}O_{19}$ 846.918

A mixture of sucrose esters with a composition approximating to the diacetate hexaisobutyrate. Clouding agent, stabiliser and specific gravity control agent for beverages, esp. fruit drinks.

Phillips, J.C. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 375-380 (*metab*)
Reynolds, R.C. *et al., Food Chem. Toxicol.*, 1998, **36**, 81-93; 95-99 (***rev, use, tox, metab***)
Chanamai, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 5561-5565 (*use*)

Sucrose 1′,4′-(4,4′-dihydroxy-3,3′-dimethoxy-β-truxinate) S-265

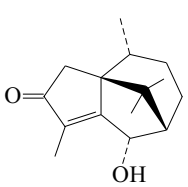


$C_{32}H_{38}O_{17}$ 694.642
Constit. of oat grains (*Avena sativa*). Off-white solid. λ_{max} 208 ; 283 (MeOH).

Dimberg, L.H. *et al., Phytochemistry*, 2001, **56**, 843-847

Sugeonol S-266

[19419-58-0]

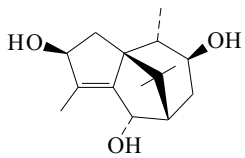


$C_{15}H_{22}O_2$ 234.338
Constit. of *Cyperus rotundus* (nutgrass). Needles (Et_2O). Mp 181-182.5°. $[\alpha]_D$ +87.5 (c, 3.8 in $CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1968, **16**, 52; 1088 (*isol, pmr*)

Sugetriol S-267

[18067-36-2]

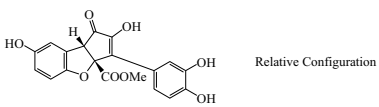


$C_{15}H_{24}O_3$ 252.353
Cryst. Mp 221-222°. $[\alpha]_D$ +62.4 (EtOH).

Tri-Ac: [17928-62-0] ***Sugetriol triacetate***
$C_{21}H_{30}O_6$ 378.464
Constit. of *Cyperus rotundus* (nutgrass). Cryst. Mp 132°. $[\alpha]_D$ +60.5 ($CHCl_3$).

Hikino, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1433 (*isol, pmr*)

Suillusin S-268

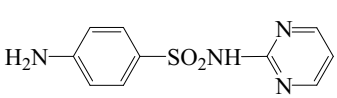


$C_{19}H_{14}O_8$ 370.315
Isol. from the mushroom *Suillus granulatus* (granulated bolete). Yellow powder. $[\alpha]_D$ +4 (c, 1 in MeOH). λ_{max} 223 (sh) (log ϵ 3.56); 261 (log ϵ 3.21); 311 (sh) (log ϵ 3.3); 348 (log ϵ 3.42) (MeOH).

Yun, B.-S. *et al., J. Nat. Prod.*, 2001, **64**, 1230-1231

Sulfadiazine, INN S-269

[68-35-9]
4-Amino-N-2-pyrimidinylbenzenesulfonamide, 9CI. N′-(2-Pyrimidinyl)sulfanilamide, 8CI. 2-(4-Aminobenzenesulfonamido)pyrimidine. Sulphadiazine, BAN. Coco-Diazine. Cremodiazine. Eskadiazine. Adiazine. Sulfapyrimidine. Sulfazin (Russian pharmaceutical). Debenal. Theradiazine



$C_{10}H_{10}N_4O_2S$ 250.281
Antibacterial agent. Used in some countries for control of bacterial disease in farmed fish. Not approved for aquacultural use in the USA. Yellowish-white or pinkish-white powder, darkens on exp. to light. Spar. sol. hot H_2O. Mp 255-256° dec. pK_{a1} 2.38; pK_{a2} 6.25 (25°). Log P 0.07 (calc). Component of Trisulfapyrimidines, USAN.

▶ Adverse renal effects when used therapeutically. LD_{50} (mus, orl) 1500 mg/kg. Exp.

reprod. and teratogenic effects. WP1925000

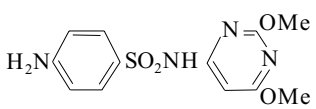
Na salt: [547-32-0] ***Sulfadiazine sodium, INN, USAN.*** *Solu-Diazine*
Yellowish-white powder, darkens on exp. to light, absorbs CO_2. V. sol. H_2O.
▶ LD_{50} (mus, orl) 1700 mg/kg. Exp. reprod. effects. WP2000000

Ag salt: [22199-08-2] ***Silver sulfadiazine, USAN.*** *Sulfadiazine silver, JAN. Silvadene. Flamazine*
$C_{10}H_9AgN_4O_2S$ 357.141
▶ WP1950000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 392A (*nmr*)
Roblin, R.O. *et al., J.A.C.S.*, 1940, **62**, 2002 (*synth*)
Fox, C.L. *et al., Arch. Surg. (Chicago)*, 1968, **96**, 184 (*Ag salt*)
Bass, A.D. *et al., Drill's Pharmacol. Med.*, 4th edn., McGraw-Hill, New York, 1971, 1657 (*rev, pharmacol*)
Chang, C.J. *et al., J. Med. Chem.*, 1975, **18**, 505 (*pmr*)
Kracmar, J. *et al., Pharmazie*, 1975, 30; 447 (*uv*)
Przybylski, M. *et al., Adv. Mass Spectrom. Biochem. Med., Proc. Int. Symp. Mass Spectrom. Biochem. Med. 2nd, 3rd*, 1976, **1**, 309 (*ms*)
Stober, H. *et al., Anal. Profiles Drug Subst.*, 1982, **11**, 523; 1984, **13**, 553 (*rev, synth, pharmacol, anal*)
Cai, E. *et al., CA*, 1982, **96**, 57702 (*synth*)
Sigel, C.W. *et al., Handb. Exp. Pharmacol.*, 1983, **64**, 163 (*rev, metab*)
Joshi, V.V. *et al., Indian J. Phys., A*, 1983, **57**, 79 (*cryst struct*)
Bult, A. *et al., Pharm. Weekbl., Sci. Ed.*, 1983, **5**, 77 (*cmr, tautom*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1477
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 201; 206
Kokila, M.K. *et al., Acta Cryst. C*, 1995, **51**, 333 (*cryst struct*)
Gehring, T.A. *et al., J. Agric. Food Chem.*, 1996, **44**, 3164-3169 (*anal*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MRM250; SNI425; PPP500

Sulfadimethoxine, INN S-270

[122-11-2]
*4-Amino-*N*-(2,6-dimethoxy-4-pyrimidinyl)benzenesulfonamide, 9CI.* N′*-(2,6-Dimethoxy-4-pyrimidinyl)sulfanilamide, 8CI. 4-*p*-Aminobenzenesulfonamido-2,6-dimethoxypyrimidine.* ***Sulphadimethoxine, BAN.*** *Albon†. Agribon. Chemiosalfa. Deltin. Madribon. Risulpir. Sulfadren. Sulfathox*



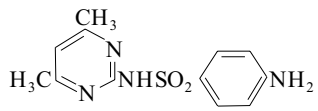
$C_{12}H_{14}N_4O_4S$ 310.333
Long-acting sulfonamide, antibacterial agent. Potential food contaminant in animal products arising from its veterinary use. Cryst. (EtOH aq.). Mp 201-203°. Log P 1.1 (calc).
▶ LD_{50} (mus, ipr) 866 mg/kg. Exp. reprod. and teratogenic effects (large doses). WO9030000

N^4*-Ac:*
$C_{14}H_{16}N_4O_5S$ 352.37
Spar. sol. H_2O. Mp 220-223°.

Bretschneider, H. *et al., Monatsh. Chem.*, 1956, **87**, 136; 1961, **92**, 128 (*synth*)
Shepherd, R.G. *et al., J.O.C.*, 1961, **26**, 2764 (*synth*)
Boehni, E. *et al., Chemotherapy (Basel)*, 1969, **14**, 195 (*pharmacol*)
Edwards, D. *et al., J. Pharm. Pharmacol.*, 1971, **23**, 956 (*ir*)
Okui, K. *et al., J. Het. Chem.*, 1972, **9**, 821 (*synth*)
Shefter, E. *et al., J. Pharm. Sci.*, 1972, **61**, 872 (*pharmacol*)
Kracmar, J. *et al., Pharmazie*, 1975, **30**, 447 (*uv*)
Bult, A. *et al., Pharm. Weekbl., Sci. Ed.*, 1983, **5**, 77 (*cmr, tautom*)
Narula, P. *et al., Indian J. Phys., A*, 1987, **61**, 132 (*cryst struct*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2351
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 876 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 207
Combs, M.T. *et al., J. Agric. Food Chem.*, 1997, **45**, 1779-1783 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SNN300

Sulfadimidine, INN S-271

[57-68-1]
*4-Amino-*N*-(4,6-dimethyl-2-pyrimidinyl)-benzenesulfonamide, 9CI.* N′*-(4,6-Dimethyl-2-pyrimidinyl)sulfanilamide, 8CI. Sulfamethazine. Sulphadimidine, BAN. Sulphamezathine. Sulfadimerazine. Sulfadimesine. Sulfadimethylpyrimidine. Sulfadimezine. Superseptil. Sulfodimezine. Sulphamethazine*



$C_{12}H_{14}N_4O_2S$ 278.334
Widely-used, short acting sulfonamide. Potential food contaminant in animal products arising from its veterinary use. Creamy-white powder; cryst. (dioxan aq.). Sol. H_2O (increasing with pH). Mp 176° (197.8-198.8°). Log P 1.07 (calc). Dec. on exposure to light. Component of Trisulfapyrimidines, USAN.
▶ Exp. thyroid effects from chronic administration. WO9275000

$N^{4'}$*-Ac:* [100-90-3] N-*[4-[[(4,6-Dimethyl-2-pyrimidinyl)amino]sulfonyl]phenyl]acetamide, 9CI*
$C_{14}H_{16}N_4O_3S$ 320.371
Mp 245.2-246.2°.

[1981-58-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 836C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 393C (*nmr*)
Visconti, M. *et al., Helv. Chim. Acta*, 1962, **45**, 615 (*synth*)
U.S. Pat., 1968, 3395141; *CA*, 77276b (*synth, $N^{4'}$-Ac*)
Cambon, A. *et al., Bull. Soc. Chim. Fr.*, 1970, 567 (*ms*)
Turczan, J. *et al., J. Pharm. Sci.*, 1972, **61**, 434 (*pmr*)
McMahon, K.A. *et al., J. Pharm. Sci.*, 1972, **61**, 518 (*pharmacol*)
Kracmar, J. *et al., Pharmazie*, 1975, **30**, 447 (*uv*)
Papastephanou, C. *et al., Anal. Profiles Drug Subst.*, 1978, **7**, 401 (*rev, synth, metab*)
Haley, T.J. *et al., Dangerous Prop. Ind. Mater. Rep.*, 1982, **2**, 5 (*rev*)
Tiwari, R.K. *et al., Acta Cryst. C*, 1984, **40**, 655 (*cryst struct*)
Maury, L. *et al., J. Pharm. Sci.*, 1985, **74**, 422 (*struct*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2343
Littlefield, N.A. *et al., Food Chem. Toxicol.*, 1989, **27**, 455; 1990, **28**, 157 (*tox*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **2**, 876 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 207
Doerge, D.R. *et al., Chem. Res. Toxicol.*, 1994, **7**, 164 (*bibl*)
Combs, M.T. *et al., J. Agric. Food Chem.*, 1997, **45**, 1779-1783 (*occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SJW500; SNJ000

Sulfamic acid, 11CI S-272

[5329-14-6]
Amidosulfonic acid
$H_2NS(O)_2OH$
H_3NO_3S 97.095
Interatomic distance: N–S 174 pm. Food contaminant arising from its use as an ingredient of paper and paperboard products used in packaging. Non-hygroscopic white cryst. solid. V. sol. H_2O, liq. NH_3, formamide. Mp 205° dec. pK_a 0.99 (25°).
▶ Irritant, corrosive, poison. WO5950000

Na salt: [13845-18-6] *Sodium sulfamate*
H_2NNaO_3S 119.077
Cryst. Mp 250°.

NH_4 salt: [7773-06-0] *Ammonium sulfamate. AMS. Amcide. Ammate*
$H_6N_2O_3S$ 114.125
Hygroscopic cryst. Sol. H_2O, liq. NH_3, formamide, glycerol. Mp 131-132°. Dec. at 160°.
▶ Powerful oxidiser. WO6125000

*Co(*II*) salt (2:1):* See Cobalt(*II*) sulfamate in *The Combined Chemical Dictionary.*

*Ni(*II*) salt (2:1):* See Nickel(*II*) sulfamate in *The Combined Chemical Dictionary.*

*Cu(*II*) salt (2:1):* See Copper(*II*) sulfamate in *The Combined Chemical Dictionary.*

Ag salt:Silver sulfamate
AgH_2NO_3S 203.955

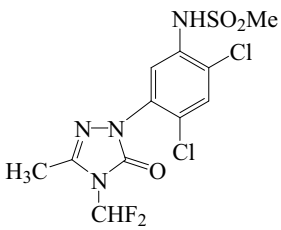
[15853-39-1, 50979-18-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1230C; 1231A (*ir*)
Chem. Rev., 1940, **26**, 49 (*rev*)
Inorg. Synth., 1946, **2**, 176; 1978, **18**, 201 (*synth, props, Ag salt*)
Gmelin Handbook Inorg. Chem., Syst. No, 9, 1963, **B3**, 1582 (*bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1117 (*use*)
Analyst (London), 1972, **97**, 740 (*microanal*)

Fadrus, H. *et al., Acta Hydrochim. Hydrobiol.*, 1975, **3**, 334; *CA*, **85**, 10196n ($NO_2^{\ominus}$ *removal*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 487 (*synth*)
Bats, J.W. *et al., Acta Cryst. B*, 1976, **32**, 1563 (*cryst struct*)
Shoi, O. *et al., CA*, 1976, **85**, 171281b (*detn,* $NO_2^{\ominus}$)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **21**, 949
Benson, G.A. *et al., Chem. Rev.*, 1980, **80**, 151 (*rev*)
Manickkavachagam, R. *et al., Z. Kristallogr.*, 1984, **168**, 179-185 (*Na salt, cryst struct*)
Pesticide Manual, 8th edn., 1987, 360 (NH_4 *salt, use*)
Canagaratna, M. *et al., J.A.C.S.*, 1996, **118**, 5290 (*microwave*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2704-2705
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANU650; SNK500

Sulfentrazone, ANSI, BSI S-273

[122836-35-5]
N-*[2,4-Dichloro-5-[4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl]phenyl]methanesulfonamide, 9CI. Authority. Boral. F 6285. FMC 6285. FMC 97285*



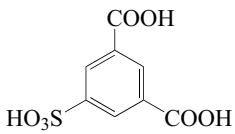
$C_{11}H_{10}Cl_2F_2N_4O_3S$ 387.193
Herbicide used against broad-leaved weeds in soya beans. Tan solid. Mp 121-123°.
▶ LD_{50} (rat, orl) 2855 mg/kg.

U.S. Pat., 1989, 4 818 275, (*FMC*); *CA*, **111**, 153817g (*synth, activity*)
Van Saun, W.A. *et al., Brighton Crop Prot. Conf. - Weeds*, 1991, 77-82 (*activity, use*)
Leung, L.Y. *et al., J. Agric. Food Chem.*, 1991, **39**, 1509-1514 (*metab*)
Theodoridis, G. *et al., ACS Symp. Ser.*, 1992, **504**, 134-146 (*synth, activity, sar*)
Vidrine, R.R. *et al., Weed Technol.*, 1996, **10**, 762-765 (*use*)
Dayan, F.E. *et al., J. Agric. Food Chem.*, 1998, **46**, 2024-2029 (*activity*)
Pesticide Manual, 12th edn., 2000, No. 711

5-Sulfo-1,3-benzenedicarboxylic acid, 9CI, 8CI S-274

[22326-31-4]

[6362-79-4]
5-Sulfoisophthalic acid, 8CI



$C_8H_6O_7S$ 246.197
FDA approved for use in food-contact polyester resins. Cryst. or cryst. + $2H_2O$. Mp 60-70° (dec.) (dihydrate) Mp 258° (anhyd.). pK_{a1} 1.87; pK_{a2} 2.68; pK_{a3} 11.42 (25°,H_2O). Mp >300° (anhyd.).

1,3-Di-Me ester: [138-25-0]

[3965-55-7]
$C_{10}H_{10}O_7S$ 274.251
Cryst. (H_2O).

Didodecyl ester: [79965-15-4]
$C_{32}H_{54}O_7S$ 582.84
Powder + $^1/_2H_2O$ (as Na salt). Mp 203-210° (Na salt). CAS no. refers to Na salt.

Dihydrazide: [56767-62-5]

[52235-84-4]
$C_8H_{10}N_4O_5S$ 274.257Mp >300° (as Na salt).

[7800-91-1, 56896-98-1]

Aldrich Library of FT-NMR Spectra, **2**, 1602B (*nmr*)
U.S. Pat., 1959, 2 895 986; *CA*, **54**, 1447a (*synth*)
Ger. Pat., 1962, 1 133 722; *CA*, **57**, 15016i (*synth*)
Czech. Pat., 1966, 119 642; *CA*, **68**, 12727j (*di-Me ester*)
Malek, J. *et al., Chem. Prum.*, 1970, **20**, 117-120 (*esters*)
Nissen, D. *et al., J. Appl. Polym. Sci.*, 1974, **18**, 1953-1968 (*dihydrazide*)
Okahota, Y. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1981, **85**, 789-798 (*synth, esters*)
Kosugi, Y. *et al., Anal. Sci.*, 1989, **5**, 253-255 (*S-33 nmr*)
Japan. Pat., 1996, 96 099 951; *CA*, **125**, 57988 (*synth, pmr, di-Me ester*)
Food Chem. News, 2002, **43(47)**, 22 (*use*)

Sulfobutanedioic acid, 9CI S-275

[5138-18-1]
Sulfosuccinic acid
$HOOCCH_2C(SO_3H)COOH$
$C_4H_6O_7S$ 198.153

(±)-*form*
Present in can-end cements. Syrup. Dec. without melting on heating. The esters listed are *C,C*-diesters. They are rather poorly documented.

Dihexyl ester: [23243-42-7]

[3006-15-3, 41925-28-4] *Acrosol MA*
$C_{16}H_{30}O_7S$ 366.475
Liq. d_4^{20} 1.09. Bp 149° Bp 153°. n_D^{20} 1.4524.

Dioctyl ester: [2373-23-1]

[1639-66-3, 14380-16-6, 33918-25-1] *Aerosol OT-N*
$C_{20}H_{38}O_7S$ 422.582
Cryst. (EtOH aq.) (as Na salt).

Didodecyl ester: [3700-71-8]

[4229-35-0, 41925-29-5]
$C_{28}H_{54}O_7S$ 534.796Used as Na salt, no phys. props. reported.

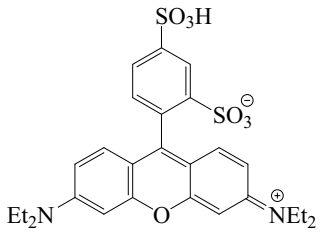
Bis(tridecyl) ester: [2673-22-5]
$C_{30}H_{58}O_7S$ 562.85
Mp 70-75°.

[20526-58-3, 54949-98-3]

Backer, H.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1927, **46**, 473 (*synth*)
U.K. Pat., 1957, 760 121; *CA*, **51**, 7044i (*bistridecyl ester*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 12 (*use, esters*)

Sulforhodamine B S-276

[2609-88-3]
*3,6-Bis(diethylamino)-9-(2,4-disulfophenyl)xanthylium hydroxide inner salt, 9CI. [6-(Diethylamino)-9-(2,4-disulfophenyl)-3*H*-xanthen-3-ylidene]diethylammonium, 8CI. C.I. Acid Red 52. Food Red 106. Lissamine Rhodamine B. C.I. 45100*



$C_{27}H_{30}N_2O_7S_2$ 558.675
Some synonyms strictly refer to the Na salt. Food dye. λ_{max} 558 (no solvent reported).

Na salt: [3520-42-1]

[53918-45-9]
$C_{27}H_{29}N_2NaO_7S_2$ 580.657
λ_{max} 554 (no solvent reported).

4′-Chloride: See 9-[4-(Chlorosulfonyl)-2-sulfophenyl]-3,6-bis(diethylamino)xanthylium in *The Combined Chemical Dictionary.*

4′-Anilide:
$C_{33}H_{35}N_3O_6S_2$ 633.788
Violet-brown needles (EtOH aq.). Dec. without melting.

Chadwick, C.S. *et al., Immunology*, 1958, **1**, 315-327 (*chloride, synth, use*)
Ioffe, I.S. *et al., Zh. Obshch. Khim.*, 1962, **32**, 1489-1492 (*chloride, anilide, synth, uv*)
Colour Index, 3rd edn., 1971, **4**, 4419 (*synth*)
Gurr, E. *et al., Synthetic Dyes in Biology, Medicine and Chemistry*, Academic Press, 1971, 372-373 (*uv, props*)
Metrione, R.M. *et al., J. Chromatogr.*, 1986, **363**, 337-344 (*chloride, use*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 956; **15**, 20 (*use*)
Konishi, N. *et al., J. Toxicol. Pathol.*, 1992, **5**, 157-165 (*tox*)

Sulfur dioxide, 11CI S-277

[7446-09-5]

[12624-32-7]
Sulfur oxide (SO_2). Sulfurous anhydride. Sulfurous oxide. E220. FEMA 3039

SO_2 (C_{2v})
O_2S 64.065
Occurs naturally in the atmosphere and as a pollutant gas from combustion processes. Implicated in formation of acid rain. Interatomic distances: S–O 143.2 pm; angle OSO 119.5°. Food preservative. Sanitising agent for food containers and fermentation equipment. Also used in foods as stabiliser, moisture control

agent, flavour modifier and texturiser. Colourless nonflammable gas with strong odour. Sol. H_2O, soly. decreases with temp. Mp -75.48°. Bp -10.02°. T_{crit} 157.6°, P_{crit} 78 atm, V_{crit} 122 cm^3g^{-1}. Catalytically oxidised by air to SO_3.

▶ Severe irritant of the eyes, skin and mucous membranes. Exposure of the eyes to liq. can cause permanent damage. OES: long-term 2 ppm; OES: short-term 5 ppm. WS4550000

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1690B (*ir*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 9, 1953, **1**, ; 1960, **2**, ; 1963, **3**, ; *Suppl. Vol.*, 1980, 70 (*rev, bibl*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1122; 1979, **7**, 346; 1969, **2**, 392; 1981, **9**, 440; 1980, **8**, 464; 1974, **4**, 469; 1984, **11**, 495; 1977, **6**, 558; 1975, **5**, 633 (*uses*)
Clark, A.H. *et al., Trans. Faraday Soc.*, 1971, **67**, 2216 (*struct*)
Hamada, Y. *et al., Can. J. Phys.*, 1974, **52**, 1443 (*struct*)
Ryan, R.R. *et al., Struct. Bonding (Berlin)*, 1981, **46**, 47 (*transition metal complexes*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **23**, 299
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4688-4693 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 732
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2706-2707
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1168
Proctor and Hughes' Chemical Hazards of the Workplace, 4th edn., (eds. Hathaway, G.J. et al), Van Nostrand Reinhold, 1996, 571
Bretherick's Handbook of Reactive Chemical Hazards, 6th edn., (ed. Urben, P.G.), Butterworth-Heinemann, 1999, 4837
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, SOH500

Sulfuric acid, 11CI S-278

[7664-93-9]
Oil of vitriol. E513
$(HO)_2SO_2$
H_2O_4S 98.079
Used in food processing as a pH control agent and a flavour modifier. Viscous colourless liq. Misc. H_2O, EtOH. d^{25} 1.83. Mp 10.36°. Bp 279.6°. pK_{a1} 3; pK_{a2} 1.99 (25°).

▶ Oxidant, v. corrosive, has great affinity for H_2O. Injurious to skin, eyes, mucosa. WS5600000

Di-NH_4 salt: [7783-20-2] *Ammonium sulfate. E517*
$H_8N_2O_4S$ 132.14
Used in foods as a dough strengthener, firming agent and processing aid. White rhombic cryst. V. sol. H_2O. Mp 513° (sealed tube).

▶ BS4500000

[8014-95-7, 13814-01-2, 43086-58-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1261B (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1930, **10**, 351 (*rev*)
Gmelin Handbook Inorg. Chem., *Syst. No.* 9, 1960, **B2**, 622 (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 869 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 190 (*manuf*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 145-146; 2708-2709
Pesticide Manual, 12th edn., 2000, No. 717
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANU750; SOI500; SOI520; SOI530

Sulfurous acid, 11CI S-279

[7782-99-2]
Sulfuric(IV) acid (H_2SO_3). Sulfur dioxide solution
$O{=}S(OH)_2$ or $HOS(O)_2H$
H_2O_3S 82.08
Probably exists in aq. soln. as the unsymmetrical struct. Known as many salts. Food additive listed on the EAFUS Food Additive Database (Jan. 2001). Present in aq. solns. of SO_2. Colourless, acid liq. Oxid. in air to sulfuric acid. pK_{a1} 1.89; pK_{a2} 7.21 (25°).

▶ Suffocating odour of SO_2. Irritant. WT2775000

Mono-Na salt: Sodium hydrogen sulfite, S-132
Di-Na salt: Sodium sulfite (Na_2SO_3), S-147
Di-K salt: Potassium sulfite (K_2SO_3), P-447
Di-NH_4 salt: Diammonium sulfite, D-121
Mono-Mg salt: See Magnesium hydrogen sulfite in *The Combined Chemical Dictionary.*

Gmelin Handbook Inorg. Chem., *Syst. No.* 9, 1960, **B2**, 397 (*rev, bibl*)
Schmidt, M. *et al., Z. Anorg. Allg. Chem.*, 1960, **303**, 184 (*evidence for free acid*)
Schmidt, M. *et al., Compr. Inorg. Chem.*, Pergamon, Oxford, 1973, **2**, 878 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1139
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SOO500

Sulfuryl fluoride, 11CI S-280

[2699-79-8]
Sulfuric oxyfluoride. Difluorodioxosulfur(VI). Vikane
$S(O)_2F_2$
F_2O_2S 102.062
Interatomic distances: F–S 153, S=O 140.5 pm. Post-harvest fumigant for walnuts and raisins. Odourless, colourless, fairly inert gas. Stable to 400°. Sol. H_2O. d^{-55} 0.17. Mp -136.7° (-135.8°). Bp -55.4°.

▶ Poison by ingestion, mildly toxic by inhalation. Exposure can cause nausea, vomiting, cramps and itching. May be narcotic. WT5075000

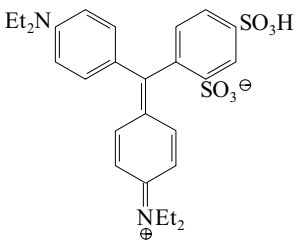
NH_3 complex: [94929-60-9] *Amminedifluorodioxosulfur(VI)*
$F_2H_3NO_2S$ 119.092
Isol. only in N_2 matrix. Weak 1:1 donor-acceptor complex.

Lide, D.R. *et al., J. Chem. Phys.*, 1957, **26**, 734 (*struct*)
Inorg. Synth., 1960, **6**, 158; 1967, **9**, 111 (*synth*)
Jolly, W.L. *et al., Prep. Inorg. React.*, 1966, **3**, 35 (*rev, ir, nmr*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 188 (*synth*)
Holloway, J.H. *et al., Adv. Inorg. Chem. Radiochem.*, 1983, **27**, 168 (*rev*)
Sass, C.S. *et al., J. Phys. Chem.*, 1985, **89**, 1002 (*ammine, ir*)
Merck Index, 11th edn., 1989, No. 8960 (*props*)
Pesticide Manual, 12th edn., 2000, No. 718
Pestic. Tox. Chem. News, 2001, **29(46)**, 8 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SOU500

Sulphan blue, BAN S-281

[116-95-0]

[129-17-9]
N-[4-[[4-(Diethylamino)phenyl](2,4-disulfophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-N-ethylethanaminium, 9CI. [4-[α-[p-(Diethylamino)phenyl]-2,4-disulfobenzylidene]-2,5-cyclohexadien-1-ylidene]-diethylammonium, 8CI. Blue VRS. Disulfine blue VNS. Alphazurine 2G. Sulfan blue. Patent blue V. C.I. 42045



$C_{27}H_{32}N_2O_6S_2$ 544.692
Strictly the name Sulphan blue applies to the sodium salt.Violet powder (as Na salt). Na salt v.sol. H_2O, sol. EtOH. λ_{max} 635 (H_2O).

▶ Hypersensitivity reactions reported incl. anaphylactic shock when used parenterally.

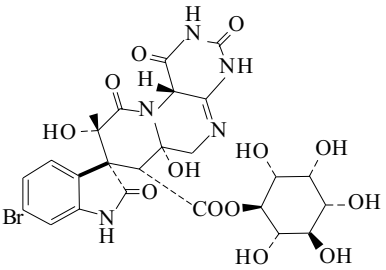
Ca salt: [3536-49-0] *C.I. Acid Blue 3. C.I. Food Blue 3. E131. CI 42051*
Colourant for beverages. Bright blue solid.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1028C (*ir*)
Holmes, W.C. *et al., Ind. Eng. Chem.*, 1923, **15**, 833 (*uv*)
Colour Index, 1971, **4**, 4383 (*synth, bibl*)
Gangolli, S.D. *et al., Food Cosmet. Toxicol.*, 1972, **10**, 449 (*pharmacol*)
Bishop, E. *et al., Indicators*, Pergamon, Oxford, 1972, 125 (*use*)
McEwen, C.N. *et al., Anal. Chem.*, 1977, **49**, 922 (*ms*)
IARC Monog., 1978, **16**, 163; *Suppl.* 7, 59 (*rev, tox*)
Newton, D.W. *et al., J. Pharm. Sci.*, 1981, **70**, 122 (*props*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1108
Nevado, B. *et al., Fresenius' Z. Anal. Chem.*, 1999, **365**, 383-388 (*anal*)
Perez-Urquiza, M. *et al., J. Chromatogr., A*, 2000, **898**, 271-275 (*anal*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 553

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADE500

Surugatoxin S-282

[40957-92-4]



$C_{25}H_{26}BrN_5O_{13}$ 684.41

Unique skeleton containing both indole and pteridine subunits. Marine toxin, causing shellfish poisoning. Prisms + $7H_2O$. Mp 300°. λ_{max} 276 (ϵ 15000) (0.1*N* HCl) (Derep). λ_{max} 279 (ϵ 19000) (0.1*N* NaOH) (Derep). λ_{max} 276 (ϵ 15000) (H_2O) (Derep).

▶ Toxic.

Kosuge, T. *et al., Tet. Lett.*, 1972, 2545 (*isol, uv, ir, cryst struct*)
Inoue, S. *et al., Tet. Lett.*, 1984, **25**, 4407 (*synth*)
Okado, K. *et al., Yakugaku Zasshi*, 1985, **105**, 375; 381 (*synth*)
Inoue, S. *et al., Tetrahedron*, 1994, **50**, 2729 (*synth*)

SW 55 Killer toxin S-283

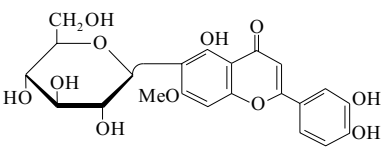
Prod. by *Candida* sp. SW55 isol. from the skin of grape berries. Killer toxin.

Yokomori, Y. *et al., Agric. Biol. Chem.*, 1988, **52**, 2791-2796 (*isol*)

Swertiajaponin S-284

[6980-25-2]

*2-(3,4-Dihydroxyphenyl)-6-β-D-glucopyranosyl-5-hydroxy-7-methoxy-4*H*-1-benzopyran-4-one, 9CI. Isoorientin 7-methyl ether. Leucanthoside*



$C_{22}H_{22}O_{11}$ 462.409

Constit. of leaves of *Gnetum gnemon* (bago). Cryst. + ½ H_2O. Mp 265° dec. $[\alpha]_D^{20}$ -2.6 (c, 0.5 in Py).

2″-O-β-D-Glucopyranoside: [77795-23-4] ***Luteoayamenin***
$C_{28}H_{32}O_{16}$ 624.551
Pale yellow cryst. (EtOH aq.). Mp 185-187°.

3′-O-β-D-Glucopyranoside:
$C_{28}H_{32}O_{16}$ 624.551

2″-O-α-L-Rhamnopyranoside: [75474-16-7]
$C_{28}H_{32}O_{15}$ 608.552

4′-O-α-L-Rhamnopyranoside: [87440-82-2]
$C_{28}H_{32}O_{15}$ 608.552

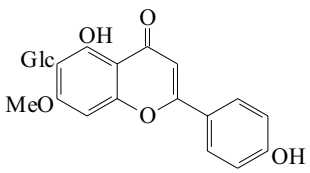
3′-O-Gentiobioside: [76166-51-3]
$C_{34}H_{42}O_{21}$ 786.693

Komatsu, M. *et al., Tet. Lett.*, 1966, 1611
Bouillant, M.L. *et al., Phytochemistry*, 1972, **11**, 1858
Vallant, K. *et al., Naturwissenschaften*, 1978, **65**, 437
Wallace, J.W. *et al., Phytochemistry*, 1978, **17**, 1809 (*uv*)
Kaldas, M. *et al., Phytochemistry*, 1978, **17**, 2083
Vallant, K. *et al., Phytochemistry*, 1978, **17**, 2136
Jay, M. *et al., Biochem. Syst. Ecol.*, 1980, **8**, 127 (*2″-rhamnoside*)
Davoust, D. *et al., Org. Magn. Reson.*, 1980, **13**, 218 (*cmr*)
Nawwar, M.A.M. *et al., Phytochemistry*, 1980, **19**, 1854 (*3′-glucosides*)
Hirose, R. *et al., Agric. Biol. Chem.*, 1981, **45**, 551 (*Luteoayamenin*)
McCormick, S. *et al., Phytochemistry*, 1983, **22**, 798 (*4′-rhamnoside*)

Swertisin S-285

[6991-10-2]

6-β-D-Glucopyranosyl-4′,5-dihydroxy-7-methoxyflavone. Flavocommelitin



$C_{22}H_{22}O_{10}$ 446.41

Pale yellow needles (H_2O). Mp 243° dec. $[\alpha]_D^{20}$ -10 (c, 0.9 in Py).

2″-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl]: [77690-93-8] ***Spinosin C***
$C_{37}H_{38}O_{17}$ 754.697
Isol. from *Zizyphus jujuba* (Chinese date).

2″-O-[4-Hydroxy-3-methoxycinnamoyl-(→6)-β-D-glucopyranosyl]: [77690-92-7] ***Spinosin B***
$C_{38}H_{40}O_{18}$ 784.723
Isol. from *Zizyphus jujuba* (Chinese date). Pale yellow powder + $2H_2O$ (MeOH). Mp 194-197°. $[\alpha]_D^{20}$ -45.2 (c, 0.38 in MeOH).

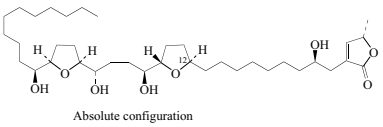
2″-O-[4-Hydroxy-3,5-dimethoxycinnamoyl-(→6)-β-D-glucopyranosyl]: [77690-91-6] ***Spinosin A***
$C_{39}H_{42}O_{19}$ 814.749
Isol. from *Zizyphus jujuba* (Chinese date). Pale yellow powder + $2H_2O$ (MeOH). Mp 198-204°. $[\alpha]_D^{20}$ -40.5 (c, 0.2 in MeOH).

Woo, W.S. *et al., Phytochemistry*, 1979, **18**, 353; 1980, **19**, 2791 (*Spinosin, derivs*)
Hirose, R. *et al., Agric. Biol. Chem.*, 1981, **45**, 551 (*Spinosin, Flavoayamenin*)

Sylvaticin S-286

[92280-14-3]

[137037-26-4]
Uleicin C



Absolute configuration

$C_{37}H_{66}O_8$ 638.924

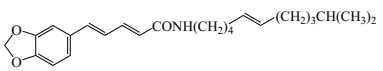
Constit. of *Rollinia mucosa* (biriba) and *Annona purpurea* (soncoya). Wax. Mp 63-64° (48 - 50°). $[\alpha]_D^{23}$ +5.9 (c, 0.524 in $CHCl_3$). λ_{max} 212 (ϵ 7270) (EtOH) (Derep). λ_{max} 207 (ϵ 9500) (MeOH) (Berdy). λ_{max} 224 (ϵ 6920) (EtOH) (Berdy).

12-Epimer: [168039-22-3] ***12,15-cis-Sylvaticin***
$C_{37}H_{66}O_8$ 638.924
Isol. from *Rollinia mucosa* (biriba). Waxy solid. Sol. MeOH, hexane; poorly sol. H_2O. Mp 63-64°. $[\alpha]_D^{23}$ +5.2 (CH_2Cl_2). λ_{max} 224 (MeOH) (Berdy).

Mikolajczak, K.J. *et al., Experientia*, 1990, **46**, 324 (*isol, pmr, cmr*)
Laprevote, O. *et al., Phytochemistry*, 1991, **30**, 2721 (*Uleicin C*)
Cortes, D. *et al., Phytochemistry*, 1993, **32**, 1467; 1475 (*rev*)
Laprevote, O. *et al., Tetrahedron*, 1994, **50**, 8479 (*ms, struct*)
Shi, G. *et al., Heterocycles*, 1995, **41**, 1785 (*isol, abs config*)
Fevrier, A. *et al., Planta Med.*, 1999, **65**, 46-49 (*isol, activity*)

Sylvatine S-287

*5-(1,3-Benzodioxol-5-yl)-*N*-(10-methyl-5-undecenyl)-2,4-pentadienamide, 9CI*



$C_{24}H_{33}NO_3$ 383.53

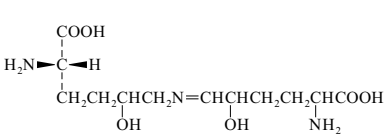
(E,E,E)-form [42438-80-2]
Alkaloid from *Piper chaba* (Javanese long pepper) and several other *Piper* spp. (Piperaceae). Needles (C_6H_6/hexane). Mp 116-117° (111-112°).

Banerji, A. *et al., Tetrahedron*, 1973, **29**, 977 (*isol, uv, ir, pmr, ms, struct*)
Patra, A. *et al., Phytochemistry*, 1974, **13**, 2889 (*isol*)
Rao, J.M. *et al., Curr. Sci.*, 1974, **43**, 76 (*isol, uv, ir, pmr*)
Dutta, C.P. *et al., Phytochemistry*, 1975, **14**, 2090 (*isol*)
Vig, O.P. *et al., Indian J. Chem.*, 1975, **13**, 225 (*synth, ir, pmr*)

Syndesine S-288

[35761-40-1]

N^6*-(5-Amino-5-carboxy-2-hydroxypentylidene)-5-hydroxy-*L*-lysine, 9CI. Dehydrodihydroxylysinonorleucine*



$C_{12}H_{23}N_3O_6$ 305.33

An intramolecular crosslink of collagen.

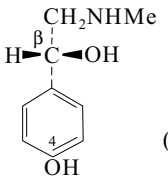
[42083-71-6, 65354-32-7]

Bailey, A.J. *et al., Biochem. J.*, 1970, **117**, 819

(*isol*)
Davis, N.R. *et al., Biochem. Biophys. Res. Commun.*, 1971, **45**, 1416 (*struct*)

Synephrine S-289

[94-07-5]
4-Hydroxy-α-[(methylamino)methyl]benzenemethanol, 9CI. 1-(p-Hydroxyphenyl)-2-methylaminoethanol. p-(α-Hydroxy-β-methylaminoethyl)phenol. Analeptin. Ethaphene. Oxedrine, BAN. Simpalon. Sympathol. Many other names



(*R*)-*form*

$C_9H_{13}NO_2$ 167.207
Log P -0.09 (calc). Was investigated as a synthetic drug before it was found naturally.
► LD_{50} (mus, ipr) 1000 mg/kg. DO7350000
(R)-form [614-35-7]
A widely distributed alkaloid, occurs in citrus leaves and juice and other plants. Plates (Me_2CO aq. or H_2O). Mp 162-164° dec. $[\alpha]_D^{25}$ -55.6 (c, 0.5 in M HCl).
► DO7175003
N,O-*Isopropylidene:* [225928-85-8] ***Synephrine acetonide***
$C_{12}H_{17}NO_2$ 207.272
Alkaloid from the seeds of *Casimiroa edulis* (Mexican apple).
(±)-form [582-84-3]
Spar. sol. org. solvs. Mp 184-185° dec. Used mainly as tartrate.
β-Me ether: [60094-92-0]
[25006-35-3] ***β-O-Methylsynephrine***
$C_{10}H_{15}NO_2$ 181.234
Obt. from tangerine leaves, poss. as artifact. Mp 182-184° (175-176°) (as hydrochloride). One isolate was definitely racemic; opt. rotn. of others not recorded, poss. enantiomeric.

[67-04-9]
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 613C (*nmr*)
Priestley, H.M. *et al., J.O.C.*, 1940, **5**, 355 (*synth*)
Corrigan, J.R. *et al., J.A.C.S.*, 1945, **67**, 1894 (*synth*)
Stewart, I.S. *et al., J. Biol. Chem.*, 1964, **239**, 930 (*isol*)
Kappe, T. *et al., J. Med. Chem.*, 1965, **8**, 368 (*uv*)
Wheaton, T.A. *et al., Phytochemistry*, 1969, **8**, 85 (*biosynth*)
McLaughlin, J.L. *et al., J. Pharm. Sci.*, 1972, **61**, 41; 1973, **62**, 408; 411; 1663 (*isol, derivs*)
Ranieri, R.L. *et al., J.O.C.*, 1976, **41**, 319 (*isol, derivs*)
Smith, T.A. *et al., Phytochemistry*, 1977, **16**, 9 (*occur*)
Hengstmann, J.H. *et al., Arzneim.-Forsch.*, 1978, **28**, 2326 (*metab*)
Dattagupta, J.K. *et al., Acta Cryst. B*, 1982, **38**, 2830 (*cryst struct*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1283
Midgley, J.M. *et al., J.C.S. Perkin 2*, 1989, 963 (*cryst struct, abs config*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1250
Kusu, F. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1158 (*resoln*)
Magos, G.A. *et al., J. Ethnopharmacol.*, 1998, **64**, 35-44; *CA*, **131**, 410 (*acetonide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HLV500; SPD000

Synergistic antifungal protein S-290

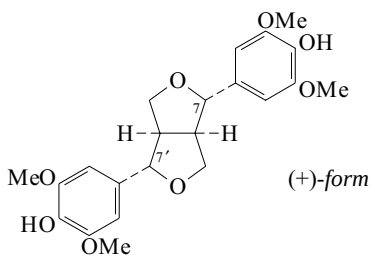
SAFP
Protein. MW approx. 19 kDa. Isol. from corn meal (*Zea mays*). Enhances the antifungal activity of polyoxins, amphotericins and, especially, nikkomycins.
Pat. Coop. Treaty (WIPO), 1989, 89 02 744; *CA*, **112**, 30639p (*isol*)

Syringacins S-291

Proteins. Prod. by *Pseudomonas syringae*. Bacteriocins with possible food uses.
Syringacin W1 [83271-78-7]
Prod. by *Pseudomonas syringae* PsW-1.
Syringacin 4A [53569-53-2]
Prod. by *Pseudomonas syringae* 4-A. Glycoprotein λ_{max} 276 (H_2O).
Haag, W.L. *et al., Antimicrob. Agents Chemother.*, 1974, **6**, 76-83 (*Syringacin 4A*)
Smidt, M.L. *et al., Can. J. Microbiol.*, 1982, **28**, 600-604; 1986, **32**, 231-236 (*Syringacin W1*)

Syringaresinol S-292

4,4′-(Tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl)bis[2,6-dimethoxyphenol], 9CI. 2,6-Bis(4-hydroxy-3,5-dimethoxyphenyl)-3,7-dioxabicyclo[3.3.0]octane. 4,4′-Dihydroxy-3,3′,5,5′-tetramethoxy-7,9′:7′,9-diepoxylignan. Lirioresinol B



$C_{22}H_{26}O_8$ 418.443
Lignan numbering shown.Sol. MeOH, $CHCl_3$. λ_{max} 217 (ε 16500); 237 (sh) (ε 11200); 273 (ε 2090) (MeOH) (Derep). λ_{max} 239 (ε 10900); 273 (ε 2800) (MeOH) (Berdy).
(+)-form [21453-69-0]
Cryst. Mp 175°. $[\alpha]_D$ +62.2 ($CHCl_3$).
Mono-O-β-D-glucopyranoside: [7374-79-0] ***Acanthoside B***
$C_{28}H_{36}O_{13}$ 580.585
Needles. Mp 174-177°.
Di-O-β-D-glucopyranoside: [573-44-4] ***Liriodendrin***
$C_{34}H_{46}O_{18}$ 742.727
Isol. from *Eleutherococcus senticosus* (Siberian ginseng). Cryst. (EtOH). Mp 269-270°. $[\alpha]_D^{18}$ -18.5 (c, 0.2 in Py). λ_{max} 268 (ε 1970) (H_2O) (Derep).
4-Me ether, 4′-O-β-D-glucopyranoside: [135743-07-6] ***Icariside E7***
$C_{29}H_{38}O_{13}$ 594.611
Needles (MeOH). Mp 88-89.5°. $[\alpha]_D^{23}$ -25 (c, 0.14 in MeOH).
Di-Me ether: See Yangambin in *The Combined Chemical Dictionary.*
5,5′-Di-O-de-Me, 4-O-β-D-glucopyranoside: ***Tortoside C***
$C_{26}H_{32}O_{13}$ 552.531
Amorph. powder. $[\alpha]_D^{15}$ -8.9 (c, 0.4 in MeOH).
7-Epimer: [21453-71-4] ***(+)-Episyringaresinol***. *Lirioresinol A. Symplicosigenol* Isol. from *Artemisia absinthium* (wormwood). Cryst. ($CHCl_3$/MeOH). Mp 210-211°. $[\alpha]_D$ +127 ($CHCl_3$). λ_{max} 217 (ε 16500); 237 (sh) (ε 11200); 273 (ε 2090) (MeOH) (Derep).
7-Epimer, 4-O-β-D-glucopyranoside: ***Tortoside A***
$C_{28}H_{36}O_{13}$ 580.585
Amorph. powder. $[\alpha]_D^{15}$ +28.3 (c, 0.3 in MeOH).
7-Epimer, 4′-O-β-D-glucopyranoside:
$C_{28}H_{36}O_{13}$ 580.585
Constit. of the roots of *Eleutherococcus senticosus* (Siberian ginseng). $[\alpha]_D^{25}$ +22 (c, 0.73 in Py). λ_{max} 207 (log ε 4); 238 (log ε 3.32) (MeOH).
7-Epimer, di-O-β-D-glucopyranoside: [79484-75-6] ***Eleutheroside D***
$C_{34}H_{46}O_{18}$ 742.727
Constit. of Siberian ginseng (*Eleutherococcus (Acanthopanax) senticosus*).
7,7′-Diepimer: [551-29-1] ***Lirioresinol C***. *Lirioresinol. Diasyringaresinol*
Mp 185-186° (174-176°). $[\alpha]_D$ +48.9 ($CHCl_3$). λ_{max} 217 (ε 16500); 237 (sh) (ε 11200); 273 (ε 2090) (MeOH) (Derep).
(-)-form [6216-81-5]
Prisms. Mp 185-186° (175-176°). $[\alpha]_D$ -5.2 ($CHCl_3$). λ_{max} 206 ; 220 ; 271 (MeOH) (Berdy).
4-O-β-D-Glucopyranoside: [137038-13-2]
$C_{28}H_{36}O_{13}$ 580.585
4-O-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]: [136997-64-3]
$C_{33}H_{44}O_{17}$ 712.7
Pale yellow powder. $[\alpha]_D$ -2.6 (MeOH).
4-O-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside], 4′-O-β-D-glucopyranoside: [136997-65-4]
$C_{39}H_{54}O_{22}$ 874.842
Pale yellow powder. $[\alpha]_D$ -23.6 (MeOH).
Di-O-[β-D-apiofuranosyl(1→2)-β-D-glucopyranoside]: [136997-66-5]
$C_{44}H_{62}O_{26}$ 1006.958
Pale yellow powder. $[\alpha]_D$ -30.7 (MeOH).
Di-O-β-D-glucopyranoside: [96038-87-8] ***Acanthoside D***. *Eleutheroside E*
$C_{34}H_{46}O_{18}$ 742.727
Isol. from Siberian ginseng (*Eleutherococcus (Acanthopanax) senticosus*). Needles. Mp 269-270°. $[\alpha]_D^{22}$ -18.5 (c, 0.54 in 50% EtOH aq.).
Di-Me ether: See Yangambin in *The Combined Chemical Dictionary.*
7-Epimer: [6216-82-6] ***(-)-Episyringaresinol***
$C_{22}H_{26}O_8$ 418.443

7-Epimer, 4′-O-[β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]: [161104-16-1] ***Albizzioside A***
$C_{33}H_{44}O_{17}$ 712.7
Oil. $[\alpha]_D^{18}$ -3.7 (c, 1.3 in MeOH).

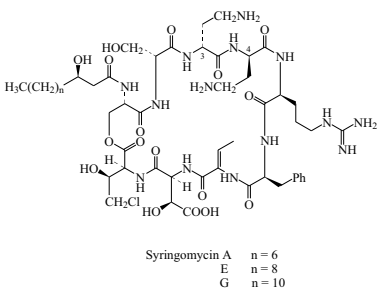
(±)-*form*
Cryst. (EtOH aq.). Mp 174-175°.

[19046-36-7, 39432-56-9, 66791-77-3]

Nimz, H. *et al., Chem. Ber.*, 1965, **98**, 538 (*isol, (±)-Syringaresinol*)
Briggs, L.H. *et al., J.C.S.(C)*, 1968, 3042
Seikel, M.F. *et al., Phytochemistry*, 1971, **10**, 2249 (*isol*)
Erickson, M. *et al., Acta Chem. Scand.*, 1972, **26**, 3085 (*synth*)
Sudo, K. *et al., CA*, 1973, **79**, 32818v (*isol*)
Bryan, R.F. *et al., J.C.S. Perkin 2*, 1976, 341 (*cryst struct, bibl*)
Fujimoto, H. *et al., CA*, 1977, **87**, 197244h (*isol*)
Bytheway, I.R. *et al., Aust. J. Chem.*, 1987, **40**, 1913 (*abs config, cryst struct*)
Abe, F. *et al., Phytochemistry*, 1988, **27**, 575 (*cmr*)
Kinjo, J. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1623 (*(-)-Syringaresinol glycosides*)
Matsushita, H. *et al., Phytochemistry*, 1991, **30**, 2025 (*Icariside E_7*)
Vermes, B. *et al., Phytochemistry*, 1991, **30**, 3087 (*synth, Acanthosides, glycosides*)
Kamel, M.S. *et al., Phytochemistry*, 1992, **31**, 2469 (*Liriodendrin*)
Chakravarty, A.K. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 405 (*isol, (-)-form*)
Ito, A. *et al., Phytochemistry*, 1994, **37**, 1455 (*Albizzioside A*)
Changzeng, W. *et al., Phytochemistry*, 1997, **45**, 159 (*Tortosides*)
Chang, F.-R. *et al., J. Nat. Prod.*, 1998, **61**, 863-866 (*Diasyringaresinol*)
Das, B. *et al., Fitoterapia*, 1999, **70**, 101-102 (*Syringaresinol, pmr*)
Li, X.-C. *et al., Planta Med.*, 2001, **67**, 776-778 (*7-epimer 4′-glucoside*)

Syringomycin S-293

[11140-67-3]



Cyclic depsipeptide antibiotic complex. Structs. of Syringomycins B, C, D and F not yet determined (2000). Prod. by a sugar cane isolate of *Pseudomonas syringae* pv. *syringae*. λ_{max} 220 (ϵ 1290); 278 (sh) (ϵ) (MeOH) (Derep).

Syringomycin A [160029-77-6]
Syringomycin A_1
$C_{51}H_{81}ClN_{14}O_{17}$ 1197.737
Sol. H_2O, DMSO, AcOH, Py; fairly sol. MeOH; poorly sol. EtOH.

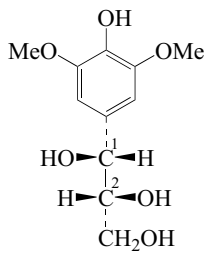
Syringomycin E [124888-22-8]
$C_{53}H_{85}ClN_{14}O_{17}$ 1225.791
Sol. H_2O, AcOH, DMSO, Py; fairly sol. MeOH; poorly sol. EtOH.

Syringomycin G [124888-23-9]
SC-10
$C_{55}H_{89}ClN_{14}O_{17}$ 1253.844
Sol. H_2O, DMSO, AcOH, Py; fairly sol. MeOH; poorly sol. EtOH.

Bidway, A.P. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1987, **84**, 6755-6759 (*Syringomycin E, activity*)
Fukuchi, N. *et al., J.C.S. Perkin 1*, 1992, 875; 1149-1157 (*isol*)
Scaloni, A. *et al., Nat. Prod. Lett.*, 1994, **4**, 159-164 (*abs config*)
Feigin, A.M. *et al., J. Membr. Biol.*, 1996, **149**, 41-47 (*Syringomycin E, activity*)
Sōrensen, K.N. *et al., J. Antibiot.*, 1998, **51**, 743-749 (*Syringomycin E, activity*)

Syringoylglycerol S-294

[4204-29-9]
1-(4-Hydroxy-3,5-dimethoxyphenyl)-1,2,3-propanetriol, 9CI. α-(4-Hydroxy-3,5-dimethoxyphenyl)glycerol. Syringylglycerol



(1*R**,2*R**)-*form*

$C_{11}H_{16}O_6$ 244.244

(1*R,2*R**)-*form*** [121748-11-6]
threo-*form*
Constit. of the roots of *Coix lachryma-jobi* (Job's tears). λ_{max} 230 (sh) ; 270 ; 278 (sh) (MeOH).

(1*R,2*S**)-*form*** [38789-97-8]
erythro-*form*
Constit. of the roots of *Coix lachryma-jobi* (Job's tears). λ_{max} 225 (sh) ; 275 (MeOH).

(1ξ,2ξ)-(A)-*form*
2-O-β-D-Glucopyranoside:
$C_{17}H_{26}O_{11}$ 406.386
Needles (MeOH). Mp 204-205°. $[\alpha]_D^{29}$ -37.7 (c, 0.5 in MeOH). Shown to have *threo* stereochem. λ_{max} 212 (log ϵ 4.18); 231 (log ϵ 3.8); 271 (log ϵ 3.11) (MeOH).
3-O-β-D-Glucopyranoside: [189456-38-0]
$C_{17}H_{26}O_{11}$ 406.386
Amorph. powder. $[\alpha]_D$ -11.9 (c, 1.4 in MeOH). λ_{max} 210 (log ϵ 4.18); 231 (log ϵ 3.75); 271 (log ϵ 2.99) (MeOH).

(1ξ,2ξ)-(B)-*form*
2-O-β-D-Glucopyranoside:
$C_{17}H_{26}O_{11}$ 406.386
Needles (MeOH). Mp 204-206°. $[\alpha]_D$ +7.9 (c, 0.6 in MeOH). Shown to have *threo* stereochem. λ_{max} 211 (log ϵ 4.11); 230 (log ϵ 3.72); 271 (log ϵ 3.03) (MeOH).

[189456-52-8]

Otsuka, H. *et al., Phytochemistry*, 1989, **28**, 883-886 (*isol, synth*)
Kijima, H. *et al., Phytochemistry*, 1997, **44**, 1551-1557 (*isol, derivs*)
Karikas, G.A. *et al., Fitoterapia*, 1998, **69**, 184-185 (*3-glucoside, pmr, ms*)

Systemin S-295

[137181-56-7]

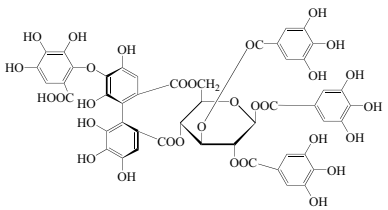
H-Ala-Val-Gln-Ser-Lys-Pro-Pro-Ser-Lys-Arg-Asp-Pro-Pro-Lys-Met-Gln-Thr-Asp-OH

$C_{85}H_{144}N_{26}O_{28}S$ 2010.296
Constit. of the leaves of tomato (*Lycopersicon esculentum*).

Pearce, G. *et al., Science (Washington, D.C.)*, 1991, **253**, 895 (*isol, struct, synth, props*)
Russell, D. J. *et al., J. Protein Chem.*, 1992, **11**, 265 (*pmr*)
Toumadje, A. *et al., J.A.C.S.*, 1995, **117**, 7023 (*struct*)
Schaller, A. *et al., BioEssays*, 1996, **18**, 27 (*rev*)
Mucha, P. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1997, **71**, 1370-1373 (*synth*)

Syzyginin A S-296

[185424-92-4]

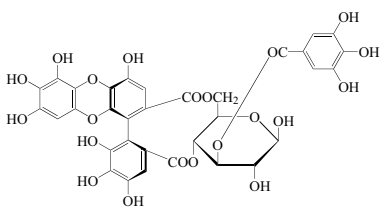


$C_{48}H_{34}O_{31}$ 1106.778
Ellagitannin isol. from *Syzygium aromaticum* (clove). Amorph. powder + $3H_2O$. $[\alpha]_D$ +21 (c, 1 in MeOH).

Tanaka, T. *et al., Phytochemistry*, 1996, **43**, 1345 (*isol, pmr, cmr*)

Syzyginin B S-297

[185424-97-9]

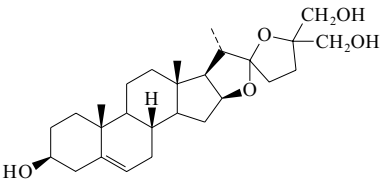


$C_{33}H_{24}O_{21}$ 756.54
Ellagitannin isol. from *Syzygium aromaticum* (clove). Powder + $4^1/_2$ H_2O (H_2O). Mp 220° (dec.). $[\alpha]_D$ +43 (c, 0.8 in MeOH).

Tanaka, T. *et al., Phytochemistry*, 1996, **43**, 1345 (*isol, pmr, cmr*)

Taccagenin T-1

22,25-Epoxyfurost-5-ene-3β,26,27-triol



$C_{27}H_{42}O_5$ 446.626

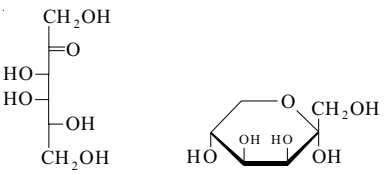
Constit. of *Tacca leontopetaloides* (Polynesian arrowroot). Cryst. (MeOH). Mp 246-248°.

Abdel-Aziz, A. *et al., Phytochemistry*, 1990, **29**, 1643 (*isol, pmr, cmr, ms*)

Tagatose, 9CI, 8CI T-2

[17598-81-1]

lyxo-*Hexulose*



D-*form* α-D-Pyranose-*form*

$C_6H_{12}O_6$ 180.157

An aq. soln. at 27° contains 79% α-pyr, 16% β-pyr, 1% α-fur, 4% β-fur and 0.6% ketone.

D-*form* [87-81-0]

GRAS status for use as a sweetener, humectant, texturiser or stabiliser in food, esp. low calorie products. Mp 134-135°. $[\alpha]_D^{20}$ -2.3 (c, 2.2 in H_2O). $[\alpha]_D^{25}$ -5 (c, 1.0 in H_2O). Sweetness ca. 0.75 - 0.92 x sucrose.

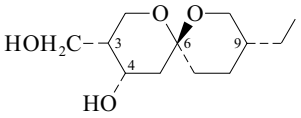
[20197-42-6, 40461-86-7, 41846-98-4, 41846-99-5, 41847-58-9, 41847-59-0]

Karabinos, J.V. *et al., Adv. Carbohydr. Chem.*, 1952, **7**, 99 (*synth, rev*)
Totton, E.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 155 (*synth, D-form*)
Jochims, J.C. *et al., Tet. Lett.*, 1967, 4363 (*pmr*)
Takagi, S. *et al., Carbohydr. Res.*, 1969, **11**, 156 (*cryst struct*)
Al-Jobore, A.A.H. *et al., Carbohydr. Res.*, 1971, **16**, 474
Heyns, K. *et al., Chem. Ber.*, 1975, **108**, 3619
Angyal, S.J. *et al., Aust. J. Chem.*, 1976, **29**, 1249 (*cmr, conformn*)
Koerner, T.A. *et al., J. Biol. Chem.*, 1976, **251**, 2983
Bock, K. *et al., Adv. Carbohydr. Chem. Biochem.*, 1983, **41**, 27 (*cmr*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)
Fessner, W.-D. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 56 (*synth*)
Barili, P. *et al., Carbohydr. Res.*, 1995, **274**, 197-208 (*synth, D-form*)
Food Chem. News, 2001, **43(40)**, 8-9 (*use, status*)

Talaromycin A T-3

[83720-10-9]

9-Ethyl-4-hydroxy-1,7-dioxaspiro[5.5]undecane-3-methanol, 9CI



$C_{12}H_{22}O_4$ 230.303

Spiroketal antibiotic. Mycotoxin prod. by the chicken litter fungus (*Talaromyces stipitatus*). Oil. Sol. $CHCl_3$, MeOH. $[\alpha]_D^{20}$ -110.2 (c, 0.83 in $CHCl_3$).

3-Epimer: [83780-27-2] ***Talaromycin B***
$C_{12}H_{22}O_4$ 230.303
From *Talaromyces stipitatus*. Oil. Sol. $CHCl_3$, MeOH.

4-Epimer: [89885-86-9] ***Talaromycin C***
$C_{12}H_{22}O_4$ 230.303
Mycotoxin from *Talaromyces stipitatus*. No phys. props. reported.

6-Epimer: [111465-44-2] ***Talaromycin F***
$C_{12}H_{22}O_4$ 230.303
Mycotoxin from *Talaromyces stipitatus*. No phys. props. reported.

3,4-Diepimer: [111465-42-0] ***Talaromycin E***
$C_{12}H_{22}O_4$ 230.303
Mycotoxin from *Talaromyces stipitatus*. No phys. props. reported.

3,6-Diepimer: [111465-43-1] ***Talaromycin D***
$C_{12}H_{22}O_4$ 230.303
Mycotoxin from *Talaromyces stipitatus*. No phys. props. reported.

4,6-Diepimer: ***Talaromycin G***
$C_{12}H_{22}O_4$ 230.303
No phys. props. reported.

Lynn, D.G. *et al., J.A.C.S.*, 1982, **104**, 7319 (*isol, struct*)
Kozikowski, A.P. *et al., J.A.C.S.*, 1984, **106**, 353 (*synth*)
Smith, A.B. *et al., J.O.C.*, 1984, **49**, 1469 (*synth*)
Kay, I.T. *et al., Tet. Lett.*, 1984, **25**, 2035 (*synth*)
Midland, M.M. *et al., J.O.C.*, 1985, **50**, 1143 (*synth*)
Schreiber, S.L. *et al., Tet. Lett.*, 1985, **26**, 17 (*synth*)
Whitby, R. *et al., Chem. Comm.*, 1987, 906 (*synth*)
Phillips, N.J. *et al., Tet. Lett.*, 1987, **28**, 1619 (*epimers*)
Iwata, C. *et al., Tet. Lett.*, 1987, **28**, 3135 (*synth*)
Mori, K. *et al., Tetrahedron*, 1987, **43**, 45 (*synth*)
Crimmins, M.T. *et al., J.O.C.*, 1989, **54**, 1157 (*synth*)
Cubero, I.I. *et al., Carbohydr. Res.*, 1990, **205**, 293 (*Talaromycin A,B, synth*)
Baker, R. *et al., J.C.S. Perkin 1*, 1990, 1415 (*synth*)
Tietze, L.F. *et al., J.O.C.*, 1991, **56**, 2476 (*synth*)
Maezaki, N. *et al., Chem. Pharm. Bull.*, 1993, **41**, 946 (*synth*)
Izquierdo, I. *et al., Eur. J. Org. Chem.*, 2002, 309-317 (*Talaromycin C,E, synth*)

Talc, 9CI T-4

[14807-96-6]

Magnesium hydroxide silicate ($Mg_3(OH)_2(Si_4O_{10})$). French chalk

$Mg_3(OH)_2(Si_4O_{10})$

$H_2Mg_3O_{12}Si_4$ 379.266

Used in foods as a masticatory agent, separation/filtration aid, material handling aid, sweetener and washing/surface removal agent. Powder. Insol. H_2O.

► VV7720000

[14378-12-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1245D (*ir*)
Deer, W.A. *et al., Rock Forming Minerals*, Longman, 1964, **3**, 121 (*mineral*)
Ghosh, S.N. *et al., J. Mater. Sci.*, 1978, **13**, 1877 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 523 (*rev*)
Perdikatsis, B. *et al., Z. Kristallogr.*, 1981, **156**, 177 (*cryst struct*)
Sanz, J. *et al., J.A.C.S.*, 1984, **106**, 4790 (*Si-29 nmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 519-521
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1096
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2717-2718
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TAB750; TAB775

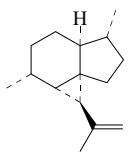
Tamarindose T-5

$C_{34}H_{58}O_{29}$ 930.815

Struct. uncertain. A hexasaccharide possibly contg. Gal + 3Glc +2Xyl. Isol. from seeds of *Tamarindus indica* (tamarind) after autolysis. Mp 228-230°. $[\alpha]_D^{30}$ +43.6 (MeOH).

Rao, P.S. *et al., CA*, 1953, **47**, 6875

Tamariscene T-6



Absolute Configuration

$C_{15}H_{24}$ 204.355

(+)-*form* [351222-68-9]
Oil.

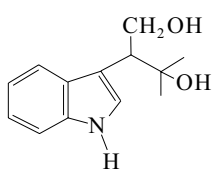
(-)-*form* [351413-96-2]
Constit. of *Valeriana officinalis* (valerian). Oil.

Paul, C. *et al., Phytochemistry*, 2001, **57**, 307-313 (*isol, pmr, cmr*)

Tanakamine T-7

[106449-17-6]

2-(1H-Indol-3-yl)-3-methyl-1,3-butanediol, 9CI



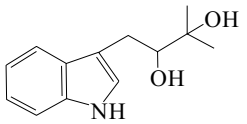
$C_{13}H_{17}NO_2$ 219.283

Alkaloid from the stems of *Limonia acidissima* (wood apple). Amorph. $[\alpha]_D^{25}$ +7.6 (c, 0.69 in MeOH).

Zarga, M.H.A. *et al., J. Nat. Prod.*, 1986, **49**, 901 (*isol, uv, pmr, cmr, ms, struct*)

Tanakine T-8

[106449-15-4]
1-(1H-Indol-3-yl)-3-methyl-2,3-butanediol, 9CI



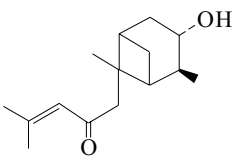
$C_{13}H_{17}NO_2$ 219.283
Alkaloid from the stems of *Limonia acidissima* (wood apple). Amorph. $[\alpha]_D^{25}$ +38 (c, 0.51 in MeOH).

N-*β*-D-*Glucopyranosyl:* [159903-55-6] ***Bruceolline F***
$C_{19}H_{27}NO_7$ 381.425
Pale yellow powder (Me_2CO/MeOH). Mp 209-211°. $[\alpha]_D^{20}$ -55.8 (c, 0.9 in Py). Stereochem. not detd. Not correlated with Tanakine.

Zarga, M.H.A. *et al., J. Nat. Prod.*, 1986, **49**, 901 (*isol, uv, pmr, ms, struct*)
Ouyang, Y. *et al., Phytochemistry*, 1994, **37**, 575 (*Bruceolline F*)

Tanavulgarol T-9

[112663-82-8]

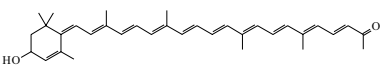


$C_{15}H_{24}O_2$ 236.353
Constit. of *Tanacetum vulgare* (tansy). Oil. $[\alpha]_D^{26}$ +80 (c, 0.3 in $CHCl_3$).

Chandra, A. *et al., Phytochemistry*, 1987, **26**, 3077

Tangeraxanthin T-10

3-Hydroxy-4,5′-retro-5′-apo-β-caroten-5′-one



$C_{34}H_{44}O_2$ 484.72
Isol. from tangerine peel. λ_{max} 484 (C_6H_6).

Curl, A.L. *et al., J. Food Sci.*, 1962, **27**, 537

Tannase, 9CI T-11

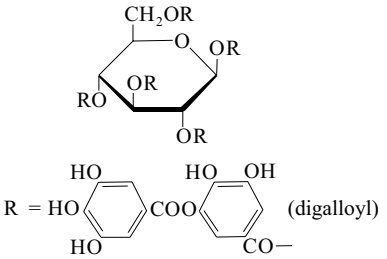
[9025-71-2]
Tannin acylhydrolase. E.C.3.1.1.20

A hydrolase. Processing aid for the manuf. of cold-water sol. tea beverages. Hydrolyses digallate to 2 gallate mols.; also hydrolyses ester links in other tannates.

Barthomeuf, C. *et al., J. Ferment. Technol.*, 1994, **77**, 320-323 (*isol*)
Lekha, P.K. *et al., Adv. Appl. Microbiol.*, 1997, **44**, 215-260 (*use*)
Lane, R.W. *et al., Food Chem. Toxicol.*, 1997, **35**, 207-212 (*safety*)

Tannin, 9CI, 8CI T-12

[1401-55-4]
Tannic acid. Gallotannic acid. Gallotannin. Chinese tannin. Glycerite. FEMA 3042



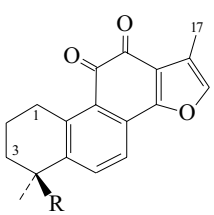
approximate composition

Chinese gallotannin is a mixt. of isomers and closely related compounds whose average composition corresponds to that of Penta-*O*-(*m*-digalloyl)-β-D-glucose. There are also some trigalloyl units. See also individual entries for separately characterised tannin components.. Clarifying agent for beer and wine; flavour enhancer, colour modifier, pH control agent. Permitted boiler water additive in generation of steam for use in food contact processes. Yellowish powder. Sol. H_2O, EtOH, Me_2CO; sl. sol. Et_2O. Mp 210-215° dec. $[\alpha]_D^{20}$ +12 → +18.4 (c, 2 in Me_2CO) (from Chinese galls, Sicilian sumach or Stagshorn sumach). $[\alpha]_D^{20}$ +21.7 → +23.2 (c, 2 in Me_2CO) (from Turkish galls). Forms precipitates with metal salts, alkaloids, albumen and gelatin.
▶ Fl. p. 199° (oc), autoignition temp. 527°.
FM3015000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 544C (*ir*)
Schoeller, W.R. *et al., Analyst (London)*, 1931, **56**, 795; 1932, **57**, 284; 1935, **60**, 284 (*use*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **2**, 142 (*use*)
Schmidt, O.T. *et al., Prog. Chem. Org. Nat. Prod.*, 1956, **13**, 70
Armitage, R. *et al., J.C.S.*, 1961, 1842
Britton, G. *et al., J.C.S.(C)*, 1966, 783
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2726
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDM250; QBJ000; MQV250; SOY500; TAD750

Tanshinone II T-13

[568-72-9]
6,7,8,9-Tetrahydro-1,6,6-trimethylphenanthro[1,2-b]furan-10,11-dione, 9CI. 14,16-Epoxy-20-nor-5(10),6,8,13,15-abietapentaene-11,12-dione. Tanshinone IIA



R = CH_3

$C_{19}H_{18}O_3$ 294.349
Bright red needles (EtOH). Mp 216° (198-200°). λ_{max} 224 ; 225 (ϵ 20500); 251 (ϵ 20000); 252 ; 268 (ϵ 25700); 269 ; 350 (ϵ 16600); 352 ; 460 (MeOH) (Berdy). λ_{max} 225 (ϵ 19500); 251 (ϵ 20400); 268 (ϵ 26300); 348 (ϵ 1740); 460 (ϵ 2950) (EtOH) (Berdy).

1,2-Didehydro: [119963-50-7] ***1,2-Didehydrotanshinone II***. *Δ^1-Dehydrotanshinone II*
$C_{19}H_{16}O_3$ 292.334
Cryst. Mp 147-148°.

1-Hydroxy: [18887-18-8] *1-Hydroxy-14,16-epoxy-20-nor-5(10),6,8,13,15-abietapentaene-11,12-dione.* ***Hydroxytanshinone***
$C_{19}H_{18}O_4$ 310.349
Minor constit. of *Salvia sclarea* (clary sage). Mp 187°. $[\alpha]_D$ 0. λ_{max} 224 ; 252 ; 269 ; 352 ; 460 (MeOH) (Berdy). λ_{max} 222 ; 252 ; 273 ; 348 ; 462 (EtOH) (Berdy).

3α-Hydroxy: [97399-71-8] *3α-Hydroxy-14,16-epoxy-20-nor-5(10),6,8,13,15-abietapentaene-11,12-dione.* ***3α-Hydroxytanshinone IIA***
$C_{19}H_{18}O_4$ 310.349
Cryst. ($CHCl_3$/MeOH). Mp 205-206°.

3α,17-Dihydroxy: ***3α,17-Dihydroxytanshinone II***
$C_{19}H_{18}O_5$ 326.348
Red cryst. Mp 209-210°.

Wessely, F. *et al., Ber.*, 1942, **75**, 958 (*struct*)
Okumura, Y. *et al., Bull. Chem. Soc. Jpn.*, 1961, **34**, 895; 1962, **35**, 2061 (*struct*)
Takiura, K. *et al., Chem. Pharm. Bull.*, 1962, **10**, 112 (*isol*)
Baillie, A.C. *et al., J.C.S.(C)*, 1968, 48 (*synth*)
Inouye, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 3318 (*synth*)
Tateishi, M. *et al., Tetrahedron*, 1971, **27**, 237 (*synth*)
Kakisawa, H. *et al., J.C.S. Perkin 1*, 1976, 1716 (*deriv*)
Luo, H.W. *et al., Phytochemistry*, 1985, **24**, 815 (*deriv*)
Luo, H.W. *et al., Yaoxue Xuebao*, 1988, **23**, 830-834 (*1,2-Didehydrotanshinone II*)
Lee, J. *et al., J.O.C.*, 1990, **55**, 4995 (*synth*)
Khetwal, K.S. *et al., J. Nat. Prod.*, 1992, **55**, 947 (*3α,17-Dihydroxytanshinone II*)
Danheiser, R.L. *et al., J.O.C.*, 1995, **60**, 8341 (*synth*)
Ryu, S.Y. *et al., Planta Med.*, 1997, **63**, 44 (*pmr, cmr*)
Jiang, Y.-Y. *et al., Tet. Lett.*, 2003, **44**, 2073-2075 (*synth*)

Tanshinonic acid T-14

[23725-04-4]
12,14-Epoxy-20-nor-11,12-dioxo-5(10),6,8,13,15-abietapentaen-19-oic acid
As Tanshinone II, T-13 with
R = COOH

$C_{19}H_{16}O_5$ 324.332
λ_{max} 223 ; 252 ; 269 ; 352 ; 465 (EtOH) (Berdy).

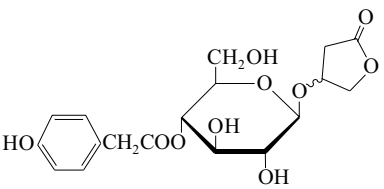
Me ester: [18887-19-9]
$C_{20}H_{18}O_5$ 338.359
Constit. of *Salvia sclarea* (Clary sage). Cryst. Mp 175-176°. $[\alpha]_D$ -139.

Kakisawa, H. *et al., Tet. Lett.*, 1968, 3231 (*isol*)
Romanova, A.R. *et al., Khim. Prir. Soedin.*, 1978, **14**, 515; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 439 (*isol, struct*)

Lee, J. *et al., J.O.C.*, 1990, **55**, 4995 (*synth*)
Haiza, M. *et al., J.O.C.*, 1990, **55**, 5008 (*synth, abs config*)

Taraxacoside T-15

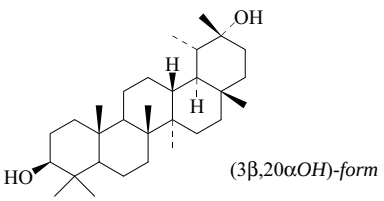
[98449-40-2]



$C_{18}H_{22}O_{10}$ 398.366
Constit. of *Taraxacum officinale* (dandelion). Cryst. ($CHCl_3$/EtOH/Me_2CO). Mp 178-180°.

Rauwald, H.-W. *et al., Phytochemistry*, 1985, **24**, 1557

3,20-Taraxastanediol T-16



$C_{30}H_{52}O_2$ 444.74

(3β,20α*OH*)-*form* [10376-47-3]
ψ-Taraxastane-3,20-diol
Constit. of *Mangifera indica* (mango). Cryst. (EtOH). Mp 270-272°. $[\alpha]_D^{23}$ -10.9 (c, 1.1 in $CHCl_3$).

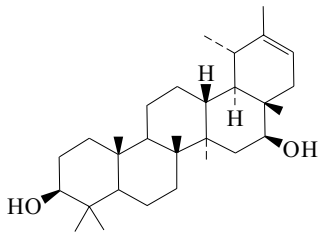
3-Ketone: [232266-07-8] *20-Hydroxy-3-taraxastanone.* ***Ψ-Taraxastanonol***
Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 275-278°. $[\alpha]_D^{30}$ -9 ($CHCl_3$).

(3β,20β*OH*)-*form* [4678-64-2]
20-Epi-ψ-taraxastane-3,20-diol
Cryst. (C_6H_6). Mp 261-263°. $[\alpha]_D$ -3 (c, 0.06 in $CHCl_3$).

3-Ketone: [388592-34-5] ***Epi-ψ-taraxastanonol***
$C_{30}H_{50}O_2$ 442.724
Cryst. (C_6H_6). Mp 257-259°. $[\alpha]_D$ +25.3 (c, 2.96 in $CHCl_3$).

Morice, M. *et al., J.C.S.*, 1940, 795; 1941, 181 (*isol, struct*)
Anjaneyulu, V. *et al., Phytochemistry*, 1985, **24**, 2359-2367 (*Ψ-Taraxastane-3,20-diol*)
Anjaneyulu, V. *et al., Phytochemistry*, 1999, **50**, 1229-1236 (*Ψ-Taraxastanonol*)
Susunaga, G.S. *et al., Fitoterapia*, 2001, 709-711 (*isol, pmr, cmr, struct*)

20-Taraxastene-3,16-diol T-17



$C_{30}H_{50}O_2$ 442.724

(3β,16β)-*form* [20554-95-4]
Faradiol. *Isoarnidendiol*
Constit. of *Tussilago farfara* (coltsfoot), *Helianthus annuus* (sunflower) and *Calendula officinalis* (pot marigold). Cryst. Mp 236-237°. $[\alpha]_D$ +44.

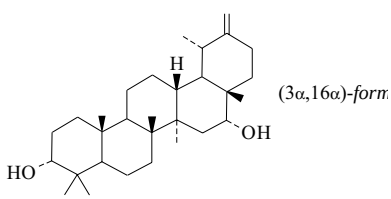
3-Dodecanoyl: [270078-40-5] *Faradiol laurate*
$C_{42}H_{72}O_3$ 625.029
Constit. of *Calendula officinalis* (pot marigold). Amorph. solid.

3-Tetradecanoyl: [193690-82-3] *Faradiol myristate*
$C_{44}H_{76}O_3$ 653.083
Constit. of *Calendula officinalis* (pot marigold).

3-Hexadecanoyl: [193690-84-5] *Faradiol palmitate*
$C_{46}H_{80}O_3$ 681.136
Constit. of *Calendula officinalis* (pot marigold).

Zimmerman, J. *et al., Helv. Chim. Acta*, 1943, **26**, 642-647 (*Faradiol, isol*)
St. Pyrek, J. *et al., Tet. Lett.*, 1973, 809-810 (*Faradiol, struct*)
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1977, **51**, 2331-2342 (*Faradiol, struct*)
St. Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1978, **52**, 97-106 (*ms*)
Zitterl-Eglseer, K. *et al., J. Ethnopharmacol.*, 1997, **57**, 139-144 (*Faradiol esters*)

20(30)-Taraxastene-3,16-diol T-18

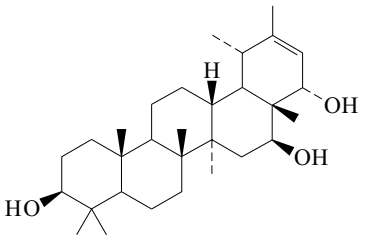


$C_{30}H_{50}O_2$ 442.724

(3β,16β)-*form* [6750-30-7]
Arnidenediol. *Arnidiol*
Found in many plants, incl. *Taraxacum officinale* (dandelion). Mp 257°. $[\alpha]_D$ +81.2.

Santer, J.O. *et al., J.O.C.*, 1962, **27**, 3204 (*isol*)
Kasprzyk, Z. *et al., Phytochemistry*, 1972, **11**, 1961 (*biosynth*)
St. Pyrek, J. *et al., Tet. Lett.*, 1973, 809 (*struct*)
St. Pyrek, J.S. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1977, **51**, 2331 (*isol, pmr*)
Cassady, J.M. *et al., Phytochemistry*, 1978, **17**, 324
St. Pyrek, J.S. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1978, **52**, 97 (*ms*)

20-Taraxastene-3,16,22-triol T-19



$C_{30}H_{50}O_3$ 458.723

(3β,16β,22α)-*form* [71876-60-3]
Heliantriol C
Constit. of *Calendula officinalis* (pot marigold) and *Helianthus annuus* (sunflower). Cryst. Mp 229-230° (220-226°). $[\alpha]_D$ +77 (MeOH).

3-Dodecanoyl: [357419-33-1]
$C_{42}H_{72}O_4$ 641.028
Amorph. solid.

3-O-*Tetradecanoyl:* [357419-34-2]
$C_{44}H_{76}O_4$ 669.082
Cryst. Mp 151-153°.

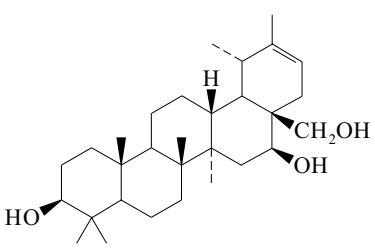
3-Hexadecanoyl: [195380-30-4]
$C_{46}H_{80}O_4$ 697.136
Mp 129-130°. $[\alpha]_D^{20}$ +51.2.

22-Me ether: [71876-67-0] *22-Methoxy-20-taraxastene-3,16-diol.* ***22α-Methoxyfaradiol***
$C_{31}H_{52}O_3$ 472.75
Mp 235-236°. $[\alpha]_D$ +24 (c, 0.2 in $CHCl_3$).

22-Me ether, 3-hexadecanoyl: [357419-35-3]
$C_{47}H_{82}O_4$ 711.162

St Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 1071 (*isol, pmr, ms*)
Wilkomorski, B. *et al., Phytochemistry*, 1985, **24**, 3066; 1986, **25**, 2667 (*isol, pmr, ms*)
Hu, L. *et al., Zhiwu Xuebao*, 1997, **39**, 85; *CA*, **127**, 231901b (*hexadecanoyl*)
Ukiya, M. *et al., J. Agric. Food Chem.*, 2001, **49**, 3187-3197 (*Chrysanthemum morifolium isolates*)

20-Taraxastene-3,16,28-triol T-20

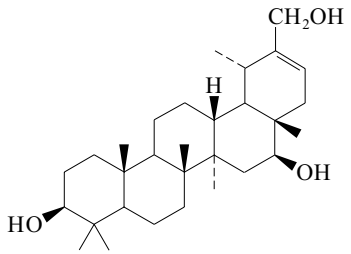


$C_{30}H_{50}O_3$ 458.723

(3β,16β)-*form* [74715-49-4]
Heliantriol B₀. *Heterobetulin*
Constit. of *Helianthus annuus* (sunflower) and *Calendula officinalis* (pot marigold). Cryst. (EtOH aq.). Mp 248-254°. $[\alpha]_D$ +33 (MeOH).

St Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 2465 (*isol, pmr, ms*)

20-Taraxastene-3,16,30-triol T-21

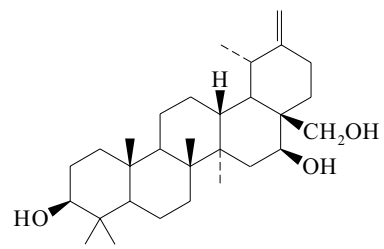


$C_{30}H_{50}O_3$ 458.723

(3β,16β)-*form* [71876-59-0]
Heliantriol F
Constit. of *Helianthus annuus* (sunflower) and *Calendula officinalis* (pot marigold). Cryst. (EtOH aq.) (as tri-Ac). Mp 190-193° (tri-Ac). $[\alpha]_D$ +53.1 (MeOH) (tri-Ac).

St Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 1071 (*isol, pmr, ms*)
Wilkomorski, B. *et al., Phytochemistry*, 1985, **24**, 3066; 1986, **25**, 2667 (*isol, pmr, ms*)

20(30)-Taraxastene-3,16,28-triol T-22

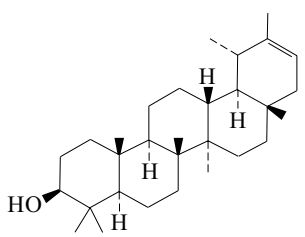


$C_{30}H_{50}O_3$ 458.723

(3β,16β)-*form* [74715-48-3]
Heliantriol B_1
Constit. of *Helianthus annuus* (sunflower) and *Calendula officinalis* (pot marigold). Cryst. (hexane) (as tri-Ac). Mp 182-187° (tri-Ac).

St Pyrek, J. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1979, **53**, 2465 (*isol, pmr*)

20-Taraxasten-3-ol T-23



$C_{30}H_{50}O$ 426.724

3β-*form* [464-98-2]
ψ-Taraxasterol. *Heterolupeol. Calendol. Pseudotaraxasterol*
Constit. of dandelion root (*Taraxacum officinale*) and germinating seeds of pot marigold (*Calendula officinalis*). Flavour component. Cryst. (EtOH). Mp 217-219°. $[\alpha]_D$ +50 ($CHCl_3$).

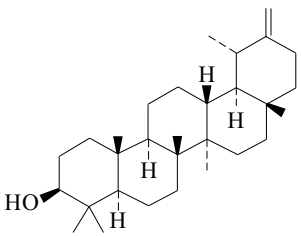
Ac: [4586-65-6]
$C_{32}H_{52}O_2$ 468.762
Constit. of *Calendula officinalis* (pot marigold). Cryst. (EtOAc). Mp 240-241°. $[\alpha]_D$ +53 ($CHCl_3$).

Ketone: [16054-73-2] *20-Taraxasten-3-one.* ***ψ-Taraxasterone***. *Pseudotaraxasterone*
$C_{30}H_{48}O$ 424.709
Constit. of dandelion root (*Taraxacum officinale*). Needles (MeOH/$CHCl_3$). Mp 174-175°.

Ames, T.R. *et al., J.C.S.*, 1954, 1905 (*struct, derivs*)
Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688 (*Ac, ms*)
Buckley, D.G. *et al., Chem. Ind. (London)*, 1971, 298 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2013 (*occur*)
Kasprzyk, Z. *et al., Phytochemistry*, 1972, **11**, 1961 (*biosynth*)
Majumder, P. *et al., J. Indian Chem. Soc.*, 1982, **59**, 881 (*cmr*)
Reynolds, W.F. *et al., Tetrahedron*, 1986, **42**, 3419 (*pmr, cmr*)

20(30)-Taraxasten-3-ol T-24

[1059-14-9]



$C_{30}H_{50}O$ 426.724

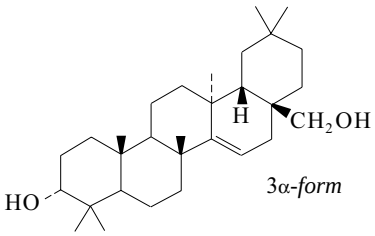
(3β,18α,19α)-*form*
Taraxasterol. *α-Lactucerol. α-Anthesterin. Taraxasterin. Inusterol A. Pyrethrol. Saussurol*
Constit. of dandelion roots (*Taraxacum officinale*), Roman chamomile flowers (*Anthemis nobilis*) and many other plants. Cryst. (EtOH). Mp 225.5-226°. $[\alpha]_D^{17}$ +95.9 ($CHCl_3$).

3-Ketone: [6786-16-9] *20(30)-Taraxasten-3-one.* ***Taraxasterone***
$C_{30}H_{48}O$ 424.709
Isol. from dandelion root *Taraxacum officinale*. Used in flavouring. Cryst. (Me_2CO). Mp 182-183°.

Ames, T.R. *et al., J.C.S.*, 1954, 1905 (*struct*)
Arthur, H.R. *et al., Aust. J. Chem.*, 1969, **22**, 597 (*isol*)
Buckley, D.G. *et al., Chem. Ind. (London)*, 1971, 298 (*pmr*)
Kasprzyk, Z. *et al., Phytochemistry*, 1972, **11**, 1961 (*biosynth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2012 (*occur*)
Patra, A. *et al., Org. Magn. Reson.*, 1981, **17**, 166 (*cmr*)
Reynolds, W.F. *et al., Can. J. Chem.*, 1985, **63**, 1048 (*cryst struct*)
Lee, H.D. *et al., Org. Mass Spectrom.*, 1985, **20**, 247 (*ms*)
Reynolds, W.F. *et al., Tetrahedron*, 1986, **42**, 3419 (*cmr*)
Anjaneyulu, V. *et al., Phytochemistry*, 1989, **28**, 1471 (*isol, pmr, cmr*)

14-Taraxerene-3,28-diol T-25

D-Friedo-14-oleanene-3,28-diol, 9CI



$C_{30}H_{50}O_2$ 442.724

3α-*form*
Isomyricadiol

3β-*form* [17884-88-7]
Myricadiol. *Myricardiol*
Cryst. (MeOH). Mp 271-273°. $[\alpha]_D$ +8 (c, 0.8 in $CHCl_3$).

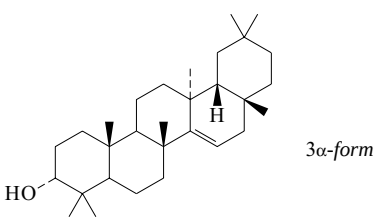
3-Ac: [97868-11-6]
$C_{32}H_{52}O_3$ 484.761
Mp 257-258°.

3-Ketone: [88717-97-9] *28-Hydroxy-14-taraxeren-3-one.* ***Miricolone***
$C_{30}H_{48}O_2$ 440.708
Isol. from *Myrica rubra* (Chinese bayberry). Cryst. ($CHCl_3$). Mp 225-227° (202-204°). $[\alpha]_D^{20}$ -0.2 (c, 1 in $CHCl_3$).

Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688 (*ms*)
Hui, W.-H. *et al., J.C.S. Perkin 1*, 1976, 23
Saltykova, I.A. *et al., Zh. Obshch. Khim.*, 1983, **53**, 2412; *J. Gen. Chem. USSR (Engl. Transl.)*, 2177
Woo, W.S. *et al., Phytochemistry*, 1985, **24**, 1116 (*acetate*)
Sakurai, N. *et al., Phytochemistry*, 1987, **26**, 217 (*ketone*)
Merfort, I. *et al., Phytochemistry*, 1992, **31**, 4031 (*Isomyricadiol, cmr*)

14-Taraxeren-3-ol T-26

[81654-73-1]
D-Friedoolean-14-en-3-ol, 9CI



$C_{30}H_{50}O$ 426.724

3β-*form* [127-22-0]
Taraxerol. *Skimmiol†. Alnulin*
Constit. of *Taraxacum officinale* (dandelion). Cryst. (C_6H_6). Mp 282-283°. $[\alpha]_D^{20}$ +0.72 (c, 0.974 in $CHCl_3$). Log P 10.66 (uncertain value) (calc). Prob. identical with Pertusarin from the lichen *Pertusaria communis* (Hesse, 1898).

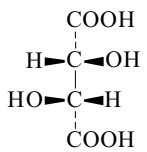
Me ether: [14021-23-9] *3-Methoxy-14-taraxerene.* ***Sawamilletin***. *Crusgallin*
$C_{31}H_{52}O$ 440.751

Constit. of *Saccharum officinarum* (sugar cane). Cryst. Mp 278°. $[\alpha]_D$ +8.2.

Brooks, C.J.W. *et al., Chem. Ind. (London)*, 1953, 1178 (*struct*)
Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688-3699 (*ms*)
Bryce, T.A. *et al., Tetrahedron*, 1967, **23**, 1283-1296 (*isol, Sawamilletin*)
Corbett, R.E. *et al., J.C.S. Perkin 1*, 1972, 2827-2829 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1970 (*occur*)
Anjaneyulu, A.S.R. *et al., Curr. Sci.*, 1974, **43**, 10 (*isol, struct*)
Sakuri, N. *et al., Phytochemistry*, 1987, **26**, 217-219 (*cmr*)
Takasaki, M. *et al., Biol. Pharm. Bull.*, 1999, **22**, 606-610 (*activity*)

Tartaric acid T-27

2,3-Dihydroxybutanedioic acid, 9CI



(2*R*,3*R*)-*form*

$C_4H_6O_6$ 150.088

DL-Nomenclature, although frequently used, is ambiguous when applied to Tartaric acid. The coml. product is normally the natural (2*R*,3*R*)-isomer. Some metal salts have separate entries. Log P -3.27 (calc).

(2*R*,3*R*)-*form* [87-69-4]

[526-83-0]
L-form. L-Threaric acid. FEMA 3044. E334
Present in many fruits, wines and coffee. Acidulant for beverages, foods and pharmaceuticals,used to enhance natural and synthetic fruit flavours, esp. in grape- and lime-flavoured drinks and candies. Firming agent, humectant. Used in leavening systems including baking powders. Stabilising agent for ground spices and cheeses to prevent discoloration. Chelating agent in fatty foods. Synergist with antioxidants, pH control agent in milk, jams and jellies, moisture-control agent. Metatartaric acid (a mixt. of polyesters obt. by the controlled dehydration of (+)-tartaric acid, together with unchanged (+)-tartaric acid) is permitted in wine in UK. Mp 169-170°. $[\alpha]_D^{20}$ +12 (c, 20.0 in H_2O). pK_{a1} 2.98; pK_{a2} 4.34 (25°). Log P -3.27 (calc).

▶ Strong solns. mildly irritant ADI 30 mg/kg b.w. (1974, 1978). WW7875000

Mono-K salt: [868-14-4] *Potassium bitartrate. Potassium acid tartrate. Cream of tartar. E336*
$C_4H_5KO_6$ 188.178
Obt. from sediment in wine manuf. Used in food processing as a nutrient, pH control agent and leavening agent. Cryst. Sol. H_2O.

Di-Na salt: [868-18-8] *Sodium tartrate. E335*
$C_4H_4Na_2O_6$ 194.052
Used in food processing as a pH control agent and emulsifier. Cryst. + $2H_2O$. Loses H_2O at 120°.

K-Na salt: [304-59-6] *Sodium potassium tartrate. Rochelle salt. E337*
$C_4H_4KNaO_6$ 210.16
Used in food processing as an emulsifier and pH control agent. Cryst. + $4H_2O$. Mp 70-80°. Loses $3H_2O$ at 100° and becomes anhyd. at 130-140°; dec. >220°.

Di-Et ester: [87-91-2] *Diethyl tartrate. FEMA 2378*
$C_8H_{14}O_6$ 206.195
Flavouring ingredient. Present in sherry, white wine and red wine. d_4^{20} 1.2. Mp 17°. Bp_{15} 155-156°. $[\alpha]_D^{20}$ +7.5 ($CHCl_3$). n_D^{20} 1.4476.

▶ Fl. p. 93°.

*Mono(4-hydroxy-*E*-cinnamoyl):* [27174-07-8]

[69222-59-9] **trans-*Coutaric acid***. trans-p-*Coumaroyltartaric acid*
$C_{13}H_{12}O_8$ 296.233
Constit. of grapes and wines. Cryst. + $1H_2O$ (H_2O). Mp 194-195° dec.

Mono(4-hydroxy-Z-cinnamoyl): [67920-37-0] **cis-*Coutaric acid***. cis-p-*Coumaroyltartaric acid*
$C_{13}H_{12}O_8$ 296.233
Constit. of grapes and wines.

Mono(3,4-dihydroxycinnamoyl): [67879-58-7] *Monocaffeoyltartaric acid.* ***Caftaric acid***. *Caffeoyltartaric acid*
$C_{13}H_{12}O_9$ 312.232
Constit. of grapes and white Riesling wine. Powder. Mp 125° dec. $[\alpha]_D$ -28.2.

(2*S*,3*S*)-*form* [147-71-7]
D-form. D-Threaric acid
Found combined as Chicoric acid (see below). Mp 169-170°. $[\alpha]_D^{20}$ -20 (c, 20.0 in H_2O). Not used commercially.

*Mono(3,4-dihydroxycinnamoyl):****Monocaffeoyl(-)-tartaric acid***
$C_{13}H_{12}O_9$ 312.232
Isol. from leaves of chicory (*Cichorium intybus*). Mp 146-147°. $[\alpha]_D$ +37 (H_2O).

(2*RS*,3*SR*)-*form* [147-73-9]
meso-*form. Racemic acid. Mesotartaric acid. Erythraric acid*
Mp 159-160°. pK_{a1} 3.17; pK_{a2} 4.91 (25°). Not found in nature.

Monobenzoyl: [65621-34-3] *Benzoyl* meso-*tartaric acid*
$C_{11}H_{10}O_7$ 254.196
Constit. of alfalfa (*Medicago sativa*). Cryst. Mp 192-196° (190-193°).

*Mono(4-hydroxy-*E*-cinnamoyl):* [27174-06-7]

[37551-71-6] *Mono*-trans-p-*coumaroylmesotartaric acid*
$C_{13}H_{12}O_8$ 296.233
Constit. of spinach leaves (*Spinacia oleracea*). Platelets + $\frac{1}{2}H_2O$ (H_2O). Mp 198-200° dec.

*2-O-(4-Hydroxy-*E*-cinnamoyl), 3-Ac:* [106928-35-2]

[35214-72-3] **2-O-*Acetyl*-trans-*coutaric acid***. *2-O-Acetyl-3-*trans-O-p-*coumaroyltartaric acid*
$C_{15}H_{14}O_9$ 338.27
Constit. of spinach. Mp 194-198° dec.

λ_{max} 226 ; 312 (MeOH).

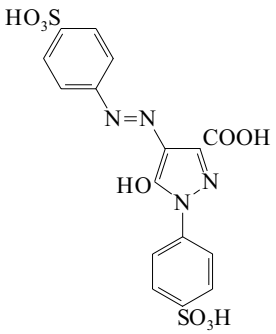
[133-48-2, 921-53-9, 1234-09-9, 3164-34-9, 3715-17-1, 6381-58-4, 6381-59-5, 14475-11-7, 18261-99-9, 38270-70-1, 40968-90-9, 84519-50-6, 117384-46-0, 174873-60-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 523A; 523C; 523D; 662D; 663A; 663C; 663D; 664A; 664C; **2**, 1286C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 813A; 813B; 813C; 859A; 1041C; 1042A; 1042B; 1179C (*nmr*)
Pasteur, L. *et al., Ann. Chim. Phys.*, 1850, **28**, 56-99 (*resoln*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **2**, 176 (*use*)
Bijvoet, J.M. *et al., Nature (London)*, 1951, **168**, 271-272 (*cryst struct*)
Van Bommel, A.J. *et al., Acta Cryst.*, 1958, **11**, 61-70 (*cryst struct*)
Scarpati, M.L. *et al., Ric. Sci.*, 1960, **30**, 1746 (*Monocaffeoyl(-)tartaric acid*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 351; **13**, 124; 276; **11**, 298 (*use*)
Tadera, K. *et al., Agric. Biol. Chem.*, 1970, **34**, 517-522; 1971, **35**, 1431-1435 (*isol, coumarates, Coutaric acid*)
Handb. Biochem. Mol. Biol., 3rd edn., 1975-1977, (Fasman, G.D., Ed.), 1975, 169
Yoshihara, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 2427-2429 (*benzoyltartaric acid*)
Stothers, J.B. *et al., Can. J. Chem.*, 1977, **55**, 841-848 (*cmr*)
Musich, J.A. *et al., J.A.C.S.*, 1978, **100**, 4865-4872 (*isopropylidene, di-Me ester, synth*)
Albertsson, J. *et al., J. Appl. Crystallogr.*, 1979, **12**, 537-544 (*cryst struct*)
Ul Hasan, B. *et al., Org. Magn. Reson.*, 1980, **14**, 309-311 (*cmr*)
Baronowski, J.D. *et al., Am. J. Enol. Vitic.*, 1981, **32**, 5-13 (*Caftaric acid, isol*)
Rossiter, B.E. *et al., J.A.C.S.*, 1981, **103**, 464-465 (*esters, use*)
Hawthorne, F.C. *et al., Acta Cryst. B*, 1982, **38**, 2461-2462 (*cryst struct*)
Buding, H. *et al., Angew. Chem., Int. Ed.*, 1985, **24**, 513 (*abs config, bibl*)
Becker, H. *et al., Z. Naturforsch., C*, 1985, **40**, 585-587 (*Chicoric acid derivs*)
Strack, D. *et al., Phytochemistry*, 1987, **26**, 107-111 (*Coutaric acids*)
Soicke, H. *et al., Planta Med.*, 1988, **54**, 175 (*Chicoric acid analogues*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TAF750
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **13**, 1071 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 522-523
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1757
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 823-824; 2280-2281; 2597-2599; 2613-2615; 2732-2735
Goetz, G. *et al., Phytochemistry*, 1999, **52**, 759-767 (*Coutaric acids*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DCH000; TAF750

Tartrazine T-28

[34175-08-1]
*4,5-Dihydro-5-oxo-1-(4-sulfophenyl)-4-[(4-sulfophenyl)azo]-1*H*-pyrazole-3-carboxylic acid, 9CI. 5-Hydroxy-1-(4-sulfophenyl)-4-[(4-sulfophenyl)azo]pyrazole-3-carboxylic acid. Hydrazine yellow. C.I.*

Food yellow 4. C.I. Acid yellow 23, 8CI. FD and C Yellow No. 5. E102



$C_{16}H_{12}N_4O_9S_2$ 468.424

Strictly the name Tartrazine applies to the trisodium salt.

Tri-Na salt: [1934-21-0]
Colour additive for desserts, candies, preserves, beverages, prepared meats and canned and frozen vegetables. Putative food allergen. Orange-yellow powder.

► UQ6400000

Al salt: [12225-21-7]

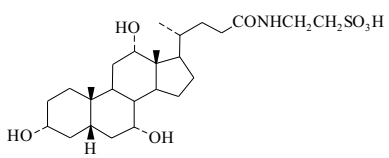
[12227-69-9, 15790-06-4, 53026-64-5] *C.I. Pigment Yellow 100, 9CI*
FDA permitted colourant for food and food contact paper or board. Lake.

Ca lake:
FDA permitted colourant for food and food contact paper or board. Lake.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1001A (*ir*)
U.K. Pat., 1947, 585 781; *CA*, **41**, 6727h (*synth*)
Freeman, K.A. *et al., J. Assoc. Off. Agric. Chem.*, 1950, **33**, 937 (*synth, uv*)
Popa, G. *et al., Zh. Anal. Khim.*, 1959, **14**, 322 (*detn, Pd*)
Colour Index, 3rd Ed, 1971, **4**, 4132
Marmino, D.M. *et al., J. Assoc. Off. Anal. Chem.*, 1974, **57**, 495 (*pmr*)
Robinson, G. *et al., Food Chem. Toxicol.*, 1988, **26**, 73; 575 (*tox, rev*)
Borzelleca, J.F. *et al., Food Chem. Toxicol.*, 1988, **26**, 179; 189 (*tox*)
Collins, T.F.X. *et al., Food Chem. Toxicol.*, 1990, **28**, 821 (*toxigenicity*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 701
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1080-1083; 1086; 1088 (*use*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 678
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG140

Taurocholic acid T-29

[81-24-3]
N-*(3,7,12-Trihydroxycholan-24-oyl)taurine. Cholyltaurine*



$C_{26}H_{45}NO_7S$ 515.71
Emulsifier in foods. Amorph. powder. Mp 125° dec. $[\alpha]_D^{20}$ +38.8 (EtOH aq.). pK_a 1.4. Log P 0.88 (uncertain value) (calc). Very hygroscopic.

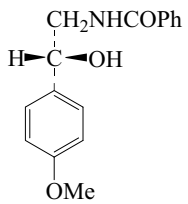
Na salt: [145-42-6]
Emulsifier in foods. Cryst. (EtOH/EtOAc). Mp 182-184° (anhyd.) Mp 235° (+ $2H_2O$).

► WX0400000

Begemann, F. *et al., Z. Klin. Chem. Klin. Biochem.*, 1972, **10**, 29 (*isol*)
Tserng, K.-Y. *et al., J. Lipid Res.*, 1977, **18**, 404 (*synth*)
Shaw, R. *et al., Lipids*, 1978, **13**, 971 (*ms*)
Lo, Y.H. *et al., Chem. Senses*, 1994, **19**, 371
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2615; 2735-2736
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKB500; TAH250

Tembamide T-30

[37791-56-3]
N-*[2-Hydroxy-2-(4-methoxypheny-l)ethyl]benzamide, 9CI*. N-*Benzoyl-2-hydroxy-2-(4-methoxyphenyl)ethylamine*



(*R*)-*form*

$C_{16}H_{17}NO_3$ 271.315

(*R*)-*form* [15298-30-3]
Cryst. (EtOH). Mp 156-157°. $[\alpha]_D^{20}$ -55.3 (c, 0.5 in $CHCl_3$). $[\alpha]_D^{21}$ +17.9 (c, 0.5 in EtOH).

Me ether:
$C_{17}H_{19}NO_3$ 285.342
Needles. Mp 88-89°. $[\alpha]_D^{25}$ +17.7 (c, 0.1 in $CHCl_3$).

(*S*)-*form* [15779-24-5]
Cryst. (EtOH). Mp 156-157°. $[\alpha]_D^{21}$ +55.8 (c, 0.5 in $CHCl_3$). $[\alpha]_D^{20}$ -18.5 (c, 0.5 in EtOH).

(±)-*form* [15298-28-9]
Alkaloid from the root of *Aegle marmelos* (bael fruit). Cryst. (EtOH, EtOAc, C_6H_6, $CHCl_3$/petrol or CH_2Cl_2/EtOH). Mp 156-157° (147-149°).

Ac: [15298-31-4] ***Tembamide acetate***
$C_{18}H_{19}NO_4$ 313.352
Needles (EtOAc or C_6H_6/petrol). Mp 159° (140-141°).

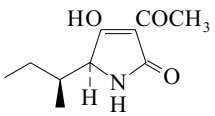
Me ether: **O-*Methyltembamide***
$C_{17}H_{19}NO_3$ 285.342
Cryst. (C_6H_6/petrol). Mp 98-99°.

[50802-66-9]

Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 2795 (*isol, ir, pmr, ms*)
Albónico, S.M. *et al., J.C.S.(C)*, 1967, 1327 (*isol, uv, ir, pmr, synth*)
Johns, S.R. *et al., Aust. J. Chem.*, 1969, **22**, 2233 (*isol*)
Della Casa de Marcano, D. *et al., Phytochemistry*, 1972, **11**, 1531 (*isol*)
Krajniak, E.R. *et al., Aust. J. Chem.*, 1973, **26**, 687 (*isol, synth, deriv*)
Shoeb, A. *et al., Phytochemistry*, 1973, **12**, 2071 (*isol, uv, ir, pmr, ms*)
Bernhard, H.O. *et al., Helv. Chim. Acta*, 1978, **61**, 2269 (*isol, ir, pmr, ms*)
Patra, A. *et al., Org. Magn. Reson.*, 1981, **16**, 65 (*cmr*)
Maxwell, A. *et al., J. Nat. Prod.*, 1989, **52**, 411 (*isol, uv, ir, pmr, cmr, ms, struct, acetate*)
Brown, R.F.C. *et al., Tetrahedron: Asymmetry*, 1993, **4**, 205 (*synth*)
De Moura, N.F. *et al., Planta Med.*, 2002, **68**, 534-538 (*isol, cmr*)

Tenuazonic acid T-31

[610-88-8]
*3-Acetyl-1,5-dihydro-4-hydroxy-5-(1-methylpropyl)-2*H*-pyrrol-2-one, 9CI. 3-Acetyl-5-*sec*-butyltetramic acid. Vivotoxin*



$C_{10}H_{15}NO_3$ 197.233

CA refers also to two tautomeric forms. Prod. by *Aspergillus* spp. Causes rice leaf rot. Viscous oil or pale-brown cryst. Sol. MeOH, Et_2O, bases; poorly sol. H_2O, hexane. Mp 74-75.5°. $Bp_{0.035}$ 117°. $[\alpha]_{Hg}^{20}$ -136 (c, 0.2 in $CHCl_3$). λ_{max} 219 (ϵ 5600); 277 (ϵ 12700) (EtOH/HCl) (Derep). λ_{max} 240 (ϵ 11700); 279 (ϵ 14800) (dil. NaOH) (Derep). λ_{max} 240 (ϵ 10800); 280 (ϵ 13500) (H_2O pH 7) (Derep). λ_{max} 240 (ϵ 11480); 280 (ϵ 14450) (MeOH) (Berdy). λ_{max} 217 (ϵ 5240); 277 (ϵ 13400) (EtOH) (Berdy). λ_{max} 240 ; 280 (MeOH-NaOH) (Berdy). λ_{max} 240 (ϵ 11480); 280 (ϵ 14450) (H_2O) (Berdy). λ_{max} 220 (ϵ 6500); 277 (ϵ 10000) (MeOH-HCl) (Berdy).

► LD_{50} (mus, orl) 225 mg/kg ; LD_{50} (mus, ivn) 125 mg/kg , LD_{50} (mus, ipr) 150 mg/kg , LD_{50} (mus, scu) 145 mg/kg. UY7425000

Na salt: [1013-59-8] *Sodium tenuazonate. NSC 525816*
$[\alpha]_{Hg}$ -96.7 (c, 2 in MeOH).

► LD_{50} (rat, orl) 168 mg/kg. UY7525000

Compd. with N,N-*Dibenzylethylenediamine (1:1):* [21327-82-2] *Benzathine tenuazonate. NSC 82260*

2,4-Dinitrophenylhydrazone:
Needles (MeOH). Mp 199-200°.

Semicarbazone:
Cryst. Mp 187-189°.

[27778-66-1, 75652-74-3]

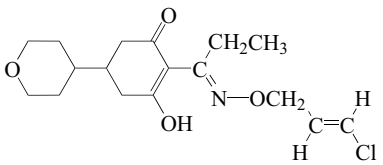
Rosett, T. *et al., Biochem. J.*, 1957, **67**, 390 (*isol*)
Stickings, C.E. *et al., Biochem. J.*, 1959, **72**, 332; 1961, **78**, 412 (*struct, biosynth*)
Harris, S.A. *et al., J. Med. Chem.*, 1965, **8**, 478 (*synth*)
Yuki, H. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1107; 1120 (*synth, props*)
Mikami, Y. *et al., Agric. Biol. Chem.*, 1971, **35**, 611
Meronuck, R.A. *et al., Appl. Microbiol.*, 1972, **23**, 613 (*isol*)
Gatenbeck, S. *et al., Acta Chem. Scand.*, 1973, **27**, 1825 (*biosynth*)

Dippenaar, A. *et al., J. Cryst. Mol. Struct.*, 1977, **7**, 189 (*cryst struct*)
Kono, Y. *et al., Agric. Biol. Chem.*, 1986, **50**, 2401 (*isol, pmr, ms*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 488
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADC250; VTA750

Tepraloxydim T-32

[151325-26-7]

[149979-41-9]
2-[1-[[(3-Chloro-2-propenyl)oxy]imino]-propyl]-3-hydroxy-5-(tetrahydro-2H-pyran-4-yl)-2-cyclohexen-1-one, 9CI. Caloxydim. BAS 620H

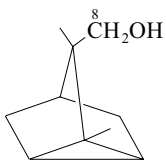


$C_{17}H_{24}ClNO_4$ 341.834

Ger. Pat., 1993, 4 222 261, (*BASF*); *CA*, **119**, 159751t (*synth, activity*)
Pesticide Manual, 11th edn., 1997, 49

Teresantalol T-33

[29550-55-8]
2,3-Dimethyltricyclo[2.2.1.0^{2,6}]heptane-3-methanol, 9CI



$C_{10}H_{16}O$ 152.236
Flavouring ingredient. Constit. of Indian sandalwood oil (*Santalum album*). Cryst. (petrol/C_6H_6). Mp 115°. Bp_9 95-98°. $[\alpha]_D$ +12.1 (EtOH).

8-Aldehyde: [59300-39-9] ***Teresantalal***
$C_{10}H_{14}O$ 150.22
Flavouring ingredient. Constit. of the oil of *Santalum album* (sandalwood).

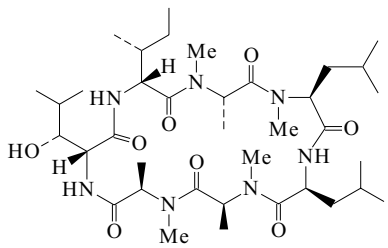
8-Carboxylic acid: [562-66-3] ***α-Teresantalic acid***
$C_{10}H_{14}O_2$ 166.219
Flavouring ingredient. Isol. from *Santalum album* (sandalwood). Cryst. (EtOH). Mp 158°. Bp_{20} 157-158°. $[\alpha]_D^{20}$ -76.6 (C_6H_6).

8-Carboxylic acid, chloride: [54793-90-7]
$C_{10}H_{13}ClO$ 184.665

Guha, P.C. *et al., J. Indian Chem. Soc.*, 1944, **59**, 271 (*isol*)
Nambara, T. *et al., J. Chromatogr.*, 1974, **100**, 180 (*use*)
Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*isol*)
Monti, S.A. *et al., J.O.C.*, 1978, **43**, 2282 (*synth*)

Ternatin T-34

[148619-41-4]

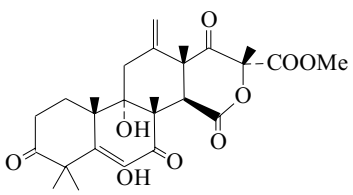


$C_{37}H_{67}N_7O_8$ 737.978
Cyclic peptide antibiotic. Isol. from culture fluids of *Didymocladium ternatum*. Agent for control of rust diseases in grain stocks. Cryst. (dioxan or 95% EtOH) (dimorph.). Sol. MeOH, Et_2O; fairly sol. hexane; poorly sol. H_2O. λ_{max} 211 (ε 9500) (EtOH) (Berdy).

U.S.S.R. Pat., 1974, N517 198 (*isol*)
Langs, D.A. *et al., Acta Cryst. D*, 1993, **49**, 158 (*cryst struct*)
Miller, R. *et al., Int. J. Pept. Protein Res.*, 1993, **42**, 539 (*cryst struct*)

Terretonin T-35

[71911-90-5]



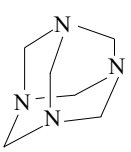
$C_{26}H_{32}O_9$ 488.533
Mycotoxin of the common soil organism *Aspergillus terreus*. Isol. from *A. terreus* infected hay. Cryst. (EtOAc/C_6H_6). Mp 260-262°. λ_{max} 276 (ε 7960) (MeOH) (Berdy).

▶ LD_{50} (mus, orl) 275-375 mg/kg.

Dorner, J.W. *et al., J.O.C.*, 1979, **44**, 4852 (*isol*)
McIntyre, C.R. *et al., J.C.S. Perkin 1*, 1989, 1987 (*pmr, cmr*)
McIntyre, C.R. *et al., Tetrahedron*, 1989, **45**, 2307 (*biosynth*)

1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane, 9CI T-36

[100-97-0]
*Hexamethylenetetramine, 8CI. **Methenamine**. Aminoform. Formamine. Formin. Herax UTS. Hexa. Hexamethylenamine. Hexamine. Metenamine. Nocceler H. Urotropin. Vulkacit H30. E239. [1^6]-Adamazane, INN*

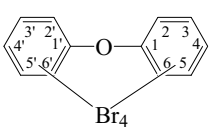


$C_6H_{12}N_4$ 140.188
Antimicrobial food preservative, but limited and declining use. Acts by releasing formaldehyde in acidic conditions. Prevents "late blowing" of hard cheese by inhibiting growth of unwanted bacteria. Presently (2002) its European use is limited to one type of Italian cheese, Provolone. Volatile, rhombohedral cryst. (EtOH). Sol. H_2O; less sol. warm H_2O. Subl. 263 *ca., in vacuo* with some dec.. pK_a 6.3 (25°). Log P 2.47 (uncertain value) (calc). The first organic structure to be determined by X-ray diffraction (1923).

▶ Dust explosion hazard in finely powdered state. Eye, skin and mucous membrane irritant. May cause skin rash. Sensitiser.. MN4725000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 378B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 596B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 471D (*ir*)
Butlerow, A. *et al., Annalen*, 1860, **115**, 322 (*synth*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1947, **3**, 124 (*synth, use*)
Vogel, A.I. *et al., Textbook of Qualitative Inorganic Analysis*, Longmans, London, 1961, (*use*)
Solinas, M. *et al., J. Chem. Phys.*, 1974, **44**, 1678 (*ir, Raman*)
Webb, G.A. *et al., Org. Magn. Reson.*, 1976, **8**, 102 (*pmr, cmr*)
Gleckman, R. *et al., Am. J. Hosp. Pharm.*, 1979, **36**, 1509
Bulusu, S. *et al., Org. Magn. Reson.*, 1981, **16**, 52 (*cmr, N-15 nmr*)
Chou, M. *et al., Acta Cryst. C*, 1987, **43**, 322 (*cryst struct*)
Hatfield, G.R. *et al., Macromolecules*, 1987, **20**, 608 (*curing agent*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 530 (*synonyms*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 173
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 2696 (*tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2325
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HEI500

Tetrabromodiphenyl ethers T-37



$C_{12}H_6Br_4O$ 485.795
Persistent environmental pollutants, detected in fish and human breast milk. Present in land-applied sewage sludge.

2,2′,4,4′-Tetrabromodiphenyl ether [5436-43-1]
1,1′-Oxybis[2,4-dibromobenzene], 9CI. PBDE 47. BDE 47
$C_{12}H_6Br_4O$ 485.795
Mp 82-82.5° (78.5-79°).

▶ Developmental neurotoxin in mice.

[40088-47-9]

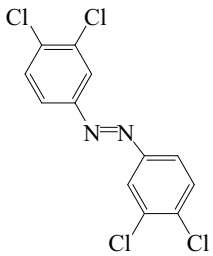
Dhanesar, S.C. *et al., J. Chromatogr.*, 1982, **252**,

91-99 (*synth, pmr*)
Environ. Health Criter., no.162, WHO, 1994, (*rev, tox, occur*)
Oern, U. *et al., Acta Chem. Scand.*, 1996, **50**, 802-807 (*synth, ms, pmr, uv*)
Strandman, T. *et al., Organohalogen Compd.*, 2000, **47**, 61-64 (*anal*)
Eriksson, P. *et al., Environ. Health Perspect.*, 2001, **109**, 903-908 (*tox*)
Hale, R.C. *et al., Nature (London)*, 2001, **412**, 140-141 (*detn, occur*)

3,3′,4,4′-Tetrachloroazobenzene, 8CI T-38

[14047-09-7]

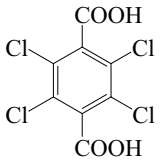
[64275-11-2]
Bis(3,4-dichlorophenyl)diazene, 9CI



$C_{12}H_6Cl_4N_2$ 320.004
Environmental pollutant arising from the soil degradn. of and related herbicides.
▶ Carcinogen, mutagen. Potent inducer of chloracne and of liver enzymes.
(E)-form [64275-12-3]
Orange cryst. (C_6H_6). Mp 158°.
N-*Oxide:* [21232-47-3] *3,3′,4,4′-Tetrachloroazoxybenzene*
$C_{12}H_6Cl_4N_2O$ 336.003
Mp 142°. Geom. isom. not determined.
▶ Carcinogen. Potent inducer of chloracne and of liver enzymes.
Corbett, J.F. *et al., J.C.S.*, 1963, 2385-2387 (*synth*)
Corbett, J.F. *et al., Chem. Comm.*, 1968, 1257-1258 (*synth, N-oxide*)
Linke, H.A.B. *et al., Z. Naturforsch., B*, 1969, **24**, 994-996; 997-999 (*synth, ir, uv, conformn*)
Bartha, R. *et al., Adv. Appl. Microbiol.*, 1970, **13**, 317-341 (*metab, rev*)
Rondestvedt, C.S. *et al., Synthesis*, 1977, 850-851 (*synth*)
Hsia, M.T. *et al., J. Assoc. Off. Anal. Chem.*, 1979, **62**, 746-750 (*N-oxide, synth, ir, ms, pmr*)
Sundstroem, G. *et al., Pergamon Ser. Environ. Sci.*, 1982, **5**, 337-353 (*rev, tox, formn*)
Worobey, B.L. *et al., Chemosphere*, 1988, **17**, 1727-1734 (*synth, props*)
Lee, J.K. *et al., J. Agric. Food Chem.*, 1995, **43**, 519-523 (*props, bibl*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 7th edn., Van Nostrand Reinhold*, 1989, TBN 500; TBN 550 (*tox*)

Tetrachloro-1,4-benzenedicarboxylic acid T-39

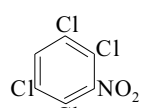
[2136-79-0]
Tetrachloroterephthalic acid. Chlorthal, BSI, ISO, WSSA



$C_8H_2Cl_4O_4$ 303.912
Environmental contaminant arising from the degradn. of the di-Me ester. Cryst. (H_2O). Mp 343-345° dec.
▶ CZ4400000
Di-Me ester: [1861-32-1] *Chlorthal-dimethyl, BSI. Dacthal. DCPA, WSSA. TCTP, JMAF. Chlorthal-methyl. Tetral*
$C_{10}H_6Cl_4O_4$ 331.966
Needles (MeOH). Mp 154-155°.
▶ LD_{50} (rat, orl) >3000 mg/kg. WZ1500000
Di-Et ester: [10497-36-6]
$C_{12}H_{10}Cl_4O_4$ 360.019
Mp 130-130.5°.
Chloride: [719-32-4]
$C_8HCl_5O_3$ 322.358
Cryst. (CCl_4). Mp 146-147°.
Amide:
$C_8H_3Cl_4NO_3$ 302.927
Cryst. (AcOH). Mp 400°.
Dinitrile: [1897-41-2] *1,2,4,5-Tetrachloro-3,6-dicyanobenzene*
$C_8Cl_4N_2$ 265.912
Rupp, E. *et al., Ber.*, 1896, **29**, 1625 (*synth*)
Rabjohn, N. *et al., J.A.C.S.*, 1948, **70**, 3518 (*synth*)
Tamborskii, C. *et al., Chem. Ind. (London)*, 1965, 2067 (*synth*)
Profft, E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1966, **299**, 577 (*synth*)
Ueda, K. *et al., Bull. Chem. Soc. Jpn.*, 1967, **40**, 688-689 (*dinitrile, synth*)
Guseinov, M.M. *et al., CA*, 1972, **76**, 99292a (*synth*)
Popova, M.F. *et al., Zh. Prikl. Khim. (Leningrad)*, 1978, **51**, 1422; *CA*, **89**, 90115f (*chlorthal-dimethyl*)
Pesticide Manual, 9th edn., 1991, No. 3090 (*chlorthal*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A89
Monokan, K. *et al., J. Agric. Food Chem.*, 1995, **43**, 2418-2423 (*anal, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBV250

1,2,4,5-Tetrachloro-3-nitrobenzene, 9CI T-40

[117-18-0]
Tecnazene, BSI, ISO. Fusarex. Folosan. Napotate. Nebulin. TCNB

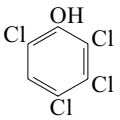


$C_6HCl_4NO_2$ 260.89
Sprout inhibitor and fungicide for stored potatoes. Cryst. Spar. sol. H_2O; sol. EtOH; v. sol. C_6H_6, CS_2, $CHCl_3$. Mp 99°.
▶ Irritant. LD_{50} (rat, orl) 7500 mg/kg. Exp. neoplastigenic data. DC0175000
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1382B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 774B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1217D (*ir*)
Berckmans, V.S.F. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1925, **44**, 851 (*synth*)
U.S. Pat., 1947, 2 615 801; *CA*, **47**, 2927h
Ripley, B.D. *et al., J. Assoc. Off. Anal. Chem.*, 1983, **66**, 1084 (*detn*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A379
Suzuki, H. *et al., Synthesis*, 1994, 841 (*synth, ir, pmr, cmr, ms*)
Bhar, A. *et al., Acta Cryst. C*, 1995, **51**, 256 (*cryst struct*)
Pesticide Manual, 11th edn., 1997, No. 685
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBR750

2,3,4,6-Tetrachlorophenol T-41

[58-90-2]

[25167-83-3]
Dowicide 6



$C_6H_2Cl_4O$ 231.892
Needles (petrol). Mp 70°. Bp_{15} 150°.
▶ LD_{50} (rat, orl) 140 mg/kg; LD_{50} (rbt, skn) 250 mg/kg. Exp. teratogenic effects. SM9275000
Ac:
$C_8H_4Cl_4O_2$ 273.929
Cryst. (EtOH). Mp 65-66°.
Benzoyl:
$C_{13}H_6Cl_4O_2$ 336
Mp 108°.
Me ether: [938-22-7] *1,2,3,5-Tetrachloro-4-methoxybenzene. 2,3,4,6-Tetrachloroanisole*
$C_7H_4Cl_4O$ 245.919
Off-odour component of flour, etc. stored in contaminated jute sacks. Needles (MeOH). Mp 64-65°.
Et ether:1,2,3,5-Tetrachloro-4-ethoxybenzene. 2,3,4,6-Tetrachlorophenetole
$C_8H_6Cl_4O$ 259.946
Needles (EtOH). Mp 55°.
Holleman, A.F. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1921, **40**, 318 (*synth*)
Tiessens, G.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1931, **50**, 112 (*synth*)
Lock, G. *et al., Monatsh. Chem.*, 1936, **67**, 320 (*synth*)
Galat, A. *et al., J.A.C.S.*, 1952, **74**, 3890 (*synth*)
Allan, E.A. *et al., J. Phys. Chem.*, 1963, **67**, 591 (*pmr*)
Rees, J. *et al., J. Chromatogr.*, 1970, **47**, 474 (*glc*)
Whitfield, F.B. *et al., Chem. Ind. (London)*, 1984, 744 (*Me ether, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBT000

Tetracosane T-42

[646-31-1]
Lignocerane
$H_3C(CH_2)_{22}CH_3$
$C_{24}H_{50}$ 338.659

Isol. from plant sources e.g. rose and orange oils. Cryst. (Et_2O). Mp 54° (51°). Bp_{10} 231°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 7A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **1**, 5D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 7A (*ir*)
Rodd's Chem. Carbon Compd. (2nd edn.) , 1964, **1A**, 367
Cambie, R.C. *et al., J.C.S.(C)* , 1966, 72 (*isol*)
Hunter, G.L.K. *et al., Phytochemistry*, 1966, **5**, 807 (*isol*)
Grant, G.G. *et al., J. Chem. Ecol.* , 1987, **13**, 345

1,24-Tetracosanediol T-43

[22513-82-2]

$HOCH_2(CH_2)_{22}CH_2OH$

$C_{24}H_{50}O_2$ 370.658

Isol. from apple wax (*Pyrus malus*). Cryst. (C_6H_6/Me_2CO). Mp 108.4-108.6°.

Di-Ac:
$C_{28}H_{54}O_4$ 454.732
Mp 73.6-73.7°. Bp_1 243°.

Bis-O-*(4-hydroxy-3-methoxy*-E-*cinnamoyl):1,24-Tetracosanediol diferulate*
$C_{44}H_{66}O_8$ 723.001
Amorph. powder.

Murray, K.E. *et al., Aust. J. Chem.* , 1955, **8**, 432
Mazliak, P. *et al., Phytochemistry*, 1962, **1**, 79 (*isol*)
Ma, C.-Y. *et al., J. Nat. Prod.* , 2002, **65**, 206-209 (*diferulate*)

4,6-Tetracosanedione T-44

$H_3C(CH_2)_{17}COCH_2COCH_2CH_2CH_3$

$C_{24}H_{46}O_2$ 366.626

Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-tetracosanone
$C_{24}H_{48}O_2$ 368.642
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

5,7-Tetracosanedione T-45

$H_3C(CH_2)_{16}COCH_2CO(CH_2)_3CH_3$

$C_{24}H_{46}O_2$ 366.626

Constit. of the pollen of *Helianthus annuus* (sunflower).

5-Alcohol:5-Hydroxy-7-tetracosanone
$C_{24}H_{48}O_2$ 368.642
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

6,8-Tetracosanedione T-46

$H_3C(CH_2)_{15}COCH_2CO(CH_2)_4CH_3$

$C_{24}H_{46}O_2$ 366.626

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

7,9-Tetracosanedione T-47

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_5CH_3$

$C_{24}H_{46}O_2$ 366.626

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

10,12-Tetracosanedione T-48

$H_3C(CH_2)_{11}COCH_2CO(CH_2)_8CH_3$

$C_{24}H_{46}O_2$ 366.626

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

20-Tetracosene-1,18-diol T-49

[151454-15-8]

$H_3CCH_2CH_2CH=CHCH_2CH(OH)CH_2(CH_2)_{15}CH_2OH$

$C_{24}H_{48}O_2$ 368.642

Constit. of the tubers of *Colocasia esculenta antiquorum*. Mp 62-63°.

Ali, M. *et al., J. Indian Chem. Soc.* , 1992, **69**, 887 (*isol*)

2-Tetracosenoic acid T-50

[26444-06-4]

$H_3C(CH_2)_{20}CH=CHCOOH$

$C_{24}H_{46}O_2$ 366.626

(E)-form [33228-63-6]
Isol. from the leaf wax of durum wheat.

(Z)-form [90377-13-2]

[335153-29-2]

Tulloch, A.P. *et al., Phytochemistry*, 1971, **10**, 871 (*isol*)
Ansari, A.A. *et al., J. Am. Oil Chem. Soc.* , 1976, **53**, 118 (*synth*)
Bohlmann, F. *et al., Rev. Latinoam. Quim.* , 1984, **14**, 103 (*isol*)
Senior, I.J. *et al., Phytochemistry*, 1993, **34**, 65 (*isol, ms*)
Popaj, K. *et al., Helv. Chim. Acta*, 2001, **84**, 180-184 (*Et ester, synth, ir, pmr, cmr*)

15-Tetracosenoic acid T-51

[26444-06-4]

$H_3C(CH_2)_7CH=CH(CH_2)_{13}COOH$

$C_{24}H_{46}O_2$ 366.626

(E)-form [14490-79-0]
Cryst. (EtOH). Mp 66-67° (61°).

Me ester:
$C_{25}H_{48}O_2$ 380.653
Cryst. (Me_2CO). Mp 36.5-37.5°.
$Bp_{0.00001}$ 180-190°.

Amide:
$C_{24}H_{47}NO$ 365.641
Mp 97-98°.

(Z)-form [506-37-6]

[31152-46-2] *Nervonic acid. Selacholeic acid*
Present in fish and rape seed oils. Cryst. (EtOH). Mp 40.5-41° Mp 44-45°.

Me ester: [2733-88-2]
Mp 14-15°. $Bp_{0.02}$ 165° approx..

Amide: [208650-37-7]
Cryst. (EtOH). Mp 86.5-87.5°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 784B (*nmr*)
Hale, J.B. *et al., J.A.C.S.* , 1930, **52**, 4536 (*synth*)
Bounds, D.G. *et al., J.C.S.* , 1954, 448 (*synth*)
Batchelor, J.G. *et al., J.A.C.S.* , 1973, **95**, 6358 (*cmr*)
Lecerf, J. *et al., J. Physiol. (Paris)* , 1975, **70**, 493
Morales, R.W. *et al., Biochim. Biophys. Acta*, 1976, **431**, 206 (*isol, biosynth*)
Bohannon, M.B. *et al., Lipids*, 1976, **11**, 157-159 (*isol*)

6,13-Tetradecadiene-1,3-diyne T-52

$HC\equiv CC\equiv CCH_2CH=CH(CH_2)_5CH=CH_2$

$C_{14}H_{18}$ 186.296

(Z)-form [37142-95-3]
Oil.

8,9-Epoxide: [122122-03-6]

[145631-83-0] *2-(6-Heptenyl)-3-(2,4-pentadiynyl)oxirane, 9CI. 8,9-Epoxy-1-tetradecene-11,13-diyne.* ***Panaxyne epoxide****. PQ 5. Panaquinquecol 5*
Isol. from ginseng. Oil. $[\alpha]_D$ -90 (c, 1 in $CHCl_3$) (-79.1).

Bohlmann, F. *et al., Chem. Ber.* , 1972, **105**, 1783 (*isol, pmr*)
Fujimoto, Y. *et al., Phytochemistry*, 1992, **31**, 3499 (*isol, pmr, cmr*)
Hirakura, K. *et al., Phytochemistry*, 1994, **35**, 963 (*epoxide*)

2,12-Tetradecadiene-4,6,8,10-tetrayne T-53

$H_3CCH=CHC\equiv CC\equiv CC\equiv CC\equiv CCH=CHCH_3$

$C_{14}H_{10}$ 178.233

Isol. from *Triticum aestivum* (wheat). λ_{max} 273 (ε 98400); 292 (ε 75300); 317 (ε 8200); 340 (ε 12100); 365 (ε 13600); 395 (ε 7300) (pentane).

Jones, E.R.H. *et al., Nature (London)* , 1951, **168**, 900 (*synth, uv*)
Schulte, H.E. *et al., Phytochemistry*, 1965, **4**, 481 (*isol, uv*)

4,6-Tetradecadiene-8,10,12-triyn-1-ol T-54

[2271-25-2]

$H_3C(C\equiv C)_3CH=CHCH=CHCH_2CH_2CH_2OH$

$C_{14}H_{14}O$ 198.264

(E,E)-form
Cryst. (Et_2O/petrol). Mp 112° (104°).

Ac: [6581-87-9] *1-Acetoxy-4,6-tetradecadiene-8,10,12-triyne*
$C_{16}H_{16}O_2$ 240.301
Isol. from roots of *Tanacetum vulgare* (tansy). Cryst. (petrol). Mp 36-37° (31.5°).

4,5-Epoxide: [17098-67-8] *4,5-Epoxy-6-tetradecene-8,10,12-triyn-1-ol*
$C_{14}H_{14}O_2$ 214.263
Cryst. Mp 74-76°.

4,5-Epoxide, Ac:
$C_{16}H_{16}O_3$ 256.301
Cryst. Mp 60-62° (45°).

[7089-15-8]

Bohlmann, F. *et al., Chem. Ber.* , 1960, **93**, 1937; 1962, **95**, 1733; 1964, **97**, 1179; 1965, **98**, 1411; 1966, **99**, 1830; 2096 (*isol, uv, pmr, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1793 (*isol, epoxide*)
Herz, W. *et al., Phytochemistry*, 1985, **24**, 89 (*isol*)

5,8-Tetradecadienoic acid T-55

[10390-16-6]

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_3COOH$

$C_{14}H_{24}O_2$ 224.342

$Bp_{0.05}$ 110-120°.

(Z,Z)-form [39039-37-7]

Goshuyic acid

Minor constit. of rape oil.

Me ester: [18829-89-5]

$C_{15}H_{26}O_2$ 238.369

Constit. of pear volatiles. n_D^{20} 1.4585. λ_{max} 230 (no solvent reported).

Et ester: [28369-25-7]

$C_{16}H_{28}O_2$ 252.396

Constit. of pear volatiles.

Sprecher, H. *et al., Lipids*, 1968, **3**, 14 (*synth, metab, uv, ms*)

Creveling, R.K. *et al., J. Agric. Food Chem.*, 1970, **18**, 19 (*isol*)

Kurono, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 559 (*isol, ir, pmr*)

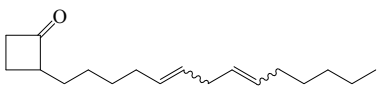
Bus, J. *et al., Chem. Phys. Lipids*, 1976, **17**, 501; 1977, **18**, 130 (*cmr*)

Sebedio, J.L. *et al., J. Am. Oil Chem. Soc.*, 1979, **56**, 15 (*isol*)

2-(5,8-Tetradecadienyl)cyclobutanone T-56

[152245-81-3]

[173074-83-4]



$C_{18}H_{30}O$ 262.434

Detected in γ-irradiated chicken, egg and papaya. Formed by dec. of linoleic acid triglycerides. Potential marker for γ-irradiation of food. No phys. props. reported.

Crone, A.V.J. *et al., J. Sci. Food Agric.*, 1993, **62**, 361-367 (*detn*)

Stewart, E.M. *et al., J. Sci. Food Agric.*, 2000, **80**, 121-130 (*detn*)

2,4,6,8,10,12-Tetradecahexaenedioic acid T-57

$HOOCCH{=}CHCH{=}CHCH{=}CHCH{=}CHCH{=}CHCOOH$

$C_{14}H_{14}O_4$ 246.262

(all-E)-form [505-53-3]

Corticrocin

Isol. from paprika (*Capsicum annuum*). Orange-red needles. Insol. most solvs. Mp 300° subl. dec. (*ca.*).

Di-Me ester: [77186-00-6]

$C_{16}H_{18}O_4$ 274.316

Orange cryst. ($CHCl_3$ or AcOH). Mp 230-232°.

Di-Et ester: [1441-61-8]

$C_{18}H_{22}O_4$ 302.369

Mp 204-205°.

1-L-Aspartic acid, 14-L-isoleucine diamide: ***Boletocrocin D***

$C_{24}H_{30}N_2O_8$ 474.51

Erdtman, H. *et al., Acta Chem. Scand.*, 1948, **2**, 209 (*isol, struct*)

Shaw, B.L. *et al., J.C.S.*, 1954, 3217 (*synth*)

Kovalev, B.G. *et al., CA*, 1963, **58**, 11209f (*synth*)

Rives-Arnau, V. *et al., Macromolecules*, 1985, **18**, 2088

Kahner, L. *et al., Phytochemistry*, 1998, **49**, 1693-1697 (*Boletocrocin D*)

Schreiner, T. *et al., Z. Naturforsch., C*, 1998, **53**, 4-8 (*isol, synth*)

Tetradecanal T-58

[124-25-4]

Myristic aldehyde. Myristaldehyde. Tetradecylaldehyde. FEMA 2763

$H_3C(CH_2)_{12}CHO$

$C_{14}H_{28}O$ 212.375

Isol. from lemon oil etc.; flavouring ingredient. Mp 30° (23°). Bp_{10} 155°. Trimerises to a white solid Mp 65°.

▶ Skin irritant. LD_{50} (rat, orl) >5000 mg/kg. XB7900000

Oxime:

$C_{14}H_{29}NO$ 227.389

Cryst. (MeOH). Mp 82-83°.

Semicarbazone:

Cryst. (MeOH). Mp 106.5°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 361C (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 470B (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 556D (*ir*)

Stephen, H. *et al., J.C.S.*, 1925, **127**, 1874 (*synth*)

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 487 (*rev, tox*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 585

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1924-1925

Aurell, M.J. *et al., Tetrahedron*, 1997, **53**, 10883-10898 (*synth, pmr*)

Wynne, J.H. *et al., Org. Prep. Proced. Int.*, 2000, **32**, 588-592 (*synth, pmr*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBX500

Tetradecanoic acid, 9CI T-59

[544-63-8]

Myristic acid, 8CI. FEMA 2764

$H_3C(CH_2)_{12}COOH$

$C_{14}H_{28}O_2$ 228.374

Occurs widely in vegetable glycerides. Major component of the lipids of nutmeg (*Myristica moschata*). Defoaming agent, lubricant used in food processing. Cryst. (petrol). Mp 54°. Bp_{100} 250.5° Bp_{16} 199°.

▶ Skin and eye irritant. LD_{50} (mus, ivn) 43 mg/kg. QH4375000

Li salt: [20336-96-3]

Stabiliser for food contact polypropylene and polypropylene copolymers.

Me ester: [124-10-7] *Methyl tetradecanoate. FEMA 2722*

$C_{15}H_{30}O_2$ 242.401

Flavour ingredient. Cryst. (Me_2CO). Mp 18.5°. Bp_7 155-157°.

Et ester: [124-06-1] *Ethyl tetradecanoate. FEMA 2445*

$C_{16}H_{32}O_2$ 256.428

Flavouring agent. Cryst. (Me_2CO). Mp 12.3°. Bp 295° Bp_4 139°.

Isopropyl ester: [110-27-0] *Isopropyl tetradecanoate. FEMA 3556*

$C_{17}H_{34}O_2$ 270.454

Flavour ingredient. Bp_{20} 188-191°.

▶ XB8600000

[822-12-8, 4086-70-8, 13429-27-1, 41669-40-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 484C; 608D; 731B (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 755C; 925C; 926A; 926B; 1197A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 576D; 628D; 629A; 629B (*ir*)

Ames, D.E. *et al., J.C.S.*, 1950, 174 (*synth*)

Marosi, L. *et al., Annalen*, 1973, 584 (*synth, struct*)

Hayashi, S. *et al., J. Chem. Phys.*, 1975, **63**, 1732 (*ir*)

Klein, W.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1975, **94**, 48 (*synth*)

Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1976, **17**, 1 (*cmr*)

Francke, W. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 796 (*isol, isopropyl ester*)

Yokoyama, I. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 400 (*ir*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1020; 1495; 1803; 1925 (*occur, use, esters*)

Food Chem. News, 2000, **41(47)**, 25 (*Li salt, use*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ENL850; IQN000; MSA250

1-Tetradecanol, 9CI, 8CI T-60

[112-72-1]

Tetradecyl alcohol. Myristyl alcohol. 1-Hydroxytetradecane

$H_3C(CH_2)_{12}CH_2OH$

$C_{14}H_{30}O$ 214.39

Flavouring ingredient. Cryst. (EtOH aq.). Mp 39-39.5°. Bp_{20} 170-173° Bp_{10} 160°.

▶ Skin irritant. XB8655000

Hydrogen sulfate: [1191-50-0]

$C_{14}H_{30}O_4S$ 294.455

Cryst. (EtOH or H_2O).

Formyl: [5451-63-8]

$C_{15}H_{30}O_2$ 242.401

Bp_{17} 166°.

▶ XB8659000

Ac: [638-59-5]

$C_{16}H_{32}O_2$ 256.428

Mp 14°.

Hexadecanoyl: [4536-26-9] *Tetradecyl palmitate. Myristyl palmitate*

$C_{30}H_{60}O_2$ 452.803

Cryst. ($CHCl_3$/MeOH). Mp 76° (48°).

[1191-50-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 112C (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 167B (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 158D (*ir*)

Watanabe, A. *et al., Bull. Chem. Soc. Jpn.*, 1961, **34**, 1728 (*synth*)

Brunnée, C. *et al., Z. Naturforsch., B*, 1967, **22**, 121 (*ms*)

Iyengar, B.T.R. *et al., Lipids*, 1969, **4**, 28-30 (*synth, esters*)

Adams, K.R. *et al., Nature (London)*, 1969, **223**, 943 (*isol*)

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 111 (*rev, tox*)

Precht, D. *et al., Fette, Seifen, Anstrichm.*, 1976, **78**, 145; 189 (*struct*)

Rossi, R. *et al., Tetrahedron*, 1982, **38**, 639 (*cmr*)

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TBY250
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1392
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1927-1928
Rani, A. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 299-300 (*Tetradecyl palmitate, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TBY250

2-Tetradecanone T-61

[2345-27-9]

$H_3C(CH_2)_{11}COCH_3$

$C_{14}H_{28}O$ 212.375

Constit. of hop oil. Cryst. (EtOH aq.). Mp 33-34°. Bp_{100} 205-206° Bp_{13} 134°.

Semicarbazone:
Mp 125-126°.

Rodd's Chem. Carbon Compd. (2nd edn.), 1965, **1**, 52
Allen, J.E. *et al., Lipids*, 1971, **6**, 448 (*synth*)
Bagnell, L. *et al., Aust. J. Chem.*, 1974, **27**, 1381 (*synth*)

2,4,8,10,12-Tetradecapentaenoic acid T-62

$H_3C(CH{=}CH)_3CH_2CH_2CH{=}CHCH{=}CHCOOH$

$C_{14}H_{18}O_2$ 218.295

(*all-E*)-*form*

2-Hydroxy-2-methylpropylamide: [127514-62-9] ***Hydroxy-γ-isosanshool***. N-*(2-Hydroxyisobutyl)-2,4,8,10,12-tetradecapentaenamide*
$C_{18}H_{27}NO_2$ 289.417
Constit. of *Zanthoxylum* spp.. Powder. λ_{max} 258 (ε 26300); 268 (ε 28900); 279 (ε 26010) (EtOH).

(2*E*,4*E*,8*Z*,10*E*,12*E*)-*form*

2-Methylpropylamide: [78886-65-4] N-*Isobutyl-2,4,8,10,12-tetradecapentaenamide.* ***γ-Sanshool***
$C_{18}H_{27}NO$ 273.417
Constit. of *Zanthoxylum piperitum* (Japanese pepper tree) and other *Zanthoxylum* spp.. Needles (hexane). Mp 88-89°. λ_{max} 260 (ε 48000); 272 (ε 57000); 280 (ε 45000) (EtOH).

2-Hydroxy-2-methylpropylamide: [78886-66-5] ***Hydroxy-γ-sanshool***
$C_{18}H_{27}NO_2$ 289.417
Constit. of *Zanthoxylum piperitum* (Japanese pepper tree). Needles ($CHCl_3$). Mp 122-123°.

2-Methylenepropylamide: ***Dehydro-γ-sanshool***
$C_{18}H_{25}NO$ 271.402
Unstable oil.

(2*E*,4*E*,8*Z*,10*Z*,12*E*)-*form*

Me ester: [114567-68-9]
$C_{15}H_{20}O_2$ 232.322
Gum. Incorrect name in ref..

2-Methylpropylamide: [114612-73-6]
$C_{18}H_{27}NO$ 273.417
Gum.

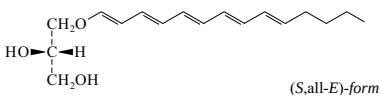
[98095-54-6, 98168-69-5, 117581-14-3]

Yasuda, I. *et al., Chem. Pharm. Bull.*, 1981, **29**, 1791-1793 (*γ-Sanshool, Hydroxy-γ-sanshool*)
Crombie, L. *et al., Tet. Lett.*, 1985, **26**, 2481 (*synth*)
Dominguez, X.A. *et al., Rev. Latinoam. Quim.*, 1987, **18**, 114 (*isol*)
Mizutani, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2362 (*isol, ir, pmr, cmr*)
Xiong, Q. *et al., Phytochemistry*, 1997, **46**, 1123-1126 (*isol, pmr, cmr, ms*)

3-(1,3,5,7,9-Tetradecapentaenyloxy)-1,2-propanediol, 9CI T-63

[84000-58-8]

1-O-(1,3,5,7,9-Tetradecapentaenyl)glycerol. ***Fecapentaene 14***



(*S*,all-*E*)-*form*

$C_{17}H_{26}O_3$ 278.391
Sol. Et_2O, $CHCl_3$; poorly sol. H_2O.

(*S*,all-*E*)-*form*
Beige plates. Mp 188-190° (sealed tube under Ar). $[\alpha]_D^{20}$ +6.5 (c, 0.46 in DMSO). Labile.
▶ Highly mutagenic.

((±)-all-*E*)-*form*
Mp 183-190° (sealed tube under Ar).
▶ Highly mutagenic.

[91379-15-6]

Gupta, I. *et al., Science (Washington, D.C.)*, 1984, **225**, 521
Baptista, J. *et al., Angew. Chem., Int. Ed.*, 1987, **26**, 1186 (*config*)
Pfaendler, R. *et al., Annalen*, 1988, 449 (*synth, ir, pmr, cmr, ms*)
Kingston, D.G.I. *et al., Chem. Res. Toxicol.*, 1990, **3**, 391 (*rev*)
Kivits, G.A.A. *et al., J. Nat. Prod.*, 1990, **53**, 42 (*uv, hplc*)

4,6,12-Tetradecatriene-8,10-diyne-1,3-diol T-64

[23414-62-2]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH(OH)CH_2CH_2OH$

$C_{14}H_{16}O_2$ 216.279

(4*E*,6*E*,12*E*)-*form* [59950-61-7]
Cryst. (CH_2Cl_2/petrol). Mp 110-112° (96-97°). $[\alpha]_D^{20}$ -19 (c, 1.1 in EtOH).

1-Ac:1-Acetoxy-4,6,12-tetradecatriene-8,10-diyn-3-ol
$C_{16}H_{18}O_3$ 258.316
Oil. λ_{max} 249 (ε 34800); 265 (ε 29700); 278 (ε 16200); 295 (ε 29100); 336 (ε 29000); 344 (ε 39800) (Et_2O).

3-Ac:3-Acetoxy-4,6,12-tetradecatriene-8,10-diyn-1-ol
$C_{16}H_{18}O_3$ 258.316
Cryst. (Et_2O/petrol). Mp 61°. $[\alpha]_{Hg}$ +31.2 (c, 1.06 in Et_2O).

Di-Ac: [29576-66-7] *1,3-Diacetoxy-4,6,12-tetradecatriene-8,10-diyne*
$C_{18}H_{20}O_4$ 300.354
Constit. of *Carthamus tinctorius* (safflower). Mp 36° Mp 58°. $[\alpha]_{Hg}^{24}$ +6.4 (c, 3.65 in Et_2O). $[\alpha]_D$ +0.4 (c, 1.0 in MeOH). Isol. as pale yellow oil by Kano *et al*.

[23414-61-1, 103994-34-9]

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 3433; 3544 (*isol, uv, ir, pmr*)
Bedford, C.T. *et al., J.C.S. Perkin 1*, 1976, 735 (*isol, uv, pmr, ms*)
Kano, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 193 (*isol, ir, uv, pmr, ms*)

6-Tetradecene-1,3-diyne-5,8-diol, 9CI T-65

$H_3C(CH_2)_5CH(OH)CH{=}CHCH(OH)C{\equiv}CC{\equiv}CH$

$C_{14}H_{20}O_2$ 220.311

(*Z*)-*form* [77769-23-4]
Isol. from tomato plants. λ_{max} 229 ; 241 ; 254 ; 284 (MeOH).

De Wit, P.J.G. *et al., Physiol. Plant Pathol.*, 1981, **18**, 143 (*isol, struct, ir, uv, pmr, ms*)
Elgersma, D.M. *et al., Physiol. Mol. Plant Pathol.*, 1989, **34**, 545 (*isol*)

13-Tetradecene-1,3-diyne-6,7-diol T-66

[122855-49-6]
Panaxyne

$H_2C{=}CH(CH_2)_5CH(OH)CH(OH)CH_2C{\equiv}CC{\equiv}CH$

$C_{14}H_{20}O_2$ 220.311
Constit. of the roots of *Panax ginseng* (ginseng).

Kim, S.I. *et al., Saengyak Hakhoechi*, 1989, **20**, 71; *CA*, **111**, 224891 (*isol*)

9-Tetradecenoic acid T-67

[26444-03-1]

$H_3C(CH_2)_3CH{=}CH(CH_2)_7COOH$

$C_{14}H_{26}O_2$ 226.358

(*E*)-*form* [50286-30-1]
Cryst. (petrol). Mp 18-18.5°.

Et ester: [68862-25-9]
$C_{16}H_{30}O_2$ 254.412
$Bp_{0.4}$ 112°.

(*Z*)-*form* [544-64-9]

[28039-98-7] *Myristoleic acid*
Occurs in natural fats, e.g. Cottonseed oil. Mp -4.5°. $Bp_{0.6}$ 144° $Bp_{0.03}$ 133°.

Me ester: [56219-06-8]
$C_{15}H_{28}O_2$ 240.385
Bp_4 125-130° (lit. gives a pressure range).

Et ester: [24880-50-0]

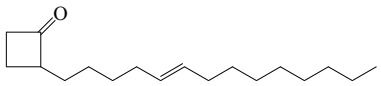
Isopropyl ester: [68862-22-6]
$C_{17}H_{32}O_2$ 268.439

Hexadecyl ester: [64660-84-0] *Cetyl myristoleate. CMO*
$C_{30}H_{58}O_2$ 450.787
Isol. from rice. Food supplement. Oil.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 782A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 587C (*ir*)
Boughton, B.W. *et al., J.C.S.*, 1952, 671 (*synth*)
Calam, D.H. *et al., Nature (London)*, 1969, **221**, 856 (*isol*)
Bestmann, H.J. *et al., Chem. Ber.*, 1975, **108**, 3582
Wawra, H. *et al., Z. Naturforsch., C*, 1978, **33**, 28 (*struct*)
Francke, W. *et al., Angew. Chem., Int. Ed.*, 1979, **18**, 796 (*isopropyl ester*)
Diehl, H.W. *et al., J. Polym. Sci.*, 1994, **83**, 296-299 (*hexadecyl ester, isol, synth*)

2-(5-Tetradecenyl)cyclobutanone T-68

[152245-80-2]
2-TDCB



(*E*)-*form*

$C_{18}H_{32}O$ 264.45

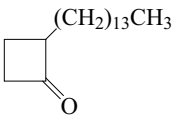
(±)-*(E)-form* [169263-76-7]
Mp 37-39°.

(±)-*(Z)-form* [173074-85-6]
Marker for γ-irradiation of foodstuffs arising from degradation of oleic acid triglycerides. Mp 25-26°.

Hamilton, L. *et al., J.C.S. Perkin 1*, 1996, 139-146 (*synth, pmr, cmr, ms*)
Miesch, M. *et al., Radiat. Phys. Chem.*, 1999, **55**, 337-344 (*synth, pmr*)
Stewart, E.M. *et al., J. Sci. Food Agric.*, 2000, **80**, 121-130 (*detn*)

2-Tetradecylcyclobutanone, 9CI T-69

[35493-47-1]
2-TCB



$C_{18}H_{34}O$ 266.466
Marker for γ-irradiation of foodstuffs esp. eggs; formed by dec. of stearic acid triglycerides.

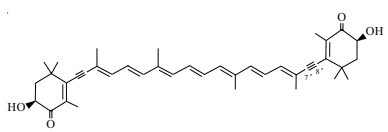
(±)-*form*
Cryst. (pentane). Mp 37°.

Ethylene acetal:
$C_{20}H_{38}O_2$ 310.519
Liq.

Crone, A.V.J. *et al., J. Sci. Food Agric.*, 1993, **62**, 361-367 (*synth, detn*)
Miesch, M. *et al., Radiat. Phys. Chem.*, 1999, **55**, 337-344 (*synth, acetal, pmr*)
Horvatovich, P. *et al., J. Chromatogr., A*, 2000, **897**, 259-268 (*detn, glc*)
Stewart, E.M. *et al., J. Sci. Food Agric.*, 2000, **80**, 121-130 (*detn*)

7,7′,8,8′-Tetradehydroastaxanthin T-70

[31687-79-3]
7,7′,8,8′-Tetradehydro-3,3′-dihydroxy-β,β-carotene-4,4′-dione. Diketotetrahydrozeaxanthin. 4,4′-Diketocynthiaxanthin



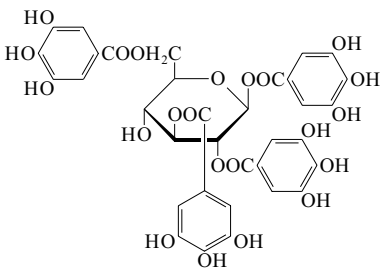
$C_{40}H_{48}O_4$ 592.817
Bluish cryst. (Et_2O). Mp 210°.

7′,8′-Dihydro: [19866-02-5] *7,8-Didehydro-3,3′-dihydroxy-β,β-carotene-4,4′-dione.*

7,8-Dehydroastaxanthianthin
$C_{40}H_{50}O_4$ 594.833
Found in lobster eggs. Violet plates (CH_2Cl_2/diisopropyl ether). Mp 211-212°. Asterinic acid was a mixt. of this with 7,7′,8,8′-Tetradehydroastaxanthin above.

Francis, G.W. *et al., Acta Chem. Scand.*, 1970, **24**, 3050 (*isol, struct*)
Thommen, H. *et al., Biochem. Syst. Ecol.*, 1976, **4**, 131 (*isol, deriv*)
Bernhard, K. *et al., Helv. Chim. Acta*, 1980, **63**, 1473 (*synth, ir, uv, pmr, cmr, ms, cd*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 400 (*bibl*)

1,2,3,6-Tetragalloylglucose T-71



$C_{34}H_{28}O_{22}$ 788.582

β-D-Pyranose-*form* [79886-50-3]
Isol. from *Ceratonia siliqua* (carob). Fine needles (H_2O). Mp 250°. $[\alpha]_D^{20}$ +41 (c, 0.8 in MeOH).

O-*(3,4,5-Trihydroxybenzoyl)(1):* [99907-48-9] *3-O-Digalloyl-1,2,6-tri-O-galloyl-β-D-glucopyranose*
$C_{41}H_{32}O_{26}$ 940.688
Amorph. powder. Sol. MeOH, EtOAc, H_2O; poorly sol. Et_2O, hexane. $[\alpha]_D^{31}$ +60 (c, 0.53 in Me_2CO). Contains a digalloyl (galloylgalloyl) residue at C-3 λ_{max} 280 (MeOH) (Berdy).

O-*(3,4,5-Trihydroxybenzoyl)(2):* [86709-52-6] *6-O-Digalloyl-1,2,3-tri-O-galloyl-β-D-glucopyranose*
$C_{41}H_{32}O_{26}$ 940.688
Light brown amorph. powder. $[\alpha]_D^{20}$ +44.1 (c, 0.54 in Me_2CO). Contains a digalloyl (galloylgalloyl) residue at C-6.

O-*Bis(3,4,5-trihydroxybenzoyl):2,6-Bis-O-digalloyl-1,3-di-O-galloyl-β-D-glucopyranose*
$C_{48}H_{36}O_{30}$ 1092.794
Light brown amorph. powder. $[\alpha]_D^{20}$ +39.4 (c, 0.33 in Me_2CO). Contains galloylgalloyl residues at C-2 and C-6.

O-*(Galloylgalloyl):6-O-Trigalloyl-1,2,3-tri-O-galloyl-β-D-glucopyranose*
$C_{48}H_{36}O_{30}$ 1092.794
Light brown amorph. powder. $[\alpha]_D^{20}$ +43.4 (c, 0.35 in Me_2CO). Contains a trigalloyl (galloylgalloylgalloyl) residue at C-6.

3D-Deoxy:1,2,3-Tri-O-galloyl-6-O-protocatechuoyl-β-D-glucopyranose. ***Monacanthin B***
$C_{34}H_{28}O_{21}$ 772.583
Off-white powder.

Haddock, E.A. *et al., J.C.S. Perkin 1*, 1982, 2515 (*isol, struct, pmr, cmr*)
Nishizawa, M. *et al., J.C.S. Perkin 1*, 1983, 961 (*derivs*)
Nishizawa, M. *et al., Phytochemistry*, 1985, **24**, 2411 (*deriv*)
Hagenah, S. *et al., Phytochemistry*, 1993, **32**, 637 (*biosynth*)
Kandil, F.E. *et al., Phytochemistry*, 2001, **58**, 611-613 (*Monacanthin B*)

1,2,4,6-Tetragalloylglucose T-72

$C_{34}H_{28}O_{22}$ 788.582

β-D-Pyranose-*form* [84297-49-4]
Isol. from *Bergenia crassifolia* (Siberian tea) and *Bergenia cordifolia*. Fine needles (H_2O). Mp 250°. $[\alpha]_D^{20}$ -2 (c, 0.5 in MeOH).

Haddock, E.A. *et al., J.C.S. Perkin 1*, 1982, 2515 (*isol, struct, pmr, cmr*)

2,3,4,6-Tetragalloylglucose T-73

$C_{34}H_{28}O_{22}$ 788.582

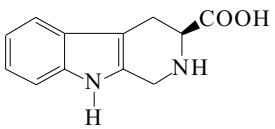
D-Pyranose-*form* [40410-95-5]
Isol. from the root and rhizome of *Sanguisorba officinalis* (burnet bloodwort). Off-white amorph. powder. $[\alpha]_D^{20}$ +67.7 (c, 1.18 in 50% Me_2CO aq.). Exists as an equilibrated mixt. of α- and β-anomers.

β-D-Pyranose-*form*
Me glycoside: Methyl 2,3,4,6-tetra-O-galloyl-β-D-glucopyranoside
$C_{35}H_{30}O_{22}$ 802.609
Gallotannin constit. of *Sanguisorba officinalis* (burnet bloodwort). Tan amorph. powder + $2^1/_2$ H_2O. $[\alpha]_D^{29}$ +33.8 (c, 0.9 in Me_2CO).

Armitage, R. *et al., J.C.S.(C)*, 1961, 1842 (*struct*)
Tanaka, T. *et al., Phytochemistry*, 1983, **22**, 2575 (*pmr, cmr*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 117 (*deriv*)
Khanbabaee, K. *et al., Tetrahedron*, 1997, **53**, 10725 (*synth, uv, pmr, cmr*)

1,2,3,4-Tetrahydro-β-carboline-3-carboxylic acid T-74

2,3,4,9-Tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic acid



$C_{12}H_{12}N_2O_2$ 216.239

(*S*)-*form* [42438-90-4]
L-*form*
Widespread in many foodstuffs especially fruit juices, jams and fermented foods or beverages. Formed by Pictet-Spengler condensation of L-tryptophan and formaldehyde in nature or during food processing. Mp 282-284°. $[\alpha]_D^{20}$ -124.6 (c, 0.2 in 0.1*M* NaOH).

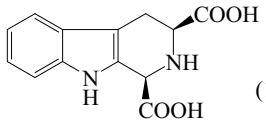
[129848-94-8]

Herraiz, T. *et al., J. Agric. Food Chem.*, 1996, **44**, 3057-3065; 1998, **46**, 3484-3490 (*hplc, occur*)

1,2,3,4-Tetrahydro-β-carboline-1,3-dicarboxylic acid T-75

[59132-30-8]

[192180-80-6, 192180-81-7]
*2,3,4,9-Tetrahydro-1*H*-pyrido[3,4-*b*]indole-1,3-dicarboxylic acid, 9CI*



(1*R*,3*S*)-*form*

$C_{13}H_{12}N_2O_4$ 260.249
Present in fruit syrups, beer, wines, vinegar and most fermented sauces. Cryst. Mp 270°.

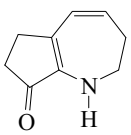
(1*R*,3*S*)-*form*
Mp 269-271°. Probable config. One set of authors gives the Mp but does not assign a config., the other authors show that the main prod. of condensation of, with Glyoxylic acid is the *cis*-isomer, but do not give a Mp..

[123771-30-2, 123771-45-9]

Bobbitt, J.M. *et al., J.O.C.*, 1980, **45**, 1978-1984 (*synth*)
Gutsche, B. *et al., J. Agric. Food Chem.*, 1997, **45**, 2458-2462 (*isol, pmr, ms, synth, config*)

2,3,6,7-Tetrahydrocyclopent[-*b*]azepin-8(1*H*)-one T-76

[97826-65-8]

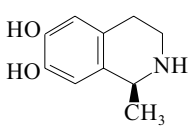


$C_9H_{11}NO$ 149.192
Proline-specific Maillard product. Characterised spectroscopically.

Tressl, R. *et al., Annalen*, 1985, 2017-2027 (*isol, pmr, ms*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137; 1993, **41**, 547-563 (*isol, pmr, ms*)
Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

1,2,3,4-Tetrahydro-6,7-dihydroxy-1-methylisoquinoline T-77

[525-72-4]
1,2,3,4-Tetrahydro-1-methyl-6,7-isoquinolinediol, 9CI. ***Salsolinol***



(*S*)-*form*

$C_{10}H_{13}NO_2$ 179.218

(R)-form [53622-83-6]
Mp 174-174° (as hydrobromide). $[\alpha]_D$ +30 (MeOH) (hydrobromide).

6-Me ether: See 1,2,3,4-Tetrahydro-7-hydroxy-6-methoxy-1-methylisoquinoline in *The Combined Chemical Dictionary.*

7-Me ether: See 1,2,3,4-Tetrahydro-6-hydroxy-7-methoxy-1-methylisoquinoline in *The Combined Chemical Dictionary.*

Di-Me ether: See 1,2,3,4-Tetrahydro-6,7-dimethoxy-1-methylisoquinoline in *The Combined Chemical Dictionary.*

(*S*)-*form* [27740-96-1]
Cryst. (EtOH/Et_2O) (as hydrobromide). Mp 174-175° (hydrobromide). $[\alpha]_D$ -30.9 (MeOH).

(±)-*form*

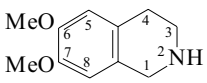
Me ether, N-*Me:* [176329-46-7] **O-*Demethylcarnegine***. O-*Norcarnegine*
$C_{12}H_{17}NO_2$ 207.272
Oil. Site of methylation not known. Identical with either (±)-*N*-Methylsalsoline or (±)-*N*-Methylisosalsoline.

(ξ)-*form*
Alkaloid from *Annona reticulata* (custard apple), *Musa paradisiaca* (banana) and *Theobroma cacao* (cocoa).

Teitel, S. *et al., J. Med. Chem.*, 1972, **15**, 845 (*synth, uv, cd, ord, pmr, abs config*)
Riggin, R.M. *et al., J. Agric. Food Chem.*, 1976, **24**, 189; 900 (*occur*)
Forgacs, P. *et al., Plant. Med. Phytother.*, 1981, **15**, 10 (*occur*)
Chen, D. *et al., Yaoxue Xuebao*, 1982, **17**, 792; *CA*, **98**, 40465k
El-Shazly, A. *et al., Phytochemistry*, 1996, **42**, 225 (*O-Demethylcarnegine*)
Francisco, M. *et al., Phytochemistry*, 2003, **62**, 1265-1270 (*isol, pmr, cmr*)

1,2,3,4-Tetrahydro-6,7-dimethoxyisoquinoline, 9CI T-78

[1745-07-9]
Heliamine



$C_{11}H_{15}NO_2$ 193.245
Mp 84-85°. Log P 0.98 (calc). Readily forms carbonate on exp. to air.

▶ NX5015000

Hydrochloride: [2328-12-3]
Cryst. (EtOH/Et_2O). Mp 255° (248°, 252°).

Picrate:
Cryst. (EtOH). Mp 223-225°.

N-*Me:* [16620-96-5] *1,2,3,4-Tetrahydro-6,7-dimethoxy-2-methylisoquinoline.* **O-*Methylcorypalline***. N-*Methylheliamine*
$C_{12}H_{17}NO_2$ 207.272
Alkaloid from *Nelumbo nucifera* (East Indian lotus). Cryst. (MeOH or petrol/cyclohexane), cryst. + ½ H_2O (Et_2O). Mp 69-70° Mp 82° (hemihydrate).

▶ NX5018510

N-*Me, hydrochloride:* [16135-43-6]
Cryst. (2-propanol). Mp 219-221° (215°, 210°).

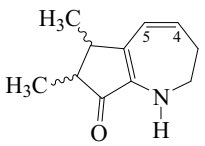
N-*Me, picrate:* [28332-96-9]
Cryst. (C_6H_6/MeOH). Mp 160°.

N,N-*Di-Me:*

[19626-05-2, 83527-64-4] *1,2,3,4-Tetrahydro-6,7-dimethoxy-2,2-dimethylisoquinolinium.* **N-*Dimethylheliamine***
$C_{13}H_{20}NO_2^{\oplus}$ 222.307
Mp 242-243° (as iodide).

Buck, J.S. *et al., J.A.C.S.*, 1934, **56**, 1769-1771 (*synth*)
Manske, R.H.F. *et al., Can. J. Res., Sect. B*, 1937, **15**, 159-167 (*synth*)
Bobbitt, J.M. *et al., J.O.C.*, 1965, **30**, 2247-2250 (*synth*)
Yang, T.H. *et al., J. Chin. Chem. Soc. (Taipei)*, 1970, **17**, 54-56; 235-242 (*N-Me, isol, struct*)
Hughes, D.W. *et al., Can. J. Chem.*, 1976, **54**, 2252-2260; 1977, **55**, 3304-3311 (*cmr*)
Von Weigrebe, W. *et al., Helv. Chim. Acta*, 1976, **59**, 949 (*synth*)
Lindgren, J.E. *et al., J. Nat. Prod.*, 1976, **39**, 464-466 (*N-Me, occur, ms*)
Strömbom, J. *et al., Acta Pharm. Suec.*, 1978, **15**, 127-132; *CA*, **89**, 126107w (*isol*)
Strömbom, J. *et al., J. Chromatogr.*, 1978, **147**, 513-515 (*N-Me, hplc*)
Shamma, M. *et al., J. Nat. Prod.*, 1978, **41**, 169-178 (*N-Me, isol, uv, ir, pmr, ms*)
Miller, L.L. *et al., J.O.C.*, 1978, **43**, 1580-1586 (*synth, pmr, ms*)
Mata, R. *et al., Phytochemistry*, 1980, **19**, 673-678; 1983, **22**, 1263-1270 (*isol, ir, uv, pmr, cmr, ms, N-Me*)
Pummangura, S. *et al., J. Nat. Prod.*, 1982, **45**, 277-282 (*isol*)
Theuns, H.G. *et al., Phytochemistry*, 1983, **22**, 247-250 (*N-Me, occur, synth, pmr, ms*)
Ruchirawat, S. *et al., Synth. Commun.*, 1984, **14**, 1221-1228 (*synth, pmr, ms*)
Murahashi, S.I. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 2968 (*pmr, cmr*)
Takano, S. *et al., Heterocycles*, 1993, **35**, 47-52 (*synth*)
Shakirov, R. *et al., Khim. Prir. Soedin.*, 1996, **32**, 410-512; *Chem. Nat. Compd. (Engl. Transl.)*, 1996, **32**, 386-512 (*N-Dimethylheliamine*)
Shinohara, T. *et al., Chem. Pharm. Bull.*, 1997, **45**, 813-819 (*synth*)

2,3,6,7-Tetrahydro-6,7-dimethylcyclopent[*b*]azepin-8(1*H*)-one T-79



$C_{11}H_{15}NO$ 177.246
Proline-specific Maillard product.

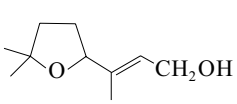
4,5-Dihydro:2,3,4,5,6,7-Hexahydro-6,7-dimethylcyclopent[b]azepin-8(1H)-one
$C_{11}H_{17}NO$ 179.261
Proline-specific Maillard product.

[97826-70-5, 97826-71-6, 97826-75-0, 97826-76-1]

Tressl, R. *et al., Annalen*, 1985, 2017-2027 (*isol, ms, pmr*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137 (*isol, ms, pmr*)
Chen, C.-W. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur*)

3-(Tetrahydro-5,5-dimethyl-2-furanyl)-2-buten-1-ol, 9CI T-80

4,7-Epoxy-3,7-dimethyl-2-octen-1-ol



$C_{10}H_{18}O_2$ 170.251

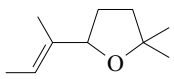
(E)-form [84184-43-0]
Constit. of peppermint oil. Oil with dry grassy hay odour.

[84184-42-9]

Sakurai, K. *et al., Agric. Biol. Chem.*, 1983, **47**, 1249

Tetrahydro-2,2-dimethyl-5-(1-methyl-1-propenyl)furan, 9CI T-81

[7416-35-5]
2,2-Dimethyl-5-(1-methyl-1-propenyl)tetrahydrofuran. Ocimen quintoxide. FEMA 3665



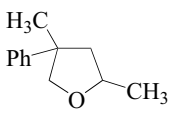
$C_{10}H_{18}O$ 154.252
Flavouring ingredient. Present in lime oil (*Citrus aurantifolia*). Oil. Sl. sol. H_2O. d^{20} 0.87. Bp_{10} 65°. $[\alpha]_D^{20}$ 0. n_D^{20} 1.4662.

[56058-69-6, 56058-70-9]

Kováts, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2705; 1966, **49**, 2055 (*isol*)
Corbier, B. *et al., Recherches*, 1974, **19**, 235 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 183
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, **1**, 863-864

Tetrahydro-2,4-dimethyl-4-phenylfuran T-82

[82461-14-1]
2,4-Dimethyl-4-phenyltetrahydrofuran. Rhubafuran

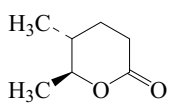


$C_{12}H_{16}O$ 176.258
Stereochem. not reported. Fragrance/flavoring agent ingredient. Liq. with a grapefruit-like aroma and fruity rhubarb undertones.

Eur. Pat., 1982, 49 543; *CA*, **97**, 60836q (*synth*)
Murahashi, S. *et al., J.O.C.*, 1988, **53**, 4489-4495 (*synth, pmr*)

Tetrahydro-5,6-dimethyl-2*H*-pyran-2-one, 9CI T-83

[10413-18-0]
γ,δ-Dimethyl-δ-valerolactone. 4-Methyl-5-hexanolide

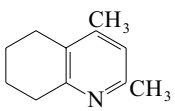


(5*R*,6*S*)-*form*

$C_7H_{12}O_2$ 128.171
(5R,6S)-form [139164-07-1]
(-)-trans-*form*
Needles (hexane). Mp 25-25.5°. $[\alpha]_D^{22}$ -6.5 (c, 0.32 in $CHCl_3$).
(5S,6R)-form [82467-25-2]
(+)-trans-*form*
Liq. Bp_1 80-82° $Bp_{0.15}$ 70° (bath). $[\alpha]_D^{20}$ +18 (c, 1.2 in $CHCl_3$).
Di-Et ketal: [101977-88-2] *2,2-Diethoxytetrahydro-5,6-dimethyl-2H-pyran, 9CI*
$C_{11}H_{22}O_3$ 202.293
Liq. $Bp_{0.08}$ 70° (bath). $[\alpha]_D^{20}$ +22.2 (c, 1.03 in $CHCl_3$).
(5RS,6RS)-form [24405-15-0] *(±)*-cis-*form*
Unstable liq. Bp_5 99-102°.
(5RS,6SR)-form [82045-40-7]
[24405-16-1] *(±)*-trans-*form*
Mp 26-28° subl. Bp_5 100-102°.
(5R*,6S*)-form
Minor flavour constit. of milk (*trans*-form of undetd. abs. config.).
Honkanen, E. *et al., Acta Chem. Scand.*, 1968, **22**, 2041; 1969, **23**, 531 (*isol, synth, ms*)
Honkanen, E. *et al., Finn. Chem. Lett.*, 1975, 129 (*cmr*)
Cooke, E. *et al., Can. J. Chem.*, 1982, **60**, 29 (*synth, spectra*)
Williams, D.R. *et al., J.A.C.S.*, 1982, **104**, 4708 (*synth*)
Schow, S.R. *et al., J.A.C.S.*, 1986, **108**, 2662 (*synth, pmr*)
Kocieński, P.J. *et al., J.C.S. Perkin 1*, 1987, 2171 (*synth, ir, pmr*)
Ley, S.V. *et al., Tetrahedron*, 1989, **45**, 7161-7194 (*synth, ir, pmr*)
Pinyarat, W. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 419-421 (*synth, ir, pmr*)

5,6,7,8-Tetrahydro-2,4-dimethylquinoline T-84

[60169-66-6]



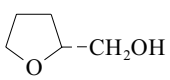
$C_{11}H_{15}N$ 161.246
Alkaloid from the roots of *Glycyrrhiza uralensis* (Chinese licorice). Mp 19-20°. Bp 250-251° Bp_{12} 122-123°.

Hydrochloride:
Mp 195°.
Picrate:
Mp 144°.
Methiodide:
Mp 157°.

v. Braun, J. *et al., Ber.*, 1923, **56**, 1346 (*synth*)
Yamaguchi, K. *et al., Yakugaku Zasshi*, 1926, **533**, 53 (*synth*)
Shaw, J.E. *et al., J. Het. Chem.*, 1987, **24**, 1477 (*synth*)
Han, Y.N. *et al., Arch. Pharmacal Res.*, 1990, **13**, 101; *CA*, **113**, 227984 (*isol*)

Tetrahydro-2-furanmethanol, 9CI T-85

[97-99-4]
Tetrahydrofurfuryl alcohol, 8CI. Oxolan-2-methanol. 2-Hydroxymethyltetrahydrofuran. FEMA 3056



(*R*)-*form*

$C_5H_{10}O_2$ 102.133
▶ Eye, skin and respiratory tract irritant. LD_{50} (rat, orl) 2500 mg/kg. Fl. p. 70/71°, autoignition temp. 280/282°. LU2450000
(±)-form [72074-94-3]
Solvent for fats, waxes, resins, etc. Flavouring ingredient. Bp_{750} 177-178° Bp_{20} 80-82°.
Ac: [637-64-9] *FEMA 3055*
Flavouring ingredient. d_{20}^{20} 1.06. Bp_{740} 192-194° Bp_{18} 88-90°. n_D^{20} 1.4475.
▶ Fl. p. 88°.
Propanoyl: [637-65-0] *FEMA 3058*
$C_8H_{14}O_3$ 158.197
Flavouring ingredient. d 1.04. Bp 204-207° Bp_3 85-87°. n_D^{23} 1.4370.
Butanoyl: [92345-48-7]

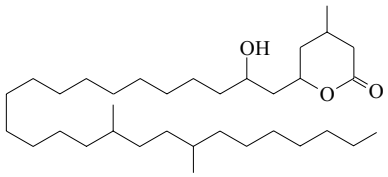
[2217-33-6] *Tetrahydrofurfuryl butyrate. FEMA 3057*
$C_9H_{16}O_3$ 172.224
Flavouring agent with heavy sweet odour resembling apricot/pineapple. Liq. Insol. H_2O. d 1.01. Bp 227°.

Cinnamoyl: [65505-25-1] *Tetrahydrofurfuryl cinnamate. FEMA 3320*
$C_{14}H_{16}O_3$ 232.279
Flavouring agent with sweet vinous odour. Sl. viscous liq. Insol. H_2O. d 1.11. Bp >300°.
(ξ)-form
Found in fermented soya hydrolysate (shoyu).
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 240B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 384A; 1089B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 317B (*ir*)
Kirner, W.R. *et al., J.A.C.S.*, 1930, **52**, 3251-3256 (*synth*)
Burdick, H.E. *et al., J.A.C.S.*, 1934, **56**, 438-442 (*synth*)
Fein, M.L. *et al., J.A.C.S.*, 1944, **66**, 1201-1203 (*2-propenoyl*)
Hartman, F.C. *et al., J.O.C.*, 1964, **29**, 873-877 (*synth*)
Defaye, J. *et al., J. Het. Chem.*, 1969, **6**, 229-234 (*synth*)
Butler, J.D. *et al., J.C.S.(C)*, 1969, 173-176 (*synth*)
Durette, P.L. *et al., Chem. Ber.*, 1974, **107**, 937-950 (*synth*)
Lloyd, R.A. *et al., Tob. Sci.*, 1976, **20**, 125-133 (*isol*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **11**, 520 (*rev*)
Descours, D. *et al., Helv. Chim. Acta*, 1991, **74**, 1757-1763 (*abs config*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 743-744 (*esters*)
Alajarin, R. *et al., J. Med. Chem.*, 1995, **38**, 2830-2841 (***synth, pmr***)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2758-2762 (*esters*)
Mravik, A. *et al., Chem. Eur. J.*, 1998, **4**, 1621-1627 (*resoln*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TCT000

Tetrahydro-6-(2-hydroxy-16,19-dimethylhexacosyl)-4-methyl-2*H*-pyran-2-one, 9CI T-86

[60797-23-1]
7-Hydroxy-3,21,24-trimethylhentriacontan-

5-olide



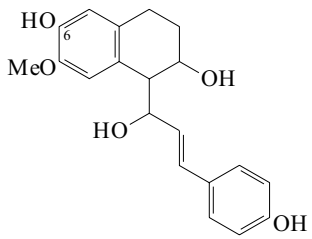
$C_{34}H_{66}O_3$ 522.894
Found in flowers of *Grewia asiatica* (phalsa). Needles. Mp 70-71°. $[\alpha]_D^{20}$ -10.3 ($CHCl_3$).

Ac:
Mp 68°.

Lakshmi, V. *et al., Phytochemistry*, 1976, **15**, 1397

1,2,3,4-Tetrahydro-1-[1-hydroxy-3-(4-hydroxyphenyl)-2-propenyl]-7-methoxy-2,6-naphthalenediol T-87

[163811-77-6]



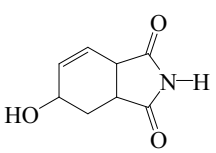
$C_{20}H_{22}O_5$ 342.391
Isol. from the rhizomes of *Musa acuminata* (dwarf banana) infected with *Fusarium oxysporum*. Cryst. (C_6H_6/hexane). Mp 112-115°. $[\alpha]_D^{25}$ -52.6 (c, 0.1 in $CHCl_3$). λ_{max} 272 ; 352 ; 378 ; 382 (EtOH).

6-Me ether: [163811-76-5] *1,2,3,4-Tetrahydro-1-[1-hydroxy-3-(4-hydroxyphenyl)-2-propenyl]-6,7-dimethoxy-2-naphthalenol*
$C_{21}H_{24}O_5$ 356.418
From *Musa acuminata* (dwarf banana) infected with *Fusarium oxysporum*. Cryst. (C_6H_6/hexane). Mp 82-84°. $[\alpha]_D^{25}$ -51.2 (c, 0.1 in $CHCl_3$). λ_{max} 274 ; 351 ; 382 (EtOH).

Luis, J.G. *et al., Tetrahedron*, 1995, **51**, 4117 (*isol, uv, ir, pmr, cmr*)

3*a*,4,5,7*a*-Tetrahydro-5-hydroxy-1*H*-isoindole-1,3(2*H*)-dione, 9CI T-88

1,2,3,4-Tetrahydro-4-hydroxyphthalimide



$C_8H_9NO_3$ 167.164
Potential food contaminant arising from the metabolism of Captan. Detected in milk.

[161961-44-0, 161961-46-2]

Kukla, D. *et al., J. Agric. Food Chem.*, 1995, **43**, 1224-1229

3*a*,4,7,7*a*-Tetrahydro-4-hydroxy-1*H*-isoindole-1,3(2*H*)-dione, 9CI T-89

1,2,3,6-Tetrahydro-3-hydroxyphthalimide

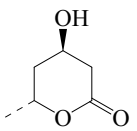
$C_8H_9NO_3$ 167.164
Potential food contaminant arising from the metabolism of Captan. Detected in milk.

[161961-43-9, 161961-45-1]

Kukla, D. *et al., J. Agric. Food Chem.*, 1995, **43**, 1224-1229

3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2*H*-pyran-2-one, 9CI T-90

3-Hydroxy-5-hexanolide



(4*R*,6*R*)-*form*

$C_6H_{10}O_3$ 130.143

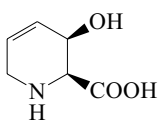
(4*S*,6*S*)-*form* [33275-54-6]
Constit. of *Osmunda japonica* (zenmai). Prisms (Et_2O). Mp 67-70°.

[87172-73-4, 87172-74-5]

Tschesche, R. *et al., Chem. Ber.*, 1971, **104**, 1420
Numata, A. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2815
Weinges, K. *et al., Eur. J. Org. Chem.*, 1998, 189-192 (*cryst struct, Parasorboside*)

1,2,3,6-Tetrahydro-3-hydroxy-2-pyridinecarboxylic acid, 9CI T-91

1,2,3,6-Tetrahydro-3-hydroxypicolinic acid. ***3-Hydroxybaikiain***



$C_6H_9NO_3$ 143.142

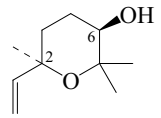
(2*S*,3*R*)-*form* [112269-85-9]
Needles (MeOH aq.). Mp 300-302°. $[\alpha]_D^{20}$ -332.7 (c, 0.3 in H_2O). $[\alpha]_D^{20}$ -324 (c, 0.3 in 1*M* HCl).

Kusano, G. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3482 (*isol, ir, pmr, cmr, ms, struct*)

Tetrahydro-3-hydroxy-2,2,6-trimethyl-6-vinylpyran T-92

[14049-11-7]

[1365-19-1]
*6-Ethenyl-3,4,5,6-tetrahydro-2,2,6-trimethyl-2*H*-pyran-3-ol. 3-Hydroxy-2,2,6-trimethyl-6-vinyltetrahydropyran.* ***Cnidiol C****. Linalool 3,7-oxide*



(3*R*,6*R*)-*form*

$C_{10}H_{18}O_2$ 170.251
Stereochem. of naturally occurring material not yet detd. (2001). Constit. of *Citrus* spp.. Oil. Bp_{10} 97-98°. $[\alpha]_D^{20}$ +15.8. Normally occurs with Linalyl oxide, L-91, see that entry for further synonyms and references. Linalool oxide C and Linalool oxide D refer to the *trans*- and *cis*-forms respectively.

O-*[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]:*

[184488-16-2, 184488-17-3]
$C_{21}H_{36}O_{11}$ 464.509
Constit. of the leaves of *Camellia sinensis* var. *sinensis* (China tea). Occurs as *cis*- and *trans*-isomers.

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:Linalool 3,7-oxide β-primeveroside*
$C_{21}H_{36}O_{11}$ 464.509
Constit. of *Camellia sinensis* var. *sinensis* (China tea). *trans*-Isomer isol..

Ac: [67674-42-4]
$C_{12}H_{20}O_3$ 212.288
Oil. Bp_{10} 98-99°. $[\alpha]_D^{20}$ +17.5.

3-Ketone: [33933-72-1] *Tetrahydro-2,2,6-trimethyl-6-vinyl-3*H*-pyran-3-one*
$C_{10}H_{16}O_2$ 168.235
Oil. $[\alpha]_D^{20}$ -9.3.

3-Ketone, 2,4-dinitrophenylhydrazone:
Cryst. Mp 111-112.5°.

(3*R*,6*R*)-*form* [24048-52-0]
Mp 94-95°. $[\alpha]_D^{20}$ +1.9 (c, 0.5 in CH_2Cl_2).

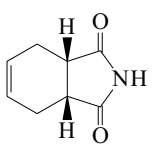
(3*S*,6*R*)-*form* [10448-31-4]
Semisolid oil. $[\alpha]_D^{20}$ +11 (c, 0.5 in CH_2Cl_2).

[11063-77-7, 11063-78-8, 14009-71-3, 39028-58-5]

Klein, E. *et al., Tet. Lett.*, 1983, 1109 (*synth*)
Dembitskii, A.D. *et al., Khim. Prir. Soedin.*, 1985, **21**, 332; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 310 (*isol*)
Meou, A. *et al., Synthesis*, 1991, 681 (*synth*)
Moon, J.-H. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1815 (*isol, glycoside*)
Nishikitani, M. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1631-1633 (*primeveroside*)
Vidari, G. *et al., Tetrahedron: Asymmetry*, 1999, **10**, 3547-3557 (*3R,6R-form, 3S,6R-form*)

3*a*,4,7,7*a*-Tetrahydro-1*H*-isoindole-1,3(2*H*)-dione, 9CI T-93

[85-40-5]
1,2,3,6-Tetrahydrophthalimide. 4-Cyclohexene-1,2-dicarboximide



$C_8H_9NO_2$ 151.165
Potential food contaminant arising from the metabolism of Captan.

► GW4660000
(3*aRS*,7*aSR*)-*form* [1469-48-3]
cis-*form*
Cryst. (EtOH). Mp 136-138°.
Ag salt: [62506-08-5]
Tan powder.
N-*Me:* [62950-21-4]
$C_9H_{11}NO_2$ 165.191
Cryst. (C_6H_6/hexane). Mp 72.5-73° (60-62°).

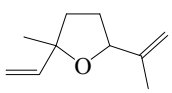
[2015-58-9, 5167-69-1, 27813-21-4]

Rice, L.M. *et al., J.O.C.*, 1954, 884 (*synth, deriv*)
Christol, H. *et al., Bull. Soc. Chim. Fr.*, 1966, 1315 (*synth*)
Kirfel, A. *et al., Acta Cryst.*, 1976, 1556 (*cryst struct*)
Evans, D.L. *et al., J.O.C.*, 1979, **44**, 497 (*deriv, pmr*)
Crockett, G.C. *et al., Synth. Commun.*, 1981, 447 (*synth*)
Wijnberg, B.P. *et al., Tetrahedron*, 1982, **38**, 209 (*synth*)
Caswell, L.R. *et al., J.O.C.*, 1984, **49**, 696 (*synth*)
Mori, M. *et al., Tet. Lett.*, 1987, 6187
Kukla, D. *et al., J. Agric. Food Chem.*, 1995, **43**, 1224-1229 (*detn in milk*)

Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran, 8CI T-94

[13679-86-2]

[54750-69-5, 54750-70-8, 145165-90-8, 145165-94-2]
2-Ethenyltetrahydro-2-methyl-5-(1-methylethenyl)furan, 9CI. 5-Isopropenyl-2-methyl-2-vinyltetrahydrofuran, 9CI. FEMA 3759

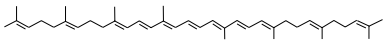


$C_{10}H_{16}O$ 152.236
Flavouring ingredient. Present in coriander oil, clary sage oil, wine, brandy, coffee and muscat grape juice. Also isol. from passionfruit and sour cherry extracts as artifact from terpene alcohol precursors. Bp_{11} 54-55°.

Ohloff, G. *et al., Helv. Chim. Acta*, 1964, **47**, 602-626 (*synth, pmr*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1974, **57**, 2055-2061 (*cmr*)
Engel, K.-H. *et al., J. Agric. Food Chem.*, 1983, **31**, 998-1002 (*occur*)
Lamparsky, D. *et al., Perfum. Flavor.*, 1988, **13**, 17-18; **13(5)**, 20-25 (*occur*)
Burdock, G.A. *et al., Food Technol. (Chicago)*, 1990, **44**, 78; **44(2)**, 80; 82; 84; 86 (*use*)
Schwab, W. *et al., Z. Lebensm.-Unters. -Forsch.*, 1990, **190**, 228-231 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 408 (*use*)
Konstantinovic, S. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 1169-1170 (*synth*)

7,7′,8,8′-Tetrahydrolycopene T-95

[13587-06-9]
7,7′,8,8′-Tetrahydro-ψ,ψ-carotene. 2,6,10,14,19,23,27,31-Octamethyl-2,6,10,12,14,16,18,20,22,26,30-dotriacontaundecaene. ζ-Carotene



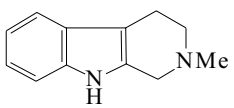
$C_{40}H_{60}$ 540.914
Constit. of carrot oil and many other natural products. Cryst. ($CHCl_3$/MeOH). Mp 42-46°. λ_{max} 360 ; 380 ; 401 ; 425 (no solvent reported).

1ξ,2ξ-Epoxide: [93861-35-9] *1,2-Epoxy-1,2-dihydro-ζ-carotene.* ***ζ-Carotene epoxide***
$C_{40}H_{60}O$ 556.913
Isol. from cherry tomato (*Lycopersicon esculentum*). Cryst. (CH_2Cl_2/MeOH). λ_{max} 232 ; 359 ; 378 ; 400 ; 425 (hexane).
(9*Z*,9′*Z*)-*form* [72746-33-9]
Isol. from cherry tomato *Lycopersicon esculentum* var. 'Tangella'. Viscous orange oil. λ_{max} 284 ; 294 ; 361 ; 379 ; 401 ; 427 (hexane).

Davis, J.B. *et al., J.C.S.(C)*, 1966, 2154 (*pmr, uv, ir, bibl*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759 (*isol, epoxide*)
Davies, B.H. *et al., Phytochemistry*, 1974, **13**, 1209 (*ms*)
Clough, J.M. *et al., J.C.S. Perkin 1*, 1983, 3011 (*cmr*)
Arm, C. *et al., Helv. Chim. Acta*, 1984, **67**, 1540 (*synth, epoxide*)
Frecknell, E.A. *et al., Phytochemistry*, 1984, **23**, 1707 (*isol, occur*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 38 (*bibl*)

1,2,3,4-Tetrahydro-2-methyl-β-carboline T-96

[13100-00-0]
*2,3,4,9-Tetrahydro-2-methyl-1*H*-pyrido[3,4-*b*]indole, 9CI*



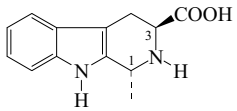
$C_{12}H_{14}N_2$ 186.256
Alkaloid from *Elaeagnus angustifolia* (Russian olive). Cryst. (MeOH). Mp 216-218°.

Hydrochloride:
Cryst. (EtOH/Et_2O). Mp 245-247°.
Picrate:
Cryst. (EtOH). Mp 195-197°.
Methiodide:
Cryst. (EtOH). Mp 265-266°.

Bockelheide, V. *et al., J.A.C.S.*, 1950, **72**, 2132 (*synth*)
Platonova, T.F. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1958, **28**, 3159 (*isol*)
Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 1737 (*isol, uv, ir, pmr, ms*)
Agurell, S. *et al., Acta Chem. Scand.*, 1969, **23**, 903 (*isol, ms*)
Allen, J.R.F. *et al., Phytochemistry*, 1980, **19**, 1573 (*rev, bibl*)
Kawanishi, K. *et al., Phytochemistry*, 1985, **24**, 1373 (*occur*)
Kumar, S. *et al., Planta Med.*, 1985, 466 (*isol, pmr, cmr, ms*)

1,2,3,4-Tetrahydro-1-methyl-β-carboline-3-carboxylic acid T-97

[5470-37-1]
*2,3,4,9-Tetrahydro-1-methyl-1*H*-pyrido[3,4-*b*]indole-3-carboxylic acid, 9CI*



(1*R*,3*S*)-*form*

$C_{13}H_{14}N_2O_2$ 230.266
(1*R*,3*S*)-*form*
Mp 242-244° (225-228° dec.). $[\alpha]_D$ -69 (c, 1 in 1*M* HCl/MeOH 1:1).
(1*S*,3*S*)-*form*
Amorph. solid. Mp 293° (276-280° dec.). $[\alpha]_D^{25}$ -106.6 (c, 1 in 1*M* HCl/MeOH 1:1).
(1ξ,3ξ)-*form*
Widespread in many foodstuffs especially fruit juices, jams and fermented foods or beverages including beer and soy sauce. Also present in the toxic fly agaric mushroom (*Amanita muscaria*). Formed by Pictet-Spengler condensation between acetaldehyde and L-tryptophan in nature or during food processing. Needles (H_2O). Mp 290° dec. $[\alpha]_D$ -142.8 (50 % Py aq.).

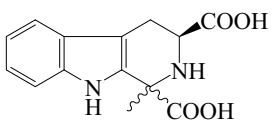
[22677-22-1]

Matsumoto, T. *et al., Helv. Chim. Acta*, 1969, **52**, 716 (*isol, uv, ir, struct*)
Brossi, A. *et al., J. Med. Chem.*, 1973, **16**, 418 (*synth, pharmacol, ord*)
Bobbitt, J.M. *et al., J.O.C.*, 1980, **45**, 1978 (*synth*)
Bosin, T.R. *et al., J. Agric. Food Chem.*, 1986, **34**, 843 (*isol*)
Herraiz, T. *et al., J. Agric. Food Chem.*, 1996, **44**, 3057-3065; 1998, **46**, 3484-3490 (*hplc, occur*)
Kicha, A.A. *et al., Tet. Lett.*, 2003, **44**, 1935-1937 (*Lethasterias alkaloid, isol, pmr, cmr*)

1,2,3,4-Tetrahydro-1-methyl-β-carboline-1,3-dicarboxylic acid T-98

[18070-61-6]

[192180-82-8, 192180-83-9]
*2,3,4,9-Tetrahydro-1-methyl-1*H*-pyrido[3,4-*b*]indole-1,3-dicarboxylic acid, 9CI. 1,2,3,4-Tetrahydroharman-1,3-dicarboxylic acid*

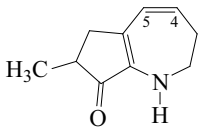


$C_{14}H_{14}N_2O_4$ 274.276
(1ξ,3*S*)-*form*
Present in fruit syrups, beer, vinegar and fermented syrups. Mp 225° dec. $[\alpha]_D^{24.6}$ -102 (c, 1 in 50% Py aq.).

Tschesche, R. *et al., Chem. Ber.*, 1958, **91**, 1732-1744 (*synth*)
Bobbitt, J.M. *et al., J.O.C.*, 1980, **45**, 1978-1984 (*synth*)
Gutsche, B. *et al., J. Agric. Food Chem.*, 1997, **45**, 2458-2462 (*isol, pmr, ms*)

2,3,6,7-Tetrahydro-7-methylcyclopent[*b*]azepin-8(1*H*)-one T-99

[97826-67-0]



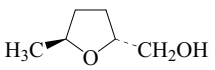
$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product with bitter taste. Present in roasted malt, wort and beer. Taste threshold 10 ppm in H_2O. Characterised spectroscopically.

4,5-Dihydro: [97826-66-9] *2,3,4,5,6,7-Hexahydro-7-methylcyclopent[b]azepin-8(1H)-one*
$C_{10}H_{15}NO$ 165.235
Proline-derived Maillard product. Mp 61-63°.

Tressl, R. *et al., Annalen*, 1985, 2017-2027 (*isol, pmr, cmr, ms*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 1132-1137; 1993, **41**, 547-553 (*isol, ms, pmr*)

Tetrahydro-5-methyl-2-furanmethanol, 9CI T-100

[6126-49-4]
2-(Hydroxymethyl)-5-methyltetrahydrofuran



(2*R*,5*S*)-*form*

$C_6H_{12}O_2$ 116.16
(2*R*,5*S*)-*form* [41869-37-8]
(+)-trans-*form*
$[\alpha]_D^{25}$ +33.7 (c, 11.5 in EtOH).
3,5-Dinitrobenzoyl:
Mp 75-76°.
(2*S*,5*S*)-*form* [41869-03-8] *(+)*-cis-*form*
$[\alpha]_D^{25}$ +11.1 (c, 9.3 in EtOH).
3,5-Dinitrobenzoyl:
Cryst. (EtOH). Mp 85-86°.
(2*RS*,5*RS*)-*form* [123931-60-2] *(±)*-cis-*form*
d_4^{25} 0.99. Bp_{14} 74°. n_D^{25} 1.4440.
(2*RS*,5*SR*)-*form* [123931-61-3] *(±)*-trans-*form*

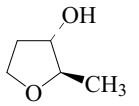
[16015-08-0, 54774-28-6, 140459-81-0, 140460-02-2]

Descotes, G. *et al., Bull. Soc. Chim. Fr.*, 1967, 2466-2472 (*synth, pmr*)
Cook, M.M. *et al., J.A.C.S.*, 1973, **95**, 3678-3686 (*synth, pmr, ir*)
Brown, H.C. *et al., J.O.C.*, 1981, **46**, 930-939 (*synth*)
Inoki, S. *et al., Chem. Lett.*, 1990, 67-70 (*synth*)
Ames, J.M. *et al., Phytochemistry*, 1990, **29**, 1201-1207 (*occur*)
Keim, W. *et al., J. High Resol. Chromatogr.*, 1991, **14**, 507-529 (*chiral glc*)

Tetrahydro-2-methyl-3-furanol, 9CI, 8CI T-101

[29848-44-0]

[20086-87-7, 20086-88-8, 50403-34-4, 114611-74-4]
3-Hydroxy-2-methyltetrahydrofuran



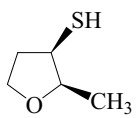
(2*R*,3*S*)-*form*

$C_5H_{10}O_2$ 102.133
Constit. of roasted peanut volatiles and cooked meat aroma model systems.
(2*R*,3*S*)-*form* [114580-34-6]
(+)-trans-*form*
$[\alpha]_D$ +29 (c, 1 in MeOH) (72% ee).
(2*RS*,3*SR*)-*form* [50403-32-2]
(±)-trans-*form*
Bp_{15} 91-92°. n_D^{20} 1.4415.

Coxon, J.M. *et al., Aust. J. Chem.*, 1973, **26**, 2521-2526 (*synth*)
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*isol, ms*)
Ho, C.-T. *et al., J. Food Sci.*, 1981, **47**, 127-133 (*occur*)
Brown, H.C. *et al., J.O.C.*, 1985, **50**, 1582-1589; 1988, **53**, 2911-2916 (*trans-form, synth, ir, pmr, cmr, ms*)
Amouroux, R. *et al., Heterocycles*, 1993, **36**, 1965-1969 (*2R,3S-form*)

Tetrahydro-2-methyl-3-furanthiol, 9CI T-102

[57124-87-5]
3-Mercapto-2-methyltetrahydrofuran



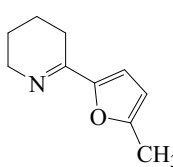
(2*RS*,3*RS*)-*form*

$C_5H_{10}OS$ 118.199
Flavour enhancer for meat-like foods.
(2*RS*,3*RS*)-*form* [26548-76-5]
(±)-cis-*form*
Bp_{13} 64-65°. n_D^{20} 1.4904.
(2*RS*,3*SR*)-*form* [26548-78-7]
(±)-trans-*form*
Bp_{20} 62°. n_D^{20} 1.4798.

Ger. Pat., 1970, 1 932 800; *CA*, **72**, 90265d (*synth, use*)
Austrian Pat., 1977, 340 748; *CA*, **88**, 120972g (*synth, use*)

2,3,4,5-Tetrahydro-6-(5-methyl-2-furanyl)pyridine T-103

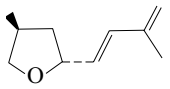
[104704-35-0]
2-(5-Methyl-2-furyl)-3,4,5,6-tetrahydropyridine



$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., Dev. Food Sci.*, 1986, **13**, 235-244 (*occur, ms, ir*)
Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 405-410 (*synth, ms, ir*)

Tetrahydro-4-methyl-2-(3-methyl-1,3-butadienyl)furan, 9CI T-104



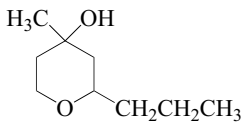
(2*R*,4*S*)-(*E*)-*form*

$C_{10}H_{16}O$ 152.236
(2*R*,4*S*,*E*)-*form* [89103-55-9]
Marmelo oxide A
Flavour component of quince fruit. Oil. $[\alpha]_D$ -33.4 (c, 0.18 in Et_2O).
(2*R*,4*R*,*E*)-*form* [89103-56-0]
Marmelo oxide B
Flavour component of quince fruit. Oil. $[\alpha]_D^{23}$ +23.5 (c, 0.15 in Et_2O).

Tsuneya, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 957 (*isol, struct*)
Nishida, Y. *et al., Agric. Biol. Chem.*, 1983, **47**, 2969 (*synth, abs config*)

Tetrahydro-4-methyl-2-propyl-2*H*-pyran-4-ol, 9CI T-105

[57094-41-4]
4-Hydroxy-4-methyl-2-propyltetrahydrofuran



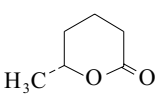
$C_9H_{18}O_2$ 158.24
Stereochem. not reported.

Ac: [131766-73-9] *Clarycet*
$C_{11}H_{20}O_3$ 200.277
Fragrance ingredient with a fruity aroma.

Arakelyan, A.S. *et al., Zh. Org. Khim.*, 1987, **23**, 2323-2326; *CA*, **109**, 22801h (*synth*)
Eur. Pat., 1990, 383 446; *CA*, **114**, 81584r (*Ac*)

Tetrahydro-6-methyl-2*H*-pyran-2-one, 9CI T-106

[823-22-3]
5-Hexanolactone. 5-Caprolactone. 5-Hydroxyhexanoic acid lactone. 5-Hexanolide. 5-Methyl-δ-valerolactone. Dihydrosorbinol. δ-Hexalactone. FEMA 3167



(*R*)-*form*

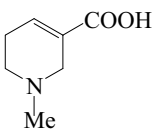
$C_6H_{10}O_2$ 114.144
Isol. from coconut oil (*Cocos nucifera*), heated milk fat, butter, chicken fat and yoghurt. Also in various fruits e.g. papaya, pineapple, raspberry, strawberry and plums.
(*R*)-*form* [43112-32-9]
Mp 22-24°. Bp_3 85-90°. $[\alpha]_D^{20}$ +37.2 (c, 1.825 in EtOH).
(*S*)-*form* [16320-13-1]
Mp 31°. $Bp_{11.5}$ 103-104° (lit. gives a pressure range). $[\alpha]_D^{19}$ -51 (EtOH). n_D^{22} 1.4426.
(±)-*form* [26991-67-3]
Flavour ingredient. Needles. Misc. H_2O.

Mp 17-19°. Bp 230-231° Bp_5 100-100.5°. Polymerises on standing.

Kuhn, R. *et al., Chem. Ber.*, 1962, **95**, 2009 (*abs config*)
Allen, R.R. *et al., Chem. Ind. (London)*, 1965, 1560 (*isol*)
Parliment, T.H. *et al., Chem. Ind. (London)*, 1966, 1845 (*synth*)
Taub, D. *et al., Tetrahedron*, 1968, **24**, 2443 (*synth*)
Sturtz, G. *et al., Tet. Lett.*, 1976, 47 (*synth*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 707 (*rev, tox*)
Seebach, D. *et al., Helv. Chim. Acta*, 1985, **68**, 2342 (*synth, ir, pmr*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 541 (*synth, uv, pmr, isomers*)
Giese, B. *et al., J.O.C.*, 1986, **51**, 3726 (*synth*)
White, J.D. *et al., J.A.C.S.*, 1995, **117**, 1908 (*synth, ir, pmr, cmr, bibl*)
Ljubovic, E. *et al., Synthesis*, 2001, 423-426 (*R-form, synth*)

1,2,5,6-Tetrahydro-1-methyl-3-pyridinecarboxylic acid, 9CI T-107

[499-04-7]
Arecaidine. *Arecaine*



$C_7H_{11}NO_2$ 141.169
Alkaloid from nuts of *Areca catechu* (betel nuts). Mp 223-224° dec. (anhyd. 232° dec.). pK_a 9.07 (25°). Log P -1.74 (calc). Strong base.
▶ QT2070800

Hydrochloride:
Mp 262-263° (rapid heat) (250.5-262°).

Me ester: [63-75-2] ***Arecoline***
$C_8H_{13}NO_2$ 155.196
Isol. from betel nuts. Liq. Bp_{17} 94° Bp_7 74°. pK_a 7.64 (25°). Log P 1.05 (calc).
▶ LD_{50} (dog, scu) 5 mg/kg. LD_{50} (rat, orl) 2500 mg/kg. QT2100000

Me ester, hydrochloride: [61-94-9]
Mp 157-158°.
▶ QT2150000

Me ester, hydrobromide: [300-08-3]
Mp 172°.
▶ QT2275000

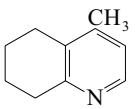
Et ester: [28125-84-0]

[6027-10-7, 17210-50-3] ***Homoarecoline***
$C_9H_{15}NO_2$ 169.223
Isol. from betel nuts. Oil.

Jahns, E. *et al., Ber.*, 1888, **21**, 3404 (*isol*)
Wohl, A. *et al., Ber.*, 1907, **40**, 4712 (*struct, synth*)
Chemnitius, F. *et al., J. Prakt. Chem.*, 1927, **117**, 147 (*isol, deriv*)
Mannich, C. *et al., Ber.*, 1942, **75**, 1480 (*synth*)
Lyle, R.E. *et al., J.O.C.*, 1955, **20**, 1761 (*synth, uv*)
Ma, J.C.N. *et al., Can. J. Chem.*, 1965, **43**, 1849 (*pmr*)
Spiteller-Friedmann, M. *et al., Monatsh. Chem.*, 1965, **96**, 104 (*ms*)
Nery, R. *et al., Biochem. J.*, 1971, **122**, 503 (*metab, tox, bibl*)
Burrows, R.B. *et al., Prog. Drug Res.*, 1973, **17**, 108 (*rev*)
Kozello, I.A. *et al., Khim.-Farm. Zh.*, 1979, **13**, 61; *CA*, **92**, 110798y (*synth*)
Strunz, G.M. *et al., Alkaloids (N.Y.)*, 1985, **26**, 89 (*rev*)
Hollander, E. *et al., Br. Med. Bull.*, 1986, **42**, 97 (*pharmacol*)
Kurihara, T. *et al., Heterocycles*, 1990, **30**, 885-896 (*Et ester, synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 39
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQT625; AQU000; AQU250; AQT750

5,6,7,8-Tetrahydro-4-methylquinoline T-108

[28971-03-1]
5,6,7,8-Tetrahydrolepidine



$C_{10}H_{13}N$ 147.219
Alkaloid from the roots of *Glycyrrhiza uralensis* (Chinese licorice). Liq. Spar. sol. H_2O. Bp_{11} 122°.

Hydrochloride:
Mp 203-204°.

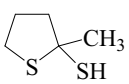
Picrate: [60166-61-2]
Mp 178-181° (170°).

Methiodide:
Mp 183°.

v. Braun, J. *et al., Ber.*, 1923, **56**, 1343 (*synth*)
Booth, H. *et al., J.C.S. Perkin 2*, 1976, 759 (*pmr*)
Reimann, E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 210 (*synth*)
Koyama, J. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2601 (*synth*)
Konno, K. *et al., Tet. Lett.*, 1986, **27**, 3865 (*synth*)
Murahashi, S.-I. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 2968 (*synth*)
Han, Y.N. *et al., Arch. Pharmacal Res.*, 1990, **13**, 101; *CA*, **113**, 227984 (*isol*)

Tetrahydro-2-methyl-2-thiophenethiol, 9CI T-109

[62308-60-5]
2-Mercapto-2-methyltetrahydrothiophene



$C_5H_{10}S_2$ 134.266
Component of cooked meat aroma model systems. Characterised spectroscopically.

Ger. Pat., 1975, 2 624 696; *CA*, 139836w (*synth, use*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, isol, pmr, ms*)

Tetrahydro-2-methyl-3-thiophenethiol, 9CI T-110

[57067-07-9]

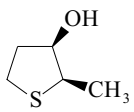
[26548-79-8, 26548-80-1]
3-Mercapto-2-methyltetrahydrothiophene

$C_5H_{10}S_2$ 134.266
Present as a mixt. of *cis*- and *trans* isomers in meat aroma model systems. Possesses a meaty, savoury odour. Characterised spectroscopically.

Ger. Pat., 1970, 1 932 800; *CA*, **72**, 90265d (*synth, use*)
Van den Ouweland, G.A.M. *et al., J. Agric. Food Chem.*, 1975, **23**, 501-505 (*occur, ms, ir*)

Tetrahydro-2-methylthiophen-3-ol T-111

Tetrahydro-3-hydroxy-2-methylthiophene



(2R,3R)-form

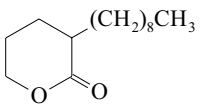
$C_5H_{10}OS$ 118.199
Found in wine. Compd. responsible for "off" taste in some wines. All four opt. active forms and both racemates obt. and characterised spectroscopically.

[121054-77-1, 121054-78-2, 121153-33-1, 121249-25-0]

Mosandl, A. *et al., Annalen*, 1989, 859 (*synth, resoln, pmr, ms*)

Tetrahydro-3-nonyl-2*H*-pyran-2-one, 9CI T-112

[77488-49-4]

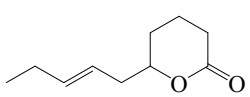


$C_{14}H_{26}O_2$ 226.358
(ξ)-*form*
Present in aroma of date palm fruit (*Phoenix dactylifera*).

Kikuchi, N. *et al., Mikrochim. Acta*, 1981, **1**, 249

Tetrahydro-6-(2-pentenyl)-2*H*-pyran-2-one, 9CI T-113

[34686-71-0]
7-Decen-5-olide. 5-Hydroxy-7-decenoic acid lactone. ***Jasmine lactone***†. *2-Pentenyltetrahydro-α-pyrone. δ-Jasmolactone*



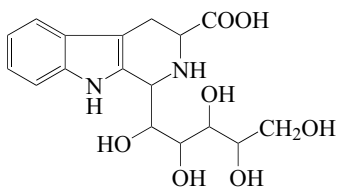
$C_{10}H_{16}O_2$ 168.235
(-)-(*Z*)-*form* [25524-95-2]
FEMA 3745
Flavouring ingredient. Present in peppermint oil and various types of tea. $Bp_{0.3}$ 95-96.5°. $[\alpha]_D^{16}$ -30.4 (neat). $n_D^{14.9}$ 1.4773.

p-*Bromobenzylisothiouronium salt:*
Mp 120-120.5°.
(±)-(*Z*)-*form* [66972-29-0]
$Bp_{0.001}$ 70-73°. $n_D^{22.5}$ 1.4751.
Winter, M. *et al., Helv. Chim. Acta*, 1962, **45**, 1250 (*isol*)

Demole, E. *et al., Helv. Chim. Acta*, 1962, **45**, 1256 (*synth*)
Ijima, A. *et al., Chem. Pharm. Bull.*, 1972, **20**, 197 (*synth*)
de Clercq, P. *et al., Bull. Soc. Chim. Belg.*, 1978, **87**, 495 (*synth*)
Dubs, P. *et al., Helv. Chim. Acta*, 1978, **61**, 998 (*isol*)
Yamanishi, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 2139 (*isol*)
Naoshima, Y. *et al., Agric. Biol. Chem.*, 1981, **45**, 2639 (*synth*)
Fehr, C. *et al., Helv. Chim. Acta*, 1981, **64**, 1247 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 362
Haffner, T. *et al., Helv. Chim. Acta*, 1996, **79**, 2088 (*biosynth, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1368-1369

Tetrahydropentoxyline T-114

[154204-09-8]
1-C-*(3-Carboxy-2,3,4,9-tetrahydro-1*H-*pyrido[3,4-*b*]indol-1-yl)pentitol, 9CI. 1,2,3,4-Tetrahydro-1-(1,2,3,4,5-pentahydroxypentyl)-β-carboline-3-carboxylic acid*

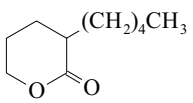


$C_{17}H_{22}N_2O_7$ 366.37
Isol. from various fruit juices and jams. The fruit juice isolate Charactised as two stereoisomers having *cis*- and *trans*-stereochem. at the tetrahydrocarboline ring, but with undetermined pentitol config..

Horiuchi, K. *et al., J. Biochem. (Tokyo)*, 1994, **115**, 362-366 (*isol, pmr, cmr*)
Herraiz, T. *et al., J. Agric. Food Chem.*, 2002, **50**, 4690-4695 (*isol, pmr, cmr, ms*)

Tetrahydro-3-pentyl-2*H*-pyran-2-one, 9CI T-115

[32821-72-0]



$C_{10}H_{18}O_2$ 170.251
(ξ)-*form*
Present in aroma of date palm fruit (*Phoenix dactylifera*).

Sarkisyan, P.A. *et al., Arm. Khim. Zh.*, 1971, **24**, 245 (*synth*)
Kurata, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 538 (*synth*)
Kikuchi, N. *et al., Mikrochim. Acta*, 1981, **1**, 249 (*occur*)

Tetrahydro-6-pentyl-2*H*-pyran-2-one, 9CI T-116

[705-86-2]
δ-Decalactone. 5-Decanolide. 5-Hydroxydecanoic acid lactone. FEMA 2361

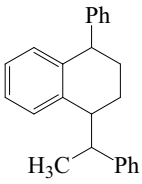
$C_{10}H_{18}O_2$ 170.251
Present in coconut oil, butter oil, apricots, peaches, cheese, cane sugar, pork fat, margarine, lavender oil, and other substances. Fragrance raw material and flavouring agent. Oil with peach odour and taste. Low oral toxicity.
▶ Eye and skin irritant. UQ1355000
(*R*)-*form* [2825-91-4]
Liq. Bp_5 160-170°. $[\alpha]_D$ +48.2 (c, 3.69 in MeOH). $[\alpha]_D$ +60.2 (c, 1.74 in THF).
(*S*)-*form* [59285-67-5]
Liq. $[\alpha]_D$ -60.2.
(±)-*form* [35221-79-5]
Liq. Mp -27°. Bp_3 121-122°. n_D^{25} 1.4550. n_D^{25} 1.4675.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1152B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 756A (*ir*)
Meijer, T.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1940, **59**, 191 (*synth*)
Crombie, L. *et al., J.C.S.*, 1955, 1007 (*synth*)
Allen, R.R. *et al., Chem. Ind. (London)*, 1965, 1560 (*isol, ir*)
Parliemerit, T.H. *et al., Chem. Ind. (London)*, 1966, 1845 (*synth, ir*)
Lardelli, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 481 (*synth*)
Kohver, O. *et al., Tetrahedron*, 1970, **26**, 2391 (*abs config, ord, cd*)
Ijima, A. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1053; 1972, **20**, 197; 1973, **21**, 215 (*synth*)
Tahara, S. *et al., Agric. Biol. Chem.*, 1975, **39**, 281 (*isol*)
Pyysalo, H. *et al., Finn. Chem. Lett.*, 1975, 129; 136 (*synth, cmr, ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 739 (*rev, tox*)
Kaiser, R. *et al., Tet. Lett.*, 1976, 1659 (*isol, struct*)
Bacardit, R. *et al., J. Chem. Ecol.*, 1983, **9**, 703 (*synth, props*)
Griese, B. *et al., Chem. Ber.*, 1984, **117**, 859 (*synth*)
Francotte, E. *et al., Helv. Chim. Acta*, 1987, **70**, 1569 (*resoln*)
Utaka, M. *et al., J.O.C.*, 1987, **52**, 4363 (*synth*)
Gessner, M. *et al., Z. Naturforsch., C*, 1987, **42**, 1159 (*synth*)
Mosandl, A. *et al., Z. Lebensm.-Unters. -Forsch.*, 1988, **187**, 40 (*synth, props*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, DAF200
Inokouchi, T. *et al., J.O.C.*, 1990, **55**, 462 (*synth*)
Fronza, G. *et al., J.C.S. Perkin 1*, 1991, 2977 (*synth*)
Cardillo, R. *et al., J.O.C.*, 1991, **56**, 5237 (*synth*)
Albrecht, W. *et al., J.O.C.*, 1992, **57**, 1954 (*synth*)
Parker, S.R. *et al., J. Agric. Food Chem.*, 1997, **45**, 2774-2776 (*activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAF200

1,2,3,4-Tetrahydro-1-phenyl-4-(1-phenylethyl)naphthalene, 9CI T-117

[26681-79-8]

[233748-71-5, 233748-72-6, 233748-73-7, 233748-74-8]
1-Phenyl-4-(1-phenylethyl)tetralin



$C_{24}H_{24}$ 312.454
Packaging migration residue. $Bp_{10.3}$ 190-200°. Bp. data refers to mixed stereoisomers. Individual stereoisomers have been characterised spectroscopically and are comly. available.
▶ Shows *in vitro* estrogenic activity.

Kauffman, H.F. *et al., Makromol. Chem.*, 1979, **180**, 2649-2663; 2681-2693 (*ms*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; 390-398; *CA*, **129**, 42008w; **130**, 251409 (*anal*)
Moriguchi, K. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1999, **48**, 623-629; *CA*, **131**, 129609h (*isol, conformn, pmr, cmr*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox, bibl*)

1,2,3,4-Tetrahydro-1-phenyl-4-(2-phenylethyl)naphthalene, 9CI T-118

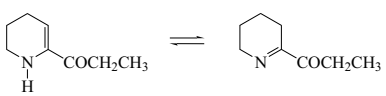
[40542-33-4]
1-Phenyl-4-(2-phenylethyl)tetralin

$C_{24}H_{24}$ 312.454
Packaging migration residue.
(1*RS*,4*RS*)-*form* [304641-44-9]
(±)-trans-*form*Characterised spectroscopically.
(1*RS*,4*SR*)-*form* [304641-43-8]
(±)-cis-*form*Characterised spectroscopically.

Wiesner, J. *et al., Makromol. Chem.*, 1973, **165**, 1-9
Yamada, T. *et al., Bunseki Kagaku (Jpn. Anal.)*, 2000, **49**, 493-501; 857-868; *CA*, **133**, 330626w; **134**, 146562s (*occur, synth, tox*)
Japan. Pat., 2000, 327 597; *CA*, **134**, 4774p (*synth, pmr*)

1,2,3,4-Tetrahydro-6-propanoylpyridine T-119

[80933-74-0, 80933-75-1]
1-(1,4,5,6-Tetrahydro-2-pyridinyl)-1-propanone, 9CI. 1-(3,4,5,6-Tetrahydro-2-pyridinyl)-1-propanone, 9CI. 2-Propionyltetrahydropyridine. PTP



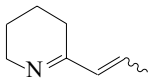
$C_8H_{13}NO$ 139.197
Tautomeric. Formed by thermal treatment of proline and glucose mixtures. Liq. with intense roast-smelling odour. Bp_7 71-76°.

De Kimpe, N. *et al., J. Agric. Food Chem.*, 1996, **44**, 1515-1519 (*synth, pmr*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 2721-2726 (*occur, ms*)

2,3,4,5-Tetrahydro-6-(1-propenyl)pyridine T-120

[16543-92-3]

[16543-93-4]
2-(1-Propenyl)-Δ¹-piperideine



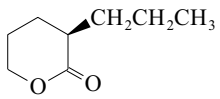
$C_8H_{13}N$ 123.197

Incorr. named as 2-(2-propenyl)-Δ¹-piperideine in the lit.. Isol. from pomegranate (leaves). Cryst. (as hydrochloride). Mp 112-114° (hydrochloride). Unstable, only obt. from fresh extracts. Hydrochloride dec. in moist air.

Roberts, M.F. *et al., Phytochemistry*, 1967, **6**, 711 (*isol, ir, pmr, struct*)

Tetrahydro-3-propyl-2*H*-pyran-2-one, 9CI T-121

[22791-77-1]
2-Propylvalerolactone



(*R*)-*form*

$C_8H_{14}O_2$ 142.197

(*R*)-*form* [73746-80-2]
Liq. Bp_{12} 115-120°. $[\alpha]_D^{23}$ -47 (c, 2.98 in MeOH).

(±)-*form*
Liq. d_4^{20} 0.99. Bp_{10} 118-120°. n_D^{20} 1.4585.

(ξ)-*form*
Detected in date aroma (*Phoenix dactylifera*).

Sarkisyan, P.A. *et al., Arm. Khim. Zh.*, 1971, **24**, 245 (*synth*)
Kurata, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 538 (*synth*)
Meyers, A.I. *et al., J.O.C.*, 1980, **45**, 2792 (*synth, ir, pmr*)
Kikuchi, N. *et al., Mikrochim. Acta*, 1981, **1**, 249 (*occur*)

Tetrahydro-6-propyl-2*H*-pyran-2-one, 9CI T-122

[698-76-0]
δ-Octalactone. 5-Octanolide. 5-Hydroxyoctanoic acid lactone. FEMA 3214

$C_8H_{14}O_2$ 142.197

► UQ1355500

(*R*)-*form* [108943-45-9]
Bp_{18} 130-140°. $[\alpha]_D^{20}$ +58.4 (c, 2.2 in MeOH). $[\alpha]_D$ +66.5 (c, 1.7 in THF).

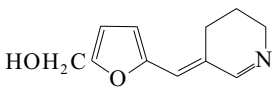
(*S*)-*form* [108943-46-0]
Bp_2 70-80°. $[\alpha]_D^{25}$ -58.8 (c, 1 in THF).

(±)-*form* [104426-32-6]
Liq. Mp -13°. Bp_{15} 126°. n_D^{25} 1.4535. n_D^{25} 1.4527. n_D^{25} 1.4700.

(ξ)-*form*
Used in food flavouring. Isol. from many substances incl. coconut and butter oils, fruits (e.g. strawberry, pineapple) and cooked meats.

Lukes, R. *et al., Coll. Czech. Chem. Comm.*, 1959, **24**, 2722 (*synth*)
Allen, R.R. *et al., Chem. Ind. (London)*, 1965, 1560 (*isol, ir*)
Parliment, T.H. *et al., Chem. Ind. (London)*, 1966, 1845 (*synth*)
Landelli, G. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 481 (*synth*)
Lamberti, V. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1967, **86**, 504 (*synth*)
Ansell, M.F. *et al., J.C.S.(C)*, 1968, 217 (*synth*)
Ijima, A. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1053; 1973, **21**, 215 (*synth*)
Pyssalo, H. *et al., Finn. Chem. Lett.*, 1975, 129; 136 (*synth, pmr, cmr, ms*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 783 (*rev, tox*)
Giese, B. *et al., Chem. Ber.*, 1984, **117**, 859 (*synth*)
Utaka, M. *et al., J.O.C.*, 1987, **52**, 4363 (*synth, ir, pmr*)
Cardillo, R. *et al., J.O.C.*, 1989, **54**, 4979 (*biosynth*)
Aquino, M. *et al., Tetrahedron*, 1991, **47**, 7887 (*synth*)
Huffer, M. *et al., Tetrahedron: Asymmetry*, 1991, **2**, 1157 (*resoln*)
Tsantrizos, Y.S. *et al., J.O.C.*, 1995, **60**, 6922 (*pmr, cmr*)

5-(3,4,5,6-Tetrahydro-3-pyridylidenemethyl)-2-furanmethanol T-123



$C_{11}H_{13}NO_2$ 191.229

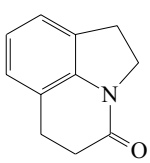
(*E*)-*form*
Prod. of reacn. between glucose and lysine in sl. acid soln.. Cryst. (toluene). Mp 104-105°.

Picrate:
Mp 162-165.5°.

Miller, R. *et al., Acta Chem. Scand., Ser. B*, 1984, **38**, 689; 1987, **41**, 208 (*isol, ms, pmr, synth, cryst struct*)

1,2,5,6-Tetrahydro-4*H*-pyrrolo[3,2,1-*ij*]quinolin-4-one, 9CI T-124

[57369-32-1]
Pyroquilon, BSI, ISO. 4-Oxolilidine. Fongoren



$C_{11}H_{11}NO$ 173.214

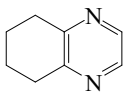
Fungicide against rice blast disease. Needles (EtOH/petrol). Mp 112-113°.

► LD_{50} (rat, orl) 321 mg/kg. UY9480000

Bass, R.J. *et al., J. Agric. Food Chem.*, 1981, **29**, 576 (*synth, use*)
Crabb, T.A. *et al., Tetrahedron*, 1986, **42**, 5407 (*synth*)
Somei, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3146 (*synth, ir, pmr, ms*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A984
Pesticide Manual, 11th edn., 1997, No. 633

5,6,7,8-Tetrahydroquinoxaline T-125

[34413-35-9]
FEMA 3321



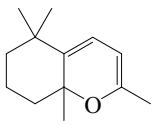
$C_8H_{10}N_2$ 134.18

Flavour ingredient. Present in wheat bread, cocoa, coffee, roasted filbert, roasted peanut, pork and roasted sesame. Mp 29-30°. Bp 108-111°. n_D^{48} 1.6231.

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **3**, 400C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1558A (*ir*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 273 (*ir, nmr, ms*)

6,7,8,8*a*-Tetrahydro-2,5,5,8*a*-tetramethyl-5*H*-1-benzopyran, 9CI T-126

[5552-30-7]
Cycloionone. FEMA 3822



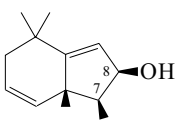
$C_{13}H_{20}O$ 192.3

Present in cognac. Food flavouring ingredient. Bp_1 70-71° $Bp_{0.1}$ 42-45°. n_D^{25} 1.4992.

Buchi, G. *et al., J.A.C.S.*, 1957, **79**, 2318-2323 (*synth, pmr*)
Kurata, S. *et al., J.C.S. Perkin 1*, 1976, 532-535 (*synth, ir, uv, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 370 (*use*)

2,4,5,7*a*-Tetrahydro-1,4,4,7*a*-tetramethyl-1*H*-inden-2-ol, 9CI T-127

[99901-23-2]
2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4-dien-8-ol



$C_{13}H_{20}O$ 192.3

Constit. of quince fruit flavour (*Cydonia oblonga*). Oil. $[\alpha]_D^{26}$ -40 (c, 0.67 in MeOH).

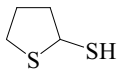
8-Ketone: [99901-22-1] *1,4,5,7a-Tetrahydro-1,4,4,7a-tetramethyl-2H-inden-2-one, 9CI. 2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4-dien-8-one*
$C_{13}H_{18}O$ 190.285
From quince (*Cydonia oblonga*). Oil. $[\alpha]_D^{26}$ +11 (c, 0.2 in MeOH).

7α-Hydroxy: [99901-24-3] *2,4,5,7a-Tetrahydro-1,4,4,7a-tetramethyl-1H-indene-1,2-diol, 9CI. 2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4-diene-7,8-diol*
$C_{13}H_{20}O_2$ 208.3
From quince (*Cydonia oblonga*). Oil. $[\alpha]_D^{26}$ -6 (c, 0.35 in MeOH).

Ishihara, M. *et al., J.O.C.*, 1986, **51**, 491

Tetrahydro-2-thiophenethiol, 9CI T-128

[61477-08-5]
2-Mercaptotetrahydrothiophene



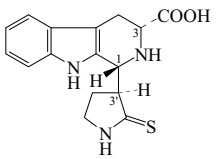
$C_4H_8S_2$ 120.239

(±)-*form*
Bp_{15} 135°.

(ξ)-*form*
Component of meat aroma model systems.

Gais, H.J. *et al., Angew. Chem., Int. Ed.*, 1977, **89**, 201-202 (*synth, pmr, ms*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, ms, pmr*)

1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-β-carboline-3-carboxylic acid T-129



(1*R**,3*R**,3'*S**)-*form*

$C_{16}H_{17}N_3O_2S$ 315.395

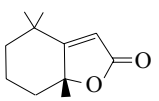
(1*R*,3*R*,3′*S*)-*form*
Alkaloid from fermented radish roots.

(1*R*,3*S*,3′*R*)-*form*
Alkaloid from fermented radish roots.

Ozawa, Y. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 216-219

5,6,7,7*a*-Tetrahydro-4,4,7*a*-trimethyl-2(4*H*)-benzofuranone, 9CI T-130

[15356-74-8]
2-Hydroxy-2,6,6-trimethylcyclohexylidene-1-acetic acid lactone. ***Dihydroactinidiolide***



(*R*)-*form*

$C_{11}H_{16}O_2$ 180.246
Has been isolated from tea, coffee and fruits. An important aroma constit. of tea. The prod. from plant sources is largely racemic (from tobacco (*R*)-isomer of 30% ee, from *A. polygama* (*S*)-isomer of 6% ee).

(*R*)-*form* [38273-56-2]
Mp 41° Mp 69-71°. $[\alpha]_D^{20}$ -119.9 (c, 0.01 in $CHCl_3$).

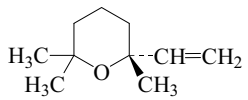
(*S*)-*form* [17092-92-1]
Mp 71-72° (40-41°). $[\alpha]_D^{15}$ +7.1 (natural). $[\alpha]_D^{22}$ +122.7 ($CHCl_3$) (synthetic). Not active as a fire ant pheromone.

(±)-*form* [19432-05-4]
Cryst. (Et_2O/petrol at -15°). Mp 42°. $Bp_{0.001}$ 90°.

Mousseron-Canet, M. *et al., Bull. Soc. Chim. Fr.*, 1967, 608 (*synth*)
Sakan, T. *et al., Tet. Lett.*, 1967, 1623 (*isol, synth*)
Isoe, S. *et al., Tet. Lett.*, 1972, 2517 (*abs config*)
Eschenmoser, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1722 (*synth*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1978, **61**, 2616 (*synth*)
Chakraborty, T.K. *et al., Tet. Lett.*, 1984, **25**, 2895 (*synth*)
Mori, K. *et al., Tetrahedron*, 1986, **42**, 283 (*synth*)
Cain, C.M. *et al., Tet. Lett.*, 1987, **28**, 3723 (*synth*)
Subbaraju, G.V. *et al., Tet. Lett.*, 1991, **32**, 4871 (*synth*)
Mori, K. *et al., Annalen*, 1993, 77 (*synth*)
Irie, O. *et al., Chem. Lett.*, 1995, 53 (*synth*)

Tetrahydro-2,2,6-trimethyl-6-vinylpyran, 8CI T-131

[7392-19-0]
2-Ethenyltetrahydro-2,6,6-trimethylpyran, 9CI. 2,2,6-Trimethyl-6-vinyltetrahydropyran. Linaloyl oxide. FEMA 3735



(*R*)-*form*

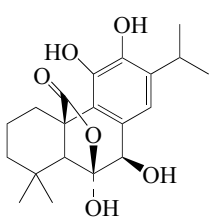
$C_{10}H_{18}O$ 154.252
Flavouring and fragrence ingredient. Present in roselle tea, muscat grapes, lime oil, alfalfa, Riesling wine, grapefruit, yellow passion fruit, apricot, blackberry, blueberry, nectarine, cherimoya, papaya and curuba fruits. Liq. with musty, earthy, terpineolic odour.

(*R*)-*form* [13226-34-1]
d_{20}^{20} 0.88. $[\alpha]_D^{20}$ +5.7 ($CHCl_3$ or EtOH). n_D^{20} 1.4479.

(±)-*form* [13837-56-4]
d_4^{25} 0.87. $Bp_{2.5}$ 22°. n_D^{25} 1.4490.

Strickler, H. *et al., Helv. Chim. Acta*, 1966, **49**, 2157-2161 (*R-form, synth, abs config*)
Torii, S. *et al., J.O.C.*, 1974, **39**, 3645-3648 (*synth*)
Audin, P. *et al., Bull. Soc. Chim. Fr.*, Part II, 1984, 297-306 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 777 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2849 (*occur, props*)
Dugo, P. *et al., Flavour Fragrance J.*, 1998, **13**, 93-97 (*glc, detn, lime oil*)
Werkhoff, P. *et al., J. Agric. Food Chem.*, 1998, **46**, 1076-1093 (*occur*)
Chen, S.-H. *et al., J. Agric. Food Chem.*, 1998, **46**, 1101-1105 (*glc, detn, roselle tea*)

6,7,11,12-Tetrahydroxy-8,11,13-abietatrien-20,6-olide T-132



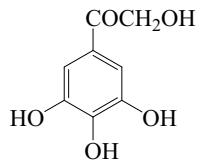
$C_{20}H_{26}O_6$ 362.422

(6α*OH*,7β)-*form*
6,7-Di-Me ether: [194425-48-4] ***6,7-Di-methoxy-7-epirosmanol***
$C_{22}H_{30}O_6$ 390.475
Constit. of *Salvia officinalis* (sage). Yellow cryst. Mp 183-188°. $[\alpha]_D^{25}$ -30 (c, 0.02 in $CHCl_3$).

Tada, M. *et al., Phytochemistry*, 1997, **45**, 1475-1477 (*isol, pmr, cmr*)

2,3′,4′,5′-Tetrahydroxyacetophenone T-133

2-Hydroxy-1-(3,4,5-trihydroxyphenyl)ethanone, 9CI. 3,4,5-Trihydroxyphenacyl alcohol



$C_8H_8O_5$ 184.148

Tetra-Ac:
$C_{16}H_{16}O_9$ 352.297
Cryst. (EtOH). Mp 124-125°.

α-Me ether, tri-Ac:
$C_{15}H_{16}O_8$ 324.287
Cryst. (EtOH). Mp 132-133°.

3′,5′-Di-Me ether: [90426-22-5] *2,4′-Dihydroxy-3′,5′-dimethoxyacetophenone. α-Hydroxyacetosyringone.* ***Danielone***
$C_{10}H_{12}O_5$ 212.202
Phytoalexin isol. from the fruits of papaya (*Carica papaya*). Powder. Mp 145°. λ_{max} 227 ; 298 (MeOH).

Tetra-Me ether:2,3′,4′,5′-Tetramethoxyacetophenone
$C_{12}H_{16}O_5$ 240.255
Needles (C_6H_6/petrol). Mp 54°. Bp_{15} 212°.

Pratt, D.D. *et al., J.C.S.*, 1925, 166
Levy, L.F. *et al., J.C.S.*, 1931, 2701
Reynolds, T.M. *et al., J.C.S.*, 1934, 1039
Echeverri, F. *et al., Phytochemistry*, 1997, **44**, 255 (*Danielone*)
Luis, J.G. *et al., J. Chem. Res., Synop.*, 1999, 220-221 (*Danielone, synth*)

2′,3′,4′,6′-Tetrahydroxyacetophenone T-134

[63635-39-2]
1-(2,3,4,6-Tetrahydroxyphenyl)ethanone, 9CI

$C_8H_8O_5$ 184.148
Pale yellow needles (EtOH or AcOH aq.). Mp 236-238° (204-205°).

Phenylhydrazone:
Red prismatic needles. Mp 248-251° dec.

2′-O-β-D-Glucopyranoside: [116964-03-5] ***Lalioside***
$C_{14}H_{18}O_{10}$ 346.29
Amorph. powder. $[\alpha]_D^{23}$ +62.5 (c, 0.8 in MeOH).

3′-O-β-D-Glucopyranoside: [110906-84-8] ***Polygoacetophenoside***
$C_{14}H_{18}O_{10}$ 346.29
Plates (EtOH). Mp 214-216°.

6′-Me ether, 3′-O-β-D-glucopyranoside: [241814-63-1]

$C_{15}H_{20}O_{10}$ 360.317
Constit. of *Crocus sativus* (saffron). Needles. Mp 188-189°. $[\alpha]_D$ +83.5 (c, 0.08 in MeOH).

3′,4′,6′-Tri-Me ether: [7507-98-4] *2′-Hydroxy-3′,4′,6′-trimethoxyacetophenone*
$C_{11}H_{14}O_5$ 226.229
Prisms (MeOH aq.). Mp 112-113° (110-112°). λ_{max} 212 (ϵ 11700); 232 (ϵ 7900); 285 (ϵ 12140); 328 (ϵ 2680) (EtOH) (Berdy).

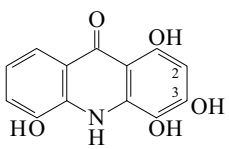
Tetra-Me ether: [7508-05-6] *2′,3′,4′,6′-Tetramethoxyacetophenone*
$C_{12}H_{16}O_5$ 240.255
Needles (EtOH). Mp 53-54°. Bp 310°.

4′-O-(3-Methyl-2-butenyl), 2′,6′-di-Me ether:3-Hydroxy-2′,6-dimethoxy-4′-prenyloxyacetophenone. 1-Acetyl-3-hydroxy-4-isopentenyl-2,6-dimethylphloroglucinol
$C_{15}H_{20}O_5$ 280.32
Viscous oil.

[116964-20-6]

Bargellini, G. *et al., Gazz. Chim. Ital.*, 1911, **41**, 18; 1919, **49**, 47; 1934, **64**, 192
Nierenstein, M. *et al., J.C.S.*, 1917, **111**, 4
Morita, N. *et al., Yakugaku Zasshi*, 1968, **88**, 1214; *CA*, **70**, 26401 (*isol, deriv*)
Obara, H. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 3627 (*synth, pmr, derivs*)
De Pascual Teresa, J. *et al., Phytochemistry*, 1982, **21**, 791 (*deriv*)
Yoshizaki, M. *et al., Planta Med.*, 1987, **53**, 273 (*Polygoacetophenoside*)
Takeda, Y. *et al., J. Nat. Prod.*, 1988, **51**, 725 (*Lalioside*)
Lorimer, S.D. *et al., Planta Med.*, 1994, **60**, 386 (*deriv*)
Rycroft, D.S. *et al., Phytochemistry*, 1998, **48**, 1351-1356 (*isol, derivs*)
Gao, W.-Y. *et al., Planta Med.*, 1999, **65**, 425-427 (*6′-Me 3′-glucoside*)

1,3,4,5-Tetrahydroxyacridone T-135



$C_{13}H_9NO_5$ 259.218

4-Me ether, N-*Me:* [86680-33-3] *1,3,5-Trihydroxy-4-methoxy-10-methylacridone.* ***Citrusinine II***
$C_{15}H_{13}NO_5$ 287.271
Alkaloid from the root bark of *Citrus sinensis* var. *brasiliensis* (navel orange). Yellow needles (Me_2CO). Mp 244-246°.

3,4-Di-Me ether, N-*Me:* [86680-32-2] *1,5-Dihydroxy-3,4-dimethoxy-10-methylacridone.* ***Citrusinine I***
$C_{16}H_{15}NO_5$ 301.298
Alkaloid from the root bark of *Citrus sinensis* var. *brasiliensis* (navel orange) and *Citrus grandis* (pummelo). Orange needles (Me_2CO). Mp 206-207°. λ_{max} 222 ; 265 ; 319 ; 331 ; 416 (EtOH) (Berdy).

Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1983, **31**, 901 (*isol, uv, ir, pmr, cmr, ms, struct*)
Wu, T.-S. *et al., Phytochemistry*, 1983, **22**, 1493 (*isol*)
Kato, N. *et al., Chem. Pharm. Bull.*, 1993, **41**, 445 (*synth, Citrusinine I*)

1,3,5,6-Tetrahydroxyacridone T-136

$C_{13}H_9NO_5$ 259.218

5-Me ether, N-*Me:1,3,6-Trihydroxy-5-methoxy-10-methylacridine.* ***Grandisine III***
$C_{15}H_{13}NO_5$ 287.271
Alkaloid from roots of several hybrid seedlings resulting from a cross of Pummelo (*Citrus grandis* cv. May Pummelo x Marsh grapefruit (*Citrus paradisi*)) (Rutaceae). Yellow amorph. powder.

3,5-Di-Me ether: [96910-77-9] *1,6-Dihydroxy-3,5-dimethoxyacridone.* ***Natsucitrine I***. *Des*-N-*methylcitpressine I*
$C_{15}H_{13}NO_5$ 287.271
Light yellow prisms (MeOH). Mp 292-293°.

3,5-Di-Me ether, N-*Me:* [81525-58-8] *1,6-Dihydroxy-3,5-dimethoxy-10-methylacridone.* ***Citpressine I***
$C_{16}H_{15}NO_5$ 301.298
Alkaloid from the root of bark of *Citrus depressa* (Shekwasha mandarin). Yellow needles + ½ H_2O (Me_2CO). Mp 183-185°.

3,6-Di-Me ether, N-*Me:* [87959-97-5] *1,5-Dihydroxy-3,6-dimethoxy-10-methylacridone.* ***Grandisine I***
$C_{16}H_{15}NO_5$ 301.298
Pale yellow needles (Me_2CO). Mp 262-264°.

5,6-Di-Me ether, N-*Me:* [87959-99-7] *1,3-Dihydroxy-5,6-dimethoxy-10-methylacridone.* ***Grandisine II***
$C_{16}H_{15}NO_5$ 301.298
Yellow needles (Me_2CO). Mp 266-268°.

3,5,6-Tri-Me ether: [96910-78-0] *1-Hydroxy-3,5,6-trimethoxyacridone.* ***Natsucitrine II***. *Des*-N-*methylcitpressine II*
$C_{16}H_{15}NO_5$ 301.298
Light yellow needles (C_6H_6/Me_2CO). Mp 246-247°.

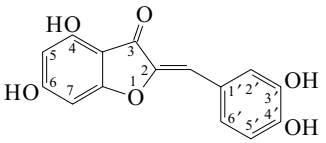
3,5,6-Tri-Me ether, N-*Me:* [81525-59-9] *1-Hydroxy-3,5,6-trimethoxy-10-methylacridone.* ***Citpressine II***
$C_{17}H_{17}NO_5$ 315.325
Alkaloid from the root of bark of *Citrus depressa* (Shekwasha mandarin). Yellow needles (Et_2O). Mp 168-170°.

5,6-Methylene, 3-Me ether, N-*Me:* [160927-87-7] *1-Hydroxy-3-methoxy-10-methyl-5,6-methylenedioxyacridone.* ***Marshdine***
$C_{16}H_{13}NO_5$ 299.282
Alkaloid from roots of marsh grapefruit *Citrus paradisi* (Rutaceae). Yellow cubes. Mp 210-213°.

Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1983, **31**, 895 (*isol, uv, ir, pmr, ms, struct, Citpressines*)
Wu, T.-S. *et al., Phytochemistry*, 1983, **22**, 1493 (*isol, uv, ir, cmr, pmr, ms, struct, Grandisines*)
Ju-ichi, M. *et al., Heterocycles*, 1985, **23**, 1131 (*isol, uv, ir, pmr, cmr, ms, struct, synth, Natsucitrines*)
Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2123; 1994, **39**, 315 (*Grandisine II, Marshdine*)

3′,4,4′,6-Tetrahydroxyaurone T-137

[480-70-6]
4,6-Dihydroxy-2-[(3,4-dihydroxyphenyl)-methylene]-3(2H)-benzofuranone, 9CI. ***Aureusidin***. *Cernuine*



$C_{15}H_{10}O_6$ 286.24
Isol. from *Citrus medica* (citron). Deep-yellow cryst. + $1H_2O$ (MeOH aq.). Mp 270° Mp 295° dec. (double Mp).

Tetra-Ac:
Yellow needles (petrol). Mp 188-189°.

4-O-β-D-Glucopyranoside: [480-69-3] ***Cernuoside***
$C_{21}H_{20}O_{11}$ 448.382
Yellow cryst. (EtOH aq.). Mp 250-258°. $[\alpha]_D^{30}$ -13 (Py).

6-O-β-D-Glucopyranoside: [633-15-8] ***Aureusin***
$C_{21}H_{20}O_{11}$ 448.382
Needles (EtOAc) (as hepta-Ac). Mp 264.5-265.5° (as hepta-Ac).

6-O-Glucuronoside: [65604-87-7] *Aureusidin 6-O-glucuronoside*
$C_{21}H_{18}O_{12}$ 462.366
No phys. props. reported.

4,6-Di-O-β-D-Glucopyranoside: [89648-26-0]
$C_{27}H_{30}O_{16}$ 610.524
No phys. props. reported.

6-O-α-L-Rhamnopyranoside: [124925-02-6]
$C_{21}H_{20}O_{10}$ 432.383
Mp 264°.

4-Me ether: [54826-89-0] *3′,4′,6-Trihydroxy-6-methoxyaurone.* ***Rengasin***
$C_{16}H_{12}O_6$ 300.267
Golden-yellow cryst. Mp 314-316° dec. Originally thought to be the 6-Me ether.

Tetra-Me ether: [23053-69-2] *3′,4,4′,6-Tetramethoxyaurone*
$C_{19}H_{18}O_6$ 342.348
Greenish-yellow needles (MeOH aq.). Mp 173° (169-170°).

[38216-54-5]

Geissman, T.A. *et al., J.A.C.S.*, 1950, **72**, 5725; 1955, **77**, 4622 (*isol, struct*)
Farkas, L. *et al., Chem. Ber.*, 1961, **94**, 2221; 1964, **97**, 1044; 1969, **49**, 2221 (*synth, struct*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Harborne, J.B. *et al., Phytochemistry*, 1966, **5**, 111; 589; 1967, **6**, 1643 (*occur, Cernuoside*)
Clifford, H.T. *et al., Phytochemistry*, 1969, **8**, 123 (*occur*)
Hastings, J.S. *et al., J.C.S. Perkin 1*, 1972, 2128 (*pmr, struct*)
Deshmukh, S.W. *et al., Indian J. Chem.*, 1974, **12**, 893 (*synth*)
Ogiyama, K. *et al., Phytochemistry*, 1976, **15**, 2025 (*isol*)
Harborne, J.B. *et al., Phytochemistry*, 1983, **22**, 2741 (*diglycoside*)
Mohan, P. *et al., Phytochemistry*, 1989, **28**, 2529 (*6-rhamnoside*)
Seabra, R.M. *et al., Phytochemistry*, 1997, **45**, 839 (*Tetramethoxyaurone*)

3′,4′,6,7-Tetrahydroxyaurone T-138

[576-02-3]
6,7-Dihydroxy-2[(3,4-dihydroxyphenyl)-methylene]-3(2H)-benzofuranone, 9CI.
Maritimetin

$C_{15}H_{10}O_6$ 286.24
Used in flavouring. Orange needles (H_2O). Mp 292° dec.

7-Me ether, 6-O-β-D-glucopyranoside:
[486-23-7] ***Leptosin***
$C_{22}H_{22}O_{11}$ 462.409
Isol. from European cranberry (*Vaccinium oxycoccus*) fruits. Orange needles. Mp 229-231° dec.

Jankowski, K. *et al., J. Nat. Prod.*, 1983, **46**, 190-193 (*Leptosin, isol*)

4,4′,5,6-Tetrahydroxyaurone T-139

4,5,6-Trihydroxy-2-[(4-hydroxyphenyl)-methylene]-3(2H)-benzofuranone

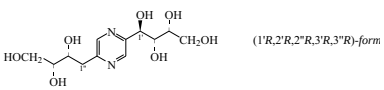
$C_{15}H_{10}O_6$ 286.24

4,4′,6-Tri-Me ether: [137648-02-3] *5-Hydroxy-4,4′,6-trimethoxyaurone*
$C_{18}H_{16}O_6$ 328.321
Isol. from the flowers of *Helianthus annuus* (sunflower).

Alfatafta, A.A. *et al., Phytochemistry*, 1992, **31**, 4109

2-(1,2,3,4-Tetrahydroxybutyl)-5-(2,3,4-trihydroxybutyl)pyrazine T-140

[68510-02-1]
1-[5-(2,3,4-Trihydroxybutyl)pyrazinyl]-1,2,3,4-butanetetrol, 9CI



(1′R,2′R,2″R,3′R,3″R)-*form*

$C_{12}H_{20}N_2O_7$ 304.299

(1′*R*,2′*R*,2″*R*,3′*R*,3″*R*)-*form* [220145-37-9]
D-lyxo-D-threo-*form*
Cryst. (MeOH). Mp 146°. $[\alpha]_D^{20}$ -14.6 (c, 0.2 in H_2O).

(1′*R*,2′*S*,2″*S*,3′*R*,3″*R*)-*form*
D-arabino-D-erythro-*form*. *Deoxyfructosazine*
Formed by reaction of ammonia and glucose. Present in ammonia caramels, soy sauce and roasted peanuts. Solid (MeOH/EtOH); cryst. (2-propanol aq.). Mp 161-162° (157-158°). $[\alpha]_D^{23.5}$ -79.8 (c, 0.2 in H_2O).

Hepta-Ac: [52057-08-6]
Oil. $[\alpha]_D^{20}$ -18 (c, 1.0 in $CHCl_3$).

(1′*R*,2′*S*,2″*S*,3′*S*,3″*S*)-*form* [220145-38-0]
L-xylo-L-threo-*form*
Beige cryst. (EtOH aq.). Mp 116°. $[\alpha]_D^{20}$ -62.4 (c, 0.5 in H_2O).

(1′*S*,2′*R*,2″*R*,3′*R*,3″*R*)-*form* [220145-36-8]
D-xylo-D-threo-*form*
Beige solid (EtOH/MeOH/Et_2O). Mp 90°. $[\alpha]_D^{20}$ +71.3 (c, 0.5 in MeOH).

(1′*S*,2′*S*,2″*S*,3′*R*,3″*R*)-*form* [220145-41-5]
D-ribo-D-erythro-*form*
Ochre cryst. (EtOH aq.). Mp 141°.

(1ξ,2ξ,2′ξ,3ξ,3′ξ)-*form* [206757-33-7] ***Pedatisectine G***

Kuhn, R. *et al., Annalen*, 1961, **644**, 122-127 (*synth*)
Chilton, W.S. *et al., J.A.C.S.*, 1967, **89**, 4129-4132 (*ord, uv*)
Tsuchida, H. *et al., Agric. Biol. Chem.*, 1973, **37**, 2571-2578; 1975, **39**, 1143-1148 (*deoxyfructosazine, isol, pmr, uv*)
Tsuchida, H. *et al., Carbohydr. Res.*, 1978, **67**, 549-563 (*ms*)
Eitelman, S.J. *et al., Carbohydr. Res.*, 1979, **77**, 205-211 (*deoxyfructosazine, synth*)
Tsuchida, H. *et al., Dev. Food Sci.*, 1986, **13**, 85-94 (*occur*)
Tsuchida, H. *et al., CA*, 1990, **113**, 229877r (*occur, soy sauce*)
Sumoto, K. *et al., Chem. Pharm. Bull.*, 1991, **39**, 792-794 (*deoxyfructosazine, synth*)
Magaletta, R.L. *et al., J. Agric. Food Chem.*, 1996, **44**, 2629-2635 (*anal, hplc*)
Wang, R. *et al., Zhongguo Zhongyao Zazhi*, 1997, **22**, 421-423; *CA*, **128**, 306181y (*Pedatisectine G*)
Pat. Coop. Treaty (WIPO), 1999, 9903842; *CA*, **130**, 139579s (*stereoisomers, synth, pmr*)
Rohovec, J. *et al., Eur. J. Org. Chem.*, 2001, 3899 (*deoxyfructosazine, synth*)

2-(1,2,3,4-Tetrahydroxybutyl)-6-(2,3,4-trihydroxybutyl)pyrazine T-141

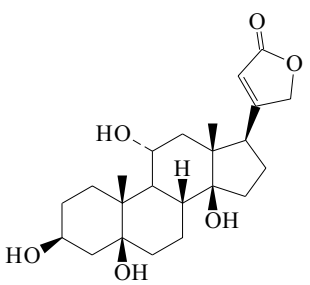
[36806-15-2]
1-[6-(2,3,4-Trihydroxybutyl)pyrazinyl]-1,2,3,4-butanetetrol, 9CI

$C_{12}H_{20}N_2O_7$ 304.299
Formed by reaction of ammonia on glucose. Present in ammonia caramels, soy sauce, roasted peanuts and flue-cured tobacco leaves. Needles (EtOH aq.). Mp 168.5-168.8°. $[\alpha]_D$ -119 (H_2O).

Hepta-Ac: [36806-18-5]
$C_{26}H_{34}N_2O_{14}$ 598.56
Needles (EtOH aq.). Mp 144-145°. $[\alpha]_D^{25}$ -8 (c, 0.73 in $CHCl_3$).

Forlane, E.A. *et al., Carbohydr. Res.*, 1972, **23**, 111-119 (*hepta-Ac*)
Tsuchida, H. *et al., Agric. Biol. Chem.*, 1973, **37**, 2571-2578 (*formn, isol, pmr, uv*)
Tsuchida, H. *et al., Carbohydr. Res.*, 1978, **67**, 549-563 (*ms*)
Shigematsu, H. *et al., CA*, 1980, **92**, 125255t (*occur, tobacco leaf*)
Tsuchida, H. *et al., Dev. Food Sci.*, 1986, **13**, 85-94 (*occur, caramels*)
Tsuchida, H. *et al., CA*, 1990, **113**, 229877r (*occur, soya sauce*)
Magaletta, R.L. *et al., J. Agric. Food Chem.*, 1996, **44**, 2629-2635 (*occur, hplc, roasted peanuts*)

3,5,11,14-Tetrahydroxycard-20(22)-enolide T-142



$C_{23}H_{34}O_6$ 406.518

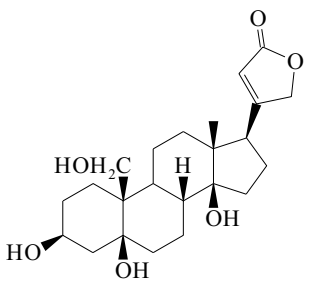
(3β,5β,11α,14β)-*form* [6246-80-6]
Bipindogenin
Cryst. (2-propanol). Mp 242-248° and 304-308°. $[\alpha]_D^{20}$ +29.6 (c, 1.22 in MeOH).

3-O-(6-Deoxy-β-D-gulopyranoside):
[53152-43-5] ***Bipindogulomethyloside***
$C_{29}H_{44}O_{10}$ 552.661
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Cryst. (2-propanol/Et_2O). Mp 150-153° and 168-170°. $[\alpha]_D^{20}$ -17.8 (c, 1.1 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→4)-2,6-dideoxy-β-D-ribo-hexopyranoside]:
[210637-15-3] ***Corchorusoside A***
$C_{35}H_{54}O_{14}$ 698.803
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{24}$ +12.8. λ_{max} 218 (log ε 4.2) (MeOH).

Yoshikawa, M. *et al., Heterocycles*, 1998, **48**, 869-873 (*Corchorusoside A*)

3,5,14,19-Tetrahydroxycard-20(22)-enolide T-143



$C_{23}H_{34}O_6$ 406.518

(3β,5β,14β)-*form* [560-54-3]
Strophanthidol
Platelets (Me_2CO/Et_2O). Mp 140-142° (138-142°). $[\alpha]_D$ +37 (MeOH).

▶ FH5325000

3-O-α-L-Rhamnopyranoside: [3253-62-1]
Convallatoxol. *Perconval*
$C_{29}H_{44}O_{10}$ 552.661
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Needles or prisms (MeOH/Et_2O). Mp 170-172°. $[\alpha]_D^{18}$ -10 (MeOH).

▶ FH4900000

3-O-(6-Deoxy-β-D-gulopyranoside):
[29336-13-8] ***Desglucocheirotoxol***. *Deglucocheirotoxol*
$C_{29}H_{44}O_{10}$ 552.661
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. No phys. props. reported.

3-O-(2,6-Dideoxy-β-D-xylo-hexopyranoside): [23838-13-3] ***Corchorosol A***
$C_{29}H_{44}O_9$ 536.661
Constit. of *Corchorus olitorius* (Jew's mallow).

3-O-[β-D-Glucopyranosyl-(1→4)-6-deoxy-β-D-gulopyranoside]: ***Cheirotoxol***
$C_{35}H_{54}O_{15}$ 714.803
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA.

3-O-[β-D-Glucopyranosyl-(1→4)-α-L-rhamnopyranoside]: ***Convallatoxoloside***
$C_{35}H_{54}O_{15}$ 714.803

Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Cryst. Mp 234-236°. $[\alpha]_D^{19}$ -16.4 (c, 0.8 in MeOH).

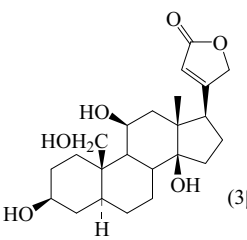
3-O-*[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranoside]:* [64766-15-0] ***Neoconvallatoxoloside***
$C_{35}H_{54}O_{15}$ 714.803
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. Amorph. Mp 161-164°. $[\alpha]_D^{20}$ -11 (c, 1.0 in EtOH).

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranoside]:* ***Glucoconvallatoxoloside***
$C_{41}H_{64}O_{20}$ 876.945
Isol. from *Convallaria majalis*. *Convallaria majalis* is banned by the FDA from food use in the USA. No phys. props, reported.

3-O-*[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-2,6-dideoxy-β-D-*xylo-*hexopyranoside]:* [210637-19-7] ***Corchorusoside E***
$C_{41}H_{64}O_{19}$ 860.945
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{26}$ -12.1 (c, 1.2 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1954, **87**, 1108 (*Convallatoxol*)
Komissarenko, N.F. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1962, **147**, 625 (*Convallatoxoloside*)
Kubelka, W. *et al., Naturwissenschaften*, 1963, **50**, 498 (*Desglucocheirotoxol, Glucoconvallatoxoloside, Cheirotoxol*)
Rao, E. *et al., Curr. Sci.*, 1973, **42**, 731; *CA*, **80**, 80068t (*Corchorosol A*)
Bochvarov, Y. *et al., Khim. Prir. Soedin.*, 1977, **13**, 537; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 448 (*Neoconvallatoxoloside*)
Yoshikawa, M. *et al., Heterocycles*, 1998, **48**, 869-873 (*Corchorusoside E*)

3,11,14,19-Tetrahydroxycard-20(22)-enolide T-144



(3β,5α,11β)-*form*

$C_{23}H_{34}O_6$ 406.518

(3β,5α,11β)-*form* [17430-51-2]
Panogenin
Mp 238-244°. $[\alpha]_D$ -25.8 (MeOH).

3-O-*α-L-Rhamnopyranoside:* [17669-76-0]
Panoside
$C_{29}H_{44}O_{10}$ 552.661
Needles (MeOH/Et_2O). Mp 274-277°. $[\alpha]_D^{24}$ -32.4 (c, 0.8 in MeOH).

► RU1700000

3-O-*[β-D-Glucopyranosyl(1→4)-α-L-rhamnopyranoside]:* ***Glucopanoside***
Amorph. Mp 225-228°. $[\alpha]_D^{27}$ -33 (c, 0.82 in MeOH).

(3β,5β,11α)-*form* *19-Hydroxysarmentogenin*

3-O-*[β-D-Glucopyranosyl-(1→4)-2,6-dideoxy-β-D-*ribo-*hexopyranoside]:* [210637-18-6] ***Corchorusoside D***
$C_{35}H_{54}O_{14}$ 698.803
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{25}$ -5.1 (c, 0.3 in MeOH). λ_{max} 217 (log ϵ 4.2) (MeOH).

Roberts, K.D. *et al., Helv. Chim. Acta*, 1966, **49**, 316
Yoshikawa, M. *et al., Heterocycles*, 1998, **48**, 869-873 (*Corchorusoside D*)

2′,3′,4,4′-Tetrahydroxychalcone, 8CI T-145

3-(4-Hydroxyphenyl)-1-(2,3,4-trihydroxyphenyl)-2-propen-1-one, 9CI

$C_{15}H_{12}O_5$ 272.257
Red-brown needles (EtOH aq.). Mp 225-225.5°.

(E)-form

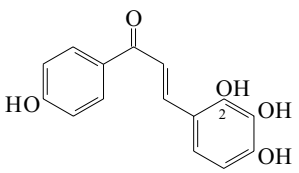
3′,4′-Di-Me ether: [193411-10-8]

[193746-16-6] *2′,4-Dihydroxy-3′,4′-dimethoxychalcone.* ***Heliannone A***
$C_{17}H_{16}O_5$ 300.31
Constit. of *Helianthus annuus* (sunflower). Yellow cryst (hexane/EtOAc). Mp 144-146° (synthetic). λ_{max} 303 (sh) ; 365 (MeOH).

Macias, F.A. *et al., Phytochemistry*, 1997, **45**, 683-687 (*Heliannone A*)
Rao, Y.K. *et al., J. Nat. Prod.*, 2001, **64**, 368-369 (*Heliannone A, synth*)

2,3,4,4′-Tetrahydroxychalcone T-146

1-(4-Hydroxyphenyl)-3-(2,3,4-trihydroxyphenyl)-2-propen-1-one



$C_{15}H_{12}O_5$ 272.257

2-Me ether: [58749-23-8] *3-(3,4-Dihydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)-2-propen-1-one. 3,4,4′-Trihydroxy-2-methoxychalcone.* ***Licochalcone B***
$C_{16}H_{14}O_5$ 286.284
Constit. of the roots of *Glycyrrhiza glabra* (licorice). Yellow needles. Mp 195-197°. Unusual 'retroflavonoid' substitution pattern λ_{max} 308 ; 364 (MeOH) (Berdy). λ_{max} 262 ; 360 (EtOH) (Berdy).

Saitoh, T. *et al., Tet. Lett.*, 1975, 4461; 4463 (*isol, struct, biosynth*)
Islam, A. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 965 (*synth*)

2′,4,4′,6′-Tetrahydroxychalcone, 8CI T-147

[5071-40-9]
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one, 9CI. ***Chalconaringenin****. Isosalipurpol*

$C_{15}H_{12}O_5$ 272.257
Isol. from tomato fruit cuticles. Cryst. (MeOH). Mp 184° (173-174°).

2′-O-*Xyloside:* [76840-08-9]
$C_{20}H_{20}O_9$ 404.373
No phys. props. reported.

2′-O-*β-D-Glucopyranoside:* [4547-85-7] ***Isosalipurposide****. Phlorizin chalcone*
$C_{21}H_{22}O_{10}$ 434.399
Mp 172-174° (anhyd.). $[\alpha]_D$ -20 (EtOH).

2′-O-*β-D-Glucopyranoside, 4′*-O-*[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:*
$C_{33}H_{42}O_{20}$ 758.683
Yellow powder. λ_{max} 243 (sh) ; 368 (MeOH).

4-O-*β-D-Glucopyranoside:* [68116-40-5]
$C_{21}H_{22}O_{10}$ 434.399
No phys. props. reported.

4-O-*(*p*-Hydroxycinnamoyl-β-D-glucopyranoside):*
$C_{30}H_{28}O_{12}$ 580.544Posn. of coumaroyl substituent in glucose residue not detd..

4′-O-*β-D-Glucopyranoside:* [25218-09-1]
$C_{21}H_{22}O_{10}$ 434.399
Mp 164-166°.

2′,4′-Di-O-*β-D-glucopyranoside:* [6198-23-8]
$C_{27}H_{32}O_{15}$ 596.541
Yellow powder. Mp 191°. λ_{max} 243 (sh) ; 368 (MeOH).

2′-O-*[Rhamnosyl-(1→4)-xyloside]:* [82344-84-1]
$C_{26}H_{30}O_{13}$ 550.515

2′-Me ether: [62014-87-3] *1-(2,4-Dihydroxy-6-methoxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one. 2′,4,4′-Trihydroxy-6′-methoxychalcone.* ***Helichrysetin***
$C_{16}H_{14}O_5$ 286.284
Yellow-orange cryst. ($CHCl_3$). Mp 248°.

2′-Me ether, 4-O-*β-D-glucopyranoside:* [155913-99-8]
$C_{22}H_{24}O_{10}$ 448.426
Yellow oil with fluor.

2′-Me ether, 4′-O-*β-D-glucopyranoside:* [61826-89-9] ***Helichrysin****. Gnaphalin*†*. Dehydro-*p*-asebotin*
$C_{22}H_{24}O_{10}$ 448.426
Yellow needles. Mp 199-200° (sinters at 140-160°) Mp 246° dec. $[\alpha]_D^{30}$ -85.2 (c, 0.71 in MeOH). Identity of the isolates apparently not conclusively establ..

2′-Me ether, 4,4′-di-O-*β-D-glucopyranoside:*
$C_{28}H_{34}O_{15}$ 610.568
Yellow cryst. (MeOH). Mp 186-188°.

4-Me ether: [56927-09-4] *2′,4′,6′-Trihydroxy-4-methoxychalcone*
$C_{16}H_{14}O_5$ 286.284
No phys. props. reported.

4′-Me ether: [81719-04-2] *1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one, 9CI. 2′,4,6′-Trihydroxy-4′-methoxychalcone.* ***Neosakuranetin***
$C_{16}H_{14}O_5$ 286.284
Cryst. ($CHCl_3$). Mp 138-140°.

4′-Me ether, 2′-O-*β-D-glucopyranoside:* [31187-54-9] ***Neosakuranin****. Chalconosakuranetin*
$C_{22}H_{24}O_{10}$ 448.426
Isol. from *Prunus cerasoides* (wild Himalayan cherry). Yellow prisms. Mp

110-112°.

2′,4-Di-Me ether:2′,4′-Dihydroxy-4,6′-dimethoxychalcone
$C_{17}H_{16}O_5$ 300.31
Yellow cryst. (Me_2CO). Mp 170-172°.

2′,4′-Di-Me ether: [37308-75-1] ***Flavokawain C****. 2′,4-Dihydroxy-4′,6′-dimethoxychalcone*
$C_{17}H_{16}O_5$ 300.31
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Pale orange needles (EtOH). Mp 194-195°.

2′,4′-Di-Me ether, 4-O-β-D-glucopyranoside: [68984-71-4]
$C_{23}H_{26}O_{10}$ 462.452
Mp 156-158°.

*2′,6′-Di-Me ether:****4,4′-Dihydroxy-2′,6′-dimethoxychalcone***
$C_{17}H_{16}O_5$ 300.31
Isol. from *Humulus lupulus* (hops). Cryst. (EtOAc/hexane). Mp 192-193°.

4,4′-Di-Me ether: [20621-49-2] *2′,6′-Dihydroxy-4,4′-dimethoxychalcone.* ***Gymnogrammene***
$C_{17}H_{16}O_5$ 300.31
Red prisms (C_6H_6). Mp 156-157°.

*4′,6′-Di-Me ether, 4-O-β-D-glucopyranoside:****2′,4-Dihydroxy-4′,6-dimethoxychalcone 4-glucoside***
$C_{23}H_{26}O_{10}$ 462.452
Yellowish needles. Mp 166-168°.

2′,4,4′-Tri-Me ether: [3420-72-2] *2′-Hydroxy-4,4′,6′-trimethoxychalcone.* ***Flavokawain A***
$C_{18}H_{18}O_5$ 314.337
Found in kava (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Yellow needles (EtOH). Mp 113°.

2′,4,6′-Tri-Me ether:4′-Hydroxy-2′,4,6′-trimethoxychalcone
$C_{18}H_{18}O_5$ 314.337
Yellow needles (MeOH). Mp 208-210°.

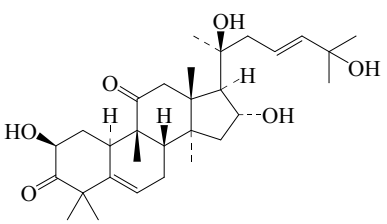
Tetra-Me ether: [25163-67-1] *2′,4,4′,6-Tetramethoxychalcone*
$C_{19}H_{20}O_5$ 328.364
Pale yellow cryst. (EtOH aq.). Mp 119-121°.

4′-O-(3-Methyl-2-butenyl): [94393-11-0] ***2′,4,6′-Trihydroxy-4′-prenyloxychalcone***
$C_{20}H_{20}O_5$ 340.375
Gum.

[25515-46-2, 73692-50-9]

Puri, B. *et al., CA*, 1955, **49**, 4942 (*Neosakuranin*)
Nilsson, M. *et al., Acta Chem. Scand.*, 1961, **15**, 211 (*Gymnogrammene*)
Guise, G.B. *et al., Aust. J. Chem.*, 1962, **15**, 314 (*isol, deriv*)
Mahanthy, P. *et al., Indian J. Chem.*, 1965, **3**, 121 (*ir*)
Harborne, J.B. *et al., Phytochemistry*, 1966, **5**, 111 (*Isosalipurposide*)
Ramakrishnan, V.T. *et al., J.O.C.*, 1970, **35**, 2901 (*synth*)
Dutta, C.P. *et al., Indian J. Chem.*, 1973, **11**, 509 (*Flavokawain C*)
Aritomi, M. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1800 (*Dehydroasebotin*)
Maruyama, M. *et al., Phytochemistry*, 1974, **13**, 286 (*Gnaphalin*)
Lam, J. *et al., Phytochemistry*, 1975, **14**, 1621 (*isol, deriv*)
Wright, W.G. *et al., J.C.S. Perkin 1*, 1976, 1819 (*Helichrysin*)
De Vlaming, P. *et al., Phytochemistry*, 1976, **15**, 348 (*isol*)
Imperato, F. *et al., Phytochemistry*, 1978, **17**, 822; 1982, **21**, 480 (*glycosides*)
Duddeck, H. *et al., Phytochemistry*, 1978, **17**, 1369 (*pmr*)
Becker, H. *et al., Z. Naturforsch., C*, 1978, **33**, 771 (*glycoside*)
Vinokurov, I.I. *et al., Khim. Prir. Soedin.*, 1979, **15**, 355 (*coumaroylglucoside*)
Bohlmann, L. *et al., Phytochemistry*, 1979, **18**, 889; 1338 (*isol*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1979, **34**, 1289 (*isol*)
Hunt, G.M. *et al., Phytochemistry*, 1980, **19**, 1415 (*isol*)
Norbedo, C. *et al., J. Nat. Prod.*, 1982, **45**, 635 (*2,4,4′-Trihydroxy-6′-methoxychalcone*)
Hitz, C. *et al., Z. Naturforsch., C*, 1982, **37**, 337 (*Neosakuranetin*)
Bohlmann, F. *et al., Phytochemistry*, 1984, **23**, 1338 (*2′,4,6′-Trihydroxy-4′-prenyloxychalcone*)
McCormick, S. *et al., Phytochemistry*, 1985, **24**, 1614 (*2′,4′,6′-Trihydroxy-4-methoxychalcone*)
Fukunaga, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3292 (*cmr, deriv*)
Babber, S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 797 (*synth*)
Mizuno, M. *et al., Phytochemistry*, 1987, **26**, 2071 (*deriv*)
von Puyvelde, L. *et al., J. Nat. Prod.*, 1989, **52**, 629 (*Helichrysetin*)
Sun, S.-S. *et al., Phytochemistry*, 1989, **27**, 1776 (*4,4′-Dihydroxy-2′,6′-dimethoxychalcone*)
Messana, I. *et al., Phytochemistry*, 1990, **29**, 329 (*Neosakuranetin*)
Roy, R. *et al., Phytochemistry*, 1994, **37**, 1775 (*2′-Me ether diglucoside*)
Bilia, A.R. *et al., Tetrahedron*, 1994, **50**, 5181 (*2′-Me ether 4-glucoside*)
Lin, L.-C. *et al., Chin. Pharm. J. (Taipei)*, 1995, **47**, 501 (*2′,4′-diglucoside*)
Thuy, T.T. *et al., Phytochemistry*, 1998, **49**, 2603-2605 (*Vitex leptobotrys chalcones*)
Iwashima, T. *et al., Phytochemistry*, 2000, **55**, 971-974 (*Asarum canadense glucosides*)

2,16,20,25-Tetrahydroxycucurbita-5,23-diene-3,11-dione T-148

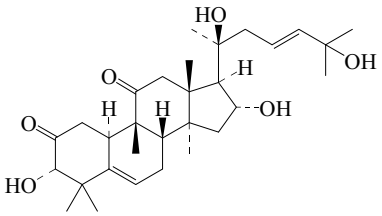


$C_{30}H_{46}O_6$ 502.69

(2β,16α,20*R*,23*E*)-*form* [15371-78-5]
22-Deoxocucurbitacin D
Constit. of *Lagenaria siceraria* (bottle gourd). Amorph. $[\alpha]_D$ +103 (c, 1 in $CHCl_3$).

Enslin, P.R. *et al., J.C.S.(C)*, 1967, 964

3,16,20,25-Tetrahydroxycucurbita-5,23-diene-2,11-dione T-149

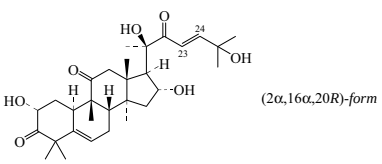


$C_{30}H_{46}O_6$ 502.69

(3α,16α,20*R*,23*E*)-*form* [15371-77-4]
22-Deoxoisocucurbitacin D
Constit. of *Lagenaria siceraria* (bottle gourd). Amorph. $[\alpha]_D$ +76 (c, 1 in $CHCl_3$).

Enslin, P.R. *et al., J.C.S.(C)*, 1967, 964

2,16,20,25-Tetrahydroxycucurbita-5,23-diene-3,11,22-trione T-150



(2α,16α,20*R*)-*form*

$C_{30}H_{44}O_7$ 516.673
▶ RC6170000

(2β,16α,20*R*)-*form* [3877-86-9]
Cucurbitacin D*. Elatericin A*
Isol. from plants of the Cucurbitaceae. Cryst. + $\frac{1}{2}H_2O$ (EtOH). Sol. EtOAc, Et_2O; poorly sol. H_2O, C_6H_6, bases. Mp 151-152°. $[\alpha]_D$ +52 (EtOH). λ_{max} 230 (ε 13000) (EtOH).
▶ LD_{50} (rat, orl) 8.2 mg/kg.

*O-[β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-D-arabinoside]:****Cucurbitacide E***
$C_{47}H_{72}O_{21}$ 973.073
Glycoside from leaves and fruit of *Cucumis sativus* (cucumber). Mp 158-160°. Posn. of glycosidation not detd..

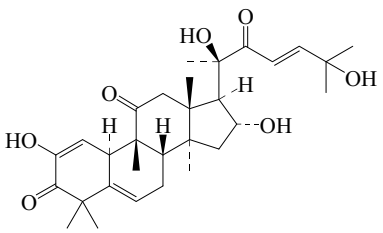
25-Ac: [6199-67-3] ***Cucurbitacin B****. Amarin*†
$C_{32}H_{46}O_8$ 558.711
Together wth other cucurbitacins, is responsible for the bitter taste and toxic props. of spoilt cucumbers. Cryst. (EtOH). Mp 180-182°. $[\alpha]_D^{25}$ +87.5 (96% EtOH). λ_{max} 229 (ε 29500) (MeOH) (Berdy). λ_{max} 229 (ε 13300) (EtOH) (Berdy).
▶ RC6190000

De Kock, W.T. *et al., J.C.S.*, 1963, 3828-3845 (*pmr*)
Lavie, D. *et al., J.O.C.*, 1963, **28**, 1790 (*struct*)
Audier, H.E. *et al., Tet. Lett.*, 1966, 2205 (*ms*)
Lavie, D. *et al., Prog. Chem. Org. Nat. Prod.*, 1971, **29**, 307-362 (*rev*)
Kintya, P.K. *et al., Khim. Prir. Soedin.*, 1972, **8**, 306; *Chem. Nat. Compd. (Engl. Transl.)*, 1972, **8**, 303 (*Cucurbitacide E*)
Bull, J.R. *et al., S. Afr. J. Chem.*, 1979, **32**, 27 (*cmr*)
Velde, D.D. *et al., Tetrahedron*, 1983, **39**, 317 (*cmr*)

Che, C.-T. *et al., J. Nat. Prod.*, 1985, **24**, 429-434 (*pmr*)
Jacobs, H. *et al., J. Nat. Prod.*, 1990, **53**, 1600 (*cmr*)
Fujita, S. *et al., Phytochemistry*, 1995, **38**, 465 (*cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EAH100

2,16,20,25-Tetrahydroxycucurbita-1,5,23-triene-3,11,22-trione T-151

16,20,25-Trihydroxycucurbita-5,23-diene-2,3,11,22-tetrone



$C_{30}H_{42}O_7$ 514.658

Exists in hydroxyenol form illus..λ_{max} 234 (ϵ 11400); 314 (ϵ 6750) (NaOH) (Berdy). λ_{max} 234 (ϵ 11000); 269 (ϵ 6850) (EtOH) (Berdy).

► RC6200000

(16α,20*R*,23*E*)-*form* [2222-07-3] ***Cucurbitacin I***. *Elatericin B*
Cryst. Sol. bases, EtOAc, Et_2O; poorly sol. H_2O, hexane, C_6H_6. Mp 148-149° dec. $[\alpha]_D^{20}$ -58.5 (MeOH).

2-O-β-D-Glucopyranoside: [29803-94-9]
$C_{36}H_{52}O_{12}$ 676.8
Constit. of *Citrullus lanatus*. Mp 241-243°. $[\alpha]_D^{20}$ -72.6 (EtOH).

► RC6191000

20-Ac: [38308-89-3] ***Datiscacin***†
$C_{32}H_{44}O_8$ 556.695
Mp 208-212°. $[\alpha]_D^{23}$ -18 (c, 0.87 in $CHCl_3$). Log P 0.32 (uncertain value) (calc). λ_{max} 231 (ϵ 9600); 268 (ϵ 5400) (EtOH) (Berdy).

25-Ac: [18444-66-1] ***Cucurbitacin E***. *α-Elaterin*
$C_{32}H_{44}O_8$ 556.695
Mp 234°. $[\alpha]_D^{20}$ -64.3 ($CHCl_3$). λ_{max} 233 (ϵ 11700); 234 ; 267 (ϵ 8400); 269 (EtOH) (Berdy).

► LD_{50} (mus, ipr) 2 mg/kg. RC6305500

25-Ac, 2-O-β-D-glucopyranoside: [1398-78-3] ***Elaterinide***. *Colocynthin*. *Gratiotoxin*
$C_{38}H_{54}O_{13}$ 718.837
Constit. of *Citrullus lanatus*. Sol. EtOH, $CHCl_3$, Me_2CO; fairly sol. Et_2O, H_2O. Mp 148-150°. $[\alpha]_D^{20}$ -63.5 ($CHCl_3$). λ_{max} 235 (ϵ 12900) (EtOH) (Berdy).

► RC6192500

23,24-Dihydro: [1110-02-7] *2,16,20,25-Tetrahydroxycucurbita-1,5-diene-3,11,22-trione*. *16,20,25-Trihydroxycucurbit-5-ene-2,3,11,22-tetrone*. ***Cucurbitacin L***
$C_{30}H_{44}O_7$ 516.673
Cryst. + ½H_2O (MeOH aq.). Mp 122-127°. $[\alpha]_D^{28}$ -41 (EtOH). λ_{max} 270 (ϵ 8050) (EtOH) (Berdy).

23,24-Dihydro, 2-O-β-D-glucopyranoside: [61105-51-9] ***Bryoamaride***
$C_{36}H_{54}O_{12}$ 678.815
Mp 228-235°. $[\alpha]_D^{20}$ -85.7 (c, 0.82 in EtOH).

23,24-Dihydro, 2,25-di-O-β-D-glucopyranoside: [142674-88-2] ***Brydioside A***
$C_{42}H_{64}O_{17}$ 840.957
Cryst. Mp 180-181.5°. $[\alpha]_D$ -28.6 (c, 0.8 in MeOH).

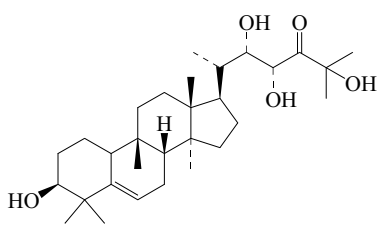
23,24-Dihydro, 25-Ac, 2-O-β-D-glucopyranoside: [61014-18-4] ***25-O-Acetylbryoamaride***
$C_{38}H_{56}O_{13}$ 720.853
$[\alpha]_D^{20}$ -34.3 (c, 1.04 in $CHCl_3$).

23,24-Dihydro, 2-O-[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [415710-99-5] ***Khekadaengoside A***
$C_{42}H_{64}O_{16}$ 824.958
Amorph. powder. $[\alpha]_D^{23}$ -109.4 (c, 3.1 in MeOH).

23,24-Dihydro, 2-O-[α-D-glucopyranosyl-(1→4)-β-D-glucopyranoside]: [415711-00-1] ***Khekadaengoside B***
$C_{42}H_{64}O_{17}$ 840.957
Amorph. powder. $[\alpha]_D^{23}$ -37 (c, 2.7 in MeOH).

Kupchan, S.M. *et al., J.O.C.*, 1973, **38**, 1420-1421 (*Datiscacin*)
Ripperger, H. *et al., Tetrahedron*, 1976, **32**, 1567-1569 (*Bryoamaride, 25-Acetylbryoamaride*)
Nielsen, J.K. *et al., Phytochemistry*, 1977, **16**, 1519-1522 (*Cucurbitacin E, Cucurbtacin I*)
Yamada, Y. *et al., Phytochemistry*, 1978, **17**, 1798 (*Cucurbitacin E, Cucurbitacin I, Cucurbitacin L*)
Bull, J.R. *et al., S. Afr. J. Chem.*, 1979, **32**, 27-33 (*cmr*)
Che, C.-T. *et al., J. Nat. Prod.*, 1985, **48**, 429-434 (*pmr*)
Oobayashi, K. *et al., Phytochemistry*, 1992, **31**, 943-946 (*Brydioside A*)
Musza, L.L. *et al., J. Nat. Prod.*, 1994, **57**, 1498-1502 (*activity*)
Kanchanapoom, T. *et al., Phytochemistry*, 2002, **59**, 215-228 (*Khekadaengosides*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, COE250

3,22,23,25-Tetrahydroxycucurbit-5-en-24-one T-152



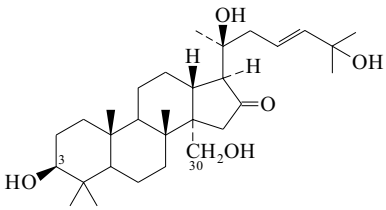
$C_{30}H_{50}O_5$ 490.722

(3β,22*S*,23*R*)-*form*

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [333333-19-0] ***Goyaglycoside h***
$C_{42}H_{70}O_{15}$ 815.006
Constit. of *Momordica charantia* (bitter melon). Powder. $[\alpha]_D^{24}$ +0.7 (c, 0.5 in Py).

Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 54-63 (*isol, pmr, cmr*)

3,20,25,30-Tetrahydroxydammar-23-en-16-one T-153



$C_{30}H_{50}O_5$ 490.722

(3β,20*S*,23*E*)-*form*

3-O-α-L-Arabinopyranoside, 30-O-β-D-glucopyranoside: [154971-10-5] ***Hoduloside VI***
$C_{41}H_{68}O_{14}$ 784.98
Constit. of *Hovenia dulcis* (raisin tree). Amorph. powder. $[\alpha]_D$ -38.6 (c, 2.5 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranoside], 30-O-β-D-glucopyranoside: [154971-11-6] ***Hoduloside VII***
$C_{47}H_{78}O_{18}$ 931.122
Constit. of *Hovenia dulcis* (raisin tree). Amorph. powder. $[\alpha]_D$ -52.1 (c, 5.2 in MeOH).

3-O-α-L-Arabinopyranoside, 30-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [154971-12-7] ***Hoduloside VIII***
$C_{46}H_{76}O_{18}$ 917.096
Constit. of *Hovenia dulcis* (raisin tree). Amorph. powder. $[\alpha]_D$ -34.4 (c, 4.6 in MeOH).

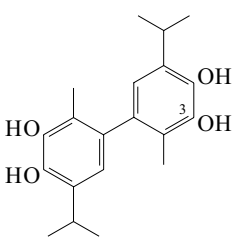
3-O-[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranoside], 30-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [154971-13-8] ***Hoduloside IX***
$C_{52}H_{86}O_{22}$ 1063.238
Constit. of *Hovenia dulcis* (raisin tree). Amorph. powder. $[\alpha]_D$ -37.6 (c, 1.8 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-[α-L-rhamnopyranosyl-(1→2)]-α-L-arabinopyranoside], 30-O-β-D-glucopyranoside: [154971-14-9] ***Hoduloside X***
$C_{53}H_{88}O_{23}$ 1093.264
Constit. of *Hovenia dulcis* (raisin tree). Amorph. powder. $[\alpha]_D$ -35 (c, 1.8 in MeOH).

Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1722 (*isol, pmr, cmr*)

3,3′,4,4′-Tetrahydroxy-5,5′-diisopropyl-2,2′-dimethylbiphenyl T-154

[120901-51-1]



$C_{20}H_{26}O_4$ 330.423
Constit. of *Thymus vulgaris* (thyme). Light

brown powder. Mp 104°. $[\alpha]_D$ -9.2 (c, 0.8 in $CHCl_3$).

3-Deoxy: [123132-69-4] *3,4,4′-Trihydroxy-5,5′-diisopropyl-2,2′-dimethylbiphenyl*
$C_{20}H_{26}O_3$ 314.424
Constit. of *Thymus vulgaris* (thyme). Pale brown needles (C_6H_6). Mp 75°. $[\alpha]_D^{25}$ -48 (c, 0.21 in $CHCl_3$).

Miura, K. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1816 (*isol, pmr, cmr*)
Miura, K. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 1159 (*synth*)
Haraguchi, H. *et al., Planta Med.*, 1996, **62**, 217 (*isol, cmr, props*)

3′,4′,5,7-Tetrahydroxy-3,6-dimethoxyflavone T-155

[5188-73-8]
*2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-3,6-dimethoxy-4*H*-1-benzopyran-4-one, 9CI. **Axillarin**. Quercetagetin 3,6-dimethyl ether*

$C_{17}H_{14}O_8$ 346.293
Cryst. (MeCN). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 211-213°. λ_{max} 260 (ϵ 23400); 270 (ϵ 21700); 358 (ϵ 26300) (MeOH) (Berdy). λ_{max} 259 (ϵ 18200); 296 (ϵ 8300); 355 (ϵ 21900) (EtOH) (Berdy). λ_{max} 273 (ϵ 18600); 299 (ϵ 8800); 369 (ϵ 17800) (EtOH/NaOH) (Berdy).

7-Sulfate:Axillarin 7-sulfate. ***Centaradixin***
$C_{17}H_{14}O_{11}S$ 426.357
Amorph. yellow solid (as Na salt).

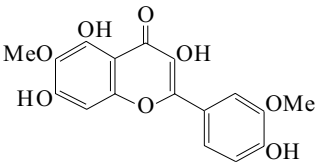
7-O-β-D-Glucopyranoside: [41749-40-0] *Axillarin 7-glucoside.* ***Axillaroside***
$C_{23}H_{24}O_{13}$ 508.435

4′-O-β-D-Glucuronopyranoside: [65039-74-9] *Axillarin 4′-glucuronide.* ***Spinatoside***
$C_{23}H_{22}O_{14}$ 522.418
Isol. from spinach (*Spinacia oleracea*) leaves. Cryst. (MeOH aq.). Mp 159° (153°). $[\alpha]_D^{25}$ -80 (c, 0.11 in MeOH).

Herz, W. *et al., Chem. Ber.*, 1966, **99**, 3539 (*isol, struct*)
Fukui, K. *et al., Experientia*, 1968, **24**, 769 (*synth*)
Jefferies, P.R. *et al., Aust. J. Chem.*, 1974, **27**, 221 (*isol*)
Oganesyan, E.T. *et al., Khim. Prir. Soedin.*, 1976, **12**, 599; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 537 (*Axillaroside*)
Wagner, H. *et al., Tetrahedron*, 1977, **33**, 1405 (*Spinatoside*)
Goudard, M. *et al., Phytochemistry*, 1978, **17**, 145 (*ms*)
Bacon, J.D. *et al., Phytochemistry*, 1978, **17**, 1939 (*Axillaroside*)
Misra, K. *et al., Indian J. Chem., Sect. B*, 1979, **18**, 88 (*isol*)
Kerr, K.M. *et al., Phytochemistry*, 1981, **20**, 791 (*Axillaroside*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Aritomi, M. *et al., Phytochemistry*, 1986, **25**, 231 (*Spinatoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Bergman, M. *et al., Phytochemistry*, 2001, **58**, 143-152 (*Spinatoside, pmr, cmr*)
Flamini, G. *et al., Phytochemistry*, 2001, **58**, 1229-1233 (*Centaradixin*)

3,4′,5,7-Tetrahydroxy-3′,6-dimethoxyflavone T-156

[3153-83-1]
*3,5,7-Trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-methoxy-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-3′,6-dimethoxyflavonol.* ***Spinacetin***. *Quercetagetin 3′,6-dimethyl ether*



$C_{17}H_{14}O_8$ 346.293
Isol. from spinach (*Spinacia oleracea*). Cryst. Mp 235-236°.

3-O-Sulfate: [111348-30-2]
$C_{17}H_{14}O_{11}S$ 426.357

3-O-β-D-Glucopyranoside: [81563-84-0]
$C_{23}H_{24}O_{13}$ 508.435
Isol. from *Artemisia absinthium* (wormwood).

7-O-β-D-Glucopyranoside: [60048-89-7]
$C_{23}H_{24}O_{13}$ 508.435

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [101021-29-8] *Spinacetin 3-gentiobioside*
$C_{29}H_{34}O_{18}$ 670.577
Isol. from spinach (*Spinacia oleracea*). Yellow needles + $1H_2O$ (MeOH). Mp 192-194°. $[\alpha]_D^{26}$ -19 (MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:Spinacetin 3-rutinoside
$C_{29}H_{34}O_{17}$ 654.577
Isol. from *Artemisia absinthium* (wormwood).

3-O-[4-Hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{39}H_{42}O_{21}$ 846.748
Constit. of spinach leaves (*Spinacia oleracea*).

3-O-[β-D-Apiofuranosyl-(1→2)[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside]:
$C_{34}H_{42}O_{22}$ 802.693
Constit. of spinach leaves (*Spinacia oleracea*). λ_{max} 257 ; 272 (sh) ; 349 (MeOH).

3-O-[4-Hydroxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→6)-[β-D-apiofuranosyl-(1→2)]-β-D-glucopyranoside]:
$C_{43}H_{48}O_{24}$ 948.838
Constit. of spinach (*Spinacia oleracea*). λ_{max} 258 ; 275 ; 300 (sh) ; 319 ; 356 (sh) (MeOH).

3-O-[4-Hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→6)-[β-D-apiofuranosyl-(1→2)]-β-D-glucopyranoside]:
$C_{44}H_{50}O_{25}$ 978.864
Constit. of spinach (*Spinacia oleracea*). λ_{max} 255 ; 275 ; 300 (sh) ; 336 ; 373 (sh) (MeOH).

3-O-[4-Hydroxy-3-methoxy-E*-cinnamoyl-(→2)-β-D-xylopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]:* ***Mesembryanthin***
$C_{44}H_{50}O_{25}$ 978.864
Constit. of the famine food *Mesembryanthemum crystallinum* (ice plant) exposed to high intensities of white light.

Zane, A. *et al., J.O.C.*, 1961, **26**, 4718 (*isol*)
Dreyer, D.L. *et al., Tetrahedron*, 1964, **20**, 2977 (*synth*)
Saunders, J. *et al., Phytochemistry*, 1976, **15**, 809 (*occur*)
Bacon, J.D. *et al., Phytochemistry*, 1978, **17**, 1939 (*isol*)
Ulubelen, A. *et al., J. Nat. Prod.*, 1979, **42**, 624 (*3-rutinoside*)
Mues, R. *et al., Phytochemistry*, 1979, **18**, 1379 (*isol*)
Bohm, B.A. *et al., Phytochemistry*, 1981, **20**, 1053 (*7-glucoside*)
Hoffmann, B. *et al., Z. Lebensm.-Unters. -Forsch.*, 1982, **174**, 211 (*3-glucoside*)
Aritomi, M. *et al., Phytochemistry*, 1986, **25**, 231 (*3-gentiobioside*)
Barron, D. *et al., Phytochemistry*, 1987, **26**, 2085 (*3-sulfate*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Ferreres, F. *et al., Phytochemistry*, 1997, **45**, 1701 (*3-gentiobiosides*)
Vogt, T. *et al., Phytochemistry*, 1999, **52**, 583-592 (*Mesembryanthin*)

3,4′,5,7-Tetrahydroxy-3′,8-dimethoxyflavone T-157

[489-33-8]
*3,5,7-Trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-8-methoxy-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-3′,8-dimethoxyflavonol.* ***Limocitrin***. *Gossypetin 3′,8-dimethyl ether. Sedoflorigenin*

$C_{17}H_{14}O_8$ 346.293
Constit. of citrus fruit peels. Yellow cryst. (Me_2CO aq.). Mp 274-275°.

3-O-β-D-Glucopyranoside: [38836-51-0] *Limocitrin 3-glucoside*
$C_{23}H_{24}O_{13}$ 508.435
Constit. of *Citrus* spp. fruit peels. Cryst. (H_2O). Mp 150° (resolidifies and remelts at 240-245°).

7-O-β-D-Glucopyranoside: [119628-58-9] *Limocitrin 7-glucoside*
$C_{23}H_{24}O_{13}$ 508.435
Light yellow needles (MeOH aq.). Mp 265-268°.

7-O-(6-O-Acetyl-β-D-glucopyranoside): [97744-93-9]
$C_{25}H_{26}O_{14}$ 550.472
Mp 231-233°. $[\alpha]_D^{20}$ -19.35.

3-O-β-D-Galactopyranoside: [103839-19-6] *Limocitrin 3-galactoside*
$C_{23}H_{24}O_{13}$ 508.435

3-O-α-L-Rhamnopyranoside: [90456-56-7] *Limocitrin 3-rhamnoside*
$C_{23}H_{24}O_{12}$ 492.435
Isol. from *Citrus* spp. fruit peels.

7-O-α-L-Rhamnopyranoside: [136561-50-7] *Limocitrin 7-rhamnoside*
$C_{23}H_{24}O_{12}$ 492.435

3,7-Di-O-β-D-glucopyranoside: [111133-91-6] *Limocitrin 3,7-diglucoside*
$C_{29}H_{34}O_{18}$ 670.577
Yellow needles (MeOH aq.). Mp 262-264°.

7-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [97744-91-7] ***Haploside E***. *Limocitrin 7-neohesperidoside*
$C_{29}H_{34}O_{17}$ 654.577
Mp 184-186°. $[\alpha]_D^{20}$ -25 (c, 0.4 in MeOH).

3-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [79384-27-3] *Limocitrin 3-rutinoside*
$C_{29}H_{34}O_{17}$ 654.577
Isol. from citrus fruit peels. Yellow powder.

3-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 7*-O-*β-D-glucopyranoside:* [301647-86-9]
$C_{35}H_{44}O_{22}$ 816.719
Yellow powder. $[\alpha]_D$ -23 (c, 1 in MeOH). λ_{max} 257 (log ε 4.13); 270 (sh) (log ε 4.05); 360 (log ε 4.01) (MeOH).

7-O-*[α-L-Rhamnopyranosyl-(1→2)-6*-O-*acetyl-β-D-glucopyranoside]:* [108279-04-5] ***Haploside C***
$C_{31}H_{36}O_{18}$ 696.615
Yellow cryst. (EtOH aq.). Mp 143-145°. $[\alpha]_D^{22}$ 0 (c, 0.35 in MeOH).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [114882-19-8] *Limocitrin 3-sophoroside*
$C_{29}H_{34}O_{18}$ 670.577
$[\alpha]_D^{20}$ -10 (c, 0.1 in MeOH).

3,4′,7-Tri-Ac:
Cryst. (Me_2CO/MeOH). Mp 188-189°.

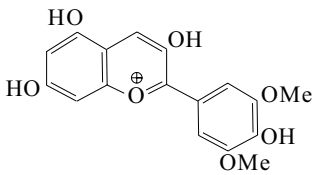
7-O-*(3-Methyl-2-butenyl):* [232932-39-7] *3,4′,5-Trihydroxy-3′,8-dimethoxy-7-prenyloxyflavone. 4′,5-Dihydroxy-3′,8-dimethoxy-7-prenyloxyflavonol.* ***7-O-(3-Methyl-2-butenyl)limocitrin***
$C_{22}H_{22}O_8$ 414.411
Amorph. yellow solid. λ_{max} 259 ; 287 (EtOH).

Horowitz, R.M. *et al., J.O.C.*, 1960, **25**, 2183; 1961, **26**, 2899 (*isol, struct*)
Gentili, B. *et al., Tetrahedron*, 1964, **20**, 2313 (*glucoside*)
Dreyer, D.L. *et al., Tetrahedron*, 1964, **20**, 2977 (*synth*)
Krishnamurti, M. *et al., Tetrahedron*, 1966, **22**, 941 (*synth*)
Pangon, J.F. *et al., Phytochemistry*, 1974, **13**, 1883 (*isol*)
Jay, M. *et al., Phytochemistry*, 1978, **17**, 827 (*isol*)
Harborne, J.B. *et al., Phytochemistry*, 1981, **20**, 1117 (*3-rutinoside*)
Ulubelen, A. *et al., Phytochemistry*, 1984, **23**, 2941 (*3-glucoside 3-rutinoside*)
Matsubara, Y. *et al., Agric. Biol. Chem.*, 1985, **49**, 909 (*3-rhamnoside 3-glucoside*)
Yuldashev, M.P. *et al., Khim. Prir. Soedin.*, 1985, **21**, 192; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 179 (*7-acetylglucoside, Haploside E*)
Agnese, A.M. *et al., J. Nat. Prod.*, 1986, **49**, 528 (*3-galactoside*)
Batirov, E.K. *et al., Khim. Prir. Soedin.*, 1987, **23**, 66; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 54 (*Haploside C*)
Stosic, D. *et al., Helv. Chim. Acta*, 1988, **71**, 348 (*3-sophoroside*)
Wolbis, M. *et al., Phytochemistry*, 1988, **27**, 3941 (*7-glucoside, 3,7-diglucoside*)
Sultana, N. *et al., Phytochemistry*, 1999, **50**, 1249-1253 (*7-Methylbutenyllimocitrin*)
Ito, H. *et al., Phytochemistry*, 2000, **54**, 695-700 (*3-rhamnosylglucoside 7-glucoside*)
Yuldashev, M.P. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2001, **37**, 288-289 (*Haploside C*)
Pat. Coop. Treaty (WIPO), 2001, 19 998; *CA*, **132**, 260708c (*Limocitrin, synth*)

3,4′,5,7-Tetrahydroxy-3′,5′-dimethoxyflavylium(1+) T-158

[10463-84-0]

[643-84-5]
3,5,7-Trihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-1-benzopyrilium(1+), 9CI. ***Malvidin****. 3′,5′-Dimethyldelphinidin. Denidin. Syringidin. Malvidol. Enidin. Oenidin. Primulidin. Malvinidin*



$C_{17}H_{15}O_7^{\oplus}$ 331.301
Occurs free and as glycosides in a wide variety of foodstuffs esp. blueberries, raspberries and red wine. Apparently present as free aglycone in *Lathyrus sativus* (chickling pea). Dark brown prisms or needles + $1H_2O$ (EtOH/HCl aq.) (as chloride). Chloride is red by transmitted light, green by reflected light.

▶ LD_{50} (mus, ivn) 18 mg/kg. Exp. reprod. effects (male). LK9840000

3-O-*β-D-Galactopyranoside:* [30113-37-2] *Malvidin 3-galactoside.* ***Primulin****. Uliginosin*
$C_{23}H_{25}O_{12}^{\oplus}$ 493.443
Isol. from many plant spp. inc. *Vaccinium myrtillus* (bilberry) and *Vaccinium corymbosum* (blueberry). Bronze needles or prisms + $5\frac{1}{2}H_2O$ (MeOH/HCl) (as chloride).

3-O-*β-D-Glucopyranoside:* [7228-78-6] *Malvidin 3-glucoside. Oenin. Ligulin. Enin. Enoside*
$C_{23}H_{25}O_{12}^{\oplus}$ 493.443
Pigment of skins of black grapes, also in other plants. Found in red wine. Violet cryst. with yellow metallic cast by transmitted light, bronze by reflected light (as chloride). $[\alpha]_D$ -421 (0.1% HCl aq.).

3-O-*(6*-O-*Acetyl-β-D-glucopyranoside):* [101072-66-6] *Malvidin 3-(6-acetylglucoside)*
$C_{25}H_{27}O_{13}^{\oplus}$ 535.48
Isol. from grape skins of port wine.

3-O-*(6*-O-*Malonyl-β-D-glucopyranoside), 5*-O-*β-D-glucopyranoside: Malvidin 3-(6*-O-*malonylglucoside) 5-glucoside*
$C_{32}H_{37}O_{20}^{\oplus}$ 741.632
Isol. from *Malva sylvestris* (high mallow).

3-O-*[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside]:* [34693-53-3] *Malvidin 3-(6-coumaroylglucoside)*
$C_{32}H_{31}O_{14}^{\oplus}$ 639.588
Pigment of skins of black grapes, found in red wine.

3-O-*[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside], 5*-O-*β-D-glucopyranoside:* [51939-51-6] ***Tibouchinin***
$C_{38}H_{41}O_{19}^{\oplus}$ 801.73
Isol. from grapes. λ_{max} 280 ; 305 ; 536 (MeOH/HCl).

3-O-*(4-Hydroxycinnamoylrutinoside), 5*-O-*β-D-glucopyranoside:* ***Negretein****. Nigretein*
$C_{44}H_{51}O_{23}^{\oplus}$ 947.873
Isol. from violet potatoes. Violet-brown globules or red needles + $1H_2O$ (HCl aq.) (as chloride).

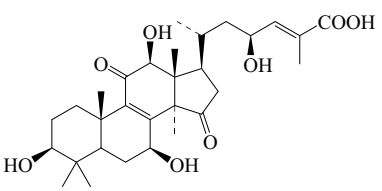
3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 5*-O-*β-D-glucopyranoside:* [61811-04-9] *Malvidin 5-glucoside 3-sophoroside*
$C_{35}H_{45}O_{22}^{\oplus}$ 817.727
Isol. from grapes.

3-O-*[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]:* [55463-07-5] *Malvidin 3-laminaribioside*
$C_{29}H_{35}O_{17}^{\oplus}$ 655.585
Isol. from *Eugenia jambolana* (jambolan).

[90276-14-5, 148154-67-0]

Bradley, W. *et al., J.C.S.*, 1928, 1541 (*synth*)
Levy, L.P. *et al., J.C.S.*, 1931, 2701 (*synth, bibl*)
Leon, A. *et al., J.C.S.*, 1932, 2221 (*synth*)
Robinson, R. *et al., J.C.S.*, 1932, 2299 (*Malvin*)
Pecket, R.C. *et al., New Phytol.*, 1960, **59**, 138 (*occur*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Harborne, J.B. *et al., Phytochemistry*, 1964, **3**, 151 (*Tibouchinin*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1746 (*occur*)
Pomilio, A.B. *et al., Phytochemistry*, 1973, **12**, 218 (*isol*)
Brouillard, R. *et al., J.A.C.S.*, 1977, **99**, 8461 (*isol*)
Srivastava, B.S. *et al., Planta Med.*, 1977, **32**, 138 (*isol*)
Hoshino, T. *et al., Phytochemistry*, 1981, **20**, 1971 (*cd*)
Hoshino, T. *et al., Tet. Lett.*, 1981, **22**, 3621 (*Malvin, Enin*)
Iacobucci, G.A. *et al., Tetrahedron*, 1983, **39**, 3005 (*rev*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Takeda, K. *et al., Phytochemistry*, 1989, **28**, 499 (*deriv*)
Santos, H. *et al., Phytochemistry*, 1993, **33**, 1227 (*Malvin*)
Merlin, J.-C. *et al., Phytochemistry*, 1994, **35**, 227 (*Raman*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MAO600

3,7,12,23-Tetrahydroxy-11,15-dioxolanosta-8,24-dien-26-oic acid T-159



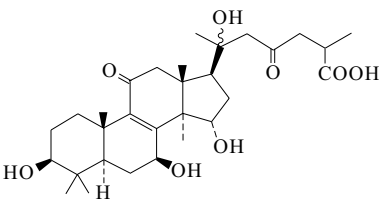
$C_{30}H_{44}O_8$ 532.673

(3β,7β,12β,23*S*,24*E*)-*form* [294674-12-7]
Ganoderic acid η
Constit. of *Ganoderma lucidum* (reishi). Yellow needles (MeOH aq.). Mp 212-214°. $[\alpha]_D$ +128 (c, 0.1 in EtOH). λ_{max} 209 (log ϵ 4.1); 257 (log ϵ 3.8) (no solvent reported).

7-Ketone: [294674-15-0] *3,12,23-Trihydroxy-7,11,15-trioxolanosta-8,24-dien-26-oic acid*. ***Ganoderic acid θ***
$C_{30}H_{42}O_8$ 530.657
Constit. of *Ganoderma lucidum* (reishi). Yellow needles (MeOH aq.). Mp 131-133°. $[\alpha]_D$ +71.3 (c, 0.1 in EtOH).

Min, B.-S. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1026-1033 (*isol, pmr, cmr*)

3,7,15,20-Tetrahydroxy-11,23-dioxolanost-8-en-26-oic acid T-160



$C_{30}H_{46}O_8$ 534.689

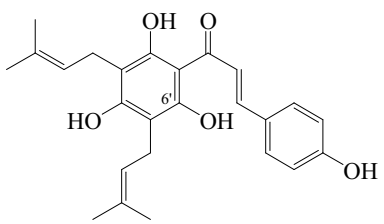
(3β,7β,15α,20ξ)-*form* [102607-24-9]
Ganoderic acid L
Metab. of *Ganoderma lucidum* (reishi).

Me ester:
Cryst. Mp 228-230°. $[\alpha]_D^{23}$ +66 (c, 0.2 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 809

2′,4,4′,6′-Tetrahydroxy-3′,5′-diprenylchalcone T-161

3-(4-Hydroxyphenyl)-1-[2,4,6-trihydroxy-3,5-bis(3-methyl-2-butenyl)]-2-propen-1-one. 3′,5′-Diprenylchalconaringenin



$C_{25}H_{28}O_5$ 408.493

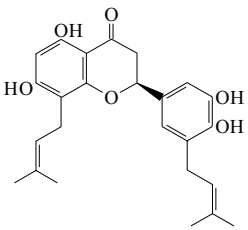
(*E*)-*form*
Constit. of hops (*Humulus lupulus*). λ_{max} 371 (MeOH).

6′-Me ether: [189299-04-5] *2′,4,4′-Trihydroxy-6′-methoxy-3′,5′-diprenylchalcone.* ***5′-Prenylxanthohumol***
$C_{26}H_{30}O_5$ 422.52
Constit. of *Humulus lupulus* (hops). Dark yellow powder.

Stevens, J.F. *et al., Phytochemistry*, 1997, **44**, 1575-1585; 2000, **53**, 759-775 (*isol, pmr, cmr, ms*)

3′,4′,5,7-Tetrahydroxy-5′,8-diprenylflavanone T-162

2-[3,4-Dihydroxy-5-(3-methyl-2-butenyl)-phenyl]-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI. ***Gancaonin E***



(*S*)-*form*

$C_{25}H_{28}O_6$ 424.493

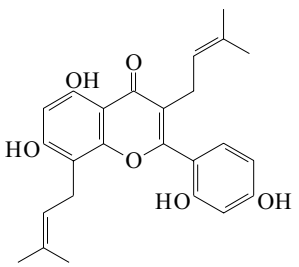
(*S*)-*form* [124596-89-0]
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Prisms. Mp 203-207°. $[\alpha]_D^{24}$ -16.8 (c, 0.8 in $CHCl_3$).

Fukai, T. *et al., Heterocycles*, 1989, **29**, 1369 (*isol*)

Dawidar, A.M. *et al., Phytochemistry*, 1994, **36**, 803 (*isol, pmr*)

2′,4′,5,7-Tetrahydroxy-3,8-diprenylflavone T-163

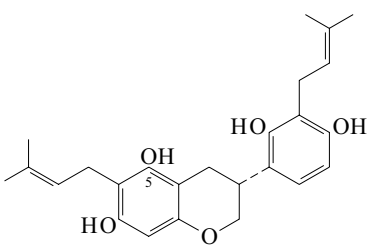
[62949-79-5]
2-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-3,8-bis(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI. ***Mulberrin***. *Kuwanon C*



$C_{25}H_{26}O_6$ 422.477
Constit. of the root bark of *Morus alba* (white mulberry). Cryst. (Et_2O/C_6H_6). Mp 148-150°. Mulberrin formerly assigned 3,6-diprenyl struct..

Nomura, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 529; 1978, **26**, 1453 (*uv, pmr, isol*)
Nomura, T. *et al., Heterocycles*, 1978, **9**, 1355
Chari, V.M. *et al., Z. Naturforsch., B*, 1978, **33**, 1547 (*cmr*)
Nomura, T. *et al., Planta Med.*, 1983, **49**, 90 (*isol*)

2′,4′,5,7-Tetrahydroxy-3′,6-diprenylisoflavan T-164



$C_{25}H_{30}O_5$ 410.509

(*R*)-*form*

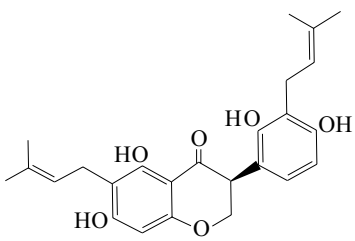
5-Me ether: [30508-27-1] *2′,4′,7-Trihydroxy-5-methoxy-3′,6-diprenylisoflavan.* ***Licoricidin***
Constit. of *Glycyrrhiza glabra* (licorice) and *Glycyrrhiza uralensis* (Chinese licorice). Cryst. ($CHCl_3/Et_2O$). Mp 154-156°. $[\alpha]_D^{22.5}$ +20 (c, 1 in MeOH). Struct. revised in 1988 (OMe group previously considered to be at 7-posn.).

5,7-Di-Me ether: [129314-37-0] *2′,4′-Dihydroxy-5,7-dimethoxy-3′,6-diprenylisoflavan*. ***Licorisoflavan A***. *7-O-Methylicoricidin*
$C_{27}H_{34}O_5$ 438.563
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Prisms (Me_2CO). Mp 65-67°. $[\alpha]_D^{20}$ +5.7 (c, 0.265 in MeOH). Identity of Licorisoflavan A (abs. config. not assigned) and 7-*O*-Methylicoricidin not establ. Phys. props. refer to Licorisoflavan A.

Shibata, S. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1932 (*isol*)
Kinoshita, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 141 (*isol*)
Shih, T.L. *et al., J.O.C.*, 1987, **52**, 2029 (*synth*)
Fukai, T. *et al., Heterocycles*, 1988, **27**, 2309 (*isol, struct, cmr*)
Zeng, L. *et al., Heterocycles*, 1992, **34**, 575 (*Licorisoflavan A*)

2′,4′,5,7-Tetrahydroxy-3′,6-diprenylisoflavanone T-165

Tetrapterol G. *Glisoflavanone*



$C_{25}H_{28}O_6$ 424.493
Constit. of *Glycyrrhiza glabra* (licorice).

(*S*)-*form*

2′-Me ether: [64280-18-8] *4′,5,7-Trihydroxy-2′-methoxy-3′,6-diprenylisoflavanone.* ***Isosophoranone***
$C_{26}H_{30}O_6$ 438.519
Cryst. (hexane). Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 189-191°. $[\alpha]_D^{22}$ -26 (c, 0.6 in $CHCl_3$). λ_{max} 293 (MeOH) (Berdy). λ_{max} 331 (MeOH-NAOH) (Berdy).

7-Me ether: [152511-45-0] *2′,4′,5-Trihydroxy-7-methoxy-3′,6-diprenylisoflavanone.* ***Kanzonol G***
$C_{26}H_{30}O_6$ 438.519
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow oil. $[\alpha]_D$ -13 (c, 0.04 in MeOH).

(±)-*form*
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Powder or needles. Mp 131° Mp 168-170°. λ_{max} 292 (log ϵ 4.26); 336 (sh) (log ϵ 3.53) (MeOH).

(ξ)-*form*

3-Hydroxy, 2′-Me ether: [202054-71-5] *3,4′,5,7-Tetrahydroxy-2′-methoxy-3′,6-diprenylisoflavanone.* ***Tomentosanol B***
$C_{26}H_{30}O_7$ 454.519
Pale yellow oil. λ_{max} 227 ; 291 ; 335 (sh) (MeOH).

Monache, G.D. *et al., Gazz. Chim. Ital.*, 1977, **107**, 189
Shirataki, Y. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2859
O'Niell, M.J. *et al., Phytochemistry*, 1986, **25**, 1315 (*isol*)
Fukai, T. *et al., Heterocycles*, 1993, **36**, 2565; 1994, **37**, 1819 (*Kanzonol G*)
Russell, G.B. *et al., Aust. J. Chem.*, 1997, **50**, 333 (*Isosophoranone*)
Tanaka, T. *et al., Phytochemistry*, 1997, **46**, 1431-1437 (*Tomentosanol B*)
Shirataki, Y. *et al., Phytochemistry*, 1999, **50**, 695-701 (*Tetrapterol G*)
Hatano, T. *et al., Phytochemistry*, 2000, **55**, 959-963 (*Glisoflavanone*)

2′,4′,5,7-Tetrahydroxy-3′,8-diprenylisoflavanone T-166

[104380-55-4]
*3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)-phenyl]-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI. 3′-(3,3-Dimethylallyl)kievitone*

$C_{25}H_{28}O_6$ 424.493

(*S*)-*form*
Yellow paste. $[\alpha]_D^{25}$ -20.3 (c, 0.01 in MeOH). λ_{max} 213 (log ε 5.3); 293 (log ε 4.15) (MeOH).

2′-Me ether: [194299-12-2] *4′,5,7-Trihydroxy-2′-methoxy-3′,8-diprenylisoflavanone.* ***Phyllanone B***
$C_{26}H_{30}O_6$ 438.519
Pale yellow oil. $[\alpha]_D$ -67 (c, 0.6 in CH_2Cl_2). Config. incorr. shown in ref. (1997) λ_{max} 293 (MeOH).

(±)-*form*
Isol. from *Phaseolus lunatus* (butter bean) seedlings under stress and from *Glycyrrhiza glabra* (licorice).

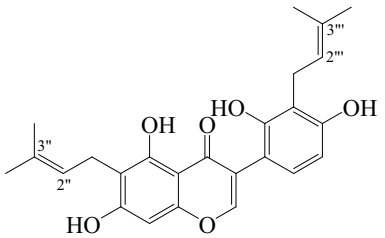
(ξ)-*form*

4′-Me ether:2′,5,7-Trihydroxy-4′-methoxy-3′,8-diprenylisoflavanone. ***Tetrapterol H***
$C_{26}H_{30}O_6$ 438.519
Yellow oil. λ_{max} 225 (sh) ; 293 ; 330 (sh) (MeOH).

O'Niell, M.J. *et al., Phytochemistry*, 1986, **25**, 1315 (*isol*)
Fukai, T. *et al., Heterocycles*, 1994, **37**, 1819 (*isol, pmr, cmr*)
Russell, G.B. *et al., Aust. J. Chem.*, 1997, **50**, 333-336 (*Phyllanone B*)
Shirataki, Y. *et al., Phytochemistry*, 1999, **50**, 695-701 (*Tetrapterol H*)
Bojase, G. *et al., Phytochemistry*, 2001, **56**, 837-841 (*isol, uv, pmr, cmr, ms*)

2′,4′,5,7-Tetrahydroxy-3′,6-diprenylisoflavone T-167

[90686-13-8]
*3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)-phenyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Angustone A****. 2′-Hydroxylupalbigenin. 3-(γ,γ-Dimethylallyl)luteone*



$C_{25}H_{26}O_6$ 422.477
Cryst. (Et_2O/petrol or $CHCl_3/C_6H_6$). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 159-160° (145-146°). λ_{max} 212 (ε 45700); 268 (ε 31400) (MeOH) (Berdy). λ_{max} 280 ; 345 (MeOH/NaOH) (Berdy).

5-O-[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranoside]: [261914-24-3]
$C_{37}H_{46}O_{14}$ 714.762
Light brown needles (Et_2O). Mp 174-175°. λ_{max} 214 (log ε 4.6); 267 (log ε 4.4) (MeOH).

2′-Me ether: [89143-44-2] *4′,5,7-Trihydroxy-2′-methoxy-3′,6-diprenylisoflavone.* ***2′-Methoxylupalbigenin***
Cryst. (EtOAc/petrol). Mp 216-217°.

7-Me ether: [156281-30-0] *2′,4′,5-Trihydroxy-7-methoxy-3′,6-diprenylisoflavone.* ***Kanzonol K***
$C_{26}H_{28}O_6$ 436.504
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow oil. λ_{max} 262 (log ε 4.05); 289 (sh) (log ε 4.04); 330 (sh) (log ε 3.46) (MeOH/$AlCl_3$).

Δ³″-Isomer, 2″-hydroxy: [121748-00-3] ***Lupinisol B***
$C_{25}H_{26}O_7$ 438.476
Gum. λ_{max} 212 (sh) ; 225 (sh) ; 268 ; 295 (sh) (MeOH).

Baruah, P. *et al., Phytochemistry*, 1984, **23**, 443-447 (*isol, pmr*)
Tahara, S. *et al., Phytochemistry*, 1984, **23**, 1889-1900 (*isol, uv, pmr, ms*)
Lane, G.A. *et al., Phytochemistry*, 1987, **26**, 295-300 (*isol, uv, pmr, cmr, ms*)
Tahara, S. *et al., Phytochemistry*, 1989, **28**, 901-911 (*Lupinisol B*)
Fukai, T. *et al., Phytochemistry*, 1994, **36**, 225-228 (*Kanzonol K*)
Yadava, R.N. *et al., Fitoterapia*, 1999, **70**, 475-477 (*5-rhamnosylrhamnoside*)

3′,4′,5,7-Tetrahydroxy-5′,6-diprenylisoflavone T-168

[129280-34-8]
*3-[3,4-Dihydroxy-5-(3-methyl-2-butenyl)-phenyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Isoangustone A***

$C_{25}H_{26}O_6$ 422.477
Isol. from the roots of *Glycyrrhiza uralensis* (Chinese licorice). Needles (Et_2O/hexane). Mp 191-193°.

Kiuchi, F. *et al., Heterocycles*, 1990, **31**, 629-636 (*isol, pmr, cmr*)

3′,4′,5,7-Tetrahydroxy-5′,8-diprenylisoflavone T-169

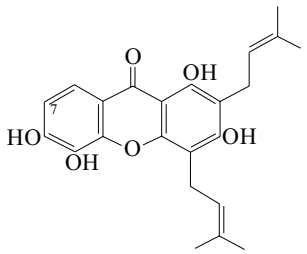
[199331-53-8]
Glyurallin B

$C_{25}H_{26}O_6$ 422.477
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Yellowish oil. λ_{max} 218 (sh) (log ε 4.6); 269 (log ε 4.46) (MeOH).

Shibano, M. *et al., Heterocycles*, 1997, **45**, 2053-2060 (*isol, uv, pmr, cmr*)

1,3,5,6-Tetrahydroxy-2,4-diprenylxanthone T-170

[103450-96-0]
*1,3,5,6-Tetrahydroxy-2,4-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one.* ***Xanthone V_{1a}***



$C_{23}H_{24}O_6$ 396.439
Brown solid (Et_2O/hexane). Mp 176-179°.

3-Me ether: [197447-28-2] *1,5,6-Trihydroxy-3-methoxy-2,4-diprenylxanthone.* ***Dulxanthone B***
$C_{24}H_{26}O_6$ 410.466
Constit. of the stem bark of *Garcinia dulcis* (mundu). Yellow oil. λ_{max} 236 (sh) ; 257 ; 282 (sh) ; 327 (MeOH).

7-Methoxy: [103450-97-1] *1,3,5,6-Tetrahydroxy-7-methoxy-2,4-diprenylxanthone.* ***Xanthone V_{2a}***
$C_{24}H_{26}O_7$ 426.465
Brown solid (Et_2O/hexane). Mp 170-173°.

Botta, B. *et al., Phytochemistry*, 1986, **25**, 1217
Ito, C. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1403-1413 (*Dulxanthone B*)

1,3,5,6-Tetrahydroxy-4,8-diprenylxanthone T-171

*1,3,5,6-Tetrahydroxy-4,8-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one*

$C_{23}H_{24}O_6$ 396.439

3,6-Di-Me ether: [4178-45-4] *1,5-Dihydroxy-3,6-dimethoxy-4,8-diprenylxanthone.* ***Dulxanthone C***
$C_{25}H_{28}O_6$ 424.493
Constit. of the stem bark of *Garcinia dulcis* (mundu). Yellow needles (Me_2CO)(synthetic) or pale yellow powder. Mp 200° dec.(synthetic). λ_{max} 236 ; 254 ; 284 (sh) ; 329 (MeOH).

Burling, E.D. *et al., Tetrahedron*, 1965, **21**, 2653-2669 (*synth*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1403-1413 (*isol, uv, ir, pmr, cmr*)

1,3,5,8-Tetrahydroxy-2,4-diprenylxanthone T-172

[33390-42-0]
*1,3,5,8-Tetrahydroxy-2,4-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one, 9CI.* ***Gartanin***

$C_{23}H_{24}O_6$ 396.439
Constit. of the fruits of *Garcinia mangostana* (mangosteen). Yellow needles. Mp 167°. λ_{max} 259 (ε 19950); 284 (ε 24000);

351 (ϵ 11200) (EtOH) (Berdy).

Govindachari, T.R. *et al., Tetrahedron*, 1971, **27**, 3919 (*isol, struct*)
Anand, S.M. *et al., Aust. J. Chem.*, 1974, **27**, 1515 (*synth*)
Gujral, V. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 3679 (*synth*)

1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone T-173

[31271-07-5]
*1,3,6,7-Tetrahydroxy-2,8-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one, 9CI.* ***γ-Mangostin****. Normangostin*

$C_{23}H_{24}O_6$ 396.439
Constit. of *Garcinia mangostana* (mangosteen). Yellow cryst. (EtOAc/petrol). Mp 207°. λ_{max} 247 ; 261 ; 314 ; 364 (MeOH) (Berdy). λ_{max} 280 ; 350 (EtOH) (Berdy).

7-Me ether: [6147-11-1] *1,3,6-Trihydroxy-7-methoxy-2,8-diprenylxanthone.* ***α-Mangostin***
$C_{24}H_{26}O_6$ 410.466
Pigment from *Garcinia mangostana* (mangosteen). Yellow needles (C_6H_6, petrol or EtOH aq.). Mp 180-181°. λ_{max} 243 ; 260 ; 314 ; 350 (MeOH) (Berdy). λ_{max} 243 (ϵ 34500); 259 (ϵ 27500); 318 (ϵ 19000); 351 (ϵ 7200) (EtOH) (Berdy).

3,6-Di-Me ether: [132031-39-1] *1,7-Dihydroxy-3,6-dimethoxy-2,8-diprenylxanthone*
$C_{25}H_{28}O_6$ 424.493
Constit. of *Garcinia mangostana* (mangosteen). Pale yellow needles (MeOH). Mp 192-194°.

3,7-Di-Me ether: [20931-37-7] *1,6-Dihydroxy-3,7-dimethoxy-2,8-diprenylxanthone.* ***β-Mangostin***
$C_{25}H_{28}O_6$ 424.493
From *Garcinia mangostana* (mangosteen). Lemon-yellow rods (EtOH). Mp 175-176°.

3,6,7-Tri-Me ether: [15404-76-9] *1-Hydroxy-3,6,7-trimethoxy-2,8-diprenylxanthone*
$C_{26}H_{30}O_6$ 438.519
Constit. of *Garcinia mangostana* (mangosteen). Cryst. (EtOH). Mp 120-121°.

3″-Hydroxy, 2″,3″-dihydro: [76996-27-5] ***Garcinone C***
$C_{23}H_{26}O_7$ 414.454
From *Garcinia mangostana* (mangosteen). Yellow solid (MeOH). Mp 216-218°.

3′-Hydroxy, 2′,3′-dihydro, O^7*-Me:* [149155-01-1] ***Cratoxylone***
$C_{24}H_{28}O_7$ 428.481
Gum.

3″-Hydroxy, 2″,3″-dihydro, O^7*-Me:* [107390-08-9] ***Garcinone D***
$C_{24}H_{28}O_7$ 428.481
From *Garcinia mangostana* (mangosteen). Light yellow needles (MeOH). Mp 202-204°.

4′-Hydroxy, 7-Me ether: ***Parvixanthone B***
$C_{24}H_{26}O_7$ 426.465
Yellow powder. Has (*Z*)-config. λ_{max} 206 (log ϵ 4.35); 242 (log ϵ 4.21); 314 (log ϵ 3.84); 353 (log ϵ 3.55) (MeOH).

*$\Delta^{1''}$-Isomer(*E*-), 3″-hydroxy, 3,7-di-Me ether:*
$C_{25}H_{28}O_7$ 440.492
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Yellow gum. λ_{max} 246 (log ϵ 4.6); 322 (log ϵ 4.29); 364 (log ϵ 4.1) (EtOH).

*$\Delta^{1''}$-Isomer(*E*-), 3″-hydroxy, 3,6,7-tri-Me ether:*
$C_{26}H_{30}O_7$ 454.519
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Pale yellow gum. λ_{max} 246 (log ϵ 4.61); 260 (log ϵ 4.56); 314 (log ϵ 4.42); 354 (log ϵ 3.96) (EtOH).

$\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 7-Me ether: [437711-43-8] ***Mangostenol***
$C_{24}H_{26}O_7$ 426.465
Constit. of the green fruit hulls of *Garcinia mangostana* (mangosteen). Yellow powder. Mp 157-159°. $[\alpha]_D^{31}$ -20 (c, 0.1 in MeOH). λ_{max} 243 (log ϵ 4.4); 319 (log ϵ 4.08); 358 (log ϵ 4) (EtOH).

$\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 3,7-di-Me ether:
$C_{25}H_{28}O_7$ 440.492
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Yellow gum. $[\alpha]_D$ +13.6 (c, 0.22 in MeOH). λ_{max} 244 (log ϵ 4.52); 256 (log ϵ 4.45); 314 (log ϵ 4.27); 354 (log ϵ 4.03) (EtOH).

$\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 6,7-di-Me ether:
$C_{25}H_{28}O_7$ 440.492
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Yellow gum. $[\alpha]_D$ -2.9 (c, 0.38 in $CHCl_3$). λ_{max} 244 (log ϵ 4.43); 260 (log ϵ 4.41); 314 (log ϵ 4.22); 352 (log ϵ 3.93) (EtOH).

$\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 3,6,7-tri-Me ether:
$C_{26}H_{30}O_7$ 454.519
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Pale yellow gum. $[\alpha]_D$ +30 (c, 0.2 in $CHCl_3$). λ_{max} 246 (log ϵ 4.29); 262 (log ϵ 4.31); 312 (log ϵ 4.15); 348 (log ϵ 3.65) (EtOH).

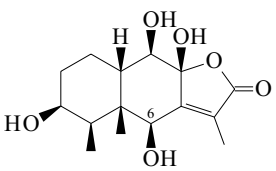
$\Delta^{3''}$-Isomer, 2″-oxo, 3,7-di-Me ether:
$C_{25}H_{26}O_7$ 438.476
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Yellow gum. λ_{max} 244 (log ϵ 4.39); 258 (log ϵ 4.28); 318 (log ϵ 4.09); 358 (log ϵ 3.99) (EtOH).

$\Delta^{3''}$-Isomer, 2″ξ-hydroxy, 3,7-di-Me ether:
$C_{25}H_{28}O_7$ 440.492
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Yellow gum. $[\alpha]_D$ +9.1 (c, 0.66 in MeOH). λ_{max} 244 (log ϵ 4.53); 258 (log ϵ 4.49); 316 (log ϵ 4.25); 356 (log ϵ 4.07) (EtOH).

$\Delta^{3''}$-Isomer, 2″ξ-hydroxy, 3,6,7-tri-Me ether:
$C_{26}H_{30}O_7$ 454.519
Constit. of the heartwood of *Garcinia mangostana* (mangosteen). Pale yellow gum. $[\alpha]_D$ +26 (c, 0.2 in $CHCl_3$). λ_{max} 244 (log ϵ 4.04); 262 (log ϵ 4.05); 314 (log ϵ 3.87); 354 (log ϵ 3.42) (EtOH).

Yates, P. *et al., J.A.C.S.*, 1958, **80**, 1691 (*struct, uv, ir, pmr*)
Stout, G.H. *et al., Chem. Comm.*, 1968, 211 (*uv, ms*)
Jefferson, A. *et al., Aust. J. Chem.*, 1970, **23**, 2539 (*isol, ir, uv, pmr, synth*)
Govindachari, T.R. *et al., Indian J. Chem.*, 1971, **9**, 505 (*isol, uv, ir, pmr*)
Govindachari, T.R. *et al., Tetrahedron*, 1971, **27**, 3919 (*isol*)
Gunasekara, S.P. *et al., Phytochemistry*, 1973, **12**, 232 (*isol*)
Lee, H.-H. *et al., J.C.S. Perkin 1*, 1981, 3205 (*synth*)
Sen, A.K. *et al., Phytochemistry*, 1982, **21**, 1747 (*Garcinone C*)
Sen, A.K. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 1157 (*Garcinone D*)
Ravikumar, K. *et al., Acta Cryst. C*, 1988, **44**, 1996 (*cryst struct*)
Bennett, G.J. *et al., J.C.S. Perkin 1*, 1990, 2671 (*biosynth*)
Chen, S.X. *et al., Planta Med.*, 1990, **62**, 381-382 (*γ- and α-Mangostin, activity*)
Bennett, G.J. *et al., Phytochemistry*, 1993, **32**, 1245 (*Cratoxylone*)
Okudaira, C. *et al., J. Enzyme Inhib.*, 2000, **15**, 129-138 (*α-Mangostin, activity*)
Xu, Y.-J. *et al., J. Nat. Prod.*, 2001, **64**, 1191-1195 (*Parvixanthone B*)
Suksamrarn, S. *et al., J. Nat. Prod.*, 2002, **65**, 761-763 (*Mangostenol*)
Nilar, *et al., Phytochemistry*, 2002, **60**, 541-548 (*Garcinia mangostana xanthones*)
Iikubo, K. *et al., Tet. Lett.*, 2002, **43**, 291-293 (*α-Mangostin*)

3,6,8,9-Tetrahydroxy-7(11)-eremophilen-12,8-olide T-174

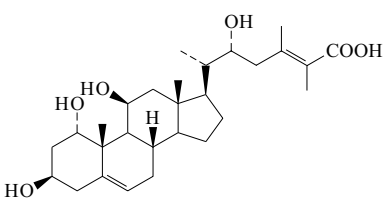


$C_{15}H_{22}O_6$ 298.335
(3β,6β,8βOH,9β,10β)-*form*
6-Angeloyl: [171422-89-2]
$C_{20}H_{28}O_7$ 380.437
Constit. of *Petasites japonicus* (sweet coltsfoot). Amorph. powder. $[\alpha]_D^{22}$ +41.2 (c, 0.4 in EtOH).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1738 (*isol, pmr, cmr*)

1,3,11,22-Tetrahydroxyergosta-5,24-dien-26-oic acid T-175

1,3,11,22-Tetrahydroxy-24-methylcholesta-5,24-dien-26-oic acid



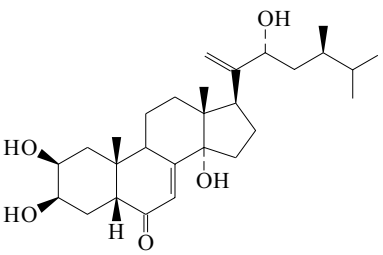
$C_{28}H_{44}O_6$ 476.652
(1α,3β,11β,22*R*,24*E*)-*form*
λ_{max} 209 (ϵ 11800); 295 (ϵ 4100) (Et_2O) (Berdy).

26-O-β-D-Glucopyranosyl ester: [155510-75-1]
$C_{34}H_{54}O_{11}$ 638.794
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. (MeOH aq.). Mp 210-211°. $[\alpha]_D^{25}$ -9.4 (c, 0.5 in MeOH).

26-O-[β-D-Glucopyranosyl-(1→2)-6-acet-

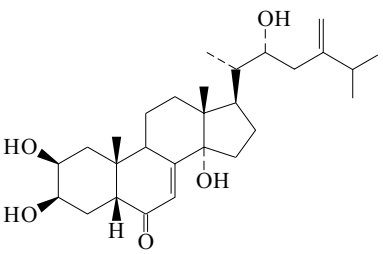
yl-β-D-glucopyranosyl] ester. [155510-76-2]
$C_{42}H_{66}O_{17}$ 842.973
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D^{25}$ -19 (c, 0.5 in MeOH).
Elliger, C.A. *et al., J. Nat. Prod.*, 1994, **57**, 348 (*isol, pmr, cmr*)

2,3,14,22-Tetrahydroxyergosta-7,20-dien-6-one T-176
2,3,14,22-Tetrahydroxy-24-methylcholesta-7,20-dien-6-one



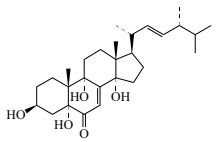
$C_{28}H_{44}O_5$ 460.653
(2β,3β,5β,14α,22*R*,24*R*)-*form* [141360-91-0]
Polyporusterone D
Constit. of *Polyporus umbellatus* (zhu ling). Amorph. powder. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 241 (ε 10230) (MeOH) (Berdy).
Ohsawa, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 143 (*isol, pmr, cmr*)

2,3,14,22-Tetrahydroxyergosta-7,24(28)-dien-6-one T-177
2,3,14,22-Tetrahydroxy-24-methylenecholest-7-en-6-one



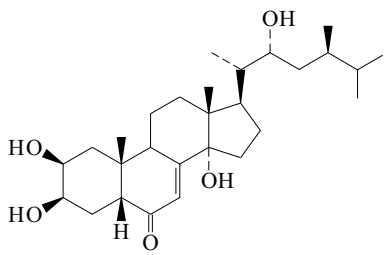
$C_{28}H_{44}O_5$ 460.653
(2β,3β,5β,14α,22*R*)-*form* [141360-94-3]
Polyporusterone G
Constit. of *Polyporus umbellatus* (zhu ling). Amorph. powder. Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 242 (ε 10470) (MeOH) (Berdy).
Ohsawa, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 143 (*isol, pmr, cmr*)

3,5,9,14-Tetrahydroxyergosta-7,22-dien-6-one T-178
3,5,9,14-Tetrahydroxy-24-methylcholesta-7,22-dien-6-one


(3β,5α,9α,14α,22*E*,24*R*)-*form*

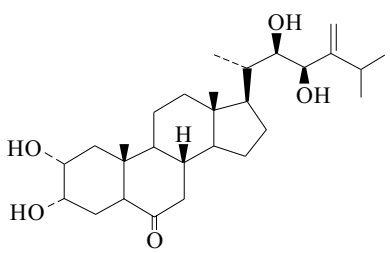
$C_{28}H_{44}O_5$ 460.653
(3β,5α,9α,14α,22*E*,24*R*)-*form* [211486-14-5]
Constit. of *Lentinus edodes* (shiitake), *Hypsizygus marmoreus* (bunashimeji), *Pleurotus ostreatus* (oyster mushroom) and *Pholiota nameko* (nameko). Amorph. powder. $[\alpha]_D^{19}$ -22.7 (c, 0.04 in $CHCl_3$). λ_{max} 225 (log ε 3.9) (MeOH).
(3β,5α,9α,14β,22*E*,24*R*)-*form* [348611-60-9]
Constit. of *Tricholoma matsutake* (matsutake). Amorph. powder. $[\alpha]_D^{18}$ -73.7 (c, 0.1 in $CHCl_3$). λ_{max} 236 (log ε 3.7) (MeOH).
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950 (*isol, pmr, cmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2001, **49**, 589-594 (*Tricholoma matsutake constit*)

2,3,14,22-Tetrahydroxyergost-7-en-6-one T-179
2,3,14,22-Tetrahydroxy-24-methylcholest-7-en-6-one



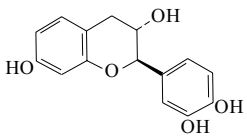
$C_{28}H_{46}O_5$ 462.668
(2β,3β,5β,14α,22*R*,24*R*)-*form* [141360-93-2]
Polyporusterone F
Constit. of *Polyporus umbellatus* (zhu ling). Needles (MeOH). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 251°. λ_{max} 242 (ε 10470) (MeOH) (Berdy).
Ohsawa, T. *et al., Chem. Pharm. Bull.*, 1992, **40**, 143 (*isol, pmr, cmr*)

2,3,22,23-Tetrahydroxyergost-24(28)-en-6-one T-180



$C_{28}H_{46}O_5$ 462.668
(2α,3α,5α,22*R*,23*R*)-*form* [85797-15-5]
Dolichosterone
Constit. of *Dolichos lablab* (hyacinth bean). Cryst. Mp 233-237°.
6-Deoxo: [87833-55-4] *5α-Ergost-24(28)-ene-2α,3α,22*R*,23*R*-tetrol, 9CI.* ***6-Deoxodolichosterone***
$C_{28}H_{48}O_4$ 448.685
Constit. of *Phaseolus vulgaris* (kidney bean) and *Dolichos lablab* (hyacinth bean). Cryst. (EtOAc/MeOH). Mp 219-220.5°. $[\alpha]_D^{23.5}$ +33.2 (c, 0.51 in MeOH).
Yukota, T. *et al., Agric. Biol. Chem.*, 1983, **47**, 2149
Baba, J. *et al., Agric. Biol. Chem.*, 1983, **47**, 659
Mori, K. *et al., Tetrahedron*, 1984, **40**, 1767 (*synth*)
Singh, H. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 989 (*rev*)
Adam, G. *et al., Phytochemistry*, 1986, **25**, 1787 (*rev*)

3,3′,4′,7-Tetrahydroxyflavan T-181
*2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-3,7-diol, 9CI. 3′,4′,7-Trihydroxy-3-flavanol*


(2*R*,3*S*)-*form*

$C_{15}H_{14}O_5$ 274.273
Quebrachocatechin, of undetd. stereochem., isol. from Quebracho in 1934.
(2*R*,3*S*)-*form* [490-49-3]
(-)-trans-*form*. ***Fisetinidol***
Light yellow cryst. (H_2O). Mp 214°. $[\alpha]_D$ -8.6 (c, 1.1 in 1:1 Me_2CO aq.).
3-O-β-D-Xylopyranoside: ***Anadanthoside.*** *Fisetinidol 3-xyloside*
$C_{20}H_{22}O_9$ 406.388
$[\alpha]_D^{25}$ +31.5 (c, 0.1 in MeOH).
Tetra-Ac:
Mp 50-60°. $[\alpha]_D$ +0.9 (c, 1.1 in tetrachloroethane).
(2*S*,3*R*)-*form* [35079-43-7] *(+)*-trans-*form*. **ent-*Fisetidinol***
Plates (H_2O). Mp 213-214°. $[\alpha]_D^{20}$ +8 (c, 0.55 in 1:1 Me_2CO aq.).
Tetra-Ac:
Amorph. Mp 55-60°. $[\alpha]_D^{20}$ -1 (c, 0.76 in tetrachloroethane).
Tetra-Me ether:3,3′,4′,7-Tetramethoxyflavan
$C_{19}H_{22}O_5$ 330.38
Cryst. (EtOH aq.). Mp 80-82°. $[\alpha]_D^{25}$ +19.2 (c, 2 in tetrachloroethane).
(2*S*,3*S*)-*form* [895-23-8] *(+)*-cis-*form*. **ent-*Epifisetinidol*.** *Epifisetinidol (obsol.)*
Mp 120-121°. $[\alpha]_D^{20}$ +82 (c, 0.5 in 50% Me_2CO aq.). Has been renamed here *ent*-Epifisetinidol in accordance with the proposals of Hemingway (1982). Formerly referred to as Epifisetinidol.
Tri-Me ether:
Mp 124°. $[\alpha]_D^{20}$ +66 (c, 0.5 in tetrachloroethane).
(2*RS*,3*SR*)-*form* *(±)*-trans-*form*
Tetra-Ac:
Cryst. (MeOH). Mp 145-146°.
(2ξ,3ξ)-*form* *Quebrachocatechin*. *Quebracho-*

catechol
Isol. from quebracho.
Freudenberg, K. *et al., Annalen*, 1934, **510**, 913 (*Quebrachocatechin*)
Weinges, K. *et al., Annalen*, 1958, **615**, 203; 1959, **627**, 229
Roux, D.G. *et al., Biochem. J.*, 1961, **78**, 120 (*isol, config*)
Dean, F.M. *et al., J.C.S.*, 1965, 828 (*isol, struct*)
Drewes, S.E. *et al., J.C.S.(C)*, 1966, 1644 (*isol*)
Weinges, K. *et al., Prog. Chem. Org. Nat. Prod.*, 1969, **27**, 158 (*rev*)
Korver, O. *et al., Tetrahedron*, 1971, **27**, 5459 (*cd*)
Kijjoa, A. *et al., Phytochemistry*, 1981, **20**, 1385 (*isol*)
Hemingway, R.W. *et al., J.C.S. Perkin 1*, 1982, 1209 (*nomencl*)
Tobiason, F.L. *et al., Tetrahedron*, 1993, **49**, 5927 (*conformn, cryst struct*)
Rossouw, W. *et al., Tetrahedron*, 1994, **50**, 12477 (*pmr, abs config*)
Piacente, S. *et al., Phytochemistry*, 1999, **51**, 709-711 (*Anadanthoside*)

3,4,4′,7-Tetrahydroxyflavan T-182

*3,4-Dihydro-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-3,4,7-triol, 9CI. 4′,7-Dihydroxy-3,4-flavandiol.* ***Guibourtacacidin***

$C_{15}H_{14}O_5$ 274.273
Solid. Mp 170° dec. (reddens at 150°). $[\alpha]_D^{21}$ +11.7 (c, 0.7 in Me_2CO aq.). Natural Guibourtacacidin contains the 2,3-*cis*-3,4-*cis*-, the 2,3-*trans*-3,4-*trans*- and the 2,3-*trans*-3,4-*cis*-diol isomers in the ratio 5:1:1.

(2*S*,3*R*,4*R*)-*form* [149820-45-1]
Constit. of the seeds of *Musa sapientum* (banana).

(2*S*,3*S*,4*R*)-*form* [149820-44-0]
Constit. of the seeds of *Musa sapientum* (banana).

[3527-02-4]

Roux, D.G. *et al., Biochem. J.*, 1963, **87**, 439 (*isol, synth*)
Saayman, H.M. *et al., Biochem. J.*, 1965, **96**, 36 (*struct, synth, config*)
Drewes, S.E. *et al., J.C.S.(C)*, 1968, 1140 (*ms*)
du Preez, I.C. *et al., J.C.S.(C)*, 1970, 1800 (*isol, pmr*)
Clark-Lewis, J.W. *et al., Aust. J. Chem.*, 1972, **25**, 1943 (*isol*)
Ferreira, D. *et al., Phytochemistry*, 1985, **24**, 2415 (*isol*)
Steynberg, J.P. *et al., J.C.S. Perkin 1*, 1987, 1705 (*isol, synth*)
Ali, M. *et al., Pharmazie*, 1993, **48**, 455 (*isol*)

3′,4′,5′,7-Tetrahydroxyflavan T-183

*3,4-Dihydro-2-(3,4,5-trihydroxyphenyl)-2*H*-1-benzopyran-7-ol. 7-Hydroxy-2-(3,4,5-trihydroxyphenyl)chroman*

$C_{15}H_{14}O_5$ 274.273

4′-Me ether:3′,5′,7-Trihydroxy-4′-methoxyflavan. Auriculin†
$C_{16}H_{16}O_5$ 288.299
Needles ($CHCl_3$/MeOH). Mp 210°. $[\alpha]_D$ -9.23 (c, 1.3 in MeOH).

*4′-Me ether, 5′-*O*-β-D-glucopyranoside:* [75871-96-4] ***Auriculoside***
$C_{22}H_{26}O_{10}$ 450.441
Mp 140°. $[\alpha]_D$ -77 (c, 1 in MeOH).

3′,4′,7-Tri-Me ether: [133342-90-2] *5′-Hydroxy-3′,4′,7-trimethoxyflavan*
$C_{18}H_{20}O_5$ 316.353
Constit. of the roots of *Muntingia calabura* (Jamaica cherry). Oil. $[\alpha]_D^{20}$ -25 (c, 0.22 in $CHCl_3$). λ_{max} 227 (ϵ 12900); 280 (ϵ 4030) (MeOH) (Berdy).
Sahai, R. *et al., Phytochemistry*, 1980, **19**, 1560
Kaneda, N. *et al., J. Nat. Prod.*, 1991, **54**, 196 (*5′-Hydroxy-3′,4′,7-trimethoxyflavan*)

3,4′,5,7-Tetrahydroxyflavan T-184

*3,4-Dihydro-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-3,5,7-triol, 9CI. 4′,5,7-Trihydroxyflavanol*

$C_{15}H_{14}O_5$ 274.273

(2*R*,3*R*)-*form* [24808-04-6] ***(-)-Epiafzelechin***
Constit. of *Actinidia chinensis* (kiwi fruit) and *Juniperus communis* (juniper). Needles (EtOH aq.). Mp 240-243° dec. (312°). $[\alpha]_D^{19}$ -58.9 (c, 3 in EtOH). $[\alpha]_D$ -4 (c, 1 in Me_2CO).

Tetra-Ac:
Prisms (AcOH aq.). Mp 126-127°.

*5-*O*-β-D-Glucopyranoside:* [94285-13-9]
$C_{21}H_{24}O_{10}$ 436.415
Buff cryst. (EtOAc). Mp 190°. $[\alpha]_D$ -38.3 (MeOH).

*3-*O*-β-D-Glucopyranoside:* [114637-87-5]
$C_{21}H_{24}O_{10}$ 436.415
Needles. Mp 234°. $[\alpha]_D^{18}$ -56.3 (c, 1.1 in MeOH).

*7-*O*-β-D-Glucopyranoside:* [126595-96-8] ***Symposide***
$C_{21}H_{24}O_{10}$ 436.415
Flat needles (EtOAc/MeOH). Mp 192-195°. $[\alpha]_D^{25}$ -102 (c, 0.2 in MeOH). $[\alpha]_D^{20}$ -58.6. λ_{max} 230 ; 275 (MeOH).

*3-*O*-β-D-Allopyranoside:* [147511-60-2] ***Propinqualin***
$C_{21}H_{24}O_{10}$ 436.415
Cryst. + $1H_2O$ (MeOH). Mp 172-174°. $[\alpha]_D^{25}$ -23.6 (c, 0.04 in MeOH).

*3-*O*-(3,4,5-Trihydroxybenzoyl):* [108907-43-3] ***3-Galloyl-(-)-epiafzelechin***. *(-)-Epiafzelechin 3-gallate*
$C_{22}H_{18}O_9$ 426.379
Isol. from *Camellia sinensis* var. *assamica* (oolong tea). Off-white powder + $1H_2O$. $[\alpha]_D^{21}$ -181.7 (c, 0.9 in Me_2CO).

4′,5,7-Tri-Me ether:
Prisms (MeOH). Mp 110°. $[\alpha]_D^{20}$ -67.4 (c, 2 in EtOH).

(2*R*,3*S*)-*form* [2545-00-8] ***Afzelechin***
Mp 221-222° dec. $[\alpha]_D^{20}$ +20.6 (5% Me_2CO aq.).

*7-*O*-β-D-Apiofuranoside:* [114590-44-2] *Afzelechin 7-apioside*
$C_{20}H_{22}O_9$ 406.388
Constit. of rhizomes of *Polypodium glycyrrhiza* (licorice fern). Powder ($CHCl_3$). Mp 135-137°. $[\alpha]_D$ -93.3 (c, 0.12 in MeOH). λ_{max} 224 (sh) (ϵ 58900); 274 (ϵ 11500) (MeOH) (Derep).

*3-*O*-β-D-Xylopyranoside:* [143458-89-3] *Afzelechin 3-xyloside.* ***Arthromerin A***
$C_{20}H_{22}O_9$ 406.388
Off-white powder. $[\alpha]_D^{25}$ -3.79 (c, 1 in MeOH). CAS name is defective.

*3-*O*-β-D-Glucopyranoside:Afzelechin 3-glucoside.* ***Arthromerin B***
$C_{21}H_{24}O_{10}$ 436.415
Off-white powder. $[\alpha]_D^{25}$ -3.03 (c, 1 in MeOH).

*4′-*O*-β-D-Glucopyranoside:* [156521-54-9] *Afzelechin 4′-glucoside*
$C_{21}H_{24}O_{10}$ 436.415
Light brown cryst. (MeOH). Mp 186-187°. $[\alpha]_D^{24}$ +37 (c, 1.2 in MeOH aq.).

*3-*O*-α-L-Rhamnopyranoside:* [142741-31-9] *Afzelechin 3-rhamnoside*
$C_{21}H_{24}O_9$ 420.415
Powder. Mp 118-120°. $[\alpha]_D^{20}$ -20.5 (c, 0.35 in MeOH).

4′,5-Di-Me ether: [67970-23-4] *3,7-Dihydroxy-4′,5-dimethoxyflavan.* ***4′,5-Di-O-methylafzelechin***
$C_{17}H_{18}O_5$ 302.326
Oil.

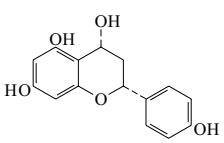
(2*S*,3*S*)-*form* [36801-69-1] ***(+)-Epiafzelechin***
$[\alpha]_D$ +66 (EtOH).

(2ξ,3ξ)-*form*

*3-*O*-α-D-Xylopyranoside:* [53549-74-9] ***Feulledin***
$C_{20}H_{22}O_9$ 406.388Unknown config..
King, F.E. *et al., J.C.S.*, 1955, 2948 (*isol, struct*)
Hillis, W.E. *et al., Aust. J. Chem.*, 1960, **13**, 390 (*isol, struct*)
Korver, O. *et al., Tetrahedron*, 1971, **27**, 5459 (*cd*)
Monache, F.D. *et al., Phytochemistry*, 1972, **11**, 2333 (*isol, bibl*)
Bhakuni, D.S. *et al., Rev. Latinoam. Quim.*, 1974, **5**, 109 (*Feulledin*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1677 (*Di-O-methylafzelechin*)
Friedrich, H. *et al., Planta Med.*, 1978, **33**, 251 (*isol*)
Waterman, P.G. *et al., Planta Med.*, 1979, **37**, 178 (*isol, cmr, pmr*)
Sethi, V.K. *et al., Phytochemistry*, 1984, **23**, 2402 (*Epiafzelechin 5-glucoside*)
Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1987, **35**, 611 (*3-Galloylepiafzelechin*)
Kim, J. *et al., Tet. Lett.*, 1987, **28**, 3655 (*apioside*)
Dhaon, R. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 982-983 (*Symposide, isol, uv, pmr, ir*)
Drewes, S.E. *et al., Phytochemistry*, 1992, **31**, 1073 (*3-rhamnoside*)
Wen-Sheng, Y. *et al., Phytochemistry*, 1992, **31**, 4385-4386 (*Arthromerins*)
Songqing, L. *et al., Phytochemistry*, 1994, **35**, 1595 (*Propinqualin*)
Baek, N.I. *et al., Phytochemistry*, 1994, **36**, 513 (*Afzelechin 4′-glucoside*)
Yamanaka, M. *et al., Phytochemistry*, 1995, **40**, 1149 (*7-glucoside, pmr, cmr, ms*)
Jin, C. *et al., Phytochemistry*, 1999, **50**, 505-508 (*Symposide, pmr, cmr*)
Min, K.R. *et al., Planta Med.*, 1999, **65**, 460-462 (*isol, pmr, cmr*)
Hwang, B.Y. *et al., J. Nat. Prod.*, 1999, **64**, 82-84 (*activity*)

4,4′,5,7-Tetrahydroxyflavan T-185

[55167-29-8]
4′,5,7-Trihydroxy-4-flavanol. ***Apiforol***



(2*RS*,4*RS*)-*form*

$C_{15}H_{14}O_5$ 274.273

(2*RS*,4*RS*)-*form*
(±)-cis-*form*

4′,5,7-Tri-Me ether: [5188-71-6]

Mp 159°.

(2*RS*,4*SR*)-*form* (±)-trans-*form*

4′,5,7-Tri-Me ether: [5188-72-7] *4-Hydroxy-4′,5,7-trimethoxyflavan. 4′,5,7-Trimethoxy-4-flavanol*
$C_{18}H_{20}O_5$ 316.353
Mp 117°.

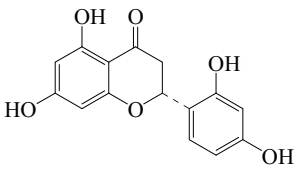
(2ξ,4ξ)-*form*
Isol. from cobs and silk of corn (*Zea mays*).

[10493-01-3, 66312-92-3]

Krishnamurty, H.G. *et al., Tet. Lett.*, 1965, 3689 (*synth*)
Kamat, M.S. *et al., Indian J. Chem.*, 1970, **8**, 119 (*synth*)
Styles, E.D. *et al., Phytochemistry*, 1975, **14**, 413 (*isol*)
Lam, J. *et al., Phytochemistry*, 1975, **14**, 1621 (*isol*)
Radford, T. *et al., Org. Mass Spectrom.*, 1979, **14**, 299 (*ms*)
Watterson, J.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 41 (*isol*)

2′,4′,5,7-Tetrahydroxyflavanone T-186

[121694-88-0]
*2-(2,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. **Norartocarpanone**. Steppogenin*



(*R*)-*form*

$C_{15}H_{12}O_6$ 288.256

(*R*)-*form*

4′-O-β-D-Glucopyranoside:
$C_{21}H_{22}O_{11}$ 450.398
Amorph. solid. Mp 259-263°. $[\alpha]_D$ -65.5 (c, 1 in MeOH). Assignment of config. dubious λ_{max} 286 ; 332 (sh) (MeOH).

(*S*)-*form* [56486-94-3]
Isol. from *Artocarpus incisus* (breadfruit). Prisms. Mp 255-257°. $[\alpha]_D$ +14.5 (c, 0.1 in MeOH).

7-O-β-D-Glucopyranoside: [20194-60-9] ***Stepposide***
$C_{21}H_{22}O_{11}$ 450.398
Needles. Mp 148-150°. $[\alpha]_D^{20}$ -52.5 (c, 1.12 in MeOH).

2′-Me ether: [57462-21-2] *4′,5,7-Trihydroxy-2′-methoxyflavanone*
$C_{16}H_{14}O_6$ 302.283
Cryst. (AcOH aq.). Mp 203° dec.

4′-Me ether, 7-O-β-D-glucopyranoside: [96157-14-1] ***Viscoside A***
$C_{22}H_{24}O_{11}$ 464.425

7-Me ether: [520-25-2] *2′,4′,5-Trihydroxy-7-methoxyflavanone*. ***Artocarpanone***
$C_{16}H_{14}O_6$ 302.283
Cryst. (Et_2O/hexane). Mp 210°.

4′,7-Di-Me ether:2′,5-Dihydroxy-4′,7-dimethoxyflavanone. ***Artocarpanone A***
$C_{17}H_{16}O_6$ 316.31
Constit. of the roots of *Artocarpus heterophyllus* (jackfruit). Needles (MeOH). Mp 159-160°. $[\alpha]_D^{23}$ -6.7 (c, 0.06 in Me_2CO). Not to be confused with Artocarpanone above.

2′,4′,5-Tri-Me ether: [64166-14-9] *7-Hydroxy-2′,4′,5-trimethoxyflavanone*. ***Cerasinone***
$C_{18}H_{18}O_6$ 330.337
Isol. from *Prunus cerasus* (cherry). Pale yellow needles (MeOH). Mp 200-201°.

2′,5,7-Tri-Me ether, 4′-O-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{30}H_{38}O_{15}$ 638.621
Light yellow cryst. Mp 213-214°. λ_{max} 288 ; 300 (sh) (MeOH).

Tetra-Me ether: [56317-22-7] *2′,4′,5,7-Tetramethoxyflavanone*. ***Arjunone***
$C_{19}H_{20}O_6$ 344.363
Mp 170°. $[\alpha]_D^{22}$ +16.6.

[73036-53-0, 116222-57-2]

Dave, K.G. *et al., J. Sci. Ind. Res., Sect. B*, 1960, **19**, 470 (*Artocarpanone*)
Sotnikova, O.M. *et al., Khim. Prir. Soedin.*, 1968, **4**, 82; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 71 (*Steppogenin, Stepposide*)
Nagarajan, G.R. *et al., Phytochemistry*, 1977, **16**, 1317 (*Cerasinone*)
Nagarajan, G.R. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 439 (*Cerasinone*)
Nagar, A. *et al., Planta Med.*, 1979, **37**, 183 (*Arjunone*)
Li, M. *et al., Zhongcaoyao*, 1985, **16**, 49; *CA*, **102**, 182423 (*Viscoside A*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1991, **46**, 325 (*2′-Me ether*)
Lin, C.-N. *et al., Phytochemistry*, 1995, **39**, 1447 (*Artocarpanone A*)
Shimizu, K. *et al., Planta Med.*, 1998, **64**, 408-412 (*isol, cd*)
El-Sohly, H.N. *et al., Phytochemistry*, 1999, **52**, 141-145 (*4′-glucoside*)
Srivastava, S.K. *et al., Fitoterapia*, 2000, **72**, 106-112 (*2′,5,7-tri-Me 4′-rutinoside*)

2,4′,5,7-Tetrahydroxyflavanone T-187

[58124-18-8]
*2,3-Dihydro-2,5,7-trihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 2-Hydroxynaringenin*

$C_{15}H_{12}O_6$ 288.256
Constit. of the bark of *Prunus avium* (wild cherry). Dec. >340°.

7-O-β-D-Glucopyranoside:
$C_{21}H_{22}O_{11}$ 450.398Natural intermed. in the conversion of methionine to cysteine via homocysteine.

[131023-26-2]

Hauteville, M. *et al., Bull. Soc. Chim. Fr.*, 1975, 1803 (*synth, uv, Raman*)
Kerscher, F. *et al., Z. Naturforsch., C*, 1987, **42**, 519
Bayer, O. *et al., Gartenbauwissenschaft*, 1989, **54**, 138 (*occur*)
Britsch, L. *et al., Arch. Biochem. Biophys.*, 1990, **282**, 152 (*synth*)
Lee, S.-S. *et al., J. Chin. Chem. Soc. (Taipei)*, 1995, **42**, 101 (*7-glucoside*)

2′,5,6,7-Tetrahydroxyflavanone T-188

$C_{15}H_{12}O_6$ 288.256
Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. λ_{max} 289 (ε 16220); 312 (EtOH) (Berdy).

(*S*)-*form*

6,7-Methylene ether: [188440-65-5] *2′,5-Dihydroxy-6,7-methylenedioxyflavanone*
$C_{16}H_{12}O_6$ 300.267
Cryst. Mp 195°. $[\alpha]_D^{21}$ -51.4 (c, 0.5 in MeOH).

6,7-Methylene, 2′,5-di-Me ether: [60132-69-6] *2′,5-Dimethoxy-6,7-methylenedioxyflavanone*. ***Betagarin***
$C_{18}H_{16}O_6$ 328.321
Constit. of the leaves of sugar beet (*Beta vulgaris*) infected with *Cercospora beticola*. Mp 187-189°. No opt. rotn. reported; abs. config. is probable λ_{max} 242 (ε 6840); 279 (ε 4790); 335 (ε 2160) (MeOH) (Berdy).

Geigert, J. *et al., Tetrahedron*, 1973, **29**, 2703 (*isol, struct, synth, Betagarin*)
Kojima, K. *et al., Phytochemistry*, 1997, **44**, 711 (*2′,5-Dihydroxy-6,7-methylenedioxyflavanone*)

3,3′,4′,7-Tetrahydroxyflavanone T-189

[101849-13-2]
*2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,7-Trihydroxydihydroflavonol. **Fustin**. Dihydrofisetin*

$C_{15}H_{12}O_6$ 288.256

(2*R*,3*R*)-*form* [20725-03-5]
(+)-trans-*form*
Needles (H_2O). Mp 228-229°. $[\alpha]_D^{23}$ +28.3 (c, 0.9 in 50% Me_2CO aq.).

3-Ac: [135607-79-3] ***3-O-Acetylfustin***
$C_{17}H_{14}O_7$ 330.293

Tetra-Ac:
Cryst. (EtOH). Mp 116-119°. $[\alpha]_D^{25}$ +24.4 (c, 0.8 in C_2Cl_4).

3-O-β-D-Glucopyranoside: [19209-93-9]
$C_{21}H_{22}O_{11}$ 450.398
Glass.

7-O-α-L-Rhamnopyranoside: [114728-43-7]
$C_{21}H_{22}O_{10}$ 434.399
Constit. of the roots of the famine food *Adansonia digitata* (baobab).

3-Me ether: [71326-00-6] *3′,4′,7-Trihydroxy-3-methoxyflavanone. 3-O-Methyl-(+)-*trans-*fustin*
$C_{16}H_{14}O_6$ 302.283
Identified as the tri-Me ether.

7-Me ether: [116822-59-4] *3,3′,4′-Trihydroxy-7-methoxyflavanone*
$C_{16}H_{14}O_6$ 302.283

7-Me ether, 3-Ac: [135607-80-6] *3-Acetoxy-3′,4′-dihydroxy-7-methoxyflavanone*
$C_{18}H_{16}O_7$ 344.32

3,7-Di-Me ether: [110559-11-0] *3′,4′-Dihydroxy-3,7-dimethoxyflavanone*
$C_{17}H_{16}O_6$ 316.31
Abs. config. of this deriv. not certain.

3′,4′,7-Tri-Me ether:3-Hydroxy-3′,4′,7-trimethoxyflavanone
$C_{18}H_{18}O_6$ 330.337
Cryst. (EtOH). Mp 141°. $[\alpha]_D^{28}$ -11 (c, 0.5 in $CHCl_3$).

3,3′,4′,7-Tetra-Me ether:3,3′,4′,7-Tetramethoxyflavanone
$C_{19}H_{20}O_6$ 344.363
Cryst. (cyclohexane/Me_2CO). Mp 148°.

$[\alpha]_D^{24}$ +39 (c, 0.3 in $CHCl_3$).

(2*S*,3*S*)-*form* [17654-28-3] *(-)*-trans-*form*
Cryst. (H_2O). Mp 228°. $[\alpha]_D^{25}$ -26 (c, 2 in 50% Me_2CO aq.).

Tetra-Ac:
Cryst. (EtOH). Mp 117-118°. $[\alpha]_D^{23}$ -25.2 (c, 0.8 in C_2Cl_4).

(2*RS*,3*RS*)-*form* *(±)*-trans-*form*
Cryst. (H_2O). Mp 223-225°.

Tetra-Ac:
Needles (EtOH). Mp 150-151°.

3-Me ether: [38681-23-1] *3′,4′,7-Trihydroxy-3-methoxyflavanone. 3*-O-*Methyl-(±)*-trans-*fustin*
$C_{16}H_{14}O_6$ 302.283

3′,4′-Methylene ether , 7-Me ether: [81855-47-2] *3-Hydroxy-7-methoxy-3′,4′-methylenedioxyflavanone*
$C_{17}H_{14}O_6$ 314.294Config. not detd..

Tetra-Me ether:
Needles (EtOH). Mp 143°.

(2*RS*,3*SR*)-*form* *(±)*-cis-*form*

3-Me ether: [38681-24-2] *3*-O-*Methyl-(±)*-cis-*fustin*
$C_{16}H_{14}O_6$ 302.283

Weinges, K. *et al., Annalen*, 1959, **627**, 229 (*isol, config*)
Roux, D.G. *et al., Biochem. J.*, 1960, **77**, 315; 1962, **84**, 416 (*isol*)
Saayman, H.M. *et al., Biochem. J.*, 1965, **97**, 794 (*biosynth*)
Markham, K.R. *et al., Tetrahedron*, 1968, **24**, 823 (*isol, struct*)
Tomas, F. *et al., An. Quim.*, 1972, **68**, 123; 1973, **69**, 1325; *CA*, **77**, 33665; **80**, 89130 (*uv, ir*)
Kingston, D.G.I. *et al., Tetrahedron*, 1973, **29**, 4083 (*ms*)
Ferreira, D. *et al., J.C.S. Perkin 1*, 1974, 1492 (*deriv*)
Malan, E. *et al., Phytochemistry*, 1974, **13**, 1575 (*3-O-Methyl-(±)-trans-fustin*)
The Flavonoids, (Eds. Harborne, J.B. *et al*), Chapman and Hall, London, 1975, 585 (*occur*)
Brandt, E.V. *et al., J.C.S. Perkin 1*, 1979, 777 (*isol, 3-Me ether*)
Burger, A.P.N. *et al., Phytochemistry*, 1983, **22**, 2813 (*isol*)
Takahashi, H. *et al., Heterocycles*, 1986, **24**, 369 (*synth*)
Crins, W.J. *et al., Phytochemistry*, 1987, **26**, 2128
Wollenweber, E. *et al., Phytochemistry*, 1991, **30**, 2445 (*derivs*)

3,4′,5,7-Tetrahydroxyflavanone T-190

[5150-32-3]
*2,3-Dihydro-3,5,7-trihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxydihydroflavonol. 3-Hydroxynaringenin. Dihydrokaempferol*

$C_{15}H_{12}O_6$ 288.256

(2*R*,3*R*)-*form* [480-20-6]
(+)-trans-*form*. ***Aromadendrin***†. *Aromadendrol. Katuranin*
Isol. from *Citrus* spp. and many other plants. Cryst. Mp 237-241° dec Mp 247-249°. $[\alpha]_D^{25}$ +26.5 (c, 2 in MeOH). $[\alpha]_D^{25}$ +45 (c, 4 in 50% Me_2CO aq.).

3,7-Di-O-*β*-D-*glucopyranoside:* [80212-10-8]
$C_{27}H_{32}O_{16}$ 612.54
Constit. of broad bean (*Vicia faba*) leaves. Config. unknown.

3-Me ether: [97231-20-4] *4′,5,7-Trihydroxy-3-methoxyflavanone*
$C_{16}H_{14}O_6$ 302.283
Constit. of *Prunus domestica* (plum). Yellow solid. Mp 182-184°.

4′-Me ether, 7-O-*α*-L-*rhamnopyranoside:* [114847-26-6]
$C_{22}H_{24}O_{10}$ 448.426
Constit. of the fruit of orange (*Citrus sinensis*). Cryst. Mp 270-272°.

(2*R*,3*S*)-*form*
cis-*form*

7-Me ether: [35815-06-6] ***Folerogenin***. *Isoauroside*
$C_{16}H_{14}O_6$ 302.283
Isol. from licorice (*Glycyrrhiza glabra*) leaves. Claimed first isoln. of a *cis*-flavonol.

[54081-49-1, 54081-50-4, 70594-44-4, 137225-59-3, 143114-80-1]

Gripenberg, J. *et al., Acta Chem. Scand.*, 1952, **6**, 1152 (*isol*)
Janes, N.P. *et al., J.C.S.*, 1960, 2560 (*isol, abs config*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Grouiller, A. *et al., Bull. Soc. Chim. Fr.*, 1967, 1938 (*pmr*)
Lutskii, V.I. *et al., Khim. Prir. Soedin.*, 1971, **7**, 203; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 197 (*ord, cd*)
Harborne, J.B. *et al., Phytochemistry*, 1971, **10**, 2727 (*occur*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 374; 583; 1635 (*occur*)
Litvinenko, V.I. *et al., Rastit. Resur.*, 1972, **8**, 35 (*Folerogenin*)
Duddeck, H. *et al., Phytochemistry*, 1978, **17**, 1369 (*cmr*)
Ayafor, J.F. *et al., J.C.S. Perkin 1*, 1981, 2563 (*derivs*)
Markham, K.R. *et al., Phytochemistry*, 1984, **23**, 2049 (*deriv*)
Grande, M. *et al., Planta Med.*, 1985, 414 (*derivs*)
Chatterjee, P. *et al., Phytochemistry*, 1988, **27**, 946 (*4′-Me ether 7-rhamnoside*)
Parmar, V.S. *et al., Phytochemistry*, 1992, **31**, 2185 (*3-Me ether*)

3′,4′,5,7-Tetrahydroxyflavanone T-191

[4049-38-1]
*2-(3,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. **Eriodictyol**. Huazhongilexone*

$C_{15}H_{12}O_6$ 288.256

Huazhongilexone originally assigned incorrect struct..Log P 1.2 (uncertain value) (calc).

(*S*)-*form* [552-58-9]
Widespread flavanone found esp. in citrus fruits (lemon, tangerine, orange, grapefruit and pummelo) and peppermint. Glycosides also widely distributed. Plates (EtOH). Mp 267°. λ_{max} 290 (ε 346); 326 (ε 140) (MeOH) (Berdy).

7-O-*α*-L-*Rhamnopyranoside:* [480-35-3] ***Eriodictin***
$C_{21}H_{22}O_{10}$ 434.399
Isol. from juice of *Citrus limettioides* (sweet lime). Cryst. (EtOAc). Mp 184-186° dec. $[\alpha]_D^{20}$ -51.5 (Py).

7-O-*β*-D-*Glucopyranoside:* [38965-51-4] ***Pyracanthoside***. *Miscanthoside*
$C_{21}H_{22}O_{11}$ 450.398
Constit. of *Pyrus communis* (pear) and *Mentha aquatica* (water mint),. Mp 175-177° Mp 215-216°. $[\alpha]_D$ -40 (60% EtOH aq.).

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [13463-28-0] ***Eriocitrin***. *Eriodictioside*
$C_{27}H_{32}O_{15}$ 596.541
Isol. from *Mentha piperita* (peppermint) leaves and from *Citrus* spp.. Mp 167-172°. $[\alpha]_D^{20}$ -62 (c, 1.4 in MeOH).

3′-Me ether, 4′-O-*(2-methylpropanoyl):* [140163-21-9] *5,7-Dihydroxy-3′-methoxy-4′*-O-*isobutanoylflavanone*
$C_{20}H_{20}O_7$ 372.374
Isol. from *Eriodictyon californicum* (yerba santa). Prisms (MeOH). Mp 149-150°.

5-Me ether, 7-O-*[xylosyl-(1→?)-galactoside]:* [79284-69-8]
$C_{27}H_{32}O_{15}$ 596.541
Isol. from the edible fern *Diplazium esculentum*. Yellow needles (EtOAc/petrol). Mp 62-64°.

5-Me ether, 7-O-*[xylosyl-(1→?)-arabinoside]:* [81074-96-6]
$C_{27}H_{32}O_{15}$ 596.541
Isol. from *Sapium sebiferum* (Chinese tallowtree). Yellow needles (Me_2CO/petrol). Mp 69°.

5-Me ether, 7-O-*[β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside]:* [114454-39-6]
$C_{28}H_{34}O_{16}$ 626.567
Constit. of the seeds of *Fagopyrum esculentum* (buckwheat). Yellow needles (EtOAc/petrol). Mp 91-93°.

4′,7-Di-Me ether: [28590-40-1] *3′,5-Dihydroxy-4′,7-dimethoxyflavanone.* ***Persicogenin***
$C_{17}H_{16}O_6$ 316.31
Isol. from *Persica vulgaris* (peach). Cryst. Mp 163-164°.

4′,7-Di-Me ether, 3′-O-*β*-D-*glucopyranoside:Persicogenin 3′-glucoside*
$C_{23}H_{26}O_{11}$ 478.452
Isol. from the stem bark of *Prunus amygdalus* (almond). Needles (MeOH). Mp 204-205°. $[\alpha]_D^{24}$ -37.2 (c, 0.1 in DMSO).

4′,7-Di-Me ether, 5-O-*β*-D-*glucopyranoside:* [28978-03-2] ***Persicoside***. *Persiconin*
$C_{23}H_{26}O_{11}$ 478.452
Isol. from *Persica vulgaris* (peach) and *Prunus* sp.. Needles (EtOH). Mp 258-260°. $[\alpha]_D$ -112.8 (EtOH).

7-O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:Eriodictyol 7-(6-galloylglucoside)*
$C_{28}H_{26}O_{15}$ 602.504
Constit. of the leaves and branches of *Phyllanthus emblica* (emblic). Amorph. yellow powder + $2\frac{1}{2}H_2O$. $[\alpha]_D^{28}$ -79.4 (c, 0.4 in MeOH). λ_{max} 281 (log ε 4.38) (EtOH).

7-O-*[4-Hydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranoside]:Eriodictyol 7-(6*-trans-p-*coumaroylglucoside)*
$C_{30}H_{28}O_{13}$ 596.543

Constit. of the leaves and branches of *Phyllanthus emblica* (emblic). Amorph. yellow powder + $2H_2O$. $[\alpha]_D^{28}$ -92.8 (c, 0.36 in MeOH). λ_{max} 286 (log ε 4.27); 315 (log ε 4.48) (EtOH).

[4250-76-4, 66568-98-7, 75917-11-2, 93012-86-3, 111322-81-7, 116301-03-2]

Power, F.B. *et al., J.C.S.*, 1907, **91**, 895 (*struct*)
Tutin, F. *et al., J.C.S.*, 1910, **97**, 2054 (*struct*)
Shinoda, J. *et al., CA*, 1929, **23**, 4210 (*synth, struct*)
Brune, W. *et al., Aust. J. Chem.*, 1965, **18**, 1649 (*deriv*)
Christiansen, K. *et al., Tet. Lett.*, 1966, 1293 (*Persicogenin*)
Hörhammer, L. *et al., Tet. Lett.*, 1966, 5133 (*deriv*)
Kowalewski, Z. *et al., Planta Med.*, 1971, **19**, 311 (*deriv*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799 (*nmr*)
Srivastava, S.K. *et al., Phytochemistry*, 1981, **20**, 862 (*xylogalactoside*)
Babber, S. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 797 (*synth*)
Nabaei-Bidhendi, G. *et al., J. Indian Chem. Soc.*, 1990, **67**, 43 (*synth*)
Liu, Y.-L. *et al., J. Nat. Prod.*, 1992, **55**, 357 (*5,7-Dihydroxy-3′-methoxy-4′-O-isobutanoylflavanone*)
Rawat, M.S.M. *et al., Phytochemistry*, 1995, **38**, 1519 (*Persicogenin 3′-glucoside*)
Garo, E. *et al., Phytochemistry*, 1996, **43**, 1265 (*isol, pmr, cmr*)
Zhang, Y.-J. *et al., Chem. Pharm. Bull.*, 2002, **50**, 841-843 (*7-6-galloylglucoside, 7-6-coumaroylglucoside*)

3′,5,5′,7-Tetrahydroxyflavanone T-192

*2-(3,5-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{12}O_6$ 288.256

(S)-form [160436-10-2] Struct. originally assigned to Huazhongilexone isol from *Ilex centrochinensis*; but proven to be, .

7-Me ether: [118024-26-3] *3′,5,5′-Trihydroxy-7-methoxyflavanone.* ***Blumeatin***
$C_{16}H_{14}O_6$ 302.283
Constit. of *Blumea balsamifera* (sambong). Mp 220-222°.

3′-Me ether: [183857-79-6] *3′,5,7-Trihydroxy-5′-methoxyflavanone.* ***Alysifolinone***
$C_{16}H_{14}O_6$ 302.283

(±)-form
Cryst. (EtOAc/heptane). Mp 208-209°.

Lin, Y. *et al., CA*, 1989, **110**, 21073f
Lin, L. *et al., Yaoxue Xuebao*, 1994, **36**, 393 (*isol*)
Topcu, G. *et al., Turk. J. Chem.*, 1996, **20**, 265-267 (*Alysifolinone*)
Anthoni, U. *et al., Acta Chem. Scand.*, 1998, **52**, 1243-1246; 1999, **53**, 375-377 (*synth, uv, pmr, cmr, struct*)

3,5,6,7-Tetrahydroxyflavanone T-193

*2,3-Dihydro-3,5,6,7-tetrahydroxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI. 5,6,7-Trihydroxydihydroflavonol*

$C_{15}H_{12}O_6$ 288.256

(2R,3R)-form

6-Me ether: [35298-89-6] *3,5,7-Trihydroxy-6-methoxyflavanone.* ***Alnustinol****. 6-Methoxypinobanksin*
$C_{16}H_{14}O_6$ 302.283
Needles (hexane). Mp 175-176°. Originally incorr. identified as the 3,5,8-trihydroxy-7-methoxy isomer.

5-Me, 6,7-methylene ether: [83532-20-1] *3-Hydroxy-5-methoxy-6,7-methylenedioxyflavanone*
$C_{17}H_{14}O_6$ 314.294
Needles (EtOAc). Mp 142-143°. $[\alpha]_D$ +29 (c, 0.5 in MeOH).

6,7-Methylene ether: [110204-44-9] *3,5-Dihydroxy-6,7-methylenedioxyflavanone*
$C_{16}H_{12}O_6$ 300.267
Constit. of sugarbeet infected with *Rhizoctonia solani*. Yellow cryst. Mp 179-180°. Stereochem. undetermined.

Asakawa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 2761 (*isol, ir, uv, pmr, ms*)
Kuroyanagi, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1602 (*isol, spectra*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 371
Takahashi, H. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 2261 (*deriv*)

4′,5,6,7-Tetrahydroxyflavanone T-194

[479-54-9]
*2,3-Dihydro-5,6,7-trihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Carthamidin****. Isocarthamidin (obsol.)*†

$C_{15}H_{12}O_6$ 288.256

Formerly named Isocarthamidin. There is still some confusion in the lit..

(S)-form
Cryst. ($CHCl_3$). Mp 220°.

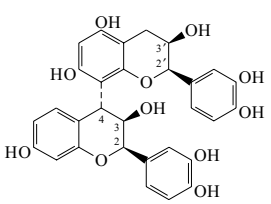
5-O-β-D-Glucopyranoside: ***Isocarthamin****. Neocarthamin*
$C_{21}H_{22}O_{11}$ 450.398
Constit. of the flowers of *Carthamus tinctorius* (safflower). Yellow cryst. + $2H_2O$. Mp 228°. Probable struct. Has been descr. as a chalcone (deriv. of 2′,3′,4,4′,6′-Pentahydroxychalcone).

6,7-Di-O-β-D-glucopyranoside:
$C_{27}H_{32}O_{16}$ 612.54
Constit. of the flowers of *Carthamus tinctorius* (safflower). Amorph. powder. Mp 207° dec. $[\alpha]_D^{25}$ -51.2 (c, 0.11 in MeOH). λ_{max} 283 ; 341 (MeOH).

[2569-77-9, 81524-08-5, 93344-58-2]

Gupta, R.K. *et al., Agric. Biol. Chem.*, 1979, **43**, 2603 (*synth, pmr, derivs*)
Kimura, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1792 (*isol, deriv*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988, 362 (*Isocarthamin*)
Li, F. *et al., Chin. J. Chem.*, 2002, **20**, 699-702 (*6,7-diglucoside*)

3,3′,4′,7-Tetrahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan T-195



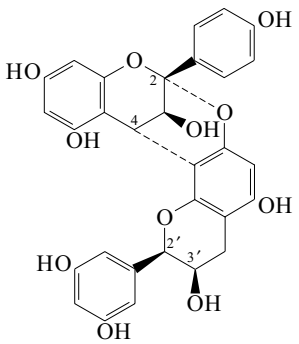
(*all-R*)-*form*

$C_{30}H_{26}O_{11}$ 562.529

(2R,2′R,3R,3′S,4R)-form
Epifisetinidol(4β→8)catechin
Constit. of *Pithecellobium dulce* (manila tamarind).

Drewes, S.E. *et al., J.C.S.(C)*, 1967, 1302 (*isol*)
Botha, J.J. *et al., J.C.S. Perkin 1*, 1981, 1235 (*synth*)
Viviers, P.M. *et al., J.C.S. Perkin 1*, 1983, 2555 (*isol*)
Young, D.A. *et al., J.C.S. Perkin 1*, 1985, 2521 (*synth*)
Young, E. *et al., J.C.S. Perkin 1*, 1986, 1737 (*isol*)
Steynberg, J.P. *et al., J.C.S. Perkin 1*, 1988, 3323; 1989, 1709 (*isol*)
Nunes, D.S. *et al., Phytochemistry*, 1989, **28**, 2183 (*isol*)
Steynberg, J.P. *et al., Phytochemistry*, 1990, **29**, 275 (*isol*)
Hatano, T. *et al., Phytochemistry*, 1996, **46**, 893-900 (*isol, uv, pmr, cmr*)
Steynberg, P.J. *et al., J.C.S. Perkin 1*, 1997, 1943-1950 (*isol, synth, pmr*)

3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,3′,5,5′,7-pentahydroxyflavan T-196

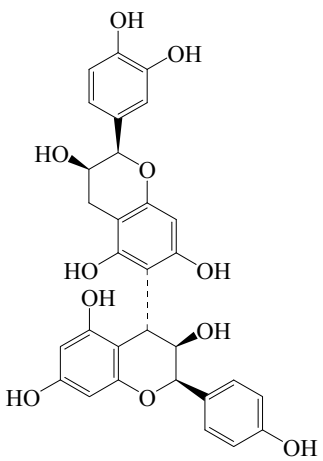


$C_{30}H_{24}O_{11}$ 560.513

(2S,2′R,3S,3′R,4S)-form [148843-32-7]
Constit. of the branches of *Prunus spinosa* (sloe).

Gonzalez Gonzalez, A. *et al., Rev. Latinoam. Quim.*, 1991, **22**, 91 (*isol*)

3,4′,5,7-Tetrahydroxyflavan(4→6)-3,3′,4′,5,7-pentahydroxyflavan T-197



$C_{30}H_{26}O_{11}$ 562.529

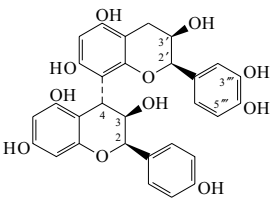
(all-R)-form

Epiafzelechin(4β→6)epicatechin

3,3′-Bis(3,4,5-trihydroxybenzoyl):
[252185-32-3]
$C_{44}H_{34}O_{19}$ 866.741
Constit. of green tea, *Camellia sinensis*. Powder.

Lakenbrink, C. *et al., J. Agric. Food Chem.*, 1999, **47**, 4621-4624 (*isol, pmr, cmr*)

3,4′,5,7-Tetrahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan T-198



(*all-R*)-*form*

$C_{30}H_{26}O_{11}$ 562.529

(all-R)-form [114715-49-0]

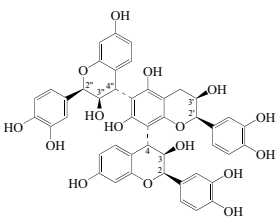
Epiafzelechin(4β→8)epicatechin
Powder. $[\alpha]_D$ +42.3 (c, 1.3 in MeOH).

3,3′-Bis(3,4,5-trihydroxybenzoyl):
$C_{44}H_{34}O_{19}$ 866.741
Constit. of green tea, *Camellia sinensis*. Powder.

Lakenbrink, C. *et al., J. Agric. Food Chem.*, 1999, **47**, 4621-4624 (*3,3′-digalloyl*)

3,3′,4′,7-Tetrahydroxyflavan(4→8)-3,3′,4′,6,8-pentahydroxyflavan(6→4)-3,3′,4′,7-tetrahydroxyflavan T-199

2,2′,2″-Tris(3,4-dihydroxyphenyl)-3,3′,3″,4,4′,4″-hexahydro-[4,6′:8′,4″-ter-2H-1-benzopyran]-3,3′,3″,5′,7,7′,7″-heptol, 9CI



(*all-R*)-*form*

$C_{45}H_{38}O_{16}$ 834.786

(all-R)-form

Epifisetinidol(4β→8)epicatechin(6→4β)epifisetinidol
Constit. of *Pithecellobium dulce* (manila tamarind).

(2R,2′R,2″R,3R,3′S,3″R,4R,4″R)-form

Epifisetinidol(4β→8)catechin(6→4β)epifisetinidol
Constit. of *Pithecellobium dulce* (manila tamarind).

(2R,2′R,2″R,3S,3′R,3″R,4S,4″R)-form

Fisetinidol(4α→8)epicatechin(6→4β)epifisetinidol
Constit. of *Pithecellobium dulce* (manila tamarind).

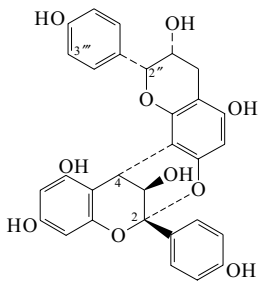
(2R,2′R,2″R,3S,3′S,3″R,4S,4″R)-form

Fisetinidol(4α→8)catechin(6→4β)epifisetinidol
Constit. of *Pithecellobium dulce* (manila tamarind).

Botha, J.J. *et al., J.C.S. Perkin 1*, 1982, 527; 535 (*isol, synth*)
Viviers, P.M. *et al., J.C.S. Perkin 1*, 1983, 2555
Steynberg, P.J. *et al., J.C.S. Perkin 1*, 1997, 1943-1950 (*isol, synth, pmr*)

3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,4′,5,7-tetrahydroxyflavan T-200

3,4-Dihydro-2,8-bis(4-hydroxyphenyl)-8,14-methano-2H,14H-1-benzopyrano-[7,8-d][1,3]benzodioxocin-3,5,11,13,15-pentol, 9CI



(all-*R*)-*form*

$C_{30}H_{24}O_{10}$ 544.514

(2R,2″R,3S,3″S,4R)-form [83944-96-1]

Afzelechin(2β→7,4β→8)afzelechin. ***Prunus inhibitor a***. *PIa*
Isol. from *Prunus persica* roots. Needles. Mp 256-257° dec. $[\alpha]_D^{16}$ -102.9 (c, 0.88 in MeOH).

(2S,2″R,3S,3″R,4S)-form [82765-89-7]

ent-*Epiafzelechin(2α→7,4α→8)epiafzelechin*. ***Mahuannin A***
From *Prunus* spp.. Amorph. powder.

3-O-(4-Hydroxybenzoyl):
$C_{37}H_{28}O_{12}$ 664.621
Constit. of *Prunus armeniaca* (apricot). Amorph. solid. λ_{max} 280 (log ϵ 4.06) (MeOH).

(2S,2″R,3S,3″S,4S)-form

Constit. of *Prunus armeniaca* (apricot). Amorph. powder. Mp >300°.

3‴-Hydroxy: [83889-81-0] *3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan*. ent-*Epiafzelechin(2α→7,4α→8)catechin*. ***Prunus inhibitor b***. *PIb*
$C_{30}H_{24}O_{11}$ 560.513
Isol. from *Prunus persica* roots.

(2S,2″S,3S,3″R,4S)-form

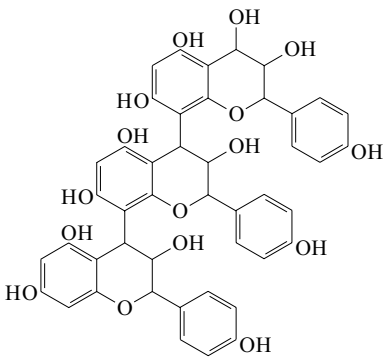
Constit. of *Prunus armeniaca* (apricot). Amorph. powder. Mp >300° λ_{max} 278 (log ϵ 4.08) (MeOH).

Ohigashi, H. *et al., Agric. Biol. Chem.*, 1982, **46**, 2555 (*derivs*)
Hikino, H. *et al., Heterocycles*, 1982, **19**, 1381
Kolodziej, H. *et al., Phytochemistry*, 1991, **30**, 2041 (*isol*)
Pant, G. *et al., Magn. Reson. Chem.*, 1992, **30**, 5142 (*isol, cmr, deriv*)
Gonzalez, A.G. *et al., Phytochemistry*, 1992, **31**, 1432 (*isol, pmr, cmr, struct*)
Drewes, S.E. *et al., Phytochemistry*, 1992, **31**, 2491 (*isol, pmr, cmr*)
Prasad, D. *et al., J. Nat. Prod.*, 1998, **61**, 1123-1125 (*Prunus armeniaca deriv*)
Rawat, M.S.M. *et al., Phytochemistry*, 1999, **50**, 321-324 (*isol, uv, ir, cd, pmr, cmr*)

3,4′,5,7-Tetrahydroxyflavan(4→8)-3,4′,5,7-tetrahydroxyflavan(4→8)-3,4,4′,5,7-pentahydroxyflavan T-201

[25713-96-6]

[4,8″:4″,8‴″-Terflavan]-3,3″,3‴″,4′,4‴,4‴″,4‴″″,5,5″,5‴″,7,7″,7‴-″,7,7″,7‴″-tridecol, 8CI



$C_{45}H_{38}O_{16}$ 834.786
Isol. from heartwood and bark of *Tamarindus indica* (tamarind).

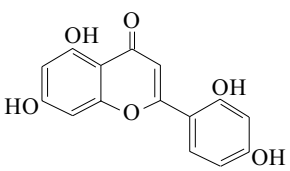
Trideca-Ac: [25664-13-5]
Mp 171-173°. $[\alpha]_D$ +92 (c, 1 in MeOH).

Bhatia, V.K. *et al., Indian J. Chem.*, 1969, **7**, 123 (*isol, struct, derivs*)

2′,4′,5,7-Tetrahydroxyflavone T-202

[520-30-9]

2-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. ***Norartocarpetin***



$C_{15}H_{10}O_6$ 286.24
Constit. of the heartwood of *Artocarpus heterophyllus* (jackfruit). Pale-yellow needles (Me_2CO, EtOH or AcOH). Mp 332-335° (230-232). Descr. under the name of Lotoflavin (aglycone of Lotusin); this was shown to be a mixt. contg. mostly Quercetin.

7-Me ether:2′,4′,5-Trihydroxy-7-methoxyflavone. ***Artocarpetin***
$C_{16}H_{12}O_6$ 300.267
Mp 310°.

7-Me ether, 4′-O-β-D-glucopyranoside:
[142009-24-3]
$C_{22}H_{22}O_{11}$ 462.409

2′-Me ether: [78709-55-4] *4′,5,7-Trihydroxy-2′-methoxyflavone*
$C_{16}H_{12}O_6$ 300.267

2′,4′,7-Tri-Me ether: [132718-84-4] *5-Hydroxy-2′,4′,7-trimethoxyflavone*
$C_{18}H_{16}O_6$ 328.321

Tetra-Me ether: [72357-29-0] *2′,4′,5,7-Tetramethoxyflavone*
$C_{19}H_{18}O_6$ 342.348
Needles (EtOH). Mp 179-180°.

Robinson, R. *et al., J.C.S.*, 1929, 65 (*synth*)
Doporto, M.L. *et al., J.C.S.*, 1955, 4249 (*synth*)
Wheeler, T.S. *et al., CA*, 1960, **54**, 13112 (*Lotoflavin*)
Dave, K.G. *et al., J. Sci. Ind. Res., Sect. B*, 1960, **19**, 470; *CA*, **55**, 16531 (*isol, struct, synth*)
Radhakrishnan, P.V. *et al., Tet. Lett.*, 1965, 663 (*isol, struct*)
Nagar, A. *et al., Phytochemistry*, 1979, **18**, 1245 (*2′,4′,5,7-Tetramethoxyflavone*)
Dogot, A.V. *et al., Farm. Zh. (Kiev)*, 1981, 78 (*isol*)
Mukherjee, K.S. *et al., Fitoterapia*, 1990, **61**, 366 (*5-Hydroxy-2′,4′,7-trimethoxyflavone*)
Shaifulla, K.M. *et al., Indian Drugs Pharm. Ind.*, 1991, **29**, 83 (*7-Me ether 4′-glucoside*)
Lin, C.-N. *et al., Phytochemistry*, 1995, **39**, 1447-1451 (*isol, cmr*)
Likhitwitayawuid, K. *et al., Planta Med.*, 2000, **66**, 275-277 (*activity*)

2′,5,6,6′-Tetrahydroxyflavone T-203

[24457-44-1]
*2-(2,6-Dihydroxyphenyl)-5,6-dihydroxy-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{10}O_6$ 286.24

Formerly assigned the 2′,5,6,7-tetrahydroxy struct..

2′,6,6′-Tri-Me ether: [14813-20-8] *5-Hydroxy-2′,6,6′-trimethoxyflavone.* ***Zapotinin***
$C_{18}H_{16}O_6$ 328.321
Constit. of *Casimiroa edulis* (Mexican apple). Yellow needles (MeOH). Mp 224-225°.

Tetra-Me ether: [14813-19-5] *2′,5,6,6′-Tetramethoxyflavone.* ***Zapotin***
$C_{19}H_{18}O_6$ 342.348
Constit. of the bark of *Casimiroa edulis* (Mexican apple). Prisms (Me_2CO or MeOH). Mp 150-151°.

Kincl, F.A. *et al., J.C.S.*, 1956, 4163 (*isol*)
Iriarte, J. *et al., J.C.S.*, 1956, 4170 (*isol*)
Sondheimer, F. *et al., Tetrahedron*, 1960, **9**, 139 (*isol*)
Garrett, P.J. *et al., Tetrahedron*, 1967, **23**, 2413 (*struct*)
Dreyer, D.L. *et al., Tetrahedron*, 1967, **23**, 4607 (*struct*)
Farkas, L. *et al., Tet. Lett.*, 1968, 3993 (*synth*)
Datta, S.C. *et al., Indian J. Chem., Sect. B*, 1969, **7**, 746 (*synth*)
Meyer, B.N. *et al., J. Nat. Prod.*, 1985, **48**, 952 (*Zapotin*)

3,3′,4′,7-Tetrahydroxyflavone T-204

[528-48-3]
*2-(3,4-Dihydroxyphenyl)-3,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,7-Trihydroxyflavonol.* ***Fisetin***

$C_{15}H_{10}O_6$ 286.24
Yellow cryst. Sol. MeOH, EtOH, Me_2CO, bases, AcOH; poorly sol. H_2O, Et_2O, $CHCl_3$, hexane, C_6H_6. Mp 330°. Shows brilliant yellow fluor. λ_{max} 252 ; 320 ; 360 (EtOH) (Berdy).

► LD_{50} (mus, ivn) 180 mg/kg. LK9250000

4′-Me ether: [57396-72-2] *3,3′,7-Trihydroxy-4′-methoxyflavone*
$C_{16}H_{12}O_6$ 300.267
Isol. from quebracho heartwood. Pale yellow needles (2-propanol). Mp 288° (282-285°).

3′,4′-Methylene, 3,7-di-Me ether: [1668-33-3] *3,7-Dimethoxy-3′,4′-methylenedioxyflavone.* ***Demethoxykanugin***. *Desmethoxykanugin*
$C_{18}H_{14}O_6$ 326.305
Isol. from *Rhus chinensis* (Chinese gall). Needles (EtOH). Mp 147°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 96A (*ir*)
v. Auwers, K. *et al., Ber.*, 1915, **48**, 85-90 (*bibl, synth*)
Allan, J. *et al., J.C.S.*, 1926, 2334-2336 (*synth*)
Kirby, K.S. *et al., Biochem. J.*, 1955, **60**, 582-590 (*isol, synth*)
Mittal, O.P. *et al., J.C.S.*, 1956, 2176-2178 (*Demethoxykanugin*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428-439 (*pmr*)
Ferreira, D. *et al., J.C.S. Perkin 1*, 1974, 1492-1498 (*3,3′,4′-7-tetramethoxyflavone, isol*)
Ahmad, J. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 420-421 (*Demethoxykanugin*)
Plant Flavonoids in Biology and Medicine, (eds. Cody, V. *et al*), A.R. Liss, N.Y., 1986, (*biochem*)
Elgindi, M.R. *et al., Asian J. Chem.*, 1999, **11**, 1525-1527 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FBW000

3′,4′,5,7-Tetrahydroxyflavone T-205

[491-70-3]
*2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI.* ***Luteolin***. *Digitoflavone. Daphneflavonol. Flavopurpol. Luteolol*

$C_{15}H_{10}O_6$ 286.24

Various methyl and methylene ethers have separate entries. Flavone v. widespread in plant world; found esp. in celery, peppermint, rosemary, thyme and Queen Anne's Lace leaves (wild carrot). Potential nutriceutical. Yellow needles. Mp 328-330° (325°). Log P 0.38 (calc). λ_{max} 255 ; 351 (MeOH) (Berdy).

► LD_{50} (mus, ipr) 180 mg/kg. Exp. reprod. effects. LK9275210

4′-O-Sulfate: [60889-07-8] *Luteolin 4′-sulfate*
$C_{15}H_{10}O_9S$ 366.305
Isol. from *Daucus carota* (carrot).

7-O-Sulfate: [56857-57-9] *Luteolin 7-sulfate*
$C_{15}H_{10}O_9S$ 366.305
Isol. from *Bixa orellana* (annatto).

7-O-β-D-Galactopyranoside: [68321-11-9] *Luteolin 7-galactoside*
$C_{21}H_{20}O_{11}$ 448.382
Isol. from *Capsella bursa-pastoris* (shepherd's purse).

4′-O-β-D-Glucopyranoside, 7-O-β-D-galacturonopyranoside: [126207-52-1] *Luteolin 4′-glucoside 7-galacturonide*
$C_{27}H_{28}O_{17}$ 624.508
Isol. from *Cuminum cyminum* (cumin).

7-O-β-D-Glucopyranoside: [5373-11-5] *Luteolin 7-glucoside.* ***Glucoluteolin***. *Cinaroside. Cynaroside. Daphneflavonoloside. Flavopurposide. Luteoloside*
$C_{21}H_{20}O_{11}$ 448.382
Constit. of the leaves of *Capsicum annuum* (red pepper). Needles + $1\frac{1}{2}H_2O$ (EtOH), yellow needles + $2H_2O$ (Me_2CO aq.). Sol. MeOH, butanol; fairly sol. H_2O; poorly sol. hexane. Mp 256-258° (254°). λ_{max} 253 (ϵ 13800); 254 (ϵ 18700); 256 ; 265 (ϵ 17000); 347 (ϵ 19200) (MeOH) (Berdy). λ_{max} 256 (ϵ 20000); 350 (ϵ 22400) (EtOH) (Berdy). λ_{max} 262 ; 264 (ϵ 20000); 267 ; 388 ; 393 ; 398 (ϵ 21000) (MeOH-NAOH) (Berdy).

► DJ3009400

7-O-(Disulfoglucoside): [121283-87-2]
$C_{21}H_{20}O_{17}S_2$ 608.511
Isol. from *Phoenix dactylifera* (date).

7-O-[4-Hydroxybenzoyl-(→6)-β-D-glucopyranoside]: ***Neobignonoside***
$C_{28}H_{24}O_{13}$ 568.49
Constit. of *Vitex agnus-castus* (agnus castus). Yellow powder (MeOH). $[\alpha]_D$ -78.6 (c, 0.03 in MeOH). Mp >300° λ_{max} 255 ; 349 (MeOH).

7-O-[3,4-Dihydroxycinnamoyl-(→?)-β-D-glucopyranoside]: [79366-63-5] *Luteolin 7-(caffeoylglucoside)*
$C_{30}H_{26}O_4$ 450.533
Isol. from *Perilla frutescens* (perilla).

3′-O-(4-O-Acetyl-β-D-glucuronopyranoside):
$C_{23}H_{20}O_{13}$ 504.403
Constit. of the leaves of *Rosmarinus officinalis* (rosemary). Yellow powder. Mp 220-230° dec.

3′-O-(O-Acetyl-β-D-glucuronopyranoside):
$C_{23}H_{20}O_{13}$ 504.403
Isol. from *Rosmarinus officinalis* (rosemary). Dark yellow powder. Mp 177-180°.

7-O-[D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]: [63808-23-1]

[34464-64-7] ***Graveobioside A***
$C_{26}H_{28}O_{15}$ 580.498
Isol. from *Apium graveolens* (celery seeds) and *Petroselinum crispum* (parsley). Mp 259-261° (251-252°).

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [20633-84-5] ***Scolymoside***. *Luteolin 7-rutinoside. Skolimoside*
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Capsella bursa-pastoris* (shepherd's purse) *Cynara scolymus* (globe artichoke). Cryst. + $1H_2O$ (MeOH). Mp 192-196° (186-189°). $[\alpha]_D^{27}$ -50.98 (Py). Log P -3.3 (uncertain value) (calc).

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 4′-O-β-D-glucopyranoside: [20056-21-7] *Luteolin 4′-glucoside 7-rutinoside.* ***Cynarotrioside***
$C_{33}H_{40}O_{20}$ 756.667
Isol. from *Cynara scolymus* (artichoke). Cryst. (Me_2CO aq.). Mp 274-276°.

7-O-[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]: [31511-92-9] *Luteolin 7-diglucoside*
$C_{27}H_{30}O_{16}$ 610.524
Isol. from the leaves of *Capsicum annuum* (red pepper).

*7-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 4′-O-β-D-glucuronopyranoside:*
$C_{43}H_{42}O_{27}$ 990.789

Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 214-215° dec. $[\alpha]_D^{20}$ -38.4 (c, 0.1 in MeOH). λ_{max} 247 ; 328 (MeOH).

[18695-03-9, 54985-16-9, 62804-16-4, 98716-92-8, 102506-55-8]

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Schulz, M. *et al., Phytochemistry*, 1985, **24**, 343 (*glucuronosides*)
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Hirobe, C. *et al., Phytochemistry*, 1997, **46**, 521-524 (*7-hydroxybenzoylglucoside*)
Stochmal, A. *et al., J. Agric. Food Chem.*, 2001, **49**, 753-758 (*alfalfa glucuronide*)

3,4′,5,7-Tetrahydroxyflavone T-206

[520-18-3]

3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxyflavonol. ***Kaempferol****. Campherol. Populnetin. Robigenin. Rhamnolutin. Trifolitin. Nimbecetin. Kampherol. Swartziol*

$C_{15}H_{10}O_6$ 286.24

Various methyl ethers and major glycosides have separate entries. Very widespread in the plant world, e.g. in Brassicaceae, Apocynaceae, Dilleniaceae, Ranunculaceae, Leguminosae, etc. Found esp. in broccoli, capers, chives, kale, garden cress, fennel, lovage, dill weed and tarragon. Yellow needles (EtOH aq.). Sol. EtOH, MeOH, Et_2O, bases; poorly sol. H_2O. Mp 276-278°. Log P 0.31 (calc). λ_{max} 204 ; 265 ; 365 (MeOH) (Berdy). λ_{max} 265 ; 365 (EtOH) (Berdy).

▶ LK9275200

3-O-[4-Hydroxy-3-methoxycinnamoyl-(→?)-apioside]: [185066-55-1] *Kaempferol 3-(feruloylapioside)*
$C_{30}H_{26}O_{13}$ 594.528
Constit. of the bracken fern *Pteridium aquilinum*. λ_{max} 265 ; 300 (sh) ; 321 (MeOH).

3-O-α-L-Arabinofuranoside: [5041-67-8] *Kaempferol 3-α-L-arabinofuranoside.* ***Juglanin***†. *Euglanin*
$C_{20}H_{18}O_{10}$ 418.356
From leaves of English walnut (*Juglans regia*). Pale yellow scales + $1^1/_2H_2O$. Mp 224-225°. $[\alpha]_D^{23}$ -169.

3-O-α-L-Arabinofuranoside, 7-O-α-L-rhamnofuranoside: [27509-67-7] *Kaempferol 3-arabinofuranoside 7-rhamnofuranoside.* ***Ternoside***
$C_{26}H_{28}O_{14}$ 564.499
Isol. from leaves of sloe (*Prunus spinosa*). Log P -3.14 (uncertain value) (calc).

3-O-α-L-Rhamnofuranoside: [5041-73-6] *Kaempferol 3-O-α-L-rhamnofuranoside*
$C_{21}H_{20}O_{10}$ 432.383
Constit. of *Prunus spinosa* (sloe). Mp 172-175°. $[\alpha]_D$ -170.

7-O-L-Rhamnofuranoside: [5041-74-7] ***α-Rhamnorobin****. Kaempferol 7-rhamnofuranoside*
$C_{21}H_{20}O_{10}$ 432.383
Isol. from bean *Phaseolus atropurpureum*, leaves of sloe (*Prunus spinosa*) and others. Light yellow needles. Mp 231-234° (222-224°). $[\alpha]_D$ -147 (c, 1.04 in EtOH).

3-O-α-L-Rhamnopyranoside, 4′-O-β-D-xylopyranoside: [132536-65-3] *Kaempferol 3-rhamnoside 4′-xyloside*
$C_{26}H_{28}O_{14}$ 564.499
Isol. from *Chenopodium ambrosioides* (Mexican tea). Pale yellow powder. Mp 262-263°.

3-O-α-L-Rhamnopyranoside, 7-O-β-D-xylopyranoside: [132618-21-4] *Kaempferol 3-rhamnoside 7-xyloside*
$C_{26}H_{28}O_{14}$ 564.499
Isol. from fruit of Mexican tea (*Chenopodium ambrosioides*). Pale yellow powder. Mp 300°.

3-O-α-L-Rhamnopyranoside, 7-O-β-D-galacturonopyranoside: [124167-98-2]
$C_{27}H_{28}O_{16}$ 608.509
Isol. from *Silybum marianum* (milk thistle).

3-O-α-L-Rhamnopyranoside, 7-O-[α-L-rhamnopyranosyl-β-D-glucopyranoside]: [111138-29-5]
$C_{33}H_{40}O_{19}$ 740.668
Isol. from seeds of lentil (*Lens culinaris*).

3-O-α-L-Rhamnopyranoside, 7-O-[β-D-glucopyranosyl-(→?)-α-L-rhamnopyranoside]: [110850-50-5]
$C_{33}H_{40}O_{19}$ 740.668
Constit. of the seeds of lentil (*Lens esculenta*).

3-O-[4-Hydroxycinnamoyl-(→4)-2,3-di-O-acetyl-α-L-rhamnopyranoside]: [128941-61-7]
$C_{34}H_{30}O_{14}$ 662.603
Isol. from leaves of bog myrtle (*Myrica gale*). Amorph.

3-O-α-D-Glucopyranoside: [31159-41-8] *Kaempferol 3-α-D-glucoside.* ***Isoastragalin***
$C_{21}H_{20}O_{11}$ 448.382
Isol. from *Gossypium hirsutum* (cotton) and other plant spp.. Mp 245-246°.

3-O-[3,6-Di-O-acetyl-2,4-di-O-(4-hydroxycinnamoyl)-β-D-glucopyranoside]: [94474-72-3]
$C_{43}H_{36}O_{17}$ 824.747
Constit. of leaves of *Quercus ilex* (holly oak). Needles (MeOH aq.). Mp 280° dec.

5-O-β-D-Glucopyranoside: [34157-80-7] *Kaempferol 5-glucoside*
$C_{21}H_{20}O_{11}$ 448.382
Isol. from *Pteridium aquilinum* (bracken fern). Mp 213°. $[\alpha]_D$ -15 (c, 0.19 in MeOH).

3-O-β-D-Glucuronopyranoside: [22688-78-4]
$C_{21}H_{18}O_{12}$ 462.366
Isol. from the leaves of *Phaseolus vulgaris* (kidney bean). Mp 189-190.5°.

3-O-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]: Astragalin, A-478

3-O-[Xylosyl-(→?)-glucoside]: [29322-07-4] *Kaempferol 3-xylosylglucoside*
$C_{26}H_{28}O_{15}$ 580.498
Isol. from various plant spp. incl. *Armoracia* sp..

3-O-[Rhamnosyl-(1→?)-galactoside], 7-O-α-L-rhamnopyranoside: [74561-73-2]
$C_{33}H_{40}O_{19}$ 740.668
Constit. of Chinese chives (*Allium tuberosum*) and *Phaseolus* sp..

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-galactopyranoside]: [17297-56-2] *Kaempferol 3-robinobioside.* ***Biorobin***
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Medicago* spp., *Trigonella* spp. and other plant spp.. Yellow needles (Me_2CO aq.). Mp 224-226° (sinters at 198°). $[\alpha]_D$ -75 (c, 1 in Py).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [32602-81-6] *Kaempferol 3-neohesperidoside*
$C_{27}H_{30}O_{15}$ 594.525
Isol. from hop (*Humulus lupulus*). Pale yellow needles. Mp 197-200°. $[\alpha]_D^{22}$ -58.8 (c, 1.36 in MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 7-O-β-D-galactopyra-

noside: [111137-46-3]

[33906-91-1] *Kaempferol 7-galactoside 3-rutinoside*
$C_{33}H_{40}O_{20}$ 756.667
Constit. of the seeds of lentil (*Lens esculenta*). The *O. regia* isolate (no phys. props reported) was an older isolate which was not fully characterised but which was prob. identical.

3-O-[α-L-Rhamnopyranosyl-(1→6)-[4-hydroxycinnamoyl-(→4)]-β-D-glucopyranoside]: [78510-18-6] *Kaempferol 2^G-coumaroylrutinoside*
$C_{36}H_{36}O_{17}$ 740.67
Isol. from leaves of European chestnut (*Castanea sativa*). Dec. at 185°.

3-O-[β-D-Galactopyranosyl-(1→6)-β-D-glucopyranoside], 7-O-[α-L-rhamnopyranosyl-(1→3)-α-L-rhamnopyranoside]: [81944-31-2] ***Melitin***
$C_{39}H_{50}O_{24}$ 902.81
Isol. from *Melilotus alba* (white melilot).

3-O-[β-D-Glucopyranosyl-β-D-xylofuranoside]: ***Rustoside***†
$C_{26}H_{28}O_{15}$ 580.498
Isol. from leaves of horseradish (*Armoracia rusticana*).

3-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-α-L-rhamnopyranoside]: [107190-70-5]
$C_{36}H_{36}O_{17}$ 740.67
Isol. from *Ginkgo biloba* (ginkgo).

3-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranoside]: [102231-39-0]
$C_{36}H_{36}O_{17}$ 740.67
Isol. from *Ginkgo biloba* (ginkgo). Pale yellow solid. Mp 337°. $[\alpha]_D^{20}$ -60 (c, 1 in EtOH).

7-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:Kaempferol 7-sophoroside
$C_{27}H_{30}O_{16}$ 610.524
Constit. of saffron (*Crocus sativus*). $[\alpha]_D$ -33 (c, 0.1 in MeOH) (as octa-Ac).

3-O-[(4-Hydroxycinnamoyl)sophorotrioside]: [60302-65-0]
$C_{42}H_{46}O_{23}$ 918.812
Isol. from *Pisum* spp..

3-O-(Feruloylsophorotrioside): [60302-63-8]
$C_{43}H_{48}O_{24}$ 948.838
Isol. from aerial parts of pea seedlings (*Pisum sativum*).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]: [80714-53-0] *Kaempferol 3-sophorotrioside*
$C_{33}H_{40}O_{21}$ 772.666
Isol. from aerial parts of pea seedlings (*Pisum sativum*).

[27638-32-0, 28384-70-5, 69501-06-0, 124027-49-2]

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3,4′,6,7-Tetrahydroxyflavone T-207

3,6,7-Trihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. 4′,6,7-Trihydroxyflavonol

$C_{15}H_{10}O_6$ 286.24
Yellow cryst. Mp 320°.

3-Me ether:4′,6,7-Trihydroxy-3-methoxyflavone
$C_{16}H_{12}O_6$ 300.267Not isol. in pure form.

4′-Me ether:3,6,7-Trihydroxy-4′-methoxyflavone
$C_{16}H_{12}O_6$ 300.267
Yellow needles (MeOH). Mp 290°.

4′-Me ether, 7-O-α-L-rhamnopyranoside:
$C_{22}H_{22}O_{10}$ 446.41
Constit. of the leaves of *Setaria italica* (Foxtail millet). Pale yellow needles ($CHCl_3$/MeOH). Mp 300-301°. λ_{max} 255 (sh) ; 287 ; 340 (no solvent reported).

3,6-Di-Me ether: [68007-24-9] ***4′,7-Dihydroxy-3,6-dimethoxyflavone***
$C_{17}H_{14}O_6$ 314.294

6,7-Di-Me ether: [123442-39-7] *3,4′-Dihydroxy-6,7-dimethoxyflavone*
$C_{17}H_{14}O_6$ 314.294
Yellow needles. Mp 182°. This struct. originally assigned to Hortensin, but revised in 1992 to 4′,5-Dihydroxy-6,7-dimethoxyflavone and then again in 1995 to 5,7-Dihydroxy-4′,6-dimethoxyflavone.

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Jain, N. *et al., J. Chem. Res., Synop.*, 1995, 265 (*4′-Me ether 7-rhamnoside*)
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3,4′,7,8-Tetrahydroxyflavone T-208

[1429-28-3]
3,7,8-Trihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. 4′,7,8-Trihydroxyflavonol

$C_{15}H_{10}O_6$ 286.24
Pale-yellow prisms + $1H_2O$ (MeOH/EtOAc). Mp 310-319° (295-305° dec.).

3-Me ether: [57499-05-5] *4′,7,8-Trihydroxy-3-methoxyflavone*
$C_{16}H_{12}O_6$ 300.267
Cryst. (MeOH/C_6H_6). Mp 245-252° dec.

7,8-Di-Me ether: [57499-07-7] *3,4′-Dihydroxy-7,8-dimethoxyflavone*
$C_{17}H_{14}O_6$ 314.294
Mp 225-227°.

3,4′,8-Tri-Me ether:7-Hydroxy-3,4′,8-trimethoxyflavone
Constit. of the leaves of the famine food *Parkia clappertoniana*. Yellow cryst. Mp 187.5-188°.

Clark-Lewis, J.W. *et al., Aust. J. Chem.*, 1967, **20**, 2191 (*isol*)
Chumbalov, T.K. *et al., Khim. Prir. Soedin.*, 1968, **4**, 67; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 59 (*isol*)
Malan, E. *et al., Phytochemistry*, 1975, **14**, 1835 (*isol, ms, pmr, uv*)
Lemmich, E. *et al., Phytochemistry*, 1996, **42**, 1011 (*7-Hydroxy-3,4′,8-trimethoxyflavone*)

3,5,7,8-Tetrahydroxyflavone T-209

[74693-69-9]
3,5,7,8-Tetrahydroxy-2-phenyl-4H-1-benzopyran-4-one. 5,7,8-Trihydroxyflavonol. 8-Hydroxygalangin

$C_{15}H_{10}O_6$ 286.24
Cryst. Mp 231-233°.
▶ LK9275250
3-Me ether: [33910-28-0] *5,7,8-Trihydroxy-*

3-methoxyflavone
$C_{16}H_{12}O_6$ 300.267
Cryst. (MeOH). Mp 244-248°.

▶LK8748100

3-Me ether, 8-angeloyl: [128508-15-6]
$C_{21}H_{18}O_7$ 382.369
Pale yellow solid. Mp 148-150°.

3-Me ether, 8-tigloyl: [221231-14-7]
$C_{21}H_{18}O_7$ 382.369
Cryst. (hexane). Mp 177-179°. λ_{max} 208 ; 322 ; 364 ($CHCl_3$).

*3-Me ether, 8-*O*-(2-methylbutanoyl):* [128508-14-5]
$C_{21}H_{20}O_7$ 384.385
Yellow solid.

7-Me ether: [32484-00-7] *3,5,8-Trihydroxy-7-methoxyflavone*
$C_{16}H_{12}O_6$ 300.267
Fine yellow needles. Mp 175-177° Mp 246°.

7-Me ether, 8-Ac: [69312-51-2]
$C_{18}H_{14}O_7$ 342.304
No phys. props. reported.

7-Me ether, 8-butanoyl: [69306-82-7]
$C_{20}H_{18}O_7$ 370.358
No phys. props. reported.

8-Me ether: [5928-42-7] *3,5,7-Trihydroxy-8-methoxyflavone. 5,7-Dihydroxy-8-methoxyflavonol*
$C_{16}H_{12}O_6$ 300.267
Needles (EtOAc). Mp 221-222°.

3,7-Di-Me ether: [33803-31-5] *5,8-Dihydroxy-3,7-dimethoxyflavone.* ***Isognaphaliin***
$C_{17}H_{14}O_6$ 314.294
Mp 216-218°.

3,7-Di-Me ether, 8-Ac: [98204-86-5] *8-Acetoxy-5-hydroxy-3,7-dimethoxyflavone*
$C_{19}H_{16}O_7$ 356.331
Mp 244-246°.

3,8-Di-Me ether: [33803-42-8] *5,7-Dihydroxy-3,8-dimethoxyflavone.* ***Gnaphaliin***
$C_{17}H_{14}O_6$ 314.294
Constit. of *Helichrysum italicum* (curry plant). Mp 174-175°. λ_{max} 270 ; 305 (MeOH) (Berdy).

*3,8-Di-Me ether, 7-*O*-(2,3-epoxy-3-methylbutyl):* [94390-13-3] ***7-(2,3-Epoxy-3-methylbutoxy)-5-hydroxy-3,8-dimethoxyflavone***
$C_{22}H_{22}O_7$ 398.412
No phys. props. reported.

5,8-Di-Me ether:3,7-Dihydroxy-5,8-dimethoxyflavone
$C_{17}H_{14}O_6$ 314.294
Yellow plates (Me_2CO). Mp 256°.

7,8-Di-Me ether: [22399-73-1] ***3,5-Dihydroxy-7,8-dimethoxyflavone.*** *5-Hydroxy-7,8-dimethoxyflavonol*
$C_{17}H_{14}O_6$ 314.294
Isol. from above-ground parts of *Helichrysum italicum* (curry plant). Yellow needles ($EtOH/CHCl_3$). Mp 204-205°.

3,5,8-Tri-Me ether: [71706-62-2] *7-Hydroxy-3,5,8-trimethoxyflavone*
$C_{18}H_{16}O_6$ 328.321
Cryst. (EtOAc/petrol). Mp 247-248°.

3,7,8-Tri-Me ether: [22399-74-2] *5-Hydroxy-3,7,8-trimethoxyflavone.* ***Methylgnaphaliin***
$C_{18}H_{16}O_6$ 328.321
Yellow cryst. Mp 176-177°.

5,7,8-Tri-Me ether: [103393-10-8] *3-Hydroxy-5,7,8-trimethoxyflavone*
$C_{18}H_{16}O_6$ 328.321
Pale yellow cryst. (MeOH). Mp 189-190°.

Tetra-Me ether: [103450-99-3] *3,5,7,8-Tetramethoxyflavone*
$C_{19}H_{18}O_6$ 342.348
Cryst. (EtOH). Mp 164-165° (156-158°).

Rao, P.R. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1945, **22**, 157; *CA*, **40**, 1832 (*synth*)
Krishnamurti, M. *et al., Tetrahedron*, 1966, **22**, 941 (*synth*)
Hänsel, R. *et al., Tet. Lett.*, 1969, 431 (*synth, uv, pmr, ms*)
Asakawa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 297 (*isol, uv, ir, ms, 3,5,8-tri-Me ether*)
Wagner, H. *et al., Chem. Ber.*, 1971, **104**, 2381 (*Gnaphaliin, Isognaphaliin*)
Opitz, L. *et al., Phytochemistry*, 1971, **10**, 1948 (*Gnaphaliin*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1978, **33**, 831 (*8-acyl derivs, 3,5,8-Trihydroxy-7-methoxyflavone*)
Dwivedi, P. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 77 (*synth, pmr*)
Proksch, M. *et al., Phytochemistry*, 1982, **21**, 1835 (*isol*)
Norbedo, C. *et al., Phytochemistry*, 1984, **23**, 2698 (*5,7,8-Trihydroxy-3-methoxyflavone, Gnaphaliin, Isognaphaliin, 7-Epoxymethylbutyl ether*)
Ferraro, G.E. *et al., J. Nat. Prod.*, 1985, **48**, 817 (*3,5-Dihydroxy-7,8-dimethoxyflavone*)
Wollenweber, E. *et al., Phytochemistry*, 1985, **24**, 965; 1493 (*Isognaphaliin, deriv*)
Mesquita, A.A.L. *et al., Phytochemistry*, 1986, **25**, 1255 (*Gnaphaliin, 3,5,8-tri-Me ether, tetra-Me ether*)
Saxena, M. *et al., Planta Med.*, 1986, **52**, 502 (*3-Hydroxy-5,7,8-trimethoxyflavone*)
Kaouadji, M. *et al., J. Nat. Prod.*, 1988, **51**, 353 (*deriv*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Urzua, A. *et al., Phytochemistry*, 1990, **29**, 1342 (*8-methylbutanoates*)
Urzua, A. *et al., J. Nat. Prod.*, 1999, **62**, 381-382 (*3-Me ether 8-tigloyl*)

4′,5,6,7-Tetrahydroxyflavone T-210

[529-53-3]
*5,6,7-Trihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Scutellarein.*** *6-Hydroxyapigenin*

$C_{15}H_{10}O_6$ 286.24
Yellow leaflets (MeOH). Mp 347-349°.

*4′-*O*-α-L-Arabinopyranoside:* [41383-43-1]
$C_{20}H_{18}O_{10}$ 418.356

*6-*O*-β-D-Xylopyranoside:* [65876-68-8]
$C_{20}H_{18}O_{10}$ 418.356
Isol. from *Juniperus communis* (juniper).

*6-*O*-β-D-Glucopyranoside:* [10289-41-5]
$C_{21}H_{20}O_{11}$ 448.382
No phys. props. reported.

*7-*O*-β-D-Glucopyranoside:* [26046-94-6] ***Plantaginin***
$C_{21}H_{20}O_{11}$ 448.382
Pale yellow powder (MeOH). Yellow needles + $2H_2O$ (MeOH). Mp 213-215°. $[\alpha]_D^{26}$ -71.9 (c, 0.51 in Py).

*7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside):* [127350-67-8] ***Scutellerein 7-(6-malonylglucoside)***
$C_{24}H_{22}O_{14}$ 534.429

*7-*O*-[3-Hydroxy-3-methylglutaroyl-(1→6)-β-D-glucopyranoside]:* [151750-82-2]
$C_{27}H_{28}O_{15}$ 592.509

*5-*O*-β-D-Glucuronopyranoside:* [27740-02-9]
$C_{21}H_{18}O_{12}$ 462.366

*6-*O*-β-D-Glucuronopyranoside:* [62023-92-1] ***Isoscutellarin***
$C_{21}H_{18}O_{12}$ 462.366

*7-*O*-β-D-Glucuronopyranoside:* [27740-01-8] ***Scutellarin***
$C_{21}H_{18}O_{12}$ 462.366
Straw-yellow needles (EtOH). Mp 300°. $[\alpha]_D^{25}$ -122 (c, 0.52 in Py).

*7-*O*-α-L-Rhamnopyranoside:* [24512-68-3] ***Sorbarin***
$C_{21}H_{20}O_{10}$ 432.383
Pale yellow needles. Mp 300°.

*4′-*O*-α-L-Rhamnopyranoside:* [28071-06-9] ***Sorbarioside***
$C_{21}H_{20}O_{10}$ 432.383
Yellow needles (EtOH). Mp 269°. $[\alpha]_D$ -113 (c, 1 in Py). λ_{max} 284 ; 337 (EtOH).

*6-*O*-β-D-Xylopyranoside, 7-*O*-α-L-rhamnoside:* [83531-16-2] ***Triumboidin***
$C_{26}H_{28}O_{14}$ 564.499
Light yellow needles. Mp 220-222°.

*4′,7-Di-*O*-α-L-rhamnofuranoside:* [35128-73-5]
$C_{27}H_{30}O_{14}$ 578.526

*7-*O*-[β-D-Xylopyranosyl-(1→2)-β-D-xylopyranoside]:*
$C_{25}H_{26}O_{14}$ 550.472

*7-*O*-[β-D-Xylopyranosyl-(1→4)-α-L-rhamnopyranoside]:* [28620-94-2] ***Sorbifolin***†
$C_{26}H_{28}O_{14}$ 564.499
Mp 230-234° Mp 320-330° (double Mp). $[\alpha]_D^{23}$ -133 (c, 0.4 in DMF).

*7-*O*-[β-D-Xylopyranosyl-(1→6)-β-D-galactopyranoside]:* [151767-51-0]
$C_{26}H_{28}O_{15}$ 580.498

*7-*O*-[β-D-Xylopyranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{26}H_{28}O_{15}$ 580.498

*6-*O*-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranoside]:* [137182-32-2]
$C_{27}H_{30}O_{15}$ 594.525
Shiny yellow needles ($CHCl_3$). Mp 319-320°.

*7-*O*-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [85852-24-0] *Scutellarein 7-neohesperidoside*
$C_{27}H_{30}O_{15}$ 594.525
Mp 232-233°. $[\alpha]_D^{28}$ -80 (DMSO).

*6-*O*-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [91485-76-6] *Scutellarein 6-rutinoside*
$C_{27}H_{30}O_{15}$ 594.525

*7-*O*-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [36285-12-8] *Scutellarein 7-rutinoside*
$C_{27}H_{30}O_{15}$ 594.525
Cryst. (EtOH aq.). Mp 185-188° Mp 318°. $[\alpha]_D^{25}$ -109 (c, 0.28 in EtOH).

*7-*O*-[β-D-Glucopyranosyl-(1→4)-α-L-*

rhamnopyranoside]: [104602-65-5] *Scutellarein 7-scillabioside*
$C_{27}H_{30}O_{15}$ 594.525

7-O-*[α-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [76754-41-1] *Scutellarein 7-sophoroside*
$C_{27}H_{30}O_{16}$ 610.524

7-O-*[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:*
$C_{27}H_{30}O_{16}$ 610.524
No phys. props. reported.

7-O-*[β-D-Mannopyranosyl-(1→2)-β-D-glucopyranoside]:* [35835-03-1] ***Stachyflaside***
$C_{27}H_{30}O_{16}$ 610.524
Mp 220-224°. $[\alpha]_D^{20}$ -60 (MeOH).

7-O-*[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [150641-65-9]
$C_{27}H_{26}O_{18}$ 638.492
Constit. of *Perilla frutescens* (perilla).

Glycoside: ***Isolignoside***
Mp 230-232°. $[\alpha]_D^{20}$ -147.3 (c, 0.038 in DMF). Appears to be an isomer of Lignoside with substituent at C-8.

6-O-*(4-Hydroxy-3-methoxycinnamoyl), 7*-O-*β-D-glucuronopyranoside:* [97165-28-1] ***6-O-Feruloylscutellarin***
$C_{31}H_{26}O_{15}$ 638.537
No phys. props. reported.

3-O-*(4-Hydroxy-3,5-dimethoxycinnamoyl), 7*-O-*β-D-glucuronopyranoside:* [29276-60-6]
$C_{32}H_{28}O_{16}$ 668.564

4′-Me ether: See 5,6,7-Trihydroxy-4′-methoxyflavone in *The Combined Chemical Dictionary.*

6-Me ether: See 4′,5,7-Trihydroxy-6-methoxyflavone in *The Combined Chemical Dictionary.*

7-Me ether: [23130-22-5] *4′,5,6-Trihydroxy-7-methoxyflavone.* ***Sorbifolin***†. *Ladanetin*
$C_{16}H_{12}O_6$ 300.267
Yellow needles. Mp 290-292°.

7-Me ether, 6-O-*β-D-glucopyranoside:* [89647-63-2]
$C_{22}H_{22}O_{11}$ 462.409
Yellow cryst. (MeOH). Mp 208-211°. λ_{max} 276 ; 332 (MeOH).

7-Me ether, 6-O-*β-D-galactopyranoside:* [107194-92-3]
$C_{22}H_{22}O_{11}$ 462.409
Mp 300° dec.

7-Me ether, 6-O-*[α-L-arabinopyranosyl-(1→2)-β-D-glucopyranoside]:* [157945-44-3]
$C_{27}H_{30}O_{15}$ 594.525

7-Me ether, 6-O-*[β-D-glucopyranosyl-(1→4)-α-L-rhamnopyranoside]:* [53011-71-5] ***Flavosorbin***
$C_{28}H_{32}O_{15}$ 608.552

7-Me ether, 4′-O-*[2,3-dihydroxy-3-(4-hydroxy-3-methoxyphenyl)propanoyl], 6*-O-*(O-acetylglucoside):* ***Lignoside***
$C_{34}H_{34}O_{17}$ 714.632
Mp 245-247°. $[\alpha]_D^{20}$ -91.6 (DMF).

4′,5-Di-Me ether: [168706-15-8] *6,7-Dihydroxy-4′,5-dimethoxyflavone.* ***Strigaflavone***
$C_{17}H_{14}O_6$ 314.294

4′,5-Di-Me ether, 7-O-*β-D-glucopyranoside:* [186466-61-5]
$C_{23}H_{24}O_{11}$ 476.436

4′,5-Di-Me ether, 7-O-*[4*-O-*acetyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [186466-62-6]
$C_{31}H_{36}O_{16}$ 664.616

4′,6-Di-Me ether: See 5,7-Dihydroxy-4′,6-dimethoxyflavone in *The Combined Chemical Dictionary.*

4′,7-Di-Me ether: See 5,6-Dihydroxy-4′,7-dimethoxyflavone in *The Combined Chemical Dictionary.*

6,7-Di-Me ether: See 4′,5-Dihydroxy-6,7-dimethoxyflavone in *The Combined Chemical Dictionary.*

4′,5,6-Tri-Me ether, 7-O-*β-D-glucopyranoside:* [17680-85-2]
$C_{24}H_{26}O_{11}$ 490.463
Constit. of *Juniperus communis* (juniper). Needles (MeOH). Mp 172-175° (semisynthetic).

4′,5,7-Tri-Me ether: [6938-19-8] *6-Hydroxy-4′,5,7-trimethoxyflavone*
$C_{18}H_{16}O_6$ 328.321
Yellow prisms. Mp 220-221° (synthetic).

4′,6,7-Tri-Me ether: See 5-Hydroxy-4′,6,7-trimethoxyflavone in *The Combined Chemical Dictionary.*

5,6,7-Tri-Me ether: [6938-18-7] *4′-Hydroxy-5,6,7-trimethoxyflavone*
$C_{18}H_{16}O_6$ 328.321
Cryst. (EtOAc). Mp 226-227° (synthetic).

5,6,7-Tri-Me ether, 4′-O-*β-D-glucopyranoside:* [169503-25-7]
$C_{24}H_{26}O_{11}$ 490.463

Tetra-Me ether: [1168-42-9] *4′,5,6,7-Tetramethoxyflavone. Tetra*-O-*methylscutellarein*
$C_{19}H_{18}O_6$ 342.348
Isol. from *Salvia officinalis* (sage) leaves. Cryst. (EtOH) in 2 forms. Mp 142° Mp 166-167° (dimorph.).

[28297-24-7, 83088-04-4]

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Sastri, V.D. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1946, **23**, 262 (*isol*)
Jouanne, M. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1966, **263**, 1022 (*synth*)
Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1969, **269**, 646-649 (*Sorbarioside*)
Bandyukova, V.A. *et al., Khim. Prir. Soedin.*, 1969, **5**, 324; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 274 (*5-O-glucuronide*)
Borodin, L.I. *et al., Khim. Prir. Soedin.*, 1969, **5**, 437; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 363 (*Isolignoside*)
Zaitsev, V.G. *et al., Khim. Prir. Soedin.*, 1969, **5**, 504; 598; 1974, **10**, 92; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 423; 516 (*Sorbarin, Flavosorbin, Sorbifolin*)
Boikova, A. *et al., Khim. Prir. Soedin.*, 1969, **5**, 596; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 513 (*7-O-glucuronide*)
Arisawa, M. *et al., Chem. Pharm. Bull.*, 1970, **18**, 916 (*uv, isol*)
Borodin, L.I. *et al., Farm. Zh. (Kiev)*, 1970, **25**, 62; *CA*, **73**, 120453 (*Lignoside*)
Nakayama, M. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 1143 (*synth, uv, pmr*)
Chumbalev, T.K. *et al., Khim. Prir. Soedin.*, 1971, **7**, 525; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 504 (*4′,7-dirhamnoside*)
Kamissarenko, N. *et al., Khim. Prir. Soedin.*, 1971, **7**, 721; 1976, **12**, 98; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 700 (*Stachyflaside*)
Subramanian, S.S. *et al., J. Indian Chem. Soc.*, 1972, **49**, 1061 (*4′-O-arabinoside*)
Farkas, L. *et al., Chem. Ber.*, 1974, **107**, 3878 (*Plantaginin 7-rutinoside, Scutellarin, synth*)
Okigawa, M. *et al., J.C.S. Perkin 1*, 1975, 1563 (*isol, deriv*)
Gumenyuk, L.A. *et al., Khim. Prir. Soedin.*, 1975, **11**, 428; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 444 (*7-rutinoside*)
Nair, A.G.R. *et al., Curr. Sci.*, 1977, **46**, 14 (*Isoscutellarin*)
Schels, H. *et al., Phytochemistry*, 1978, **17**, 523 (*ms*)
Ulubelen, A. *et al., J. Nat. Prod.*, 1981, **44**, 294 (*6-O-glucoside*)
Nair, A.G.R. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 1135; 1985, **24**, 323 (*Neohesperidoside, Ferulylscutellarin*)
Prakach, S. *et al., Phytochemistry*, 1982, **17**, 2992 (*isol*)
Markham, K.R. *et al., Phytochemistry*, 1983, **22**, 316 (*isol, struct*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1006 (*synth*)
Harborne, J.B. *et al., Z. Naturforsch., C*, 1984, **39**, 18 (*7-glucoside*)
Washington, J.S. *et al., J. Indian Chem. Soc.*, 1986, **63**, 226 (*7-glucosylrhamnoside*)
Alam, M.S. *et al., Phytochemistry*, 1986, **25**, (*Sorbifolin 6-galactoside*)
Nair, A.G.R. *et al., Phytochemistry*, 1986, **25**, 768 (*Triumboidin*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Stein, W. *et al., Z. Naturforsch., C*, 1990, **45**, 25 (*7-malonylglucoside*)
Ahmad, N.J.M. *et al., J. Chem. Res., Synop.*, 1991, 218 (*6-rhamnosylgalactoside*)
Alam, M.S. *et al., Fitoterapia*, 1993, **64**, 239 (*7-xylosylgalactoside*)
Yoshida, K. *et al., Phytochemistry*, 1993, **33**, 917 (*7-diglucuronide*)
Kraut, L. *et al., Phytochemistry*, 1993, **34**, 211; 1999, **52**, 749 (*7-HMG glucoside*)
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Shafiullah, M.P. *et al., J. Chem. Res., Synop.*, 1994, 320 (*7-rutinoside*)
Aqil, M. *et al., CA*, 1995, **123**, 251219f; 1997, **126**, 129250f (*Strigaflavone glycosides*)
Krishnaswamy, N.R. *et al., Indian J. Chem., Sect. B*, 1995, **34**, 750 (*7-Me 6-glucoside*)
Garcia, E. *et al., Nat. Prod. Lett.*, 1997, **11**, 67-72 (*synth*)
Manthey, J.A. *et al., Curr. Med. Chem.*, 2001, **8**, 135-153 (*Scutellarein, rev, activity*)
Mitchell, K.A. *et al., Phytochemistry*, 2001, **56**, 453-461 (*7-2-xylosylglucoside, 7-2-xylosylxyloside*)

4′,5,7,8-Tetrahydroxyflavone T-211

[41440-05-5]
5,7,8-Trihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Isoscutellarein****. 8-Hydroxyapigenin*

$C_{15}H_{10}O_6$ 286.24
Yellow needles (AcOH aq.). Mp 247-248° Mp 300-301°. λ_{max} 286 ; 339 (MeOH) (Berdy).

7-O-*β-D-Xylopyranoside:* [126771-29-7]
$C_{20}H_{18}O_{10}$ 418.356

7-O-*β-D-Glucopyranoside:* [63317-86-2]
$C_{21}H_{20}O_{11}$ 448.382

8-O-*β*-D-*Glucopyranoside:* [53761-83-4]
$C_{21}H_{20}O_{11}$ 448.382

8-O-*[4-Hydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranoside]:* ***Isoscutellarein 8-O-(6-coumaroylglucoside)***
$C_{30}H_{26}O_{13}$ 594.528
Amorph. powder. λ_{max} 270 ; 318 (MeOH).

7-O-*β*-D-*Glucuronopyranoside:* [141642-01-5]
$C_{21}H_{18}O_{12}$ 462.366

8-O-*β*-D-*Glucuronopyranoside:* [56317-09-0]
$C_{21}H_{18}O_{12}$ 462.366

8-O-*β*-D-*Glucuronopyranoside, Me ester:*
$C_{22}H_{20}O_{12}$ 476.393
Amorph. yellow solid. $[\alpha]_D^{26}$ +40.9 (c, 0.69 in MeOH). λ_{max} 211 (log ε 3.83); 274 (log ε 3.78); 346 (log ε 3.7) (MeOH).

8-O-*(2,4-Di*-O-*sulfo-β-D-glucuronopyranoside):*
$C_{21}H_{18}O_{18}S_2$ 622.494
Amorph. yellow powder. $[\alpha]_D^{21}$ -82.4 (c, 0.43 in H_2O). λ_{max} 270 (log ε 4.1); 298 (log ε 3.94); 333 (log ε 4.06) (H_2O).

7-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [123063-33-2] *Isoscutellarein 7-neohesperidoside*
$C_{27}H_{30}O_{15}$ 594.525

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [91485-77-7] *Isoscutellarein 7-rutinoside*
$C_{27}H_{30}O_{15}$ 594.525

7-O-*[β-D-Allopyranosyl-(1→2)-β-D-glucopyranoside]:* [96627-12-2]
$C_{27}H_{30}O_{16}$ 610.524

7-O-*[6*-O-*Acetyl-β-D-allopyranosyl-(1→2)-β-D-glucopyranoside]:* [80666-75-7]
$C_{29}H_{32}O_{17}$ 652.562

7-O-*[6*-O-*Acetyl-β-D-allopyranosyl-(1→2)-6*-O-*acetyl-β-D-glucopyranoside]:* [108706-08-7]
$C_{31}H_{34}O_{18}$ 694.599

4′-O-*[β-D-Mannopyranosyl-(1→2)-β-D-glucopyranoside]:* [68321-32-4] ***Isostachyflaside***
$C_{27}H_{30}O_{16}$ 610.524

4′-O-*[2*-O-*Acetyl-β-D-mannopyranosyl-(1→2)-β-D-glucopyranoside]:* [83323-89-1] ***Acetylisostachyflaside***
$C_{29}H_{32}O_{17}$ 652.562
Mp 174-178°.

4′-O-*[β-D-Mannopyranosyl-(1→2)-3,4-di*-O-*acetyl-β-D-glucopyranoside]:* [83323-88-0] ***Diacetylisostachyflaside***
$C_{31}H_{34}O_{18}$ 694.599
Mp 186-188°.

7-O-*[β-D-Glucopyranosyl-(1→2)-β-D-xylopyranoside]:*
$C_{26}H_{28}O_{15}$ 580.498
λ_{max} 203 ; 273 ; 302 (MeOH).

7-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [59379-75-8] ***Palustaside***. *Isoscutellarein 7-sophoroside*
$C_{27}H_{30}O_{16}$ 610.524
Mp 193-195°.

7-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], Ac:* [59379-76-9]
$C_{29}H_{32}O_{17}$ 652.562
Mp 167-169°. $[\alpha]_D^{22}$ +80 (c, 0.25 in MeOH aq.). Posn. of acetylation not detd..

4′-Me ether: 5,7,8-Trihydroxy-4′-methoxyflavone, T-619

7-Me ether: [56595-23-4] *4′,5,8-Trihydroxy-7-methoxyflavone. Salvitin*†
$C_{16}H_{12}O_6$ 300.267
Yellow needles (MeOH). Mp 304-305° (277-279°). The name Salvitin is no longer used.

8-Me ether: [57096-02-3] *4′,5,7-Trihydroxy-8-methoxyflavone. 4′-Hydroxywogonin*
$C_{16}H_{12}O_6$ 300.267
Yellow powder (EtOH). Mp 300°.

8-Me ether, 7-O-*[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [110011-53-5]
$C_{28}H_{32}O_{15}$ 608.552
Yellow needles (MeOH). Mp 320° dec.

4′,7-Di-Me ether: [89456-41-7] *5,8-Dihydroxy-4′,7-dimethoxyflavone.* ***4′,7-Di-O-methylisoscutellarein***
$C_{17}H_{14}O_6$ 314.294
Bright yellow cryst. (MeOH). Mp 261° dec.

4′,8-Di-Me ether: [65501-87-3] *5,7-Dihydroxy-4′,8-dimethoxyflavone.* ***Bucegin***. *Galangustin*
$C_{17}H_{14}O_6$ 314.294
Cryst. (MeOH). Mp 225°. Struct. formerly assigned to 4′,5-Dihydroxy-6,7-dimethoxyflavone.

4′,8-Di-Me ether, 7-O-*β-D-glucuronopyranoside:*
$C_{23}H_{22}O_{12}$ 490.42

7,8-Di-Me ether: [6608-33-9] *4′,5-Dihydroxy-7,8-dimethoxyflavone*
$C_{17}H_{14}O_6$ 314.294
Obt. from leaves and stems of *Scutellaria* spp. and from peel of *Citrus reticulata* (mandarin). Cryst. (EtOH). Mp 292-294°.

4′,5,7-Tri-Me ether: [21919-71-1] *8-Hydroxy-4′,5,7-trimethoxyflavone*
$C_{18}H_{16}O_6$ 328.321
Yellow prisms (MeOH). Mp 235°.

4′,7,8-Tri-Me ether: [57096-03-4] *5-Hydroxy-4′,7,8-trimethoxyflavone*
$C_{18}H_{16}O_6$ 328.321
From the peel of *Citrus reticulata* (mandarin). Yellow needles (EtOAc). Mp 220-221°.

Tetra-Me ether: [6601-66-7] *4′,5,7,8-Tetramethoxyflavone*
$C_{19}H_{18}O_6$ 342.348
Needles (MeOH). Mp 207-208°.

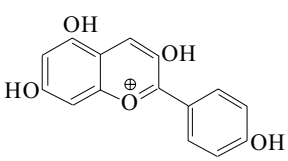
[107347-36-4, 129946-98-1]

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Combier, H. *et al., CA*, 1975, **83**, 177579 (*uv*)
Gupta, H.C. *et al., Indian J. Chem.*, 1975, **13**, 215 (*Salvitin*)
Markham, K.R. *et al., Phytochemistry*, 1975, **14**, 1093 (*8-glucuronoside*)
Bishara, S.A.R. *et al., CA*, 1976, **85**, 2514 (*Palustaside*)
Chhabra, S.C. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 651 (*4′,5,7-Trihydroxy-8-methoxyflavone*)
Komissarenko, N.F. *et al., Khim. Prir. Soedin.*, 1978, **14**, 521; 1980, **16**, 172; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 445; 1980, **16**, 128 (*Isostachyflaside*)
Tatum, J.H. *et al., Phytochemistry*, 1978, **17**, 447 (*4′,5,7,8-Tetramethoxyflavone*)
Goudard, M. *et al., Phytochemistry*, 1979, **18**, 186 (*ms*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 708; 717 (*isol, cmr, ms, deriv*)
Chari, V.M. *et al., Phytochemistry*, 1981, **20**, 1977 (*deriv*)
Savona, G. *et al., Heterocycles*, 1982, **19**, 1581 (*isol*)
Kostyuchenko, O.I. *et al., Khim. Prir. Soedin.*, 1982, **18**, 254; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 235 (*Acetylisostachyflasides*)
Tomimori, T. *et al., Yakugaku Zasshi*, 1982, **102**, 388 (*4′,5,7-Trihydroxy-8-methoxyflavone*)
Horie, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 3773 (*synth*)
Dommisse, R.A. *et al., Bull. Soc. Chim. Belg.*, 1983, 497 (*cmr*)
Reynaud, J. *et al., Pharmazie*, 1983, **38**, 628 (*4′,5,7-Trihydroxy-8-methoxyflavone*)
Markham, K.R. *et al., Phytochemistry*, 1983, **22**, 143 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Nakayama, M. *et al., Yakugaku Zasshi*, 1983, **103**, 675 (*5,7-Dihydroxy-4′,8-dimethoxyflavone*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1006 (*synth*)
Lenherr, A. *et al., Phytochemistry*, 1984, **23**, 2343 (*deriv*)
Iinuma, M. *et al., Yakugaku Zasshi*, 1984, **104**, 691 (*synth, 4′,5,7-Trimethoxy-8-methoxyflavone*)
Barberan, F.A.T. *et al., J. Nat. Prod.*, 1985, **48**, 28 (*7*-O-*allosylglucoside*)
Lenherr, A. *et al., Phytochemistry*, 1987, **26**, 1185 (*7-acetylallosylacetylglucoside*)
Alam, M.S. *et al., Phytochemistry*, 1987, **26**, 1843 (*8-Me ether, 7-neohesperidoside*)
Markham, K.R. *et al., Phytochemistry*, 1988, **27**, 2843; 1990, **29**, 501 (*7-glucoside, 7-xyloside*)
Ramesh, P. *et al., J. Nat. Prod.*, 1995, **58**, 1242 (*5,8-Dihydroxy-4′,7-dimethoxyflavone*)
Palomino, O.M. *et al., Phytochemistry*, 1996, **42**, 101 (*7-glucosylxyloside*)
Sharaf, M. *et al., Fitoterapia*, 1998, **69**, 355-357 (*8-coumaroylglucoside*)
Tezuka, Y. *et al., Helv. Chim. Acta*, 1999, **82**, 408-417 (*8-glucuronoside Me ester*)
Kamiya, K. *et al., Phytochemistry*, 2001, **57**, 297-301 (*8-2,4-disulfoglucuronoside*)

3,4′,5,7-Tetrahydroxyflavylium(1+), 8CI T-212

[7690-51-9]

[134-04-3]
3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-1-benzopyrylium(1+), 9CI. ***Pelargonidin***



$C_{15}H_{11}O_5^{\oplus}$ 271.249
Anthocyanin pigment present in many plants, flowers and fruits, e.g. cherries, raspberries, radishes, orchids, brassicas, *Petunia* spp. Glycosides also widely dis-

tributed. Red-brown prisms (HCl aq.) (as chloride). Mod. sol. H_2O. Mp 350° (chloride). Ms unsuitable as analytical technique λ_{max} 530 (ϵ 32000) (MeOH/HCl) (Berdy).

3-O-*α-L-Rhamnopyranoside:* [56190-03-5] *Pelargonidin 3-rhamnoside*
$C_{21}H_{21}O_9^{\oplus}$ 417.391
Isol. from *Ficus* sp. and others.

3-O-*α-L-Rhamnopyranoside, 5*-O-*β-D-glucopyranoside:* [53925-32-9] *Pelargonidin 5-glucoside 3-rhamnoside*
$C_{27}H_{31}O_{14}^{\oplus}$ 579.533
Isol. from *Pisum* spp..

3-O-*β-D-Galactopyranoside:* [125410-44-8] ***Fragarin***
$C_{21}H_{21}O_{10}^{\oplus}$ 433.391
Found in strawberry anthocyanin pigments used as fruit material in jam processing. Dark red cryst. with orange reflex + $4H_2O$ (as chloride).

5-O-*β-D-Galactopyranoside:* [157526-28-8] *Pelargonidin 5-galactoside*
$C_{21}H_{21}O_{10}^{\oplus}$ 433.391
Isol. from matara tea (*Cassia auriculata*).

3-O-*[4-Hydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranoside], 5*-O-*(4,6-di*-O-*malonyl-β-D-glucopyranoside):* [73545-87-6] ***Monardein***. *Monardaein*
$C_{42}H_{41}O_{23}^{\oplus}$ 913.772
Colouring matter of golden balm (*Monarda didyma*). Red powder (as chloride). $[\alpha]_D$ -374.5 (0.1% HCl, as chloride). CAS no. refers to chloride.

3,5-Di-O-*β-D-glucopyranoside:* [17334-58-6] ***Pelargonin***†. *Monardin*. *Salvinin*†. *Punicin*
$C_{27}H_{31}O_{15}^{\oplus}$ 595.533
Prob. occurs in pomegranate (*Punica granatum*). Fine red needles + $4H_2O$ (as chloride). Sol. H_2O. Mp 180° dec. (anhyd.) (chloride). $[\alpha]_D$ -244. Orange-red soln. in H_2O turning viol. on standing. MeOH soln. red with green fluor. The identity with Punicin from pomegranate is tentative.

3-O-*[α-L-Rhamnopyranosyl-(1→6)-[4-hydroxycinnamoyl-(→?)]-β-D-glucopyranoside], 5*-O-*β-D-glucopyranoside:* [51922-18-0] ***Pelanin***
$C_{42}H_{47}O_{21}^{\oplus}$ 887.821
Isol. from potato.

3-O-*[4-Hydroxy-3-methoxy*-E-*cinnamoyl-(→4)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 5*-O-*β-D-glucopyranoside:*
$C_{43}H_{49}O_{22}^{\oplus}$ 917.847
Constit. of red potatoes (*Solanum tuberosum*).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]:* [54542-60-8] *Pelargonidin 3-sophoroside*
$C_{27}H_{31}O_{15}^{\oplus}$ 595.533
Isol. from petals of *Papaver rhoeas* (corn poppy). λ_{max} 268 ; 505 (MeOH/HCl).

3-O-*[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 5*-O-*β-D-glucopyranoside:* [75093-88-8] ***Rubrobrassicin***
$C_{33}H_{41}O_{20}^{\oplus}$ 757.675
Present in roots of radish (*Raphanus sativus*) and *Brassica oleracea*. Cryst. + $4H_2O$. Apparently present as acylated derivs. in *R. sativus*, known as Raphanusins.

3-O-*[β-D-Glucopyranosyl-(1→2)-[4-hydroxycinnamoyl-(→6)]-β-D-glucopyranoside]*(E-)*, 5*-O-*β-D-glucopyranoside:* [218963-78-1]
$C_{42}H_{47}O_{22}^{\oplus}$ 903.82
Constit. of radish (*Raphanus sativus*).

3-O-*[β-D-Glucopyranosyl-(1→2)-[4-hydroxycinnamoyl-(→6)]-β-D-glucopyranoside]*(E-)*, 5*-O-*(6*-O-*malonyl-β-D-glucopyranoside):* [218963-76-9]
$C_{45}H_{49}O_{25}^{\oplus}$ 989.867
Constit. of radish (*Raphanus sativus*).

3-O-*[β-D-Glucopyranosyl-(1→2)-[4-hydroxy-3-methoxycinnamoyl-(→6)]-β-D-glucopyranoside]*(E-)*, 5*-O-*β-D-glucopyranoside:* [185027-87-6]
$C_{43}H_{49}O_{23}^{\oplus}$ 933.846
Constit. of radish (*Raphanus sativus*).

3-O-*[β-D-Glucopyranosyl-(1→2)-[4-hydroxy-3-methoxycinnamoyl-(→6)]-β-D-glucopyranoside]*(E-)*, 5*-O-*(6*-O-*malonyl-β-D-glucopyranoside):* [218963-77-0]
$C_{46}H_{51}O_{26}^{\oplus}$ 1019.893
Constit. of radish (*Raphanus sativus*).

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:Pelargonidin 3-(2*^{glu}*glucosylrutinoside)*
$C_{33}H_{41}O_{19}^{\oplus}$ 741.675
Isol. from fruits of raspberry (*Rubus idaeus*). λ_{max} 275 ; 508 (MeOH/HCl).

3-O-*(3,4-Dihydroxycinnamoyl), 5*-O-*β-D-glucopyranoside:* [100595-03-7] *3-Caffeoylpelargonidin 5-glucoside*
$C_{30}H_{27}O_{13}^{\oplus}$ 595.535
Isol. from red radish (*Raphanus* sp.).

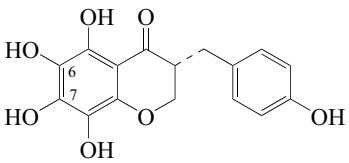
3-O-*(4-Hydroxy-3-methoxycinnamoyl), 5*-O-*β-D-glucopyranoside:* [100595-04-8] *3-Feruylpelargonidin 5-glucoside*
$C_{31}H_{29}O_{13}^{\oplus}$ 609.562
Isol. from red radish (*Raphanus* sp.).

[101752-18-5, 101752-19-6]

Karrer, P. *et al., Helv. Chim. Acta*, 1927, **10**, 67; 1928, **12**, 292 (*isol, Monardein*)
Robertson, A. *et al., J.C.S.*, 1928, 1460; 1533 (*isol*)
Léon, A. *et al., J.C.S.*, 1931, 2673 (*synth, glucosides*)
Nair, P.V. *et al., J.C.S.*, 1934, 1611 (*3-galactoside*)
Harborne, J.B. *et al., Phytochemistry*, 1963, **2**, 85; 1964, **3**, 151; 453; 1966, **5**, 589 (*derivs*)
Ishikura, N. *et al., CA*, 1965, **64**, 2411 (*Raphanusins, Rubrobrassicins*)
Timberlake, C.F. *et al., Nature (London)*, 1966, **212**, 158 (*uv*)
Nilson, E. *et al., Chem. Scr.*, 1973, **4**, 49 (*pmr*)
Timberlake, C.F. *et al., The Flavonoids*, (Eds. Harborne, J.B. *et al*), Chapman and Hall, London, 1975, 215 (*rev*)
Hoshino, T. *et al., Tet. Lett.*, 1981, **22**, 3621 (*cd, uv*)
Iacobucci, G.A. *et al., Tetrahedron*, 1983, **39**, 3005 (*rev*)
Saito, N. *et al., Heterocycles*, 1985, **23**, 2709 (*cryst struct*)
Lu, X. *et al., Shipin Yu Fajiao Gongye*, 1985, 19-25; *CA*, **104**, 106243n (*derivs, isol, red radish*)
Kondo, T. *et al., Tet. Lett.*, 1985, **26**, 5879; 1989, **30**, 6729 (*struct, Monardein, Salvianin*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Rai, K.N. *et al., Asian J. Chem.*, 1994, **6**, 696 (*5-galactoside*)
Merlin, J.-C. *et al., Phytochemistry*, 1994, **35**, 227 (*Raman*)
Giusti, M.M. *et al., J. Agric. Food Chem.*, 1998, **46**, 4858-4863 (*Raphanus sativus anthocyanins*)
Naito, K. *et al., Phytochemistry*, 1998, **47**, 109-112 (*Solanum anthocyanins*)

5,6,7,8-Tetrahydroxy-3-(4-hydroxybenzyl)-4-chromanone T-213

*2,3-Dihydro-5,6,7,8-tetrahydroxy-3-[(4-hydroxyphenyl)methyl]-4*H-*1-benzopyran-4-one*



$C_{16}H_{14}O_7$ 318.282

(R)-form

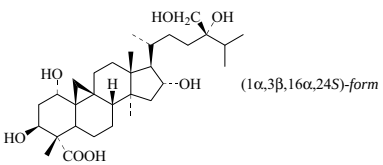
6,7-Di-Me ether: [96910-98-4] *5,8-Dihydroxy-3-(4-hydroxybenzyl)-6,7-dimethoxy-4-chromanone.* ***Muscomin***
$C_{18}H_{18}O_7$ 346.336
Isol. from *Muscari comosum* (tassel hyacinth). Cryst. ($CHCl_3$). Mp 144.7° (131-132°). $[\alpha]_D$ -71 (c, 0.6 in dioxan).

6,7,8-Tri-Me ether: [187527-48-6] *5-Hydroxy-3-(4-hydroxybenzyl)-6,7,8-trimethoxy-4-chromanone*
$C_{19}H_{20}O_7$ 360.363
Yellow cryst. Mp 59.7°. $[\alpha]_D^{25}$ -46.2 (c, 0.9 in MeOH).

Adinolfi, M. *et al., Phytochemistry*, 1985, **24**, 624
Amschler, G. *et al., Planta Med.*, 1996, **62**, 534 (*isol, uv, cd, pmr, cmr, ms*)

1,3,16,24-Tetrahydroxy-24-(hydroxymethyl)cycloartan-28-oic acid T-214

1,3,16,24,31-Pentahydroxy-24-methylcycloartan-28-oic acid



(1α,3β,16α,24*S*)-*form*

$C_{31}H_{52}O_7$ 536.748

(1α,3β,16α,24S)-form [239794-30-0]

[301540-77-2]
Cyclotricuspidogenin C. *Cyclopassifloic acid G*
Isol. from *Passiflora edulis* (passion fruit). $[\alpha]_D^{23}$ +12.1 (c, 1 in MeOH). $[\alpha]_D^{25}$ +39.3 (c, 3.0 in MeOH).

28-O-*β-D-Glucopyranosyl ester:* [301540-82-9] ***Cyclopassifloside X***
$C_{37}H_{62}O_{12}$ 698.89
Constit. of *Passiflora edulis* (passion fruit). Needles. Mp 167-169°. $[\alpha]_D^{25}$ +36.8

(c, 2.1 in MeOH).

31-O-*β*-D-*Glucopyranoside, 28*-O-*β*-D-*glucopyranosyl ester:* [239794-23-1]

[301644-34-8] ***Cyclotricuspidoside C***. *Cyclopassifloside XI*
$C_{43}H_{72}O_{17}$ 861.032
Constit. of *Passiflora edulis* (passion fruit). Needles. Mp 171-173°. $[\alpha]_D^{23}$ +28.2 (c, 1 in MeOH). $[\alpha]_D^{25}$ +13.6 (c, 2.7 in MeOH).

(1α,3β,16β,24*S*)-*form* [239794-27-5]

[301540-76-1]
Cyclotricuspidogenin B. *Cyclopassifloic acid F*
Isol. from *Passiflora edulis* (passion fruit). Amorph. powder. $[\alpha]_D^{23}$ +17 (c, 0.8 in MeOH). $[\alpha]_D^{25}$ +48.2 (c, 5.1 in MeOH).

28-O-*β*-D-*Glucopyranosyl ester:* [301540-81-8] ***Cyclopassifloside VIII***
$C_{37}H_{62}O_{12}$ 698.89
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{25}$ +38.6 (c, 1.3 in MeOH).

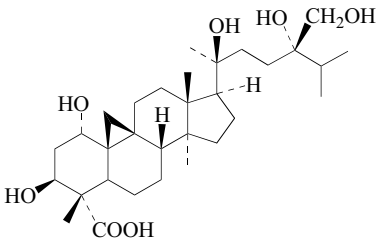
31-O-*β*-D-*Glucopyranoside, 28*-O-*β*-D-*glucopyranosyl ester:* [239794-22-0]

[301644-33-7] ***Cyclotricuspidoside B***. *Cyclopassifloside IX*
$C_{43}H_{72}O_{17}$ 861.032
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{23}$ +35.9 (c, 1 in MeOH). $[\alpha]_D^{25}$ +19 (c, 1.3 in MeOH).

Kasai, R. *et al., Phytochemistry*, 1999, **51**, 803-808 (*Cyclotricuspidogenins, Cyclotricuspidosides*)
Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 1377-1380 (*Cyclopassifloic acids, Cyclopassiflosides*)

1,3,20,24-Tetrahydroxy-24-(hydroxymethyl)cycloartan-28-oic acid T-215

1,3,20,24,31-Pentahydroxy-24-methylcycloartan-28-oic acid



$C_{31}H_{52}O_7$ 536.748

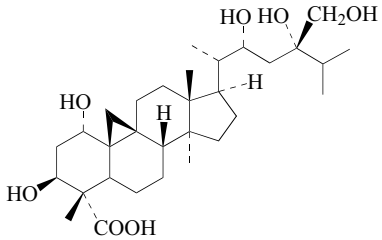
(1α,3β,20*S*,24*S*)-*form* [292167-36-3]
Cyclopassifloic acid C
Constit. of *Passiflora edulis* (passion fruit). Amorph. powder. $[\alpha]_D^{25}$ +23.8 (c, 2.1 in MeOH).

28-O-*β*-D-*Glucopyranosyl ester:* [292167-41-0] ***Cyclopassifloside IV***
$C_{37}H_{62}O_{12}$ 698.89
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{25}$ +33.1 (c, 6.3 in MeOH).

31-O-*β*-D-*Glucopyranoside, 28*-O-*β*-D-*glucopyranosyl ester:* [292167-42-1] ***Cyclopassifloside V***
$C_{43}H_{72}O_{17}$ 861.032
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{25}$ +16.5 (c, 6.8 in MeOH).
Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 1229-1234 (*isol, pmr, cmr*)

1,3,22,24-Tetrahydroxy-24-(hydroxymethyl)cycloartan-28-oic acid T-216

1,3,22,24,31-Pentahydroxy-24-methylcycloartan-28-oic acid



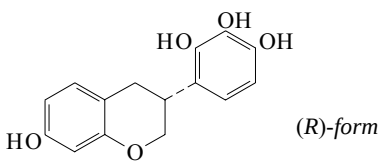
$C_{31}H_{52}O_7$ 536.748

(1α,3β,22*R*,24*S*)-*form* [292167-34-1]
Cyclopassifloic acid A
Constit. of *Passiflora edulis* (passion fruit). Needles. Mp 229-231°. $[\alpha]_D^{25}$ +56.6 (c, 1.5 in MeOH).

28-O-*β*-D-*Glucopyranosyl ester:* [292167-38-5] ***Cyclopassifloside I***
$C_{37}H_{62}O_{12}$ 698.89
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{25}$ +54.5 (c, 0.2 in MeOH).
Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 1229-1234 (*isol, pmr, cmr*)

2′,3′,4′,7-Tetrahydroxyisoflavan T-217

*3,4-Dihydro-7-hydroxy-3-(2,3,4-trihydroxyphenyl)-2*H*-1-benzopyran*



(*R*)-*form*

$C_{15}H_{14}O_5$ 274.273

(*R*)-*form*

3′,4′-Di-Me ether: [64474-51-7] *2′,7-Dihydroxy-3′,4′-dimethoxyisoflavan*. ***Isomucronulatol***. *Astraisoflavan*
$C_{17}H_{18}O_5$ 302.326
Isol. from *Glycyrrhiza glabra* (licorice). Cryst. (MeOH aq.). Mp 152-153°. $[\alpha]_D^{20}$ -19.4 (c, 0.24 in EtOH). λ_{max} 271 (ε 4160) (EtOH) (Berdy). λ_{max} 222 ; 294 (EtOH/NaOH) (Berdy).

2′,3′,4′-Tri-Me ether: [136027-12-8] *7-Hydroxy-2′,3′,4′-trimethoxyisoflavan*
$C_{18}H_{20}O_5$ 316.353
Constit. of *Medicago sativa* (alfalfa). Mp 168-170°. $[\alpha]_D^{27}$ +6.5 (c, 1.15 in $CHCl_3$). Unusual + ve opt. rotn..

(±)-*form*

2′,3′-Di-Me ether: [52305-06-3] ***Laxifloran***. *(±)-Sphaerosin*
Isol. from *Lablab niger* (hyacinth bean). Cryst. (MeOH). Mp 170-171°. λ_{max} 213 ; 281 (MeOH) (Berdy). λ_{max} 211 ; 282 ; 290 (EtOH) (Berdy). λ_{max} 213 ; 245 ; 294 (EtOH/NaOH) (Berdy). λ_{max} 219 ; 291 (MeOH/NaOH) (Berdy).

[27973-50-8, 52250-35-8]

Pelter, A. *et al., J.C.S.(C)*, 1969, 887 (*Laxifloran*)
Farkas, L. *et al., J.C.S. Perkin 1*, 1974, 305 (*Laxifloran*)
Al-Ani, H.A.M. *et al., Phytochemistry*, 1985, **24**, 55 (*biosynth, bibl, Isomucronulatol*)
He, Z.Q. *et al., J. Nat. Prod.*, 1991, **54**, 810
Subarnas, A. *et al., Phytochemistry*, 1991, **30**, 2777
Spencer, G.F. *et al., Phytochemistry*, 1991, **30**, 4147 (*7-Hydroxy-2′,3′,4′-trimethoxyisoflavan*)

2′,4′,5′,7-Tetrahydroxyisoflavan T-218

*3,4-Dihydro-7-hydroxy-3-(2,4,5-trihydroxyphenyl)-2*H*-1-benzopyran*
$C_{15}H_{14}O_5$ 274.273

(*R*)-*form*

2′,4′,5′-Tri-Me ether: [122577-99-5] *7-Hydroxy-2′,4′,5′-trimethoxyisoflavan*. ***5′-Methoxysativan***
$C_{18}H_{20}O_5$ 316.353
Isol. from the leaves of *Medicago sativa* (alfalfa). $[\alpha]_D^{25}$ -12.7 (c, 2.7 in MeOH).

[22091-12-9]

Miller, R.W. *et al., J. Nat. Prod.*, 1989, **52**, 634 (*5′-Methoxysativan*)

2′,4′,6,7-Tetrahydroxyisoflavan T-219

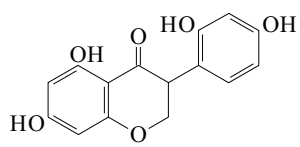
*3,4-Dihydro-3-(2,4-dihydroxyphenyl)-6,7-dihydroxy-2*H*-1-benzopyran*
$C_{15}H_{14}O_5$ 274.273

4′,6-Di-Me ether: [56752-02-4] *2′,7-Dihydroxy-4′,6-dimethoxyisoflavan*. ***6-Methoxyvestitol***
$C_{17}H_{18}O_5$ 302.326
Isol. from cultures of *Fusarium solani* growing on *Pisum sativum* (pea).

Pueppke, S.G. *et al., Physiol. Plant Pathol.*, 1976, **8**, 51

2′,4′,5,7-Tetrahydroxyisoflavanone T-220

[30368-42-4]
*2,3-Dihydro-5,7-dihydroxy-3-(2,4-dihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*. ***Dalbergioidin***



$C_{15}H_{12}O_6$ 288.256
Isol. from *Dolichos biflorus* (papadi), *Lablab niger* (hyacinth bean) and *Phaseolus vulgaris* (kidney bean). λ_{max} 201 ; 289 ; 291 (ε 7000) (MeOH) (Berdy). λ_{max} 288 (ε 22000) (EtOH) (Berdy). λ_{max} 323 (MeOH-NaOH) (Berdy).

2′-Me ether: [76656-75-2] *4′,5,7-Trihydroxy-2′-methoxyisoflavanone*. ***Isoferreirin***

$C_{16}H_{14}O_6$ 302.283
Constit. of *Dolichos biflorus* (papadi). λ_{max} 212 ; 229 ; 289 (MeOH) (Berdy). λ_{max} 214 ; 244 ; 324 (MeOH-NaOH) (Berdy). λ_{max} 225 ; 288 ; 330 (EtOH) (Berdy).

4′-Me ether: [32898-79-6] *2′,5,7-Trihydroxy-4′-methoxyisoflavanone.* ***Ferreirin***
$C_{16}H_{14}O_6$ 302.283
Isol. from *Cajanus cajan* (pigeon pea). Prisms (MeOH aq. or petrol). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 210-212°. λ_{max} 288 (MeOH) (Berdy). λ_{max} 324 (MeOH-NaOH) (Berdy).

7-Me ether:2′,4′,5-Trihydroxy-7-methoxyisoflavanone. ***Dihydrocajanin***
$C_{16}H_{14}O_6$ 302.283
Cryst. Mp 214-216°. Racemic λ_{max} 211 (ϵ 31600); 287 (ϵ 20900) (EtOH) (Berdy).

2′,4′-Di-Me ether: [482-01-9] *5,7-Dihydroxy-2′,4′-dimethoxyisoflavanone.* ***Homoferreirin***
$C_{17}H_{16}O_6$ 316.31
Isol. from *Cicer arietinum* (chickpea). Rectangular plates (C_6H_6/petrol or MeOH aq.). Mp 168-169°.

2′,4′-Di-Me ether, di-Ac:
Long needles. Mp 132-133°.

2′,5-Di-Me ether: [99965-02-3] *4′,7-Dihydroxy-2′,5-dimethoxyisoflavanone*
$C_{17}H_{16}O_6$ 316.31
Isol. from *Phaseolus coccineus* (scarlet runner bean). Sol. MeOH, EtOAc; poorly sol. H_2O. λ_{max} 205 ; 286 (EtOH) (Berdy). λ_{max} 206 ; 245 ; 322 (EtOH-NaOH) (Berdy).

2′,7-Di-Me ether: [61020-70-0] *4′,5-Dihydroxy-2′,7-dimethoxyisoflavanone.* ***Cajanol***
$C_{17}H_{16}O_6$ 316.31
Isol. from fungus-infected stems of *Cajanus cajan* (pigeon pea). Revised struct. Formerly considered to be 2′,6-Dihydroxy-4′,7-dimethoxyisoflavanone λ_{max} 214 ; 229 ; 287 (MeOH) (Berdy). λ_{max} 215 ; 244 ; 287 (NaOH) (Berdy).

Tetra-Me ether: [28812-39-7] *2′,4′,5,7-Tetramethoxyisoflavanone*
$C_{19}H_{20}O_6$ 344.363
Cryst. (C_6H_6). Mp 163°.

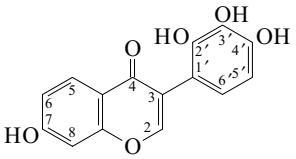
4′-O-β-D-Glucopyranoside:Dalbergioidin 4′-glucoside
$C_{21}H_{22}O_{11}$ 450.398
Amorph. powder. $[\alpha]_D$ -16.2 (c, 0.07 in MeOH).

[66152-08-7]

King, F.E. *et al., J.C.S.*, 1952, 4580; 4752 (*Ferreirin, Homoferreirin*)
Farkas, L. *et al., J.C.S.(C)*, 1971, 1994 (*synth*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1976, **31**, 504; 1977, **32**, 1018; 1980, **35**, 923 (*isol, spectra, biosynth, derivs*)
Woodward, M.D. *et al., Phytochemistry*, 1979, **18**, 363 (*isol*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1979, **34**, 159 (*Cajanol*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Adensanya, S.A. *et al., Phytochemistry*, 1985, **24**, 2699 (*4′,7-Dihydroxy-2′,5-dimethoxyisoflavanone*)
Osawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2970 (*Dihydrocajanin*)
Iinuma, M. *et al., Phytochemistry*, 1994, **37**, 889 (*4′-glucoside*)

2′,3′,4′,7-Tetrahydroxyisoflavone T-221

[148356-26-7]
7-Hydroxy-3-(2,3,4-trihydroxyphenyl)-4H-1-benzopyran-4-one



$C_{15}H_{10}O_6$ 286.24
Mp 261-263°.

3′,4′-Methylene ether: [65242-64-0] *2′,7-Dihydroxy-3′,4′-methylenedioxyisoflavone.* ***Glyzaglabrin***
$C_{16}H_{10}O_6$ 298.251
Isol. from root of *Glycyrrhiza glabra* (licorice).

Bhardwaj, D.K. *et al., Curr. Sci.*, 1977, **46**, 753 (*Glyzaglabrin*)

2′,4′,5,7-Tetrahydroxyisoflavone T-222

[1156-78-1]
3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. ***2′-Hydroxygenistein***

$C_{15}H_{10}O_6$ 286.24
Isol. from *Cajanus cajan* (pigeon pea), *Dolichos biflorus* (papadi), *Lablab niger* (hyacinth bean), *Phaseolus vulgaris* (kidney bean) and *Phaseolus coccineus* (scarlet runner bean). Cryst. ($CHCl_3$/MeOH). Mp 270-273°. λ_{max} 209 ; 262 ; 288 (MeOH) (Berdy).

4′-O-β-D-Glucopyranoside: [137351-14-5]
$C_{21}H_{20}O_{11}$ 448.382

7-O-β-D-Glucopyranoside: [137351-12-3]
$C_{21}H_{20}O_{11}$ 448.382
Mp 208-210°.

4′,7-Di-O-β-D-glucopyranoside: [147879-69-4]
$C_{27}H_{30}O_{16}$ 610.524
Powder. $[\alpha]_D^{25}$ -19.7 (c, 0.6 in DMSO).

7-O-(6-O-Malonyl-β-D-glucopyranoside): [137351-13-4]
$C_{24}H_{22}O_{14}$ 534.429
Isol. from the roots of *Lupinius albus* (white lupin).

4′-Me ether: [32884-35-8] *2′,5,7-Trihydroxy-4′-methoxyisoflavone.* ***Dehydroferreirin****. 2′-Hydroxybiochanin A*
$C_{16}H_{12}O_6$ 300.267
Needles (MeOH aq.). Mp 215-216° (201-203°).

5-Me ether: [101691-27-4] *2′,4′,7-Trihydroxy-5-methoxyisoflavone.* ***Barpisoflavone A****. 2′-Hydroxyisoprunetin*
$C_{16}H_{12}O_6$ 300.267
Constit. of *Phaseolus coccineus* (scarlet runner bean). Needles. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 290° dec.
The name 2′-Hydroxyisoprunetin is not recommended λ_{max} 206 ; 256 ; 290 (EtOH) (Berdy). λ_{max} 210 ; 273 ; 320 (EtOH/NaOH) (Berdy).

7-Me ether: [32884-36-9] *2′,4′,5-Trihydroxy-7-methoxyisoflavone.* ***Cajanin***
$C_{16}H_{12}O_6$ 300.267
Isol. from *Cajanus cajan* (pigeon pea), *Canavalia ensiformis* (jack bean). Sol. EtOAc. Mp 208-210°. λ_{max} 216 ; 260 (ϵ 22400); 288 (MeOH) (Berdy). λ_{max} 272 (MeOH/NaOH) (Berdy). λ_{max} 269 ; 306 (HCl) (Berdy).

2′,4′-Di-Me ether: [61243-75-2] *5,7-Dihydroxy-2′,4′-dimethoxyisoflavone. 2′-Methoxybiochanin A*
$C_{17}H_{14}O_6$ 314.294
Cryst. (MeOH). Mp 222-223°.

2′,5-Di-Me ether:4′,7-Dihydroxy-2′,5-dimethoxyisoflavone
$C_{17}H_{14}O_6$ 314.294
From *Phaseolus coccineus* (scarlet runner bean).

4′,7-Di-Me ether: [61020-69-7] *2′,5-Dihydroxy-4′,7-dimethoxyisoflavone*
$C_{17}H_{14}O_6$ 314.294
Isol. from *Cajanus cajan* (pigeon pea) (fungus-infected stems). Struct. not confirmed.

5,7-Di-Me ether: [131862-36-7] ***2′,4′-Dihydroxy-5,7-dimethoxyisoflavone***
$C_{17}H_{14}O_6$ 314.294

2′,4′,7-Tri-Me ether: [54443-60-6] *5-Hydroxy-2′,4′,7-trimethoxyisoflavone*
$C_{18}H_{16}O_6$ 328.321
Cryst. Mp 160-162°.

Tetra-Me ether: [1100-15-8] *2′,4′,5,7-Tetramethoxyisoflavone*
$C_{19}H_{18}O_6$ 342.348
Cryst. (C_6H_6/petrol or MeOH). Mp 203-204° (197-199°).

King, F.E. *et al., J.C.S.*, 1952, 4752-4756 (*4′-Me ether, 2′,4′-di-Me ether, synth*)
Farkas, L. *et al., J.C.S.(C)*, 1971, 1994-2000 (*4′-Me ether, synth*)
Braz Filho, R. *et al., Phytochemistry*, 1976, **15**, 1029-1030 (*isol, uv, ir, pmr, ms, 2′-Me ether, 2′,7-di-Me ether*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1976, **31**, 504-508; 1977, **32**, 1018-1022 (*isol*)
Prasad, J.S. *et al., Phytochemistry*, 1977, **16**, 1120 (*isol, uv, pmr, struct*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1-266 (*rev, occur*)
Sanduja, R. *et al., J. Chem. Res., Synop.*, 1985, 56 (*2′,4′,7-tri-Me ether, tetra-Me ether*)
Parmar, V.S. *et al., Org. Mass Spectrom.*, 1985, **20**, 265-266 (*ms*)
Adeesanya, S.A. *et al., Phytochemistry*, 1985, **24**, 2699-2702 (*isol, 5-Me ether, 2′,5-di-Me ether*)
Tahara, S. *et al., Agric. Biol. Chem.*, 1986, **50**, 1809-1819 (*Barpisoflavone A*)
Souleles, C. *et al., J. Nat. Prod.*, 1990, **53**, 1340-1341 (*2′,4′-Dihydroxy-5,7-dimethoxyisoflavone*)
Shibuya, Y. *et al., Z. Naturforsch., C*, 1991, **46**, 513-518 (*glucosides*)
Watanabe, K. *et al., Chem. Pharm. Bull.*, 1993, **41**, 394-396 (*4′,7-diglucoside*)
Waffo, A.K. *et al., Phytochemistry*, 2000, **53**, 981-985 (*Cajanin*)

2′,5,6,7-Tetrahydroxyisoflavone T-223

5,6,7-Trihydroxy-3-(2-hydroxyphenyl)-4H-1-benzopyran-4-one

$C_{15}H_{10}O_6$ 286.24

2′,6-Di-Me ether, 7-O-α-L-rhamnopyranoside: [275816-77-8]
$C_{23}H_{24}O_{10}$ 460.437
Constit. of the roots of *Sesbania grandiflora* (agati).

6,7-Methylene, 5-Me ether, 2′-O-β-D-xylopyranoside: [160485-40-5] ***Betavulgarin xyloside***
$C_{22}H_{20}O_{10}$ 444.394
Constit. of *Beta vulgaris* (sugar beet) infected with *Rhizoctonia solani*. Cryst. (EtOH). Mp 144-146°.

6,7-Methylene, 5-Me ether, 2′-O-β-D-glucopyranoside: ***Betavulgarin glucoside***
$C_{23}H_{22}O_{11}$ 474.42
Isol. from *Beta vulgaris* (sugar beet) infected with *Rhizoctonia solani* as a phytoalexin. Cryst. (MeOH). Mp 259-261°.

Geigert, J. *et al., Tetrahedron*, 1973, **29**, 2703 (*Betavulgarin*)
Elliger, C.A. *et al., Phytochemistry*, 1994, **37**, 691 (*Betavulgarin glycosides*)
Saxena, V.K. *et al., CA*, **133**, 40508t (*2′,6-di-Me 7-rhamnoside*)

3′,4′,5,7-Tetrahydroxyisoflavone T-224

[480-23-9]
3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4H-1-benzopyran-4-one, 9CI. ***Orobol****. Norsantal. Isoluteolin*

$C_{15}H_{10}O_6$ 286.24
Pale yellow cryst. (AcOH). Sol. MeOH, EtOAc. Mp 212°. All isolations of isoflavonoids from microorganisms are considered doubtful λ_{max} 263 (ϵ 27500); 290 (ϵ 11400) (MeOH) (Derep). λ_{max} 234 (ϵ 25000); 263 (E1%/1cm 960); 290 (E1%/1cm 400) (MeOH) (Berdy).

► DJ2982400

4′-Me ether: [2284-31-3] *3′,5,7-Trihydroxy-4′-methoxyisoflavone.* ***Pratensein***
$C_{16}H_{12}O_6$ 300.267
Constit. of *Cicer arietinum* (chickpea). Cryst. (EtOH). Mp 272-273°. λ_{max} 262 (MeOH) (Berdy). λ_{max} 270 ; 320 (MeOH-NaOH) (Berdy).

4′-Me ether, 3′-O-β-D-glucopyranoside:
$C_{22}H_{22}O_{11}$ 462.409
Constit. of the skins of peanuts, *Arachis hypogaea*. Needles (MeOH). Mp 236-239°.

7-Me ether: [529-60-2] *3′,4′,5-Trihydroxy-7-methoxyisoflavone.* ***Santal***
$C_{16}H_{12}O_6$ 300.267
Constit. of *Pterocarpus soyauxii*. Cryst. (EtOH). Mp 222-223°.

3′,7-Di-Me ether: [104668-88-4] *4′,5-Dihydroxy-3′,7-dimethoxyisoflavone. 3′,7-Di-O-methylorobol*
$C_{17}H_{14}O_6$ 314.294
Constit. of *Pterocarpus soyauxii*. Mp 179° (as di-Ac).

Akisanya, A. *et al., J.C.S.*, 1959, 2679 (*isol*)
Wong, E. *et al., J.O.C.*, 1963, **28**, 2336 (*isol, struct, synth*)
Markham, K.R. *et al., Phytochemistry*, 1968, **7**, 791 (*isol*)
Dement, A.W. *et al., Phytochemistry*, 1972, **11**, 1089 (*isol*)
Adinarayana, D. *et al., Indian J. Chem.*, 1974, **12**, 911 (*synth*)
Leite de Almeida, M.E. *et al., Phytochemistry*, 1974, **13**, 751 (*isol*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Asres, K. *et al., Z. Naturforsch., C*, 1985, **40**, 617 (*isol*)
Jain, A.C. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 488 (*synth*)
Nishiyama, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 107 (*synth*)
Hou, A.-J. *et al., J. Nat. Prod.*, 2001, **64**, 65-70 (*activity*)
Lou, H. *et al., Planta Med.*, 2001, **67**, 345-349 (*4′-Me 3′-glucoside*)

3′,4′,7,8-Tetrahydroxyisoflavone T-225

3-(3,4-Dihydroxyphenyl)-7,8-dihydroxy-4H-1-benzopyran-4-one, 9CI

$C_{15}H_{10}O_6$ 286.24

4′,8-Di-Me ether: [53947-99-2] *3′,7-Dihydroxy-4′,8-dimethoxyisoflavone*
$C_{17}H_{14}O_6$ 314.294
Isol. from *Myroxylon balsamum* (Tolu balsam). Cryst. (EtOH). Mp 212-213°.

Harper, S.H. *et al., Phytochemistry*, 1976, **15**, 1019 (*4′,8-di-Me ether*)
Albuquerque, F.B. *et al., Phytochemistry*, 1981, **20**, 235 (*4′,8-di-Me ether*)

4′,5,7,8-Tetrahydroxyisoflavone T-226

[13539-27-0]
5,7,8-Trihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 8-Hydroxygenistein

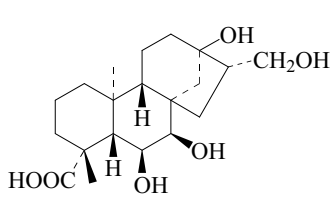
$C_{15}H_{10}O_6$ 286.24
Cryst. (EtOH). Sol. MeOH. Mp 330° dec. All isolations of isoflavones from microorganisms are considered suspect λ_{max} 272 (E1%/1cm 813); 310 (MeOH) (Berdy).

► DJ3100260

8-Me ether, 4′-O-β-D-glucopyranoside, 7-O-α-L-rhamnopyranoside:
$C_{28}H_{32}O_{15}$ 608.552
Constit. of the aerial parts of *Salvia triloba* (greek sage). Amorph. yellow solid. λ_{max} 274 ; 321 (MeOH).

El-Sayed, N.H. *et al., Fitoterapia*, 2001, **72**, 850-853 (*8-Me 7-rhamnoside 4′-glucoside*)

6,7,13,17-Tetrahydroxy-19-kauranoic acid T-227



$C_{20}H_{32}O_6$ 368.469

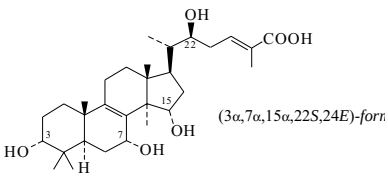
(ent-6α,7α,16αH)-form [333334-48-8]
Pisuminic acid
Powder. $[\alpha]_D^{25}$ -30.5 (c, 0.1 in MeOH).

19-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl] ester: [333334-43-3] ***Pisumoside B***
$C_{32}H_{52}O_{16}$ 692.753
Constit. of *Pisum sativum* (pea). Powder. $[\alpha]_D^{25}$ -31.5 (c, 0.2 in MeOH).

17-O-β-D-Glucopyranoside, 19-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl] ester: [333334-42-2] ***Pisumoside A***
$C_{38}H_{62}O_{21}$ 854.895
Constit. of *Pisum sativum* (pea). Powder. $[\alpha]_D^{26}$ -18.8 (c, 0.9 in MeOH).

Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 73-77 (*isol, pmr, cmr*)

3,7,15,22-Tetrahydroxylanosta-8,24-dien-26-oic acid T-228



$C_{30}H_{48}O_6$ 504.706

(3α,5α,7α,15α,22S,24E)-form

3,15,22-Tri-Ac:3α,15α,22S-Triacetoxy-7α-hydroxylanosta-8,24E-dien-26-oic acid. ***Ganoderic acid O***†
$C_{36}H_{54}O_9$ 630.817
Constit. of cultured mycelium of *Ganoderma lucidum* (reishi). Needles. Mp 156-158°. Not the same as Ganoderic acid O in 7,20-Dihydroxy-3,11,15,23-tetraoxolanost-8-en-26-oic acid, D-697.

3,15,22-Tri-Ac, 7-Me ether:3α,15α,22S-Triacetoxy-7α-methoxylanosta-8,24E-dien-26-oic acid. ***O-Methylganoderic acid O***
$C_{37}H_{56}O_9$ 644.844
Constit. of cultured mycelium of *Ganoderma lucidum* (reishi). Cryst. Mp 228-229.5°.

(3α,5α,7α,15α,22ξ,24E)-form

3,15,22-Tri-Ac:3α,15α,22-Triacetoxy-7α-hydroxylanosta-8,24E-dien-26-oic acid. ***Ganoderic acid Mb***
$C_{36}H_{54}O_9$ 630.817
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{27}$ -4 (c, 0.2 in MeOH).

3,7,22-Tri-Ac:3α,7α,22-Triacetoxy-15α-hydroxylanosta-8,24E-dien-26-oic acid. ***Ganoderic acid Mc***
$C_{36}H_{54}O_9$ 630.817
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{27}$ -23 (c, 0.2 in MeOH).

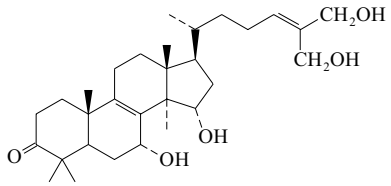
3,22-Di-Ac, 7-Me ether: [110042-11-0] *3α,22-Diacetoxy-15α-hydroxy-7α-methoxylanosta-8,24E-dien-26-oic acid.* ***Ganoderic acid Mg***
$C_{35}H_{54}O_8$ 602.807
Metab. *Ganoderma lucidum* (reishi). Amorph. powder. Mp 126-129°. $[\alpha]_D^{23}$ -23 (c, 0.2 in MeOH).

3,22-Di-Ac: [110024-17-4] *3α,22-Diacetoxy-7α,15α-dihydroxylanosta-8,24E-dien-26-oic acid.* ***Ganoderic acid Mh***
$C_{34}H_{52}O_8$ 588.78

Syrup. $[\alpha]_D^{23}$ +2 (c, 0.2 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 619; 1149 (*isol*)
Hirotani, H. *et al., Phytochemistry*, 1987, **26**, 2797 (*isol*)

7,15,26,27-Tetrahydroxylanosta-8,24-dien-3-one T-229



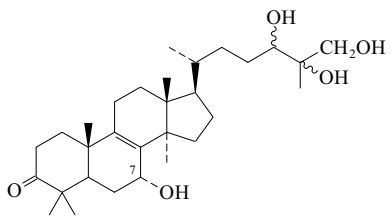
$C_{30}H_{48}O_5$ 488.706

(7α,15α)-*form*

7-Me ether: [114567-49-6] *15α,26,27-Trihydroxy-7α-methoxy-8,24-lanostadien-3-one.* ***Ganoderiol I***
$C_{31}H_{50}O_5$ 502.733
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{22}$ +53 (c, 0.1 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 367 (*isol, pmr, cmr*)

7,24,25,26-Tetrahydroxylanost-8-en-3-one T-230



$C_{30}H_{50}O_5$ 490.722

(7α,24ξ,25ξ)-*form*

7-Me ether: [114567-48-5] *24,25,26-Trihydroxy-7α-methoxy-8-lanosten-3-one.* ***Ganoderiol G***
$C_{31}H_{52}O_5$ 504.749
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{24}$ +34 (c, 0.1 in MeOH).

7-Et ether: [114567-44-1] *7α-Ethoxy-24,25,26-trihydroxy-8-lanosten-3-one.* ***Ganoderiol C***
$C_{32}H_{54}O_5$ 518.776
Metab. of *Ganoderma lucidum* (reishi). Syrup (as di-Ac). $[\alpha]_D^{23}$ +54 (c, 0.1 in EtOH) (di-Ac).

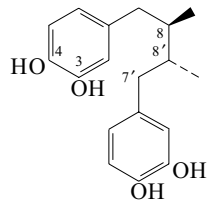
7-Ketone: [114567-45-2] *24,25,26-Tetrahydroxy-8-lanostene-3,7-dione.* ***Ganoderiol D***
$C_{30}H_{48}O_5$ 488.706
Metab. of *Ganoderma lucidum* (reishi). Syrup (as di-Ac). $[\alpha]_D^{21}$ +8 (c, 0.1 in MeOH) (di-Ac).

7-Ketone, 3β-alcohol: [114612-72-5] *3β,24,25,26-Tetrahydroxy-8-lanosten-7-one.* ***Ganoderiol H***
$C_{30}H_{50}O_5$ 490.722
Metab. of *Ganoderma lucidum* (reishi). Needles. Mp 200-201.5°. $[\alpha]_D^{24}$ +22 (c, 0.1 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 367 (*isol, pmr, cmr*)

3,3′,4,4′-Tetrahydroxylignan T-231

[500-38-9]
1,4-Bis(3,4-dihydroxyphenyl)-2,3-dimethylbutane. 2,3-Bis(3,4-dihydroxybenzyl)butane. Bisdemethyldihyroguaiaretic acid. Nordihydroguaiaretic acid. Norhydroguaiaretic acid. NDGA



(8*R*,8′*R*)-*form*

$C_{18}H_{22}O_4$ 302.369

Lignan numbering shown. Antioxidant. Formerly approved as a food additive; now banned by FDA (USA). Log P 3.92 (calc).

▶ UX1750000

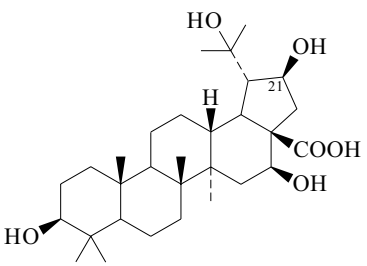
(8*S*,8′*R*)-*form*

3,4-Methylene, 3′-Me ether: [107534-93-0] ***Macelignan***. *Anwulignan. Calophyn*
$C_{20}H_{24}O_4$ 328.407
Constit. of *Myristica fragrans* (nutmeg). Cryst. (hexane). Mp 70-72°. $[\alpha]_D^{20}$ +5.28 (c, 1.8 in $CHCl_3$). Information on abs. config. and identity of the various samples not fully clear. One sample of Anwulignan appears to be racemic.

[68964-82-9, 90365-59-6, 103185-28-0, 119182-23-9, 119584-40-6, 124649-80-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1119D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 325A (*nmr*)
Perry, C.W. *et al., J.O.C.*, 1972, **37**, 4371 (*bibl, uv, ir, pmr*)
Gisvold, O. *et al., J. Pharm. Sci.*, 1974, **63**, 1905 (*isol*)
Liu, J.-S. *et al., Can. J. Chem.*, 1981, **59**, 1680
Liu, J.S. *et al., CA*, 1984, **101**, 3913 (*Anwulignan*)
Woo, W.S. *et al., Phytochemistry*, 1987, **26**, 1542 (*isol, cryst struct, Macelignan*)
Alvarez, V. *et al., CA*, 1988, **108**, 183594 (*Calophyn*)
Liu, J.S. *et al., Youji Huaxue*, 1988, **8**, 227 (*Anwulignan*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, NBR000

3,16,20,21-Tetrahydroxy-28-lupanoic acid T-232



$C_{30}H_{50}O_6$ 506.721

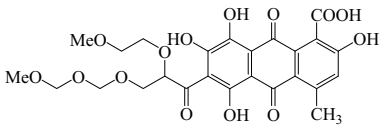
(3β,16β,21β)-*form*

28→21 Lactone: [152218-60-5] *3β,16β,20-Trihydroxy-28,21β-lupanolide.* ***16β-Hydroxystellatogenin***
$C_{30}H_{48}O_5$ 488.706
Constit. of *Stenocereus stellatus* (pitaya). Cryst. Mp 255-258°. $[\alpha]_D^{20}$ +15 (c, 0.0008 in $CHCl_3$).

Koyama, K. *et al., J. Nat. Prod.*, 1993, **56**, 2201 (*isol, pmr, cmr*)

2,5,7,8-Tetrahydroxy-6-[2-(2-methoxyethoxy)-3-[(methoxymethoxy)methoxy]propanoyl]-4-methylanthraquinone-1-carboxylic acid T-233

[245343-12-8]

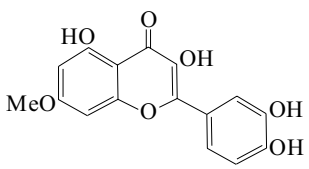


$C_{25}H_{26}O_{14}$ 550.472
Potential food colourant.

Pat. Coop. Treaty (WIPO), 1999, 99 50 434; *CA*, **131**, 271009f

3,3′,4′,5-Tetrahydroxy-7-methoxyflavone T-234

[90-19-7]
2-(3,4-Dihydroxyphenyl)-3,5-dihydroxy-7-methoxy-4H-1-benzopyran-4-one, 9CI. 3′,4′,5-Trihydroxy-7-methoxyflavonol. ***Rhamnetin***. *Quercetin 7-methyl ether. β-Rhamnocitrin*



$C_{16}H_{12}O_7$ 316.267
Yellow cryst. (EtOH). Sol. MeOH, Et_2O, bases; poorly sol. H_2O. Mp 294-296°. λ_{max} 256 (ε 42200); 371 (ε 43500) (EtOH) (Berdy).

▶ LK8748000

3′-O-α-L-Rhamnopyranoside, 3-O-arabinoside: ***Peumoside***
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Peumus boldus* (boldo). Needles (EtOAc/MeOH). Mp 195-197°.

3-O-[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranoside]: [105755-71-3] *Rhamnetin 3-(4-rhamnosylrhamnoside)*
$C_{28}H_{32}O_{15}$ 608.552
Isol. from *Cyperus rotundus* (nutgrass).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [259234-17-8] *Rhamnetin 3-sophoroside*
$C_{28}H_{32}O_{17}$ 640.551
Constit. of *Nasturtium officinale* (water cress). Pale yellow oil. λ_{max} 255 ; 298 ; 355 (MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]:Rhamnetin 3-laminaribioside

$C_{28}H_{32}O_{17}$ 640.551
Constit. of *Pteridium aquilinum* (bracken fern). λ_{max} 258 (sh) ; 265 ; 355 (MeOH).

[1324-63-6, 55196-43-5, 62858-07-5]

Kuhn, R. *et al., Ber.*, 1944, **77**, 211 (*synth*)
Krug, H. *et al., Pharmazie*, 1965, **20**, 692 (*Peumoside*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799 (*cmr*)
Tripathi, V.D. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 89 (*isol, deriv*)
Averett, J.E. *et al., Phytochemistry*, 1986, **25**, 1995 (*derivs*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Izumi, T. *et al., J.C.S. Perkin 1*, 1992, 1265 (*synth*)
Ozipek, M. *et al., Phytochemistry*, 1994, **37**, 249 (*deriv*)
Imperato, F. *et al., Phytochemistry*, 1997, **45**, 1729 (*3-laminaribioside*)
Goda, Y. *et al., Biol. Pharm. Bull.*, 1999, **22**, 1319-1326 (*Glucorhamnin, 3-sophoroside*)

3,3′,4′,7-Tetrahydroxy-5-methoxyflavone T-235

[529-51-1]
*2-(3,4-Dihydroxyphenyl)-3,7-dihydroxy-5-methoxy-4*H*-1-benzopyran-4-one, 9CI. 3′,4′,7-Trihydroxy-5-methoxyflavonol.* ***Azaleatin***

$C_{16}H_{12}O_7$ 316.267
Bright yellow needles (MeOH aq.). Mp 322° (318°). λ_{max} 252 ; 368 (no solvent reported).

3-O-*Arabinoside:* [63742-73-4]
$C_{21}H_{20}O_{11}$ 448.382
Isol. from pecan nuts *Carya pecan*. Mp 150° dec.

3-O-*β*-D-*Glucopyranoside:* [23598-17-6]
$C_{22}H_{22}O_{12}$ 478.409
Isol. from apples and pecan nuts. Needles + $1H_2O$ (EtOH). Mp 195-196°. $[\alpha]_D^{24}$ -24.4 (c, 1 in Py).

3-O-*β*-D-*Galactopyranoside:*
$C_{22}H_{22}O_{12}$ 478.409
Isol. from pecan nuts *Carya pecan* and apples. Deep yellow needles (MeOH aq.). Mp 196-197°. $[\alpha]_D^{21}$ -42.8 (c, 0.65 in Py).

3-O-*β*-D-*Glucuronopyranoside:*
$C_{22}H_{20}O_{13}$ 492.392Probable struct..

3-O-*α*-L-*Rhamnopyranoside:* [29028-02-2] ***Azalein***
$C_{22}H_{22}O_{11}$ 462.409
Light yellow needles + $5H_2O$. Mp 181-185°.

3-O-*[Xylosyl-(1→?)-arabinoside]:*
$C_{26}H_{28}O_{15}$ 580.498

3-O-*[Arabinosyl-(1→?)-galactoside]:* [28680-35-5]
$C_{27}H_{30}O_{16}$ 610.524

3-O-*[β*-D-*Glucopyranosyl-(1→?)-β*-D-*glucopyranoside]:* [28680-36-6] *Azaleatin diglucoside*
$C_{28}H_{32}O_{17}$ 640.551

3-O-*[Rhamnosyl-(1→?)-arabinoside]:* [60961-96-8]
$C_{27}H_{30}O_{15}$ 594.525

3-O-*[α*-L-*Rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [63764-79-4] *Azaleatin 3-rutinoside*
$C_{28}H_{32}O_{16}$ 624.551
Isol. from pecan nuts *Carya pecan*. Mp 200-204° dec.

[28454-85-5]

Wada, E. *et al., J.A.C.S.*, 1956, **78**, 4725 (*isol*)
Jurd, L. *et al., J.O.C.*, 1957, **22**, 1618 (*Azaleatin, Azalein*)
Pacheco, H. *et al., Bull. Soc. Chim. Fr.*, 1965, 779 (*synth*)
Grouiller, A. *et al., Bull. Soc. Chim. Fr.*, 1967, 1938 (*pmr*)
Bate-Smith, E.C. *et al., Phytochemistry*, 1967, **6**, 1407 (*isol*)
Hoerhammer, L. *et al., Chem. Ber.*, 1969, **102**, 792 (*3-galactoside*)
Harborne, J.B. *et al., Phytochemistry*, 1969, **8**, 419 (*isol*)
Harborne, J.B. *et al., Phytochemistry*, 1969, **8**, 763 (*3-glucuronide*)
Mitchell, R.E. *et al., Phytochemistry*, 1971, **10**, 1559 (*3-rutinoside*)
Matlawska, I. *et al., Herba Pol.*, 1976, **22**, 11 (*3-rhamnosylarabinoside*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799 (*cmr*)
El-Ansari, M.A. *et al., Z. Naturforsch., C*, 1977, **32**, 444 (*3-arabinoside-3-rutinoside*)
Ishak, M.S. *et al., Phytochemistry*, 1980, **19**, 2512 (*3-glucoside*)

3,3′,5,7-Tetrahydroxy-4′-methoxyflavone T-236

[603-61-2]
*3,5,7-Trihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-1-benzopyran-4-one. 3′,5,7-Trihydroxy-4′-methoxyflavonol.* ***Tamarixetin***

$C_{16}H_{12}O_7$ 316.267
Isol. from *Gossypium hirsutum* (cotton) and other plants. Bright yellow prisms. Mp 260° (256-257°).

► LK8745000

[29297-73-2, 50838-09-0]

Jurd, L. *et al., J.O.C.*, 1962, **27**, 1294-1297 (*synth*)
Audier, H. *et al., Bull. Soc. Chim. Fr.*, 1966, 2892-2899 (*ms*)
Bahl, C.P. *et al., Indian J. Chem.*, 1967, **5**, 171-172 (*Tamarixetin*)
Rao, K.V. *et al., J. Het. Chem.*, 1976, **13**, 1293-1295 (*synth, pmr*)
Norbedo, C. *et al., Phytochemistry*, 1984, **23**, 2698-2708 (*isol*)
McCormick, S. *et al., Phytochemistry*, 1985, **24**, 2133 (*isol*)

3′,4′,5,6-Tetrahydroxy-7-methoxyflavone T-237

[22384-63-0]
*2-(3,4-Dihydroxyphenyl)-5,6-dihydroxy-7-methoxy-4*H*-1-benzopyran-4-one, 9CI.* ***Pedalitin***

$C_{16}H_{12}O_7$ 316.267
Isol. from *Sesamum indicum* (sesame). Yellow needles (MeOH). Mp 300-301° dec. λ_{max} 284 (ε 12000); 343 (ε 19400) (EtOH) (Berdy).

► LK9275430

Tetra-Ac:
Needles (MeOH). Mp 242-243°.

6-O-*β*-D-*Glucopyranoside:* [22860-72-6] ***Pedaliin***
$C_{22}H_{22}O_{12}$ 478.409
From leaves of *Sesamum indicum* (sesame). Pale-yellow needles (Py aq.). Mp 254° dec. $[\alpha]_D^{19}$ +27.2 (c, 0.294 in Py/EtOH).

6-O-*β*-D-*Galactopyranoside:* [76449-91-7]
$C_{22}H_{22}O_{12}$ 478.409

3-O-*[β*-D-*Galactopyranosyl-β*-D-*glucopyranoside]:* [77139-23-2]
$C_{28}H_{32}O_{17}$ 640.551

[75423-06-2]

Morita, N. *et al., Chem. Pharm. Bull.*, 1960, **8**, 59 (*isol*)
Kupchan, S.M. *et al., Tetrahedron*, 1969, **25**, 1303 (*rev, struct, pmr, uv*)
Krishnaswamy, N.R. *et al., Indian J. Chem.*, 1970, **8**, 1074 (*struct*)
Horie, T. *et al., Nippon Kagaku Zasshi*, 1978, 748 (*synth*)
Soltis, D.E. *et al., Biochem. Syst. Ecol.*, 1980, **8**, 149 (*6-galactosides*)
Neuman, P. *et al., J. Nat. Prod.*, 1981, **44**, 50 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Horie, T. *et al., Chem. Pharm. Bull.*, 1986, **34**, 30 (*Pedaliin*)

3,4′,5,7-Tetrahydroxy-3′-methoxyflavone T-238

[480-19-3]
*3,5,7-Trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-3′-methoxyflavonol.* ***Isorhamnetin****. Isorhamnetol. Quercetin 3′-methyl ether*

$C_{16}H_{12}O_7$ 316.267
Widespread flavonol found especially in bee pollen, chives, corn poppy leaves, garden cress, fennel, hartwort, red onions, pears, dillweed, parsley and tarragon. Greenish-yellow cryst. (AcOH). Spar. sol. EtOH, AcOH; insol. C_6H_6, $CHCl_3$. Mp 305° dec.

► LK9275450

7-O-*α*-L-*Rhamnopyranoside, 3*-O-*α*-L-*arabinopyranoside:* [69760-70-9]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Peumus boldus* (boldo). Cryst. (MeOH). Mp 211°.

3-O-*β*-D-*Glucofuranoside, 4′*-O-*α*-L-*rhamnopyranoside:* [10576-85-9] ***Pasternoside***
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Pastinaca sativa* (parsnip). Mp 235-237°. $[\alpha]_D^{20}$ -120 (c, 1.3 in Py).

4′-O-*β*-D-*Glucopyranoside:* [58902-89-9] ***Alliumoside A****. Isorhamnetin 4′-glucoside*
$C_{22}H_{22}O_{12}$ 478.409
Present in onions. Yellow cryst. (MeOH). Mp 262-266° (252-254°). $[\alpha]_D^{20}$ +28 (c, 0.2 in EtOH). $[\alpha]_D^{27}$ -40 (c, 0.1 in Py). λ_{max} 254 ; 365 (MeOH).

7-O-*β*-D-*Glucopyranoside:* [6743-96-0] ***Brassicin***
$C_{22}H_{22}O_{12}$ 478.409
Isol. from various plants inc. *Brassica napus* (oilseed rape). Mp 253-255°. $[\alpha]_D^{20}$ +40.5 (c, 0.1 in MeOH).

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-α*-L-*rhamnopyranoside]:* [121064-69-5] ***Calendoflaside***
$C_{28}H_{32}O_{15}$ 608.552
Isol. from *Calendula officinalis* (pot marigold).

3-O-*[α-L-Rhamnopyranosyl-(1→?)-α-L-rhamnopyranoside]:Isorhamnetin 3-dirhamnoside*
$C_{28}H_{32}O_{15}$ 608.552
Glucoside present in the leaves of *Peumus boldus* (boldo). Mp 230-233°. Tentative struct..

3-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-galactopyranoside]:* [107740-46-5] ***Keioside***. *Isorhamnetin 3-robinobioside*
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Pyrus communis* (pear). Yellow needles (EtOH aq.). Mp 183-186° (178-181°). $[\alpha]_D^{20}$ -21.4 (c, 0.84 in MeOH). λ_{max} 255 ; 267 ; 356 (MeOH) (Berdy). λ_{max} 273 ; 412 (MeOH-NaOH) (Berdy).

4′-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [139742-27-1] ***Crosatoside A***
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Crocus sativus* (saffron).

3-O-*[β-D-Galactopyranosyl-(1→?)-α-L-rhamnopyranoside]:* [38784-66-6]
$C_{28}H_{32}O_{17}$ 640.551
Isol. from *Convallaria majalis* . *Convallaria majalis* is banned by the FDA from food use in the USA. Mp 175-177°. $[\alpha]_D^{25}$ -70.2 (c, 0.69 in Py).

3-O-*[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranoside]:*
$C_{28}H_{32}O_{16}$ 624.551
Constit. of *Ginkgo biloba* (ginkgo). Mp 170-172°. λ_{max} 254 (log ϵ 4.24); 357 (log ϵ 4.03) (MeOH).

3-O-*[4-Hydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranosyl-(1→2)-α-L-rhamnopyranoside]:*
$C_{37}H_{38}O_{18}$ 770.696
Constit. of the leaves of *Gingko biloba* (ginkgo). Pale yellow powder. λ_{max} 253 ; 265 (sh) ; 315 ; 365 (MeOH).

3-O-*[β-D-Glucopyranosyl-(1→?)-α-L-rhamnopyranoside]:* [64812-31-3]
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Anethum graveolens* (dill).

3-O-*[β-D-Xylopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:*
$C_{33}H_{40}O_{20}$ 756.667
Constit. of peanut skins (*Arachis hypogaea*). Yellowish powder (MeOH). $[\alpha]_D^{25}$ -49 (MeOH).

3-O-*[β-D-Galactopyranosyl-(1→?)-α-L-rhamnopyranosyl-(1→?)-α-L-rhamnopyranoside]:* [64808-85-1] *Isorhamnetin 3-(galactosylrhamnosylrhamnoside)*
$C_{34}H_{42}O_{20}$ 770.694
Isol. from *Convallaria majalis* (lily of the valley). *Convallaria majalis* is banned by the FDA from food use in the USA.

3-O-*[β-D-Glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:*
$C_{34}H_{42}O_{21}$ 786.693
Constit. of peanut skins (*Arachis hypogaea*). Yellowish powder (MeOH). $[\alpha]_D^{25}$ -48 (MeOH).

[63109-33-1]

Heap, T. *et al., J.C.S.*, 1926, 2336-2344 (*synth*)
Kuhn, R. *et al., Chem. Ber.*, 1948, **81**, 363-367 (*isol*)
Pacheco, H. *et al., Bull. Soc. Chim. Fr.*, 1965, 779-785 (*synth, ir, uv*)
Pelter, A. *et al., J. Het. Chem.*, 1965, **2**, 262-271 (*ms*)
Krug, H. *et al., Pharmazie*, 1965, **20**, 692-697 (*3,7-dirhamnoside*)
Maksyutina, N.P. *et al., Khim. Prir. Soedin.*, 1966, **2**, 20-26; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 16-20 (*Pasternoside*)
Hörhammer, L. *et al., Tet. Lett.*, 1966, 567-571 (*synth, 3-xylopyranoside, Cacticin, Brassicin*)
Hörhammer, L. *et al., Chem. Ber.*, 1967, **100**, 2301-2305 (*synth, Cacticin, Brassicin*)
Maksyutina, N.P. *et al., Khim. Prir. Soedin.*, 1970, **6**, 201-204; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 196-198 (*Alliosidin*)
Burasheva, G.S. *et al., Khim. Prir. Soedin.*, 1975, **11**, 254-255; 1976, **12**, 391-392; 663; 1977, **13**, 280-281; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 261; 1976, **12**, 342-343; 596; 1977, **13**, 242 (*derivs*)
Bombardelli, E. *et al., Fitoterapia*, 1976, **47**, 3-5 (*3-arabinoside-7-rhamnoside*)
Kowalewski, Z. *et al., Herba Pol.*, 1978, **24**, 5-10; 1979, **25**, 183-187 (*3-arabinoside, 7-rhamnoside*)
Song, C. *et al., Huaxue Xuebao*, 1991, **49**, 917; *CA*, **116**, 148197d (*Crosatoside A*)
Park, Y.-K. *et al., J. Agric. Food Chem.*, 1996, **44**, 34-36 (*4′-glucoside, isol, pmr*)
Tang, Y.-P. *et al., Yaoxue Xuebao*, 2000, **35**, 363-366 (*3-2-glucosylrhamnoside*)
Yang, X.-H. *et al., Yaoxue Xuebao*, 2000, **35**, 752-755 (*Alliumoside A*)
Tang, Y. *et al., Phytochemistry*, 2001, **58**, 1251-1256 (*Ginkgo biloba glycoside*)
Lou, H. *et al., Planta Med.*, 2001, **67**, 345-349 (*Arachis glycosides*)

3′,4′,5,7-Tetrahydroxy-3-methoxyflavone T-239

[1486-70-0]
*2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-3-methoxy-4*H*-1-benzopyran-4-one, 9CI. 3-*O*-Methylquercetin. Quercetin 3-methyl ether*

$C_{16}H_{12}O_7$ 316.267
Yellow cryst. Mp 273-275° (259°).

7-O-*[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranoside]:*
$C_{28}H_{32}O_{17}$ 640.551
Constit. of the stems of *Acacia catechu* (black catechu). Yellow needles (EtOH). Mp 283-284°. λ_{max} 257 ; 356 (MeOH).

Yadava, R.N. *et al., J. Asian Nat. Prod. Res.*, 2002, **4**, 11-15 (*7-4-galactosylglucoside*)

3,4′,5,7-Tetrahydroxy-6-methoxyflavone T-240

[32520-55-1]
*3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-6-methoxy-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-6-methoxyflavonol. 6-Methoxykaempferol*

$C_{16}H_{12}O_7$ 316.267
Constit. of the buds of the wild cherry *Prunus avium*. Yellow needles (EtOH). Mp 270°.

Rodriguez, E. *et al., Phytochemistry*, 1972, **11**, 3509 (*isol*)
Wollenweber, E. *et al., Z. Naturforsch., B*, 1972, **27**, 567 (*isol, struct*)
Combier, H. *et al., Bull. Liaison-Groupe Polyphenols*, 1974, **5**, 20; *CA*, **83**, 177579 (*uv*)
Goudard, M. *et al., Phytochemistry*, 1978, **17**, 145 (*ms*)
Merfort, I. *et al., Planta Med.*, 1984, 107; 1985, 136 (*isol*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1986, **41**, 87 (*isol*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,

3′,4′,5,7-Tetrahydroxy-6-methoxyflavone T-241

[520-11-6]
*2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-6-methoxy-4*H*-1-benzopyran-4-one, 9CI. **Eupafolin**. Nepetin. 6-Methoxyluteolin*

$C_{16}H_{12}O_7$ 316.267
Yellow needles (EtOH or MeOH). Mp 258-262° Mp 272-274° Mp 280-281°.

7-O-*β-D-Glucopyranoside:* [569-90-4] ***Nepitrin***
$C_{22}H_{22}O_{12}$ 478.409
Constit. of rosemary (*Rosmarinus officinalis*). Pale yellow needles (EtOH). Mp 172-174° Mp 252-256°.
▶ LD_{50} (mus, ipr) 794 mg/kg. DJ3009500

3′-O-*β-D-Glucopyranoside:* [112208-84-1]
$C_{22}H_{22}O_{12}$ 478.409
Constit. of rosemary *Rosmarinus officinalis*.

4′-O-*β-D-Glucopyranoside:* [112208-83-0] *Eupafolin 4′-glucoside. Nepetin 4′-glucoside*
$C_{22}H_{22}O_{12}$ 478.409
Constit. of rosemary (*Rosmarinus officinalis*). Pale yellow powder. λ_{max} 275 ; 335 (MeOH).

7-O-*β-D-Glucuronopyranoside:* [82657-12-3]
$C_{22}H_{20}O_{13}$ 492.392
Isol. from Greek sage (*Salvia triloba*).

[27923-79-1]

Krishnaswamy, N.R. *et al., Indian J. Chem.*, 1968, **6**, 676 (*Nepitrin*)
Hiermann, A. *et al., Planta Med.*, 1982, **45**, 59 (*7-glucuronosides*)
Iwashina, T. *et al., Phytochemistry*, 1999, **51**, 1109-1111 (*4′-glucoside*)

3,4′,5,7-Tetrahydroxy-8-methoxyflavone T-242

[571-74-4]
*3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-8-methoxy-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-8-methoxyflavonol. **Sexangularetin**. 8-Methoxykaempferol*

$C_{16}H_{12}O_7$ 316.267

3-O-*Sophoroside:* [114882-17-6]
$C_{28}H_{32}O_{17}$ 640.551
Isol. from *Prunus amygdalus* (almond). $[\alpha]_D^{20}$ -18 (c, 0.1 in MeOH).

3-O-*β-D-Glucopyranoside, 7*-O-*α-L-rhamnopyranoside:* [47850-51-1]
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Gossypium hirsutum* (cottonseed). Cryst. (MeOH aq.). Mp 184-186°.

Elliger, C.A. *et al., Phytochemistry*, 1984, **23**, 1199 (*3-glucoside-7-rhamnoside*)
Stosic, D. *et al., Helv. Chim. Acta*, 1988, **71**, 348 (*3-sophoroside*)
Ferreres, F. *et al., Phytochemistry*, 1989, **28**, 1901 (*3-sophoroside*)

3′,5,7,8-Tetrahydroxy-4′-methoxyflavone T-243

*5,7,8-Trihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. Hypolaetin 4′-methyl ether*

$C_{16}H_{12}O_7$ 316.267

8-O-*β*-D-*Glucopyranoside:* [80756-87-2]
$C_{22}H_{22}O_{12}$ 478.409
Isol. from *Althaea officinalis* (marsh mallow).

8-O-*β*-D-*Glucopyranoside, 3′*-O-*sulfate:* [131622-65-6]
$C_{22}H_{22}O_{15}S$ 558.473
Isol. from *Althaea officinalis* (marsh mallow) (as K salt).

8-O-*β*-D-*Glucuronopyranoside:* [135010-46-7]
$C_{22}H_{20}O_{13}$ 492.392
Isol. from *Malva sylvestris* (high mallow).

8-O-*β*-D-*Glucuronopyranoside, Me ester:*
$C_{23}H_{22}O_{13}$ 506.419
Amorph. yellow solid. $[\alpha]_D^{26}$ +38.4 (c, 0.12 in MeOH). λ_{max} 213 (log ϵ 4.18); 275 (log ϵ 4.16); 343 (log ϵ 3.92) (MeOH).

7-O-*[β*-D-*Allopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [114611-04-0]
$C_{28}H_{32}O_{17}$ 640.551Not specifically stated to be a β-D-sugar, but this seems probable.

7-O-*[6*-O-*Acetyl-β*-D-*allopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [93753-29-8]
$C_{30}H_{34}O_{18}$ 682.588
No phys. props. reported.

7-O-*[6*-O-*Acetyl-β*-D-*allopyranosyl-(1→2)-6*-O-*acetyl-β*-D-*glucopyranoside]:* [108706-09-8]
$C_{32}H_{36}O_{19}$ 724.625

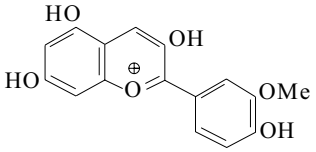
7-O-*[6*-O-*Acetyl-β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [162110-44-3]
$C_{30}H_{34}O_{18}$ 682.588
Constit. of *Sideritis syriaca* (Greek mountain tea). Cryst. (MeOH). Mp 270-272°.

[80756-88-3]

Lenherr, A. *et al., Phytochemistry*, 1984, **23**, 2343-2345; 1987, **26**, 1185-1188 (*7-allosylglucosides*)
Gudej, J. *et al., Acta Pol. Pharm.*, 1985, **42**, 192-198 (*8-glucosides*)
Manez, S. *et al., Planta Med.*, 1986, **52**, 525 (*7-allosylglucoside*)
Billeter, M. *et al., Phytochemistry*, 1991, **30**, 987-990 (*8-glucuronoside*)
Venturella, P. *et al., Phytochemistry*, 1995, **38**, 527-530 (*7-acetyldiglucoside*)
Tezuka, Y. *et al., Helv. Chim. Acta*, 1999, **82**, 408-417 (*8-glucuronoside Me ester*)

3,4′,5,7-Tetrahydroxy-3′-methoxyflavylium(1+) T-244

[134-01-0]
3,5,7-Trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-1-benzopyrylium(1+), 9CI. ***Peonidin****. Paeonidin*



$C_{16}H_{13}O_6^{\oplus}$ 301.275
Widespread anthocyanin found esp. in concord grapes, blueberries, cherries and red table wines. Reddish-brown needles + $2H_2O$ (as chloride). CAS no. refers to chloride. Forms a sesquihydrate showing dimorphism.

3-O-*Arabinoside:* [27214-74-0] *Peonidin 3-arabinoside*
$C_{21}H_{21}O_{10}^{\oplus}$ 433.391
Isol. from grapes and many other plant spp..

3-O-*α*-L-*Rhamnopyranoside:* [72551-79-2] *Peonidin 3-rhamnoside*
$C_{22}H_{23}O_{10}^{\oplus}$ 447.418
Isol. from legumes.

3-O-*α*-L-*Rhamnopyranoside, 5*-O-*β*-D-*glucopyranoside:* [53859-11-3] *Peonidin 5-glucoside 3-rhamnoside*
$C_{28}H_{33}O_{15}^{\oplus}$ 609.56
Isol. from peas.

3-O-*β*-D-*Glucopyranoside:* [6906-39-4] ***Oxycoccicyanin****. Peonidin 3-glucoside*
$C_{22}H_{23}O_{11}^{\oplus}$ 463.417
Isol. from grapes and many other plant spp. Present in red wine. Dark brown needles + $2H_2O$ (as chloride).

3-O-*[4-Hydroxycinnamoyl-(→?)-β*-D-*glucopyranoside]:* [71802-54-5]
$C_{31}H_{29}O_{13}^{\oplus}$ 609.562
Isol. from grapes.

3-O-*[4-Hydroxycinnamoyl-(→6)-β*-D-*glucopyranoside], 5*-O-*β*-D-*glucopyranoside:* [51939-65-2]
$C_{37}H_{39}O_{18}^{\oplus}$ 771.704
Isol. from concord grapes.

3-O-*[β*-D-*Xylopyranosyl-(1→2)-β*-D-*galactopyranoside]:* [155380-00-0] *Peonidin 3-lathyroside*
$C_{27}H_{31}O_{15}^{\oplus}$ 595.533
Constit. of leaf and stem cultures of Japanese asparagus (*Aralia cordata*).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside], 5*-O-*β*-D-*glucopyranoside:* [79549-69-2] *Peonidin 5-glucoside 3-sophoroside.* ***YGM 0B***
$C_{34}H_{43}O_{21}^{\oplus}$ 787.701
Constit. of purple sweet potato tubers (*Ipomea batatas* cv. Yamagawamrasaki).

3-O-*[4-Hydroxybenzoyl-(→6)-β*-D-*glucopyranosyl-(1→2)-[3,4-dihydroxy*-E-*cinnamoyl-(→6)]-β*-D-*glucopyranoside], 5*-O-*β-glucopyranoside:* ***YGM 5A***
$C_{50}H_{53}O_{26}^{\oplus}$ 1069.953
Isol. from sweet potato roots.

3-O-*[β*-D-*Glucopyranosyl-(1→2)-[3,4-dihydroxycinnamoyl-(→6)]-β*-D-*glucopyranoside]*(E-*), 5*-O-*β*-D-*glucopyranoside:* ***YGM 5B***
$C_{43}H_{49}O_{24}^{\oplus}$ 949.846
Constit. of purple sweet potato tubers (*Ipomoea batatas* cv. Yamagawamrasaki). Struct. revised (1997); Lu *et. al.* (1992) assigned an isomeric struct..

3-O-*[3,4-Dihydroxy*-E-*cinnamoyl-(→6)-β*-D-*glucopyranosyl-(1→2)-[3,4-dihydroxy*-E-*cinnamoyl-(→6)]-β*-D-*glucopyranoside], 5*-O-*β*-D-*glucopyranoside:* ***YGM 4B***
$C_{52}H_{55}O_{27}^{\oplus}$ 1111.99
Constit. of sweet potato roots.

3-O-*[4-Hydroxy-3-methoxy*-E-*cinnamoyl-(→6)-β*-D-*glucopyranosyl-(1→2)-[3,4-dihydroxy*-E-*cinnamoyl-(→6)]-β*-D-*glucopyranoside], 5*-O-*β*-D-*glucopyranoside:* ***YGM 6***
$C_{53}H_{57}O_{27}^{\oplus}$ 1126.017
Isol. from sweet potato roots.

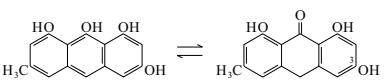
3-O-*[β*-D-*Glucopyranosyl-(1→6)-[4-hydroxy-3,5-dimethoxycinnamoyl-(→4)]-β*-D-*glucopyranoside]:* [131189-51-0] *Peonidin 3-(4-sinapoylgentiobioside).* ***Alatanin 2***
$C_{39}H_{43}O_{20}^{\oplus}$ 831.757
Isol. from tubers of king yam (*Dioscorea alata*). Purple-red powder (as chloride).

[140447-88-7]

Nolan, T.J. *et al., J.C.S.*, 1926, 1968 (*synth*)
Murakami, S. *et al., J.C.S.*, 1928, 1537 (*synth*)
Robinson, R. *et al., J.C.S.*, 1931, 2715; 2722; 1932, 2493 (*glycosides*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1725 (*occur*)
Pomilio, A.B. *et al., Phytochemistry*, 1973, **12**, 218 (*isol*)
Fong, R.A. *et al., Phytochemistry*, 1974, **13**, 1001 (*isol*)
Hrazdina, G. *et al., Lebensm.-Wiss. Technol.*, 1975, **8**, 111-113 (*Vitis derivs*)
Melin, D. *et al., Phytochemistry*, 1975, **14**, 2363 (*isol*)
Iacobucci, G.A. *et al., Tetrahedron*, 1983, **39**, 3005 (*rev*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Shoyama, Y. *et al., Phytochemistry*, 1990, **29**, 2999 (*Alatanin 2*)
Merlin, J.-C. *et al., Phytochemistry*, 1994, **35**, 227 (*Raman*)
Asada, Y. *et al., Phytochemistry*, 1994, **35**, 1471 (*3-lathyroside*)
Goda, Y. *et al., Phytochemistry*, 1997, **44**, 183 (*Ipomoea batatas deriv*)
Terahara, N. *et al., Biosci., Biotechnol., Biochem.*, 1999, **63**, 1420-1424; 2002, **66**, 2483-2486 (*YGM pigments*)

1,3,8,9-Tetrahydroxy-6-methylanthracene T-245

[491-60-1]
*1,3,8-Trihydroxy-6-methyl-9(10*H*)-anthracenone. 6-Methyl-1,3,8,9-anthracenetetrol.* ***Emodinanthranol****. Emodinol. Protophyscihydrone. Frangulaemodinanthrone. Emodinanthrone. Frangulaemodinanthranol. Emodin anthrone*



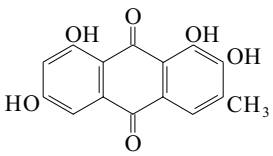
$C_{15}H_{12}O_4$ 256.257
Tautomeric. Isol. from *Hypericum perforatum* (St. John's wort). Yellow platelets.

Mp 250-258° dec. (236°).

Perkin, A.G. *et al., J.C.S.*, 1894, **65**, 937 (*isol*)
Tutin, F. *et al., J.C.S.*, 1912, **101**, 290 (*isol, struct*)
Jacobson, R.A. *et al., J.A.C.S.*, 1924, **46**, 1312 (*synth*)
Brockmann, H. *et al., Naturwissenschaften*, 1953, **40**, 509 (*isol*)
v. Mühlemann, H. *et al., Pharm. Acta Helv.*, 1955, **30**, 350

1,2,6,8-Tetrahydroxy-3-methylanthraquinone T-246

[641-90-7]
1,2,6,8-Tetrahydroxy-3-methyl-9,10-anthracenedione, 9CI. ***Alaternin***



$C_{15}H_{10}O_6$ 286.24
Brick-red plates (AcOH). Mp 310°.

▶ CB7920500

1-O-β-D-Glucopyranoside:
$C_{21}H_{20}O_{11}$ 448.382
Yellow needles (MeOH). Mp 254-255°.

2-O-β-D-Glucopyranoside:
$C_{21}H_{20}O_{11}$ 448.382
Constit. of the seeds of *Cassia tora* (charota). Amorph. powder.

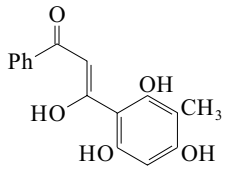
1-Me ether:2,6,8-Trihydroxy-1-methoxy-3-methylanthraquinone
$C_{16}H_{12}O_6$ 300.267
Yellow needles (EtOAc/hexane). Mp 292-294°. λ_{max} 228 (log ϵ 4.36); 284 (log ϵ 4.42); 311 (log ϵ 4.08); 393 (log ϵ 3.92) (MeOH).

6-Me ether: [14717-90-9] *1,2,8-Trihydroxy-6-methoxy-3-methylanthraquinone*
$C_{16}H_{12}O_6$ 300.267
Orange-yellow needles (Py). Mp 267-268°.

Tetra-Me ether:1,2,6,8-Tetramethoxy-3-methylanthraquinone
$C_{19}H_{18}O_6$ 342.348
Yellow needles (AcOH). Mp 181-182°.

Briggs, L.H. *et al., J.C.S.*, 1953, 3069 (*isol, struct*)
Dave, K.G. *et al., Tet. Lett.*, 1959, **No. 6**, 22 (*isol, struct*)
Lovie, I.C. *et al., J.C.S.*, 1961, 485 (*synth*)
Stoessl, A. *et al., Can. J. Chem.*, 1969, **47**, 767; 1983, **61**, 372 (*isol, pmr, ir, uv, cmr*)
Banks, H.J. *et al., Aust. J. Chem.*, 1976, **29**, 1509 (*isol*)
Suemitsu, R. *et al., Agric. Biol. Chem.*, 1977, **41**, 207 (*isol, uv, ir, ms*)
Van Eijk, G.W. *et al., J. Chromatogr.*, 1984, **295**, 497 (*glc, ms*)
Kitanaka, S. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1274
Lee, H.J. *et al., Phytochemistry*, 1998, **49**, 1403-1404 (*2-glucoside*)
Lin, L.-C. *et al., J. Nat. Prod.*, 2001, **64**, 674-676 (*1-Me ether, isol*)

β,2,4,6-Tetrahydroxy-3-methylchalcone T-247

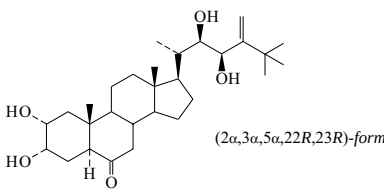


$C_{16}H_{14}O_5$ 286.284
Enolised β-diketone.

4′,6′-Di-Me ether: [109845-46-7] *β,2-Dihydroxy-4,6-dimethoxy-3-methylchalcone*
$C_{18}H_{18}O_5$ 314.337
Constit. of *Leptospermum scoparium* (red tea). Yellow prisms and pale yellow needles (Et_2O). Mp 119-126° (enol) Mp 126-128° (dioxo). The two cryst. modifications correspond to the enol (illus.) and dioxo forms respectively. They interconvert on further recryst..

Mayer, R. *et al., Planta Med.*, 1993, **59**, 269

2,3,22,23-Tetrahydroxy-25-methylergost-24(28)en-6-one, 9CI T-248



(2α,3α,5α,22*R*,23*R*)-form

$C_{29}H_{48}O_5$ 476.695

(2α,3α,5α,22*R*,23*R*)-*form* [111618-87-2] ***25-Methyldiolichosterone***
Constit. of the immature seeds of *Phaseolus vulgaris* (kidney bean). Needles (MeOH). Mp 254° (246-247°). $[\alpha]_D^{22}$ +4.3 (c, 0.13 in MeOH).

(2β,3α,5α,22*R*,23*R*)-*form* [121398-03-6]
Constit. of the immature seeds of *Phaseolus vulgaris* (kidney bean).

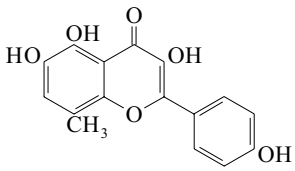
(2β,3β,5α,22*R*,23*R*)-*form* [114958-54-2]
Constit. of the immature seeds of *Phaseolus vulgaris* (kidney bean). Prisms (MeOH). Mp 248°. $[\alpha]_D^{22}$ +4.6 (c, 0.18 in $CHCl_3$). Sinters at 243°.

[121398-03-6]

Kim, S.K. *et al., Agric. Biol. Chem.*, 1987, **51**, 2303 (*isol*)
Mori, K. *et al., Annalen*, 1988, 815 (*synth*)
Japan. Pat., 1988, 88 255 297; *CA*, **111**, 36804 (*isol*)

3,4′,5,6-Tetrahydroxy-8-methylflavone T-249

[65501-43-1]
*3,5,6-Trihydroxy-2-(4-hydroxyphenyl)-8-methyl-4*H*-1-benzopyran-4-one. 4′,5,6-Trihydroxy-8-methylflavonol. Demethylsilpin*



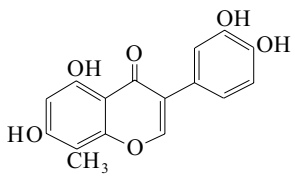
$C_{16}H_{12}O_6$ 300.267
Yellow acicular cryst. (MeOH). Mp 290°.

3-Me ether: [65501-41-9] *4′,5,6-Trihydroxy-3-methoxy-8-methylflavone.* ***Sylpin***. *Silpin*
$C_{17}H_{14}O_6$ 314.294
Isol. from *Pinus sylvestris* (Scotch pine). Yellow acicular cryst. Mp 301-303°.

Medvedeva, S.A. *et al., Khim. Prir. Soedin.*, 1977, 650; *Chem. Nat. Compd. (Engl. Transl.)*, 539 (*isol*)
Zapeschnaya, G.G. *et al., Khim. Prir. Soedin.*, 1984, 306; *Chem. Nat. Compd. (Engl. Transl.)*, 284 (*uv, ms, pmr*)

3′,4′,5,7-Tetrahydroxy-8-methylisoflavone T-250

*3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-8-methyl-4*H*-1-benzopyran-4-one*



$C_{16}H_{12}O_6$ 300.267

7-O-β-D-Glucopyranoside: [263839-32-3]
$C_{22}H_{22}O_{11}$ 462.409

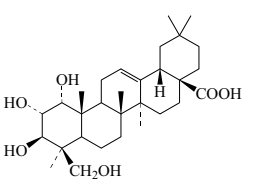
3′,4′,7-Tri-Me ether: [87592-97-0] *5-Hydroxy-3′,4′,7-trimethoxy-8-methylisoflavone*
Mp 159°.

3′,4′,7-Tri-Me ether, 5-Ac:
Cryst. Mp 159°.

3′,4′,7-Tri-Me ether, 5-O-[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [87611-94-7]
$C_{31}H_{38}O_{15}$ 650.632
Constit. of seeds of *Dolichos biflorus* (papadi). Cryst. Mp 184°.

Mitra, J. *et al., Phytochemistry*, 1983, **22**, 1063 (*tri-Me ether neohesperidoside*)
Elgindi, M.R. *et al., Asian J. Chem.*, 1999, **11**, 1534-1536 (*7-glucoside*)

1,2,3,24-Tetrahydroxy-12-oleanen-28-oic acid T-251



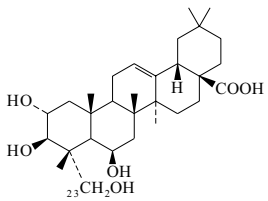
(1α,2α,3β)-form

$C_{30}H_{48}O_6$ 504.706

(1α,2α,3β)-*form* [157528-78-4]
Needles (MeOH). Mp 298.5-300.5° dec. $[\alpha]_D^{25}$ +47.6 (c, 0.3 in MeOH).

(1β,2α,3α)-*form* [254098-66-3]
Constit. of nectarine fruits (*Prunus persica* cv. Fantasia). Powder.
Zhang, Y.-J. *et al., Phytochemistry*, 1994, **36**, 997 (*isol, pmr, cmr, ms*)
El Lahlou, H. *et al., Phytochemistry*, 1999, **52**, 623-629 (*Prunus persica constit*)

2,3,6,23-Tetrahydroxy-12-oleanen-28-oic acid T-252



(2α,3β,6β)-*form*

$C_{30}H_{48}O_6$ 504.706

(2α,3β,6β)-*form* [564-13-6]
Terminolic acid†
Cryst. (Me_2CO). Mp 347°. $[\alpha]_D$ +42 (c, 0.11 in EtOH).

Me ester:
Prisms. Mp 165-168°. $[\alpha]_D$ +40 (c, 0.78 in $CHCl_3$).

28-O-β-D-Glucopyranosyl ester: [149475-28-5] ***Chebuloside II***
$C_{36}H_{58}O_{11}$ 666.848
Cryst. (MeOH). Mp 215°. $[\alpha]_D$ +25 (c, 0.75 in MeOH).

28-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [125265-68-1] ***Asiaticoside B***
$C_{48}H_{78}O_{20}$ 975.132
Constit. of *Centella asiatica* (Asiatic pennywort).

3-O-β-D-Glucopyranoside, 28-O-[β-D-apiofuranosyl-(1→3)-[α-L-rhamopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)]-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [220788-69-2] ***Beciumecine 1***
$C_{63}H_{102}O_{31}$ 1355.48
Amorph. powder. $[\alpha]_D^{19}$ -31.8 (c, 1.7 in MeOH).

23-Carboxylic acid: [71832-46-7] *2,3,6-Trihydroxy-12-oleanene-23,28-dioic acid.* ***Barringtonic acid***
$C_{30}H_{46}O_7$ 518.689
Cryst. (MeOH). Mp 285°. $[\alpha]_D^{30}$ +19.6 (c, 0.8 in MeOH).

(2β,3β,6α)-*form* [98985-56-9] ***Butyracic acid***
Needles ($CHCl_3$/MeOH). Mp 332-334°.

Me ester: [98990-10-4]
Needles (CH_2Cl_2/Et_2O). Mp 200-202°. $[\alpha]_D$ +47.1 (c, 0.5 in $CHCl_3$).

(2β,3β,6β)-*form* [37905-13-8] ***Protobassic acid***
Constit. of the famine food *Madhuca longifolia*. Cryst. (MeOH). Mp 310-312°. $[\alpha]_D$ +22.7 (c, 0.11 in Py).

Me ester: [37867-31-5]
Needles (Me_2CO). Mp 198-201°. $[\alpha]_D$ +42.4 (c, 0.5 in MeOH).

28-O-α-L-Arabinopyranosyl ester: [67258-70-2] ***Madlongiside C***
$C_{35}H_{56}O_{10}$ 636.821
Constit. of the famine food *Madhuca longifolia*. Needles. Mp 196-198°. $[\alpha]_D^{25}$ +32 (c, 1.2 in MeOH).

28-O-[α-L-Rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [58019-21-9] ***Madlongiside D***
$C_{41}H_{66}O_{14}$ 782.964
Constit. of the famine food *Madhuca longifolia*. Needles. Mp 230-232°. $[\alpha]_D^{25}$ -12.9 (c, 1.8 in MeOH).

28-O-[β-D-Xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[β-D-apiofuranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [161995-30-8] ***Sideroxyloside C***
$C_{57}H_{92}O_{26}$ 1193.338
Amorph. powder (MeOH). $[\alpha]_D^{24}$ -42.8 (c, 0.6 in MeOH).

3-O-β-D-Glucopyranoside: [53840-47-4]
$C_{36}H_{58}O_{11}$ 666.848
Powder (MeOH). $[\alpha]_D$ +26 (c, 0.95 in MeOH).

3-O-β-D-Glucopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [173792-52-4] ***Mimusopside A***
$C_{47}H_{76}O_{19}$ 945.106
Amorph. powder. Mp 245-248° dec. $[\alpha]_D$ -20.9 (c, 0.22 in MeOH).

3-O-β-D-Glucopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-xylopyranosyl] ester: [155740-08-2] ***Sideroxyloside A***
$C_{58}H_{94}O_{27}$ 1223.364
Powder (MeOH). $[\alpha]_D$ -19 (c, 0.31 in MeOH).

3-O-β-D-Glucopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [54328-42-6] ***Mi-saponin A***
$C_{58}H_{94}O_{27}$ 1223.364
Amorph. powder. Mp 232-235°. $[\alpha]_D$ -33.1 (MeOH).

3-O-β-D-Glucopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [171674-85-4] ***Mimusopin***
$C_{64}H_{104}O_{31}$ 1369.507
Amorph. solid. $[\alpha]_D^{21}$ -17.9 (c, 0.12 in MeOH).

3-O-β-D-Glucopyranoside, 28-O-[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→4)-[β-D-apiofuranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [161995-29-5] ***Sideroxyloside B***
$C_{68}H_{110}O_{35}$ 1487.596
Amorph. powder (MeOH). $[\alpha]_D^{24}$ -49.4 (c, 1.6 in MeOH).

3-O-β-D-Glucopyranoside, 28-O-[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [144425-22-9] ***Arganine F***. *Butyroside A*. *Mi-saponin B*
$C_{57}H_{92}O_{27}$ 1209.338
Needles (MeOH). Mp 242-243° dec. $[\alpha]_D^{22}$ -48.2 (c, 0.36 in MeOH).

3-O-β-D-Glucuronopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [159803-58-4] ***Butyroside C***
$C_{58}H_{92}O_{28}$ 1237.348
Powder (MeOH). Mp 216-220° dec. $[\alpha]_D^{16}$ -20 (c, 0.8 in MeOH).

3-O-β-D-Glucuronopyranoside, 28-O-[α-L-rhamnopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→3)]-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [173614-95-4]
$C_{64}H_{102}O_{32}$ 1383.491
$[\alpha]_D$ -37.7 (c, 0.3 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside], 28-O-[α-L-rhamnopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [171674-86-5] ***Mimusopsin***
$C_{64}H_{104}O_{32}$ 1385.506
Amorph. solid. $[\alpha]_D^{21}$ -17.9 (c, 0.12 in MeOH). $[\alpha]_D$ -31.5 (c, 0.45 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside], 28-O-[α-L-rhamnopyranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [144442-85-3] ***Mimusin***. *Arganine D*
$C_{64}H_{104}O_{32}$ 1385.506
Amorph. solid. Mp 227° dec. $[\alpha]_D$ +20 (c, 0.09 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside], 28-O-[β-D-apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyl] ester: [144442-86-4] ***Arganine E***
$C_{63}H_{102}O_{32}$ 1371.48

2-Ketone:3,6,23-Trihydroxy-2-oxo-12-oleanen-28-oic acid
$C_{30}H_{46}O_6$ 502.69

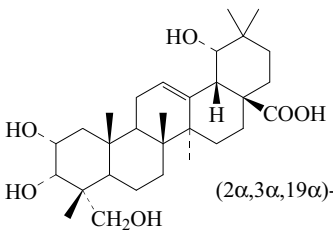
2-Ketone, 28-α-L-arabinopyranosyl ester: [312959-40-3] ***Madlongiside A***
$C_{35}H_{54}O_{10}$ 634.806
Needles. Mp 202-204°. $[\alpha]_D^{25}$ +34.5 (c, 0.8 in MeOH).

2-Ketone, 3-O-β-D-glucopyranoside, 28-O-α-L-arabinopyranosyl ester: [312959-41-4] ***Madlongiside B***
$C_{41}H_{64}O_{15}$ 796.948
Needles. Mp 212-214°. $[\alpha]_D^{25}$ +15.7 (c, 1.5 in MeOH).

King, F.E. *et al., J.C.S.*, 1955, 1333; 1956, 4469 (*Terminolic acid*)
Raw, L.R. *et al., Indian J. Chem.*, 1964, **2**, 463 (*isol*)
Yosioka, I. *et al., Tetrahedron*, 1974, **30**, 707 (*Protobassic acid*)
Anjaneyulu, A.S.R. *et al., J. Indian Chem. Soc.*, 1978, **55**, 1169 (*struct*)
Banerjee, R. *et al., Planta Med.*, 1985, 280 (*Butyracic acid*)
Toyota, M. *et al., Phytochemistry*, 1990, **29**, 2849-2851 (*cmr, Mi-saponins*)
Massiot, G. *et al., Bull. Soc. Chim. Fr.*, 1991, **127**, 100 (*isol, pmr, cmr*)
Charrouf, Z. *et al., Phytochemistry*, 1992, **31**, 2079-2086 (*Arganines, Mi-saponin A*)
Nigam, S.K. *et al., Phytochemistry*, 1992, **31**, 3169-3172 (*Butyroside A*)

Kundu, A.P. *et al., Phytochemistry*, 1993, **32**, 999-1002 (*cmr, Chebuloside II*)
Jiang, Y. *et al., Phytochemistry*, 1994, **35**, 1013 (*Sideroxyloside A*)
Li, X.-C. *et al., Phytochemistry*, 1994, **37**, 827 (*Butyroside C*)
Nicolas, G. *et al., Phytochemistry*, 1995, **38**, 225 (*Sideroxylosides*)
Sahu, N.P. *et al., Tetrahedron*, 1995, **51**, 13435 (*Mimusopin, Mimusopsin*)
Sahu, N.P.L. *et al., Phytochemistry*, 1996, **41**, 883 (*Mimusopside A*)
Lavaud, C. *et al., Phytochemistry*, 1996, **41**, 887 (*Mimusops saponins*)
Sahu, N.P. *et al., Phytochemistry*, 1997, **44**, 1145 (*Mimusin*)
Burger, I. *et al., Phytochemistry*, 1998, **49**, 2087-2095 (*Beciumecine 1*)
Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 1679-1681 (*Madlongisides*)

2,3,19,23-Tetrahydroxy-12-oleanen-28-oic acid T-253



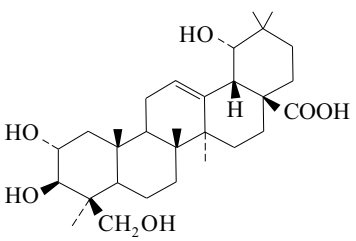
(2α,3α,19α)-*form*

$C_{30}H_{48}O_6$ 504.706

(2α,3β,19β)-*form* [6753-23-7]
Tomentosic acid
Constit. of *Bixa orellana* (annatto). Cryst. (Me_2CO). Mp 328-330°. $[\alpha]_D^{31}$ +64 (EtOH).

Row, L.R. *et al., Tetrahedron*, 1962, **18**, 827-838 (*isol, Tomentosic acid*)
Schneider, W.P. *et al., J.O.C.*, 1965, **30**, 2856-2857 (*struct, Tomentosic acid*)
Mahato, S. *et al., J.C.S. Perkin 2*, 1990, 1445-1450 (*cryst struct, Tomentosic acid*)

2,3,19,24-Tetrahydroxy-12-oleanen-28-oic acid T-254



$C_{30}H_{48}O_6$ 504.706
Log P 3.28 (calc).

(2α,3β,19α)-*form* [55306-03-1]
Sericic acid
Constit. of *Quercus ilex* (holly oak). Cryst. (EtOH). Mp 282°. $[\alpha]_D^{30}$ +38 (c, 0.32 in EtOH).

β-D-Glucopyranosyl ester: [55306-04-2]
Sericoside
$C_{36}H_{58}O_{11}$ 666.848
Constit. of *Quercus ilex* (holly oak). Cryst. (MeOH). Mp 209°. $[\alpha]_D^{30}$ +5.4 (c, 2 in Py).

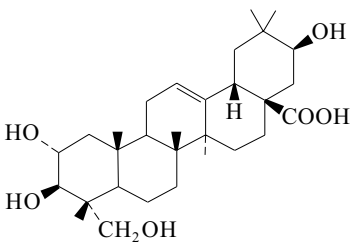
2,3,23-Tri-Ac: [58096-15-4]
$C_{36}H_{54}O_9$ 630.817
Isol. from *Quercus ilex* (holly oak).

24-Aldehyde:2α,3β,19α-Trihydroxy-24-oxo-12-oleanen-28-oic acid
$C_{30}H_{46}O_6$ 502.69

24-Aldehyde, β-D-glucopyranosyl ester: [177413-34-2] ***Paradrymonoside***. *Paradrymoniside. Paradrymonin*
$C_{36}H_{56}O_{11}$ 664.832
Amorph. powder. Mp 197-200°. $[\alpha]_D$ +24 (c, 0.11 in MeOH).

Bombardelli, E. *et al., Phytochemistry*, 1974, **13**, 2559
Romussi, G. *et al., Pharmazie*, 1983, **38**, 787 (*triacetate*)
Terreaux, C. *et al., Phytochemistry*, 1996, **42**, 495-499 (*isol, pmr, cmr*)
Yeo, H. *et al., Phytochemistry*, 1998, **48**, 1399-1401 (*Sericic acid, pmr, cmr*)

2,3,21,23-Tetrahydroxy-12-oleanen-28-oic acid T-255



$C_{30}H_{48}O_6$ 504.706

(2α,3β,21β)-*form* [29623-64-1]
Caccigenin
Cryst. (MeOH). Mp 267-270°. $[\alpha]_D$ +24 (c, 0.4 in MeOH).

β-D-Glucopyranosyl ester: [54526-93-1]
Poterioside
$C_{36}H_{58}O_{11}$ 666.848
Cryst. Mp 270-279°. $[\alpha]_D$ +38.4.

3-O-β-Glucopyranoside: [206270-86-2] ***Lucyoside R***
$C_{36}H_{58}O_{11}$ 666.848
Constit. of *Luffa cylindrica* (smooth luffa). Cryst. Mp 234-236°. $[\alpha]_D$ +35.7 (c, 0.4 in MeOH).

21-O-β-D-Glucopyranoside: [86425-63-0] ***Anchusoside 3***
$C_{36}H_{58}O_{11}$ 666.848
Cryst. (MeOH). Mp 270° (dec.).

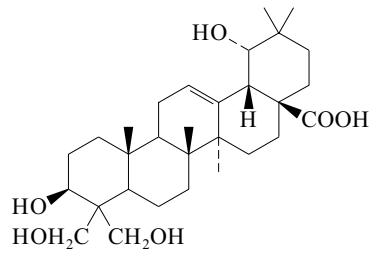
21-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [94491-24-4] ***Anchusoside 9***. *Caccigenin 21-sophoroside*
$C_{42}H_{68}O_{16}$ 828.99
Amorph.

21-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside], 3-O-β-D-xylopyranoside: [94474-71-2] ***Anchusoside 8***
$C_{47}H_{76}O_{20}$ 961.105
Mp 300° dec.

28→21 Lactone: [29623-52-7] ***Caccigenin lactone***
$C_{30}H_{46}O_5$ 486.69
Cryst. (MeOH). Mp 203-205°. $[\alpha]_D$ -44 (c, 0.4 in $CHCl_3$).

Tewari, N.C. *et al., Indian J. Chem.*, 1970, **8**, 593 (*struct*)
Shukyurov, D.N. *et al., Khim. Prir. Soedin.*, 1974, **10**, 531; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 546 (*Poterioside*)
Romussi, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 499-504 (*Anchusoside 3*)
Romussi, G. *et al., Annalen*, 1984, 1869 (*Anchusosides*)
Liang, L. *et al., Yaoxue Xuebao*, 1997, **32**, 761-764 (*Lucyoside R*)

3,19,23,24-Tetrahydroxy-12-oleanen-28-oic acid T-256



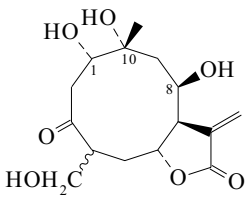
$C_{30}H_{48}O_6$ 504.706

(3β,19α)-*form*
Constit. of the wild guava *Alibertia edulis*.

Me ester, 3,23,24-tri-Ac: [157469-23-3]
Cryst. (MeOH). Mp 181-183°.

Brochini, C.B. *et al., Phytochemistry*, 1994, **36**, 1293 (*isol, pmr, cmr*)

1,8,10,15-Tetrahydroxy-3-oxo-11(13)-germacren-12,6-olide T-257

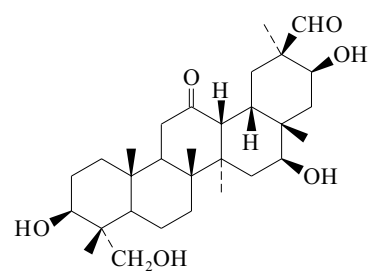


$C_{15}H_{22}O_7$ 314.335

(1α,4ξ,6α,8β,10*R*)-*form*
*1,10-Di-Me ether, 8-angeloyl:8β-Angeloyloxy-15-hydroxy-1α,10*R*-dimethoxy-3-oxo-11(13)-germacren-12,6α-olide*
$C_{22}H_{32}O_8$ 424.49
Constit. of *Helianthus annuus* (sunflower).

Alfatafta, A.A. *et al., Phytochemistry*, 1992, **31**, 4109 (*isol, pmr*)

3,16,21,23-Tetrahydroxy-12-oxo-30-oleananal T-258



$C_{30}H_{48}O_6$ 504.706

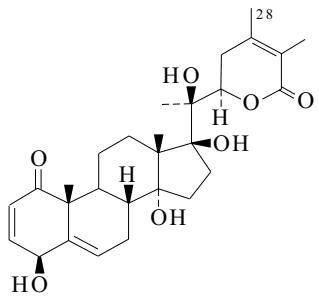
(3β,16β,21β)-*form*

21-Benzoyl: [90578-34-0] ***Avenestergenin A2***
$C_{37}H_{52}O_7$ 608.814
Aglycone from oat root. Needles (MeOH aq.). Mp 189-190°.

21-(2-Methylaminobenzoyl): [90578-35-1] ***Avenestergenin A1***
$C_{38}H_{55}NO_7$ 637.855
Aglycone from oat root. Microneedles (MeOH aq.). Mp 210-211°.

Begley, M.J. *et al., J.C.S. Perkin 1*, 1986, 1905 (*isol, pmr, cmr, cryst struct*)

4,14,17,20-Tetrahydroxy-1-oxowitha-2,5,24-trienolide T-259



$C_{28}H_{38}O_7$ 486.604

(4β,14α,17β,20*R*,22*R*)-*form* [74799-65-8] ***Withaphysanolide***
Cryst. (MeOH). Mp 215°. $[\alpha]_D$ +95 (c, 2.63 in dioxan). Struct. revised in 1984 although still indexed by CAS as the 5-hydroxy-8(14)-dehydro compd. (4β,5α,17β,20*R*-Tetrahydroxy-1-oxo-22*R*-witha-2,8(14),24-trienolide).

4-Ac:
Cryst. (MeOH aq.). $[\alpha]_D^{22}$ +95.9 (c, 1.74 in MeOH).

*28-Hydroxy:4β,14,17β,20*R*,28-Pentahydroxy-1-oxo-22*R*-witha-2,5,24-trienolide.* ***28-Hydroxywithaphysanolide***
$C_{28}H_{38}O_8$ 502.603
Cryst. (MeOH). Mp 234°.

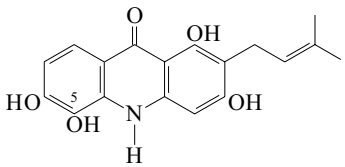
28-Hydroxy, 4,28-Di-Ac:
Cryst. (MeOH aq.). Mp 204°. $[\alpha]_D^{22}$ +89.6 (c, 1.894 in $CHCl_3$).

(4β,14α,17β,20*S*,22*R*)-*form* ***Physapruin A***
Constit. of *Physalis pruinosa* (strawberry tomato). Needles ($CHCl_3$/MeOH). Mp 207-209°. $[\alpha]_D$ +159.1 (c, 0.46 in MeOH).

Maslennikova, V.A. *et al., Khim. Prir. Soedin.*, 1980, **16**, 214; *Chem. Nat. Compd. (Engl. Transl.)*, 1980, **16**, 167 (*isol*)
Abdullaev, N.D. *et al., Khim. Prir. Soedin.*, 1984, **20**, 197; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 182 (*struct*)
Shingu, K. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1873 (*isol, pmr, cmr*)

1,3,5,6-Tetrahydroxy-2-prenylacridone T-260

*1,3,5,6-Tetrahydroxy-2-(3-methyl-2-butenyl)-9*H*-acridin-9-one*



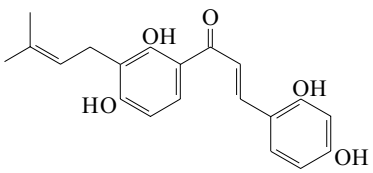
$C_{18}H_{17}NO_5$ 327.336

5-Me ether, N-*Me:* [119116-85-7] *1,3,6-Trihydroxy-5-methoxy-10-methyl-2-prenylacridone.* ***Buntanine***
$C_{20}H_{21}NO_5$ 355.39
Alkaloid from the root bark of *Citrus grandis* (pummelo). Yellow plates (Me_2CO). Mp 247-249°.

Wu, T.-S. *et al., Phytochemistry*, 1988, **27**, 3717 (*isol, uv, ir, pmr, cmr, ms, struct*)

2,2′,4,4′-Tetrahydroxy-3′-prenylchalcone T-261

1-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)-phenyl]-3-(2,4-dihydroxyphenyl)-2-propen-1-one



$C_{20}H_{20}O_5$ 340.375

(*E*)-*form* [76472-88-3] ***Morachalcone A***
Constit. of *Morus alba* (white mulberry). Mp 204-205° (138°).

Takasugi, M. *et al., Chem. Lett.*, 1980, 1573 (*isol*)
Batirov, E.K. *et al., Khim. Prir. Soedin.*, 1987, **23**, 516; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 429 (*cmr*)
Hano, Y. *et al., Heterocycles*, 1989, **29**, 807 (*isol*)
Delle Monache, G. *et al., Phytochemistry*, 1995, **39**, 575 (*isol, pmr, cmr*)

2,3′,4,4′-Tetrahydroxy-3-prenylchalcone T-262

3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)-phenyl]-1-(3,4-dihydroxyphenyl)-2-propen-1-one

$C_{20}H_{20}O_5$ 340.375

(*E*)-*form*

2-Me ether:3′,4,4′-Trihydroxy-2-methoxy-3-prenylchalcone. ***Licoagrochalcone C***
$C_{21}H_{22}O_5$ 354.402
Isol. from hairy root cultures of *Glycyrrhiza glabra* (licorice). Yellow powder. λ_{max} 247 (log ϵ 4.1); 360 (log ϵ 4.38) (MeOH).

Li, W. *et al., Phytochemistry*, 2000, **55**, 447-456

2′,4,4′,6′-Tetrahydroxy-3′-prenylchalcone T-263

[115063-39-3]
3-(4-Hydroxyphenyl)-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propen-1-one. ***Desmethylxanthohumol***

$C_{20}H_{20}O_5$ 340.375

Chalcone numbering shown. Constit. of *Humulus lupulus* (hops).

4′-Me ether: [265659-35-6] *2′,4,6′-Trihydroxy-4′-methoxy-3′-prenylchalcone.* ***Xanthogalenol***
$C_{21}H_{22}O_5$ 354.402
Isol. from *Humulus lupulus* (hops).

6′-Me ether: [6754-58-1]

[569-83-5] *2′,4,4′-Trihydroxy-6′-methoxy-3′-prenylchalcone.* ***Xanthohumol***
$C_{21}H_{22}O_5$ 354.402
Isol. from *Humulus lupulus* (hops). Orange-yellow cryst. (EtOH aq.). Sol. MeOH; poorly sol. H_2O. Mp 172°.

4′,6′-Di-Me ether: [123316-63-2] *2′,4-Dihydroxy-4′,6′-dimethoxy-3′-prenylchalcone*
$C_{22}H_{24}O_5$ 368.429
Isol. from *Humulus lupulus* (hops). Cryst. (EtOAc/hexane). Mp 152-153°.

2′,4,4′-Tri-Me ether: [70872-21-8]
$C_{23}H_{26}O_5$ 382.455
Cryst. (EtOAc). Mp 137-138°.

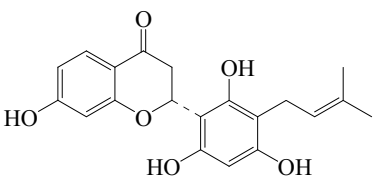
4,4′,6′-Tri-Me ether: [70872-24-1]
Cryst. (EtOAc/petrol). Mp 131-132° (126-127°).

Δ$^{3''}$-Isomer, 2′′-hydroxy, 6′-Me ether: [274675-25-1] ***Xanthohumol D***
$C_{21}H_{22}O_6$ 370.401
Isol. from *Humulus lupulus* (hops). λ_{max} 369 (log ϵ 4.42) (MeOH).

α,β-Dihydro, 6′-Me ether: [102448-00-0] *2′,4,4′-Trihydroxy-6′-methoxy-3′-prenyldihydrochalcone.* ***α,β-Dihydroxanthohumol***
$C_{21}H_{24}O_5$ 356.418
Constit. of hops (*Humulus lupulus*).

Verzele, M. *et al., Bull. Soc. Chim. Belg.*, 1957, **66**, 452-475 (*isol, Xanthohumol*)
Hubner, H. *et al., Chem. Ber.*, 1960, **93**, 312-317 (*4′,6′-di-Me ether, synth*)
Vanderwalle, M. *et al., Bull. Soc. Chim. Belg.*, 1961, **70**, 163-167 (*struct, synth*)
Orth, W.A. *et al., Annalen*, 1963, **663**, 74-82 (*struct*)
Jain, A.C. *et al., Tetrahedron*, 1978, **34**, 3563-3567 (*4,4′,6′-tri-Me ether, 2′,4,4′-tri-Me ether, synth*)
Sun, S.-S. *et al., Phytochemistry*, 1989, **28**, 1776-1777 (*Xanthohumol, 4′,6′-di-Me ether, isol*)
Tabata, N. *et al., Phytochemistry*, 1997, **46**, 683-687 (*Xanthohumol, isol, pmr, cmr*)
Etteldorf, N. *et al., Z. Naturforsch., C*, 1999, **54**, 610-612 (*Dihydroxanthohumol*)
Stevens, J.F. *et al., Phytochemistry*, 2000, **53**, 759-775 (*Xanthohumol D, isol, occur*)

2′,4′,6′,7-Tetrahydroxy-3′-prenylflavanone T-264



$C_{20}H_{20}O_6$ 356.374

(R)-form

2′,4′-Di-Me ether:6′,7-Dihydroxy-2′,4′-dimethoxy-3′-prenylflavanone. ***Glicoisoflavanone***

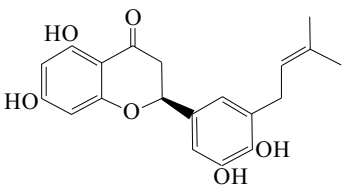
$C_{22}H_{24}O_6$ 384.428

Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Needles. Mp 102°. $[\alpha]_D$ -3 (c, 2 in MeOH).

Hatano, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1286-1292

3′,4′,5,7-Tetrahydroxy-5′-prenylflavanone T-265

*2-[3,4-Dihydroxy-5-(3-methyl-2-butenyl)-phenyl]-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI.* ***Sigmoidin B.*** *Uralenin*



$C_{20}H_{20}O_6$ 356.374

λ_{max} 325 (ϵ 21800) (MeOH/NaOH) (Derep). λ_{max} 288 (ϵ 12900) (MeOH) (Derep).

(S)-form [87746-47-2]

Cryst. Mp 217-218°. $[\alpha]_D^{28}$ -54 (c, 3 in MeOH).

3′,4′-Di-Me ether: [147047-03-8] *5,7-Dihydroxy-3′,4′-dimethoxy-5′-prenylflavanone*

$C_{22}H_{24}O_6$ 384.428

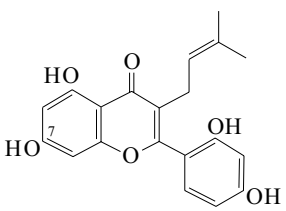
Constit. of *Melilotus alba* (white melilot).

Souleles, C. *et al., Sci. Pharm.*, 1992, **60**, 101 (*3′,4′-di-Me ether*)

2′,4′,5,7-Tetrahydroxy-3-prenylflavone T-266

[73343-42-7]

*2-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-3-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Albanin A***



$C_{20}H_{18}O_6$ 354.359

Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*. Cryst. (hexane). Mp 220-227°. λ_{max} 257 (ϵ 20600); 294 (ϵ 9600); 326 (ϵ 9610) (MeOH) (Berdy).

7-Me ether: [60791-49-3] *2′,4′,5-Trihydroxy-7-methoxy-3-prenylflavone.* ***Integrin***†

$C_{21}H_{20}O_6$ 368.385

Constit. of heartwood of *Artocarpus integer* (champeduk). Pale-yellow needles (C_6H_6). Mp 165°.

Tetra-Me ether:

Yellow needles (MeOH). Mp 138°.

Pendse, A.D. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 69

Takasugi, M. *et al., CA*, 1980, **92**, 160450 (*isol*)

Ferrari, F. *et al., Planta Med.*, 1989, **55**, 70 (*isol, pmr, cmr, uv*)

2′,4′,5,7-Tetrahydroxy-6-prenylflavone T-267

[3162-09-2]

*2-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Artocarpesin***

$C_{20}H_{18}O_6$ 354.359

Constit. of the heartwood of *Artocarpus heterophyllus* (jackfruit). Yellow needles (Me_2CO). Mp 275-276° (250°).

Δ1′′-Isomer:2′,4′,5,7-Tetrahydroxy-6-(3-methyl-1-butenyl)flavone. ***Isoartocarpesin***

$C_{20}H_{18}O_6$ 354.359

Constit. of *Artocarpus incisus* (breadfruit). Yellow powder.

2′′,3′′-Dihydro, 3′′-hydroxy: [23806-62-4] ***Oxidihydroartocarpesin***

$C_{20}H_{20}O_7$ 372.374

Isol. from *Artocarpus heterophyllus* (jackfruit).

Radharakrishnan, P.V. *et al., Tet. Lett.*, 1965, 663

Parthasarathy, P.C. *et al., Indian J. Chem.*, 1969, **7**, 101 (*Oxidihydroartocarpesin*)

Rao, A.V.R. *et al., Indian J. Chem.*, 1972, **10**, 905; 989 (*isol, ms*)

Young, H.S. *et al., Arch. Pharmacal Res.*, 1989, **12**, 39 (*isol*)

Monache, G.D. *et al., Phytochemistry*, 1994, **37**, 893 (*isol, uv, pmr, cmr, ms*)

Shimizu, K. *et al., Planta Med.*, 1998, **64**, 408-412 (*Isoartocarpesin*)

2′,4′,5,7-Tetrahydroxy-8-prenylflavone T-268

*2-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI*

$C_{20}H_{18}O_6$ 354.359

7-Me ether: [167319-12-2] *2′,4′,5-Trihydroxy-7-methoxy-8-prenylflavone.* ***Artocarpetin A***†

$C_{21}H_{20}O_6$ 368.385

Constit. of *Artocarpus heterophyllus* (jackfruit). Pale yellow needles ($CHCl_3$/MeOH). Mp 270-271°. Not to be confused with, 7-Me ether. Incorrectly named as an isoflavone in CA. λ_{max} 207 (log ϵ 4.76); 252 (log ϵ 4.36); 269 (log ϵ 4.45); 288 (log ϵ 4.2); 356 (log ϵ 4.43) (MeOH).

2′,7-Di-Me ether: [170894-22-1] *4′,5-Dihydroxy-2′,7-dimethoxy-8-prenylflavone.* ***Artocarpetin B***

$C_{22}H_{22}O_6$ 382.412

Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow needles ($CHCl_3$). Mp 253-257°. λ_{max} 209 (log ϵ 4.53); 252 (sh) (log ϵ 4.16); 270 (log ϵ 4.3); 288 (sh) (log ϵ 4.08); 345 (log ϵ 4.23) (MeOH).

Lin, C.-N. *et al., Phytochemistry*, 1995, **39**, 1447 (*isol, uv, pmr, cmr, ms*)

Chung, M.-I. *et al., Phytochemistry*, 1995, **40**, 1279-1282 (*Artocarpetin B*)

3,4′,5,7-Tetrahydroxy-3′-prenylflavone T-269

[94805-83-1]

*3,5,7-Trihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-3′-prenylflavonol.* ***Isolicoflavonol***

$C_{20}H_{18}O_6$ 354.359

Constit. of *Glycyrrhiza uralensis* (Chinese licorice) and *Glycyrrhiza glabra* (licorice). Pale yellow needles. Mp 119°. Log P 2.31 (calc).

Hatano, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2090; 2286 (*isol*)

3,4′,5,7-Tetrahydroxy-6-prenylflavone T-270

[60197-60-6]

*3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-6-prenylflavonol.* ***Licoflavonol***

$C_{20}H_{18}O_6$ 354.359

Isol. from the roots of *Glycyrrhiza uralensis* (Chinese licorice). Yellow needles ($CHCl_3$/MeOH). Mp 185-187° dec. Log P 2.31 (calc).

3-Me ether: [109605-79-0] *4′,5,7-Trihydroxy-3-methoxy-6-prenylflavone.* ***Topazolin***

$C_{21}H_{20}O_6$ 368.385

Pale yellow rods (Me_2CO/EtOAc). Mp 227-228.5°. λ_{max} 215 (ϵ 31100); 272 (ϵ 25600); 336 (ϵ 19000) (MeOH) (Berdy). λ_{max} 277 ; 330 ; 401 (MeOH/NaOH) (Berdy).

2′′,3′′-Dihydro, 3′′-hydroxy: [143724-79-2] *3,4′,5,7-Tetrahydroxy-6-(3-hydroxy-3-methylbutyl)flavone*

$C_{20}H_{20}O_7$ 372.374

Yellow needles. Mp 223-224°. Struct. revised in 1992.

2′′,3′′-Dihydro, 3′′-hydroxy, 3-Me ether: [109605-84-7] ***Topazolin hydrate***

$C_{21}H_{22}O_7$ 386.401

Pale-yellow rods (EtOAc/hexane). Mp 239-241°.

Saitoh, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1242 (*isol, struct*)

Tahara, S. *et al., Agric. Biol. Chem.*, 1987, **51**, 1039

Fukai, T. *et al., Heterocycles*, 1992, **34**, 1213

3′,4′,5,7-Tetrahydroxy-6-prenylflavone T-271

[129145-53-5]

*2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Gancaonin O***

$C_{20}H_{18}O_6$ 354.359

Constit. of *Glycyrrhiza uralensis* (Chinese licorice) and *Hypericum perforatum* (St. John's Wort). Yellow needles (Me_2CO/hexane). Mp 245-248°.

3′-Me ether: [76735-58-5] *4′,5,7-Trihydroxy-3′-methoxy-6-prenylflavone.* ***Cannflavin B.*** *Canniflavone 1*

$C_{21}H_{20}O_6$ 368.385

Cryst. Mp 234°.

Crombie, L. *et al., J.C.S. Perkin 1*, 1982, 1455

Fukai, T. *et al., Heterocycles*, 1990, **31**, 373 (*isol, pmr, cmr*)
Ngadjui, B.T. *et al., Phytochemistry*, 1998, **48**, 349-354 (*isol, uv, pmr, cmr*)
Dias, A.C.P. *et al., Phytochemistry*, 1998, **48**, 1165-1168 (*isol, uv, pmr, cmr, ms*)

3,4′,5,7-Tetrahydroxy-8-prenylflavone T-272

[28610-31-3]
*3,5,7-Trihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI. 4′,5,7-Trihydroxy-8-prenylflavonol.* ***Noranhydroicaritin****. 8-*C*-Prenylkaempferol*

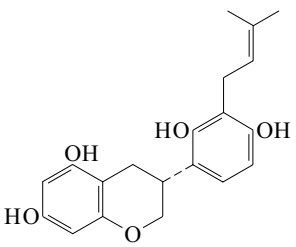
$C_{20}H_{18}O_6$ 354.359
Yellow cryst. (EtOAc/petrol). Mp 226°. λ_{max} 272 (ϵ 23500); 376 (ϵ 19000) (EtOH) (Berdy).

*4′-Me ether, 3-*O*-[α-*L*-rhamnopyranosyl-(1→6)-β-*D*-galactopyranoside], 7-*O*-β-*D*-galactopyranoside:*
$C_{39}H_{50}O_{20}$ 838.812
Constit. of *Sesbania grandiflora* (agati). Cryst. Mp 214-217°. λ_{max} 266 ; 348 (MeOH).

[119708-36-0, 119708-38-2, 156216-77-2, 156216-78-3]

Das, K.C. *et al., Fitoterapia*, 1998, **69**, 477-478 (*Sesbania grandiflora constit*)

2′,4′,5,7-Tetrahydroxy-3′-prenylisoflavan T-273



$C_{20}H_{22}O_5$ 342.391

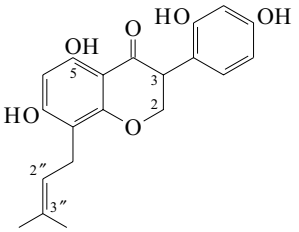
(R)-form

4′,5-Di-Me ether: [156250-73-6] *2′,7-Dihydroxy-4′,5-dimethoxy-3′-prenylisoflavan.* ***Kanzonol R***
$C_{22}H_{26}O_5$ 370.444
Constit. of *Glycyrrhiza glabra* (licorice). Granules (C_6H_6/Me_2CO). Mp 69-72°. $[\alpha]_D$ -25 (c, 0.04 in MeOH). λ_{max} 214 (ϵ 57540); 272 (ϵ 8130); 280 (sh) (ϵ 7413); 295 (sh) (ϵ 4466) (MeOH).

Fukai, T. *et al., Heterocycles*, 1994, **38**, 1089 (*isol, uv, ms, cd, pmr, cmr*)

2′,4′,5,7-Tetrahydroxy-8-prenylisoflavanone T-274

[40105-60-0]
*3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Kievitone****. Vignatin. Phaseolus substance II*



$C_{20}H_{20}O_6$ 356.374
Isol. from *Dolichos biflorus* (papadi), *Lablab niger* (hyacinth bean), *Phaseolus aureus* (mung bean), *Phaseolus calcaratus* (rice bean), *Phaseolus lunatus* (butter bean), *Phaseolus vulgaris* (kidney bean) and *Vigna unguiculata* (all Leguminosae, Papilionoideae). Sol. MeOH, bases, Et_2O; poorly sol. H_2O, hexane. λ_{max} 210 ; 293 (ϵ 16600); 330 (ϵ 3800); 340 (MeOH) (Berdy).

4′-Me ether:2′,5,7-Trihydroxy-4′-methoxy-8-prenylisoflavanone. ***4′-O-Methylkievitone***
$C_{21}H_{22}O_6$ 370.401
Isol. from *Phaseolus mungo* (mung bean). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 292 ; 345 (MeOH) (Berdy).

5-Deoxy: [74161-24-3] *2′,4′,7-Trihydroxy-8-prenylisoflavanone.* ***5-Deoxykievitone***
$C_{20}H_{20}O_5$ 340.375
Isol. from pods of *Phaseolus vulgaris* (kidney bean) and *Phaseolus mungo* (mung bean). λ_{max} 286 (MeOH) (Berdy). λ_{max} 340 (MeOH-NaOH) (Berdy).

2,3-Didehydro: 2′,4′,5,7-Tetrahydroxy-8-prenylisoflavone, T-277

2″,3″-Dihydro, 3″-hydroxy: [62682-11-5] ***Kievitone hydrate***
$C_{20}H_{22}O_7$ 374.39
Isol. from *Phaseolus mungo* (mung bean). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 210 ; 293 (MeOH) (Berdy).

2″,3″-Dihydro, 4″-hydroxy: [104363-14-6] ***Kievitol***
$C_{20}H_{22}O_7$ 374.39
Isol. from *Phaseolus lunatus* (butter bean).

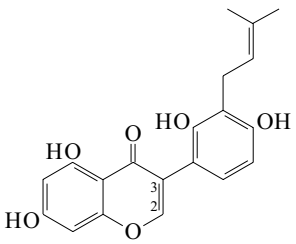
5-Deoxy, 2″,3″-dihydro, 3″-hydroxy: ***5-Deoxykievitone hydrate***
$C_{20}H_{22}O_6$ 358.39
Isol. from *Phaseolus mungo* (mung bean). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 284 (MeOH) (Berdy).

5-Deoxy, 4″-hydroxy: [104380-54-3] ***5-Deoxykievitol***
$C_{20}H_{20}O_6$ 356.374
Isol. from *Phaseolus lunatus* (butter bean).

Burden, R.S. *et al., Tet. Lett.*, 1972, 4175 (*isol*)
Smith, D.A. *et al., Physiol. Plant Pathol.*, 1973, **3**, 293 (*ms, ir, uv*)
Kuhn, P.J. *et al., Phytochemistry*, 1977, **16**, 296 (*Kievitone hydrate*)
Granamanickam, S.S. *et al., Experientia*, 1979, **35**, 323 (*isol*)
Woodward, M.D. *et al., Phytochemistry*, 1979, **18**, 363 (*occur*)
Woodward, M.D. *et al., Phytochemistry*, 1979, **18**, 2007 (*5-Deoxykievetone*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
O'Neill, M.J. *et al., Z. Naturforsch., C*, 1983, **38**, 693 (*derivs*)
Adesanya, S.A. *et al., Z. Naturforsch., C*, 1984, **39**, 888 (*derivs*)
O'Neill, M.J. *et al., Phytochemistry*, 1986, **25**, 1315 (*Kievitol, 5-Deoxykievitol*)

2′,4′,5,7-Tetrahydroxy-3′-prenylisoflavone T-275

[66056-19-7]
*[2,4-Dihydroxy-3-(3-methyl-2-butenyl)-phenyl]-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′-Isopentenyl-2′,4′,5,7-tetrahydroxyisoflavone.* ***Licoisoflavone A****. Phaseoluteone*



$C_{20}H_{18}O_6$ 354.359
Constit. of *Phaseolus vulgaris* (kidney bean). Pale yellow prisms (MeOH aq.).

Tetra-Ac:
Mp 136-138°.

*7-*O*-β-*D*-Glucopyranoside:* [137351-16-7]
$C_{26}H_{28}O_{11}$ 516.501

*4′-*O*-β-*D*-Glucopyranoside:* [137351-17-8]
$C_{26}H_{28}O_{11}$ 516.501

2,3-Dihydro, 2′-Me ether: [69573-59-7] *4′,5,7-Trihydroxy-2′-methoxy-3′-prenylisoflavanone.* ***Sophoraisoflavanone A***
$C_{21}H_{22}O_6$ 370.401
Needles. Mp 178-180°. $[\alpha]_D^{22}$ -17.3 (EtOH). λ_{max} 291 (ϵ 27000); 330 (ϵ 11000) (EtOH) (Berdy).

Kinoshita, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 141 (*isol, struct*)
Komatsu, M. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3863 (*Sophoraisoflavanone A*)
Woodward, M.D. *et al., Phytochemistry*, 1979, **18**, 363 (*isol, uv, pmr, ir*)
Tsukayama, M. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 136 (*synth*)
Shibuya, Y. *et al., Z. Naturforsch., C*, 1991, **46**, 513 (*glucosides*)

2′,4′,5,7-Tetrahydroxy-6-prenylisoflavone T-276

[41743-56-0]
*3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Luteone***†

$C_{20}H_{18}O_6$ 354.359
Constit. of *Lupinus* spp.. Pale yellow plates (MeOH). Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 225-227°. λ_{max} 266 (ϵ 28300); 290 (ϵ 14100) (MeOH) (Berdy). λ_{max} 223 ; 279 ; 337 (MeOH-NAOH) (Berdy).

*7-*O*-β-*D*-Glucopyranoside:* [137351-15-6]
$C_{26}H_{28}O_{11}$ 516.501
Isol. from the roots of *Lupinus albus*

(white lupin).

4′-Me ether: [129145-52-4] *2′,5,7-Trihydroxy-4′-methoxy-6-prenylisoflavone.* ***Gancaonin N***
$C_{21}H_{20}O_6$ 368.385
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Prisms (Me_2CO/C_6H_6/hexane). Mp 159-162°.

2′,4′,7-Tri-Me ether:
Mp 134-135°.

[91681-62-8]

Harborne, J.B. *et al., Phytochemistry*, 1976, **15**, 1485 (*occur*)
Jain, A.C. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 611; 613 (*struct, synth*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1980, **35**, 197; 1983, **38**, 194 (*isol*)
Hashidoko, Y. *et al., Agric. Biol. Chem.*, 1986, **50**, 1797 (*isol, pmr*)
Fukai, T. *et al., Heterocycles*, 1990, **31**, 373 (*Gancaonin N*)
Shibuya, Y. *et al., Z. Naturforsch., C*, 1991, **46**, 513 (*7-glucoside*)

2′,4′,5,7-Tetrahydroxy-8-prenylisoflavone T-277

[74161-25-4]
2,3-Dehydrokievitone

$C_{20}H_{18}O_6$ 354.359
Isol. from *Phaseolus lunatus* (butter bean) and *Phaseolus vulgaris* (kidney bean). λ_{max} 265 (MeOH) (Berdy). λ_{max} 281 (MeOH/NaOH) (Berdy).

► LD_{50} (mus, ivn) .83 mg/kg , LD_{50} (mus, ipr) 3.2 mg/kg. DJ2982700

5-Me ether: [104703-88-0] *2′,4′,7-Trihydroxy-5-methoxy-8-prenylisoflavone.* ***Barpisoflavone B***
$C_{21}H_{20}O_6$ 368.385
Pale yellow plates. Mp 208-210°.

4″-Hydroxy: [104363-17-9] *2′,4′,5,7-Tetrahydroxy-8-(4-hydroxy-3-methyl-2-butenyl)isoflavone.* ***2,3-Dehydrokievitol***
$C_{20}H_{18}O_7$ 370.358
Isol. from *Phaseolus lunatus* (butter bean) induced with aq. $CuCl_2$.

2″,3″-Dihydro, 3″-hydroxy: [104691-93-2] *2′,4′,5,7-Tetrahydroxy-8-(3-hydroxy-3-methylbutyl)isoflavone.* ***2,3-Dehydrokievitone hydrate***
$C_{20}H_{20}O_7$ 372.374
Yellow needles. Mp 134-136°.

Woodward, M.D. *et al., Phytochemistry*, 1979, **18**, 2007 (*isol*)
O'Neill, M.J. *et al., Z. Naturforsch., C*, 1983, **38**, 693 (*isol*)
Hashidoko, Y. *et al., Agric. Biol. Chem.*, 1986, **50**, 1797 (*2,3-Dehydrokievitone hydrate*)
Tahara, S. *et al., Agric. Biol. Chem.*, 1986, **50**, 1809 (*Barpisoflavone B*)
O'Neill, M.J. *et al., Phytochemistry*, 1986, **25**, 1315 (*2,3-Dehydrokievitol*)
Tsukayama, M. *et al., Chem. Lett.*, 1994, 2101 (*synth*)

2′,4′,6′,7-Tetrahydroxy-3′-prenylisoflavone T-278

*7-Hydroxy-3-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one*

$C_{20}H_{18}O_6$ 354.359

2′-Me ether: [161099-37-2] *2′,4′,7-Trihydroxy-6′-methoxy-3′-prenylisoflavone.* ***Glicoricone***
$C_{21}H_{20}O_6$ 368.385
Constit. of *Glycyrrhiza* sp.. Needles $+\frac{1}{2}H_2O$. Mp 192°. λ_{max} 209 (log ϵ 4.55); 240 (sh) (log ϵ 4.27); 247 (log ϵ 4.24); 285 (log ϵ 4.02); 305 (sh) (log ϵ 3.94) (MeOH).

2′,4′-Di-Me ether: [51847-92-8] *2′,7-Dihydroxy-4′,6′-dimethoxy-3′-prenylisoflavone.* ***Licoricone***
$C_{22}H_{22}O_6$ 382.412
Constit. of the root of *Glycyrrhiza uralensis* (Chinese licorice). Mp 250-251°. Log P 3.77 (calc).

Tetra-Me ether:
Mp 179.5-181°.

Kaneda, M. *et al., Acta Cryst. B*, 1973, **29**, 2827 (*cryst struct*)
Kaneda, M. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1338 (*isol, struct*)
Saitoh, T. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1242 (*isol*)
Tsukayama, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2369 (*synth*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1238-1243 (*Glicoricone*)

3′,4′,5,7-Tetrahydroxy-6-prenylisoflavone T-279

[66777-71-7]
*3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one*

$C_{20}H_{18}O_6$ 354.359

3′-Me ether: [85966-81-0] *4′,5,7-Trihydroxy-3′-methoxy-6-prenylisoflavone.* ***Lupisoflavone***
$C_{21}H_{20}O_6$ 368.385
Sol. MeOH, EtOAc. Not to be confused with Lupinisoflavones λ_{max} 269 (MeOH) (Berdy). λ_{max} 281 (MeOH-NaOH) (Berdy).

4′-Me ether: [124596-86-7] *3′,5,7-Trihydroxy-4′-methoxy-6-prenylisoflavone.* ***Gancaonin B***
$C_{21}H_{20}O_6$ 368.385
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow prisms (C_6H_6). Mp 206-209°.

3′,4′-Methylene ether: [22044-58-2] *3′,4′-Methylenedioxy-6-prenylisoflavone.* ***Derrubone***
$C_{21}H_{18}O_6$ 366.37
Yellow prisms (MeOH). Mp 210-212°.

3′,4′-Methylene ether, 5,7-di-Ac:
Needles (MeOH). Mp 204-206°.

East, A.J. *et al., J.C.S.(C)*, 1969, 365 (*isol, struct, Derrubone*)
Jain, A.C. *et al., Tetrahedron*, 1972, **28**, 5063 (*synth, Derrubone*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1983, **28**, 194 (*Lupisoflavone*)
McCormick, S. *et al., Phytochemistry*, 1986, **25**, 1723 (*Lupisoflavone, isol*)
Fukai, T. *et al., Heterocycles*, 1989, **29**, 1369; 1761 (*Gancaonin B*)

3′,4′,5,7-Tetrahydroxy-8-prenylisoflavone T-280

[129145-50-2]
*3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Gancaonin L***

$C_{20}H_{18}O_6$ 354.359
Isol. from the aerial parts of *Glycyrrhiza uralensis* (Chinese licorice). Prisms (Me_2CO/hexane). Mp 189-192°.

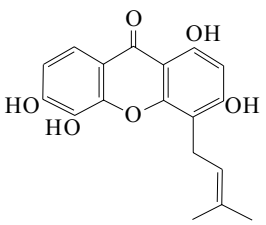
3′-Me ether: [120727-35-7] *4′,5,7-Trihydroxy-3′-methoxy-8-prenylisoflavone*
$C_{21}H_{20}O_6$ 368.385

2″,3″-Dihydro, 3″-hydroxy, 3′,4′-di-Me ether, 7-O-β-D-glucopyranoside:
$C_{28}H_{34}O_{12}$ 562.569
Constit. of soybean molasses (*Glycine* sp.). Amorph. yellow powder. $[\alpha]_D^{20}$ +6.1 (c, 0.54 in Py aq.). λ_{max} 234 (log ϵ 4.51); 282 (log ϵ 4.33) (MeOH).

Fukai, T. *et al., Heterocycles*, 1989, **29**, 1369; 1990, **31**, 373 (*isol, pmr, cmr*)
Bohm, B.A. *et al., Phytochemistry*, 1989, **28**, 501 (*3′-Me ether*)
Hosny, M. *et al., J. Nat. Prod.*, 1999, **62**, 853-858 (*Glycine glucoside*)

1,3,5,6-Tetrahydroxy-4-prenylxanthone T-281

[13179-11-8]
*1,3,5,6-Tetrahydroxy-4-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, 9CI.* ***Ugaxanthone***



$C_{18}H_{16}O_6$ 328.321
Constit. of *Garcinia dulcis* (mundu). Pale yellow cryst. λ_{max} 242 ; 312 (MeOH).

3-Me ether:1,5,6-Trihydroxy-3-methoxy-4-prenylxanthone. ***Dulxanthone A***
$C_{19}H_{18}O_6$ 342.348
Constit. of the stem bark of *Garcinia dulcis* (mundu). Yellow powder. λ_{max} 236 (sh) ; 253 ; 285 ; 328 (MeOH).

5-Me ether:1,3,6-Trihydroxy-5-methoxy-4-prenylxanthone
$C_{19}H_{18}O_6$ 342.348
Yellow powder. λ_{max} 242 ; 322 ; 362 (MeOH).

3,5,6-Tri-Me ether:1-Hydroxy-3,5,6-trimethoxy-4-prenylxanthone
$C_{21}H_{22}O_6$ 370.401
Pale yellow cryst. Mp 162°.

Burling, E.D. *et al., Tetrahedron*, 1965, **21**, 2653 (*synth*)
Locksley, H.D. *et al., J.C.S.(C)*, 1966, 2265 (*isol*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1403-1413 (*isol, Dulxanthone A*)
Wu, Q.-L. *et al., Phytochemistry*, 1998, **49**, 1395-1402 (*isol, uv, ir, pmr, cmr, ms*)
Gonda, R. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1219-1222 (*5-Me ether*)

1,3,5,8-Tetrahydroxy-2-prenylxanthone T-282

[127716-76-1]
1,3,5,8-Tetrahydroxy-2-(3-methyl-2-butenyl)xanthone. ***Morusignin B***

$C_{18}H_{16}O_6$ 328.321
Constit. of *Morus insignis* (mangosteen). Yellow needles (hexane/Me_2CO). Mp 259-261°.

3-Me ether: [110187-11-6] *1,5,8-Trihydroxy-3-methyl-2-prenylxanthone*
$C_{19}H_{18}O_6$ 342.348
Constit. of *Garcinia mangostana* (mangosteen). Cryst. Mp 193-195°.

3,5-Di-Me ether: [132031-40-4] *1,8-Dihydroxy-3,5-dimethoxy-2-prenylxanthone*
$C_{20}H_{20}O_6$ 356.374
Constit. of *Garcinia mangostana* (mangosteen). Yellow needles (MeOH). Mp 178-181°.

Perveen, M. *et al., Phytochemistry*, 1988, **27**, 3695
Hano, Y. *et al., Heterocycles*, 1990, **31**, 1345 (*Morusignin B*)
Bennett, G.J. *et al., J.C.S. Perkin 1*, 1990, 2671

1,4,5,6-Tetrahydroxy-7-prenylxanthone T-283

1,4,5,6-Tetrahydroxy-7-(3-methyl-2-butenyl)-9H-xanthen-9-one, 9CI

$C_{18}H_{16}O_6$ 328.321

5-Me ether: [160623-47-2] *1,4,6-Trihydroxy-5-methoxy-7-prenylxanthone*
$C_{19}H_{18}O_6$ 342.348
Constit. of the branches of *Garcinia dulcis* (mandu).

Harrison, L.J. *et al., Nat. Prod. Lett.*, 1994, **5**, 111

2,3,6,8-Tetrahydroxy-1-prenylxanthone T-284

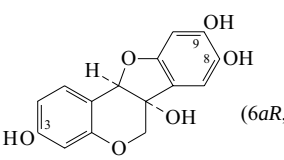
[70786-45-7]
2,3,6,8-Tetrahydroxy-1-(3-methyl-2-butenyl)-9H-xanthen-9-one, 9CI. 1-(3,3-Dimethylallyl)-2,3,6,8-tetrahydroxyxanthone

$C_{18}H_{16}O_6$ 328.321
Yellow cryst. (C_6H_6/Me_2CO). Mp 203-206°.

2-Me ether:3,6,8-Trihydroxy-2-methoxy-1-prenylxanthone. ***Dulxanthone D***
$C_{19}H_{18}O_6$ 342.348
Constit. of the stem bark of *Garcinia dulcis* (mundu). Yellow powder. λ_{max} 241 ; 252 ; 312 ; 350 (MeOH).

Nielsen, H. *et al., J. Nat. Prod.*, 1979, **42**, 301 (*isol*)
Ishiguro, K. *et al., Phytochemistry*, 1995, **38**, 867 (*isol, pmr, cmr*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1403-1413 (*Dulxanthone D*)

3,6*a*,8,9-Tetrahydroxypterocarpan T-285



(6*aR*,11*aR*)-form

$C_{15}H_{12}O_6$ 288.256

(6aR,11aR)-form

8,9-Methylene ether: [14602-93-8] *3,6a-Dihydroxy-8,9-methylenedioxypterocarpan.* ***6a-Hydroxymaackiain.*** *6a-Hydroxyinermin*
$C_{16}H_{12}O_6$ 300.267
Isol. from leaves of *Trifolium pratense* (red clover) as a phytoalexin. Mp 178-181° dec. $[\alpha]_D^{21}$ +337 (c, 0.944 in EtOH).

3-Me, 8,9-methylene ether: [469-01-2]

[20186-22-5] *6a-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan.* ***Pisatin***
$C_{17}H_{14}O_6$ 314.294
Stress metab. from *Pisum sativum* (pea) and *Trifolium pratense* (red clover). Cryst. (EtOH or C_6H_6). Sol. MeOH, CCl_4, CS_2, Et_2O; fairly sol. H_2O, hexane. Mp 61°. $[\alpha]_D^{20}$ +280 (c, 0.11 in EtOH). λ_{max} 213 (ε 56230); 280 (ε 4170); 282 ; 286 (ε 4800); 287 ; 309 (ε 7244); 310 (MeOH) (Berdy). λ_{max} 286 (ε 4800); 309 (ε 7250) (EtOH) (Berdy).

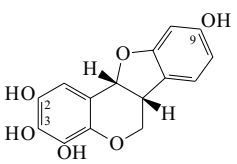
(±)-form

3-Me, 8,9-methylene ether:
Mp 188-190°.

[61218-44-8, 73068-87-8]

Perrin, D.R. *et al., J.A.C.S.*, 1962, **84**, 1919; 1922 (*isol*)
Bevan, C.W.L. *et al., J.C.S.*, 1964, 5991 (*synth*)
Fukui, K. *et al., Tet. Lett.*, 1966, 1805 (*synth*)
Kelsey, T.C. *et al., Phytochemistry*, 1975, **14**, 1103 (*isol, struct*)
Bilton, J.N. *et al., Phytochemistry*, 1976, **15**, 1411 (*isol*)
de Martinis, C. *et al., J. Cryst. Mol. Struct.*, 1978, **8**, 247 (*struct*)
Ingham, J.L. *et al., Phytochemistry*, 1980, **19**, 1203 (*abs config*)
Banks, S.W. *et al., Phytochemistry*, 1982, **21**, 1605; 2235; 1983, **22**, 1591 (*biosynth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*occur*)
Mori, K. *et al., Annalen*, 1989, 35 (*synth*)
Pinard, E. *et al., Tet. Lett.*, 1998, **39**, 2739-2742 (*synth*)

2,3,4,9-Tetrahydroxypterocarpan T-286



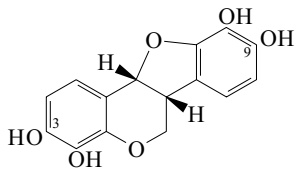
Absolute configuration

$C_{15}H_{12}O_6$ 288.256

2,3,9-Tri-Me ether: [56841-82-8] *4-Hydroxy-2,3,9-trimethoxypterocarpan. 6a,11a-Dihydro-2,3,9-trimethoxy-6H-benzofuro[3,2-c][1]benzopyran-4-ol, 9CI*
$C_{18}H_{18}O_6$ 330.337
Isol. from *Pisum sativum* (pea). Needles (Me_2CO aq.). Mp 141-145°. $[\alpha]_D^{23}$ -185 (EtOH).

Pueppke, S.G. *et al., J.C.S. Perkin 1*, 1975, 946 (*isol*)

3,4,9,10-Tetrahydroxypterocarpan T-287



$C_{15}H_{12}O_6$ 288.256

3,9-Di-Me ether: [83013-81-4] *4,10-Dihydroxy-3,10-dimethoxypterocarpan.* ***Melilotocarpan D***
$C_{17}H_{16}O_6$ 316.31
From *Melilotus alba* (white melilot). Needles (MeOH). Mp 161-162.5°. $[\alpha]_D^{23}$ -210 (c, 1.0 in dioxan).

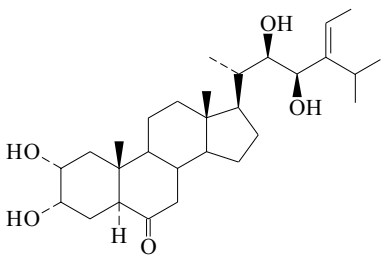
3,10-Di-Me ether: [83013-80-3] *4,9-Dihydroxy-3,10-dimethoxypterocarpan.* ***Melilotocarpan E***
$C_{17}H_{16}O_6$ 316.31
From *Melilotus alba* (white melilot). Needles ($CHCl_3$/MeOH). Mp 197-199°. $[\alpha]_D^{22}$ -169 (c, 3.51 in dioxan).

3,4,9-Tri-Me ether: [101153-42-8] *10-Hydroxy-3,4,9-trimethoxypterocarpan.* ***Odoricarpan***
$C_{18}H_{18}O_6$ 330.337

3,9,10-Tri-Me ether: [83013-82-5] *4-Hydroxy-3,9,10-trimethoxypterocarpan.* ***Melilotocarpan C***
$C_{18}H_{18}O_6$ 330.337
From *Melilotus alba* (white melilot). Needles (Me_2CO). Mp 160-162.5°. $[\alpha]_D^{18}$ -219 (c, 1.40 in dioxan).

Miyase, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1986 (*Melilotocarpans*)
Goda, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 5606; 1992, **40**, 2452 (*Odoricarpan*)

2,3,22,23-Tetrahydroxystigmast-24(28)-en-6-one T-288



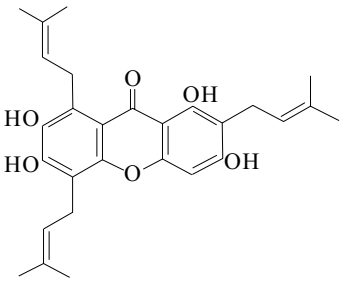
$C_{29}H_{48}O_5$ 476.695
λ_{max} 280 (ε 10230); 310 (ε 1860) (EtOH) (Berdy).

(2α,3α,5α,22R,23R)-form [85797-14-4] ***Homodolichosterone***
Constit. of *Dolichos lablab* (hyacinth bean) seed. Cryst. (MeOH/$CHCl_3$). Mp 225-226° (204-208°) Mp 222° (sinters). $[\alpha]_D^{22}$ -9.8 (c, 0.598 in $CHCl_3$).

Yokota, T. *et al., Agric. Biol. Chem.*, 1984, **48**, 2529 (*isol, hplc*)
Sakakibara, M. *et al., Agric. Biol. Chem.*, 1984, **48**, 745 (*synth*)
Mori, K. *et al., Tetrahedron*, 1984, **40**, 1767 (*synth*)

1,3,6,7-Tetrahydroxy-2,5,8-triprenylxanthone T-289

[112649-21-5]
Garcinone E

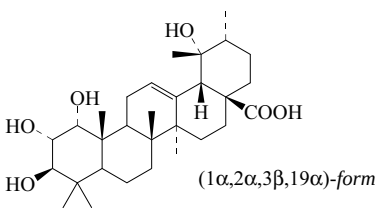


$C_{28}H_{32}O_6$ 464.557
Constit. of the fruit of *Garcinia mangostana* (mangosteen). Yellow cryst. (EtOAc/hexane). Mp 152.5-155.5°.

7-Me ether: [194090-67-0] *1,3,6-Trihydroxy-7-methoxy-2,5,8-triprenylxanthone.* ***7-O-Methylgarcinone E***
$C_{29}H_{34}O_6$ 478.584
Yellow powder. λ_{max} 244 (log ϵ 4.44); 260 (log ϵ 4.37); 320 (log ϵ 4.32); 362 (log ϵ 3.9) (MeOH).

Sakai, S. *et al., Chem. Pharm. Bull.*, 1993, **41**, 958-960 (*isol, pmr, cmr*)
Likhitwitayawuid, K. *et al., Phytochemistry*, 1997, **45**, 1299-1301 (*7-O-Methylgarcinone E*)
Ho, C.-K. *et al., Planta Med.*, 2002, **68**, 975-979 (*isol, activity*)

1,2,3,19-Tetrahydroxy-12-ursen-28-oic acid T-290



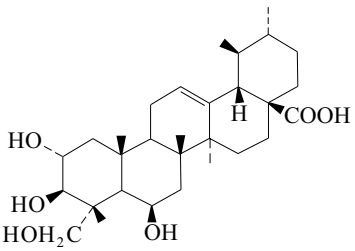
(1α,2α,3β,19α)-*form*

$C_{30}H_{48}O_6$ 504.706
(1β,2α,3β,19α)-*form*

*28-*O*-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranosyl] ester:* [211944-25-1]
$C_{42}H_{68}O_{16}$ 828.99
Constit. of *Acorus calamus* (sweet flag). Cryst. ($CHCl_3$). Mp 94°.

Rai, R. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 473-476 (*Acorus calamus saponin*)

2,3,6,23-Tetrahydroxy-12-ursen-28-oic acid T-291



$C_{30}H_{48}O_6$ 504.706
(2α,3β,6β)-*form* [18449-41-7]
Madecassic acid. *Brahmic acid. 6β-Hydroxyasiatic acid*
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. (MeOH). Mp 285-288° Mp 293°. $[\alpha]_D$ +31 (c, 1.5 in MeOH). Isobrahmic acid was a mixt..

*28-*O*-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [386223-75-2]
Centellasaponin B
$C_{42}H_{68}O_{16}$ 828.99
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. ($CHCl_3$/MeOH). Mp 223-224°. $[\alpha]_D^{25}$ +13.2 (c, 0.3 in MeOH).

*28-*O*-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [34540-22-2]

[17669-86-2] ***Madecassoside***. *Asiaticoside A*
$C_{48}H_{78}O_{20}$ 975.132
Isol. from whole plants of *Centella asiatica* (Ji Xue Cao). Cryst. (butanol). Mp 220-223°. $[\alpha]_D$ -19 (c, 2 in H_2O).

*3-*O*-α-L-Arabinopyranoside:* [325687-48-7]
$C_{35}H_{56}O_{10}$ 636.821

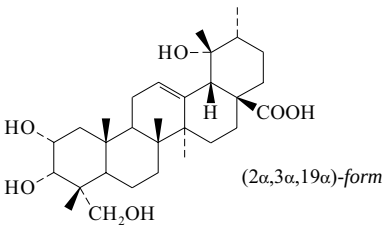
Triglycoside: ***Brahmoside***
$C_{47}H_{78}O_{19}$ 947.122
Isol. from whole plants of *Centella asiatica* (Ji Xue Cao). Needles. Mp 242-246°. $[\alpha]_D^{32}$ -38 (c, 0.71 in Py). Acid hydrol. yields glucose, arabinose and rhamnose (1:1:1).

Tetraglycoside: ***Brahminoside***
$C_{53}H_{88}O_{24}$ 1109.264
Isol. from *Centella asiatica* (Asiatic pennywort). Cryst. Mp 221-223°. $[\alpha]_D^{32}$ -19 (c, 0.7 in Py). Acid hydrol. yields glucose, arabinose and rhamnose (2:1:1).

Me ester: [23140-81-0]
Mp 210-213°.

Rastogi, R.P. *et al., Indian J. Chem.*, 1963, **1**, 267-269 (*Brahmoside, Brahminoside*)
Pinhas, H. *et al., Bull. Soc. Chim. Fr.*, 1967, 1888-1890; 1890-1895 (*Madecassic acid, Madecassoside*)
Singh, B. *et al., Phytochemistry*, 1968, **7**, 1385-1393 (*Brahmic acid*)
Luo, S. *et al., Zhongcaoyao*, 1981, **12**, 5-6 (*Madecassoside*)
Sahu, N.P. *et al., Phytochemistry*, 1989, **28**, 2852-2854 (*Asiaticoside A*)
Shukla, Y.N. *et al., Pharm. Biol.*, 2000, **38**, 262-267 (*arabinoside*)
Matsuda, H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1368-1371 (*Centellasaponin B*)

2,3,19,23-Tetrahydroxy-12-ursen-28-oic acid T-292



(2α,3α,19α)-*form*

$C_{30}H_{48}O_6$ 504.706
(2α,3α)-*form* [89786-84-5]
Myrianthic acid
Constit. of *Coleus amboinicus* (Cuban oragano). Mp 126° (as Me ester). $[\alpha]_D^{17}$ +25.3 (c, 1.05 in MeOH). Revised struct., originally considered to be 24-hydroxy.

(2α,3β)-*form* [70868-78-9]
23-Hydroxytormentic acid
Constit. of *Quercus ilex* (holly oak). Cryst. (EtOH). Mp 283-285°. $[\alpha]_D^{20}$ +27.9 (c, 0.54 in MeOH).

α-D-Glucopyranosyl ester: [87340-30-5]
Quercilicoside A
$C_{36}H_{58}O_{11}$ 666.848
Constit. of *Quercus ilex* (holly oak). Cryst. (EtOH aq.). Mp 247° dec.

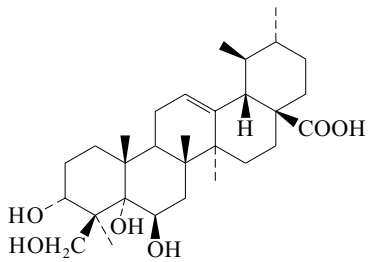
*23-(4-Hydroxy-*E*-cinnamoyl):* [144604-14-8] ***23-trans-p-Coumaroyloxytormentic acid***
$C_{39}H_{54}O_8$ 650.851
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ +18.2 (c, 1 in MeOH). Incorrectly named as 23-*trans*-*p*-Coumaroyltormentic acid in ref..

23-(4-Hydroxy-Z-cinnamoyl): [144604-15-9] ***23-cis-p-Coumaroyloxytormentic acid***
$C_{39}H_{54}O_8$ 650.851
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ +13.3 (c, 1 in MeOH). Incorrectly named as 23-*cis*-*p*-Coumaroyltormentic acid in ref..

[65669-84-3, 82843-98-9]

Teresa, J. de P. *et al., An. Quim.*, 1979, **75**, 135
Higuchi, R. *et al., Phytochemistry*, 1982, **21**, 907
Romussi, G. *et al., Annalen*, 1983, 1448
Seto, T. *et al., Phytochemistry*, 1984, **23**, 2829 (*isol, pmr, cmr*)
Gao, I. *et al., Chem. Pharm. Bull.*, 1985, **33**, 37 (*cmr*)
Gopalsamy, N. *et al., Phytochemistry*, 1988, **27**, 3593 (*deriv*)
Kojima, H. *et al., Phytochemistry*, 1989, **28**, 1703 (*pmr, struct*)
Gupta, D. *et al., Phytochemistry*, 1990, **29**, 1945 (*isol, pmr, cmr*)
De Tommasi, N. *et al., J. Nat. Prod.*, 1992, **55**, 1067 (*p-coumaroyl esters*)
Reher, G. *et al., Phytochemistry*, 1992, **31**, 3909 (*deriv*)
Kamperdick, C. *et al., Z. Naturforsch., C*, 1997, **52**, 295-300 (*Myrianthic acid, pmr, cmr*)
Hirai, N. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1707-1712 (*Myrianthic acid, isol, activity*)

3,5,6,24-Tetrahydroxy-12-ursen-28-oic acid T-293

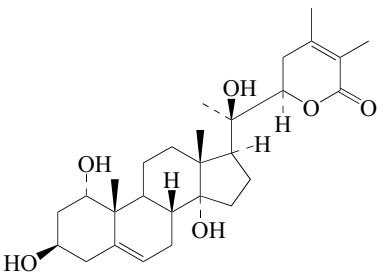


$C_{30}H_{48}O_6$ 504.706

(3α,5α,6β)-*form* [22882-19-5]
Isothankunic acid
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. Mp 288-290°. $[\alpha]_D^{30}$ +23.9 ($CHCl_3$).

Dutta, T. *et al., Indian J. Chem.*, 1968, **6**, 543-545 (*isol*)

1,3,14,20-Tetrahydroxywitha-5,24-dienolide T-294



$C_{28}H_{42}O_6$ 474.636

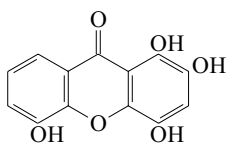
(1α,3β,14α,20*R*,22*R*)-*form*

3-O-*β*-D-*Glucopyranoside, 1-Ac:* [227179-07-9]
$C_{36}H_{54}O_{12}$ 678.815
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. powder. $[\alpha]_D^{25}$ +16.5 (c, 0.49 in MeOH). λ_{max} 228 (log ε 3.89) (MeOH).

Ahmad, S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 477-480 (*isol, pmr, cmr*)

1,2,4,5-Tetrahydroxyxanthone T-295

*1,2,4,5-Tetrahydroxy-9*H*-xanthen-9-one*



$C_{13}H_8O_6$ 260.203

1-Me ether: [115713-07-0] *2,4,5-Trihydroxy-1-methoxyxanthone.* ***BR-Xanthone B***
$C_{14}H_{10}O_6$ 274.229
Constit. of the dry fruit hulls of *Garcinia mangostana* (mangosteen). Greenish-yellow cryst. Mp 308-310°.

Balasubramanian, K. *et al., Phytochemistry*, 1988, **27**, 1552

1,3,5,6-Tetrahydroxyxanthone T-296

[5084-31-1]
*1,3,5,6-Tetrahydroxy-9*H*-xanthen-9-one, 9CI*

$C_{13}H_8O_6$ 260.203
Cryst. (Py aq.). Mp 320° (357°) dec. λ_{max} 250 (ε 42500); 283 (ε 9900); 324 (ε 20700) (MeOH) (Berdy).

5-Me ether: [41357-84-0] *1,3,6-Trihydroxy-5-methoxyxanthone*
$C_{14}H_{10}O_6$ 274.229
Constit. of *Garcinia dulcis* (mundu). Pale yellow needles (MeOH). Mp 290-291°.

Ghosal, S. *et al., J. Pharm. Sci.*, 1973, **62**, 137-138 (*5-Me ether*)

1,3,6,7-Tetrahydroxyxanthone T-297

[3542-72-1]
*1,3,6,7-Tetrahydroxy-9*H*-xanthen-9-one, 9CI.* ***Mangiferitin****. Norathyriol*

$C_{13}H_8O_6$ 260.203
Yellow-brown needles. Mp 270° dec. (323°).

1-O-*(6-Deoxy-β-*D*-glucopyranoside):* [104669-03-6] ***Gymnocarposide****. Norathyriol 1-quinovoside*
$C_{19}H_{18}O_{10}$ 406.345
Mp 263-265°. $[\alpha]_D$ -73.

6-O-*β*-D-*Glucopyranoside:* [82855-00-3] ***Tripteroside***
$C_{19}H_{18}O_{11}$ 422.345
Pale yellow needles (MeOH). Mp 263-265°.

3-Me ether: [28283-84-3] *1,6,7-Trihydroxy-3-methoxyxanthone.* ***Athyriol***
$C_{14}H_{10}O_6$ 274.229
Yellow-brown needles. Mp 300° dec.

6-Me ether: [59092-97-6] *1,3,7-Trihydroxy-6-methoxyxanthone.* ***Isoathyriol***
$C_{14}H_{10}O_6$ 274.229
Mp 325°.

7-Me ether: [67370-97-2] *1,3,6-Trihydroxy-7-methoxyxanthone.* ***Alloathyriol***
$C_{14}H_{10}O_6$ 274.229
Constit. of *Garcinia dulcis* (mundu). Pale yellow-brown needles (EtOH aq.). Mp 304° dec.

7-Me ether, 6-O-*[α-*L*-rhamnopyranosyl-(1→2)-β-*D*-glucopyranoside]:* ***Polygalaxanthone V***
$C_{26}H_{30}O_{15}$ 582.514
Yellow powder. Mp 232-235°. $[\alpha]_D^{23}$ -81.7 (c, 0.7 in MeOH). λ_{max} 238 (log ε 4.34); 256 (log ε 4.38); 309 (log ε 4.03); 360 (log ε 4) (MeOH).

7-Me ether, 3,6-di-Ac: [64767-74-4] ***Laxanthone II***
$C_{18}H_{14}O_8$ 358.304
Mp 180-181°.

1,3-Di-Me ether:6,7-Dihydroxy-1,3-dimethoxyxanthone
$C_{15}H_{12}O_6$ 288.256
Yellow needles (CH_2Cl_2/MeOH). Mp >300° λ_{max} 240 (sh) (log ε 4.11); 303 (log ε 3.84); 350 (log ε 3.78); 400 (sh) (log ε 2.85) (MeOH).

1,7-Di-Me ether:3,6-Dihydroxy-1,7-dimethoxyxanthone
$C_{15}H_{12}O_6$ 288.256
Yellow powder. Mp 251-252° dec. λ_{max} 212 (log ε 4.17); 250 (log ε 4.03); 302 (log ε 3.65); 348 (log ε 3.61) (MeOH).

3,6-Di-Me ether: [42833-92-1] *1,7-Dihydroxy-3,6-dimethoxyxanthone*
$C_{15}H_{12}O_6$ 288.256
Yellow needles (MeOH). Mp 237-240°.

3,7-Di-Me ether: [69618-09-3] *1,6-Dihydroxy-3,7-dimethoxyxanthone*
$C_{15}H_{12}O_6$ 288.256
Yellow needles (EtOH). Mp 264-265°.

3,7-Di-Me ether, 6-O-*[α-*L*-rhamnopyranosyl-(1→2)-β-*D*-glucopyranoside]:* ***Polygalaxanthone IV***
$C_{27}H_{32}O_{15}$ 596.541
Yellow powder. Mp 273-275°. $[\alpha]_D^{23}$ -60 (c, 0.7 in MeOH). λ_{max} 237 (log ε 4.35); 256 (log ε 4.38); 309 (log ε 4.02); 361 (log ε 4.02) (MeOH).

3,7-Di-Me ether, 6-Ac: [69618-06-0] ***Laxanthone III***
$C_{17}H_{14}O_7$ 330.293
Yellow needles (EtOAc/petrol). Mp 210-211°.

6,7-Di-Me ether: [34318-15-5] *1,3-Dihydroxy-6,7-dimethoxyxanthone.* ***Laxanthone I***
$C_{15}H_{12}O_6$ 288.256
Mp 286-287°.

1,3,7-Tri-Me ether: [72991-50-5] *6-Hydroxy-1,3,7-trimethoxyxanthone*
$C_{16}H_{14}O_6$ 302.283
Yellow cryst. (EtOH). Mp 274-276°.

3,6,7-Tri-Me ether: [2054-36-6] *1-Hydroxy-3,6,7-trimethoxyxanthone*
$C_{16}H_{14}O_6$ 302.283
Yellow cryst. (MeOH). Mp 219.5-221° (232-233°).

Tetra-Me ether: [3542-74-3] *1,3,6,7-Tetramethoxyxanthone*
$C_{17}H_{16}O_6$ 316.31
Cream solid. Mp 210-212°.

Yates, P. *et al., J.A.C.S.*, 1958, **80**, 1691 (*synth*)
Ueno, A. *et al., Yakugaku Zasshi*, 1962, **82**, 1482; 1486 (*isol*)
Quillinan, A.J. *et al., J.C.S. Perkin 1*, 1973, 1329 (*synth*)
Owen, P.J. *et al., J.C.S. Perkin 1*, 1974, 1018 (*isol*)
Hj Idris, M.S.B. *et al., J.C.S. Perkin 1*, 1977, 2158 (*synth*)
Bhardwaj, D.K. *et al., Phytochemistry*, 1977, **16**, 1616; 1978, **17**, 1440 (*Laxanthones*)
Bhardwaj, D.K. *et al., Curr. Sci.*, 1978, **47**, 336 (*Alloathyriol*)
Miura, I. *et al., Nouv. J. Chim.*, 1978, **2**, 653 (*cmr*)
Bhardwaj, D.K. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 288 (*synth, derivs*)
Murakami, T. *et al., Yakugaku Zasshi*, 1986, **106**, 378 (*Gymnocarposide*)
Lin, C.-N. *et al., Phytochemistry*, 1989, **21**, 948 (*Tripteroside*)
Ikeya, Y. *et al., Phytochemistry*, 1991, **30**, 2061 (*isol, derivs*)
Fujita, T. *et al., Phytochemistry*, 1992, **31**, 3997-4000 (*tetra-Me ether*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1744 (*Alloathyriol*)
Lin, C.N. *et al., J. Pharm. Pharmacol.*, 1996, **48**, 532 (*Mangiferitin, activity*)
Chung, M.-I. *et al., J. Nat. Prod.*, 1999, **62**, 1033-1035 (*1,3-di-Me ether*)
Hu, L. *et al., Phytochemistry*, 1999, **52**, 1371-1373 (*3,6-Dihydroxy-1,7-dimethoxyxanthone*)

Jiang, Y. *et al., Phytochemistry*, 2002, **60**, 813-816 (*Polygalaxanthones IV,V*)

1,4,5,7-Tetrahydroxyxanthone T-298

*1,4,5,7-Tetrahydroxy-9*H*-xanthen-9-one, 9CI*

$C_{13}H_8O_6$ 260.203

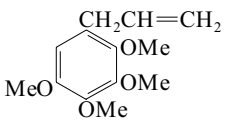
1,4,5-Tri-Me ether:7-Hydroxy-1,4,5-trimethoxyxanthone
$C_{16}H_{14}O_6$ 302.283
Mp 257°.

*1,4,5-Tri-Me ether, 7-*O*-[β-*D*-glucopyranosyl-(1→2)-β-*D*-galactopyranoside]:* [258885-35-7]
$C_{28}H_{34}O_{16}$ 626.567
Constit. of the rhizomes of *Acorus calamus* (sweet flag). Cryst. (EtOAc). Mp 270°. λ_{max} 220 ; 240 ; 255 ; 265 ; 360 (MeOH).

Rai, R. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1143-1144

1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene T-299

[15361-99-6]
1-Allyl-2,3,4,5-tetramethoxybenzene

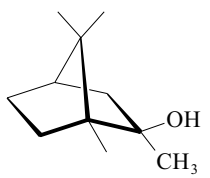


$C_{13}H_{18}O_4$ 238.283
Isol. from parsley oil and other *Petroselinum* spp.. Tablets (EtOH aq.). Mp 25°. Bp_{12} 145°.

Baker, W. *et al., J.C.S.*, 1934, 1681
Shulgin, A.T. *et al., J. Chromatogr.*, 1967, **30**, 54 (*isol, synth*)
Brophy, J.J. *et al., J. Essent. Oil Res.*, 1992, **4**, 315

1,2,7,7-Tetramethylbicyclo[2.2.1]heptan-2-ol, 9CI T-300

1,2,7,7-Tetramethylnorbornan-2-ol, 8CI. 2-Methyl-2-bornanol. 2-Methylisoborneol



$C_{11}H_{20}O$ 168.278

(1R,2R)-form
Found in polluted water, causes objectionable odour of water supplies. Implicated in off-flavour of freshwater fish and shellfish. Mp 170°. $[\alpha]_D^{20}$ -11.8 (c, 10 in EtOH).

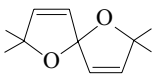
4-Nitrobenzoyl: [13389-79-2]
Mp 138°.

[2371-42-8, 28405-88-1, 68330-44-9]

Capmau, M.L. *et al., Bull. Soc. Chim. Fr.*, 1968, 3233 (*synth*)
Toivonen, H. *et al., Tet. Lett.*, 1968, 3041 (*synth*)
Gerber, N.N. *et al., J. Antibiot.*, 1969, **22**, 508 (*isol*)
Gerber, N.N. *et al., J. Chem. Ecol.*, 1977, **3**, 475
Wood, N.F. *et al., J. Chromatogr.*, 1977, **132**, 405
Croteau, R. *et al., J. Nat. Prod.*, 1981, **44**, 261 (*biosynth*)
Kimura, T. *et al., Appl. Environ. Microbiol.*, 1982, **43**, 654 (*isol*)
Karahadian, C. *et al., J. Agric. Food Chem.*, 1985, **33**, 339
Toyota, M. *et al., Phytochemistry*, 1990, **29**, 2334 (*isol, pmr, cmr, synth*)
Conte, E.D. *et al., J. Agric. Food Chem.*, 1996, **44**, 829-835 (*occur, anal*)

2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene T-301

[15129-55-2]



$C_{11}H_{16}O_2$ 180.246
Constit. of hops. Oil. Bp_{11} 74-76°.

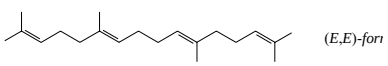
Dihydro: [15031-05-7] *2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]non-3-ene*
$C_{11}H_{18}O_2$ 182.262
Constit. of hops. Oil.

Tetrahydro: [15031-07-9] *2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nonane*
$C_{11}H_{20}O_2$ 184.278
Oil. Bp 178.5°.

Naya, Y. *et al., Tet. Lett.*, 1967, 1715 (*isol, struct*)
Burgstahler, A.W. *et al., J.O.C.*, 1973, **38**, 3652 (*synth*)

2,6,11,15-Tetramethyl-2,6,10,14-hexadecatetraene, 9CI T-302

[3294-76-6]
2,6,10,14-Phytatetraene



$C_{20}H_{34}$ 274.489

(E,E)-form [35162-77-7]
Digeranyl
Isol. from bergamot oil. Bp_{10} 190°. n_D^{20} 1.4825. n_D^{20} 1.4837.

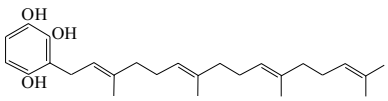
(Z,Z)-form [35162-83-5]
Dineryl
Oil.

[35162-81-3]

Souček, M. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 2551 (*isol*)
Biellmann, J.F. *et al., Tetrahedron*, 1971, **27**, 5861 (*synth, pmr*)
Kitagawa, Y. *et al., Tet. Lett.*, 1975, 1859 (*synth*)
Schurtenberger, H. *et al., Helv. Chim. Acta*, 1983, **66**, 2346 (*synth, pmr, cmr*)
Momose, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 1840 (*synth*)

3-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-1,2,4-benzenetriol, 9CI T-303

3-Geranylgeranyl-1,2,4-trihydroxybenzene



$C_{26}H_{38}O_3$ 398.584

(all-E)-form [103538-10-9]

2-Ac: [126398-82-1]
$C_{28}H_{40}O_4$ 440.622
Isol. from *Suillus granulatus* (granulated bolete).

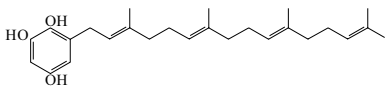
4-Ac: [103538-03-0] ***Suillin***
$C_{28}H_{40}O_4$ 440.622
Metab. of *Suillus* spp.. Cryst. Mp 108°. λ_{max} 275 (ϵ 14100) (MeOH) (Derep).

4-Me ether: [126398-83-2]
$C_{27}H_{40}O_3$ 412.611
Isol. from *Suillus granulatus* (granulated bolete). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 283 (ϵ 2120) (EtOH) (Berdy).

Jägers, E. *et al., Z. Naturforsch., B*, 1986, **41**, 645 (*Suillin, isol, pmr, cmr, uv*)
Tringali, C. *et al., J. Nat. Prod.*, 1989, **52**, 941 (*isol, derivs*)

6-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-1,2,4-benzenetriol T-304

6-Geranylgeranyl-1,2,4-benzenetriol



$C_{26}H_{38}O_3$ 398.584

(all-E)-form

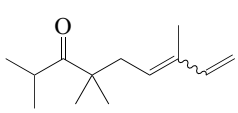
1-Ac: [123941-64-0] *4-Acetoxy-5-geranylgeranyl-1,3-benzenediol.* ***Bolegrevilol***
$C_{28}H_{40}O_4$ 440.622
Isol. from *Suillus grevillei* (larch bolete). Oil. λ_{max} 209 (ϵ 30600); 280 (ϵ 2500) (MeOH) (Berdy).

1-Me ether: [126398-85-4] *4-Methoxy-5-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)-1,3-benzenediol*
$C_{27}H_{40}O_3$ 412.611
Isol. from *Suillus granulatus* (granulated bolete). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 285 (ϵ 2200) (EtOH) (Berdy).

Hayashi, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1424 (*Bolegrevilol*)
Tringali, C. *et al., J. Nat. Prod.*, 1989, **52**, 941 (*derivs*)

2,4,4,7-Tetramethyl-6,8-nonadien-3-one, 9CI T-305

[81782-89-0]

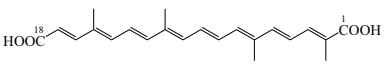


$C_{13}H_{22}O$ 194.316

Oxime: [81783-01-9] *Labienoxime*

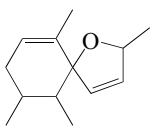
$C_{13}H_{23}NO$ 209.331
Fragrance ingredient with a blackcurrant-like aroma.
Eur. Pat., 1982, 45 861; *CA*, **98**, 53177t (*synth*)

2,6,11,15-Tetramethyl-2,4,6,8,10,12,14,16-octadecaoctaenedioic acid T-306
6,8′-Diapo-6,8′-carotenedioic acid



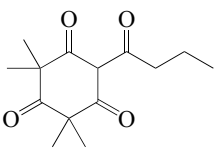
$C_{22}H_{26}O_4$ 354.445
(all-*E*)-*form*
18-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenoyl) ester, 1-Me ester:
[247030-33-7]
$C_{43}H_{60}O_4$ 640.945
Constit. of *Bixa orellana* (annatto) seeds. λ_{max} 330 ; 416 ; 441 ; 469 (2-methoxy-2-methylpropane).
Mercadante, A.Z. *et al., Phytochemistry*, 1999, **52**, 135-139 (*isol, pmr, cmr*)

2,6,9,10-Tetramethyl-1-oxaspiro[4.5]deca-3,6-diene, 9CI T-307
[71078-31-4]
Isospirene



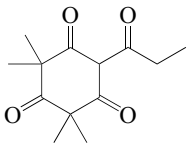
$C_{13}H_{20}O$ 192.3
Fragrance ingredient with a blackcurrant-like aroma.
U.K. Pat., 1980, 1 560 286; *CA*, **93**, 101378e (*synth, use*)

2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione T-308
2-Butanoyl-4,4,6,6-tetramethyl-1,3,5-cyclohexanetrione



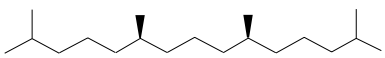
$C_{14}H_{20}O_4$ 252.31
Constit. of the essential oil of *Leptospermum scoparium* (red tea). Tentative indentification.
Porter, N.G. *et al., Phytochemistry*, 1999, **50**, 407-415 (*isol, ms*)

2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione T-309
2,2,4,4-Tetramethyl-6-propanoyl-1,3,5-cyclohexanetrione



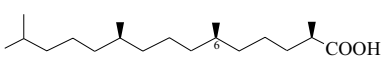
$C_{13}H_{18}O_4$ 238.283
Tentative identification. Constit. of the essential oil *Leptospermum scoparium* (red tea).
Porter, N.G. *et al., Phytochemistry*, 1999, **50**, 407-415 (*isol, ms*)

2,6,10,14-Tetramethylpentadecane T-310
[1921-70-6]
Pristane. *Norphytane. Bute hydrocarbon*



$C_{19}H_{40}$ 268.525
▶ Skin irritant. RZ1880000
(6*RS*,10*SR*)-*form*
meso-*form*
Isol. from fish liver oil. Oil. Mp -100°. Bp 296° Bp_{10} 158°. Chiral forms may also occur naturally; in most cases the opt. rotn. of isol. samples has not been measured.
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 16C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 12B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 16C (*ir*)
Hallgren, B. *et al., Acta Chem. Scand.*, 1963, **17**, 543
Kates, M. *et al., Biochemistry*, 1967, **6**, 3329 (*abs config, bibl*)
Jain, T.C. *et al., Can. J. Chem.*, 1969, **47**, 4359 (*isol*)
Goodman, R.A. *et al., J.A.C.S.*, 1973, **95**, 7553 (*cmr*)
Carman, C.J. *et al., Macromolecules*, 1973, **6**, 719 (*cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PMD500

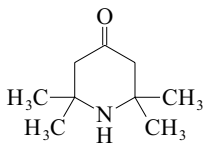
2,6,10,14-Tetramethylpentadecanoic acid T-311
[1189-37-3]
Pristanic acid



$C_{19}H_{38}O_2$ 298.508
Component of butterfat and sheep perinephric fat. Oil. A mixture of 6*R*- and 6*S*-forms occurs in nature.
Cason, J. *et al., Tetrahedron*, 1965, **21**, 471 (*isol, struct*)
Eldjarn, L. *et al., Acta Chem. Scand.*, 1966, **20**, 2313 (*synth*)
Nakajima, K. *et al., Agric. Biol. Chem.*, 1974, **38**, 1859 (*biosynth*)
Cox, R.E. *et al., Biochim. Biophys. Acta*, 1974, **360**, 166 (*biosynth, stereochem*)

2,2,3,4-Tetramethylpentane T-312
[1186-53-4]
$(H_3C)_2CHCH(CH_3)C(CH_3)_3$
C_9H_{20} 128.257
Constit. of *Jasminum sambac* (Arabian Jasmine) and *Humulus lupulus* (hops).
(±)-*form*
Bp 134°.
Hellman, S. *et al., Chem. Ber.*, 1983, **116**, 2219 (*synth, ir, pmr, cmr, ms*)
Zhu, L. *et al., Zhiwu Xuebao*, 1984, **26**, 189 (*isol*)
Tanaka, T. *et al., CA*, 1990, **113**, 187684t (*isol*)
Yaws, C.L. *et al., Hydrocarbon Process. Int. Ed.*, 1990, **69**, 87

2,2,6,6-Tetramethyl-4-piperidinone, 9CI T-313
[826-36-8]
4-Oxo-2,2,6,6-tetramethylpiperidine. 2,2,6,6-Tetramethyl-γ-piperidone. Triacetonamine. Odoratin†. Vincubine

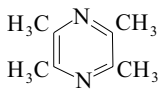


$C_9H_{17}NO$ 155.239
Isol. from *Viola odorata* (sweet violet). Plates + $1H_2O$ (Et_2O); anhyd. needles (dry Et_2O). Mp 34.9° (anhyd.). Bp 205°. The hydrochloride of the alkaloid from *Salsola tetrandra* was reported to have $[\alpha]_D$ +14.3° (EtOH) which makes the struct. assignment highly dubious. Artifact.
▶ TO0127900
Monohydrate: [10581-38-1]
Mp 61-63° (58°). Bp_{18} 102-105°.
Hydrochloride: [33973-59-0]
Mp 198° dec.
Oxime: [4168-79-0]
$C_9H_{18}N_2O$ 170.254
Prisms (EtOH). Mp 153°.
▶ LD_{50} (mus, ivn) 180 mg/kg. TO0128000
Semicarbazone:
Cryst. (EtOH). Mp 219-220°.
N,N-*Di-Me:*
[113308-50-2, 195864-37-0] *1,1,2,2,6,6-Hexamethyl-4-oxopiperidinium, 9CI. 1,1,2,2,6,6-Hexamethyl-4-piperidinone*
$C_{11}H_{22}NO^{\oplus}$ 184.301
N-*Benzyl:* [52981-86-9]
$C_{16}H_{23}NO$ 245.364
Plates or prisms (EtOH/Et_2O) (as hydrochloride). Mp 137-138° (hydrochloride).
N-*Bromo:*
$C_9H_{16}BrNO$ 234.135
Cryst. (petrol). Mp 44°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 461C; 461D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 720C; 721A (*nmr*)

Frenclowa, I. *et al., Acta Pol. Pharm.*, 1961, **18**, 187; 1964, **21**, 145; *CA*, **57**, 7381; **62**, 10817 (*isol*)
Rees, B. *et al., Acta Cryst. B*, 1971, **27**, 932 (*cryst struct*)
Karawya, M.S. *et al., Phytochemistry*, 1971, **10**, 3303 (*isol*)
Sosnovsky, G. *et al., Synthesis*, 1976, 735 (*synth*)
Ermakov, A.I. *et al., Khim. Geterotsikl. Soedin.*, 1979, 507 (*ms*)
Ozinskas, A.J. *et al., Helv. Chim. Acta*, 1980, **63**, 1407 (*pmr*)
Parameswaran, P.S. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 449 (*isol, pmr, cmr*)
Shimoi, N. *et al., Fish Sci.*, 1997, **63**, 650-651 (*Hexamethylpiperidone*)
Koenig, G.M. *et al., Planta Med.*, 1998, **64**, 88-89 (*isol, pmr, cmr*)
Bond, A.D. *et al., Acta Cryst. C*, 2002, **58**, o115-o116 (*monohydrate, cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TDU000

Tetramethylpyrazine T-314

[1124-11-4]
Chuanxiongzine. *FEMA 3237*



$C_8H_{12}N_2$ 136.196
Isol. from Galbanum oil. Present in french fries, bread, cooked meats, tea, cocoa, coffee, beer, spirits, peanuts, filberts, dairy products and soy products. Fragrance and flavouring ingredient. Trihydrate; cryst. (H_2O). Mp 74-77° (hyd.) Mp 86° (anhyd.). Bp 190°. pK_{a1} 3.61; pK_{a2} -2.73 (25°, H_2O). pK_{a1} 3.55; pK_{a2} -2.7 (27°, H_2SO_4 aq.). Log P 1.58 (calc). Odour threshold 10^4 ppb in H_2O λ_{max} 294 (ε 8500) (MeOH) (Berdy).
► LD_{50} (rat, orl) 1910 mg/kg. UQ3905000

Hydrochloride:
Mp 91° (dihydrate) Mp 156° (anhyd.).

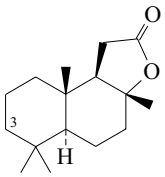
Dipicrate:
Needles. Mp 194-195°.

1,4-Dioxide:
$C_8H_{12}N_2O_2$ 168.195
Mp 224°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 402A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 841C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1559A (*ir*)
Piloty, O. *et al., Ber.*, 1910, **43**, 489
Kipping, F.B. *et al., J.C.S.*, 1929, 2891
Gnitchtel, H. *et al., Chem. Ber.*, 1972, **105**, 1865
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
Eiermann, U. *et al., Chem. Ber.*, 1990, **123**, 523 (*uv*)
Ozaki, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 954 (*isol, pharmacol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TDV725

13,14,15,16-Tetranor-12,8-labdanolide T-315

[1216-84-8]



$C_{16}H_{26}O_2$ 250.38
8α-*form* [564-20-5]
Norambreinolide. *Sclareolide. FEMA 3794*
Used to enhance the flavour of beverages and foodstuffs. Flavouring ingredient. Constit. of labdanum oil and clary sage (*Salvia sclarea*). Cryst. (petrol or MeOH aq.) with musky wood odour. Mp 122-125°. $[\alpha]_D$ +42 (c, 0.25 in $CHCl_3$).

3α-Hydroxy: [123844-63-3] *3α-Hydroxy-13,14,15,16-tetranor-12,8-labdanolide.* ***3α-Hydroxynorambreinolide***
$C_{16}H_{26}O_3$ 266.38
Cryst. (Et_2O/hexane). Mp 190-191°. $[\alpha]_D$ +22.2 (c, 1.08 in $CHCl_3$).

6α-Hydroxy:6α-Hydroxy-13,14,15,16-tetranor-12,8-labdanolide. ***6α-Hydroxynorambreinolide***
$C_{16}H_{26}O_3$ 266.38
$[\alpha]_D$ +61 (c, 0.35 in $CHCl_3$).

(*ent*-8α)-*form* [95406-08-9] **ent-*Norambreinolide***
Cryst. (EtOAc/petrol). Mp 120-122°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1142C (*nmr*)
Carman, R.M. *et al., Aust. J. Chem.*, 1966, **19**, 1535 (*synth, bibl*)
Fernández, C. *et al., Phytochemistry*, 1985, **24**, 188 (*isol*)
Gonzalez, M.S. *et al., Tetrahedron*, 1989, **45**, 3575 (*3α-Hydroxynorambreinolide*)
Barrero, A.F. *et al., Tetrahedron*, 1994, **50**, 6653 (*synth*)
Dolmazon, R. *et al., Phytochemistry*, 1995, **38**, 917 (*isol, pmr, cmr*)
Topcu, G. *et al., J. Nat. Prod.*, 1996, **59**, 113 (*6α-Hydroxynorambreinolide*)
Eur. Pat., 1998, 821 055; *CA*, **128**, 153392r (*use*)
Weyerstahl, P. *et al., Flavour Fragrance J.*, 1998, **13**, 295-318 (*8α-form, isol, labdanum oil*)
Adams, T.B. *et al., Food Chem. Toxicol.*, 1998, **36**, 249-278 (*8α-form, tox*)
Koga, T. *et al., Tetrahedron: Asymmetry*, 1998, **9**, 3819-3823 (*8α-form, synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1626-1627 (*8α-form, use*)
De La Torre, M.C. *et al., Tet. Lett.*, 2002, **43**, 6351-6353 (*synth*)

Panax ginseng Tetrapeptide T-316

[178553-95-2]
Valyl-D-γ-glutamyl-D-arginylglycine
H-Val-D-γ-Glu-Arg-Gly-OH
$C_{18}H_{33}N_7O_7$ 459.501
Constit. of *Panax ginseng* (ginseng). $[\alpha]_D^{22}$ +26 (c, 0.2 in H_2O).

[178738-27-7]

Yagi, A. *et al., Planta Med.*, 1996, **62**, 115 (*isol, synth, pmr, cmr*)

1,2,4,5-Tetrathiane, 9CI T-317

[291-22-5]
1,2,4,5-Tetrathiacyclohexane

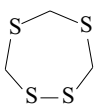


$C_2H_4S_4$ 156.318
Found in shiitake mushrooms (*Lentinus edodes*). Food flavouring agent. Needles (petrol). Mp 132-133°.

Böhme, H. *et al., Chem. Ber.*, 1965, **98**, 1455 (*synth*)
Japan. Pat., 1970, 70 23 580; *CA*, **74**, 63330 (*use*)
Allinger, N.L. *et al., J.A.C.S.*, 1976, **98**, 2741 (*conform*)
Chen, C.C. *et al., Agric. Food Chem. : Past, Present, Future [Pap. Am. Chem. Soc. Centen. Meet.], 1976 (1978)*, 1986, **34**, 830 (*isol*)
Chen, C.C. *et al., J. Chromatogr.*, 1986, **356**, 455 (*hplc*)
Stradella, O.G. *et al., THEOCHEM*, 1986, **28**, 7 (*conform*)
Takikawa, Y. *et al., Chem. Lett.*, 1988, 1517 (*ir, ms, pmr, synth*)

1,2,4,6-Tetrathiepane T-318

[292-45-5]
1,2,4,6-Tetrathiacycloheptane

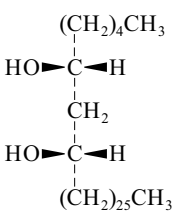


$C_3H_6S_4$ 170.344
Isol. from shiitake mushroom (*Lentinus edodes*). Mp 79°.

4,4-Dioxide: [58966-89-5]
$C_3H_6O_2S_4$ 202.343
Prisms ($CHCl_3$). Mp 154-155°.

Morita, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 998 (*synth, isol*)
Wratten, S.J. *et al., J.O.C.*, 1976, **41**, 2465 (*isol*)
Weissflog, E. *et al., Phosphorus Sulfur Relat. Elem.*, 1980, **8**, 157 (*synth*)
Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521
Still, I.W.J. *et al., Tet. Lett.*, 1981, 1939 (*synth*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)

6,8-Tetratriacontanediol T-319



$C_{34}H_{70}O_2$ 510.926
(6*R,8*S**)-*form*** [155800-91-2]
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 84-85°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

7,9-Tetratriacontanediol T-320

$C_{34}H_{70}O_2$ 510.926

(7R*,9S*)-form [193419-74-8]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 74-78°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

1-Tetratriacontanol, 9CI, 8CI T-321

[28484-70-0]
Sapiol

$H_3C(CH_2)_{32}CH_2OH$

$C_{34}H_{70}O$ 494.926
Isol. from cotton wax. Mp 92°. Bp_1 200-250° subl..

Hexadecanoyl: [84461-48-3] *Tetratriacontyl hexadecanoate. Tetratriacontyl palmitate*
$C_{50}H_{100}O_2$ 733.339
Cryst. (C_6H_6). Mp 69°.

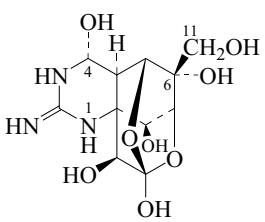
Octacosanoyl: [86989-35-7] *Tetratriacontyl octacosanoate*
$C_{62}H_{124}O_2$ 901.66
Cryst. (Me_2CO/MeOH). Mp 66-68°.

[103215-66-3]

Chibnall, A.C. *et al., Biochem. J.*, 1934, **28**, 2189 (*isol*)
Mazliak, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1960, **251**, 2393 (*isol*)
Wanatabe, A. *et al., Bull. Chem. Soc. Jpn.*, 1961, **34**, 1728 (*synth*)
Tasumi, M. *et al., Spectrochim. Acta*, 1964, **20**, 629 (*ir*)
Japan. Pat., 1980, 80 129 292; *CA*, **94**, 120844r (*synth*)
Shukla, Y.N. *et al., Phytochemistry*, 1983, **22**, 973 (*Tetratriacontyl octacosanoate*)
Singh, M. *et al., Z. Naturforsch., B*, 1984, **39**, 1425 (*hexadecanoyl*)

Tetrodotoxin T-322

[4368-28-9]
Tarichatoxin. Spheroidine. Tetrodontoxin. Fugu poison. Maculotoxin. Araregai toxin



$C_{11}H_{17}N_3O_8$ 319.271
Potent neurotoxin isol. from ovaries and liver of Japanese puffer fish and skin of Californian newt. Cause of accidental poisoning in Japan. Cryst. Sol. acids; fairly sol. H_2O; poorly sol. EtOAc, hexane. $[\alpha]_D^{25}$ -8.64 (c, 8.55 in AcOH aq.). pK_a 8.76. Darkens at 225° but does not melt.

▶ LD_{50} (mus, orl) 435 µg/kg. LD_{50} (mus, ivn) 9 µg/kg. Highly toxic to mammals, birds, reptiles, amphibians and fish. IO1450000

Hydrobromide:
Prisms (EtOH aq.). No definite Mp.

Picrate:
Yellow needles + $1H_2O$ (H_2O). Darkens >200° without melting.

Penta-Ac:
Mp 205.5-207°.

Hepta-Ac:
Mp 188.5-191.5°. $[\alpha]_D^{30}$ +15.8 (c, 0.39 in $CHCl_3$).

4-Epimer: [98242-82-1] ***4-Epitetrodotoxin***
$C_{11}H_{17}N_3O_8$ 319.271
Amorph.

6-Epimer: [112318-40-8] ***6-Epitetrodotoxin***
$C_{11}H_{17}N_3O_8$ 319.271
Amorph. $[\alpha]_D^{21}$ -4.8 (c, 0.3 in AcOH aq.).
▶ LD_{50} (mus, ipr) .6 mg/kg.

11-Deoxy: [112174-24-0] ***11-Deoxytetrodotoxin***
$C_{11}H_{17}N_3O_7$ 303.271
Needles (AcOH aq.). Mp 202° (dec.). $[\alpha]_D^{25}$ +5.4 (c, 0.3 in AcOH aq.).
▶ LD_{50} (mus, ipr) .71 mg/kg.

11-Deoxy, 4-epimer: [113564-23-1] ***11-Deoxy-4-epitetrodotoxin***
$C_{11}H_{17}N_3O_7$ 303.271
Amorph.

11-Hydroxy: [123665-88-3] ***11-Hydroxytetrodotoxin***
$C_{11}H_{17}N_3O_9$ 335.27
Amorph. Exists as covalent hydrate.

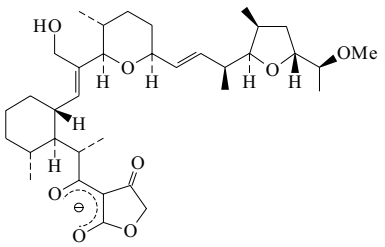
6-De(hydroxymethyl): [156336-07-1] ***11-Nortetrodotoxin***. *11-Nortetrodotoxin-6S-ol*
$C_{10}H_{15}N_3O_7$ 289.244

6-De(hydroxymethyl), 6-epimer: [81520-41-4] ***6-Epi-11-nortetrodotoxin***. *6-De(hydroxymethyl)-6-epitetrodotoxin. 11-Nortetrodotoxin-6R-ol*
$C_{10}H_{15}N_3O_7$ 289.244
Amorph.

Yakoo, A. *et al., Nippon Kagaku Kaishi*, 1950, **71**, 590 (*isol*)
Tomiie, Y. *et al., Tet. Lett.*, 1963, 2101 (*struct*)
Woodward, R.B. *et al., Pure Appl. Chem.*, 1964, **9**, 49 (*struct*)
Goto, T. *et al., Tetrahedron*, 1965, **21**, 2059 (*isol, ir, pmr, struct*)
Tsuda, K. *et al., Naturwissenschaften*, 1966, **53**, 171 (*rev*)
Furusaki, A. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 3332 (*cryst struct*)
U.S. Pat., 1971, 3 966 934; *CA*, **85**, 87545 (*use*)
Kishi, Y. *et al., J.A.C.S.*, 1972, **94**, 9219 (*synth*)
Yasumoto, T. *et al., Agric. Biol. Chem.*, 1986, **50**, 793 (*isol*)
Tetrodotoxin, Saxitoxin and the Molecular Biology of the Sodium Channel, (eds. Kao, C.Y. *et al*), New York Academy of Sciences, 1986, (*book*)
Yasumoto, T. *et al., J.A.C.S.*, 1988, **110**, 2344-2345 (*derivs, isol, pmr, cmr*)
Endo, A. *et al., Tet. Lett.*, 1988, **29**, 4127-4128 (*6-Epi-11-nortetrodotoxin*)
Khora, S.S. *et al., Tet. Lett.*, 1989, **30**, 4393-4394 (*11-Hydroxytetrodotoxin*)
Yotsu, M. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 370-371 (*11-Nortetrodotoxin-6S-ol*)
Arakawa, O. *et al., Fish Sci.*, 1994, **60**, 769-771 (*11-Oxotetrodotoxin, 11-Nortetrodotoxin-6R-ol*)
Yasumoto, T. *et al., J. Toxicol., Toxin Rev.*, 1996, **15**, 81-90 (*rev*)
Dyakonov, A.L. *et al., Khim. Prir. Soedin.*, 1997, **33**, 297-351; *Chem. Nat. Compd. (Engl. Transl.)*, 1997, **33**, 221-267 (*rev*)
Isobe, M. *et al., Tetrahedron*, 2001, **57**, 4543-4558 (*5,11-Dideoxytetrodotoxin, synth*)
Nishikawa, T. *et al., J.A.C.S.*, 2002, **124**, 7847-7852 (*11-Deoxytetrodotoxin, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FOQ000

Tetronasin, BAN, INN T-323

[75139-06-9]
Antibiotic M 139603. ICI 139603. M 139603



$C_{35}H_{53}O_8^{\ominus}$ 601.799
Polyether antibiotic. Isol. from *Streptomyces longisporoflavus*. Investigated as ruminant feed additive. Sol. MeOH, C_6H_6; poorly sol. H_2O. λ_{max} 234 (ε 13000); 270 (ε 11000) (MeOH) (Berdy). λ_{max} 234 (ε 12900); 272 (ε 10800) (EtOH/NaOH) (Berdy).

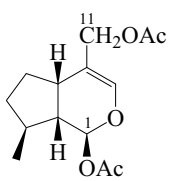
Na salt: [75139-05-8]
Cryst. Mp 176-178°. $[\alpha]_D^{23}$ -82 (c, 0.2 in MeOH).

K salt: [75139-07-0]
Mp 146-150°.

U.K. Pat., 1980, 2 027 013, (*ICI*); *CA*, **93**, 184292 (*isol, props*)
Davies, D.H. *et al., Chem. Comm.*, 1981, 1073 (*cryst struct*)
Eur. Pat., 1983, 70 622, (*ICI*); *CA*, **99**, 158138 (*derivs*)
Grandjean, J. *et al., Tet. Lett.*, 1983, 3319 (*conformn*)
Doherty, A.M. *et al., Tet. Lett.*, 1986, **27**, 105
Newbold, J.C. *et al., Appl. Environ. Microbiol.*, 1988, **54**, 544 (*pharmacol*)
Riddell, F.G. *et al., Biochim. Biophys. Acta*, 1989, **984**, 6 (*activity*)
Ley, S.V. *et al., Tet. Lett.*, 1994, **35**, 307; 311; 315; 319; 323 (*biosynth, synth*)
Ley, S.V. *et al., Farmaco*, 1996, **51**, 147 (*rev*)
Ley, S.V. *et al., J.C.S. Perkin 1*, 1998, 2259-2276 (*synth, bibl*)

Teucrein T-324

[89289-90-7]



$C_{14}H_{20}O_5$ 268.309
Oil. $Bp_{0.5}$ 125-130°. $[\alpha]_D^{20}$ -73.5 (c, 0.3 in C_6H_6).

1-O-De-Ac, 1-O-(3-methylbutanoyl):
[162232-32-8] ***Valdiate***
$C_{17}H_{26}O_5$ 310.389
Constit. of *Valeriana officinalis* var.

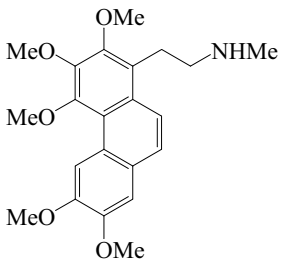
sambucifolia.

Di-O-*de-Ac, 11*-O-*(3,4-dihydroxy*-E-*cinnamoyl):* [182261-53-6]
$C_{19}H_{22}O_6$ 346.379
Gum. $[\alpha]_D$ -65.5 (c, 0.1 in MeOH). Assigned incorrect trivial name in ref..

Bellesia, F. *et al., J. Chem. Res., Synop.*, 1983, 328-329 (*Teucrein*)
Gränicher, F. *et al., Phytochemistry*, 1995, **38**, 103-105 (*Valdiate*)
Bolzani, V. da S. *et al., J. Braz. Chem. Soc.*, 1996, **7**, 157-160 (*Tocoyena isolate*)

Thalicpureine T-325

[218900-91-5]
2,3,4,6,7-Pentamethoxy-N-*methyl-1-phenanthrenemethanamine, 9CI. 2,3,4,6,7-Pentamethoxy-1-(2-methylaminoethyl)phenanthrene*

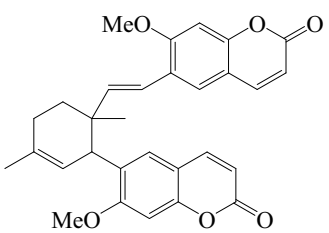


$C_{22}H_{27}NO_5$ 385.459
Alkaloid from the leaves of *Annona purpurea* (soncoya). Yellow needles ($CHCl_3$). Mp 196-197°. λ_{max} 220 ; 264 ; 308 ; 326 ; 345 ; 358 (sh) (EtOH).

Chang, F.-R. *et al., J. Nat. Prod.*, 1998, **61**, 1457-1461 (*isol, uv, pmr, cmr, ms*)

Thamnosin T-326

[18458-66-7]
*7-Methoxy-6-[2-[2-(7-methoxy-2-oxo-2*H-*1-benzopyran-6-yl)-1,4-dimethyl-3-cyclohexen-1-yl]ethenyl]-2*H-*1-benzopyran-2-one, 9CI. Cyclobisuberodiene*



$C_{30}H_{28}O_6$ 484.548
Constit. of *Citrus grandis* (pummelo). Cryst. (C_6H_6 or EtOAc). Mp 244-246°.

[128571-88-0]

Dreyer, D.L. *et al., Tetrahedron*, 1966, **22**, 2923 (*isol*)
Kutney, J.P. *et al., J.A.C.S.*, 1968, **90**, 813
Kutney, J.P. *et al., Tetrahedron*, 1970, **26**, 3171 (*struct*)
Wu, T.S. *et al., Phytochemistry*, 1988, **27**, 585 (*isol*)
Reisch, J. *et al., Annalen*, 1990, 931 (*synth, ir, pmr, ms*)

Thaumatin T-327

[53850-34-3]

[62168-98-3]
Talin. E957. FEMA 3732

Protein consisting of 207 amino acid residues with 8 disulfide bridges, M = 22,000. Obt. from ripe miracle berry fruits (*Thaumatococcus daniellii*). Sweetener (5,000 times sweeter than sucrose), flavour enhancer for coffee, peppermint flavours etc. Permitted in EU at 50-400 ppm in chewing gum, vitamin preparations and some other sugar-free products. Use limited by slow contact and persistence of sensation. Cryst.

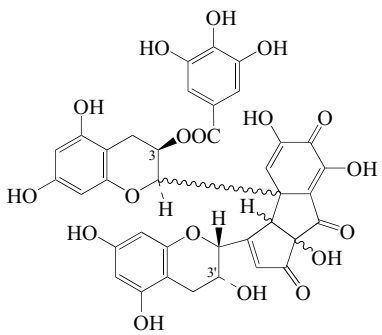
Recombinant-*form*
Thaumatin B-recombinant. r-Thaumatin. Cotour. FEMA 3814
Flavour enhancer, non-nutritive sweetener.

[62168-98-3, 71396-29-7, 83271-81-2, 93616-28-5]

Van der Wel, H. *et al., Eur. J. Biochem.*, 1972, **31**, 221; 1984, **144**, 41 (*isol, struct, disulfide bridges*)
Van der Wel, H. *et al., FEBS Lett.*, 1975, **56**, 316-317 (*cryst struct*)
Iyengar, R.B. *et al., Eur. J. Biochem.*, 1979, **96**, 193 (*struct*)
Van der Wel, H. *et al., Chem. Ind. (London)*, 1983, 19 (*rev*)
Higginbotham, J.D. *et al., Food Chem. Toxicol.*, 1983, **21**, 815-823 (*tox*)
Lee, J.H. *et al., Biochemistry*, 1988, **27**, 5101 (*cloning, struct*)
Ko, T.-P. *et al., Acta Cryst. D*, 1994, **50**, 813-825 (*cryst struct*)
Faus, I. *et al., Appl. Microbiol. Biotechnol.*, 1998, **49**, 393-398 (*r-Thaumatin*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1691; 1692 (*use*)

Theacitrin A T-328

[201998-49-4]



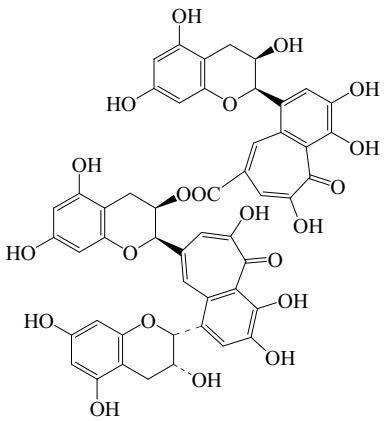
$C_{37}H_{28}O_{18}$ 760.617
Constit. of the fermented leaves of *Camellia sinensis* (black tea). Yellow solid. λ_{max} 277 ; 379 (no solvent reported).

3′-O-*(3,4,5-Trihydroxybenzoyl):* ***Theacitrin C***
$C_{44}H_{32}O_{22}$ 912.724
Constit. of fermented leaves of *Camellia sinensis* (black tea). Struct. requires confirmation.

Isomer: ***Theacitrin B***
$C_{37}H_{28}O_{18}$ 760.617
Constit. of fermented leaves of *Camellia sinensis* (black tea). Prob. the isomer of Theacitrin A having the trihydroxybenzoyl residue on the 3′ oxygen. Struct. requires confirmation.

Davis, A.L. *et al., Phytochemistry*, 1997, **46**, 1397-1402 (*isol, uv, ir, pmr, cmr*)

Theadibenzotropolone A T-329

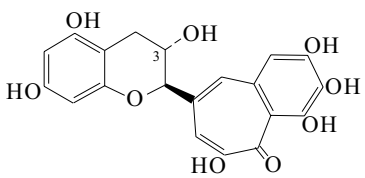


$C_{50}H_{38}O_{21}$ 974.838
Constit. of black tea (*Camellia sinensis*).

Sang, S. *et al., Tet. Lett.*, 2002, **43**, 7129-7133 (*isol, synth, pmr, cmr, ms*)

Theaflagallin T-330

[102208-15-1]



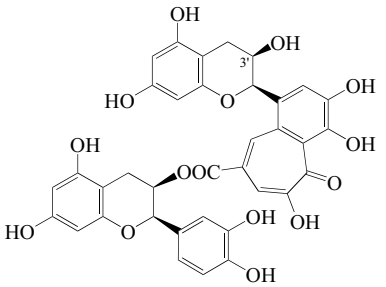
$C_{20}H_{16}O_9$ 400.341
Red pigment from black tea (*Camellia sinensis* var. *assamica*). Red cryst. powder (MeOH aq.). Mp 203-204°. $[\alpha]_D^{18}$ -27.5 (c, 0.1 in Me_2CO).

3-Epimer: [102208-16-2] ***Epitheaflagallin***
$C_{20}H_{16}O_9$ 400.341
Pigment from black tea. Red needles (MeOH aq.). Mp 170-171°. $[\alpha]_D^{25}$ -150.1 (c, 0.2 in Me_2CO).

3-Epimer, 3-O-*(3,4,5-trihydroxybenzoyl):* [102067-92-5] *Epitheaflagallin 3*-O-*gallate*
$C_{27}H_{20}O_{13}$ 552.447
Pigment from black tea. Red cryst. powder + $2H_2O$ (MeOH aq.). Mp 218-220°. $[\alpha]_D^{23}$ -383.2 (c, 0.4 in Me_2CO).

Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1986, **34**, 61 (*isol, struct, synth*)

Theaflavate B T-331



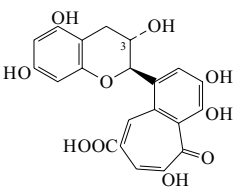
$C_{36}H_{28}O_{15}$ 700.608
Constit. of black tea (*Camellia sinensis*). Amorph. orange-red powder. λ_{max} 284 ; 406 (no solvent reported).

3′-O-(3,4,5-Trihydroxybenzoyl): [152542-70-6] ***Theaflavate A***
$C_{43}H_{32}O_{19}$ 852.714
Constit. of black tea (*Camellia sinensis*).

Wan, X. *et al., J. Sci. Food Agric.*, 1997, **74**, 401-408 (*isol, pmr, cmr*)
Lewis, J.R. *et al., Phytochemistry*, 1998, **49**, 2511-2519 (*isol, uv, pmr, cmr*)

Theaflavic acid T-332

[30407-93-3]



Relative configuration

$C_{21}H_{16}O_{10}$ 428.351
Isol. from black tea (*Camellia sinensis*).

3-Epimer: [30407-94-4] ***Epitheaflavic acid***
$C_{21}H_{16}O_{10}$ 428.351
Isol. from black tea *Camellia sinensis*.

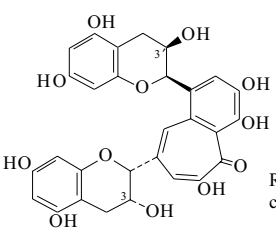
3-Epimer, 3-O-(3,4,5-trihydroxybenzoyl): [34218-97-8] ***Epitheaflavic acid 3′-gallate***
$C_{28}H_{20}O_{14}$ 580.458
Isol. from black tea *Camellia sinensis*.

[41001-95-0, 41002-04-4]

Coxon, D.T. *et al., Tet. Lett.*, 1970, 5237; 5247 (*isol, struct*)
Collier, P.D. *et al., Tetrahedron*, 1973, **29**, 125 (*isol, cd, ms, pmr*)

Theaflavin T-333

[4670-05-7]
1,8-Bis(3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl)-3,4,6-trihydroxy-5H-benzocyclohepten-5-one, 9CI



Relative configuration

$C_{29}H_{24}O_{12}$ 564.501
Constit. of black tea (*Camellia sinensis*). Cryst. (H_2O). Poorly sol. hexane. Mp 237-240° dec. λ_{max} 216 (ϵ 35000); 271 (ϵ 19500); 384 (ϵ 8700); 470 (ϵ 3600) (EtOH) (Berdy).

▶ DE8382900

Nona-Ac:
Pale yellow needles (MeOH). Mp 167-168°.

3-O-(3,4,5-Trihydroxybenzoyl): [30462-34-1] ***Theaflavin 3-gallate***
$C_{36}H_{28}O_{16}$ 716.608
Constit. of black tea and commercial oolong tea. Brown amorph. powder.

3′-O-(3,4,5-Trihydroxybenzoyl): [28543-07-9] ***Theaflavin 3′-gallate***
$C_{36}H_{28}O_{16}$ 716.608
Constit. of black tea and commercial oolong tea. Brown amorph. powder.

3,3′-Bis-O-(3,4,5-trihydroxybenzoyl): [30462-35-2] ***Theaflavin 3,3′-digallate***
$C_{43}H_{32}O_{20}$ 868.714
Constit. of black tea and commercial oolong tea. Brown cryst. Mp 226-230° dec.

3-Epimer: [31701-93-6] ***Isotheaflavin***
$C_{29}H_{24}O_{12}$ 564.501
Present in black tea.

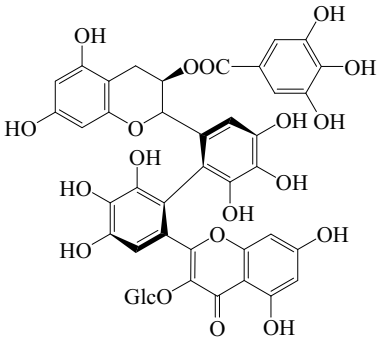
3′-Epimer, 3-O-(3,4,5-trihydroxybenzoyl):- ***Neotheaflavin 3-gallate***
$C_{36}H_{28}O_{16}$ 716.608
Constit. of black tea. λ_{max} 277 ; 373 ; 451 (no solvent reported).

3-Epimer, 3′-O-(3,4,5-trihydroxybenzoyl): ***Isotheaflavin 3′-gallate***
$C_{36}H_{28}O_{16}$ 716.608
Constit. of black tea. λ_{max} 284 ; 375 ; 455 (no solvent reported).

Roberts, E.A.H. *et al., J. Sci. Food Agric.*, 1957, **8**, 72; 1958, **9**, 212; 217; 1959, **10**, 167; 172 (*isol*)
Takino, Y. *et al., Agric. Biol. Chem.*, 1963, **27**, 319; 1964, **28**, 255 (*isol*)
Brown, A.G. *et al., Tet. Lett.*, 1966, 1193 (*struct*)
Takino, Y. *et al., Tet. Lett.*, 1966, 4024 (*struct*)
Coxon, D.T. *et al., Tet. Lett.*, 1970, 5241 (*Isotheaflavin*)
Collier, P.D. *et al., Tetrahedron*, 1973, **29**, 125 (*isol, config, uv, ms, pmr, cd*)
Japan. Pat., 1978, 78 12 897; *CA*, **89**, 75349 (*synth*)
Davis, A.L. *et al., Magn. Reson. Chem.*, 1995, **33**, 549 (*pmr, cmr*)
Lewis, J.R. *et al., Phytochemistry*, 1998, **49**, 2511-2519 (*Isotheaflavin 3′-gallate, Neotheaflavin 3-gallate*)

Theaflavonin T-334

[144207-59-0]



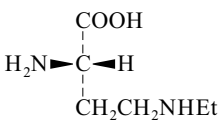
$C_{43}H_{36}O_{24}$ 936.743
Fermentation prod. isol. from black tea. Yellow brown powder + $2H_2O$. $[\alpha]_D^{22}$ -179.4 (c, 1 in Me_2CO). λ_{max} 253 (log ϵ 4.42); 260 (sh) (log ϵ 4.41); 301 (log ϵ 4.02); 345 (log ϵ 4.08) (MeOH).

De-O-(3,4,5-trihydroxybenzoyl): [143833-95-8] ***Degalloyltheaflavonin***
$C_{36}H_{32}O_{20}$ 784.637
Fermentation prod. isol. from black tea. Yellow brown powder + $2H_2O$. $[\alpha]_D^{18}$ -63.9 (c, 1 in Me_2CO). λ_{max} 254 (sh) (log ϵ 4.34); 261 (sh) (log ϵ 4.34); 297 (log ϵ 4); 345 (log ϵ 3.91) (MeOH).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1383-1389 (*isol, uv, cd, pmr, cmr, ms*)

Theanine T-335

N-*Ethylglutamine, 9CI. 2-Amino-4-(ethylamino)butanoic acid*



$C_7H_{14}N_2O_3$ 174.199

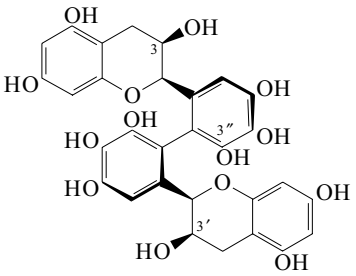
(S)-form [3081-61-6]
L-form
Constit. of tea (*Thea sinensis*) and of the fungus *Xerocomus badius* (kostanjevka). Cryst. (EtOH aq.). Mp 217-218° dec. $[\alpha]_D$ +8.7 (c, 1.74 in H_2O).

Lichtenstein, N. *et al., J.A.C.S.*, 1942, **64**, 1021 (*synth, abs config*)
Sakato, Y. *et al., Nippon Nogei Kagaku Kaishi*, 1950, **23**, 262 (*isol*)
Sakato, Y. *et al., Nippon Nogei Kagaku Kaishi*, 1950, **23**, 269 (*synth*)
Hashizume, T. *et al., Nippon Nogei Kagaku Kaishi*, 1951, **25**, 25 (*synth*)
Cartwright, R.A. *et al., J. Sci. Food Agric.*, 1954, **5**, 597 (*isol*)
Casimir, J. *et al., Biochim. Biophys. Acta*, 1960, **39**, 462 (*isol*)
Furuyama, T. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 1078 (*synth*)
Vitzthum, O. *et al., J. Chromatogr.*, 1974, **95**, 39 (*glc, ms*)
Takeo, T. *et al., Phytochemistry*, 1974, **13**, 1401 (*biosynth*)
Kawagishi, H. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 689 (*synth, bibl*)

Theasinensin C T-336

[89013-69-4]

*6,6′-Bis(3,4-dihydro-3,5,7-trihydroxy-2*H*-1-benzopyran-2-yl)-[1,1′-biphenyl]-2,2′,3,3′,4,4′-hexol, 9CI*



$C_{30}H_{26}O_{14}$ 610.527

Isol. from oolong tea (*Camellia sinensis* var. *viridis*). Powder + $1\frac{1}{2}H_2O$. $[\alpha]_D^{18}$ -20.4 (c, 0.75 in Me_2CO).

3-O-*(3,4,5-Trihydroxybenzoyl):* [89064-32-4] ***Theasinensin B***

$C_{37}H_{30}O_{18}$ 762.633

Isol. from leaves of green tea (*Thea sinensis*). Pale brown powder + $\frac{1}{2}H_2O$. $[\alpha]_D^{21}$ -147.2 (c, 0.5 in Me_2CO).

3,3′-Bis(3,4,5-trihydroxybenzoyl): [89064-31-3] ***Theasinensin A***

$C_{44}H_{34}O_{22}$ 914.739

Isol. from green tea *Thea sinensis*. Pale brown powder $+1\frac{1}{2}H_2O$. $[\alpha]_D^{15}$ -226.8 (c, 0.73 in Me_2CO).

3″-Deoxy, 3,3′-bis-O-*(3,4,5-trihydroxybenzoyl):* [116329-55-6] ***Theasinensin F***

$C_{44}H_{34}O_{21}$ 898.74

From oolong tea *Camellia sinensis* var. *viridis*. Off-white powder + $5H_2O$. $[\alpha]_D^{26}$ -263.6 (c, 1 in Me_2CO).

Atropisomer: [116348-81-3] ***Theasinensin E***

$C_{30}H_{26}O_{14}$ 610.527

From oolong tea *Camellia sinensis* var. *viridis*. Off-white powder + $\frac{2}{3}H_2O$. $[\alpha]_D^{23}$ +22.6 (c, 1 in Me_2CO). Opposite chirality of the biaryl system.

Atropisomer, 3,3′-bis-O-*(3,4,5-trihydroxybenzoyl):* [116403-62-4] ***Theasinensin D***

$C_{44}H_{34}O_{22}$ 914.739

From oolong tea *Camellia sinensis* var. *viridis*. Off-white powder + $5H_2O$. $[\alpha]_D^{28}$ -158.6 (c, 1 in Me_2CO).

Atropisomer, 3″-deoxy, 3,3′-bis-O-*(3,4,5-trihydroxybenzoyl):* [116403-61-3] ***Theasinensin G***

$C_{44}H_{34}O_{21}$ 898.74

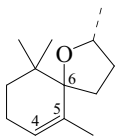
From oolong tea *Camellia sinensis* var. *viridis*. Off-white powder + $5H_2O$. $[\alpha]_D^{26}$ -103 (c, 1 in Me_2CO).

Nonaka, G. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3906; 1988, **36**, 1676 (*isol, struct, pmr, cmr*)

Theaspirane T-337

[36431-72-8]

2,6,10,10-Tetramethyl-1-oxaspiro[4.5]dec-6-ene, 9CI. 6,9-Epoxy-4-megastigmene. FEMA 3774



$C_{13}H_{22}O$ 194.316

Numbering systems vary. Natural theaspirane is a mixt. of the (6*R*) and (6*S*) compds. (Theaspirane B and Theaspirane A resp.). Constit. of raspberry, yellow passion fruit, tea, wine grape, white wine, quince, cherimoya and black chokeberry. Flavouring ingredient. Oil with fruity, woody, sweetish, camphorous odour. Bp_6 91-96°.

4,5-Dihydro, 5-hydroxy: [53398-90-6] *2,6,10,10-Tetramethyl-1-oxaspiro[4.5]-decan-6-ol, 9CI. 6-Hydroxydihydrotheaspirane. FEMA 3549*

$C_{13}H_{24}O_2$ 212.331

Flavouring ingredient with camphoraceous, woody, green odour. Constit. of black tea. d_4^{20} 1. Bp_{16} 130°. n_D^{20} 1.4840.

4,5-Dihydro, 5-acetoxy: [72541-09-4] *5-Acetoxydihydrotheaespirane. FEMA 3651*

$C_{15}H_{26}O_3$ 254.369

Flavouring ingredient. Semicryst. mass. Obt. only as a mixt. of 5-epimers.

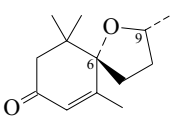
[43126-21-2, 43126-22-3, 66537-39-1, 66965-88-6, 66965-89-7, 130404-01-2, 130404-02-3]

Schulte-Elte, K.H. *et al., Helv. Chim. Acta*, 1978, **61**, 1125 (*synth*)
Ohloff, G. *et al., Prog. Chem. Org. Nat. Prod.*, 1978, **35**, 431 (*isol*)
Okawara, H. *et al., Heterocycles*, 1979, **13**, 191 (*synth*)
Torii, S. *et al., Tet. Lett.*, 1981, **22**, 2291 (*synth*)
Masuda, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 861 (*synth*)
Uneyama, K. *et al., Tet. Lett.*, 1985, **26**, 4637 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1369; 2770-2771 (*occur, props*)
Boulin, B. *et al., Tetrahedron*, 2000, **56**, 3927-3932 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 16; 814 (*4,5-dihydro-5-hydroxy, 4,5-dihydro-5-acetoxy, use, props*)

Theaspirone T-338

[19377-59-4]

2,6,10,10-Tetramethyl-1-oxaspiro[4.5]dec-6-en-8-one, 9CI. 6,9-Epoxy-4-megastigmen-3-one



(6*R*,9*R*)-*form*

$C_{13}H_{20}O_2$ 208.3

Terpenoid numbering shown.

(6*R*,9*R*)-*form* [50763-74-1]

Theaspirone B

Constit. of quince fruit. Oil. $[\alpha]_D^{22}$ +23.4 (c, 1.2 in $CHCl_3$).

(6*R*,9*S*)-*form* [24399-19-7]

Theaspirone A

Constit. of the aroma of black tea. Also in other plants. Oil. $[\alpha]_D^{22}$ -4.9 (c, 1.01 in $CHCl_3$).

(6*S*,9*S*)-*form* [153925-96-3]

Constit. of quince fruit. Characterised spectroscopically.

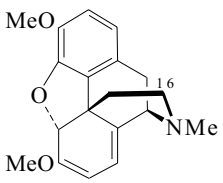
[23131-48-8, 57760-39-1]

Ina, K. *et al., Tet. Lett.*, 1968, 2777 (*isol*)
Nakatani, T. *et al., Agric. Biol. Chem.*, 1970, **34**, 152 (*synth*)
Weiss, G. *et al., Chem. Comm.*, 1973, 565 (*synth, abs config*)
Marx, J.N. *et al., Tetrahedron*, 1975, **31**, 1251 (*synth*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1978, **61**, 387 (*synth, cd*)
Etoh, H. *et al., Agric. Biol. Chem.*, 1980, **44**, 2871 (*synth*)
Koenst, W.M.B. *et al., Synth. Commun.*, 1980, **10**, 899 (*synth*)
Herion, P. *et al., Phytochem. Anal.*, 1993, **4**, 235-239 (*isol, cd*)
Weyerstahl, P. *et al., Annalen*, 1994, 415 (*synth*)
Anderson, P.G. *et al., Tetrahedron*, 1994, **50**, 559 (*synth*)
Paquette, L.A. *et al., J.O.C.*, 1996, **61**, 1119 (*synth*)
Nilsson, Y.I.M. *et al., J.O.C.*, 1996, **61**, 1825 (*synth*)

Thebaine T-339

[115-37-7]

6,7,8,14-Tetradehydro-4,5-epoxy-3,6-dimethoxy-17-methylmorphinan, 9CI. Codeinone methyl enol ether. Paramorphine



(−)-*form*

$C_{19}H_{21}NO_3$ 311.38

Log P 1.49 (uncertain value) (calc).

▶ LD_{50} (mus, ipr) 20 mg/kg. QD2975000

(-)-*form*

Minor constit. of opium. Rectangular plates (EtOH); needles by subl.; also obt. in cubes and prisms. Sol. C_6H_6, $CHCl_3$, v. spar. sol. petrol. Mp 192.5°. $[\alpha]_D^{16}$ -221 (c, 0.35 in MeOH). Log P 1.49 (uncertain value) (calc). Pharmacol. active isomer.

O^3-*De-Me:* [467-04-9] *6,7,8,14-Tetradehydro-4,5-epoxy-6-methoxy-17-methylmorphinan-3-ol.* ***Oripavine***

$C_{18}H_{19}NO_3$ 297.353

Alkaloid from opium poppy (*Papaver somniferum*). Needles (EtOH). Mp 201-202°. $[\alpha]_D^{20}$ -216.9 (c, 3.44 in $CHCl_3$). Log P 0.91 (uncertain value) (calc).

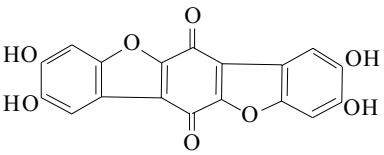
▶ QD2097500

Kiselev, V.V. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1948, **18**, 142; 855 (*Oripavine*)
Bentley, K.W. *et al., Chemistry of the Morphine Alkaloids*, Oxford Univ. Press, 1954, 184 (*isol, props*)
Okuda, S. *et al., Chem. Pharm. Bull.*, 1964, **12**, 104 (*pmr*)
Brochmann-Hanssen, E. *et al., J. Pharm. Sci.*, 1964, **53**, 1549 (*glc, tlc*)
Barton, D.H.R. *et al., J.C.S.*, 1965, 2423 (*biosynth*)

Rapoport, H. *et al., J.A.C.S.*, 1967, **89**, 1942 (*synth*)
Wheeler, D.M.S. *et al., J.A.C.S.*, 1967, **89**, 4494 (*ms*)
Kametani, T. *et al., J.C.S.(C)*, 1969, 2030 (*synth, uv, ord, cd*)
Barber, R.B. *et al., J. Med. Chem.*, 1975, **18**, 1074 (*synth*)
Terui, Y. *et al., Tet. Lett.*, 1975, 2853 (*cmr*)
Weller, D.D. *et al., J. Med. Chem.*, 1976, **19**, 1171 (*synth*)
Shaffie, A. *et al., J. Polym. Sci.*, 1977, **66**, 1050 (*Oripavine, isol, uv, ir*)
Neilsen, B. *et al., Planta Med.*, 1983, **48**, 205 (*Oripavine, isol, pmr, ms*)
Rice, K.C. *et al., Chem. Biol. Isoquinoline Alkaloids, Int. Symp., Phytochem. Soc. Eur., Abstr. Pap.*, 1985, 191 (*rev, synth*)
Mahler, C.H. *et al., Acta Cryst. C*, 1996, **52**, 3193-3195 (*(-)-form, cryst struct*)
Coop, A. *et al., Heterocycles*, 1998, **49**, 43-47 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEN000

Thelephoric acid T-340

[479-64-1]
2,3,8,9-Tetrahydroxybenzo[1,2-b:4,5-b′]bisbenzofuran-6,12-dione, 9CI

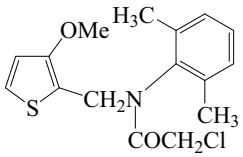


$C_{18}H_8O_8$ 352.256
Constit. of the cap skin of *Suillus grevillei* (larch bolete). Black powder with metallic reflex. Almost insol. org. solvs. except Py. Mp 300°. λ_{max} 217 (log ϵ 4.33); 264 (log ϵ 4.27); 305 (log ϵ 4.3); 390 (sh) (log ϵ 3.48); 483 (log ϵ 3.86) (EtOH).

Gripenberg, J. *et al., Tetrahedron*, 1960, **10**, 135 (*isol, struct, synth*)
Lounasmaa, M. *et al., Acta Chem. Scand.*, 1965, **19**, 540 (*synth*)
Sullivan, G. *et al., J. Pharm. Sci.*, 1971, **60**, 1727 (*isol*)
Edwards, R.L. *et al., J.C.S. Perkin 1*, 1973, 1921 (*isol*)
Gill, M. *et al., Prog. Chem. Org. Nat. Prod.*, 1987, **51**, 13; 31 (*rev, occur*)
Jokela, R. *et al., Planta Med.*, 1997, **63**, 381-383 (*pmr, cmr*)
Kwak, J.-Y. *et al., J. Microb. Biotechnol.*, 1999, **9**, 798-803; *CA*, **132**, 276370x (*isol, activity*)

Thenylchlor, BSI T-341

[96491-05-3]
2-Chloro-N-(2,6-dimethylphenyl)-N-[(3-methoxy-2-thienyl)methyl]acetamide, 9CI. 2-Chloro-N-(3-methoxy-2-thenyl)-2′,6′-dimethylacetamilide

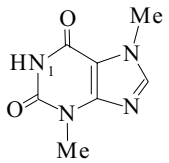


$C_{16}H_{18}ClNO_2S$ 323.842
Brown solid. Mp 72-74°. $Bp_{0.5}$ 173-175°.
▶ LD_{50} (rat, orl) >5000 mg/kg.

Japan. Pat., 1985, 60 202 803, (*Tokuyama*); *CA*, **104**, 83807h (*synth, activity*)
Okamoto, H. *et al., Bull. Chem. Soc. Jpn.*, 1991, **64**, 2128-2130 (*synth, ir, pmr*)
Pesticide Manual, 11th edn., 1997, No. 700

Theobromine, BAN T-342

[83-67-0]
3,7-Dihydro-3,7-dimethyl-1H-purine-2,6-dione, 9CI. 3,7-Dimethylxanthine. Diurobromine. Santheose. Thesal. FEMA 3591. Many other names



$C_7H_8N_4O_2$ 180.166
Constit. of tea leaves (*Camellia thea*), cocoa *Theobroma cacao*, cola nut (*Cola acuminata*) and guarana (*Paullinia cupana*); flavouring ingredient with a bitter taste. Monoclinic needles. Mp 351°. Subl. 290. pK_{a1} 1; pK_{a2} 10 (25°). Log P -0.69 (calc).
▶ Human systemic effects by ingestion (CNS and gastrointestinal). LD_{50} (rat, orl) 1265 mg/kg. Exp. reprod. and teratogenic effects (large dose). XH2275000

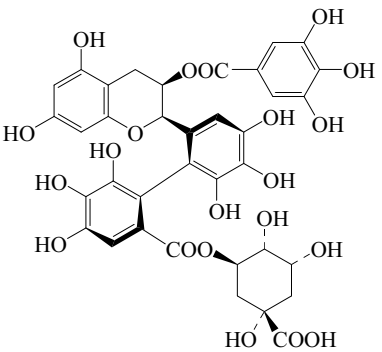
Perchlorate:
Mp 271-273° dec.

1-Hexyl: [1028-33-7] ***Pentifylline, BAN, INN.*** *Cosaldon. Hexyltheobromine. SK 7*
$C_{13}H_{20}N_4O_2$ 264.327
Mp 82-83°. Log P 2.59 (uncertain value) (calc).
▶ UO8450000

Blout, E.R. *et al., J.A.C.S.*, 1950, **72**, 479 (*ir*)
Lockhart, E.L. *et al., J.A.C.S.*, 1950, **72**, 5328 (*uv*)
Spiteller, G. *et al., Monatsh. Chem.*, 1962, **93**, 632 (*ms*)
Twanmoh, L.-M. *et al., J. Het. Chem.*, 1973, **10**, 187 (*pmr*)
Nicolau, C. *et al., Z. Naturforsch., C*, 1974, **29**, 475 (*cmr*)
Bergmann, F. *et al., J.O.C.*, 1977, **42**, 2470 (*synth*)
Royer, R.F. *et al., Actual. Pharmacol.*, 1982, **191**, 36 (*rev, pharmacol*)
Ueda, T. *et al., Heterocycles*, 1982, **19**, 2291 (*synth*)
Tarka, S.M. *et al., Prog. Clin. Biol. Res.*, 1984, **158**, 9 (*props, isol, biosynth*)
Shively, C.A. *et al., Toxicol. Appl. Pharmacol.*, 1986, **84**, 593 (*metabol, toxicol, rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 688 (*synonyms*)
Atta-ur-Rahman, *et al., The Alkaloids*, 1990, **38**, 230 (*spectral props*)
Fujii, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2833 (*synth, uv, pmr*)
IARC Monog., 1991, **51**, 421 (*rev, tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1318
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 751
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2771-2772
Ford, K.A. *et al., Acta Cryst. C*, 1998, **54**, 1980-1983 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEO500

Theogallinin T-343

[144207-58-9]

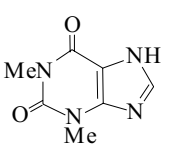


$C_{36}H_{32}O_{21}$ 800.636
Fermentation prod. isol. from black tea. Pale brown powder + $7H_2O$. $[\alpha]_D^{19}$ -79.2 (c, 0.5 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1383-1389 (*isol, cd, pmr, cmr*)

Theophylline, BAN, JAN, USAN T-344

[58-55-9]
3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione, 9CI. 1,3-Dimethylxanthine. Austyn. Elan. Elixophyllin. Euphyllin. Nuelin. Spophyllin retard. Teonova. Theocin. Theodel. Theo-Dur. Theograd. Theolair. Theona P. Theotard. Uniphyllin. Many other names



$C_7H_8N_4O_2$ 180.166
Constit. of tea leaves (*Camellia thea*) and maté (*Ilex paraguariensis*). Mp 268° Mp 264°. pK_{a1} 1; pK_{a2} 8.6 (25°). Log P -0.06 (uncertain value) (calc).
▶ Adverse effects reported when used therapeutically incl. gastrointestinal and CNS

changes. Overdosage can cause death. LD_{50} (rat, orl) 244 mg/kg. Exp. reprod. and teratogenic effects. XH3850000

[5967-84-0, 8002-89-9, 49746-06-7, 85531-28-8]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **3**, 214B (*nmr*)
Blout, E.R. *et al., J.A.C.S.* , 1950, **72**, 479 (*ir*)
Spiteller, G. *et al., Monatsh. Chem.* , 1962, **93**, 632 (*ms*)
Twanmoh, L.-M. *et al., J. Het. Chem.* , 1973, **10**, 187 (*pmr*)
Takayama, S. *et al., Chem. Pharm. Bull.* , 1974, **22**, 1200 (*synth, uv*)
Cohen, J.L. *et al., Anal. Profiles Drug Subst.* , 1975, **4**, 466 (*rev, ir, pmr, uv, ms, anal*)
Goeber, B. *et al., Pharmazie*, 1978, **33**, 717 (*ms*)
Naqvi, A.A. *et al., J. Appl. Crystallogr.* , 1981, **14**, 464 (*cryst struct*)
Atta-ur-Rahman, *et al., The Alkaloids*, 1990, **38**, 232 (*spectra*)
IARC Monog. , 1991, **51**, 391 (*rev, tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1314; 1315; 1319
Ebisuzaki, Y. *et al., Acta Cryst. C*, 1997, **53**, 777-779 (*cryst struct*)
Markham, A. *et al., Drugs*, 1998, **56**, 1081-1091 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEP000; TEP500

Thermocins T-345

Prod. by *Bacillus stearothermophilus*. Bacteriocins with potential food uses.

Thermocin 10 [88232-99-9]

Thermocin 93 [71950-65-7]
Prod. by *Bacillus stearothermophilus* RS93.

Sharp, R.J. *et al., J. Gen. Microbiol.* , 1979, **111**, 449-451 (*Thermocin 93*)
Fikes, J.D. *et al., Can. J. Microbiol.* , 1983, **29**, 1576-1582 (*Thermocin 10*)

Thermoleovorin T-346

Thermoleovorin S2 [144378-02-9]
Prod. by *Bacillus thermoleovorans* S-II.

Thermoleovorin NR 9 [144378-01-8]
Prod. by *Bacillus thermoleovorans* NR-9.

Novotny, J.F. *et al., Appl. Environ. Microbiol.* , 1992, **58**, 2393-2396 (*isol*)

Thermophilin 1 T-347

Protein. Prod. by *Streptococcus thermophilus* CNCM I-1351. Bacteriocin, can be used to inhibit bacterial growth in foods.

Eur. Pat. , 1995, 643 136; *CA* , **123**, 79465v (*isol*)

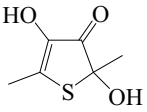
Thermophilin A T-348

Glycoprotein. Bacteriocin. Prod. by *Streptococcus thermophilus* ST134.

Ward, D.J. *et al., Appl. Microbiol. Biotechnol.* , 1995, **43**, 330-335 (*isol*)

Thiacremonone T-349

[96504-28-8]
2,4-Dihydroxy-2,5-dimethyl-3(2H)-thiophenone, 9CI

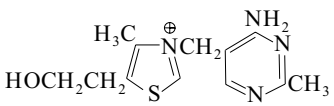


$C_6H_8O_3S$ 160.193
Formed in the Maillard reaction of Cystine and 4-Hydroxy-2,5-dimethyl-3(2*H*)-furanone, H-407. Oil. Racemic λ_{max} 364 (ϵ 6000) (MeOH).

Shu, C.K. *et al., J. Agric. Food Chem.* , 1985, **33**, 638-641 (*occur*)
Gehrt, A. *et al., Nat. Prod. Lett.* , 2000, **14**, 281-284

Thiamine, BAN, INN T-350

[70-16-6]
3-[(4-Amino-2-methyl-5-pyrimidinyl)-methyl]-5-(2-hydroxyethyl)-4-methylthiazolium(1+), 9CI, 8CI. Vitamin B_1. Torulin. Oryzanin. Aneurine. Vitaneurin. Many other names



$C_{12}H_{17}N_4OS^{\oplus}$ 265.358
Essential vitamin. Present in yeast, eggs, liver, milk, green vegetables, roots, tubers and cereals, esp. rice husks. Dietary supplement esp. in baked goods and grain products. Sol. H_2O; sl. sol. EtOH. pK_a 5.17. Log P -3.91 (uncertain value) (calc). Labile in acid or alkaline soln. or on heating. In alkaline soln. the thiazolium ring is reversibly opened to thiols. In therapy thiamine can be replaced by various ring-opened analogues, e.g. Benfotiamine.

Chloride: [59-43-8] *Thiamine monochloride. Thiacrat*
$C_{12}H_{17}ClN_4OS$ 300.811
Nutrient supplement. Cryst. + $1H_2O$ (H_2O). Mp 120-122° dec., 163-165° dec. (anhyd.). Infrequently encountered, hydrochloride more stable.
▶ XI6550000

Chloride; hydrochloride: [67-03-8] ***Thiamine hydrochloride, USAN***. *Bewon. Betaxin. Betalin S. Vinothiam. FEMA 3322*
$C_{12}H_{18}Cl_2N_4OS$ 337.272
Nutrient supplement; flavouring ingredient with a bitter taste. Plates or cryst. (EtOH). V. sol. H_2O; spar. sol. EtOH; insol. Et_2O, C_6H_6. Mp 248° dec. Mp is not a good criterion of purity.
▶ XI7350000

Nitrate: [532-43-4] ***Thiamine mononitrate, USAN***
$C_{12}H_{17}N_5O_4S$ 327.363
Nutrient supplement, used for the enrichment of flour mixes. Mp 164-165° Mp 196-200°.
▶ XI7400000

O-*Phosphate, chloride:* [532-40-1] *Monophosphothiamine chloride*
$C_{12}H_{18}ClN_4O_4PS$ 380.791
Mp 200°.

O-*Diphosphate:* See Thiamine diphosphate in *The Combined Chemical Dictionary.*

O-*Triphosphate:* [15666-52-1] *Thiamine triphosphate. Thiamine triphosphoric acid. TTP*†
$C_{12}H_{20}N_4O_{13}P_3S$ 553.296
Cryst. (EtOH aq.). CAS no. refers to chloride.

[7019-71-8]

Aldrich Library of NMR Spectra, 2nd edn. , 1983, **2**, 515C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **2**, 647A (*ir*)
Todd, A.R. *et al., J.C.S.* , 1937, 364; 1938, 26 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta* , 1946, **29**, 711 (*phosphate*)
Lenormant, H. *et al., Bull. Soc. Chim. Fr.* , 1954, 375 (*ir, uv*)
Greiling, H. *et al., Nature (London)* , 1958, **13**, 251 (*isol, triphosphate*)
Kotera, K. *et al., Chem. Pharm. Bull.* , 1965, **13**, 440 (*pmr*)
Hesse, M. *et al., Helv. Chim. Acta* , 1967, **50**, 808 (*ms*)
Linnett, P.E. *et al., J.C.S.(C)* , 1967, 796 (*biosynth*)
Pletcher, J. *et al., Acta Cryst. B* , 1972, **28**, 2928 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe* , 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2609
Holzbecher, J. *et al., Anal. Chim. Acta* , 1973, **64**, 147 (*detn, P*)
Dwidevi, B.K. *et al., J. Agric. Food Chem.* , 1973, **21**, 54 (*props*)
Gallo, A.A. *et al., J. Biol. Chem.* , 1974, **249**, 1382 (*cmr*)
Thiamine, [Proc. Pap. Discuss. U.S.-Jpn. Semin.], 2nd , Wiley, N.Y., 1976, (*book*)
Oka, Y. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley* , 1978, **24**, 124 (*synth*)
Penttinen, H.K. *et al., Methods Enzymol.* , 1979, **62**, 112 (*triphosphate*)
Brown, G.M. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.* , 1982, **53**, 345 (*biosynth*)
Sable, H.Z. *et al., Ann. N.Y. Acad. Sci.* , 1982, **378**, 78; 378; 454 (*book, nmr, cryst struct, conformn*)
Uray, G. *et al., Monatsh. Chem.* , 1982, **113**, 1475 (*synth*)
Davis, R.E. *et al., Adv. Clin. Chem.* , 1983, **23**, 93 (*chemistry*)
Ishida, T. *et al., Acta Cryst. C*, 1984, **40**, 437 (*cryst struct*)
Gubler, C.J. *et al., Handbook of Vitamins* , (Machlin, L.J. Ed.), M. Dekker, New York, 1984, 245 (*rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag* , 1987, 2515; 2540; 4574
Al-Rashood, K.A.M. *et al., Anal. Profiles Drug Subst.* , 1989, **18**, 413 (*rev*)
Contant, P. *et al., Helv. Chim. Acta* , 1990, **73**, 1300 (*synth*)
Hu, N. *et al., Acta Cryst. C*, 1992, **48**, 1951 (*cryst struct*)
Bender, D.A. *et al., Nutritional Biochemistry of the Vitamins* , Cambridge University Press, Cambridge, 1992, 128 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1053
Casas, J.S. *et al., Acta Cryst. C*, 1994, **50**, 1265 (*cryst struct, acetate*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 1797
Estramareix, B. *et al., New J. Chem.* , 1996, **20**, 607 (*rev, biosynth*)
Spenser, I.D. *et al., Angew. Chem., Int. Ed.* , 1997, **36**, 1033-1046 (*rev, biosynth*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2772-2778 (*rev, use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TES750; TET300; TET500

Thiazole, 9CI, 8CI T-351

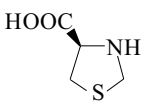
[288-47-1]
FEMA 3615



C_3H_3NS 85.129
Flavouring ingredient. Liq. with characteristic unpleasant odour. d^{17} 1.2. Bp 117-118.5°. n_D^{25} 1.5371. pK_a 2.52 (25°). Forms azeotrope with H_2O.
▶ LD_{50} (mus, orl) 983 mg/kg. XJ1290000
Hydrobromide: [39657-68-6]
Cryst. (EtOH/Et_2O). Mp 188-189°.
Picrate salt: [99066-95-2]
Yellow needles (H_2O or EtOH). Mp 159-160° dec. Sinters at 150°.
Methiodide: [31766-74-2] *3-Methylthiazolium iodide, 9CI*
C_4H_6INS 227.069
Needles (EtOH). Mp 150-150.5°.
Metho(4-methylbenzenesulfonate): [16183-01-0]
Cryst. (EtOH). Mp 159°.
N-*Oxide:*
C_3H_3NOS 101.129
Light yellow glass.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 642D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 108B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1491C (*ir*)
McLean, J. *et al., J.C.S.*, 1942, 383 (*synth*)
Hafferl, W. *et al., Biochemistry*, 1963, **2**, 1298 (*deriv*)
Iversen, P.E. *et al., Synthesis*, 1972, 484 (*synth*)
Salmona, G. *et al., Org. Mass Spectrom.*, 1978, **13**, 119 (*ms*)
Metzger, J.V. *et al., Chem. Heterocycl. Compd.*, Pt. 1-3, Wiley-Interscience, 1979, **34**, (*rev*)
Brandsma, L. *et al., Synthesis*, 1985, 948 (***synth***)
Tseng, C.K. *et al., Magn. Reson. Chem.*, 1987, **25**, 105 (*cmr, pmr*)
Pérez-Peña, J. *et al., Coll. Czech. Chem. Comm.*, 1989, **54**, 28 (*ir, Raman*)
Begtrup, M. *et al., Acta Chem. Scand.*, 1992, **46**, 372 (*oxide*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 752
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2778

4-Thiazolidinecarboxylic acid T-352

[444-27-9]
Thioproline. ***Timonacic, INN.*** *γ-Thiaproline. Heparegen. NSC 25855. Many other names*



(*R*)-*form*

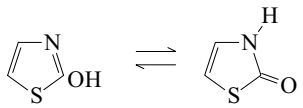
$C_4H_7NO_2S$ 133.171
pK_{a1} 1.51; pK_{a2} 6.21 (25°).
▶ Human systemic effects by ingestion incl. somnolence, tremors, altered renal function. LD_{50} (rat, orl) 875 mg/kg. XJ5425000
(*R*)-*form* [34592-47-7]
L-form
Needles (H_2O). Mp 196-197° dec Mp 205-209°. $[\alpha]_D^{20}$ -141 (c, 1.3 in H_2O). $[\alpha]_D^{22}$ -100 (1*M* HCl). $[\alpha]_D$ -203 (1*M* NaOH).
▶ XJ5425500
Hydrochloride: [67089-84-3]
Prisms (dil. HCl). Mp 184-185° dec.
Me ester: [42258-90-2]
$C_5H_9NO_2S$ 147.198
Bp_1 75°. $[\alpha]_D^{23}$ -83 (H_2O). $[\alpha]_D^{21}$ -106.3 (C_6H_6).
Me ester; hydrochloride: [65983-36-0]
Plates (MeOH/Et_2O). Mp 164-165° dec.
N-*Benzoyl:* [111390-63-7]
$C_{11}H_{11}NO_3S$ 237.279
Syrup. $[\alpha]_D^{20}$ -153 (c, 10.9 in DMSO).
N-*Carbethoxy:* See Telmesteine in *The Combined Chemical Dictionary.*
N-*Nitroso:* [86594-16-3]
$C_4H_6N_2O_3S$ 162.169
Non-mutagenic contaminant of smoked cured meats. A marker for *in vivo N*-nitrosations. Cryst. (CH_2Cl_2/pentane). Mp 86-88° Mp 105-106° (101-102°) Mp 180°.
(±)-*form* [19291-02-2]
Prisms (H_2O). Mp 183-184° dec Mp 195°. Log P -0.79 (calc).
▶ XJ5425300
Et ester: [51977-21-0]
$C_6H_{11}NO_2S$ 161.224
Bp_{13} 125°.

[45521-09-3]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 506B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 596D (*ir*)
Ratner, S. *et al., J.A.C.S.*, 1937, **59**, 200-206 (*synth*)
Martin, R.B. *et al., J.A.C.S.*, 1965, **87**, 1065-1070 (*pmr, conformn*)
Rambacher, P. *et al., Chem. Ber.*, 1968, **101**, 2595-2597 (*synth*)
Bollier, F. *et al., Gazz. Med. Ital.*, 1972, **131**, 251-255 (*pharmacol, tox*)
Loscalzo, J. *et al., Arch. Biochem. Biophys.*, 1973, **157**, 426-430 (*cryst struct*)
Chacko, K.K. *et al., Cryst. Struct. Commun.*, 1974, **3**, 561-564 (*cryst struct*)
Vestling, M.M. *et al., J. Het. Chem.*, 1975, **12**, 243-246 (*synth, ir, pmr, ms*)
Parthasarathy, R. *et al., J.A.C.S.*, 1976, **98**, 6634-6643 (*cryst struct, pmr*)
Kamo, J. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 706-710 (*abs config*)
Weber, H.U. *et al., Arch. Gerontol. Geriatr.*, 1982, **1**, 299-310 (*rev, pharmacol*)
Naulet, N. *et al., Org. Magn. Reson.*, 1983, **21**, 564-566 (*N-15 nmr*)
Howard-Lock, H.E. *et al., Can. J. Chem.*, 1986, **64**, 1215-1219 (*synth, ir, pmr, cmr*)
Shiraiwa, T. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 3277-3283; 1989, **62**, 109-113 (*resoln, synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 207
Lin, I.-N.C. *et al., Food Addit. Contam.*, 1990, **7**, 357-368 (*N-nitroso*)
Tsuda, M. *et al., IARC Sci. Publ.*, 1991, **109**, 123-128 (*N-nitroso*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1421
Refouvelet, B. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1076-1083 (*Et ester, synth, ir, pmr*)
Pellegrini, N. *et al., Chem. Pharm. Bull.*, 1999, **47**, 950-955 (*synth, ir, pmr*)
Braibante, M.E.F. *et al., Synthesis*, 1999, 943-946 (*synth, ir*)
Refouvelet, B. *et al., J. Het. Chem.*, 2000, **37**, 1425-1430 (*R-form, synth, pmr*)
Kaupp, G. *et al., J. Prakt. Chem.*, 2000, **342**, 269-280 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEV000

2(3*H*)-Thiazolone T-353

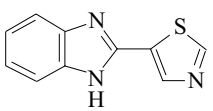
[6039-97-0]
4-Thiazolin-2-one. 2-Hydroxythiazole. 2-Thiazolol



C_3H_3NOS 101.129
Exists in soln. entirely or predominantly in the oxo-form.
OH-form
O-*Et:* [15679-19-3] *2-Ethoxythiazole. FEMA 3340*
C_5H_7NOS 129.182
Flavouring ingredient. Oil. $Bp_{3.7}$ 35°.
Cornwell, S.P. *et al., J.C.S. Perkin 1*, 1981, 2340 (*uv, ir, pmr, cmr*)
Al-Awadi, N. *et al., J.C.S. Perkin 2*, 1986, 1589 (*O-Et*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 213 (*O-Et*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 939 (*O-Et*)

2-(4-Thiazolyl)-1*H*-benzimidazole, 9CI T-354

[148-79-8]
Thiabendazole, BAN, BSI, ISO, JMAF, USAN. *Tiabendazole, INN. Mintezol. Thiprazole. Equizole. Thiabendole. Thibendole. Thibenzole. TBZ. Mertect. Tecto. Storite. Many other names*



$C_{10}H_7N_3S$ 201.251
Anthelmintic, pre- and postharvest fungicide, also freq. for vet. use. Used as a postharvest treatment for bananas, plantains and oranges. Registered in Canada for control of silver scurf in stored potatoes. Mp 304-305°. Log P 2.34 (calc). Component of Ranizole.
▶ Shows teratogenic activity in mice. LD_{50} (rat, orl) 3100 mg/kg. Exp. teratogen. Exp. nephrotoxic effects. DE0700000
Benzoyl:
$C_{17}H_{11}N_3OS$ 305.359
Mp 147°.

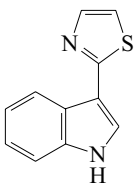
1-N-*Me:* [32594-70-0]
$C_{11}H_9N_3S$ 215.278
Mp 139-140°.

[50933-50-1]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 187C (*nmr*)
Brown, H.D. *et al., J.A.C.S.*, 1961, **83**, 1764 (*synth*)
Grenda, V.J. *et al., J.O.C.*, 1965, **30**, 259 (*synth, uv*)
Trus, B.L. *et al., Acta Cryst. B*, 1973, **29**, 2298 (*cryst struct*)
Daldrup, T. *et al., Fresenius' Z. Anal. Chem.*, 1981, **308**, 413 (*detn*)
Kapoor, V.K. *et al., Anal. Profiles Drug Subst.*, 1987, **16**, 611 (*pharmacol*)
Tsuchiya, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2985 (*metab, tox*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1403
Tada, Y. *et al., Food Chem. Toxicol.*, 1989, **27**, 307 (*rev, tox*)
Fujitani, T. *et al., Food Chem. Toxicol.*, 1991, **29**, 265 (*rev, tox*)
Pesticide Manual, 9th edn., 1991, No. 11500
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A391
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 54
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TEX000

3-(2-Thiazolyl)-1*H*-indole, 9CI T-355

[135531-86-1]
Camalexin. *2-(3-Indolyl)thiazole*



$C_{11}H_8N_2S$ 200.264
Alkaloid from the leaves of *Camelina sativa* (false flax) infected by the fungus *Alternaria brassicae*. Cryst. (MeOH). Mp 134-137°. λ_{max} 214 (ϵ 22200); 274 (ϵ 7900); 318 (ϵ 13800) (MeOH) (Derep).

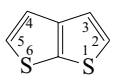
N^1-*Me:* [194155-86-7] *1-Methyl-3-(2-thiazolyl)-1*H*-indole, 9CI*. ***1-Methylcamalexin***
$C_{12}H_{10}N_2S$ 214.29
From *Capsella bursa-pastoris* (shepherd's purse) infected with *Alternaria brassicae*.

6-Methoxy: [135531-87-2] *6-Methoxy-3-(2-thiazolyl)-1*H*-indole.* ***Methoxycamalexin***
$C_{12}H_{10}N_2OS$ 230.29
From *Camelina sativa* (false flax) infected with *Alternaria brassicae*. Cryst. (MeOH/hexane). Mp 157-159°. λ_{max} 218 (ϵ 21700); 296 (ϵ 11500); 324 (ϵ 11300) (MeOH) (Derep).

Browne, L.M. *et al., Tetrahedron*, 1991, **47**, 3909 (*isol, uv, ir, pmr, cmr, ms, struct*)
Ayer, W.A. *et al., Tetrahedron*, 1992, **48**, 2919 (*synth*)
Fürstner, A. *et al., Tetrahedron*, 1995, **51**, 773 (*synth*)
Sakamoto, T. *et al., J.C.S. Perkin 1*, 1996, 1927 (*synth, pmr*)
Pedras, M.S.C. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 2255-2260 (*metab*)
Jimenez, L.D. *et al., Phytoprotection*, 1997, **78**, 99-103 (*1-Methylcamalexin*)
Pedras, M.S.C. *et al., Phytochemistry*, 2000, **53**, 161-176 (*rev*)
Dzurilla, M. *et al., Molecules*, 2001, **6**, 716-720 (*synth*)

Thieno[2,3-*b*]thiophene T-356

[250-84-0]
Liquid thiophthene. 1,6-Thiophthene



$C_6H_4S_2$ 140.23
Maillard product. Yellow oil. Bp_1 75-80°.

Picrate:
Mp 135-136°.

Gronowitz, S. *et al., Acta Chem. Scand.*, 1967, **22**, 812 (*synth*)
Boicelli, C.A. *et al., J.C.S. Perkin 2*, 1972, 599 (*pmr*)
Litvinov, V.P. *et al., Adv. Heterocycl. Chem.*, 1976, **19**, 123 (*rev*)
de Jong, R.L.P. *et al., Chem. Comm.*, 1983, 1056 (*synth*)
Jacobsen, J.P. *et al., J. Mol. Struct.*, 1984, **118**, 345 (*pmr*)
de Jong, R.L.P. *et al., Synth. Commun.*, 1991, **21**, 145 (*synth*)
Otsubo, T. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 2033 (*synth*)
Comel, A. *et al., J. Het. Chem.*, 2001, **38**, 1167-1171 (*synth, uv, pmr, cmr*)

1-(2-Thienyl)-1-butanone, 9CI T-357

[5333-83-5]
2-Butyrylthiophene. 2-Butyrothienone. Propyl 2-thienyl ketone



$C_8H_{10}OS$ 154.232
Flavour enhancer for coffee. Liq. Bp_{745} 240° Bp_3 97°.

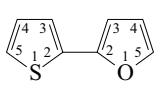
Semicarbazone:
Cryst. Mp 173.5-174°.

2,4-Dinitrophenylhydrazone:
Cryst. Mp 167°.

Org. Synth., Coll. Vol., 2, 1943, 8 (*synth*)
Nakhmanovich, A.S. *et al., Khim. Geterotsikl. Soedin.*, 1970, 894; *CA*, **74**, 87722 (*synth*)
U.S. Pat., 1976, 4 000 328; *CA*, **86**, 87910u (*use*)
Konishi, H. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 957

2-(2-Thienyl)furan T-358

[27521-80-8]
2-(2-Furanyl)thiophene



C_8H_6OS 150.201
Component of yeast extract volatiles and cooked meat flavour model systems. Yellow oil.

Wynberg, H. *et al., J.O.C.*, 1971, **36**, 1011
Carpita, A. *et al., Tetrahedron*, 1985, **41**, 1919 (*synth, pmr, ir, cmr*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*isol, ms, pmr*)
Werkhoff, P. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1991, **131**, 30-57 (*occur, yeast*)

1-(2-Thienyl)-1-heptanone, 9CI T-359

[30711-40-1]
2-Heptanoylthiophene

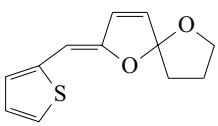


$C_{11}H_{16}OS$ 196.313
Constit. of roast beef aroma. d_4^{20} 1.03. Bp_{10} 150°.

Grey, T.F. *et al., J.C.S.*, 1960, 1502-1508 (*synth*)
Hsu, C.-M. *et al., J. Food Sci.*, 1982, **47**, 2068-2069 (*occur*)

2-(2-Thienylmethylene)-1,6-dioxaspiro[4.4]non-3-ene T-360

[124442-15-5]

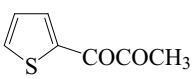


$C_{12}H_{12}O_2S$ 220.292
Isol. from *Chrysanthemum coronarium* (chop-suey greens). Yellowish oil.

Sanz, J.F. *et al., Annalen*, 1990, 303 (*isol, pmr, cmr*)
Gao, Y. *et al., Tet. Lett.*, 1996, **37**, 893 (*synth*)

1-(2-Thienyl)-1,2-propanedione, 9CI, 8CI T-361

[13678-69-8]
2-Pyruvoylthiophene

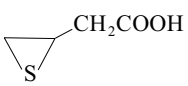


$C_7H_6O_2S$ 154.189
Flavouring ingredient. Component of flavourants produced by reaction of H_2S and glucose. Yellow cryst. with woody odour. Bp_{12} 101-105°.

Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628-694 (*synth, ms, uv, ir*)
U.S. Pat., 1975, 3 924 015; *CA*, **84**, 164364g (*synth, use*)
Sakaguchi, M. *et al., J. Agric. Food Chem.*, 1978, **26**, 1260-1262 (*occur*)

Thiiraneacetic acid T-362

3,4-Epithiobutanoic acid



$C_4H_6O_2S$ 118.156

Parent acid unknown.

Nitrile: [58130-93-1] *Thiiraneacetonitrile, 9CI. 1-Cyano-2,3-epithiopropane. (Cyanomethyl)thiirane*
C_4H_5NS 99.156
Hydrol. prod. from seeds of *Brassica campestris*.

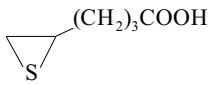
► Mutagenic.

[76786-80-6]

Cole, R.A. *et al., Phytochemistry*, 1975, **14**, 2293
Luethy, L. *et al., Phytochemistry*, 1979, **18**, 2028 (*isol*)
Luethy, L. *et al., Int. J. Vitam. Nutr. Res.*, 1980, **50**, 423 (*synth, tox*)
Petroski, R.J. *et al., Phytochemistry*, 1985, **24**, 213 (*biosynth*)

Thiiranebutanoic acid, 9CI T-363

5,6-Epithiohexanoic acid



$C_6H_{10}O_2S$ 146.21

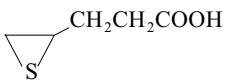
Nitrile: [58130-94-2] *Thiiranebutanenitrile, 9CI. 1-Cyano-4,5-epithiopentane. (3-Cyanopropyl)thiirane*
C_6H_9NS 127.21
Hydrol. prod. from seeds of *Brassica campestris*.

[76786-82-8]

Cole, R.A. *et al., Phytochemistry*, 1975, **14**, 2293
Luethy, L. *et al., Int. J. Vitam. Nutr. Res.*, 1980, **50**, 423 (*synth*)

Thiiranepropanoic acid, 9CI T-364

3,4-Epithiopentanoic acid



$C_5H_8O_2S$ 132.183

(ξ)-form

Nitrile: [54096-45-6] *Thiiranepropanenitrile, 9CI. 1-Cyano-3,4-epithiobutane*
C_5H_7NS 113.183
Hydrol. prod. from seeds of *Brassica campestris*.

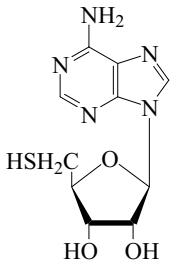
► LD_{50} (rat, scu) 109 mg/kg. Exp. reprod. and teratogenic effects. YV8525000

[76786-81-7]

Kirk, J.T.O. *et al., Phytochemistry*, 1974, **13**, 2611
Luethy, L. *et al., Int. J. Vitam. Nutr. Res.*, 1980, **50**, 423 (*synth*)
Brocker, E.R. *et al., Phytochemistry*, 1983, **22**, 770 (*biosynth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, EBD600

5′-Thioadenosine, 9CI T-365

[67805-97-4]
6-Amino-9-(5-thioribofuranosyl)purine



$C_{10}H_{13}N_5O_3S$ 283.31
Cryst. (H_2O). Mp 75-77°.

S-*Me:* [2457-80-9] *5′-S-Methyl-5′-thioadenosine, 9CI, 8CI. Adenine thiomethylpentoside*
$C_{11}H_{15}N_5O_3S$ 297.337
Needles (MeOH aq.). Mp 213-214°. $[\alpha]_D$ +12.2 (1% H_2SO_4 aq.).

► AU7410000

S-*Me, 2′,3′*-O-*isopropylidene:*
$C_{14}H_{19}N_5O_3S$ 337.402
Mp 143°.

S-*Me, tritosyl:* [80860-53-3]
$C_{32}H_{33}N_5O_9S_4$ 759.905
Mp 158-160°.

S-*Me,* S-*oxide(*R-*):* [897-42-7]

[3387-65-3] *5′-Deoxy-5′-(methylsulfinyl)adenosine, 9CI*
$C_{11}H_{15}N_5O_4S$ 313.337
Prod. by *Ganoderma lucidum* (reishi). Cryst. Sol. H_2O, MeOH. Mp 185-187°. $[\alpha]_D^{20}$ -23.5 (c, 1.4 in H_2O). λ_{max} 270 (H_2O) (Berdy).

S-*Me,* S-*oxide(*S-*):* [737-74-6]
$C_{11}H_{15}N_5O_4S$ 313.337
Prod. by *Ganoderma lucidum* (reishi). Cryst. Mp 210-211°. $[\alpha]_D$ -93.3 (c, 1 in H_2O).

S-*(2-Methylpropyl):* [35899-54-8]
$C_{14}H_{21}N_5O_3S$ 339.418
Cryst. (EtOH). Mp 126-128°. $[\alpha]_D^{24}$ 0 (c, 0.85 in MeOH).

3′-Epimer, S-*Me:* [53458-29-0] ***9-(5-S-Methyl-5-thio-β-D-xylofuranosyl)adenine***
$C_{11}H_{15}N_5O_3S$ 297.337
Glass. Mp 199-201° (as picrate).

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 219C (*nmr*)

Weygand, F. *et al., Ber.*, 1951, **84**, 633 (*synth*)
Baddiley, J. *et al., J.C.S.*, 1951, 1348 (*synth*)
Satoh, K. *et al., Nature (London)*, 1951, **167**, 238 (*S-Me struct, S-Me tritosyl, S-Me isopropylidene*)
Trauth, O. *et al., Nature (London)*, 1951, **167**, 359 (*S-Me, synth*)
Kuhn, R. *et al., Chem. Ber.*, 1965, **98**, 1699-1704 (*synth*)
Zappia, V. *et al., J. Biol. Chem.*, 1969, **244**, 4499 (*S-Me, biochem*)
Hildesheim, J. *et al., Biochimie*, 1971, **53**, 1067-1071 (*S-2-methylpropyl*)
Montgomery, J.A. *et al., J. Med. Chem.*, 1974, **17**, 1197-1207 (*synth*)
Sugimoto, Y. *et al., Arch. Microbiol.*, 1976, **108**, 175
Borkakoti, N. *et al., Acta Cryst. B*, 1978, **34**, 867 (*S-Me, cryst struct*)
Porcelli, M. *et al., Adv. Exp. Med. Biol.*, 1988, **250**, 219-228 (*3′-epimer-S-Me*)
Porcelli, M. *et al., Biochem. J.*, 1989, **263**, 635-640 (*3′-epimer-S-Me*)
Marriott, J.H. *et al., Tet. Lett.*, 1990, **31**, 7485 (*synth, pmr*)
Robins, M.J. *et al., Can. J. Chem.*, 1991, **69**, 1468 (*S-Me, uv, pmr, cmr, ms*)
Kawagishi, H. *et al., Phytochemistry*, 1993, **32**, 239-241 (*S-Me-S-oxide*)
Pignot, M. *et al., Eur. J. Org. Chem.*, 2000, 549-555 (*synth, pmr, cmr*)

4,4′-Thiobis-2-butanone, 9CI T-366

[40790-04-3]
Bis(3-oxobutyl) sulfide. FEMA 3335
$H_3CCOCH_2CH_2SCH_2CH_2COCH_3$
$C_8H_{14}O_2S$ 174.263
Flavouring and perfumery ingredient. Liq. with spicy, fresh green odour. Bp_2 100-105° (kugelrohr).

Disemicarbazone:
Mp 189-191°. Also forms an anhydroform semicarbazide with Mp 227-228°.

McGinnis, N.A. *et al., J.C.S.*, 1941, 404-408 (*synth*)
Swiss Pat., 1973, 531 559; *CA*, **78**, 115134z (*synth, use*)
Del Mazza, D. *et al., J.O.C.*, 1981, **46**, 128-134 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 155 (*props, use*)

1,1′-Thiobisethanethiol, 9CI T-367

[53897-59-9]
Bis(1-mercaptoethyl) sulfide
$H_3CCH(SH)SCH(SH)CH_3$
$C_4H_{10}S_3$ 154.321
Volatile constit. of cooked mutton. Liq. with allium, meaty odour. Bp_5 77°. n_D^{20} 1.5659. Props. doubtless refer to a mixt. of diastereomers.

Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*synth, ms, pmr*)
Nixon, L.N. *et al., J. Agric. Food Chem.*, 1979, **27**, 355-359 (*occur, mutton*)

1,1′-Thiobis[2-methyl-1-propanethiol], 9CI T-368

Bis(1-mercaptoisobutyl) sulfide
$(H_3C)_2CHCH(SH)SCH(SH)CH(CH_3)_2$
$C_8H_{18}S_3$ 210.428
Liq. with allium-mushroom odour. Bp_4 120°. n_D^{20} 1.5352. Props. doubtless refer to a mixt. of diastereomers.

Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*synth, ms, pmr*)

1,1′-Thiobis-1-propanethiol, 9CI T-369

[53897-60-2]
Bis(1-mercaptopropyl) sulfide
$H_3CCH_2CH(SH)$-S-$CH(SH)CH_2CH_2CH_3$
$C_6H_{14}S_3$ 182.375
Liq. with green, fruity, allium odour. Bp_5 110°. n_D^{20} 1.5489. Props. doubtless refer to a mixt. of diastereomers.

Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*synth, ms, pmr*)

3,3′-Thiobispropanoic acid, 9CI T-370

[111-17-1]
3,3′-Thiodipropionic acid, 8CI. Thiodihy-

dracrylic acid. Diethyl sulfide β,β′-dicarboxylic acid. Bis(2-carboxyethyl) sulfide. 4-Thiaheptanedioic acid

$HOOCCH_2CH_2SCH_2CH_2COOH$

$C_6H_{10}O_4S$ 178.209

Antioxidant used in food packaging materials. Sol. H_2O, EtOH. Mp 134° (129-130°). pK_{a1} 3.84; pK_{a2} 4.66 (25°, 0.1*M* $NaClO_4$). pK_{a1} 4.15; pK_{a2} 4.8 (25°).

▶ Skin and eye irritant. LD_{50} (rat, orl) 3980 mg/kg. UF7990000

Di-Me ester: [4131-74-2]
$C_8H_{14}O_4S$ 206.262
Oil. Mp 7.8°. Bp_{10} 158-159°.

Di-Et ester: [673-79-0]
$C_{10}H_{18}O_4S$ 234.316
Oil. Mp -20°. Bp_7 148°.

Dibutyl ester: [6975-31-1]
$C_{14}H_{26}O_4S$ 290.423
Oil. Bp_2 131°.

Didodecyl ester: [123-28-4] *Didodecyl thiobispropanoate. Dilauryl thiodipropionate. Carstab DLTDP. Ipognox 89. Irganox PS 800. Neganox DLTP*
$C_{30}H_{58}O_4S$ 514.852
Preservative for foods. Cryst. Mp 43-44° (39°).

▶ UF8000000

Ditridecyl ester: [10595-72-9]
$C_{32}H_{62}O_4S$ 542.905
d 0.94. n_D^{20} 1.4700.

Ditetradecyl ester: [16545-54-3]
$C_{34}H_{66}O_4S$ 570.959
Cryst. (Me_2CO). Mp 52-53°.

Dioctadecyl ester: [693-36-7] *Dioctadecyl thiobispropanoate. Naugard DSTDP. Irganox PS 802. Yoshinox DSTDP*
$C_{42}H_{82}O_4S$ 683.173
Cryst. Mp 61°.

▶ UF8010000

Dichloride: [18733-39-6]
$C_6H_8Cl_2O_2S$ 215.099
Oil. Bp_1 120-121°.

Diamide: [5459-10-9]
$C_6H_{12}N_2O_2S$ 176.239
Plates (EtOH). Mp 182°.

Dianilide: [41798-68-9]
$C_{18}H_{20}N_2O_2S$ 328.434
Cryst. (EtOH). Mp 165°.

Dinitrile: [111-97-7] *3,3′-Thiobispropanenitrile. 2,2′-Dicyanodiethyl sulfide*
$C_6H_8N_2S$ 140.209
Needles (Et_2O). Sl. sol. H_2O, EtOH; sol. Me_2CO, $CHCl_3$, C_6H_6. d^{30} 1.11. Mp 28°. Bp_3 178-180°.

▶ Skin and eye irritant. LD_{50} (rat, orl) 4500 mg/kg. UG4375000

S-*Oxide:* [3680-08-8] *3,3′-Sulfinylbispropanoic acid, 9CI*
$C_6H_{10}O_5S$ 194.208
Cryst. (H_2O). Mp 112°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 465A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 529C (*ir*)
Sadtler Standard C-13 NMR Spectra, 4827 (*cmr*)
Sadtler Standard NMR Spectra, 6200 (*pmr*)
MacGregor, J.H. *et al., J.C.S.*, 1950, 736 (*synth, dinitrile, dianilide*)
U.K. Pat., 1965, 980 219; *CA*, **62**, 7645h (*esters*)
Ger. Pat., 1971, 1 935 759, (*Lentia*); *CA*, **75**, 5278e (*esters*)
Laing, D.K. *et al., J.C.S. Dalton*, 1975, 2297 (*synth*)
Prout, K. *et al., Acta Cryst. B*, 1982, **38**, 338 (*cryst struct*)
Kumar, A. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 880 (*esters*)
Srinivas, R. *et al., Org. Mass Spectrom.*, 1989, **24**, 128 (*ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 835; 2781
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BHM000; TFD500; DGS600

1-Thiocyanato-4-(methylthio)-butane T-371

[41756-12-1]
4-(Methylthio)butyl thiocyanate, 9CI

$MeSCH_2CH_2CH_2CH_2SCN$

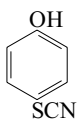
$C_6H_{11}NS_2$ 161.292

Isol. from *Eruca sativa* (rocket). Oil. $Bp_{0.5}$ 105-110°.

Schluter, M. *et al., Phytochemistry*, 1972, **11**, 3427 (*isol*)
Benn, M.H. *et al., Can. J. Chem.*, 1986, **64**, 940 (*synth, ir, pmr, cmr*)

4-Thiocyanatophenol T-372

[3774-52-5]
4-(Hydroxyphenyl) thiocyanate, 9CI



C_7H_5NOS 151.189

Constit. of cucumber root. Long needles (C_6H_6/hexane). Mp 62-63°.

Me ether: [5285-90-5] *1-Methoxy-4-thiocyanatobenzene. 4-Methoxyphenyl thiocyanate*
C_8H_7NOS 165.215
Needles. Mp 31-32°.

Bordwell, F.G. *et al., J.A.C.S.*, 1956, **78**, 854-860 (*synth, uv*)
Schmitz, E. *et al., J. Prakt. Chem.*, 1971, **313**, 1125-1130 (*synth, ir*)
Fujio, M. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2127-2133 (*pmr*)
Yu, J.Q. *et al., Chem. Express*, 1993, **8**, 577-580 (*isol*)
Bangher, A. *et al., Spectrochim. Acta A*, 1995, **51**, 1703-1713 (*pmr, cmr*)
Kita, Y. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1887-1890 (*synth, ir, pmr*)
Still, I.W.J. *et al., Synth. Commun.*, 2001, **31**, 1355-1359 (*Me ether*)

3-Thiocyanato-1-propene T-373

[764-49-8]
2-Propenyl thiocyanate, 9CI. Allyl thiocyanate. Allylrhodamide

$H_2C{=}CHCH_2SCN$

C_4H_5NS 99.156

Present in seeds of *Brassica juncea*.. Pungent oil. d^{15} 1.06. Bp 161°. Rearr. on standing to 3-Isothiocyanato-1-propene, I-194.

▶ XL2000000

Gmelin, R. *et al., Acta Chem. Scand.*, 1959, **13**, 1474 (*isol*)
Kirk, L.D. *et al., J. Am. Oil Chem. Soc.*, 1964, **41**, 599
Emerson, D.W. *et al., J. Chem. Educ.*, 1971, **48**, 81 (*synth*)
Fenwick, G.R. *et al., CRC Crit. Rev. Food Sci. Nutri.*, 1983, **18**, 123 (*occur*)
Gurudutt, K.N. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 343 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGS750

Thiocyanic acid, 9CI T-374

[463-56-9]
Sulfocyanic acid. Hydrogen thiocyanate

$HSC{\equiv}N$

CHNS 59.092

V. strong acid. Various metallic salts (thiocyanates) have ndividual entries. Present in Cruciferae e.g. *Brassica* spp.. Sol. H_2O, EtOH, Et_2O. Mp -110°. pK_a -1.85 (25°). Polymerises at -90°, stable in dil. aq. soln..

NH_4 salt: See Ammonium thiocyanate (NH_4SCN) in *The Combined Chemical Dictionary.*

Me ester: [556-64-9] *Methyl thiocyanate*
C_2H_3NS 73.118
Liq. d^{15} 1.08. Fp -91. Bp_{756} 130.5°. n_D^{15} 1.0765.

▶ LD_{50} (rat, orl) 60 mg/kg. LD_{50} (mus, ipr) 23 mg/kg. XL1575000

Et ester: [542-90-5] *Ethyl thiocyanate, 9CI. Thiocyanatoethane*
C_3H_5NS 87.145
Liq. Insol. H_2O. d^{16} 1.02. Bp 146°.

▶ LD_{50} (mus, ipr) 10 mg/kg. XK9900000

Propyl ester: [4251-16-5] *Propyl thiocyanate. 1-Thiocyanatopropane*
C_4H_7NS 101.172
Liq. with unpleasant odour. Bp 163°.

2-Propenyl ester: 3-Thiocyanato-1-propene, T-373

Ph ester: See Phenyl thiocyanate in *The Combined Chemical Dictionary.*

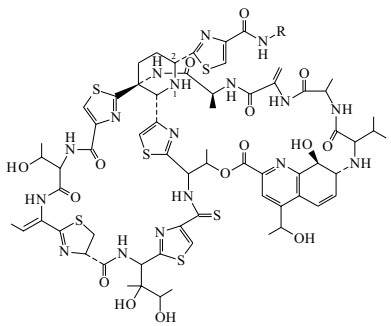
[302-04-5, 593-84-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 873C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1408B; 1408C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 825D; 826A (*ir*)
Kaufmann, H.P. *et al., Ber.*, 1926, **59**, 187 (*synth*)
Dienske, J.W. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1927, **46**, 154
Allen, P. *et al., J.A.C.S.*, 1935, **57**, 198 (*synth*)
Org. Synth., Coll. Vol., 2, 1943, 366 (*synth*)
Brintzinger, H. *et al., Chem. Ber.*, 1952, **85**, 455 (*synth, Me ester*)
Gmelin, R. *et al., Acta Chem. Scand.*, 1960, **14**, 507 (*isol, biosynth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 954
Knoke, D. *et al., Pharmazie*, 1973, **28**, 574; 617 (*rev, synth, Me ester*)
Newman, A.A. *et al., Chem. Biochem. Thiocyanic Acid Its Derivs.*, 1975, (*rev*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 635 (*synth*)
Reeves, W.P. *et al., Synth. Commun.*, 1976, **6**, 509 (*synth, Et ester*)

Katritzky, A.R. *et al., Chem. Comm.*, 1978, 133 (*synth, Et ester*)
Harpp, D.N. *et al., Synthesis*, 1979, 181 (*synth, Me ester*)
Fenwick, G.R. *et al., CRC Crit. Rev. Food Sci. Nutri.*, 1983, **18**, 123; *CA*, **98**, 70391a (*glucosinate dec*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGS750; EPP000; MPT000

Thiopeptin B_a T-375

[70606-90-5]
Thiofeed



R = C(=CH_2)CONHC(=CH_2)COOH

$C_{71}H_{84}N_{18}O_{18}S_6$ 1669.95

Cyclic depsipeptide antibiotic. Used as a feed additive. Faintly yellow cryst. Sol. DMF, dioxan, Py, THF, $CHCl_3$, DMSO; fairly sol. MeOH, Me_2CO, EtOAc; poorly sol. C_6H_6, H_2O, hexane. Mp 219-222°. $[\alpha]_D^{23}$ -80 (c, 1 in $CHCl_3$). λ_{max} 248 (E1%/1cm 430); 250 (E1%/1cm 327) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 40 - 80 mg/kg , LD_{50} (mus, scu) 3600 mg/kg.

Me ester: [70591-36-5] ***Thiopeptin A_{1a}***
$C_{72}H_{86}N_{18}O_{18}S_6$ 1683.977
Yellow plates (EtOAc). Sol. DMSO, DMF, $CHCl_3$, dioxan, Py; fairly sol. MeOH, Me_2CO, EtOAc; poorly sol. C_6H_6, hexane, H_2O. Mp *ca.* 200 (browns). $[\alpha]_D$ -71 ($CHCl_3$). Data refers to inseparable mixt. of Thiopeptins A_{1a} and A_1 λ_{max} 295 ; 305 (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 500 mg/kg.

1,2-Didehydro: [70591-33-2] ***Thiopeptin B_b***
$C_{71}H_{82}N_{18}O_{18}S_6$ 1667.935

1,2-Didehydro, Me ester: [70591-34-3] ***Thiopeptin A_{1b}***
$C_{72}H_{84}N_{18}O_{18}S_6$ 1681.961
Sol. $CHCl_3$; poorly sol. H_2O. λ_{max} 250 (E1%/1cm 335) (MeOH) (Berdy).

[12789-58-1]

Miyairi, N. *et al., J. Antibiot.*, 1970, **23**, 113 (*isol*)
Miyaira, N. *et al., Antimicrob. Agents Chemother.*, 1972, **1**, 192 (*isol, uv, ir*)
Hensens, O.D. *et al., J. Antibiot.*, 1983, **36**, 799; 814; 832 (*struct, bibl*)

Thiophene, 9CI, 8CI T-376

[110-02-1]
Thiofuran. Thiacyclopentadiene. Thiaphene



C_4H_4S 84.142
Maillard product. Liq. d_4^{20} 1.06. Mp -38.3°. Bp 84°. n_D^{20} 1.5246. Stable to at least 340°.

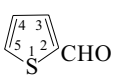
▶ Highly flammable, fl. p. -1/-6°. Reacts violently with fuming HNO_3. Severe eye irritant. LD_{50} (rat, orl) 1400 mg/kg.
XM7350000

S,S-*Dioxide:* [27092-46-2]
$C_4H_4O_2S$ 116.14
Cryst,. Mp *ca.* 6. Melt solidifies at r.t. to form dimeric and trimeric compds..

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 591B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 42C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1466B (*ir*)
Meyer, V. *et al., Ber.*, 1883, **16**, 1465 (*isol*)
Org. Synth., Coll. Vol., 2, 1943, 578 (*synth*)
Hartough, H.D. *et al., Thiophene Its Deriv.*, Interscience, N.Y., 1952, (*rev*)
Adv. Chem. Ser., 1955, **15**, 183 (***props***)
Bonham, R.A. *et al., J. Phys. Chem.*, 1963, **67**, 2474 (*struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 965 (*rev*)
Satonaka, H. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 2463 (*pmr*)
Fraser, R.R. *et al., Can. J. Chem.*, 1985, **63**, 3505 (*cmr*)
Nyulászi, L. *et al., Chem. Scr.*, 1986, **26**, 629 (*uv*)
Nagasawa, H. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 1919-1926 (*dioxide*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1358
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1207
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFM250

2-Thiophenecarboxaldehyde, 9CI, 8CI T-377

[98-03-3]
Thiophene-2-aldehyde. 2-Formylthiophene. 2-Thienal. α-Thenaldehyde. 2-Thienylaldehyde



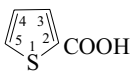
C_5H_4OS 112.152
Flavour ingredient. Liq. Bp_{756} 198° Bp_1 44-45°. n_D^{20} 1.5917. Rapidly oxid. in air.

▶ XM8225000

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 57A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 599C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1475B (*ir*)
Campaigne, E. *et al., J.A.C.S.*, 1953, **75**, 989 (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 915 (*synth, bibl*)
Bag, S.P. *et al., J. Indian Chem. Soc.*, 1975, **52**, 30 (*pKa*)
Hoshika, Y. *et al., J. Chromatogr.*, 1977, **136**, 253 (*use*)
Pavskii, V.I. *et al., Zh. Fiz. Khim.*, 1977, **51**, 2733; *Russ. J. Phys. Chem. (Engl. Transl.)*, 1977, **51**, 1597 (*uv*)
Satonaka, H. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 2463 (*pmr*)
Archer, W.J. *et al., J.C.S. Perkin 2*, 1983, 813 (*synth*)
Lunazzi, L. *et al., J.C.S. Perkin 2*, 1984, 819 (*cmr, conformn*)
Tenhosaari, A. *et al., Org. Mass Spectrom.*, 1988, **23**, 236 (*ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFM500

2-Thiophenecarboxylic acid, 9CI, 8CI T-378

[527-72-0]
α-Thiophenic acid. α-Thienoic acid. α-Thenoic acid



$C_5H_4O_2S$ 128.151
Needles (H_2O). V. sol. hot H_2O; spar. sol. petrol. Mp 129-130°. pK_a 3.49 (25°).

▶ XM8330200

Me ester: [5380-42-7]
$C_6H_6O_2S$ 142.178
Maillard product. Liq. d^{20} 1.23. $Bp_{0.5}$ 40°.

Et ester: [2810-04-0]
$C_7H_8O_2S$ 156.205
Liq. d_4^{16} 1.16. Bp_{18} 96° $Bp_{0.4}$ 45°.

Ph ester: [881-89-0]
$C_{11}H_8O_2S$ 204.249
Cryst. (petrol). Mp 59° (54°).

Chloride: [5271-67-0]
C_5H_3ClOS 146.597
Oil. Bp 190°.

Amide: [5813-89-8]
C_5H_5NOS 127.167
Cryst. (EtOH). Mp 180°.

▶ XM8290000

Anilide: [6846-13-5] N-*Phenyl-2-thiophenecarboxamide, 9CI*
$C_{11}H_9NOS$ 203.264
Cryst. (EtOH). Mp 141-142°.

Hydrazide: [2361-27-5]
$C_5H_6N_2OS$ 142.181
Mp 136-139°.

Nitrile: [1003-31-2] *2-Cyanothiophene. 2-Thienylcarbonitrile*
C_5H_3NS 109.151
Oil. Bp 192° Bp_1 46°. n_D^{20} 1.5612. n_D^{20} 1.5630. Steam-volatile.

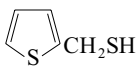
Anhydride: [25569-97-5]
$C_{10}H_6O_3S_2$ 238.288
Needles (petrol). Mp 62°. Bp_{15} 218-220°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 59A; 62B; 65A; 65B; 65C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 600D; 603A; 605B; 605C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1477D; 1479A (*ir*)
Steinkopf, W. *et al., Annalen*, 1924, **437**, 14 (*anhydride, nitrile*)
Gilman, H. *et al., J.A.C.S.*, 1949, **71**, 1870 (*synth*)

Gross, H. *et al., Chem. Ber.*, 1963, **96**, 1382 (*synth*)
Gronowitz, S. *et al., Chem. Scr.*, 1975, **7**, 76 (*cmr*)
Fisichella, S. *et al., Phosphorus Sulfur Relat. Elem.*, 1982, **13**, 59 (*ms*)
Chadwick, D.J. *et al., J.C.S. Perkin 1*, 1985, 173 (*synth, pmr*)
van Soolingen, J. *et al., Synth. Commun.*, 1990, **20**, 3153 (*nitrile*)
Vorbrüggen, H. *et al., Tetrahedron*, 1994, **50**, 6549 (*nitrile*)

2-Thiophenemethanethiol, 9CI, 8CI T-379

[6258-63-5]
2-(Mercaptomethyl)thiophene. 2-Thenylthiol. 2-Thenyl mercaptan



$C_5H_6S_2$ 130.234
Flavouring ingredient. $d_4^{19.5}$ 1.17. Bp_{15} 86°.

S-*Me:* [22906-17-8] *2-[(Methylthio)-methyl]thiophene. Methyl 2-thenyl sulfide*
$C_6H_8S_2$ 144.261
Liq. with strong disagreeable odour. $d_4^{20.5}$ 1.15. Bp_{15} 101-103° Bp_2 56-60°. n_D^{20} 1.5775.

S-*Me,* S,S-*dioxide:* [18185-60-9] *2-[(Methylsulfonyl)methyl]thiophene. Methyl 2-thenyl sulfone*
$C_6H_8O_2S_2$ 176.26
Cryst. (EtOH). Mp 94-95°.

S-*Et:* [19175-56-5] *2-[(Ethylthio)-methyl]thiophene. Ethyl 2-thenyl sulfide*
$C_7H_{10}S_2$ 158.288
Liq. Bp_9 93-94° Bp_3 66-69°.

S-*Et,* S,S-*dioxide:2-[(Ethylsulfonyl)-methyl]thiophene. Ethyl 2-thenyl sulfone*
$C_7H_{10}O_2S_2$ 190.287
Cryst. Mp 55-56°.

S-*Ph:* [69639-48-1] *2-[(Phenylthio)-methyl]thiophene. Phenyl 2-thenyl sulfide*
$C_{11}H_{10}S_2$ 206.332
Liq. $Bp_{2.5}$ 155°.

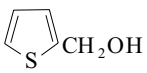
S-*Ph,* S-*oxide:* [20894-79-5] *2-[(Phenylsulfinyl)methyl]thiophene. Phenyl 2-thenyl sulfoxide*
$C_{11}H_{10}OS_2$ 222.331
Mp 80°. Racemate.

S-*Ph,* S,S-*dioxide:* [20894-80-8] *2-[(Phenylsulfonyl)methyl]thiophene. Phenyl 2-thenyl sulfone*
$C_{11}H_{10}O_2S_2$ 238.331
Mp 138°.

Cagniant, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1949, **229**, 1342-1343 (*synth, S-Me*)
Kipnis, F. *et al., J.A.C.S.*, 1949, **71**, 3571 (*S-Et*)
Kametani, T. *et al., Yakugaku Kenkyu*, 1959, **31**, 125-131; *CA*, **54**, 11018i (*synth*)
Fedorov, B.P. *et al., Zh. Obshch. Khim.*, 1962, **32**, 1518; *CA*, **58**, 4495h (*S-Et*)
U.K. Pat., 1967, 1 069 379; *CA*, **68**, 39472j (*S-Me, S-Me dioxide*)
Lapkin, I.I. *et al., Khim. Geterotsikl. Soedin.*, 1968, 53; *CA*, **70**, 11448y (*S-Ph, oxides*)
Ger. Pat., 1979, 2 824 249; *CA*, **92**, 207080n (*synth*)
McCrindle, R. *et al., J.C.S. Perkin 1*, 1981, 3070 (*S-Me*)
Guindon, Y. *et al., J.O.C.*, 1983, **48**, 1357 (*S-Ph*)
Torisawa, Y. *et al., Tet. Lett.*, 1988, **29**, 1729 (*S-Me*)
Patel, V.F. *et al., J.C.S. Perkin 1*, 1990, 2729 (*S-Ph, synth, pmr, cmr*)
Dass Gupta, R. *et al., J.C.S. Perkin 2*, 1990, 537 (*S-Ph, synth, pmr, ms, dioxide*)
Nakamura, T. *et al., Synth. Commun.*, 1999, **29**, 201-210 (*synth, ir, pmr, ms*)

2-Thiophenemethanol, 9CI T-380

[636-72-6]
2-Hydroxymethylthiophene. Thenyl alcohol



C_5H_6OS 114.168
Maillard product. Liq. $d_4^{14.5}$ 1.22. Bp_{12} 94.5-96°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 50A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 595B (*ir*)
Steinkopf, W. *et al., Annalen*, 1939, **540**, 14
Kriscke, R. *et al., Annalen*, 1974, 1486

3-Thiophenemethanol, 9CI T-381

[71637-34-8]
3-Hydroxymethylthiophene

C_5H_6OS 114.168
Maillard product. Bp_{10} 86-88°. n_D^{20} 1.5640.

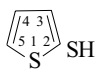
Ac:
$C_7H_8O_2S$ 156.205
Bp_{16} 105.5°. n_D^{25} 1.5138.

Me ether:3-(Methoxymethyl)thiophene
C_6H_8OS 128.195
Bp_{10} 78°.

Campaigne, E. *et al., J.A.C.S.*, 1954, **76**, 2445 (*synth*)
Raich, W.J. *et al., J.A.C.S.*, 1957, **79**, 3800 (*synth*)
Tserng, K. *et al., J.O.C.*, 1975, **40**, 172 (*synth, derivs, pmr*)
Bures, E. *et al., J.O.C.*, 1997, **62**, 8741-8749 (*synth, ir, pmr*)

2-Thiophenethiol, 9CI, 8CI T-382

[7774-74-5]
2-Mercaptothiophene. 2-Thienyl mercaptan. FEMA 3062



$C_4H_4S_2$ 116.208
Flavouring ingredient. Yellow oil with unpleasant burnt caramel/sulfuraceous odour and flavour. d_4^{20} 1.24. Bp 166° Bp_5 53-56°. n_D^{20} 1.6130. Dimerises on standing in air.

S-*Me:* [5780-36-9] *2-(Methylthio)thiophene, 9CI. Methyl-2-thienyl sulfide*
$C_5H_6S_2$ 130.234
Liq. Bp_{22} 82-86°.

S-*Me,* S,S-*dioxide:* [38695-60-2] *2-(Methylsulfonyl)thiophene*
$C_5H_6O_2S_2$ 162.233
Plates (EtOH aq.). Mp 46-47°.

S-*Ph:* [16718-12-0] *2-(Phenylthio)thiophene, 9CI*
$C_{10}H_8S_2$ 192.305
Oil. Bp_{20} 161°.

Houff, W.H. *et al., J.A.C.S.*, 1953, **75**, 6316 (*synth*)
Cymerman-Craig, J. *et al., J.C.S.*, 1954, 237 (*deriv*)
Gronowitz, S. *et al., Ark. Kemi*, 1959, **13**, 239 (*deriv, uv*)
Peron, J.J. *et al., Spectrochim. Acta A*, 1970, **26**, 1651 (*ir*)
Voronkov, M. *et al., Khim. Geterotsikl. Soedin.*, 1974, 712; 1986, 1614 (*synth, pmr*)
Gronowitz, S. *et al., Chem. Scr.*, 1975, **7**, 76 (*deriv, cmr*)
Sadykhov, K. *et al., Zh. Org. Khim.*, 1975, **11**, 2157 (*derivs*)
Everhardus, R.H. *et al., Chem. Comm.*, 1977, 801 (*deriv*)
Org. Synth., Coll. Vol., 6, 1988, 979 (*synth*)
Vvedenskii, V.Yu. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1989, **305**, 624; *Dokl. Chem. (Engl. Transl.)*, 1989, **305**, 98 (*synth, props*)
Misharina, T. *et al., Zh. Anal. Khim.*, 1990, **45**, 535 (*ms, ir, glc*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 753
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2779-2780

3-Thiophenethiol, 9CI T-383

[7774-73-4]
3-Mercaptothiophene

$C_4H_4S_2$ 116.208
Liq. d_{25}^{25} 1.25. Bp 171° Bp_2 40-45°. n_D^{20} 1.6218. Dec. slowly at r.t..

S-*Me:* [20731-74-2] *3-(Methylthio)thiophene, 9CI. Methyl 3-thienyl sulfide*
$C_5H_6S_2$ 130.234
Maillard product, present in meat flavour. Bp_{30} 93-94°. n_D^{25} 1.6029.

S-*Me,* S,S-*dioxide:* [38695-58-8] *3-(Methylsulfonyl)thiophene. Methyl 3-thienyl sulfone*
$C_5H_6O_2S_2$ 162.233
Plates (MeOH). Mp 76-77°.

S-*(2,4-Dinitrophenyl):*
Mp 132.5-133°.

Brooks, J.W. *et al., J.A.C.S.*, 1950, **72**, 1289 (*derivs*)
Caesar, P.D. *et al., Ind. Eng. Chem.*, 1952, **44**, 122 (*synth, ir*)
Gronowitz, S. *et al., Ark. Kemi*, 1959, **13**, 269; 1961, **16**, 309 (*synth, derivs*)
Hoffman, R.A. *et al., Ark. Kemi*, 1960, **16**, 515 (*pmr*)
Gronowitz, S. *et al., J.C.S.*, 1963, 3881 (*ir, deriv*)
Gronowitz, S. *et al., Chem. Scr.*, 1975, **7**, 76; 111 (*pmr, cmr, deriv*)
Henrio, G. *et al., Tetrahedron*, 1977, **33**, 191 (*synth, derivs*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027 (*synth, glc, ms, ir, nmr*)

Thiourea, 9CI T-384

[62-56-6]
Thiocarbamide. Thiocarbonic diamide

H_2NCSNH_2

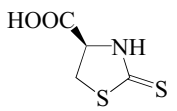
CH_4N_2S 76.122
Prohibited from use in food. Rhombohedra or needles (EtOH). Sol. H_2O, EtOH; spar. sol. Et_2O. Mp 175-177° Mp 180°. pK_a -1.19 (20°, H_2SO_4 aq.).

► Possible human carcinogen. Adverse haemopoietic effects reported by ingestion. LD_{50} (rat, orl) 125 mg/kg. Exp. carcinogen and teratogen. Exp. reprod. effects. Hepatotoxic. YU2800000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 827A; 831B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1339B; 1342B (*nmr*)
Ger. Pat., 1971, 1 957 202; *CA*, **75**, 35188t (*manuf*)
IARC Monog., 1974, **7**, 95; *Suppl*. 7, 72 (*rev, tox*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2782
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 2nd edn., Butterworths*, 1979, 313
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1209
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADD250; ISR000; TMH750; DNS800

2-Thioxo-4-thiazolidinecarboxylic acid T-385

[20933-67-9]
4-Carboxy-2-thiazolidinethione



(*S*)-form

$C_4H_5NO_2S_2$ 163.221

(*R*)-*form* [98169-56-3]
Raphanusamic acid
Isol. from etiolated seedlings of *Raphanus sativus* var. *hortensis* (Japanese radish Daikon). $[\alpha]_D^{29}$ -86 (c, 2.5 in 0.5*M* HCl).

Me ester: [80963-80-0] *4-(Methoxycarbonyl)-2-thiazolidinethione*
$C_5H_7NO_2S_2$ 177.248
Light yellow oil. $[\alpha]_D^{20}$ -68.2 ($CHCl_3$).

(*S*)-*form*
Et ester: [157832-46-7]
$C_6H_9NO_2S_2$ 191.275
Orange solid. Mp 44-46°.

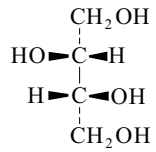
(±)-*form*
Me ester: [114180-04-0]
Prisms (CH_2Cl_2). Mp 95-96°.

[64014-03-5, 101799-35-3]

Hase, T. *et al., Rev. Latinoam. Quim.*, 1985, **16**, 1 (*synth, isol, props*)
Hsiao, C.-N. *et al., J.O.C.*, 1987, **52**, 2201 (*synth, ester, ir, pmr*)
Nagao, Y. *et al., Chem. Pharm. Bull.*, 1988, **36**, 495 (*synth, ester, uv, pmr, cmr*)
Inamori, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2854 (*synth, activity*)
U.S. Pat., 1993, 5 210 094; *CA*, **119**, 22809y (*use*)
Calo, V. *et al., Tetrahedron*, 1994, **50**, 7283 (*synth, ester, pmr*)
Dobson, A.J. *et al., Acta Cryst. C*, 1998, **54**, 1634-1637 (*R-form, cryst struct*)

Threitol T-386

[7493-90-5]
(R,R)-1,2,3,4-Butanetetrol, 9CI



(2*R*,3*R*)-form

$C_4H_{10}O_4$ 122.121

For (*R*,*S*)-*meso*-form see Erythritol, E-236. Log P -3.02 (calc).

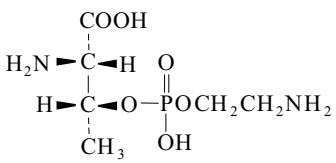
(2*R*,3*R*)-*form* [2418-52-2]
D-form
Found in the edible fungus *Armillaria mellea*. Constit. of jute (*Corchorus capsularis* and *Corchorus olitorius* (Jew's mallow)), and the pigeon pea plant (*Cajanus cajan*). Needles (EtOH). V. sol. hot EtOH. Mp 72-74° Mp 88.5-89°. $[\alpha]_D^{20}$ +6 (c, 2 in Me_2CO). $[\alpha]_D^{20}$ +4.6 (c, 6 in H_2O). $[\alpha]_D^{20}$ -11.5 (c, 5 in EtOH).

[20638-61-3, 50623-73-9, 71641-34-4, 102779-61-3, 114924-93-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 184D; 247D; 248A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 287B; 287C; 400B; 400C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 327C; 327D (*ir*)
Maquenne, L. *et al., C. R. Hebd. Seances Acad. Sci.*, 1900, **130**, 1402 (*synth*)
Ness, R.K. *et al., J.A.C.S.*, 1951, **73**, 4759 (*synth*)
Institoris, L. *et al., Arzneim.-Forsch.*, 1967, **17**, 145 (*pharmacol*)
Hilden, J. *et al., J. Antibiot.*, 1976, **29**, 58 (*use*)
Angyal, S.J. *et al., Carbohydr. Res.*, 1980, **84**, 201 (*cmr*)
Double, J.A. *et al., Br. J. Cancer*, 1983, **48**, 739 (*use*)
Hawkes, G.E. *et al., J.C.S. Perkin 2*, 1984, 2073 (*pmr, conformn*)
Andrews, M.A. *et al., J.O.C.*, 1989, **54**, 5257 (*synth*)
Jeffrey, G.A. *et al., Carbohydr. Res.*, 1992, **223**, 11 (*cryst struct, D-threitol*)
Kopf, J. *et al., Carbohydr. Res.*, 1993, **247**, 119 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 503
Corradi da Silva, M. de L. *et al., Phytochemistry*, 1993, **34**, 715 (*isol*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1999, **47**, 988-992 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFU500

Threonine ethanolamine phosphate T-387

Threonine 2-aminoethyl hydrogen phosphate, 9CI

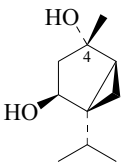


$C_6H_{15}N_2O_6P$ 242.168

(*S*)-*form* [1935-19-9]
L-form
Mp 176° dec. $[\alpha]_D$ -37.3 (c, 0.94 in H_2O).

Rosenberg, H. *et al., Biochem. J.*, 1962, **84**, 536 (*isol, synth, ir*)
Porcellati, G. *et al., Comp. Biochem. Physiol.*, 1965, **14**, 413
Allen, A.K. *et al., Comp. Biochem. Physiol.*, 1968, **27**, 695 (*biosynth*)
Rosenberg, H. *et al., Comp. Biochem. Physiol.*, 1968, **27**, 695 (*isol, synth, ir*)
v. Heyningen, R. *et al., Exp. Eye Res.*, 1976, **23**, 29

2,4-Thujanediol T-388

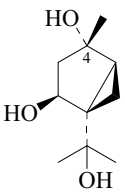


$C_{10}H_{18}O_2$ 170.251

(1*S*,2*S*,4*S*,5*S*)-*form*
4-O-β-D-Glucopyranoside: [240495-81-2]
$C_{16}H_{28}O_7$ 332.393
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{25}$ -10 (c, 0.3 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 805-808 (*isol, pmr, cmr*)

2,4,7-Thujanetriol T-389



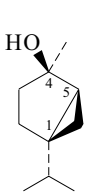
$C_{10}H_{18}O_3$ 186.25

(1*S*,2*S*,4*S*,5*S*)-*form*
4-O-β-D-Glucopyranoside: [240495-80-1]
$C_{16}H_{28}O_8$ 348.392
Constit. of *Foeniculum vulgare* (fennel). Amorph. powder. $[\alpha]_D^{25}$ -30 (c, 0.2 in MeOH).

Ishikawa, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 805-808 (*isol, pmr, cmr*)

4-Thujanol T-390

[546-79-2]
2-Methyl-5-(1-methylethyl)bicyclo[3.1.0]-hexan-2-ol, 9CI. 5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol. Sabina hydrate. Sabinene hydrate. FEMA 3239



(1*R*,4*R*,5*R*)-form

$C_{10}H_{18}O$ 154.252

(1*R*,4*R*,5*R*)-*form*

Cryst. Mp 36.5-37.2°. $[\alpha]_D^{25}$ +47.2 (c, 10 in EtOH).

(1R,4S,5R)-form

Constit. of the essential oil of American peppermint and other *Mentha* spp. Flavouring agent. Cryst. by subl. Mp 61°. $[\alpha]_D^{25}$ +32.2 (c, 4.2 in EtOH).

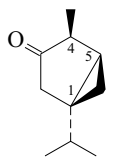
[7712-82-5, 15537-55-0, 15826-82-1, 17699-16-0, 58117-61-6]

Daly, J.W. *et al., J.A.C.S.*, 1958, **80**, 6330 (*isol, synth*)
Ohloff, G. *et al., Tetrahedron*, 1966, **22**, 309 (*abs config, synth*)
Fanta, W.I. *et al., J.O.C.*, 1968, **33**, 1656 (*synth*)
Baeckström, P. *et al., Bioorg. Med. Chem.*, 1996, **4**, 419 (*synth*)
Cheng, D. *et al., Org. Lett.*, 2001, **3**, 2121-2123 (*synth*)
Galopin, C.C. *et al., Tet. Lett.*, 2001, **42**, 5589-5591 (*synth*)

3-Thujanone T-391

[1125-12-8]

4-Methyl-1-(1-methylethyl)bicyclo[3.1.0]-hexan-3-one, 9CI. 1-Isopropyl-4-methylbicyclo[3.1.0]hexan-3-one. 3-Sabinanone. Tanacetone. Absinthone. Salvone. Chrysanthone



(1*S*,4*S*,5*R*)-*form*

$C_{10}H_{16}O$ 152.236

► LD_{50} (mus, scu) 87 mg/kg.

(1S,4S,5R)-form [471-15-8]

(+)-3-Thujone. (+)-Isothujone. (+)-β-Thujone

Liq. Bp 201-202°. $[\alpha]_D$ +72.46 (neat).

► LD_{50} (mus, scu) 442 mg/kg. XO9630000

(1R,4R,5S)-form

(-)-3-Thujone

Liq. $[\alpha]_D$ -27.8.

(1S,4R,5R)-form [546-80-5]

(-)-3-Isothujone. (-)-α-Thujone

Ingredient of absinthe. Presence in food and beverages regulated by legislation. Liq. Bp_{12} 78°. $[\alpha]_D^{23}$ -20.5 (c, 2 in $CHCl_3$).

► Absinthe abuse causes convulsions in humans. LD_{50} (rat, orl) 500 mg/kg. XO9625000

(1R,4S,5S)-form

(+)-3-Isothujone

Liq. Bp_{12} 78°. $[\alpha]_D^{25}$ +20 (c, 1 in $CHCl_3$).

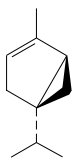
[58501-78-3]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 677A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 526A (*ir*)
v. Sydow, E. *et al., Acta Chem. Scand.*, 1964, **18**, 1099 (*ms*)
Acharya, S.P. *et al., J.O.C.*, 1969, **34**, 3015 (*synth, abs config*)
Whittaker, D. *et al., Chem. Rev.*, 1972, **72**, 305 (*rev*)
Norin, T. *et al., Acta Chem. Scand.*, 1973, **27**, 1579 (*pmr*)
Abraham, R.J. *et al., Org. Magn. Reson.*, 1974, **6**, 184 (*cmr*)
Hach, V. *et al., J.O.C.*, 1977, **42**, 1616 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1329
Micali, G. *et al., Flavour Fragrance J.*, 1995, **10**, 329-333 (*hplc*)
Oppolzer, W. *et al., Helv. Chim. Acta*, 1997, **80**, 623 (*synth*)
Hold, K.M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 3826-3831 (*bibl, pharmacol, metab*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFW000

3-Thujene T-392

[2867-05-2]

2-Methyl-5-(1-methylethyl)bicyclo[3.1.0.]hex-2-ene, 9CI. 5-Isopropyl-2-methylbicyclo[3.1.0]hex-2-ene. Origanene. α-Thujene



(−)-*form*

$C_{10}H_{16}$ 136.236

(+)-form [563-34-8]

Liq. Bp 151-153°. $[\alpha]_D$ +38.84.

(-)-form [3917-48-4]

Occurs in essential oils. Bp 150.5-152.5°. $[\alpha]_D$ -14.76. n_D^{20} 1.4559.

(ξ)-form

Isol. from Indian olibanum tree (*Boswellia serrata*), *Eucalyptus* spp., dill, juniper, coriander and many other plant oils. (Opt. rotn. frequently not reported).

Shaw, A.C. *et al., Can. J. Chem.*, 1953, **31**, 277 (*isol*)
Norin, T. *et al., Acta Chem. Scand.*, 1962, **16**, 640 (*abs config*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Wrolstad, R.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 501 (*ir*)
Acharya, S.P. *et al., J.O.C.*, 1969, **34**, 3015 (*abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 59 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 77 (*rev*)

4(10)-Thujene T-393

[3387-41-5]

4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane, 9CI. 1-Isopropyl-4-methylenebicyclo[3.1.0]hexane. ***Sabinene***



(+)-*form*

$C_{10}H_{16}$ 136.236

(+)-form [2009-00-9]

Constit. of *Myristica fragrans* (nutmeg). Bp_{160} 163-165°. $[\alpha]_D$ +95 (c, 20 in CCl_4).

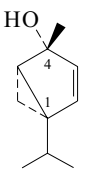
(-)-form [10408-16-9]

Constit. of *Laurus nobilis* (bay laurel) and some other plants. Liq. Bp 162-166°. $[\alpha]_D$ -89.

Jaureguiberry, G. *et al., Bull. Soc. Chim. Fr.*, 1962, 1985 (*isol, ir, pmr*)
Ryhage, R. *et al., Acta Chem. Scand.*, 1963, **17**, 2025 (*ms*)
Banthorpe, D.V. *et al., Chem. Comm.*, 1966, 177 (*biosynth*)
Fanta, W.I. *et al., J.O.C.*, 1968, **33**, 1656 (*synth*)
Acharya, S.P. *et al., J.O.C.*, 1969, **34**, 3015 (*abs config*)
Whitaker, D. *et al., Chem. Rev.*, 1972, **72**, 305 (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 60 (*occur*)
Zaidlewicz, M. *et al., Tetrahedron: Asymmetry*, 1997, **8**, 3847-3850 (*synth*)
Adam, K.-P. *et al., Phytochemistry*, 1998, **49**, 475-480 (*biosynth*)

2-Thujen-4-ol T-394

[83260-52-0]



(1*R**,4*R**)-*for*

$C_{10}H_{16}O$ 152.236

(1R*,4R*)-form [97631-68-0]

cis-*form*

Constit. of *Laurus nobilis* (bay laurel). Oil.

(1R*,4S*)-form [69651-92-9]

trans-*form*

Constit. of *Laurus nobilis* (bay laurel). Oil.

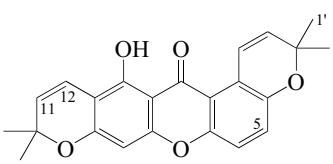
[7766-03-2]

Klein, E. *et al., Chem. Ber.*, 1965, **98**, 3045 (*synth*)
Novak, M. *et al., Phytochemistry*, 1985, **24**, 858 (*isol*)

Thwaitesixanthone T-395

[55785-61-0]

*13-Hydroxy-3,3,10,10-tetramethyl-10*H*-dipyrano[3,2-a:2′,3′-i]xanthen-14(3*H*)-one, 9CI*



$C_{23}H_{20}O_5$ 376.408

Yellow needles (EtOH aq.). Mp 221-224°.

Me ether:

Mp 160-162°.

11,12-Dihydro: [176226-40-7] ***11,12-Dihydrothwaitesixanthone***

$C_{23}H_{22}O_5$ 378.424

Yellow needles. Mp 258-259°.

1′-Hydroxy: [106897-02-3] ***Thwaitesixanthonol***

$C_{23}H_{20}O_6$ 392.407

Yellow prisms (EtOAc/petrol). Mp 176°.

5-Hydroxy: [84002-57-3] ***Padiaxanthone.*** *Brasilixanthone B*
$C_{23}H_{20}O_6$ 392.407
Yellow needles (Me_2CO/hexane). Mp 229-232° (207° dec.). λ_{max} 254 (log ϵ 4.17); 289 (log ϵ 4.53); 300 (log ϵ 4.53); 330 (log ϵ 4.31); 383 (log ϵ 3.7) (MeOH).

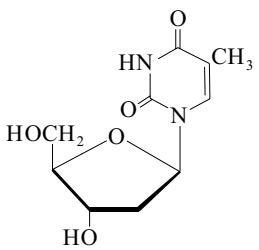
5-Hydroxy, 1,2,11,12-tetrahydro: [112649-48-6] ***BR-Xanthone A***
$C_{23}H_{24}O_6$ 396.439
Constit. of the dry fruit hulls of *Garcinia mangostana* (mangosteen). Pale-yellow needles (C_6H_6/petrol). Mp 181-182°.

5-Methoxy, 1,2-dihydro: ***Garcimangosone B***
$C_{24}H_{24}O_6$ 408.45
Constit. of the dry fruit hulls of *Garcinia mangostana* (mangosteen). Yellow powder. Mp 136-138°. λ_{max} 288 (log ϵ 4.25); 330 (log ϵ 3.92) (MeOH).

Dahanayake, M. *et al., J.C.S. Perkin 1*, 1974, 2510-2514 (*isol, struct*)
Westerman, P.W. *et al., Org. Magn. Reson.*, 1977, **9**, 631-636 (*cmr*)
Ampofo, S.A. *et al., Phytochemistry*, 1986, **25**, 2617-2620 (*Thwaitesixanthonol*)
Balasubramanian, K. *et al., Phytochemistry*, 1988, **27**, 1552 (*BR-Xanthone*)
Dharmaratne, H.R.W. *et al., Phytochemistry*, 1996, **42**, 249-250 (*Dihydrothwaitesixanthone*)
Ishiguro, K. *et al., Phytochemistry*, 1996, **42**, 435-437 (*Padiaxanthone*)
Marques, V.L.L. *et al., Phytochemistry*, 2000, **55**, 815-818 (*Brasilixanthone B*)
Huang, Y.L. *et al., J. Nat. Prod.*, 2001, **64**, 903-906 (*Garcimangosone B*)

Thymidine, 8CI T-396

[50-89-5]
*1-(2-Deoxy-β-D-*erythro*-pentofuranosyl)-5-methyl-2,4(1*H*,3*H*)-pyrimidinedione, 9CI. 1-(2-Deoxy-β-D-ribofuranosyl)-5-methyluracil. Thymine 2-desoxyriboside. Thymosine. NSC 21548*



$C_{10}H_{14}N_2O_5$ 242.231
Isol. from seedlings of *Phaseolus vulgaris* (kidney bean). Mp 186-187°. $[\alpha]_D$ +18.5 (H_2O). $[\alpha]_D^{25}$ +30.6 (c, 1.0 in H_2O). pK_{a1} 9.8; pK_{a2} 12.9 (25°). λ_{max} 207 (ϵ 9800); 267 (ϵ 9700) (no solvent reported) (pH 7.2).

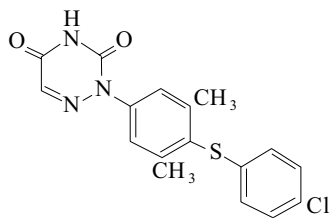
▶ Exp. reprod. and teratogenic effects (large dose), human adverse systemic effects (large dose), exp. antineoplastic agent (and in co-administration with methotrexate). LD_{50} (mus, ipr) 2512 mg/kg. XP2071000

[50-88-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 815A; 818A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 370B; 376B (*nmr*)
Levene, P.A. *et al., J. Biol. Chem.*, 1929, **83**, 793 (*isol*)
Michelson, A.M. *et al., J.C.S.*, 1955, 816 (*config*)
Fox, J.J. *et al., Adv. Carbohydr. Chem.*, 1959, **14**, 283 (*rev*)
Shaw, G. *et al., J.C.S.*, 1959, 50 (*synth*)
Lemieux, R.U. *et al., Can. J. Chem.*, 1961, **39**, 110; 116 (*conformn*)
Ulbricht, T.L.V. *et al., Tet. Lett.*, 1964, 695 (*ord*)
Young, D.W. *et al., Acta Cryst. B*, 1969, **25**, 1423 (*cryst struct*)
Gupta, V.S. *et al., Can. J. Chem.*, 1971, **49**, 719 (*synth*)
Krugh, T.R. *et al., J.A.C.S.*, 1973, **95**, 4761 (*cmr*)
Davies, D.B. *et al., J.C.S. Perkin 2*, 1975, 1703 (*pmr*)
Mathlouthi, M. *et al., Carbohydr. Res.*, 1984, **134**, 23 (*ir, Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1420
Tsuboi, M. *et al., Bull. Chem. Soc. Jpn.*, 1994, **67**, 1483 (*Raman*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFX790

Tiazuril, INN, USAN T-397

[35319-70-1]
*2-[4-[(4-Chlorophenyl)thio]-3,5-dimethylphenyl]-1,2,4-triazine-3,5(2*H*,4*H*)-dione, 9CI. CP 25673*

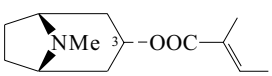


$C_{17}H_{14}ClN_3O_2S$ 359.835
Coccidiostat for poultry. Cryst. (MeCN). Mp 132-135°. Log P 6.29 (uncertain value) (calc).

U.K. Pat., 1972, 1 371 907, (*Pfizer*); *CA*, **77**, 164712z (*synth, pharmacol*)
Lynch, M.J. *et al., J. Agric. Food Chem.*, 1977, **25**, 1344 (*metab*)
Miller, M.W. *et al., J. Med. Chem.*, 1981, **24**, 1337 (*synth, pharmacol*)

3-Tigloyloxytropane T-398

2-Methyl-2-butenoic acid 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, 8CI. Tropine tiglate



3α-*form*

$C_{13}H_{21}NO_2$ 223.314
Log P 2.03 (calc). Both α- and β-forms reported to possess pharmacol. activity.

3α-*form* [495-83-0]
Tigloyltropeine. *Tropigline, BAN, INN*
Alkaloid from *Physalis alkekengi* (winter cherry) roots. Mp 181.5-183° Mp 204-207°.

Hydrochloride:
Mp 214.5-217.5°.

N-*Oxide:* ***3α-Tigloyloxytropane* N-*oxide***
$C_{13}H_{21}NO_3$ 239.314
Alkaloid from *Physalis alkekengi* (winter cherry). Mp 185-186° dec.
No longer marketed

3β-*form* [533-08-4]
Tigloidine, BAN, INN
Alkaloid from *Physalis alkekengi* (winter cherry). Syrup.

Hydrochloride:
Tabular cryst. (H_2O). Sol. $CHCl_3$, mod. sol. H_2O. Mp 234-235°.

Picrate:
Mp 239°.

Barger, G. *et al., J.C.S.*, 1937, 1820 (*isol, synth*)
Sanghvi, I.S. *et al., Eur. J. Pharmacol.*, 1968, **4**, 246 (*pharmacol*)
Evans, W.C. *et al., J.C.S. Perkin 1*, 1972, 2017 (*isol*)
Evans, W.C. *et al., Phytochemistry*, 1973, **12**, 2077; 2505 (*isol*)
Beresford, P.J. *et al., Phytochemistry*, 1974, **13**, 2143; 1975, **14**, 2205 (*isol, biosynth*)
Yamaguchi, H. *et al., Yakugaku Zasshi*, 1974, **94**, 1115 (*oxide*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 419
Witte, L. *et al., Planta Med.*, 1987, **53**, 192 (*glc-ms*)

Tin(*II*) chloride ($SnCl_2$), 9CI T-399

[7772-99-8]
Stannous chloride. Stannochlor. E512
$SnCl_2$
Cl_2Sn 189.615
Struct. may be descr. as a v. distorted $PbCl_2$ struct. Contains discernible $SnCl_3$ chains. Food additive (antioxidant) e.g. for colour retention in canned vegetables such as asparagus. White cryst. Sol. H_2O, EtOH, Et_2O, Me_2CO, EtOAc, MeOAc, Py. Mp 246°. Bp 623°.

▶ XP8700000

Dihydrate: [10025-69-1]
$Cl_2H_4O_2Sn$ 225.646
White monoclinic cryst. Sol. EtOH, Et_2O, Me_2CO; dec. in H_2O. Mp 37.7°. Struct. comprises discrete $SnCl_2(OH_2)$ groups and isolated H_2O molecules. Absorbs aerial O_2 forming the oxychloride.

▶ XP8850000

Stephen, H. *et al., J.C.S.*, 1930, 2786 (*synth*)
Lister, M.W. *et al., Trans. Faraday Soc.*, 1941, **37**, 406 (*struct*)
Williams, J.W. *et al., Org. Synth.*, 1943, **23**, 63 (*synth*)
Van den Berg, J.M. *et al., Acta Cryst.*, 1961, **14**, 1002; 1962, **15**, 1051 (*cryst struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1112 (*use*)
Buchanan, A.S. *et al., J. Phys. Chem.*, 1969, **73**, 4394 (*ms*)
Drobut, N.F. *et al., Zh. Neorg. Khim.*, 1972, **17**, 1199 (*synth*)
Kiriyama, H. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 1389 (*cryst struct, dihydrate*)
Wang, C.H. *et al., J. Chem. Phys.*, 1977, **67**, 3097 (*Raman*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 45 (*rev*)
Deans, R.A. *et al., Synth. React. Inorg. Met.-Org. Chem.*, 1978, **8**, 345 (*synth*)
Harrison, P.G. *et al., Inorg. Chim. Acta*, 1983, **75**, 265 (*Mössbauer*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2642-2643 (*use*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGC000; TGC275

Tin chloride ($SnCl_4$) T-400

[7646-78-8]
Tin tetrachloride. Tetrachlorostannane, 9CI. Stannic chloride

$SnCl_4$

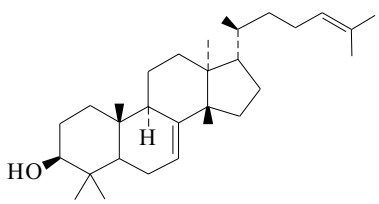
Cl_4Sn 260.521
Antioxidant in foods. Fuming liq. Sol. H_2O, CCl_4, C_6H_6. d_4^{20} 2.23. Mp -33°. Bp 114°.

▶ Caustic. XP8750000

Johnson, K.J. *et al., J. Chem. Phys.*, 1969, **51**, 4493 (*Cl-35 nmr*)
Buchanan, A.S. *et al., J. Phys. Chem.*, 1969, **73**, 4394 (*ms*)
Fujii, H. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 1933 (*struct*)
Debye, N.W.G. *et al., J. Chem. Phys.*, 1974, **61**, 4770 (*Mössbauer*)
Andrews, S.P. *et al., J. Chem. Res., Synop.*, 1978, 94 (*ir, Raman*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 47 (*rev*)
Colto, R. *et al., Inorg. Chim. Acta*, 1982, **61**, 1 (*Sn-119 nmr*)
Arthers, S.A. *et al., J.C.S. Dalton*, 1984, 819 (*ir*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGC250

Tirucalla-7,24-dien-3-ol T-401

[33755-52-1]



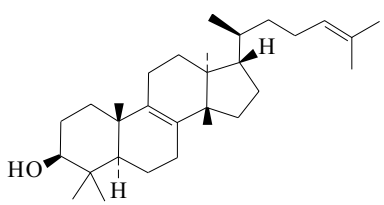
$C_{30}H_{50}O$ 426.724

3β-*form*
Constit. of the seed oil of *Thea sinensis* (tea). Cryst. Mp 95.5-97°.

Ac:
Cryst. Mp 123-124°. $[\alpha]_D^{21}$ -39 (c, 0.82 in $CHCl_3$).

Ekong, D.E.U. *et al., Chem. Comm.*, 1971, 1117 (*synth*)
Itoh, T. *et al., Lipids*, 1976, **11**, 434 (*isol, struct*)

Tirucalla-8,24-dien-3-ol T-402



$C_{30}H_{50}O$ 426.724

3β-*form* [514-46-5]
Tirucallol. *Kanzuiol. 20*-epi-*Euphol. Tirucalladienol*
Constit. of gum mastic and pistachio nut resin. Cryst. (EtOH). Mp 133-134.5°. $[\alpha]_D^{20}$ +4.5 (c, 2 in C_6H_6).

Arigoni, D. *et al., Helv. Chim. Acta*, 1955, **38**, 222 (*isol*)
Barton, D.H.R. *et al., J.C.S.*, 1956, 4150 (*isol*)
Boar, R.B. *et al., J. Chem. Res., Synop.*, 1982, 94 (*synth*)
Nes, W.D. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1984, **81**, 5896 (*cryst struct*)
Bartlett, W.R. *et al., J.O.C.*, 1990, **55**, 2215 (*synth*)
Akihisa, T. *et al., J. Nat. Prod.*, 1998, **61**, 409-412 (*pmr, cmr*)

Titanium(*IV*) oxide (TiO_2), 11CI T-403

[13463-67-7]

[1344-29-2, 51745-87-0]
Titanium oxide. Titanium dioxide, USAN. Bayertitan. Titania. Tioxide. Unitane. C.I. 77891. E171. Many other names

TiO_2

O_2Ti 79.879
Colour additive in foods; also found in foods as an indirect additive arising from its use in packaging materials, e.g. paper, cellophane. White solid. Insol. H_2O, HCl, HNO_3, dil. H_2SO_4; sol. hot conc. H_2SO_4, HF. Mp 1892° (under O_2 atm.). V. high refractive index (2.61-2.90). Loses O_2 in air to form $TiO_{1.985}$ which melts at *ca.* 1843°.

▶ OES: long-term 10 mg m^{-3} (total inhalable dust). Mild pulmonary irritant.
XR2275000

[12214-43-6]

Baur, W.H. *et al., Acta Cryst. B*, 1953, **9**, 515; 1955, **11**, 488; *Acta Cryst. A*, 1971, **27**, 2133 (*cryst struct, TiO_2*)
Czanderna, *et al., J.A.C.S.*, 1957, **79**, 5407 (*synth*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, 1366 (*synth*)
Industrial Chemicals, (Eds. Lowenheim, F.A. *et al*), 4th Ed., Wiley-Interscience, N.Y., 1975, 814 (*synth*)
Hong, S.H. *et al., Acta Cryst. B*, 1982, **38**, 2570 (*cryst struct, Ti_3O_5*)
Le Page, Y. *et al., J. Solid State Chem.*, 1982, **44**, 273 (*cryst struct, Ti_6O_{11}-Ti_9O_{17}*)
Le Page, Y. *et al., J. Solid State Chem.*, 1984, **53**, 13 (*cryst struct, Ti_4O_7*)
Lee, K.P. *et al., Toxicol. Appl. Pharmacol.*, 1985, **79**, 179 (*tox, exp*)
Brittain, H.G. *et al., Anal. Profiles Drug Subst.*, 1992, **21**, 659 (*rev*)
Qian, Y. *et al., J. Mater. Chem.*, 1993, **3**, 203 (*ultrafine, synth, manuf*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 529-531
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2796-2798
Martindale, The Extra Pharmacopoeia, 32nd edn., Pharmaceutical Press, 1999, 1093
Proctor and Hughes' Chemical Hazards of the Workplace, 4th edn., (eds. Hathaway, G.J. et al), Van Nostrand Reinhold, 1996, 603
Bretherick's Handbook of Reactive Chemical Hazards, 6th edn., (ed. Urben, P.G.), Butterworth-Heinemann, 1999, 4842
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, TGG760

TML 1 T-404

Protein; dimer with MW approx. 37000. Isol. from the edible mushroom *Tricholoma mongolicum*. Lectin. TML 2 also isol..

Wang, H.X. *et al., Int. J. Pept. Protein Res.*, 1995, **46**, 508-513 (*isol*)

ζ_2-Tocopherol T-405

[17976-95-3]
5,7-Dimethyltocol
As α-Tocopherol, T-406 with
$R^1 = R^2 = CH_3$, $R^3 = H$

$C_{28}H_{48}O_2$ 416.686
Constit. of rice. Oil. Mp -4°.

4-Phenylazobenzoyl:
Cryst. (2-propanol). Mp 61°.

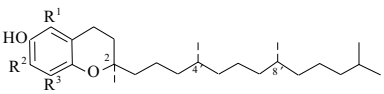
[1406-66-2]

McHale, D. *et al., J.C.S.*, 1958, 1600 (*synth*)
Green, J. *et al., J.C.S.*, 1959, 3362 (*synth*)

α-Tocopherol T-406

[59-02-9]

[364-50-1, 1431-54-5, 2074-53-5, 10191-41-0, 43119-47-7]
*3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, 9CI. 5,7,8-Trimethyltocol. Vitamin E*†*. Antisterility vitamin. Ephynal. Syntopherol. Profecundin. E307*



$R^1 = R^2 = R^3 = CH_3$

$C_{29}H_{50}O_2$ 430.713
Constit. of many vegetable oils such as soya and sunflower oils. Dietary supplement and nutrient. Nutriceutical with anticancer and antioxidant props. Added to fats and oils to prevent rancidity. The naturally-occurring tocopherol is a single stereoisomer; synthetic forms are a mixt. of all eight possible isomers. Viscous oil, cryst. (MeOH at -35°). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 2.5-3.5°. $Bp_{0.03}$ 140°. $[\alpha]_D^{25}$ +0.65 (EtOH). Log P 12.15 (uncertain value) (calc). Thermostable λ_{max} 294 (E1%/1cm 71) (MeOH) (Berdy). λ_{max} 292 (EtOH) (Berdy).

▶ DJ2900000

Ac: [58-95-7]

[54-22-8, 7695-91-2, 52225-20-4] *Alfacol. Fertilvit. Tocophrin.* ***α-Tocopherol acetate****. Vitamin E acetate. Combinal E. Many other names*

$C_{31}H_{52}O_3$ 472.75
Vitamin E supplement and antioxidant for foodstuffs. Oil. Mp 26.5-27.5°. $Bp_{0.02}$ 205° (bath). $[\alpha]_D^{25}$ +3.03 (c, 5 in EtOH). Log P 12.15 (uncertain value) (calc).

▶ GP8588000

p-*Phenylazobenzoyl:*
Cryst. Mp 62-64°. $[\alpha]_{600}$ +6.99 (c, 3.33 in $CHCl_3$).

3-Carboxypropanoyl: [4345-03-3] ***α-Toco-***

pherol succinate. *Many other names*
$C_{33}H_{54}O_5$ 530.787
Vitamin E supplement and antioxidant for foodstuffs. Needles (petrol). Mp 76-77°. Log P 11.82 (uncertain value) (calc).

3-Pyridinecarbonyl: [16676-75-8]

[51898-34-1] ***α-Tocopherol nicotinate***. *Vitamin E nicotinate. Many other names*
$C_{35}H_{53}NO_3$ 535.809
Yellow oil or solid. Mp 38°.

Ester with polyethylene glycol succinate:
[30999-06-5] ***Tocophersolan, USAN***. *Tocofersolan, INN*
Vitamin E supplement, antioxidant.

8′,12′-Dihydroxy: [159860-32-9]
$C_{29}H_{50}O_4$ 462.712
Oil. $[\alpha]_D$ -6 (c, 0.5 in $CDCl_3$).

[1406-66-2, 17407-37-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 330A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1326A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1387B (*ir*)
Baxter, J.G. *et al., J.A.C.S.*, 1943, **65**, 918-924 (*succinate*)
Praill, P.F. *et al., J.C.S.*, 1959, 3100 (*esters*)
Robeson, C.D. *et al., J.A.C.S.*, 1962, **84**, 3196-3197 (*isol*)
Meyer, H. *et al., Helv. Chim. Acta*, 1963, **46**, 650-671; 963-982 (*synth, abs config*)
Fr. Pat., 1968, M6320; *CA*, **74**, 79582 (*nicotinate*)
Nakamura, A. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2318-2324 (*synth*)
Scheppele, S.E. *et al., Lipids*, 1972, **7**, 297-304 (*ms*)
Rudy, B.C. *et al., Anal. Profiles Drug Subst.*, 1974, **3**, 111-126 (*bibl*)
Gatlin, L.A. *et al., Drug Intell. Clin. Pharm.*, 1975, **9**, 655-656 (*Tocophersolan, rev*)
Scott, J.W. *et al., Helv. Chim. Acta*, 1976, **59**, 290-306 (*synth*)
Cohen, N. *et al., J.O.C.*, 1976, **41**, 3505-3511; 1992, **57**, 5783-5785 (*synth, bibl*)
Schultz, G. *et al., Phytochemistry*, 1976, **15**, 1383-1386 (*biosynth*)
Matsuo, M. *et al., Tetrahedron*, 1976, **32**, 229-231 (*pmr*)
Nakamura, T. *et al., J. Nutr. Sci. Vitaminol.*, 1978, **24**, 459-469 (*pharmacol, esters*)
Chan, K.-K. *et al., J.O.C.*, 1978, **43**, 3435-3440 (*synth*)
Cohen, N. *et al., J.A.C.S.*, 1979, **101**, 6710-6716 (*synth*)
Akkerman, J.M. *et al., J.C.S. Perkin 1*, 1979, 2124-2129 (*synth*)
Urano, S. *et al., Chem. Pharm. Bull.*, 1980, **28**, 1992-1998 (*cmr*)
Olson, G.L. *et al., J.O.C.*, 1980, **45**, 803-805 (*synth*)
Cohen, N. *et al., Helv. Chim. Acta*, 1981, **64**, 1158-1173 (*synth, isom*)
Suzuki, N. *et al., J. Nutr. Sci. Vitaminol.*, 1983, **29**, 93-103 (*nicotinate, metab*)
Ballester-Rodes, M. *et al., Synth. Commun.*, 1984, **14**, 515-520 (*nicotinate, synth*)
Burton, G.W. *et al., Acc. Chem. Res.*, 1986, **19**, 194-201 (*rev, props*)
Inoue, S. *et al., J.O.C.*, 1987, **52**, 5495-5497 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7835; 7936; 8009
Furuya, T. *et al., Phytochemistry*, 1987, **26**, 2741-2747 (*biosynth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TGJ050; TGJ060; VSZ450
Hübscher, M. *et al., Helv. Chim. Acta*, 1990, **73**, 782-789; 1068-1086 (*bibl, hplc*)
Bourgeois, C. *et al., Determination of Vitamin E, Tocopherols and Tocotrienols*, Elsevier, 1992, (*book*)
Berger, S. *et al., Annalen*, 1994, 1239-1241 (*cmr*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 12-14
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 494-495 (*8′,12′-Dihydroxy-α-tocopherol, isol*)
Matsui, M. *et al., Bull. Chem. Soc. Jpn.*, 1995, **68**, 3569-3571; 1996, **69**, 137-139 (*synth*)
Chen, C.Y. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2153-2156 (*synth*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1391
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGJ050; TGJ060; VSZ450

β-Tocopherol T-407

[148-03-8]
*3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, 9CI. 2,5,8-Trimethyl-2-(4,8,12-trimethyltridecyl)chroman-6-ol, 8CI. 5,8-Dimethyltocol. Cumotocopherol. Neotocopherol*. p-*Xylotocopherol*
As α-Tocopherol, T-406 with
$R^1 = R^3 = CH_3$, $R^2 = H$
$C_{28}H_{48}O_2$ 416.686
Isol. from vegetable sources, e.g. spinach chloroplasts (*Spinacia oleracea*), soybean oil, corn oil and wheat germ. Antioxidant. Member of Vitamin E group. Pale yellow viscous oil. $Bp_{0.1}$ 200-210°. $[\alpha]_D^{20}$ +6.37. Thermostable; resistant to acids and alkalis.

3,5-Dinitrobenzoyl:
Mp 86-87°.

Ac:
Pale-yellow oil. $Bp_{0.3}$ 215-220°.

[1406-66-2, 16662-70-7, 16698-35-4]

Karrer, P. *et al., Helv. Chim. Acta*, 1938, **21**, 1234; 1939, **22**, 260 (*synth, struct*)
Mayer, H. *et al., Helv. Chim. Acta*, 1963, **46**, 963 (*abs config*)
Pearson, C.K. *et al., Br. J. Nutr.*, 1970, **24**, 581 (*metab*)
Nakamura, A. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2318 (*synth*)
Scheppele, S.E. *et al., Lipids*, 1972, **7**, 297 (*ms*)
Matsuo, M. *et al., Tetrahedron*, 1976, **32**, 229 (*cmr*)
Tangney, C.C. *et al., J. Chromatogr.*, 1979, **172**, 513 (*purifn*)
Burton, G.W. *et al., J.A.C.S.*, 1981, **103**, 6472 (*props*)
Pure Appl. Chem., 1982, **54**, 1507 (*nomencl*)
Urano, S. *et al., Heterocycles*, 1985, **23**, 2793 (*synth*)

δ-Tocopherol T-408

[119-13-1]
*3,4-Dihydro-2,8-dimethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, 9CI. 8-Methyltocol. E309*
As α-Tocopherol, T-406 with
$R^1 = R^2 = H$, $R^3 = CH_3$
$C_{27}H_{46}O_2$ 402.659
Widespread occurrence in vegetable oils incl. soya and sunflower oils. Used as antioxidant food additive. Member of Vitamin E group. Added to fats and oils to prevent rancidity. The naturally occurring tocopherol is a single stereoisomer; synthetic forms are a mixt. of all eight possible isomers. Pale yellow oil. $Bp_{0.001}$ 150° (bath).

p-*Phenylazobenzoyl:*
Orange-yellow leaflets. Mp 41-42°. $Bp_{0.001}$ 250°.

[1406-66-2]

Stein, M.H. *et al., J.A.C.S.*, 1947, **69**, 869 (*isol*)
Green, J. *et al., J.C.S.*, 1959, 3374 (*synth*)
Matsuo, M. *et al., Tetrahedron*, 1976, **32**, 229 (*cmr*)
Tangney, C.C. *et al., J. Chromatogr.*, 1979, **172**, 513 (*purifn*)

γ-Tocopherol T-409

[7616-22-0]
*3,4-Dihydro-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, 9CI. 7,8-Dimethyltocol. Vitamin E†. E308*
As α-Tocopherol, T-406 with
$R^1 = H$, $R^2 = R^3 = CH_3$
$C_{28}H_{48}O_2$ 416.686
Occurs in many nut and other vegetable oils such as soya and sunflower oil. Used as antioxidant food additive. Member of Vitamin E group. Added to fats and oils to prevent rancidity. The naturally occurring tocopherol is a single steroisomer; synthetic forms are a mixt. of all eight possible isomers. Viscous oil. Mp -3°. $[\alpha]_{Hg}^{25}$ +2.2 (EtOH). $[\alpha]_{Hg546}^{25}$ -2.4 (C_6H_6).

p-*Nitrophenylurethane:*
Mp 119-121°.

[1406-66-2]

Karrer, P. *et al., Helv. Chim. Acta*, 1939, **22**, 260 (*struct*)
Tsukida, K. *et al., J. Vitaminol.*, 1972, **18**, 24 (*pmr*)
Scheppele, S.E. *et al., Lipids*, 1972, **7**, 297 (*ms*)
Matsuo, M. *et al., Tetrahedron*, 1976, **32**, 229 (*cmr*)
Tangney, C.C. *et al., J. Chromatogr.*, 1979, **172**, 513 (*purifn*)

η-Tocopherol T-410

[91-86-1]
7-Methyltocol
As α-Tocopherol, T-406 with
$R^1 = R^3 = H$, $R^2 = CH_3$
$C_{27}H_{46}O_2$ 402.659
Constit. of rice. Oil.

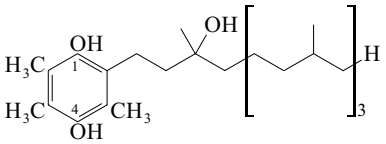
4-Phenylazobenzoyl:
Cryst. (2-propanol). Mp 55-56°.

[1406-66-2]

Marcinkiewicz, S. *et al., J.C.S.*, 1959, 3377

α-Tocopherolhydroquinone T-411

[14745-36-9]
α-Tocopheryl hydroquinone



$C_{29}H_{52}O_3$ 448.728
Viscous, golden-yellow oil.

Tri-Ac:
Cryst. Mp 75°.

1,4-Quinone: [7559-04-8] ***α-Tocopherolquinone***. α-Tocoquinone. Eutrophyl. Ipotensil. Metorena. Tensiopress. Trimina. Vitapressina. D 178. α-Tocopheryl quinone
$C_{29}H_{50}O_3$ 446.712
Isol. from spinach (*Spinacia oleracea*) chloroplasts and many other plant sources. Viscous, golden-yellow oil. $Bp_{0.002}$ 120°. Log P 9.62 (uncertain value) (calc).

► DK5170000

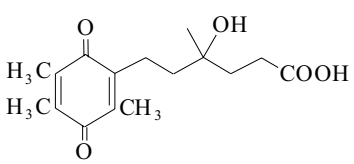
1,4-Quinone, Me ether: [137551-40-7] ***α-Tocopherolquinone methyl ether***
$C_{30}H_{52}O_3$ 460.739
Yellow oil. $[\alpha]_D$ +15 (c, 1.2 in $CHCl_3$).

*1,4-Quinone, 11′ξ,14′S-dihydroxy:**3′,11′,14′-Trihydroxy-α-tocopherolquinone***
$C_{29}H_{50}O_5$ 478.711
Cryst. Mp 113-114°. $[\alpha]_D$ -4 (c, 0.34 in $CDCl_3$).

Tishler, M. *et al., J.A.C.S.*, 1941, **63**, 1532 (*struct*)
MacKenzie, J.B. *et al., J. Biol. Chem.*, 1950, **183**, 655 (*props*)
Cairella, M. *et al., Clin. Ter. (Rome)*, 1964, **31**, 278 (*pharmacol*)
Chow, C.K. *et al., Lipids*, 1967, **2**, 390 (*metab*)
Whistace, J. *et al., Biochem. J.*, 1968, **109**, 577 (*biosynth*)
Kleeva, L.P. *et al., Zh. Org. Khim.*, 1968, **4**, 1171 (*synth*)
Rao, G.H.R. *et al., Prog. Lipids Res.*, 1981, **20**, 549 (*pharmacol*)
Rasool, N. *et al., Phytochemistry*, 1991, **30**, 2800 (α-*Tocopherolquinone methyl ether*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1422
Kobayashi, M. *et al., J. Chem. Res., Synop.*, 1994, 494 (*3′,11′,14′-Trihydroxy-α-tocopherol quinone*)

Tocopheronic acid T-412

[1948-76-1]
γ-Hydroxy-γ,2,4,5-tetramethyl-3,6-dioxo-1,4-cyclohexadiene-1-hexanoic acid, 9CI. 2-(3-Hydroxy-3-methyl-5-carboxypentyl)-3,5,6-trimethyl-1,4-benzoquinone



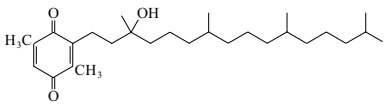
$C_{16}H_{22}O_5$ 294.347
Human metab. of α-Tocopherol, T-406.

Lactone:
Yellow plates (EtOH).

Simon, E.J. *et al., J. Biol. Chem.*, 1956, **221**, 807 (*isol*)
Green, J. *et al., Nature (London)*, 1961, **190**, 318

β-Tocopheryl quinone T-413

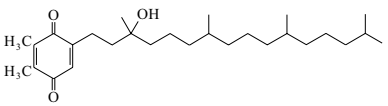
[3361-08-8]



$C_{28}H_{48}O_3$ 432.685
Isol. from vegetable sources, e.g. spinach chloroplasts (*Spinacia oleracea*). Oil. λ_{max} 261 (no solvent reported).

Henninger, M.D. *et al., Biochemistry*, 1963, **2**, 1168

γ-Tocopheryl quinone T-414

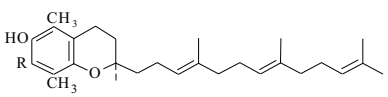


$C_{28}H_{48}O_3$ 432.685
Isol. from vegetable sources, e.g. spinach chloroplasts (*Spinacia oleracea*). Oil. λ_{max} 258 (no solvent reported).

Henninger, M.D. *et al., Biochemistry*, 1963, **2**, 1168

α-Tocotrienol T-415

[1721-51-3]
3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2H-1-benzopyran-6-ol, 9CI. ζ_1-Tocopherol. 5,7,8-Trimethyltocotrienol



R = CH_3
(*R*)-*form*

$C_{29}H_{44}O_2$ 424.665
The name α-Tocotrienol is IUPAC preferred (*Eur. J. Biochem.*, 1974, **46**, 217).

(R)-form [58864-81-6]
Occurs in wheat, barley, rye and palm oil.. Mp 30-31°. $[\alpha]_D^{25}$ -5.7 (c, 1.01 in $CHCl_3$).

p-*Phenylazobenzoyl:*
Cryst. (2-propanol). Mp 70-71°.

(±)-form
Cryst. Mp 30-31°.

p-*Phenylazobenzoyl:*
Cryst. Mp 84-85.5°.

Green, J. *et al., Chem. Ind. (London)*, 1960, 73 (*struct*)
Mayer, H. *et al., Helv. Chim. Acta*, 1963, **46**, 963 (*abs config*)
Schudel, P. *et al., Helv. Chim. Acta*, 1963, **46**, 2517 (*synth*)
Scott, J.W. *et al., Helv. Chim. Acta*, 1976, **59**, 290 (*synth*)
Guthrie, N. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C), CRC Press, 2001, 269-280
Chênevert, R. *et al., Tet. Lett.*, 2002, **43**, 7971-7973 (*synth*)

β-Tocotrienol T-416

[490-23-3]
3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-4H-1-benzopyran-6-ol, 9CI. ϵ-Tocopherol
As α-Tocotrienol, T-415 with
R = H
$C_{28}H_{42}O_2$ 410.639
Isol. from wheat bran oil. Yellow oil. $Bp_{0.00005}$ 140° (bath). Hydrogenation gives β-Tocopherol, T-407.

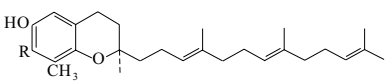
p-*Phenylazobenzoyl:*
Cryst. (2-propanol). Mp 70-71° (49-52°).

[1406-66-2]

Green, J. *et al., J.C.S.*, 1959, 3362 (*isol, struct*)
Green, J. *et al., Chem. Ind. (London)*, 1960, 73 (*struct, isol*)
Schudel, P. *et al., Helv. Chim. Acta*, 1963, **46**, 2517 (*synth*)
McHale, D. *et al., J.C.S.*, 1963, 784 (*struct*)

δ-Tocotrienol T-417

[25612-59-3]
3,4-Dihydro-2,8-dimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2H-1-benzopyran-6-ol, 9CI. 2,8-Dimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-6-chromanol. 8-Methyltocotrienol



R = H

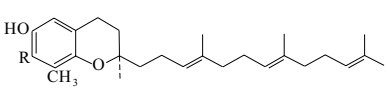
$C_{27}H_{40}O_2$ 396.612
Constit. of palm oil. Nutriceutical with anticancer props. and a positive influence on the blood lipid profile. Oil. Poorly sol. hexane.

11′,12′-Epoxide: [57576-80-4] ***Epoxy-δ-tocotrienol***. δ-Tocotrienol epoxide
$C_{27}H_{40}O_3$ 412.611

Dunphy, P.J. *et al., Nature (London)*, 1965, **207**, 521 (*isol*)
Whittle, K.J. *et al., Biochem. J.*, 1966, **100**, 138 (*ir*)
Kato, T. *et al., Chem. Lett.*, 1975, 335 (*Epoxytocotrienol*)
Vieira, P.C. *et al., Phytochemistry*, 1983, **22**, 2281 (*isol, pmr*)
Guthrie, N. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 269-280

γ-Tocotrienol T-418

[14101-61-2]
7,8-Dimethyltocotrienol. Plastochromanol 3



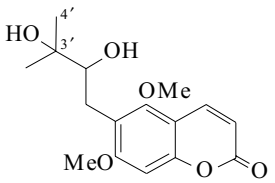
R = CH_3

$C_{28}H_{42}O_2$ 410.639
Constit. of palm oil. Nutriceutical with anticancer props. and a positive influence on the blood lipid profile. Oil.

Mayer, H. *et al., Helv. Chim. Acta*, 1967, **50**, 1376
Guthrie, N. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 269-280

Toddalolactone T-419

[483-90-9]
*6-(2,3-Dihydroxy-3-methylbutyl)-5,7-dimethoxy-2*H*-1-benzopyran-2-one, 9CI*



$C_{16}H_{20}O_6$ 308.33
Prisms. Mp 135°. $[\alpha]_D^{30}$ +55.9 ($CHCl_3$).

Di-Ac:
Needles. Mp 119°.

3′-Me ether: [85011-60-5]
$C_{17}H_{22}O_6$ 322.357
Oil.

3′-Deoxy, 2′-Ketone: [77636-08-9] ***Toddanone***
$C_{16}H_{18}O_5$ 290.315
Cryst. (CH_2Cl_2/Et_2O). Mp 116°.

3′-Deoxy, 3′,4′-didehydro: [77715-99-2] ***Toddanol***
$C_{16}H_{18}O_5$ 290.315
Mp 125°. $[\alpha]_D^{20}$ -93.3 (c, 3.0 in $CHCl_3$).

3′-Deoxy, 3′,4′-didehydro, O^5*-de-Me:* [126622-57-9] *5-Hydroxy-6-(2-hydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, 9CI*. ***5-De-O-methyltoddanol***
$C_{15}H_{16}O_5$ 276.288
Constit. of the stem bark of *Citrus grandis* (pummelo).

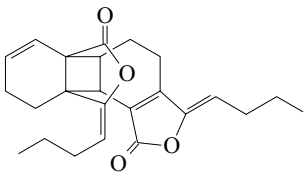
3′-Deoxy, 3′-chloro: [15575-50-5] ***6-(3-Chloro-2-hydroxy-3-methylbutyl)-5,7-dimethoxy-2H-1-benzopyran-2-one***
$C_{16}H_{19}ClO_5$ 326.776
Mp 153°. $[\alpha]_D$ +72.3 (c, 2.5 in $CHCl_3$).

[78548-01-3, 137182-34-4]

Späth, E. *et al., Ber.*, 1938, **71**, 1825; *Chem. Ber.*, 1939, **72**, 53 (*struct*)
Combes, G. *et al., Bull. Soc. Chim. Fr.*, 1961, 1609 (*synth*)
Desai, P.D. *et al., Indian J. Chem.*, 1967, **5**, 41 (*3′-Deoxy-3′-chloro*)
Sharma, P.N. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 299 (*isol*)
Sharma, P.N. *et al., Phytochemistry*, 1981, **20**, 335 (*Toddanol, Toddanone*)
Reisch, J. *et al., Pharmazie*, 1982, **37**, 862 (*deriv*)
Huang, S.C. *et al., Phytochemistry*, 1989, **28**, 3574 (*Demethyltoddanol*)
Ishii, H. *et al., Yakugaku Zasshi*, 1991, **111**, 376 (*struct*)

Tokinolide A T-420

[112899-62-4]

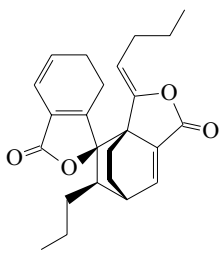


$C_{24}H_{28}O_4$ 380.483
Constit. of the roots of *Angelica acutiloba* (Dong Dang Gui). Oil. Racemic.

Tsuchida, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4460 (*isol, struct*)

Tokinolide B T-421

[112966-16-2]

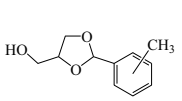


$C_{24}H_{28}O_4$ 380.483
Constit. of the roots of *Angelica acutiloba* (Dong Dang Gui). Oil. Racemic.

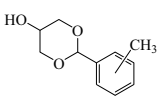
Tsuchida, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4460 (*isol, struct*)
Ogawa, Y. *et al., Heterocycles*, 1997, **45**, 1869-1872 (*synth, pmr*)

Tolualdehyde glyceryl acetal T-422

[4388-47-0, 4740-79-8, 4757-23-7, 5694-72-4, 72190-17-1, 72190-18-2, 72190-19-3, 72190-20-6, 143492-57-3, 143492-58-4, 143562-57-6, 143562-92-9]
2-(Methylphenyl)-1,3-dioxolane-4-methanol. 2-(Methylphenyl)-1,3-dioxan-5-ol. FEMA 3067



1,2-acetal



1,3-acetal

$C_{11}H_{14}O_3$ 194.23
Coml. material is a mixt. of 1,2- and 1,3-isomers in ca. 4:6 ratio and a mixt. of *o*-, *m*- and *p*- isomers. Flavouring ingredient for beverages, baked goods, puddings and candies. Sl. viscous almost odourless liq. with mild, bitter-almond flavour. Bp 292°.

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 887 (*rev, tox*)
Japan. Pat., 1987, 62 19 547; *CA*, **117**, 150998e (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1705-1706 (*use, props*)

Toluene, 8CI T-423

[108-88-3]
Methylbenzene, 9CI

$PhCH_3$

C_7H_8 92.14
Isol. from distilled tolu balsam (*Myroxylon balsamum*). Minor constit. of lime oil (*Citrus aurantifolia*). Liq. d_4^{20} 0.87. Fp -95. Bp 110.6° $Bp_{14.56}$ 14.5°. n_D^{20} 1.4967. pK_a 54 (MeCN).

▶ Highly flammable, fl. p. 4°, autoignition temp. 480°. Reacts violently with many oxidants. CNS depressant. Low conc. (100 ppm) cause eye, respiratory tract irritation, headache, dizziness. High conc. produce mental confusion, loss of coordination, and unconsciousness within minutes. Not associated with the haemopoietic effects of benzene. Chronic exposure or abuse can injure kidneys and liver, and cause teratogenic effects. OES: long-term 50 ppm; short-term 150 ppm (Sk). XS5250000

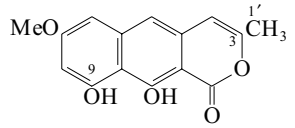
Picrate:
Pale yellow cryst. Mp 88.2°.

[1124-18-1, 2037-26-5, 6711-19-9, 18860-15-6, 34504-47-7]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 931B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 849B (*ir*)
Perkin, W.H. *et al., J.C.S.*, 1896, **69**, 1025 (*synth*)
Adv. Chem. Ser., 1955, **15**, 12 (***props***)
Davies, M. *et al., Trans. Faraday Soc.*, 1968, **64**, 847 (*ir, microwave*)
Schmid, E.D. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1971, **75**, 1334 (*Raman*)
Beynon, J.H. *et al., Org. Mass Spectrom.*, 1971, **5**, 303 (*ms*)
Proulx, T.W. *et al., J. Magn. Reson.*, 1976, **23**, 477 (*cmr*)
Breslow, R. *et al., J.A.C.S.*, 1977, **99**, 7745 (*acidity*)
Palmer, M.H. *et al., J. Mol. Struct.*, 1978, **49**, 105 (*pe*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 246 (*rev*)
Bolovinos, A. *et al., J. Chem. Phys.*, 1981, **75**, 4343 (*uv*)
Schaefer, T. *et al., Can. J. Chem.*, 1985, **63**, 2597 (*pmr*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1105
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TGK750
Antti-Poika, M. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 38 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2612
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1222

Toralactone T-424

[41743-74-2]
*9,10-Dihydroxy-7-methoxy-3-methyl-1*H*-naphtho[2,3-c]pyran-1-one, 9CI*



$C_{15}H_{12}O_5$ 272.257
Isol. from seeds of *Cassia tora* (charota). Pale yellow needles (C_6H_6/hexane). Mp 252-254°.

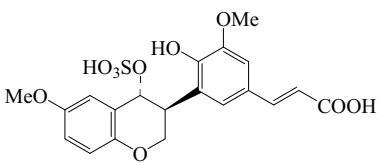
9-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: [119170-52-4] ***Cassiaside C***. *Toralactone 9-gentiobioside*
$C_{27}H_{32}O_{15}$ 596.541
Isol. from seeds of *Cassia tora* (charota). Pale yellow needles (MeOH aq.). Mp 235-237° (218-220°). $[\alpha]_D^{25}$ -56.4 (c, 0.37 in Py).

9-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Cassiaside C₂***
$C_{39}H_{52}O_{25}$ 920.825
Yellow needles (MeOH aq.). Mp 195.5-197°. $[\alpha]_D^{18}$ +5.2 (c, 0.5 in H_2O). λ_{max} 218 (log ϵ 3.03); 279 (log ϵ 3.58); 384 (log ϵ 2.64) (H_2O).

$\Delta^{3,1'}$-Isomer: [80503-54-4] *3,4-Dihydro-9,10-dihydroxy-7-methoxy-3-methylene-1H-naphtho[2,3-c]pyran-1-one, 9CI.* ***Isotoralactone***
$C_{15}H_{12}O_5$ 272.257
Pale-yellow needles (C_6H_6). Mp 233-235° dec.

Takahashi, S. *et al., Yakugaku Zasshi*, 1973, **93**, 261; *CA*, **78**, 156649q (*isol, struct*)
Kitanaka, S. *et al., Phytochemistry*, 1981, **20**, 1951 (*Isotoralactone*)
Kitanaka, S. *et al., Yakugaku Zasshi*, 1986, **106**, 302; *CA*, **105**, 85022t (*isol*)
Kitanaka, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3980; 1998, **46**, 1650-1652 (*Cassiaside C, Cassiaside C2*)
Wong, S.M. *et al., Planta Med.*, 1989, **55**, 276 (*Cassiaside C*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1121-1127 (*activity*)

Torvanol A T-425

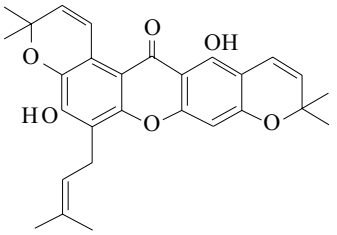


$C_{20}H_{20}O_{10}S$ 452.438
Constit. of the fruit of *Solanum torvum*. Amorph. powder (as K salt). $[\alpha]_D^{29}$ -50 (c, 0.28 in H_2O) (K salt). Mp >300° (K salt) λ_{max} 203 ; 234 ; 283 (MeOH) (K salt).

Arthan, D. *et al., Phytochemistry*, 2002, **59**, 459-463

Tovophyllin B T-426

[40738-45-2]
5,13-Dihydroxy-3,3,10,10-tetramethyl-6-(3-methyl-2-butenyl)-2H-dipyrano[2,3-a:2′,3′-i]xanthen-14-one



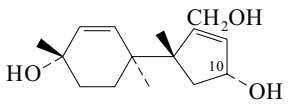
$C_{28}H_{28}O_6$ 460.526
Struct. revised in 1975. Constit. of *Garcinia mangostana* (mangosteen). Yellow needles (EtOH). Mp 190-191°.

3′,4′-Dihydro: ***Mangostenone B***
$C_{28}H_{30}O_6$ 462.541
Constit. of the green fruit hulls of *Garcinia mangostana* (mangosteen). Yellow amorph. resin. λ_{max} 293 (log ϵ 4.47); 334 (log ϵ 4.09); 366 (log ϵ 3.87) (EtOH).

Gonçalves de Oliveira, W. *et al., Phytochemistry*, 1972, **11**, 3323-3325 (*isol*)
Mesquita, A.A.L. *et al., Phytochemistry*, 1975, **14**, 803-806 (*derivs, struct*)
Suksamrarn, S. *et al., J. Nat. Prod.*, 2002, **65**, 761-763 (*isol, cmr, Mangostenone B*)

Toxin FS2 T-427

1,4-Dimethyl-4-[4-hydroxy-2-(hydroxymethyl)-1-methyl-2-cyclopentenyl]-2-cyclohexen-1-ol. FS2 Toxin



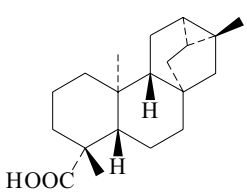
$C_{15}H_{24}O_3$ 252.353
Isol. from *Fusarium sporotrichioides*. No phys. props. reported.

10-Ketone: ***Toxin FS4***. *FS4 toxin*
$C_{15}H_{22}O_3$ 250.337
From *Fusarium sporotrichioides* and *Fusarium sambucinum*. Glass. λ_{max} 229 (ϵ 13000) (MeCN) (Berdy).

10-Epimer: ***Epi FS2***
$C_{15}H_{24}O_3$ 252.353
From *Fusarium sporotrichioides*. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. λ_{max} 194 (ϵ 12000) (MeCN) (Berdy).

Corley, D.G. *et al., J.O.C.*, 1987, **52**, 4405 (*isol, struct*)
Sanson, D.R. *et al., J.O.C.*, 1989, **54**, 4313 (*derivs*)

19-Trachylobanoic acid T-428



$C_{20}H_{30}O_2$ 302.456
ent-form
Cryst. Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 128-131°. $[\alpha]_D$ -52 (c, 0.8 in $CHCl_3$).

Thujyl ester:
$C_{30}H_{46}O_2$ 438.692
Isol. from sunflowers. Cryst. Mp 128-131°.

19-Aldehyde: [94061-33-3] ***ent-19-Trachylobanal***
$C_{20}H_{30}O$ 286.456
Isol. from sunflowers. Oil.

St Pyrek, J. *et al., J. Nat. Prod.*, 1984, **47**, 822
Faulkner, D.F. *et al., Planta Med.*, 1985, 354
Leong, Y.W. *et al., Phytochemistry*, 1997, **45**, 1457-1459 (*isol, pmr, cmr*)
Toyota, M. *et al., J.O.C.*, 2000, **65**, 4565-4570 (*synth*)

Transferrins T-429

A class of two-sited single-chain metal-binding glycoproteins. MW 76000-81000. There are three major types; serum transferrins, lactoferrins and ovotransferrins. Recombinant form is under consideration as a component of infant food. Bovine lactoferrin has GRAS status for use as a 2% antimicrobial spray application to raw beef. Red cryst. by dialysis. λ_{max} 465 (pH8.2).

Serum transferrin
Serotransferrin. Siderophilin
Commonly called transferrin.

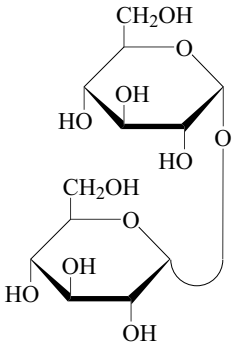
Lactoferrin
Lactotransferrin
Bovine lactoferrin has GRAS status for use as a 2% spray for application to raw beef as antimicrobial.

Ovotransferrin
Conalbumin
[166870-72-0]

Castellino, F.J. *et al., J. Biol. Chem.*, 1970, **245**, 4269 (*struct*)
Querinjean, P. *et al., Eur. J. Biochem.*, 1971, **20**, 420 (*props*)
Aisen, P. *et al., Inorg. Biochem.*, 1973, **1**, 280 (*rev*)
Bezkorovainy, A. *et al., Arzneim.-Forsch.*, 1974, **24**, 476 (*rev*)
Aisen, P. *et al., Annu. Rev. Biochem.*, 1980, **49**, 357-393 (*rev*)
Metz-Boutigue, M.H. *et al., Eur. J. Biochem.*, 1984, **145**, 659 (*struct*)
Rey, M.W. *et al., Nucleic Acids Res.*, 1990, **18**, 5288 (*cloning*)
Tomita, M. *et al., Acta Paediatr. Jpn.*, 1994, **36**, 585-591 (*rev*)
Hutchens, T.W. *et al., Adv. Exp. Med. Biol.*, 1994, **357**,
Lien, E.L. *et al., Exp. Biol. Med.*, 1997, **28**, (*use*)
Food Chem. News, no. 20, 2001, **43**, 9 (*use*)

α,α-Trehalose T-430

[99-20-7]
α-D-Glucopyranosyl-α-D-glucopyranoside, 9CI, 8CI. Mycose. Mushroom sugar. Trehalose



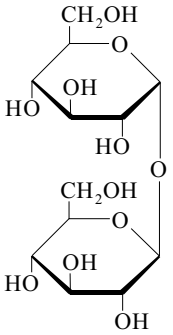
$C_{12}H_{22}O_{11}$ 342.299
Occurs in fungi. EU and USA approved sweetener. Mp 97° (hydrate) Mp 214-216° (anhyd.). $[\alpha]_D^{20}$ +178.3 (H_2O) (hydrate). $[\alpha]_D^{20}$ +199 (H_2O) (anhyd.). Sweet taste. Sweetness = 0.36 × sucrose. Fermented by yeast.

[6138-23-4]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 912C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 196A (*ir*)
Richtmyer, N.K. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 370 (*isol*)
Birch, G. *et al., Adv. Carbohydr. Chem.*, 1963, **18**, 201 (*rev*)
Birch, G. *et al., J.C.S.(C)*, 1966, 1072 (*synth*)
Pazur, J.H. *et al., The Carbohydrates*, (Eds., Pigman, W., *et al*), 2nd edn., Academic Press, 1970, **2A**, 106 (*rev*)
Taga, T. *et al., Acta Cryst. B*, 1972, **28**, 3258 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 644 (*occur*)
Usui, T. *et al., J.C.S. Perkin 1*, 1973, 2425 (*conformn, cmr*)
Elbein, A.D. *et al., Adv. Carbohydr. Chem. Biochem.*, 1974, **30**, 227 (*rev*)
Usui, T. *et al., Carbohydr. Res.*, 1974, **33**, 105 (*pmr, config*)
Hough, L. *et al., Pure Appl. Chem.*, 1977, **49**, 1069 (*rev*)
Pfeffer, P.E. *et al., J.A.C.S.*, 1979, **107**, 1265 (*cmr*)
Lee, G.K. *et al., Dev. Food Carbohydr.*, Applied Science Pub., 1980, **2**, 1 (*rev*)
Jeffrey, G.A. *et al., Carbohydr. Res.*, 1985, **137**, 21 (*cryst struct*)
Abbate, S. *et al., Carbohydr. Res.*, 1991, **210**, 1 (*ir, Raman*)
Tarelli, E. *et al., Carbohydr. Res.*, 1994, **261**, 25 (*synth, phosphates*)
Hull, S.R. *et al., Carbohydr. Res.*, 1995, **266**, 147-157 (*isol*)
Mueller, J. *et al., Plant Sci. (Limerick, Irel.)*, 1995, **112**, 1 (*rev, occur*)
Gil, A.M. *et al., Spectrochim. Acta A*, 1996, **52**, 1649-1659 (*ir, Raman, pmr, cmr*)
Food Chem. News, 2000, **42(42)**, 6; 2001, **43(20)**, 15 (*use*)
Sussich, F. *et al., Carbohydr. Res.*, 2001, **334**, 165-176 (*solution props*)
Akao, K. *et al., Carbohydr. Res.*, 2001, **334**, 233-241 (*ir, props*)

α,β-Trehalose T-431

[585-91-1]
β-D-Glucopyranosyl α-D-glucopyranoside, 9CI, 8CI. α-D-Glucopyranosyl β-D-glucopyranoside. Neotrehalose



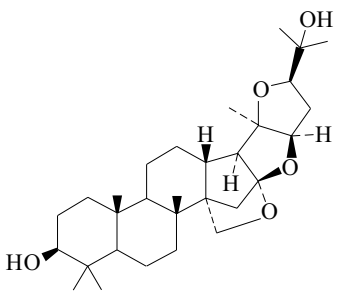
$C_{12}H_{22}O_{11}$ 342.299
Constit. of honey. Mp 149°. $[\alpha]_D^{22}$ +83.5 (c, 2 in H_2O). Considerable variations in props. reported in the lit., probably owing to variations in purity.

Octa-Ac:
$C_{28}H_{38}O_{19}$ 678.597
Mp 140-141°. $[\alpha]_D^{18}$ +79.6 (c, 0.7 in $CHCl_3$).

Burckhardt, H. *et al., Chem. Ber.*, 1956, **89**, 314 (*synth*)
Birch, G. *et al., Adv. Carbohydr. Chem.*, 1963, **18**, 201 (*rev*)
Usui, T. *et al., J.C.S. Perkin 1*, 1973, 2425 (*conformn, cmr*)
Usui, T. *et al., Carbohydr. Res.*, 1974, **33**, 105 (*config, pmr*)
Pfeffer, P.E. *et al., J.A.C.S.*, 1979, **101**, 1265 (*cmr*)
Parrish, F.W. *et al., Carbohydr. Res.*, 1987, **168**, 129 (*purifn, props, cmr, bibl*)
Taga, T. *et al., Acta Cryst. C*, 1997, **53**, 234-236 (*cryst struct*)

Trevoagenin D T-432

*16α,18:16β,22*R:*20*R,*24*R-*Triepoxydammarane-3β,25-diol*



$C_{30}H_{48}O_5$ 488.706
Cryst. (hexane). Mp 249-251°. $[\alpha]_D$ -14 (c, 0.28 in $CHCl_3$).

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galactopyranoside]: [146445-94-5] ***Jujubasaponin VI***
$C_{42}H_{68}O_{14}$ 796.991
Constit. of *Zizyphus jujuba* (Chinese date). Amorph. powder. $[\alpha]_D$ -28.1 (c, 4.5 in MeOH).

Betancor, C. *et al., Tet. Lett.*, 1982, **23**, 1125 (*cryst struct*)
Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2275 (*Jujubasaponin VI*)

Triacontanal, 9CI T-433

[22725-63-9]
$H_3C(CH_2)_{28}CHO$
$C_{30}H_{60}O$ 436.803
Isol. from wine grapes (*Vitis vinifera*), from *Brassica oleracea* leaves and from apple cuticle wax.

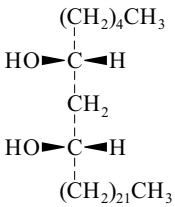
Radler, F. *et al., Aust. J. Chem.*, 1965, **18**, 1059
Schmid, H.H.O. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1969, **350**, 462 (*isol*)
Japan. Pat., 1982, 59 95 236; *CA*, **101**, 170706f (*synth*)

1,11-Triacontanediol T-434

[180005-30-5]
$H_3C(CH_2)_{18}CH(OH)(CH_2)_9CH_2OH$
$C_{30}H_{62}O_2$ 454.819
Constit. of the leaf wax of *Papaver somniferum* (opium poppy).

Jetter, R. *et al., Phytochemistry*, 1996, **42**, 1617-1620 (*isol, ms*)

6,8-Triacontanediol T-435



$C_{30}H_{62}O_2$ 454.819
(6*R,8*S**)-*form*** [155800-87-6]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 74-75°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

7,9-Triacontanediol T-436

$C_{30}H_{62}O_2$ 454.819
(7*R,9*S**)-*form*** [193419-72-6]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 59-61°.

Akihisa, Y. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, pmr, ms*)

7,9-Triacontanedione T-437

$H_3C(CH_2)_{20}COCH_2CO(CH_2)_5CH_3$
$C_{30}H_{58}O_2$ 450.787
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

10,12-Triacontanedione T-438

$H_3C(CH_2)_{17}COCH_2CO(CH_2)_8CH_3$
$C_{30}H_{58}O_2$ 450.787
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

11,13-Triacontanedione T-439

$H_3C(CH_2)_{16}COCH_2CO(CH_2)_9CH_3$
$C_{30}H_{58}O_2$ 450.787
Constit. of the pollen of *Helianthus*

annuus (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

12,14-Triacontanedione T-440

$H_3C(CH_2)_{15}COCH_2CO(CH_2)_{10}CH_3$

$C_{30}H_{58}O_2$ 450.787

Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

13,15-Triacontanedione T-441

[81116-08-7]

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_{11}CH_3$

$C_{30}H_{58}O_2$ 450.787

Constit. of coffee and the blue gum (*Eucalyptus globulus*). Antioxidant for foods.

Japan. Pat., 1981, 81 151 486; *CA*, **96**, 141433n (*isol, props*)

Ablanque, E. *et al., CA*, 1989, **110**, 209458q (*isol*)

Triacontanoic acid, 9CI, 8CI T-442

[506-50-3]

Melissic acid A

$H_3C(CH_2)_{28}COOH$

$C_{30}H_{60}O_2$ 452.803

Found in some plant waxes, e.g. cotton. Cryst. (C_6H_6/Me_2CO). Mp 93.5-94°.

Me ester: [629-83-4]
$C_{31}H_{62}O_2$ 466.83
Cryst. (petrol). Mp 71.5°.

Et ester: [7505-12-6]
$C_{32}H_{64}O_2$ 480.856
Cryst. (EtOH). Mp 70.5°.

Pentyl ester: [116044-06-5]
$C_{35}H_{70}O_2$ 522.937

Hexyl ester: [108706-11-2]
$C_{36}H_{72}O_2$ 536.964

Tetradecyl ester: [104932-41-4]
$C_{44}H_{88}O_2$ 649.178

Hentriacontyl ester: [135729-36-1]
$C_{61}H_{122}O_2$ 887.634

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 487B; 610C (*ir*)

Robinson, G.M. *et al., J.C.S.*, 1934, 1543 (*synth, esters*)

Cocker, W. *et al., J.C.S.*, 1962, 5194 (*isol*)

Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 713 (*occur*)

Odinokov, V.N. *et al., Zh. Org. Khim.*, 1990, **26**, 1209; *J. Org. Chem. USSR (Engl. Transl.)*, 1990, **26**, 1402 (*synth, Me ester, ms*)

21-Triacontenoic acid T-443

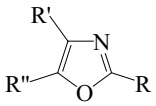
$H_3C(CH_2)_7CH{=}CH(CH_2)_{19}COOH$

$C_{30}H_{58}O_2$ 450.787

(Z)-form [67329-09-3]
Lumequic acid
Isol. from seed oil of *Ximenia americana* (tallow nut). Plates. Mp 60.8-61.2°.

Lightelm, S.P. *et al., J. Sci. Food Agric.*, 1954, **5**, 281

Trialkyloxazoles T-444



See also Trimethyloxazole, T-787.

2-Ethyl-4,5-dimethyloxazole, 9CI [53833-30-0]
FEMA 3672
$C_7H_{11}NO$ 125.17
Flavouring ingredient. Aroma constit. of French fried potatoes and Arabica coffee. d_4^{20} 1.48. Bp 150-152°. n_D^{20} 1.4574.

4-Ethyl-2,5-dimethyloxazole [30408-61-8]
$C_7H_{11}NO$ 125.17
Constit. of Arabica coffee aroma, French fries and yeast extract. Bp 148-150°. n_D^{24} 1.4442.

5-Ethyl-2,4-dimethyloxazole [33318-74-0]
$C_7H_{11}NO$ 125.17
Constit. of Arabica coffee aroma, French fries and yeast extract. Characterised spectroscopically.

2,4-Dimethyl-5-propyloxazole, 9CI [84027-86-1]
$C_8H_{13}NO$ 139.197
Constit. of roasted peanuts, French fries and boiled shrimp (*Panaeus brevistoris*) aromas. Characterised spectroscopically.

2,5-Dimethyl-4-propyloxazole [30674-60-3]
$C_8H_{13}NO$ 139.197
Bp 165-168°. n_D^{24} 1.4457.

4,5-Dimethyl-2-propyloxazole, 9CI [53833-32-2]
$C_8H_{13}NO$ 139.197
Constit. of roast beef and coffee aroma. Bp 175-185°.

4,5-Diethyl-2-methyloxazole, 9CI [94794-04-4]
$C_8H_{13}NO$ 139.197
Not reported in nature. Liq. with sweet, earthy odour. Bp_{17} 64-65°.

2,4-Diethyl-5-methyloxazole [84027-88-3]
$C_8H_{13}NO$ 139.197
Strong green, flowery odour. Characterised spectroscopically.

2-Isopropyl-4,5-dimethyloxazole [19519-45-0]
4,5-Dimethyl-2-(1-methylethyl)oxazole, 9CI
$C_8H_{13}NO$ 139.197
Volatile constit. of roasted peanuts, French fries, cocoa butter, fried bacon, fried chicken and coffee. Bp 163-164°.

2-Ethyl-4-methyl-5-propyloxazole [102586-53-8]
$C_9H_{15}NO$ 153.224
Constit. of French fries. Characterised spectroscopically.

4-Ethyl-2-methyl-5-propyloxazole, 9CI [88300-06-5]
$C_9H_{15}NO$ 153.224
Volatile constit. of French fried potato and cocoa butter. Oil with green, fatty, vegetable-like odour. Bp_{19} 82-87°.

5-Ethyl-2-isopropyl-4-methyloxazole [102586-54-9]
5-Ethyl-4-methyl-2-(1-methylethyl)oxazole, 9CI
$C_9H_{15}NO$ 153.224
Volatile constit. of French fried potato. Characterised spectroscopically.

2-Butyl-4,5-dimethyloxazole, 9CI
$C_9H_{15}NO$ 153.224
Constit. of French fries. Characterised spectroscopically.

5-Ethyl-2-methyl-4-propyloxazole, 9CI [84027-92-9]
$C_9H_{15}NO$ 153.224
Constit. of roasted peanuts. Characterised spectroscopically.

4-Ethyl-2-isopropyl-5-methyloxazole [84027-96-3]
4-Ethyl-5-methyl-2-(1-methylethyl)oxazole, 9CI
$C_9H_{15}NO$ 153.224
Constit. of yeast extracts, cocoa butter or beans and roasted peanut volatiles. Bp_{10} 74-76°.

4-Butyl-2,5-dimethyloxazole, 9CI [30408-62-9]
$C_9H_{15}NO$ 153.224
Constit. of roast beef, cocoa butter and French fried potato aroma. Liq. with green, fatty, vegetable odour. Bp 186-188°. n_D^{24} 1.4478.

4,5-Dimethyl-2-(2-methylpropyl)oxazole, 9CI [26131-91-9]
2-Isobutyl-4,5-dimethyloxazole, 8CI
$C_9H_{15}NO$ 153.224
Constit. of French fried potato volatiles. Characterised spectroscopically.

4-Ethyl-5-methyl-2-propyloxazole, 9CI [84027-94-1]
$C_9H_{15}NO$ 153.224
Not reported in nature. Oil with acidic, cheesy, sl. fruity aroma. Characterised spectroscopically.

5-Butyl-2,4-dimethyloxazole, 9CI [88300-07-6]
$C_9H_{15}NO$ 153.224
Not reported in nature. Liq. with acidic, fatty, sweet, flowery odour or herb-like odour. Bp_{19} 95-101°.

2,4-Diethyl-5-propyloxazole, 9CI [77311-03-6]
$C_{10}H_{17}NO$ 167.25
Constit. of French fries and roasted peanut. Characterised spectroscopically.

2,4-Diethyl-5-butyloxazole [84028-09-1]
$C_{11}H_{19}NO$ 181.277
Green, fruity odour. Characterised spectroscopically.

2-Butyl-5-ethyl-4-methyloxazole, 9CI [84028-02-4]
$C_{10}H_{17}NO$ 167.25
Constit. of cocoa butter. Liq. with green, sweet odour. Bp_{10} 97-101°.

5-Butyl-4-ethyl-2-methyloxazole, 9CI [84027-98-5]
$C_{10}H_{17}NO$ 167.25
Constit. of cocoa butter. Bp_{19} 94-98°.

2-Butyl-4-ethyl-5-methyloxazole, 9CI [84028-03-5]
$C_{10}H_{17}NO$ 167.25

Constit. of cocoa butter and yeast extract aromas. Bp_{10} 90-92°.

2,4-Dimethyl-5-pentyloxazole [94794-05-5]
$C_{10}H_{17}NO$ 167.25
Sweet, floral, fruity slightly green odour. No phys. props. reported.

4,5-Dimethyl-2-pentyloxazole, 9CI [84028-05-7]
$C_{10}H_{17}NO$ 167.25
Volatile constit. of French fried potato. Fennel-like, earthy, green odour. Characterised spectroscopically.

4-Butyl-2-ethyl-5-methyloxazole, 9CI [94794-06-6]
$C_{10}H_{17}NO$ 167.25
Not reported in nature. Fatty, sweet odour. No phys. props. reported.

5-Ethyl-4-methyl-2-pentyloxazole [84028-13-7]
$C_{11}H_{19}NO$ 181.277
Constit. of French fries. Characterised spectroscopically.

4-Hexyl-2,5-dimethyloxazole, 8CI [20662-86-6]
$C_{11}H_{19}NO$ 181.277
Constit. of roast beef. Characterised spectroscopically.

2-Butyl-4,5-diethyloxazole, 9CI
$C_{11}H_{19}NO$ 181.277
Constit. of French fries. Characterised spectroscopically.

2-Butyl-5-methyl-4-propyloxazole, 9CI [94794-09-9]
$C_{11}H_{19}NO$ 181.277
Constit. of French fries. Characterised spectroscopically.

2-Hexyl-4,5-dimethyloxazole, 9CI
$C_{11}H_{19}NO$ 181.277
Constit. of French fried potato. Liq. with fresh, flowery aroma. $Bp_{0.08}$ 58-60°.

5-Butyl-4-methyl-2-propyloxazole, 9CI [84028-11-5]
$C_{11}H_{19}NO$ 181.277
Not reported in nature. Characterised spectroscopically.

4-Ethyl-5-methyl-2-pentyloxazole, 9CI [84028-14-8]
$C_{11}H_{19}NO$ 181.277
Not reported in nature. Characterised spectroscopically.

2,5-Dibutyl-4-methyloxazole, 9CI [88300-08-7]
$C_{12}H_{21}NO$ 195.304
Constit. of cocoa butter. Liq. with sweet, fruity odour. Bp_{10} 116-119°.

5-Ethyl-2-hexyl-4-methyloxazole, 9CI [84028-19-3]
$C_{12}H_{21}NO$ 195.304
Volatile constit. of French fried potato. Characterised spectroscopically.

4-Methyl-2-pentyl-5-propyloxazole, 9CI [84028-17-1]
$C_{12}H_{21}NO$ 195.304
Not reported in nature. Green, nutty odour. Characterised spectroscopically.

4-Ethyl-2-hexyl-5-methyloxazole, 9CI [84028-20-6]
$C_{12}H_{21}NO$ 195.304
Not reported in nature. Fatty, sweet, French fries-like odour. Characterised spectroscopically.

4,5-Dimethyl-2-heptyloxazole, 9CI
$C_{12}H_{21}NO$ 195.304
Not reported in nature. Sweet, herbal, flowery odour. No phys. props. reported.

2,5-Diethyl-4-propyloxazole [40953-17-1]
$C_{10}H_{17}NO$ 167.25
Liq. with sweet, floral sl. green-fatty odour. Bp 193-197°. n_D^{20} 1.4491.

5-Ethyl-4-methyl-2-propyloxazole [84027-93-0]
$C_9H_{15}NO$ 153.224
Very sweet, fruity odour. Characterised spectroscopically.

2-Ethyl-5-methyl-4-pentyloxazole [84028-10-4]
$C_{11}H_{19}NO$ 181.277
Mushroom-fatty note, sweet odour. Characterised spectroscopically.

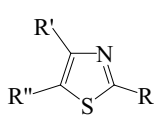
2-Ethyl-4-methyl-5-pentyloxazole [84028-08-0]
$C_{11}H_{19}NO$ 181.277
Characterised spectroscopically.

2-Butyl-4-methyl-5-propyloxazole, 9CI [94794-07-7]
$C_{11}H_{19}NO$ 181.277
Green, sweet, green pepper-like odour.

[106100-43-0]

Bredereck, H. *et al., Chem. Ber.*, 1953, **86**, 88-96 (*synth*)
Fr. Pat., 1963, 1 340 996; *CA*, **60**, 5507a (*synth*)
Wiegand, E.E. *et al., Synthesis*, 1970, 648-649 (*synth, pmr*)
Van Bergen, T.J. *et al., J.A.C.S.*, 1972, **94**, 8451-8471 (*synth, pmr*)
Wiegand, E.E. *et al., J. Chem. Eng. Data*, 1973, **18**, 237 (*synth*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, pmr, occur, coffee*)
Reddy, G.S. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 322-323 (*2-Ethyl-4,5-dimethyloxazole, synth*)
Ho, C.-T. *et al., J. Agric. Food Chem.*, 1983, **31**, 180-181; 1384-1386 (*occur, ms, synth, peanuts, beef*)
Ho, C.-T. *et al., J. Food Sci.*, 1983, **48**, 1570-1571 (*occur, ms, synth*)
Jin, Q.Z. *et al., Perfum. Flavor.*, 1984, **9(4)**, 25-28 (*synth, aroma, occur*)
Carlin, J.T. *et al., J. Agric. Food Chem.*, 1986, **34**, 621-623 (*occur, synth, ms, French fries*)
Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur, cocoa*)
Shenderuk, V.V. *et al., CA*, 1990, **112**, 177182t (*occur, shrimp*)
Ames, J.M. *et al., Flavour Fragrance J.*, 1992, **7**, 89-103 (*detn, yeast*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 227 (*2-Ethyl-4,5-dimethyloxazole, use*)

Trialkylthiazoles T-445



See also Trimethylthiazole, T-797. Maillard products which are odour ingredients of cooked foods.

2-Ethyl-4,5-dimethylthiazole, 9CI [873-64-3]
$C_7H_{11}NS$ 141.237
Component of coffee aroma. Liq. Bp 185°.

4-Ethyl-2,5-dimethylthiazole, 9CI [32272-57-4]
$C_7H_{11}NS$ 141.237
Flavour component of coffee, baked potato, fried bacon, cooked pork and yeast extract. Liq. d^{20} 1. Mp 115-116° (as picrate). Bp_{11} 66-68°. n_D^{20} 1.5053.

5-Ethyl-2,4-dimethylthiazole, 9CI [38205-61-7]
Volatile flavour ingredient of coffee, roasted peanuts, roasted lamb fat, fried chicken, cooked pork, roast beef and yeast extract; flavouring ingredient.

2,4-Dimethyl-5-propylthiazole, 9CI [41981-70-8]
$C_8H_{13}NS$ 155.263
Claimed food uses are not well documented.

2,5-Dimethyl-4-propylthiazole, 9CI
$C_8H_{13}NS$ 155.263
Claimed food uses are not well documented. Bp_{12} 90-100°.

4,5-Dimethyl-2-propylthiazole, 9CI [41981-72-0]
$C_8H_{13}NS$ 155.263
Volatile component of cooked beef flavour and yeast extract.

2-Isopropyl-4,5-dimethylthiazole [53498-30-9]
4,5-Dimethyl-2-(1-methylethyl)thiazole, 9CI
Volatile flavour component of cooked potatoes, roasted peanuts, roast beef, fried chicken and roast cocoa beans.

2,5-Diethyl-4-methylthiazole, 9CI [41981-71-9]
$C_8H_{13}NS$ 155.263
Volatile flavour component of cooked pork, roast beef and baked potatoes. Mp 87° (as picrate). Bp_{11} 81.5-82.5°.

4-Butyl-2,5-dimethylthiazole, 9CI [41981-77-5]
$C_9H_{15}NS$ 169.29
Volatile flavour component of fried chicken, roast peanuts and baked potato.

4-Ethyl-2-methyl-5-propylthiazole, 9CI [41981-75-3]
Volatile flavour component of roasted peanuts and roast beef.

5-Ethyl-2-methyl-4-propylthiazole, 9CI [4276-67-9]
Volatile flavour component of roast beef. Bp_{12} 93-95°.

4-Ethyl-5-methyl-2-propylthiazole, 9CI [86290-19-9]
Volatile flavour component of roast beef. Mp 78-79° (as picrate). Bp_{13} 102-103°. n_D^{20} 1.5000.

5-Ethyl-4-methyl-2-propylthiazole, 9CI
$C_9H_{15}NS$ 169.29
Claimed food uses are not well documented.

4-Ethyl-2-isopropyl-5-methylthiazole [87116-68-5]
4-Ethyl-5-methyl-2-(1-methylethyl)thiazole, 9CI
Volatile component of fried chicken, roast peanut and yeast extract. Liq. Mp

94° (as picrate). Bp_{11} 87°.

5-Ethyl-2-isopropyl-4-methylthiazole [53498-31-0]
5-Ethyl-4-methyl-2-(1-methylethyl)thiazole, 9CI
$C_9H_{15}NS$ 169.29
Volatile flavour component of boiled potatoes and cooked beef.

2,4-Dimethyl-5-pentylthiazole, 9CI [96693-91-3]
$C_{10}H_{17}NS$ 183.317
Claimed food uses are not well documented.

4,5-Dimethyl-2-pentylthiazole, 9CI [86290-22-4]
Volatile flavour component of roast beef and fried chicken.

4-Methyl-2,5-dipropylthiazole, 9CI [87116-71-0]
$C_{10}H_{17}NS$ 183.317
Component of roast peanut flavour.

2-Butyl-5-ethyl-4-methylthiazole, 9CI [86290-20-2]
$C_{10}H_{17}NS$ 183.317
Volatile flavour component of fried chicken, roasted peanuts and roast beef.

4-Butyl-2-ethyl-5-methylthiazole, 9CI [96693-90-2]
Claimed food uses not well documented.

2,4-Diethyl-5-propylthiazole, 9CI [87116-70-9]
$C_{10}H_{17}NS$ 183.317
Volatile component of roast peanut flavour.

2,5-Diethyl-4-propylthiazole, 9CI [4276-68-0]
$C_{10}H_{17}NS$ 183.317
Volatile component of roast peanut flavour. Bp_{16} 70-73°.

5-Ethyl-4-methyl-2-pentylthiazole, 9CI [96693-87-7]
$C_{11}H_{19}NS$ 197.344

2-Hexyl-4,5-dimethylthiazole [87262-49-5]
Volatile flavour component of cooked beef.

2-Heptyl-4,5-dimethylthiazole, 9CI [87262-50-8]
Volatile flavour component of fried chicken and cooked beef.

4,5-Dimethyl-2-octylthiazole, 9CI [87262-52-0]
Flavour component of fried chicken and roast beef.

4-Ethyl-2-heptyl-5-methylthiazole, 9CI [87262-51-9]
$C_{13}H_{23}NS$ 225.397
Aroma constituent of fried chicken and cooked beef.

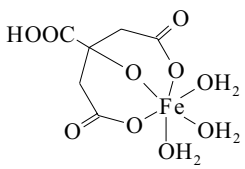
5-Ethyl-4-methyl-2-octylthiazole [192998-89-3]
Component of cooked beef aroma.

Asinger, F. *et al., Annalen*, 1957, **610**, 49-56; 1959, **634**, 131-134; 1961, **642**, 83-95; 1964, **672**, 156-178 (*synth*)
Pyl, T. *et al., Annalen*, 1964, **679**, 139-144 (*2-Et-4,5-di-Me, synth*)
Gerencevic, N. *et al., CA*, 1965, **63**, 16327a (*synth*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1973, **21**, 488-490; 1974, **22**, 912-914; 1977, **25**, 1227-1229 (*ms, occur*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264 (*5-Et-2,4-di-Me, synth*)
Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*occur, coffee*)
Haag, A. *et al., Org. Mass Spectrom.*, 1976, **11**, 511-524 (*ms*)
Coleman, E.C. *et al., J. Agric. Food Chem.*, 1980, **28**, 66-68; 1981, **29**, 42-48 (*occur, potato*)
Lee, M.H. *et al., J. Agric. Food Chem.*, 1981, **29**, 684-686 (*occur, peanuts*)
Ho, C.T. *et al., J. Agric. Food Chem.*, 1983, **31**, 336-342; 1384-1386 (*occur, bacon, peanuts*)
Hartman, G.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1030-1033 (*occur, beef*)
Tang, J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1287-1292 (*occur, chicken*)
Galt, A.M. *et al., J. Agric. Food Chem.*, 1984, **32**, 59-64 (*occur, beef*)
Ho, C.T. *et al., Perfum. Flavor.*, 1984, **9**, 15-18 (*synth, odour*)
Mottram, D.S. *et al., J. Sci. Food Agric.*, 1985, **36**, 377-382 (*occur, pork*)
Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur, cocoa*)
Vercellotti, J.R. *et al., J. Agric. Food Chem.*, 1987, **35**, 1030-1035 (*occur, beef*)
St. Angelo, A.S. *et al., J. Food Sci.*, 1987, **52**, 1163-1168 (*occur, beef*)
Silwar, R. *et al., Z. Lebensm.-Unters. -Forsch.*, 1992, **195**, 112-119 (*occur*)
Ames, J.M. *et al., ACS Symp. Ser.*, 1995, **564**, 146-159 (*occur, yeast*)
Elmore, J.S. *et al., J. Agric. Food Chem.*, 1997, **45**, 3595-3602; 3603-3607 (*occur*)

Triaqua[hydrogencitrato(3-)]iron T-446

[61927-79-5]

[2338-05-8]



$C_6H_{11}FeO_{10}$ 298.994

Compd. with choline: [1336-80-7] ***Ferrocholinate, INN***. *Ferrocholine. Ferrochelate. Chelafer. Chel-Iron. Many other names*
$C_{11}H_{24}FeNO_{11}$ 402.158
Nutrient supplement. Brown amorph. powder.

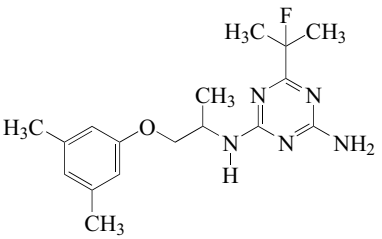
▶ LD_{50} (mus, orl) 5500 mg/kg. KH2979000

U.S. Pat., 1951, 2 575 611, (*Flint Eaton*); *CA*, **46**, 1722g (*synth, Ferrocholinate*)
Chakrabarti, J.K. *et al., Chem. Ind. (London)*, 1961, 1407 (*synth, pharmacol, Ferrocholinate*)
Miller, E.R. *et al., J. Anim. Sci.*, 1981, **52**, 783 (*use*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 976
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag*, 1994, 425 (*synonyms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1407-1408 (*Ferrocholinate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FBC100

Triaziflam, BSI T-447

[131475-57-5]

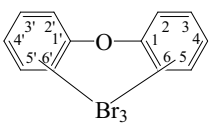
N-*[2-(3,5-Dimethylphenoxy)-1-methylethyl]-6-(1-fluoro-1-methylethyl)-1,3,5-triazine-2,4-diamine, 9CI*



$C_{17}H_{24}FN_5O$ 333.408

Pat. Coop. Treaty (WIPO), 1990, 90 09 378, (*Idemitsu Kosan*); *CA*, **114**, 42816y (*synth, activity*)
Res. Discl., 1996, **388**, 487-488 (*use*)
Pesticide Manual, 11th edn., 1997, 725

Tribromodiphenyl ethers T-448



$C_{12}H_7Br_3O$ 406.899
Persistent environmental pollutant, detected in human breast milk.

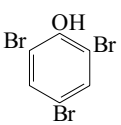
2,4,4′-Tribromodiphenyl ether [41318-75-6]
2,4-Dibromo-1-(4-bromophenoxy)benzene, 9CI. PBDE 28. BDE 28
$C_{12}H_7Br_3O$ 406.899
Mp 64-64.5°.

Environ. Health Criter., No. 162, Polybrominated Diphenyl Ethers, WHO, 1994, (*rev, tox, occur*)
Marsh, G. *et al., Environ. Sci. Technol.*, 1999, **33**, 3033-3037 (*synth, uv, pmr, ms*)
Hu, J. *et al., Magn. Reson. Chem.*, 2000, **38**, 375-378 (*pmr, cmr*)
Strandman, T. *et al., Organohalogen Compd.*, 2000, **47**, 61-64 (*occur*)

2,4,6-Tribromophenol, 9CI, 8CI T-449

[118-79-6]

[25376-38-9]
Bromol



$C_6H_3Br_3O$ 330.801
Isol. from molluscs and crustaceans. Flavour component of seafood, imparts an intense shrimp-like flavour. Needles (EtOH), prisms (C_6H_6). Sol. alkalis, EtOH, petrol. Mp 87-89°. Subl. 95-96. λ_{max} 288 ; 297 (EtOH) (Berdy).

▶ Potent irritant. LD_{50} (rat, orl) 2000 mg/kg. SN1225000

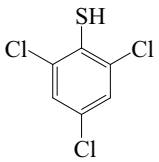
[2666-53-7, 3784-04-1, 78697-30-0]

Boyle, J.L. *et al., J. Food Sci.*, 1992, **57**, 918-922 (*occur*)

Whitfield, F.B. *et al., J. Agric. Food Chem.*, 1997, **45**, 4398-4405 (*occur*)

2,4,6-Trichlorobenzenethiol T-450

[24207-66-7]



$C_6H_3Cl_3S$ 213.514
Cryst. (EtOH). Mp 60°.

Benzoyl: [78547-39-4] S-*(2,4,6-Trichlorophenyl) benzenecarbothioate*
$C_{13}H_7Cl_3OS$ 317.622
Cryst. (xylene). Mp 170°.

S-*Me,* S,S-*dioxide:* [89692-93-3] *1,3,5-Trichloro-(2-methylsulfonyl)benzene*
$C_7H_5Cl_3O_2S$ 259.539
Isol. from lettuce, potatoes and soil.

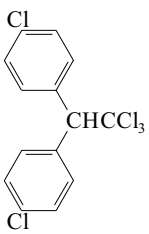
Disulfide: [89988-08-9] *Bis(2,4,6-trichlorophenyl) disulfide*
$C_{12}H_4Cl_6S_2$ 425.012
Cryst. (xylene). Mp 165°.

S-*Amino:*
$C_6H_4Cl_3NS$ 228.528
Cryst. Mp 91-92°.

Baddeley, G. *et al., J.C.S.*, 1933, 46-48 (*synth, disulfide, benzoyl*)
Reineke, C.E. *et al., J.O.C.*, 1977, **42**, 1139-1142 (*synth*)
Bergman, A. *et al., Chemosphere*, 1988, **17**, 717-725 (*S-Me S,S-dioxide*)
Mąkosza, M. *et al., J.O.C.*, 1998, **63**, 4878-4888 (*S-amino*)

1,1,1-Trichloro-2,2-bis(4-chlorophenyl)ethane T-451

[50-29-3]
1,1′-(2,2,2-Trichloroethylidene)bis(4-chlorobenzene), 9CI. ***Clofenotane, INN.*** *Chlorophenothane.* p,p′*-DDT, BSI. DDT, BSI, JMAF. Zeidane. Dicophane, BAN. Dichlorodiphenyltrichloroethane*



$C_{14}H_9Cl_5$ 354.489
Insecticide. Major component of commercial DDT (other names Gespan, Gesarol, Geverol, Chlorophenotane). Use banned or discouraged in many countries. Needles (EtOH or petrol). Mp 108.5-109°. Log P 6.76 (calc).

▶ Ingestion of large doses affects nervous system and causes paraesthesias of tongue, lips and face. Other symptoms incl. tremor, dizziness, confusion and malaise. Similar effects observed by skin absorption of acetone soln. Exp. hepatoxic, and hepatocarcinogen (in some species). Prolonged exposure results in storage of DDT and metabolites in body fat. OES: long-term 1 mg m^{-3}; short-term 3 mg m^{-3}. LD_{50} (rat, orl) 113-118 mg/kg. Induces myoclonus in rodents. KJ3325000

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 165B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1025D (*ir*)
Zeidler, O. *et al., Ber.*, 1874, **7**, 1180 (*synth*)
Läuger, P. *et al., Helv. Chim. Acta*, 1944, **27**, 892 (*sar, rev*)
Bailes, E.L. *et al., J. Chem. Educ.*, 1945, **22**, 122 (*synth*)
Haller, H.L. *et al., J.A.C.S.*, 1945, **67**, 1591 (*bibl, anal*)
Mueller, P. *et al., Helv. Chim. Acta*, 1946, **29**, 1560 (*sar*)
Downing, J.R. *et al., Ind. Eng. Chem., Anal. Ed.*, 1946, **18**, 461 (*ir*)
Forrest, J. *et al., J.C.S.*, 1946, 333 (*anal*)
Sphon, J.A. *et al., Org. Mass Spectrom.*, 1970, **3**, 51 (*ms*)
Hague, R. *et al., Biochemistry*, 1973, **12**, 2346 (*nmr*)
Maugh, T.H. *et al., Science (Washington, D.C.)*, 1973, **180**, 578 (*metab*)
Abou-Donici, M.B. *et al., Appl. Spectrosc.*, 1975, **29**, 261 (*uv*)
Baldwin, M.K. *et al., Pestic. Sci.*, 1977, **8**, 110 (*anal*)
Gold, B. *et al., Chem. Biol. Interact.*, 1982, **41**, 327 (*metab*)
Kennard, C.H.L. *et al., J. Agric. Food Chem.*, 1984, **32**, 886 (*cryst struct, activity*)
Sharpless, N.E. *et al., Appl. Spectrosc.*, 1985, **39**, 579 (*cmr*)
Dangerous Prop. Ind. Mater. Rep., 1985, **5**, 12 (*rev*)
Mellanby, K. *et al., BCPC Monogr.*, 1989, **43**, 3 (*rev*)
Mellanby, K. *et al., The DDT Story*, British Crop Protection Council, Farnham, Surrey, 1992, (*book*)
Pranzatelli, M.R. *et al., Neurotoxicology*, 1994, **15**, (*pharmacol*)
Pesticide Manual, 10th edn., 1994, No. 193
Barros, S.B.M. *et al., Toxicol. Lett.*, 1994, **70**, 33 (*tox*)
Bucholski, K.A. *et al., J. Chromatogr., A*, 1996, **754**, 479 (*gc-ms*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1434
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 203
Handbook of Pesticide Toxicology, (Eds. Hayes, W.J. *et al*), Academic Press, 1991, 743 (*tox, rev*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1242
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DAD200

Trichloroethylene, 8CI, INN T-452

[79-01-6]
Trichloroethene, 9CI. Tri-Clene. Trichloran. Chlorylen. Trilene. R 1120. Many other names

$Cl_2C{=}CHCl$

C_2HCl_3 131.388
Solvent and extractive in the manuf. of foods. Nonflammable mobile liq. with characteristic odour. Insol. H_2O; misc. EtOH, Et_2O. d_4^{20} 1.46. Mp -84.8° (-86.8). Bp 86.7° Bp_{60} 20°. n_D^{20} 1.4775. Log P 2.63 (calc). Vp 74 mmHg (25°). Widespread use declining due to toxicity. Resistant to radical homopolym. but undergoes copolym. with some vinyl monomers. Q/e values for copolym., Q 0.010, e +1.29.

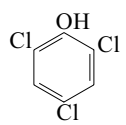
▶ Non-flammable, autoignition temp. 410/420°. Eye and severe skin irritant. High vapour conc. narcotic. Prolonged or repeated exposure can damage kidney, liver, heart and lung, and produce skin disorders and conjunctivitis. LD_{50} (mus, orl) 2402 mg/kg; LC_{50} (rat, ihl) 25700 ppm (1h exposure). MEL: long-term 100 ppm; short-term 150 ppm (Sk). KX4550000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 101B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 147C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 141D (*ir*)
Alfrey, T. *et al., J. Polym. Sci.*, 1948, **3**, 297 (*copolym*)
Breitenbach, J.W. *et al., Monatsh. Chem.*, 1950, **81**, 21 (*polymerisability*)
Japan. Pat., 1954, 6874; *CA*, **50**, 2651 (*synth*)
Shikaji, T. *et al., Chem. Eng. (Rugby, Engl.)*, 1970, **77**, 74 (*synth*)
Roberts, J.D. *et al., J.O.C.*, 1974, **39**, 1276 (*cmr*)
Stepanyants, A.U. *et al., Zh. Anal. Khim.*, 1976, **31**, 1770; *J. Anal. Chem. USSR (Engl. Transl.)*, 1976, **31**, 1333 (*pmr*)
Waters, E.M. *et al., J. Toxicol. Environ. Health*, 1977, **2**, 671 (*rev*)
IARC Monog., 1979, **20**, 545; *Suppl.* 7, 364; *Suppl.* 6, 530 (*rev, tox*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values*)
Fielder, R.J. *et al., Toxic. Rev.*, HMSO, London, 1982, (*rev, metab, tox*)
Organo-chlorine Solvents, Royal Society of Chemistry, 1986, 93 (*tox rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 32
McCunney, R.J. *et al., Br. J. Ind. Med.*, 1988, **45**, 122 (*human tox*)
Bretherick, L. *et al., Chem. Eng. News*, Dec. 12, 1988, 2 (*haz*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 40 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 920
Gribble, G.W. *et al., Prog. Chem. Org. Nat. Prod.*, 1996, **68**, 1 (*occur*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2826
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1245
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TIO750

2,4,6-Trichlorophenol, 9CI, 8CI T-453

[88-06-2]

[25167-82-2]



$C_6H_3Cl_3O$ 197.447
Needles (AcOH). Mp 69.5°. Bp 246°. pK_a 7.42 (25°). Steam-volatile.

▶ Eye and skin irritant. LD_{50} (rat, orl) 820

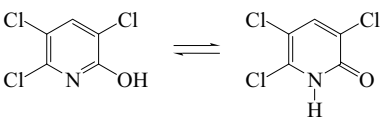
mg/kg. Exp. carcinogen. Exp. hepatotoxic and haematological effects. SN1575000

Me ether: [87-40-1] *1,3,5-Trichloro-2-methoxybenzene, 9CI. 2,4,6-Trichloroanisole*
$C_7H_5Cl_3O$ 211.474
Off-odour component found in foods etc. Responsible for 'cork taint' in wines. Needles or prisms (EtOH) with intense musty odour. Mp 61-62°. Bp_{738} 240°. Sublimes.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1050A; 1095C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 202C; 287C (*nmr*)
Whitfield, F.B. *et al., Chem. Ind. (London)*, 1984, 744 (*isol, Me ether*)
Fischer, C. *et al., J. Agric. Food Chem.*, 1997, **45**, 1995-1997 (*Me ether, occur*)

3,5,6-Trichloro-2-pyridinol, 9CI T-454

[6515-38-4]
3,5,6-Trichloro-2(1H)-pyridinone. 2,3,5-Trichloro-6-hydroxypyridine



$C_5H_2Cl_3NO$ 198.435
Environmental contaminant arising from the degradation of Chlorpyrifos and Triclopyr. Mp 208-209°.

OH-form

Me ether: [31557-34-3] *2,3,5-Trichloro-6-methoxypyridine, 9CI*
$C_6H_4Cl_3NO$ 212.462
Mp 52-53°.

NH-form

N-*Me:* [75348-52-6] *3,5,6-Trichloro-1-methyl-2(1H)-pyridinone, 9CI*
$C_6H_4Cl_3NO$ 212.462
Cryst. (EtOH). Mp 133-134°.

Berry, D.J. *et al., J.C.S.(C)*, 1971, 1227 (*O-Me*)
Giacobbe, T.J. *et al., J. Het. Chem.*, 1974, **11**, 889; 1976, **13**, 891
Giacobbe, T.J. *et al., J.O.C.*, 1974, **39**, 1685 (*synth, ir, pmr*)
Iddon, B. *et al., J.C.S. Perkin 1*, 1980, 1370 (*N-Me, cmr*)
Manclús, J.J. *et al., J. Agric. Food Chem.*, 1996, **44**, 3703-3709 (*anal*)

1,1,2-Trichloro-1,2,2-trifluoroethane T-455

[76-13-1]

[26523-64-8]
Fluorocarbon 113. Freon 113. Arcton 113. Arklone P. Asahifron 113. CFC 113. Forane 113. Fridohna. Frigen 113. Fron 113. Fronsolve 113. Genetron 113. Isceon 113

$Cl_2CFCClF_2$
$C_2Cl_3F_3$ 187.375
Used in freezing of foods. Mp -36.4°. Bp 47.7°.
▶ Incompatible with some metals. LD_{50} (rat, orl) 43000 mg/kg. Production controlled by environmental legislation. Skin irritant. OES: long-term 1000 ppm; short-term 1250 ppm. KJ4000000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 90B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 127B (*ir*)
Iwasaki, M. *et al., Bull. Chem. Soc. Jpn.*, 1959, **32**, 194 (*struct*)
Case, J.R. *et al., J.C.S.*, 1961, 2070 (*synth*)
Park, J.D. *et al., J.O.C.*, 1961, **26**, 3316; 3319; 4017 (*synth*)
Vecchio, M. *et al., Hydrocarbon Process.*, 1973, **52**, 97 (*synth*)
Naae, D.G. *et al., Org. Mass Spectrom.*, 1974, **9**, 1203 (*ms*)
Kolditz, L. *et al., Z. Anorg. Allg. Chem.*, 1977, **434**, 55 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 577-578
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1253
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FOO000

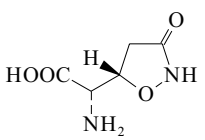
1,1,3-Trichloro-1,3,3-trifluoro-2-propanone, 9CI T-456

[79-52-7]
1,1,3-Trichloro-1,3,3-trifluoroacetone. unsym-*Trichlorotrifluoroacetone*
$Cl_2CFCOCClF_2$
$C_3Cl_3F_3O$ 215.386
Sprout-inhibiting agent for a wide variety of plants, inc. potatoes. Liq. Bp 84.2°. Not used commercially.
▶ Irritant. UC3850000

U.S. Pat., 1957, 2 807 640; 1958, 2 853 524; *CA*, **52**, 2890h; **53**, 5133h (*synth*)
Sutcliffe, L.H. *et al., Spectrochim. Acta A*, 1972, **28**, 619 (*F-19 nmr*)
Hackett, P.A. *et al., J. Chem. Phys.*, 1974, **78**, 665 (*spectra*)
In, H.J. *et al., Tet. Lett.*, 1986, **27**, 3709 (*synth*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 6th edn., Van Nostrand Reinhold*, 1984, 2633 (*haz*)

Tricholomic acid T-457

[2644-49-7]
α-Amino-3-oxo-5-isoxazolidineacetic acid, 9CI. 2-(3-Oxo-5-isoxazolidinyl)glycine



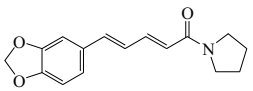
Absolute configuration

$C_5H_8N_2O_4$ 160.129
Constit. of the mushroom *Tricholoma muscarium*. Said to be useful as a flavouring substance. Cryst. (H_2O). Sol. H_2O. Mp 207° dec. $[\alpha]_D^{20}$ +80 (c, 0.20 in H_2O). λ_{max} 215 (ε 3470) (H_2O) (Berdy).

Takemoto, T. *et al., Yakugaku Zasshi*, 1964, **84**, 1183; 1230; *CA*, **62**, 7859b; 8121c (*isol, struct*)
Iwasaki, H. *et al., Chem. Pharm. Bull.*, 1965, **13**, 753 (*synth*)
Kamiya, K. *et al., Chem. Pharm. Bull.*, 1966, **14**, 1307 (*synth*)
Japan. Pat., 1969, 69 16 354; *CA*, **71**, 111463p (*manuf*)
Japan. Pat., 1979, 79 148 782; *CA*, **92**, 198384u (*synth*)

Trichostachine T-458

1-[5-(1,3-Benzodioxol-5-yl)]-1-oxo-2,4-pentadienylpyrrolidine, 9CI. 5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoic acid pyrrolidide. Piperyline. Pyrroperine



(*E,E*)-*form*

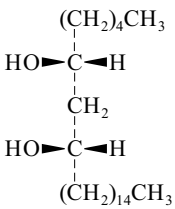
$C_{16}H_{17}NO_3$ 271.315
λ_{max} 245 (ε 10500); 261 (ε 10800); 309 (ε 19200); 343 (ε 33500) (MeOH) (Derep).

(E,E)-form [25924-78-1]
Alkaloid from *Piper nigrum* (pepper). Cryst. (EtOAc/hexane or C_6H_6/petrol). Mp 143-145°.

(2E,4Z)-form
Amorph. solid. λ_{max} 280 (ε 2890) (MeOH).

Grewe, R. *et al., Chem. Ber.*, 1970, **103**, 3752 (*isol, uv, ir, pmr, ms, struct, synth*)
Okogun, J.I. *et al., J.C.S. Perkin 1*, 1974, 2195 (*isol*)
Olsen, R.A. *et al., J. Agric. Food Chem.*, 1981, **29**, 942 (*synth, uv, ir, pmr*)
Jacobs, H. *et al., J. Indian Chem. Soc.*, 1999, **76**, 713-717 (*isol, pmr, cmr*)
Vasques da Silva, R. *et al., Phytochemistry*, 2002, **59**, 521-527 (*2E,4Z-form*)

6,8-Tricosanediol T-459



$C_{23}H_{48}O_2$ 356.631

(6R*,8S*)-form [155800-83-2]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 56-59°.

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

4,6-Tricosanedione T-460

$H_3C(CH_2)_{16}COCH_2COCH_2CH_2CH_3$
$C_{23}H_{44}O_2$ 352.599
Constit. of the pollen of *Helianthus annuus* (sunflower).

4-Alcohol:4-Hydroxy-6-tricosanone
$C_{23}H_{46}O_2$ 354.615
Constit. of the pollen of *Helianthus annuus* (sunflower).

6-Alcohol:6-Hydroxy-4-tricosanone
$C_{23}H_{46}O_2$ 354.615
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

6,8-Tricosanedione T-461

$H_3C(CH_2)_{14}COCH_2CO(CH_2)_4CH_3$
$C_{23}H_{44}O_2$ 352.599
Constit. of the pollen of *Helianthus*

annuus (sunflower).

6-Alcohol:6-Hydroxy-8-tricosanone
$C_{23}H_{46}O_2$ 354.615
Constit. of the pollen of *Helianthus annuus* (sunflower).

8-Alcohol:8-Hydroxy-6-tricosanone
$C_{23}H_{46}O_2$ 354.615
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336 (*isol, synth*)

Tricosanoic acid T-462

[2433-96-7]

$H_3C(CH_2)_{21}COOH$

$C_{23}H_{46}O_2$ 354.615
Constit. of *Citrus bergamia* (bergamot orange) oil. Cryst. (C_6H_6). Mp 79.1°.

Me ester: [2433-97-8]
$C_{24}H_{48}O_2$ 368.642
Cryst. (Me_2CO). Mp 53.4°.

Et ester: [18281-07-7]
$C_{25}H_{50}O_2$ 382.669
Cryst. (Me_2CO). Mp 51.2°.

Nitrile:
$C_{23}H_{45}N$ 335.615
Cryst. (Me_2CO). Mp 53.5-54.5°.

Heptadecyl ester: [42233-32-9] *Heptadecyl tricosanoate*
$C_{40}H_{80}O_2$ 593.071
Cryst. (MeOH). Mp 108°. Incorrect struct. diag. in ref.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 486D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 759A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 633A (*ir*)
Francis, F. *et al., J.A.C.S.*, 1939, **61**, 577
Cocker, W. *et al., Perfum. Essent. Oil Res.*, 1963, **54**, 235; 1964, **55**, 442 (*isol*)
Rowe, J.W. *et al., J.O.C.*, 1964, **29**, 1554 (*isol*)
Aleby, S. *et al., Ark. Kemi*, 1969, **31**, 267 (*ir, polymorphism*)
Marosi, L. *et al., Annalen*, 1973, 584 (*cryst struct*)
Manorajani, M. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1148-1150 (*heptadecyl ester*)

12-Tricosanol T-463

[24897-74-3]

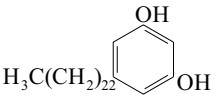
$H_3C(CH_2)_{10}CH(OH)(CH_2)_{10}CH_3$

$C_{23}H_{48}O$ 340.632
Constit. of leaf wax of *Artemisia vulgaris* (mugwort). Mp 75.5°.

Kipping, S. *et al., J.C.S.*, 1890, **57**, 980 (*synth*)
Fujita, A. *et al., CA*, 1954, **48**, 3252 (*isol*)
Streibl, V.M. *et al., Fette, Seifen, Anstrichm.*, 1972, **74**, 566 (*synth*)
Ubik, K. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 1718 (*ms*)
Dhar, D.N. *et al., Planta Med.*, 6th Ed., 1976, **29**, 91 (*isol*)

5-Tricosyl-1,3-benzenediol, 9CI T-464

[70110-60-0]
5-Tricosylresorcinol



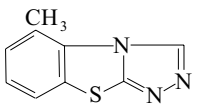
$C_{29}H_{52}O_2$ 432.729
Constit. of cereal grains.

3-Me ether: [119708-39-3] *3-Methoxy-5-tricosylphenol, 9CI.* ***Tamarixinol***
$C_{30}H_{54}O_2$ 446.755
Pale yellow cryst.(EtOH). Mp 77-78°.

Reusch, R.N. *et al., J. Bacteriol.*, 1979, **139**, 448; 1981, **145**, 889 (*isol*)
Gohil, S. *et al., J. Sci. Food Agric.*, 1988, **45**, 43 (*isol*)
Jiang, Y.Q. *et al., Yaoxue Xuebao*, 1988, **23**, 749-755 (*Tamarixinol*)
Suzuki, Y. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 480-486 (*isol, ms*)

Tricyclazole, BSI T-465

[41814-78-2]
5-Methyl-1,2,4-triazolo[3,4-b]benzothiazole, 9CI. Beam. Bim. Blascide



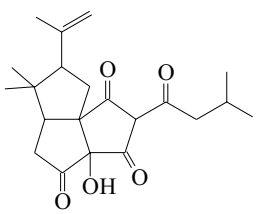
$C_9H_7N_3S$ 189.24
Rice fungicide. Cryst. solid. Sol. Me_2CO, $CHCl_2$, MeOH, EtOH; spar. sol. H_2O. Mp 187-188°.

▶ LD_{50} (rat, orl) 250 mg/kg. XZ5475000

U.K. Pat., 1971, 1 419 121; *CA*, **79**, 18721b
Day, E.W. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1980, **11**, 263 (*synth, props, detn*)
Dreikorn, B.A. *et al., J. Het. Chem.*, 1989, **26**, 1735 (*synth, bibl*)
Pesticide Manual, 11th edn., 1997, No. 734
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MQC000

Tricyclodehydroisohumulone T-466

[56143-68-1]

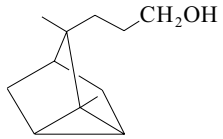


$C_{21}H_{28}O_5$ 360.449
Constit. of hops. Cryst. (petrol). Mp 163°. $[\alpha]_D^{20}$ +299 (MeOH).

Elvidge, J.A. *et al., J.C.S. Perkin 1*, 1979, 1250

Tricycloekasantalol T-467

[16933-12-3]
2,3-Dimethyltricyclo[2.2.1.0^{2,6}]heptane-3-propanol, 9CI



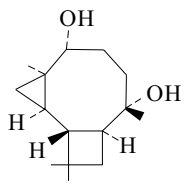
$C_{12}H_{20}O$ 180.289
Flavouring ingredient. Isol. from oil of sandalwood (*Santalum album*).

Aldehyde: [16933-18-9] ***Tricycloekasantal***
$C_{12}H_{18}O$ 178.274
Constit. of the oil of *Santalum album* (sandalwood). Oil.

Lewis, R.G. *et al., Tet. Lett.*, 1967, 401 (*synth, ir, nmr*)
Kretschmar, H.C. *et al., Tet. Lett.*, 1970, 37 (*isol*)
Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*isol*)

Tricyclohumuladiol T-468

[21446-02-6]



$C_{15}H_{26}O_2$ 238.369
Constit. of hop oil. Cryst. (Et_2O/MeOH). Mp 207°. $[\alpha]_D^{24}$ 0 (c, 2.7 in MeOH).

Naya, Y. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2405 (*isol, struct*)
Namikawa, M. *et al., Chem. Lett.*, 1978, 391 (*synth*)

1,5-Tridecadiene T-469

[136904-12-6]

$H_3C(CH_2)_6CH{=}CHCH_2CH_2CH{=}CH_2$

$C_{13}H_{24}$ 180.333

(Z)-form [84348-07-2]
Constit. of the essential oil of *Tussilago farfara* (coltsfoot).

[84348-08-3]

Hara, S. *et al., Synth. Commun.*, 1982, **12**, 813 (*synth*)
Suzuki, N. *et al., Yakugaku Zasshi*, 1992, **112**, 571 (*isol*)

1,3-Tridecadiene-5,7,9,11-tetrayne, 9CI T-470

[18668-88-7]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH{=}CH_2$

$C_{13}H_8$ 164.206

(E)-form [3760-28-9]
Unstable cryst. (petrol). λ_{max} 273 ; 290 ; 311 ; 331 ; 356 ; 382 (Et_2O).

1,2-Epoxide: [104017-81-4] *2-(1-Undecen-3,5,7,9-tetraynyl)oxirane. 1,2-Epoxy-3-tridecene-5,7,9,11-tetrayne*
$C_{13}H_8O$ 180.206
Cryst. Mp 95.5-97°. $[\alpha]_D$ +75.1 ($CHCl_3$).

(Z)-form [124604-45-1]
Isol. from safflower (*Carthamus tinc-*

torius).

Bohlmann, F. *et al., Chem. Ber.*, 1961, **94**, 3179; 1964, **97**, 809; 2125; 1965, **98**, 3081; 1966, **99**, 3201; 3433; 3544; 1968, **101**, 2056; 1975, **108**, 433 (*isol, uv, ir, synth, struct*)
Schulte, K.E. *et al., J. Nat. Prod.*, 1969, **32**, 360 (*isol, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1189; 1980, **19**, 331 (*isol*)
Washino, T. *et al., Nippon Nogei Kagaku Kaishi*, 1986, **60**, 377; *CA*, **105**, 111980a (*isol*)
Binder, R.G. *et al., J. Agric. Food Chem.*, 1990, **38**, 764; 1245 (*isol*)

1,11-Tridecadiene-3,5,7,9-tetrayne, 9CI T-471

[2345-16-6]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CH_2$

$C_{13}H_8$ 164.206

λ_{max} 252 ; 256 ; 271 ; 286 ; 315 ; 356 ; 361 ; 390 (hexane) (Berdy).

1,2-Epoxide: [65398-26-7] *12,13-Epoxy-2-tridecene-4,6,8,10-tetrayne, 8CI. 9-Undecene-1,3,5,7-tetraynyloxirane, 9CI*
$C_{13}H_8O$ 180.206Mixt. of *cis* and *trans* forms not fully separated.

11,12-Epoxide: [16697-27-1] *11,12-Epoxy-1-tridecene-3,5,7,9-tetrayne, 8CI. 2-(9-Decene-1,3,5,7-tetraynyl)-3-methyloxirane, 9CI*
$C_{13}H_8O$ 180.206
Oil.

(*E*)-*form* [26130-86-9]
Trace constituent of roots *Triticum aestivum* (wheat). Isol. from *Carthamus tinctorius* (safflower). Pale yellow needles (pentane). Dec. without melting >40°. Rapidly becomes brown in diffused daylight even at -5°.

(*Z*)-*form* [59950-58-2]
Isol. from *Carthamus tinctorius* (safflower). Oil.

[16697-26-0, 16697-36-2]

Sorensen, J.S. *et al., Acta Chem. Scand.*, 1954, **8**, 1741 (*isol, ir*)
Bohlmann, F. *et al., Chem. Ber.*, 1958, **91**, 1642; 1962, **95**, 1315; 1964, **97**, 1193; 2583; 1965, **98**, 872; 1228; 1966, **99**, 35; 1223; 3201; 3433; 1971, **104**, 961; 1975, **108**, 440; 1976, **109**, 3956 (*isol, struct, occur, biosynth*)
Jones, E.R.H. *et al., J.C.S.*, 1958, 1054 (*synth, uv, ir, glc*)
Schulte, K.E. *et al., Phytochemistry*, 1965, **4**, 481 (*isol*)
Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1966, **299**, 468; 1970, **303**, 7 (*isol, struct, ir, uv, pmr, glc*)
Bohlmann, F. *et al., Chem. Ber.*, 1967, **100**, 1944 (*epoxides, isol, struct*)
Chin, C. *et al., J.C.S.(C)*, 1970, 314 (*isol*)
Ichihana, K. *et al., Agric. Biol. Chem.*, 1975, **39**, 1103 (*isol, uv, pmr, ir*)
Bedford, C.T. *et al., J.C.S. Perkin 1*, 1976, 735 (*isol*)
Anderson, A.B. *et al., Phytochemistry*, 1977, **16**, 1829 (*isol*)
Binder, R.G. *et al., Phytochemistry*, 1978, **17**, 315 (*isol, ms, uv, pmr*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1666; 1979, **18**, 99; 1980, **19**, 692; 1983, **22**, 1281 (*isol*)

3,11-Tridecadiene-5,7,9-triyne-1,2-diol, 9CI T-472

[65398-35-8]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH(OH)CH_2OH$

$C_{13}H_{12}O_2$ 200.237

(*R,E,E*)-*form* [27978-14-9]
Safynol
Isol. from diseased *Carthamus tinctorius* (safflower). Cryst. (Et_2O/petrol or $CHCl_3$/hexane). Mp 122.5-123° (112°). $[\alpha]_D^{20}$ -17 (MeOH). An opt. rotn. of $[\alpha]_D^{23}$ +38 (MeOH) is given without explanation by Bohlmann for a prod. from saponification of the natural monoacetate. Stable in dark at -18°, resinifies in air λ_{max} 215 ; 225 ; 235 ; 246 ; 255 ; 269 (ε 61600); 290 ; 309 ; 330 ; 354 (EtOH) (Berdy).

Bohlmann, F. *et al., Chem. Ber.*, 1958, **91**, 1642; 1959, **92**, 1319; 1961, **94**, 3179; 1964, **97**, 520 (*isol, struct, biosynth*)
Thomas, C.A. *et al., Phytopathology*, 1970, **60**, 261 (*isol*)
Allen, E.H. *et al., Phytochemistry*, 1971, **10**, 1579 (*isol*)
Nakada, H. *et al., Agric. Biol. Chem.*, 1977, **41**, 1761 (*synth, abs config*)
Jente, R. *et al., Phytochemistry*, 1979, **18**, 829 (*isol, struct, ms, uv, pmr*)
MacRae, W.D. *et al., Experientia*, 1980, **36**, 1096 (*pharmacol*)

2-(1,12-Tridecadienyl)furan T-473

[34227-08-2]
Avocadienofuran



$C_{17}H_{26}O$ 246.392
Constit. of *Persea americana* (avocado).

Alves, H.M. *et al., Ann. Acad. Bras. Ci&eenc.*, 1970, **42S**, 45 (*isol, struct*)
Fraga, B.M. *et al., Phytochemistry*, 1996, **41**, 229 (*isol, pmr, cmr*)

2-(2,12-Tridecadienyl)furan T-474

[34227-09-3]
Isoavocadienofuran

$C_{17}H_{26}O$ 246.392
Component of Avocatin X, a constit. of the seeds of *Persea gratissima* (avocado).

Alves, H.M. *et al., Ann. Acad. Bras. Ci&eenc.*, 1970, **42S**, 45 (*isol, struct*)

Tridecanal T-475

[10486-19-8]
Tridecyl aldehyde
$H_3C(CH_2)_{11}CHO$
$C_{13}H_{26}O$ 198.348
Volatile flavour component of coriander leaf. Also in lemon and cucumber oils. Liq. with waxy-citrus odour. Mp 14°. Bp_{10} 126-128°. n_D^{18} 1.4384.

Oxime:
$C_{13}H_{27}NO$ 213.362
Cryst. (EtOH aq.). Mp 80.5°.

Semicarbazone:
Cryst. (EtOH). Mp 113-114°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 470A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 556C (*ir*)
Stoll, M. *et al., Helv. Chim. Acta*, 1947, **30**, 122 (*synth*)
Kummer, R. *et al., CA*, 1974, **80**, 14569f (*isol*)
Bott, K. *et al., Fette, Seifen, Anstrichm.*, 1974, **76**, 443 (*synth*)
Kemp, T.R. *et al., J. Agric. Food Chem.*, 1974, **22**, 717 (*isol*)
Mac Leod, A.J. *et al., J. Sci. Food Agric.*, 1976, **27**, 721 (*isol*)

Tridecane T-476

[629-50-5]
$H_3C(CH_2)_{11}CH_3$
$C_{13}H_{28}$ 184.364
Isol. from lime oil. Fp -5.5. Bp 234° Bp_{15} 114°.
▶ LD_{50} (mus, ivn) 1161 mg/kg. YD3025000
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 3C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 3B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 4B (*ir*)
Vogel, A.I. *et al., J.C.S.*, 1946, 13 (*synth*)
Kováts, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2705 (*isol*)
Cocker, W. *et al., J.C.S.*, 1963, 677 (*isol*)
Ivanov, C. *et al., CA*, 1972, **77**, 111474s (*isol, struct*)
Critchley, B.R. *et al., Bull. Entomol. Res.*, 1973, **63**, 1 (*tox*)
Clark, R.G. *et al., J. Sci. Food Agric.*, 1976, **27**, 713 (*glc, ms*)
Tonelli, A.E. *et al., Macromolecules*, 1976, **9**, 863
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TJH500

1,9-Tridecanediol T-477

[39516-34-2]
$H_3C(CH_2)_3CH(OH)(CH_2)_7CH_2OH$
$C_{13}H_{28}O_2$ 216.363

1-Docosanoyl: [155758-78-4]
$C_{35}H_{70}O_3$ 538.936
Constit. of *Artocarpus heterophyllus* (jackfruit). Amorph. solid ($CHCl_3$/MeOH). Mp 75-76°.

Baser, I.A. *et al., Fette, Seifen, Anstrichm.*, 1972, **74**, 524; *CA*, **78**, 57666 (*synth*)
Lu, C.-M. *et al., Phytochemistry*, 1994, **35**, 781 (*isol, ester*)

1,13-Tridecanediol, 9CI T-478

[13362-52-2]
$HOCH_2(CH_2)_{11}CH_2OH$
$C_{13}H_{28}O_2$ 216.363
Cryst. (hexane). Mp 76.5-77° Mp 81°.

Di-Ph ether: [141620-05-5] *1,1′-[1,13-Tridecanediylbis(oxy)]bisbenzene, 9CI. 1,13-Diphenoxytridecane*
$C_{25}H_{36}O_2$ 368.558
Isol. from the leaves of *Arachis hypogaea* (peanut) infected with *Puccinia arachidis*.

Guyer, A. *et al., Helv. Chim. Acta*, 1955, **38**, 976 (*synth*)
Gold'farb, Y.L. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1955, **25**, 1321 (*synth*)

Bianchetti, G. *et al., Farmaco, Ed. Sci.*, 1957, **12**, 441; *CA*, **51**, 17914 (*synth*)
Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 1248 (*synth*)
Rao, P.V.S. *et al., Oleagineux*, 1991, **46**, 501; *CA*, **116**, 252152 (*di-Ph ether*)
Mori, K. *et al., Annalen*, 1994, 695 (*synth, pmr*)
Nakamura, N. *et al., Acta Cryst. C*, 1997, **53**, 253-255 (*cryst struct*)

2-Tridecanone T-479

[593-08-8]
FEMA 3388

$H_3C(CH_2)_{10}COCH_3$

$C_{13}H_{26}O$ 198.348

Isol. from plant oils, e.g. palm oil, coconut oil. Also found in American cranberry, rabbiteye, blueberry, raspberry, grapefruit, onion, ginger and cheeses. Used as a flavouring essence. Mp 29°. Bp 260-265° Bp_{16} 160°.

►Fl. p. 107°.

Oxime:
$C_{13}H_{27}NO$ 213.362
Insol. petrol. Mp 56-57°.

Semicarbazone:
Mp 126°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 641C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 498A (*ir*)
Pickard, R.H. *et al., J.C.S.*, 1911, **55**, 45 (*synth*)
Morgan, G.T. *et al., J. Soc. Chem. Ind., London*, 1925, **44**, 108r
Allen, R.R. *et al., Chem. Ind. (London)*, 1965, 1560 (*isol*)
Regnier, F.E. *et al., J. Insect Physiol.*, 1968, **43**, 411
Hajek, M. *et al., Tet. Lett.*, 1974, **36**, 3193 (*synth*)
McDaniel, C.A. *et al., J. Chem. Ecol.*, 1987, **13**, 227

1,3,5,11-Tridecatetraene-7,9-diyne T-480

[16914-98-0]

$H_3CCH{=}CHC{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH{=}CH_2$

$C_{13}H_{12}$ 168.238

(*E,E,E*)-*form* [17091-00-8]
Isol. from *Carthamus tinctorius* (safflower). Sl. yellow cryst. (petrol). Mp 71-72°. Readily oxidises and polymerises.

(3*E*,5*Z*,11*E*)-*form* [63366-81-4]
Isol. from *Carthamus tinctorius* (safflower).

(3*Z*,5*E*,11*E*)-*form* [63366-82-5]
Isol. from *Carthamus tinctorius* (safflower). Yellowish viscous liq.

[14441-92-0]

Sorensen, J.S. *et al., Acta Chem. Scand.*, 1954, **8**, 1741 (*isol*)
Ichihara, K. *et al., Agric. Biol. Chem.*, 1975, **39**, 1103 (*isol, struct, bibl*)
Andersen, A.B. *et al., Phytochemistry*, 1977, **16**, 1829 (*isol*)
Binder, R.G. *et al., Phytochemistry*, 1978, **17**, 315 (*isol, struct, pmr, ms*)
Guillet, G. *et al., Phytochemistry*, 1997, **45**, 695 (*isol, uv, pmr, cmr*)

2,4,6,8-Tridecatetrayne T-481

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}C(CH_2)_3CH_3$

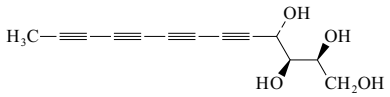
$C_{13}H_{12}$ 168.238

Metabolite of *Fistulina hepatica* (beefsteak fungus). Mp 25-26°.

Jones, E.R.H. *et al., J.C.S.(C)*, 1966, 139 (*isol, synth*)

5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol, 9CI T-482

[109958-96-5]



$C_{13}H_{12}O_4$ 232.235

(2*S*,3*S*,4*S*)-*form*
Isol. from *Fistulina hepatica* (beefsteak fungus). Silvery plates (Me_2CO). Mp 155° dec. $[\alpha]_D^{24}$ +1.8 (c, 0.11 in EtOH). λ_{max} 217 ; 227 ; 239 ; 272 ; 289 ; 308 ; 329 ; 353 (MeOH) (Berdy).

Jones, E.R.H. *et al., J.C.S.(C)*, 1966, 139 (*isol, struct, uv, ir, pmr*)
Barley, G.C. *et al., J. Chem. Res., Synop.*, 1987, 232

2,4,7-Tridecatrienal, 9CI T-483

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCH{=}CHCHO$

$C_{13}H_{20}O$ 192.3

(2*E*,4*Z*,7*Z*)-*form* [13552-96-0]
FEMA 3638
Component of cooked chicken flavour. Flavouring ingredient. $Bp_{0.33}$ 138°.

Harkes, P.D. *et al., J. Am. Oil Chem. Soc.*, 1974, **51**, 356

3,5,7-Tridecatriene-9,11-diyn-1-ol, 9CI T-484

Chamomilla alcohol
$H_3CC{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH{=}CHCH_2CH_2OH$

$C_{13}H_{14}O$ 186.253

(all-*E*)-*form*
Isol. from roots of *Matricaria chamomilla* (German chamomile) and *Matricaria discoidea* (pineapple weed). Cryst. (Et_2O/petrol). Mp 86.5°.

Ac: [506-16-1] *1-Acetoxy-3,5,7-tridecatriene-9,11-diyne.* ***Chamomilla ester***
$C_{15}H_{16}O_2$ 228.29
Cryst. (petrol). Mp 68.5°.

(3*E*,5*Z*,7*E*)-*form*
Ac:

Christensen, P.K. *et al., CA*, 1960, **54**, 6531 (*isol*)
Bohlmann, F. *et al., Chem. Ber.*, 1960, **93**, 1931; 1970, **103**, 2860 (*isol, synth, ir, uv, struct, biosynth*)

1,3,5-Tridecatriene-7,9,11-triyne T-485

[2739-64-2]

$H_3CC{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH{=}CHCH{=}CH_2$

$C_{13}H_{10}$ 166.222

(*E,E*)-*form* [6581-77-7]
Mp 88-93°.

3,4:5,6-Diepoxide:3,4:5,6-Diepoxy-1-tridecene-7,9,11-triyne. ***Annuadiepoxide***
$C_{13}H_{10}O_2$ 198.221
Unstable cryst.

(3*E*,5*Z*)-*form* [126381-91-7]
Isol. from *Artemisia vulgaris* (mugwort).

Bohlmann, F. *et al., Chem. Ber.*, 1962, **95**, 1320; 1973, **106**, 1328 (*isol, uv, ir, pmr*)
David, D. *et al., Phytochemistry*, 1974, **13**, 455 (*isol, struct*)
Kenichi, I. *et al., Agric. Biol. Chem.*, 1975, **39**, 1103 (*isol*)
Wallnoefer, B. *et al., Phytochemistry*, 1989, **28**, 2687 (*isol, pmr*)
Manns, D. *et al., J. Nat. Prod.*, 1992, **55**, 29 (*Annuadiepoxide*)

1,3,11-Tridecatriene-5,7,9-triyne T-486

[18668-89-8]

$H_3CCH{=}CH(C{\equiv}C)_3CH{=}CHCH{=}CH_2$

$C_{13}H_{10}$ 166.222

Constit. of *Carthamus tinctorius* (safflower). Oil. Partial stereochem. known for some isolates λ_{max} 224 ; 234 ; 243 ; 274 ; 289 ; 299 ; 310 ; 319 ; 331 ; 342 ; 354 ; 366 ; 382 (MeOH) (Berdy).

1,2-Epoxide: [2780-71-4] *(1,9-Undecadiene-3,5,7-triynyl)oxirane, 9CI. 12,13-Epoxy-2,10-undecadiene-4,6,8-triyne*
$C_{13}H_{10}O$ 182.221
Cryst. (petrol). Mp 76.5°. $[\alpha]_D^{20}$ +63 ($CHCl_3$). Has (3*E*,7*E*)-config., abs. config. not detd..

[50739-51-0, 58998-11-1, 61434-49-9, 124604-44-0]

Sorensen, N.A. *et al., Acta Chem. Scand.*, 1958, **12**, 756; 1959, **13**, 2101 (*isol, synth*)
Bohlmann, F. *et al., Chem. Ber.*, 1958, **91**, 1631; 1642; 1961, **94**, 3179; 1964, **97**, 1193; 2583; 1966, **99**, 3433 (*isol, synth, epoxide*)
Chin, C. *et al., J.C.S.(C)*, 1970, 314 (*isol*)
Lam, J. *et al., Planta Med.*, 1973, **24**, 107 (*isol*)
Kenichi, I. *et al., Agric. Biol. Chem.*, 1975, **39**, 1103 (*isol*)
Kogiso, S. *et al., Agric. Biol. Chem.*, 1976, **40**, 2085 (*isol, struct, uv, ir, ms, pmr activity*)
Bedford, C.T. *et al., J.C.S. Perkin 1*, 1976, 735 (*isol, synth*)
Binder, R.G. *et al., J. Agric. Food Chem.*, 1990, **38**, 764; 1053; 1245 (*isol*)

2-Tridecenal T-487

[7774-82-5]
FEMA 3082

$H_3C(CH_2)_9CH{=}CHCHO$

$C_{13}H_{24}O$ 196.332

Flavouring ingredient.

►YD4593000

(*E*)-*form* [7069-41-2]
Liq. $Bp_{0.16}$ 80°.

2,4-Dinitrophenylhydrazone:
Cryst. Mp 117°.

(*Z*)-*form* [71277-06-0]
Liq. $Bp_{0.3}$ 90-92°.

Di-Et acetal: [13043-66-8] *1,1-Diethoxy-2-tridecene*
$C_{17}H_{34}O_2$ 270.454
$Bp_{0.2}$ 111°.

Hirai, K. *et al., Tet. Lett.*, 1972, 2743 (*synth, pmr*)

Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1988, **26**, 411 (*rev, tox*)
Chang, Y.-H. *et al., Synthesis*, 1990, 1033 (*synth, pmr, ir, ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 766
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2828-2829

1-Tridecene T-488

[2437-56-1]

[25377-82-6]
1-Tridecylene

$H_3C(CH_2)_{10}CH{=}CH_2$

$C_{13}H_{26}$ 182.348
Constit. of coconut (*Cocos nucifera*) flesh. Also present in heated oils of peanut, sunflower and butter. Fp -13. Bp_{10} 102-103°.

▶ LD_{50} (mus, orl) 10000 mg/kg. YD4595000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 15B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 20B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 20B (*ir*)
Kozacik, A.P. *et al., J.A.C.S.*, 1938, **60**, 2436 (*synth*)
Hoebold, W. *et al., J. Prakt. Chem.*, 1975, **317**, 1054 (*cmr*)
Schmidt, A.W. *et al., Chem. Ber.*, 1977, **74**, 1313 (*synth*)
Prevot, A. *et al., Frying Food*, 1988, 155-165 (*anal*)
Binder, R.G. *et al., J. Agric. Food Chem.*, 1990, **38**, 764; 1245 (*isol*)

1-Tridecene-3,5,7,9,11-pentayne, 9CI, 8CI T-489

[81900-91-6]

[2060-59-5]

$H_2C{=}CHC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH_3$

$C_{13}H_6$ 162.19
Found in leaves, flowers and seeds of numerous spp. e.g. *Valeriana officinalis* (valerian). Yellow needles (pentane). V. unstable when exposed to light.

1,2S-Epoxide: [112663-83-9] *12,13-Epoxy-2,4,6,8,10-tridecapentayne. 1,3,5,7,9-Undecapentaynyloxirane, 9CI*
$C_{13}H_6O$ 178.19
Pale yellow cryst. dec. immediately becoming violet or black. Sol. Me_2CO, Et_2O, $CHCl_3$. $[\alpha]_D$ +52.8. λ_{max} 285 (ϵ 1100); 326 (ϵ 1700); 350 (ϵ 1700); 377 (ϵ 800) (MeOH) (Berdy).

[16697-28-2]

Sörensen, J.S. *et al., Acta Chem. Scand.*, 1954, **8**, 1769; 1958, **12**, 771 (*isol*)
Jones, E.R.H. *et al., J.C.S.*, 1958, 1054 (*synth, uv*)
Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1963, **296**, 273; 1964, **297**, 443; 1966, **299**, 468; 1970, **303**, 7 (*isol*)
Bohlmann, F. *et al., Chem. Ber.*, 1963, **96**, 1229; 1964, **97**, 2125; 2135; 1965, **98**, 883; 1128; 3081; 1966, **99**, 550; 590; 1648; 3194; 1967, **100**, 1910; 1944; 1971, **104**, 958; 961; 964; 1973, **106**, 382; 1337; 3035; 1975, **108**, 362
Kenichi, I. *et al., Agric. Biol. Chem.*, 1975, **39**, 1103 (*isol, tlc*)
Bohlmann, F. *et al., Phytochemistry*, 1976, **15**, 1177; 1309; 1977, **16**, 768; 1980, **19**, 692; 1981, **20**, 18; 1623; 1631; 1643; 1982, **21**, 465; 647; 1087; 1103; 1983, **22**, 1645; 1984, **23**, 1185; 1985; 1985, **24**, 1108; 1392 (*isol, uv, ir, pmr*)
Anderson, A.B. *et al., Phytochemistry*, 1977, **16**, 1829 (*isol*)
Takasugi, M. *et al., Phytochemistry*, 1987, **26**, 2957 (*isol*)
Stevens, K.L. *et al., J. Liq. Chromatogr.*, 1989, **12**, 1261 (*chromatog*)
Bittner, M. *et al., Phytochemistry*, 1989, **28**, 271 (*isol*)

12-Tridecene-4,6,8,10-tetraynal, 9CI T-490

[28789-45-9]

$H_2C{=}CHC{\equiv}CC{\equiv}CC{\equiv}CC{\equiv}CCH_2CH_2CHO$

$C_{13}H_8O$ 180.206
Isol. from the roots of *Silybum marianum* (milk thistle).

Schulte, K.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1970, **303**, 7 (*isol, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1983, **22**, 2858 (*isol*)

2-Tridecene-4,6,8-triyn-1-ol T-491

$H_3C(CH_2)_3C{\equiv}CC{\equiv}CC{\equiv}CCH{=}CHCH_2OH$

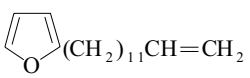
$C_{13}H_{14}O$ 186.253

(E)-form
Metabolite of *Fistulina hepatica* (beefsteak fungus). Mp 50-52°.

Jones, E.R.H. *et al., J.C.S.(C)*, 1966, 139 (*isol, synth*)

2-(12-Tridecenyl)furan T-492

[25346-24-1]
Avocadenofuran

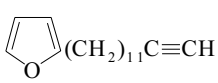


$C_{17}H_{28}O$ 248.408
Constit. of avocado.

Kashman, Y. *et al., Tetrahedron*, 1969, **25**, 4617 (*isol*)
Alves, H.M. *et al., Ann. Acad. Bras. Ci&eenc.*, 1970, **42S**, 45

2-(12-Tridecynyl)furan T-493

[24708-33-6]
Avocadynofuran

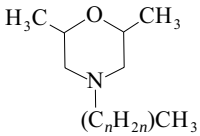


$C_{17}H_{26}O$ 246.392
Constit. of *Persea americana* (avocado).

Kashman, Y. *et al., Tetrahedron*, 1969, **25**, 4617 (*isol*)
Alves, H.M. *et al., Ann. Acad. Bras. Ci&eenc.*, 1970, **42S**, 45
Fraga, B.M. *et al., Phytochemistry*, 1996, **41**, 229 (*isol, pmr, cmr*)

Tridemorph, BSI, ISO T-494

[81412-43-3]
Calixin. Elbamorph



n = 10,11,12 or 13

Mixt. of C_{11}-C_{14} 4-alkyl-2,6-dimethylmorpholine homologues containing 60-70% of 4-tridecyl isomers. Orig. thought to be 2,6-Dimethyl-4-tridecylmorpholine. Systemic eradicant cereal fungicide. Oil. Misc. H_2O, org. solvs. $Bp_{0.5}$ 134°. pK_a 7.5 (20°,basic).

▶ LD_{50} (rat, orl) 650 mg/kg. Exp. teratogen. QE2705000

[24602-86-6]

U.K. Pat., 1968, 1 275 485; *CA*, **75**, 20415r
Rahier, A. *et al., BCPC Monogr.*, 1985, **31**, 249 (*activity*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A409
Pesticide Manual, 11th edn., 1997, 1242
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DUJ400; TJJ500

Tridodecylamine T-495

[102-87-4]
N,N-*Didodecyl-1-dodecanamine, 9CI. Trilaurylamine*

$[H_3C(CH_2)_{11}]_3N$

$C_{36}H_{75}N$ 521.995
Solvent for extraction of citric acid from fermentation liquors. Mp 15.7°. $Bp_{0.03}$ 220-228°. n_D^{25} 1.4567.

Hydrochloride: [2486-89-7] *Tridodecylammonium chloride, 9CI. Trilaurylammonium chloride*
$C_{36}H_{76}ClN$ 558.456
Cryst. (Me_2CO). Sol. toluene. Mp 84-85°.

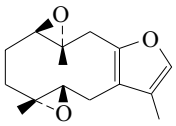
Hydrobromide: [5810-40-2] *Tridodecylammonium bromide, 9CI. Trilaurylammonium bromide*
$C_{36}H_{76}BrN$ 602.907
Cryst. (Me_2CO). Sol. common org. solvs. Mp 86-87°.

N-*Oxide:* [20587-64-8]
$C_{36}H_{75}NO$ 537.995
Cryst. (Me_2CO). Sol. C_6H_6. Mp 50-53°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 487B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 387A (*ir*)
Ralston, A. *et al., J.O.C.*, 1944, **9**, 259 (*synth*)
Mayer, I. *et al., J. Inorg. Nucl. Chem.*, 1967, **29**, 1377 (*synth, cryst struct, salts*)
Alian, A. *et al., Talanta*, 1967, **14**, 659 (*use*)
Kliger, G.A. *et al., CA*, 1973, **79**, 41815u (*synth*)
Tseryuta, Y.S. *et al., CA*, 1973, **79**, 108619d; 1974, **80**, 87883p (*detn, Mo, W*)
Muhammed, M. *et al., Chem. Scr.*, 1974, **6**, 61 (*synth*)
Chimboulev, M. *et al., J. Radioanal. Chem.*, 1976, **30**, 397 (*sepn, Hg*)
Shijo, Y. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 143; 700; 1983, **56**, 105 (*detn, V, Bi, Ga, In, Sb, W*)

Bui-The-Khai, *et al., J.O.C.*, 1981, **46**, 1759 (*synth*)
Rashid, M. *et al., Mikrochim. Acta*, 1986, **1**, 191 (*detn, Hg*)
Masana, A. *et al., Anal. Sci.*, 1988, **4**, 63 (*sepn, Zn*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2829-2830

1,10:4,5:8,12-Triepoxy-7,11-germacradiene T-496



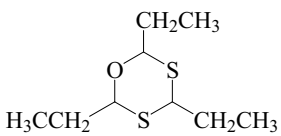
$C_{15}H_{20}O_3$ 248.321

(1β,4α,5β,10α)-*form* [38146-67-7]
Glechomafuran. *Alexandrofuran*
Constit. of *Smyrnium olusatrum* (alexanders). Cryst. (petrol). Mp 115°. $[\alpha]_D^{20}$ +151.5 ($CHCl_3$).

Stahl, E. *et al., Annalen*, 1972, **757**, 23 (*isol*)
Oksuz, A.U.S. *et al., J. Nat. Prod.*, 1983, **46**, 490 (*cryst struct*)
González, A.G. *et al., J. Nat. Prod.*, 1989, **52**, 1307 (*cryst struct*)

2,4,6-Triethyl-1,3,5-oxadithiane, 9CI T-497

[53897-57-7]

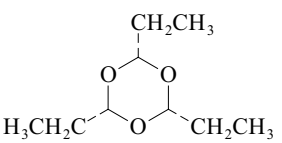


$C_9H_{18}OS_2$ 206.373
Constit. of onion like flavouring produced by reaction of H_2S with propanal. Liq. (?) with green, allium-like odour. Characterised spectroscopically.

Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*formn, ms, aroma*)
Ledl, F. *et al., Z. Lebensm.-Unters. -Forsch.*, 1975, **157**, 28-33 (*formn, glc, ms*)

2,4,6-Triethyl-1,3,5-trioxane, 9CI T-498

[2396-42-1]
Propionaldehyde trimer. Parapropionaldehyde. Parapropanal



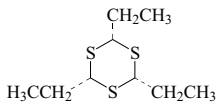
$C_9H_{18}O_3$ 174.239
Normally consists exclusively of the 2α,4α,6α-form. Synthetic onion aroma. Colourless or yellowish oil. Spar. sol. H_2O; sol. EtOH, Et_2O. Fp -20. Bp_{773} 172-173° Bp_{10} 57-57.5° (60.5-61°). n_D^{21} 1.4188. Reverts to monomer on treatment with dilute acid.
► YK0400000

[1499-04-3]

Meier, R. *et al., Chem. Ber.*, 1957, **90**, 2344 (*synth*)
Blanc, P.-Y. *et al., Helv. Chim. Acta*, 1964, **47**, 567 (*synth, props, uv*)
Jungnickel, J.L. *et al., J. Mol. Spectrosc.*, 1965, **16**, 135 (*pmr, config*)
Ward, W.R. *et al., Spectrochim. Acta*, 1965, **2**, 1311 (*ir, Raman*)
Seebald, H.J. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1973, **306**, 393 (*synth, ir, glc*)
Krasnov, V.L. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1983, **53**, 2135 (*synth, nmr*)
Abdelhader, M. *et al., Macromolecules*, 1987, **20**, 949 (*synth, pmr*)
Zhu, Z. *et al., Synthesis*, 1998, 417-422 (*synth, ir, pmr, cmr*)
Hon, Y.-S. *et al., Tetrahedron*, 2001, **57**, 6181-6188 (*synth, pmr, cmr, ir, ms*)

2,4,6-Triethyl-1,3,5-trithiane T-499

[53897-58-8]



(2α,4α,6α)-*form*

$C_9H_{18}S_3$ 222.439
Assignment of stereoisomers is not confirmed. Component of synthetic onion aroma obtained from propanal, H_2S and NH_3. Liq. or partially mass crystalline with green, allium odour. Bp_{13} 135-160°. Bp data is for mixed isomers.

(2α,4α,6α)-*form*
α-*form*
Mp 36°.

(2α,4α,6β)-*form*
β-*form*
Mp 76°.

Douglass, I.B. *et al., J.O.C.*, 1950, **15**, 795-799 (*synth*)
Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*occur, ms, pmr*)
Ledl, F. *et al., Z. Lebensm.-Unters. -Forsch.*, 1975, **157**, 28-33 (*occur, isol*)

Trifluoromethanesulfonic acid, 9CI T-500

[1493-13-6]
Triflic acid. Fluorad FC24
F_3CSO_3H
CHF_3O_3S 150.078
Catalyst used in the prodn. of cocoa butter substitute from palm oil. Liq. Misc. H_2O. d_4^{20} 1.69. Mp 34° (monohydrate). Bp 162°. Fumes in moist air; v. hygroscopic, forming monohydrate. V. strong acid. Forms various hydrates.
► Friedel-Crafts catalysed-reactions can be violent. Highly corrosive and irritating to all tissues.

[2926-27-4, 37181-39-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 898D; 899A; 899B; 901B; **2**, 1231C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 1431A; 1443B; 1443C; 1446A; 1448C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 834B; 834C; 835C (*ir*)
Sadtler Standard C-13 NMR Spectra, 19961 (*cmr*)

Haszeldine, R.N. *et al., J.C.S.*, 1954, 4228 (*synth*)
Burdon, J. *et al., J.C.S.*, 1957, 2574 (*synth*)
Robinson, E.A. *et al., Can. J. Chem.*, 1961, **39**, 247 (*ir*)
Lundgren, J.O. *et al., Acta Cryst. B*, 1973, **29**, 1923; 1978, **34**, 2428; 2432 (*cryst struct*)
Beard, C.D. *et al., J.O.C.*, 1973, **38**, 3673 (*synth*)
Howells, R.D. *et al., Chem. Rev.*, 1977, **77**, 69 (*rev*)
Varetti, E.L. *et al., Spectrochim. Acta*, 1988, **44**, 733 (*ir, Raman*)
Tordeux, M. *et al., J.O.C.*, 1989, **54**, 2452 (*synth, F-19 nmr*)
Bartmann, K. *et al., Acta Cryst. C*, 1990, **46**, 319 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2833-2834
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0357
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1272
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TKB310

Trifolianol T-501

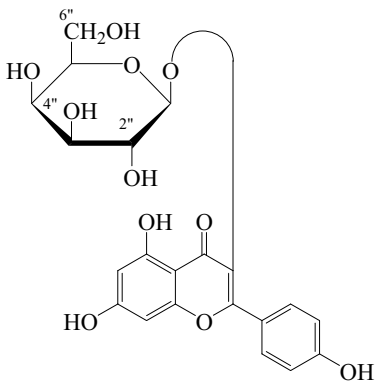
$C_{21}H_{36}O_4$ 352.513
Struct. unknown. Dihydric alcohol. Isol. from *Trifolium pratense* (red clover). Mp 295° dec.

Di-Ac:
Flat needles. Mp 165-166°. $[\alpha]_D$ -24.4.

Salway, A.H. *et al., J.C.S.*, 1911, **99**, 2148

Trifolin T-502

[23627-87-4]
3-O-β-D-Galactopyranosyloxy-4′,5,7-trihydroxyflavone. Kaempferol 3-galactoside. Trifolioside



$C_{21}H_{20}O_{11}$ 448.382
Widespread occurrence in plant world, e.g. *Pinus sylvestris* (Scotch pine) and fruits of *Scolymus hispanicus* (Spanish salsify). Yellowish needles (Py aq.). Mp 235° (229-231°).

6″-Ac:Kaempferol 3-(6-acetylgalactoside)
$C_{23}H_{22}O_{12}$ 490.42
Constit. of the flowers of *Trifolium repens* (white clover).

6″-O-*(4-Hydroxycinnamoyl):* [68170-52-5]
6″*-O-p-*Coumaroyltrifolin. *Kaempferol 3-(6-*p*-coumaroylgalactoside)*
$C_{30}H_{26}O_{13}$ 594.528
Constit. of *Pinus sylvestris* (Scotch

pine).

3″,6″-Bis-O-*(4-hydroxycinnamoyl):* [68127-12-8] ***3″,6″-Di*-O-p-*coumaroyltrifolin***
$C_{39}H_{32}O_{15}$ 740.673
Constit. of *Pinus sylvestris* (Scotch pine).

2″-O-*β-D-Apiofuranosyl:* [132294-84-9]
$C_{26}H_{28}O_{15}$ 580.498
Isol. from seeds of quinoa (*Chenopodium quinoa*). Yellow powder. Mp 166-169°. $[\alpha]_D$ -52 (c, 0.1 in MeOH).

2″-O-*β-D-Apiofuranosyl, 6″*-O-*α-L-rhamnopyranosyl:* [132185-73-0] *Kaempferol 3-(2^G-apiosylrobinobioside)*
$C_{32}H_{38}O_{19}$ 726.641
Constit. of seeds of quinoa (*Chenopodium quinoa*). Yellow powder. $[\alpha]_D$ -67 (c, 0.1 in MeOH).

2″-O-*β-D-Xylopyranosyl:* [83144-68-7] ***Rustoside***
$C_{26}H_{28}O_{15}$ 580.498
Isol. from leaves of horseradish (*Armoracia rusticana*).

2″-O-*β-D-Glucopyranosyl:* [31512-06-8] ***Panasenoside****. Lilyn*
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Panax ginseng* (ginseng). Cryst. (EtOH). Mp 225-228° dec.

2″,6″-Di-O-*α-L-rhamnopyranosyl:* [109008-28-8] ***Mauritianin****. Kaempferol 3-(2^G-rhamnosylrobinobioside)*
$C_{33}H_{40}O_{19}$ 740.668
Constit. of seeds of quinoa (*Chenopodium quinoa*). Pale yellow needles + 4½H_2O (MeCN aq.). Mp 202-204°.

2″-O-*[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranosyl], 6″*-O-*rhamnopyranosyl:* [214407-43-9]
$C_{39}H_{50}O_{24}$ 902.81
Constit. of the leaves of *Maytenus aquifolium* (tea). Brown gum. λ_{max} 266 ; 350 (MeOH).

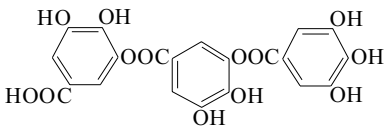
6″-O-*[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranosyl]:* [134953-94-9]
$C_{33}H_{40}O_{20}$ 756.667
Constit. of black tea (*Camellia sinensis*).

[11055-94-0, 78656-61-8, 152343-70-9]

Power, F.B. *et al., J.C.S.*, 1910, **97**, 231 (*isol*)
Schultz, G. *et al., Z. Naturforsch., B*, 1971, **26**, 972
Nair, A.G. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 1045
Roschin, Yu.V. *et al., Khim. Prir. Soedin.*, 1977, **13**, 576; *Chem. Nat. Compd. (Engl. Transl.)*, 1977, **13**, 481
Okuyama, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3071 (*cmr*)
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1978, **14**, 332 (*6″-coumaroyl derivs*)
Larsen, L.M. *et al., Phytochemistry*, 1982, **21**, 1029 (*2″-xylosyl*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
De Simone, F. *et al., Phytochemistry*, 1990, **29**, 3690 (*deriv, isol, quinoa*)
Finger, A. *et al., Phytochemistry*, 1991, **30**, 2057 (*deriv, tea*)
Foo, L.Y. *et al., Phytochemistry*, 2000, **54**, 539-548 (*6″-Ac*)
Han, Y. *et al., Phytochemistry*, 2001, **58**, 577-580 (*Panasenoside*)

m-Trigallic acid T-503

[2131-66-0]
3,4-Dihydroxy-5-[(3,4,5-trihydroxybenzoyl)oxy]benzoic acid 5-carboxy-2,3-dihydroxyphenyl ester, 9CI. Metatrigallic acid

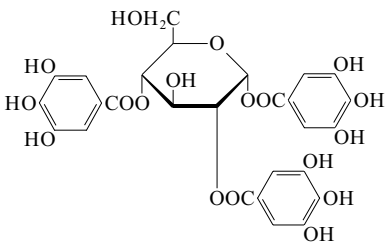


$C_{21}H_{14}O_{13}$ 474.334
Constit. of mango (*Mangifera indica*) fruit. Small needles (Me_2CO aq.). Mp 228° (217°).

Me ester:
Fine needles + 1H_2O (Me_2CO aq.). Mp 253-255°.

King, H.G.C. *et al., J.C.S.*, 1961, 3231 (*synth, ir*)
Reddy, K.K. *et al., Indian J. Chem.*, 1965, **3**, 129; *CA*, **63**, 3226a (*isol*)
Crabtree, P.W. *et al., J.C.S.*, 1965, 6888 (*synth, ir*)

1,2,4-Trigalloylglucose T-504



$C_{27}H_{24}O_{18}$ 636.476

α-D-Pyranose-*form* [111234-33-4]
Needles + 2H_2O (H_2O). Mp 208-210°. $[\alpha]_D^{31}$ +73.5 (c, 1.6 in Me_2CO). λ_{max} 278 (ε 21200) (MeOH) (Berdy). λ_{max} 278 (ε 36858) (EtOH) (Berdy).

β-D-Pyranose-*form*
Constit. of the leaves of *Punica granatum* (pomegranate). Amorph. powder. λ_{max} 277 (MeOH).

Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3127 (*isol, uv, pmr, cmr*)
Hussein, S.A.M. *et al., Phytochemistry*, 1997, **45**, 819 (*isol, uv, pmr, cmr*)

1,2,6-Trigalloylglucose T-505

$C_{27}H_{24}O_{18}$ 636.476

α-D-Pyranose-*form* [82008-89-7]
Off-white amorph. powder + 2H_2O. $[\alpha]_D$ +31 (c, 0.5 in MeOH). Struct. once assigned to a constit. of *Nuphar japonicum*; later revised to 1,2,4-trigalloyl-α-D-glucose (1989) λ_{max} 218 (log ε 4.79); 277 (log ε 4.42) (MeOH).

β-D-Pyranose-*form* [79886-49-0]
Isol. from *Rubus fruticosus* (blackberry) and *Rubus idaeus* (raspberry). Buff amorph. powder + 1H_2O. $[\alpha]_D^{20}$ +10.3 (c, 0.5 in Me_2CO).

O-*(3,4,5-Trihydroxybenzoyl):6′*-O-*Digalloyl-1,2-di*-O-*galloyl-β-D-glucopyranoside*
$C_{34}H_{28}O_{22}$ 788.582
Off-white powder. Substd. in the 6-galloyl residue to produce a digalloyl (galloylgalloyl) residue.

Haddock, E.A. *et al., J.C.S. Perkin 1*, 1982, 2515 (*isol, struct, pmr, cmr*)
Ishimatsu, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 129 (*struct*)
Nishizawa, K. *et al., Phytochemistry*, 1990, **29**, 2491 (*uv, ir, pmr, cmr*)
Nawwar, M.A.M. *et al., Phytochemistry*, 1994, **36**, 793 (*isol, pmr, cmr*)
Amakura, Y. *et al., Can. J. Chem.*, 1997, **75**, 727-733 (*isol, α-D-glucose*)

1,3,4-Trigalloylglucose T-506

1,3,4-Tris(3,4,5-trihydroxybenzoyl)glucose
$C_{27}H_{24}O_{18}$ 636.476

β-D-Pyranose-*form* [193484-86-5]
Constit. of the leaves of *Punica granatum* (pomegranate). Amorph. powder. λ_{max} 277 (MeOH).

Hussein, S.A.M. *et al., Phytochemistry*, 1997, **45**, 819-823 (*isol, uv, pmr, cmr*)

1,4,6-Trigalloylglucose T-507

$C_{27}H_{24}O_{18}$ 636.476

α-D-Pyranose-*form*
Euphormisin M$_3$
Pale brown amorph. powder. $[\alpha]_D$ +2 (c, 0.5 in MeOH).

β-D-Pyranose-*form* [94513-58-3]
Tannin isol. from green tea. Needles + 2H_2O (H_2O). Mp 204-205°. $[\alpha]_D^{24}$ +49.7 (c, 0.48 in Me_2CO).

Nonaka, G. *et al., Phytochemistry*, 1984, **23**, 1753 (*struct, pmr*)
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1803 (*Euphormisin M$_3$*)
Nawwar, M.A.M. *et al., Phytochemistry*, 1994, **36**, 793 (*isol, pmr, cmr*)

2,3,6-Trigalloylglucose T-508

$C_{27}H_{24}O_{18}$ 636.476

β-D-Pyranose-*form*

Me glycoside:Methyl 2,3,6-tri-O-*galloyl-β-D-glucopyranoside*
$C_{28}H_{26}O_{18}$ 650.503
Isol. from *Sanguisorba officinalis* (burnet bloodwort). Tan amorph. powder. $[\alpha]_D^{23}$ +84.3 (c, 1.0 in Me_2CO).

Bis-(3,4,5-trihydroxybenzoyl):2,6-Bis-O-*digalloyl-3*-O-*galloyl-β-D-glucopyranoside*
$C_{41}H_{32}O_{26}$ 940.688
Off-white powder. Substd. in 2- and 6-galloyl residues to produce *P* and *m* digalloyl (galloylgalloyl) residues λ_{max} 282 (MeOH).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 117 (*struct, pmr, cmr*)
Kandil, F.E. *et al., Phytochemistry*, 1996, **42**, 1243-1245 (*bisgalloyl, uv, cmr*)

3,4,6-Trigalloylglucose T-509

$C_{27}H_{24}O_{18}$ 636.476

D-Pyranose-*form* [99523-99-6]
Off-white amorph. powder + 1H_2O. $[\alpha]_D^{20}$ -77.4 (c, 1.06 in MeOH). Exists as an equilibrated mixt. of α- and β-anomers.

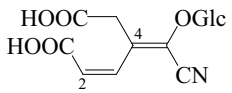
β-D-Pyranose-*form*
Me glycoside: [89927-26-4] *Methyl 3,4,6-*

tri-O-*galloyl-β-D-glucopyranoside*
$C_{28}H_{26}O_{18}$ 650.503
Isol. from underground parts of *Sanguisorba officinalis* (burnet bloodwort). Tan amorph. powder. $[\alpha]_D^{32}$ -52.7 (c, 0.6 in Me_2CO).

Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 117 (*deriv*)
Wilkins, C. *et al., Phytochemistry*, 1988, **27**, 2317 (*struct, cd, pmr*)
Lee, S.H. *et al., Phytochemistry*, 1989, **28**, 3469 (*pmr*)
He, Q. *et al., Carbohydr. Res.*, 2001, **335**, 245-250 (*synth*)

Triglochinin T-510

[28876-11-1]



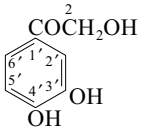
$C_{14}H_{17}NO_{10}$ 359.289
Constit. of the famine food *Alocasia macrorrhiza* (wild taro). Hygroscopic amorph. powder. $[\alpha]_D^{16.5}$ +5.5 (c, 0.2 in MeOH).

*2*E-*Isomer:* [56816-21-8] ***Isotriglochinin***
$C_{14}H_{17}NO_{10}$ 359.289
Constit. of the famine food *Alocasia macrorrhiza* (wild taro). Poss. artifact.

Eyjólfsson, R. *et al., Phytochemistry*, 1970, **9**, 845
Ettlinger, M. *et al., Chem. Comm.*, 1972, 572 (*struct*)
Nahrstedt, A. *et al., Phytochemistry*, 1975, **14**, 1339-1340; 1870-1871 (*isol*)
Jaroszewski, J.W. *et al., Phytochemistry*, 1981, **20**, 819 (*biosynth*)

2,3′,4′-Trihydroxyacetophenone, 8CI T-511

[29477-54-1]
1-(3,4-Dihydroxyphenyl)-2-hydroxyethanone, 9CI. α,3,4-Trihydroxyacetophenone. 3,4-Dihydroxyphenacyl alcohol



$C_8H_8O_4$ 168.149
Cryst. (H_2O). Mp 195°. λ_{max} 220 (log ϵ 3.7); 231 (log ϵ 3.7); 290 (sh) (log ϵ 3.6); 325 (log ϵ 3.8) (MeOH).

2-O-*(3,4-Dihydroxy*-E-*cinnamoyl):* [162616-81-1] ***Petasiphenone***. *3,4-Dihydroxyphenacyl caffeate*
$C_{17}H_{14}O_7$ 330.293
Constit. of the rhizomes of *Petasites japonicus* (sweet coltsfoot). Pale brown powder. Mp 236-238°. λ_{max} 220 (log ϵ 3.7); 231 (log ϵ 3.7); 290 (sh) (log ϵ 3.6); 325 (log ϵ 3.8) (MeOH).

Voswinckel, H. *et al., Ber.*, 1909, **42**, 4651
Robinson, R. *et al., J.C.S.*, 1925, **127**, 170
Yaoita, Y. *et al., Phytochemistry*, 1994, **37**, 1773-1774 (*Petasiphenone*)

2′,4′,6′-Trihydroxyacetophenone, 8CI T-512

[480-66-0]
1-(2,4,6-Trihydroxyphenyl)ethanone, 9CI. 2-Acetyl-1,3,5-benzenetriol. Acetophloroglucinol. Acetylphloroglucinol. Phloracetophenone. Phloroacetophenone

$C_8H_8O_4$ 168.149
Isol. from bark of *Prunus domestica* (plum). Needles (H_2O). Mp 219° (anhyd.). λ_{max} 228 (ϵ 14500); 288 (ϵ 16200) (EtOH) (Berdy).

2′-Me ether: [3602-54-8] *2′,4′-Dihydroxy-6′-methoxyacetophenone*
$C_9H_{10}O_4$ 182.176
Constit. of *Artemisia* sp.. Cryst. (Me_2CO). Mp 197-199°.

2′-Me ether, 6′-O-*β-D-glucopyranoside:* [241814-62-0]
$C_{15}H_{20}O_9$ 344.318
Constit. of *Crocus sativus* (saffron). Needles. Mp 158-160°. $[\alpha]_D$ +48.7 (c, 0.05 in MeOH).

4′-Me ether: [7507-89-3] *2′,6′-Dihydroxy-4′-methoxyacetophenone. 4*-O-*Methylphloracetophenone*
$C_9H_{10}O_4$ 182.176
Isol. from the bark of *Prunus domestica* (plum). Mp 141-142°.

4′-Me ether, O-*β-D-glucopyranoside:* [24587-97-1] ***Pleoside***. *Domesticoside*
$C_{15}H_{20}O_9$ 344.318
Isol. from the bark of *Prunus domestica* (plum). Needles (MeOH). Mp 189-191° (sinters at 183°) Mp 200-203°. $[\alpha]_D$ -41.6 (Py). Identity of samples not apparently establ. Higher Mp and opt. rotn. refer to Pleoside.

2′,4′-Di-Me ether: [90-24-4] *2′-Hydroxy-4′,6′-dimethoxyacetophenone.* ***Xanthoxylin***. *Brevifolin. 6-Methoxypaeonol*
$C_{10}H_{12}O_4$ 196.202
Obt. from *Zanthoxylum piperitum* (Japanese pepper tree) and *Sapium sebiferum* (Chinese tallowtree). Cryst. (EtOH). Mp 85-88°.

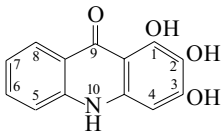
2′,4′-Di-Me ether, 6′-O-*[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [87432-28-8]
$C_{21}H_{30}O_{13}$ 490.46
Constit. of *Sapium sebiferum* (Chinese tallowtree). Needles (MeOH). Mp 188-190°. $[\alpha]_D^{26}$ -41.7 (Py). λ_{max} 225 (ϵ 14520); 273 (ϵ 7570) (EtOH).

[4547-84-6]

v. Kostanecki, S. *et al., Ber.*, 1899, **32**, 2260-2269 (*2′,4′-di-Me ether, synth*)
Dean, F.M. *et al., J.C.S.*, 1953, 1241-1249 (*2′,4′-di-Me ether, 2′,6′-di-Me ether, synth*)
Hikino, H. *et al., Yakugaku Zasshi*, 1969, **89**, 372 (*Pleoside*)
Nagarajan, G.R. *et al., Phytochemistry*, 1977, **16**, 614-615 (*isol, 4′-Me ether, 4′-Me ether 6-glucoside*)
Kokubin, T. *et al., Phytochemistry*, 1994, **35**, 331-333 (*isol, 4′-Me ether*)
Yenesew, A. *et al., Phytochemistry*, 1994, **37**, 525-528 (*2′-Me ether*)
Gao, W.-Y. *et al., Planta Med.*, 1999, **65**, 425-427 (*2′-Me 6′-glucoside*)

1,2,3-Trihydroxyacridone T-513

*1,2,3-Trihydroxy-9(10*H*)-acridinone, 9CI*



$C_{13}H_9NO_4$ 243.218

2,3-Di-Me ether: [17014-43-6] ***Xanthoxoline***. *1-Hydroxy-2,3-dimethoxyacridone*
$C_{15}H_{13}NO_4$ 271.272
Mp 256-257°.

2,3-Di-Me ether, O-*Ac:*
$C_{17}H_{15}NO_5$ 313.309
Mp 238-241°.

2,3,10-O,O,N-*Tri-Me:* [5489-57-6] ***Arborinine***
$C_{16}H_{15}NO_4$ 285.299
Alkaloid from *Ruta graveolens* (rue). Cryst. (EtOH). Mp 175-176°. Log P 1.11 (calc).

2,3,10-O,O,N-*Tri-Me,* O-*Ac:*
$C_{18}H_{17}NO_5$ 327.336
Mp 215-216°.

O,O,O,N-*Tetra-Me:* ***1,2,3-Trimethoxy-10-methylacridone***
$C_{17}H_{17}NO_4$ 299.326
Mp 169-171°.

3-O-*(3-Methyl-2-butenyl),* O^2,N-*di-Me:* [16584-45-5] *1-Hydroxy-2-methoxy-10-methyl-3-prenyloxyacridone.* ***Evoprenine***
$C_{20}H_{21}NO_4$ 339.39
Yellow needles (EtOH). Mp 143°.

2,3-Methylene, 1-Me ether: See 1-Methoxy-2,3-methylenedioxyacridone in *The Combined Chemical Dictionary.*

Hughes, G.K. *et al., Aust. J. Sci. Res., Ser. A*, 1952, **5**, 401; 406 (*isol, synth*)
Chakravati, D. *et al., J.C.S.*, 1953, 3337 (*isol, Arborinine*)
Gell, R.J. *et al., Aust. J. Chem.*, 1955, **8**, 114 (*isol, struct*)
Pakrashi, S.C. *et al., Chem. Ind. (London)*, 1961, 464 (*pmr*)
Banerjee, S.K. *et al., Tetrahedron*, 1961, **16**, 251 (*isol, ir*)
Bowie, J. *et al., Aust. J. Chem.*, 1967, **20**, 1179 (*ms*)
Diment, J.A. *et al., Aust. J. Chem.*, 1967, **20**, 1719 (*Evoprenine*)
Bergenthal, D. *et al., Phytochemistry*, 1979, **18**, 161-163 (*cmr*)
Coppola, G.M. *et al., J. Het. Chem.*, 1989, **26**, 957 (*1,2,3-Trimethoxy-10-methylacridone, synth, ir, pmr*)

1,3,5-Trihydroxyacridone T-514

*1,3,5-Trihydroxy-9(10*H*)-acridinone, 9CI*

$C_{13}H_9NO_4$ 243.218

N-*Me:* ***1,3,5-Trihydroxy-10-methylacridone***
$C_{14}H_{11}NO_4$ 257.245
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisi*) x Dancy tangerine (*Citrus tangerina*)]. Yellow oil.

O^3,N-*Di-Me:* [108598-30-7] *1,5-Dihydroxy-3-methoxy-10-methylacridone.* ***Citrusamine***
$C_{15}H_{13}NO_4$ 271.272

Orange-yellow needles ($CHCl_3$/petrol), yellow prisms (Me_2CO). Mp 140-141° Mp 243-246°. Large discrepancy in Mp between the two isolates may indicate an incorrect identity.

O^5,N-*Di-Me:* [145940-33-6] *1,3-Dihydroxy-5-methoxy-10-methylacridone.* ***Yukodine***
$C_{15}H_{13}NO_4$ 271.272
Yellow needles. Mp 246-250°.

O^3,O^5,N-*Tri-Me:* [145940-34-7] *1-Hydroxy-3,5-dimethoxy-10-methylacridone.* ***Yukodinine***
$C_{16}H_{15}NO_4$ 285.299
Pale yellow oil.

O,O,O,N-*Tetra-Me:* [52911-52-1] ***1,3,5-Trimethoxy-10-methylacridone***
$C_{17}H_{17}NO_4$ 299.326
Beige needles ($CHCl_3$/Et_2O). Mp 141°.

Vacquette, J. *et al., Plant. Med. Phytother.*, 1974, **8**, 57 (*isol, struct*)
Ju-Ichi, M. *et al., Heterocycles*, 1987, **26**, 1873 (*isol, uv, ir, pmr, ms, struct*)
Bowen, I.H. *et al., Planta Med.*, 1987, **53**, 73 (*isol, uv, ir, pmr, ms, struct*)
Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2123 (*Yukodine, Yukodinine*)
Takemura, Y. *et al., Chem. Pharm. Bull.*, 1996, **44**, 804 (*1,3,5-Trihydroxy-10-methylacridone*)

1,3,6-Trihydroxyacridone T-515

*1,3,6-Trihydroxy-9(10*H*)-acridinone, 9CI*

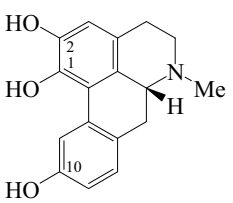
$C_{13}H_9NO_4$ 243.218

O^3,N-*Di-Me:* [145940-36-9] *1,6-Dihydroxy-3-methoxy-10-methylacridone.* ***Pummeline***
$C_{15}H_{13}NO_4$ 271.272
Alkaloid from roots of several hybrid seedlings resulting from a cross of Pummelo (*Citrus grandis* cv. May Pummelo × Marsh grapefruit (*Citrus paradisi*) (Rutaceae)). Yellow cubes. Mp 235-240°.

Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2123 (*isol, uv, ir, pmr, cmr, ms, struct*)

1,2,10-Trihydroxyaporphine T-516

*5,6,6a,7-Tetrahydro-6-methyl-4*H*-dibenzo[de,g]quinoline-1,2,10-triol, 9CI*



(*R*)-*form*

$C_{17}H_{17}NO_3$ 283.326

(*S*)-*form*

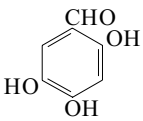
1,2-Di-Me ether, N-*de-Me,* N-*methoxycarbonyl:* [356048-25-4] ***Romucosine C***
$C_{20}H_{21}NO_5$ 355.39
Alkaloid from *Rollinia mucosa* (biriba). Amorph. powder. $[\alpha]_D^{25}$ +140 (c, 0.05 in $CHCl_3$). λ_{max} 265 (log ϵ 4.25); 280 (log ϵ 4.02); 305 (log ϵ 4.35) (MeOH).

Tri-Me ether, N-*de-Me,* N-*methoxycarbonyl:* [356048-26-5] ***Romucosine D***
$C_{21}H_{23}NO_5$ 369.416
Alkaloid from *Rollinia mucosa* (biriba). Amorph. powder. $[\alpha]_D^{25}$ +145 (c, 0.05 in $CHCl_3$). λ_{max} 263 (log ϵ 4.33); 275 (log ϵ 4.22); 307 (log ϵ 3.75) (MeOH).

Kuo, R.Y. *et al., Phytochemistry*, 2001, **57**, 421-425 (*Romucosines*)

2,4,5-Trihydroxybenzaldehyde, 9CI T-517

[35094-87-2]



$C_7H_6O_4$ 154.122
Cryst. (H_2O). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 223° Mp 229-230°. λ_{max} 241 (ϵ 14000); 282 (ϵ 11000); 350 (ϵ 8000) (MeOH) (Berdy).

2,4,5-Tri-Me ether: [4460-86-0] *2,4,5-Trimethoxybenzaldehyde, 9CI, 8CI. Asaronaldehyde. Asarylaldehyde. Gazarin. Asaraldehyde*
$C_{10}H_{12}O_4$ 196.202
Constit. of bitter principle of carrot seeds (*Daucus carota*) and sweetflag (*Acorus calamus*). Needles ($CHCl_3$ or H_2O). Mp 114°.

▶ CU8460000

Starkovsky, N.A. *et al., J.O.C.*, 1962, **27**, 3733 (*2,4,5-tri-Me ether, isol, ir*)

3,4,5-Trihydroxybenzaldehyde, 9CI T-518

[13677-79-7]
Gallaldehyde. Gallic aldehyde

$C_7H_6O_4$ 154.122
Cryst. + $1H_2O$ (H_2O). Mp 212° dec. (rapid heat).

3-O-[6-O-(3,4,5-Trihydroxybenzoyl)-β-D-glucopyranoside]: [115355-99-2] ***Castamollissin***
$C_{20}H_{20}O_{13}$ 468.37
Isol. from the leaves of *Castanea mollissima* (Chinese chestnut). Needles + $2H_2O$ (H_2O). Mp 209-211°. $[\alpha]_D^{20}$ -58.8 (c, 1.06 in Me_2CO aq.).

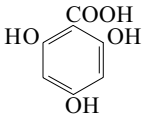
4-O-[6-O-(3,4,5-Trihydroxybenzoyl)-β-D-glucopyranoside]: [67771-96-4] ***Neocretanin***
$C_{20}H_{20}O_{13}$ 468.37
Isol. from Japanese chestnut galls (*Castanea crenata*). Needles + $2H_2O$ (H_2O). Mp 195-197° dec. $[\alpha]_D^{23}$ -63.8 (c, 0.99 in MeOH).

Ozawa, T. *et al., Agric. Biol. Chem.*, 1977, **41**, 1257; 1978, **42**, 1213 (*Neocrenatin, Neocretanin*)
Rao, D.V. *et al., Synthesis*, 1983, 308 (*synth*)
Feng, H. *et al., Phytochemistry*, 1988, **27**, 1185 (*Castamollissin*)

2,4,6-Trihydroxybenzoic acid, 9CI, 8CI T-519

[83-30-7]

[71989-93-0]
Phloroglucinolcarboxylic acid. Phloroglucinic acid



$C_7H_6O_5$ 170.121
Isol. from onion skin (*Allium* sp.). Cryst. + $1H_2O$. Mp 207-210° dec. (monohydrate).

▶ DH8750000

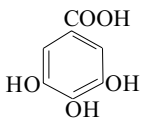
Me ester: [3147-39-5]
$C_8H_8O_5$ 184.148
Isol. from onion skin. Cryst. (EtOH aq.). Mp 174-176°.

[52578-53-7, 71989-93-0]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 434D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 461A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1419B (*ir*)
Will, W. *et al., Ber.*, 1884, **17**, 2098; 2103 (*synth*)
Saraiya, P.R. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1950, **31**, 187
Horii, Z. *et al., Yakugaku Zasshi*, 1952, **72**, 1520; *CA*, **47**, 8039 (*synth*)
Herrmann, K. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1958, **291**, 238 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TKO000

3,4,5-Trihydroxybenzoic acid T-520

[149-91-7]
Gallic acid



$C_7H_6O_5$ 170.121
Present in red wine. Japan approved food antioxidant additive. Needles (MeOH or $CHCl_3$); cryst. + $1H_2O$ (H_2O). Sol. Me_2CO, EtOH; spar. sol. H_2O; insol. C_6H_6, $CHCl_3$. Mp 253° dec Mp 235-240° (225°). pK_{a1} 3.13; pK_{a2} 8.84; pK_{a3} 12.4 (20°, 0.1*M* KNO_3). Log P 0.43 (calc).

▶ LD_{50} (rbt, orl) 5000 mg/kg. Exp. reprod. effects. LW7525000

β-D-Glucopyranosyl ester: 1-Galloylglucose, G-46

Et ester: [831-61-8] *Ethyl 3,4,5-trihydroxybenzoate. Ethyl gallate. Phyllemblin*
$C_9H_{10}O_5$ 198.175
Occurs, *inter alia*, in Indian gooseberry (*Phyllanthus emblica*). Mp 160-162° (anhyd.). Log P 1.46 (calc).

▶ LW7700000

Propyl ester: [121-79-9] *Propyl 3,4,5-trihydroxybenzoate. Propyl gallate. E310. FEMA 2947*
$C_{10}H_{12}O_5$ 212.202
Antioxidant used in foods esp. animal fats and vegetable oils. Synergistic with other antioxidants such as Butylated hydroxyanisole, B-241 and 2,6-Di-*tert*-butyl-4-methylphenol, D-148. Esp. effective with polyunsaturated fats. Indirect food additive arising from paper or board packaging, adhesives and food

contact polymers. Cryst. Sol. Me_2CO, 2-butanol. Mp 150° (147-148°).

▶ LD_{50} (rat, orl) 2100 mg/kg. Exp. reprod. and teratogenic effects (v. large doses). LW8400000

Octyl ester: [1034-01-1] *Octyl gallate. E311*
$C_{15}H_{22}O_5$ 282.336
Antioxidant used in margarine. Cryst. (C_6H_6). Mp 94-95°.

Dodecyl ester: [1166-52-5] *Dodecyl gallate. E312*
$C_{19}H_{30}O_5$ 338.443
Antioxidant used in foods esp. oil, fats, cheeses and mashed potato. Permitted for use in margarine in USA. Possesses same antioxidant effects as propyl gallate but incr. alkyl chain length gives rise to greater fat solubility. Sol. EtOH, Me_2CO. Mp 96-97°.

▶ LD_{50} (mus, orl) 1600 mg/kg. DH9100000

3-O-β-D-Glucopyranoside: [91984-84-8] ***3-Glucogallic acid***
$C_{13}H_{16}O_{10}$ 332.263
Isol. from commercial rhubarb (*Rheum* spp.). Granules. Mp 244-245°. $[\alpha]_D^{24}$ -73.6 (c, 0.5 in MeOH).

3-O-[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]: [87087-61-4] *Gallic acid 3-O-(6-galloylglucoside)*
$C_{20}H_{20}O_{14}$ 484.37
Isol. from commercial rhubarb and from the underground part of great burnet (*Sanguisorba officinalis*). Needles + $1\frac{1}{2}H_2O$. Mp 261-263° dec. $[\alpha]_D^{26}$ -19.4 (c, 0.48 in Me_2CO).

4-O-β-D-Glucopyranoside: see 4-Galloylglucose, G-48

3-Me ether: [3934-84-7] *3,4-Dihydroxy-5-methoxybenzoic acid*
$C_8H_8O_5$ 184.148
Present in hydrolysed soy protein and oak aged wines and brandies. Mp 220° (197°). Mp also reported as 131-132°.

3,5-Di-Me ether: [530-57-4] *4-Hydroxy-3,5-dimethoxybenzoic acid.* ***Syringic acid****. Cedar acid*
$C_9H_{10}O_5$ 198.175
Present in various plants free and combined, e.g. principal phenolic constit. of soyabean meal (*Glycine max*). Cryst. Mp 210°. pK_{a1} 4.34; pK_{a2} 9.49 (25°). The homopolymer has been prepd. λ_{max} 271 ; 272 (MeOH) (Berdy).

▶ DH2090000

Tri-Me ether: [118-41-2] *3,4,5-Trimethoxybenzoic acid.* ***Eudesmic acid***
$C_{10}H_{12}O_5$ 212.202
Isol. from eucalyptus oil etc.. Prisms. Mp 171-172°.

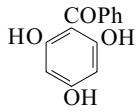
Tri-Me ether, Et ester: [6178-44-5] ***Ethyl 3,4,5-trimethoxybenzoate***
Isol. from cashew gum. Mp 50-51°.

[5995-86-8, 13405-60-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 229B; 232A; 232B; 301A; 301B; 461B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1142C; 1143A; 1147C; 1148B; 1261B; 1261C; 1352C; 1539C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1332D; 1370B; 1370C; 1419C (*ir*)
Clarke, J. *et al., J.C.S.*, 1927, 2647-2653 (*propyl ester, butyl ester*)
Morris, S.G. *et al., J.A.C.S.*, 1946, **68**, 500 (*esters*)
Welcher, J.F. *et al., Organic Analytical Reagents*, van Nostrand, N.Y., 1947, **1**, 200 (*use*)
Pearl, I.A. *et al., J.A.C.S.*, 1950, **72**, 1743-1746 (*synth, derivs*)
Van Der Kerk, G.J.M. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1951, **70**, 277 (*esters*)
Haslam, E. *et al., J.C.S.*, 1961, 1854 (*biosynth*)
Takahashi, T. *et al., Agric. Biol. Chem.*, 1966, **30**, 617 (*isol, deriv*)
Mishra, R.K. *et al., Indian J. Appl. Chem.*, 1968, **31**, 233; *CA*, **71**, 77046t (*dodecyl ester, detn, U*)
Chumbalov, T.K. *et al., Khim. Prir. Soedin.*, 1971, **6**, 120; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **6**, 112 (*isol, 3-Me ether*)
Shima, K. *et al., Phytochemistry*, 1971, **10**, 894 (*isol, deriv*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 903; 904; 909; 910 (*occur, derivs*)
Pryce, R.J. *et al., Phytochemistry*, 1972, **11**, 1911 (*isol*)
Mgebrishvili, M.A. *et al., Khim. Prir. Soedin.*, 1974, **10**, 512; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 514 (*isol*)
Shipchandler, M.T. *et al., J.C.S. Perkin 1*, 1975, 1400 (*synth*)
Rodd's Chem. Carbon Compd. (2nd edn.), 1976, **3D**, 193 (*bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **18**, 677 (*rev*)
Elford, H.L. *et al., Cancer Res.*, 1979, **39**, 844 (*activity*)
Van't Riet, B. *et al., J. Med. Chem.*, 1979, **22**, 589 (*synth, pharmacol*)
Pratt, D.E. *et al., J. Food Sci.*, 1981, **47**, 24-25 (*3-Me ether*)
U.S. Pat., 1981, 4 263 322; *CA*, **95**, 80517y (*synth*)
Gross, G.G. *et al., Z. Naturforsch., C*, 1982, **37**, 778 (*synth*)
Nonaka, G.-I. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1652; 1989, **37**, 2030 (*galloylglucosides*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 117 (*galloylglucosides*)
Puech, J.-L. *et al., J. Food Sci.*, 1987, **52**, 1280-1282 (*3-Me ether*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, PNM750; DXX200
Nielsen, B.B. *et al., Acta Cryst. C*, 1993, **49**, 810 (*cryst struct*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 402-404
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1116
Zhu, J. *et al., Synth. Commun.*, 1996, **26**, 2479 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 907; 2033; 2360-2362 (*dodecyl ester, propyl ester, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DXX200; GBE000; MKI100; PNM750

2,4,6-Trihydroxybenzophenone, 8CI T-521

[3555-86-0]
(2,4,6-Trihydroxyphenyl)phenylmethanone, 9CI. Phlorbenzophenone



$C_{13}H_{10}O_4$ 230.22
Yellow cryst. + $1H_2O$ (H_2O). Mp 165°.

2-O-β-D-Glucopyranoside: ***Garcimangosone D***
$C_{19}H_{20}O_9$ 392.362
Constit. of the dried fruit hulls of *Garcinia mangostana* (mangosteen). Yellow powder. Mp 136-138°. $[\alpha]_D^{25}$ -64 (c, 0.5 in MeOH). λ_{max} 204 (log ε 4.8); 258 (log ε 4.37) (MeOH).

2-Me ether: [81525-12-4] *2,4-Dihydroxy-6-methoxybenzophenone.* ***Isocotoin***
$C_{14}H_{12}O_4$ 244.246
Yellow needles. Mp 162°.

4-Me ether: [479-21-0] *2,6-Dihydroxy-4-methoxybenzophenone.* ***Cotoin***
$C_{14}H_{12}O_4$ 244.246
Yellowish cryst. (H_2O). Mp 130-131°. Reduces Fehling's soln. and NH_3.Ag-NO_3 slowly in the cold.

▶ DJ1050000

2,4-Di-Me ether: [34425-64-4] *2-Hydroxy-4,6-dimethoxybenzophenone.* ***Hydrocotoin***
$C_{15}H_{14}O_4$ 258.273
Light yellow prisms or needles (EtOH). Mp 97-98°.

2,6-Di-Me ether:4-Hydroxy-2,6-dimethoxybenzophenone
$C_{15}H_{14}O_4$ 258.273
Mp 178-179°.

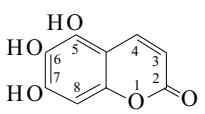
Tri-Me ether: [3770-80-7] *2,4,6-Trimethoxybenzophenone.* ***Methylhydrocotoin***
$C_{16}H_{16}O_4$ 272.3
Isol. from Cascara sagrada. Prisms or tablets (EtOH). Mp 113-115°.

4-O-(3,6-Dimethyl-2,7-octadienyl)(E-), 2-Me ether: [140158-57-2] *4-Geranyloxy-2-hydroxy-6-methoxybenzophenone*
$C_{24}H_{28}O_4$ 380.483

Karrer, P. *et al., Helv. Chim. Acta*, 1928, **11**, 789 (*struct*)
Phadke, R. *et al., J. Indian Chem. Soc.*, 1950, **27**, 349 (*synth*)
Gottleib, O.R. *et al., J.A.C.S.*, 1958, **80**, 2263 (*isol, Cotoin*)
Harris, T.M. *et al., J.A.C.S.*, 1966, **88**, 5686 (*synth*)
Randriaminahy, M. *et al., Z. Naturforsch., C*, 1992, **47**, 10 (*deriv*)

5,6,7-Trihydroxy-2*H*-1-benzopyran-2-one, 9CI T-522

[16574-13-3]
5,6,7-Trihydroxycoumarin



$C_9H_6O_5$ 194.143

6-Me ether, 7-O-β-D-glucopyranoside: [141238-32-6] *7-Glucosyloxy-5-hydroxy-6-methoxycoumarin*

$C_{16}H_{18}O_{10}$ 370.312
Isol. from *Prunus spinosa* (sloe). Cryst. Mp 135°.

6,7-Di-Me ether, 5-O-β-D-glucopyranoside: [28446-08-4] ***Tomenin***
$C_{17}H_{20}O_{10}$ 384.339
Constit. of *Prunus tomentosa* (nanking cherry). Cryst. (MeOH). Mp 206°.

González, A.G. *et al., An. Quim.*, 1973, **69**, 781 (*derivs*)
Artem'eva, M.V. *et al., Khim. Prir. Soedin.*, 1973, **9**, 493; *Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 465 (*isol*)
Murray, R.D.H. *et al., Tetrahedron*, 1975, **31**, 2966 (*struct*)
Ahluwalia, V.K. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 286; 591 (*synth, Tomenin*)
Irizar, A.C. *et al., J. Nat. Prod.*, 1992, **55**, 450 (*7-Glucosyloxy-5-hydroxy-6-methoxycoumarin*)

6,7,8-Trihydroxy-2*H*-1-benzopyran-2-one, 9CI T-523

[114371-80-1]
6,7,8-Trihydroxycoumarin

$C_9H_6O_5$ 194.143

6,8-Di-Me ether, 7-O-α-D-glucopyranoside: [16845-16-2] ***Eleutheroside B₁***
$C_{17}H_{20}O_{10}$ 384.339
From Siberian ginseng (*Eleutherococcus (Acanthopanax) senticosus*). Cryst. Mp 218°. $[\alpha]_D^{20}$ +80 (MeOH).

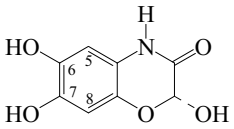
6,8-Di-Me ether, 7-O-β-D-glucopyranoside: [483-91-0] ***Calycanthoside***
$C_{17}H_{20}O_{10}$ 384.339
Constit. of *Calycanthus occidentalis* (Californian allspice). Cryst. Mp 219-220°. $[\alpha]_D^{20}$ -42 (MeOH).

6,7-Methylene, 8-Me ether: [81558-03-4] *8-Methoxy-6,7-methylenedioxycoumarin*
$C_{11}H_8O_5$ 220.181
Isol. from *Artemisia vulgaris* (mugwort). Cryst. (EtOAc/toluene). Mp 200-202°.

7,8-Methylene, 6-Me ether: [28843-40-5] *4-Methoxy-8H-1,3-dioxolo[4,5-h][1]benzopyran-8-one. 6-Methoxy-7,8-methylenedioxycoumarin.* ***Dracunculin***
$C_{11}H_8O_5$ 220.181
Constit. of *Artemisia dracunculoides* (Russian tarragon). Mp 219-221°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 326B (*ir*)
Aldrich Library of FT-NMR Spectra, 1992, **2**, 1317C (*nmr*)
Ovodov, Y.S. *et al., Khim. Prir. Soedin.*, 1967, **3**, 63-64; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 53-54 (*Eleutheroside B₁*)
Herz, W. *et al., Phytochemistry*, 1970, **9**, 891-894 (*Dracunculin*)
Stefanovic, M. *et al., CA*, 1982, **96**, 177968 (*8-Methoxy-6,7-methylenedioxycoumarin*)
Murray, R.D.H. *et al., J. Nat. Prod.*, 1986, **49**, 550-551 (*Dracunculin*)
Castillo, P. *et al., Synthesis*, 1986, 839-840 (*Dracunculin, synth*)
Zhang, D. *et al., Zhongcaoyao*, 1989, **20**, 487; *CA*, **112**, 175635 (*8-Methoxy-6,7-methylenedioxycoumarin*)
Sarker, S.D. *et al., J. Nat. Prod.*, 1994, **57**, 1549 (*8-Methoxy-6,7-methylenedioxycoumarin*)

2,6,7-Trihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one T-524



$C_8H_7NO_5$ 197.147

(R)-form

N-*Hydroxy, 6,7-di-Me ether:* [67467-45-2] *2,4-Dihydroxy-6,7-dimethoxy-2H-1,4-benzoxazin-3(4H)-one, 9CI*
$C_{10}H_{11}NO_6$ 241.2
Constit. of sweet corn (*Zea mays*).

Hofman, J. *et al., Phytochemistry*, 1973, **12**, 207-208

2,7,8-Trihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one T-525

$C_8H_7NO_5$ 197.147

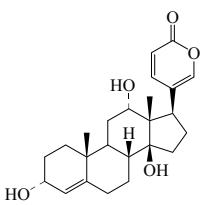
(R)-form

N-*Hydroxy, 7,8-di-Me ether:* [60032-92-0] *2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one, 9CI*
$C_{10}H_{11}NO_6$ 241.2
Constit. of wheat and sweet corn.

N-*Hydroxy, 7,8-di-Me ether, 2-O-β-D-glucopyranoside:* [40246-08-0]
$C_{16}H_{21}NO_{11}$ 403.342
Constit. of wheat and sweet corn (*Zea mays*).

Hofman, J. *et al., Phytochemistry*, 1973, **12**, 207-208

3,12,14-Trihydroxybufa-4,20,22-trienolide T-526



(3α,12α,14β)-*form*

$C_{24}H_{32}O_5$ 400.514

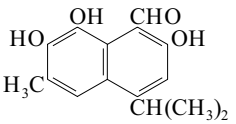
(3β,12β,14β)-*form* [21305-04-4] ***Scillipheosidin***. *Scilliphaeosidin*
Cryst. (MeOH). Mp 274-279°. $[\alpha]_D$ -2.8 (c, 0.526 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-α-L-rhamnopyranoside]: [261158-68-3]
$C_{36}H_{52}O_{14}$ 708.798
Constit. of the seeds of *Tamarindus indica* (tamarind).

Yadava, R.N. *et al., CA*, 2000, **132**, 227232v (*glucosyl(1→2)rhamnoside*)

2,3,9-Trihydroxy-14-cadalenal T-527

[54835-63-1]
2,7,8-Trihydroxy-4-isopropyl-6-methyl-1-naphthalenecarboxaldehyde. Isohemigossypol



$C_{15}H_{16}O_4$ 260.289

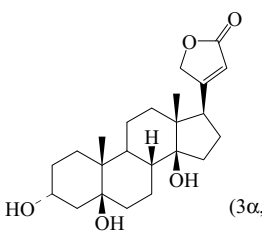
7-Me ether: [60089-74-9] *2,8-Dihydroxy-4-isopropyl-7-methoxy-6-methyl-1-naphthalenecarboxaldehyde.* ***Gossyvertin***
$C_{16}H_{18}O_4$ 274.316
Isol. from the stems of cotton plants (*Gossypium* sp.) infected with *Verticillium dahliae*. Mp 147-149°. Revised struct..

8-Me ether: [80442-49-5] *2,7-Dihydroxy-4-isopropyl-8-methoxy-6-methyl-1-naphthalenecarboxaldehyde*
$C_{16}H_{18}O_4$ 274.316
Cryst. (petrol). Mp 156-160° (153°). Revised struct. (1981) λ_{max} 204 (log ε 4.08); 232 (log ε 4.71); 275 (log ε 3.81); 363 (log ε 3.99) (MeOH).

7,8-Di-Me ether: [80442-48-4] *2-Hydroxy-4-isopropyl-7,8-dimethoxy-6-methyl-1-naphthalenecarboxaldehyde*
$C_{17}H_{20}O_4$ 288.343
Yellow cryst. (petrol). Mp 101-102°. λ_{max} 207 (log ε 4.32); 228 (log ε 4.74); 250 (log ε 4.29); 337 (log ε 4.02) (MeOH).

Karimdzhanov, A.K. *et al., Khim. Prir. Soedin.*, 1976, **12**, 238; *Chem. Nat. Compd. (Engl. Transl.)*, 211 (*isol, pmr, ms, uv*)
Sankaram, A.V.B. *et al., Phytochemistry*, 1981, **20**, 1877 (*isol, uv, ir, pmr, ms*)
Joshi, K.C. *et al., Planta Med.*, 1983, **49**, 127 (*isol, deriv*)

3,5,14-Trihydroxycard-20(22)-enolide T-528



(3α,5β,14β)-*form*

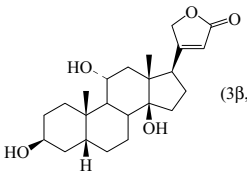
$C_{23}H_{34}O_5$ 390.519

(3β,5β,14β)-*form* [514-39-6] ***Periplogenin***
Cryst. (MeOH aq.). Mp 238° (sinters at 140°). $[\alpha]_D^{31.5}$ +27 (c, 0.667 in $CHCl_3$).
▶ Toxic. LD_{50} (cat) 0.72 mg/kg. FH5387000

*3-O-[β-D-Glucopyranosyl-(1→4)-2,6-dideoxy-β-D-*ribo*-hexopyranoside]:* [210637-17-5] ***Corchorusoside C***
$C_{35}H_{54}O_{13}$ 682.804
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{24}$ +20.6 (c, 0.5 in MeOH) (16.9). λ_{max} 217 (log ε 4.1) (MeOH).

Yoshikawa, M. *et al., Heterocycles*, 1998, **48**, 869-873 (*Corchorusoside C*)
Nakamura, T. *et al., Phytochemistry*, 1998, **49**, 2097-2101 (*Corchorus olitorius saponin*)
Goda, Y. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 1998, **40**, 371-376; *CA*, **131**, 85493j (*Corchorus olitorius constit*)

3,11,14-Trihydroxycard-20(22)-enolide T-529



(3β,5β,11α,14β)-*form*

$C_{23}H_{34}O_5$ 390.519
Cryst. (EtOH). Mp 270°. $[\alpha]_D$ +21.3 (EtOH).

(3β,5β,11α,14β)-*form* [76-28-8]
Sarmentogenin
Prisms or plates (EtOH aq.). Mp 265-267°. $[\alpha]_D^{20}$ +21.5 (EtOH).

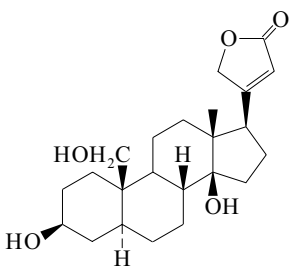
► LD_{50} (cat, ivn) 0.46 mg/kg. FH5389000

3-O-*[β-D-Glucopyranosyl-(1→4)-2,6-dideoxy-β-D*-ribo-*hexopyranoside]:* [210637-16-4] ***Corchorusoside B***
$C_{35}H_{54}O_{13}$ 682.804
Constit. of *Corchorus olitorius* (Jew's mallow). Powder. $[\alpha]_D^{26}$ +12.9 (c, 0.9 in MeOH). λ_{max} 217 (log ε 4.2) (MeOH).

[60344-07-2]

Yoshikawa, M. *et al., Heterocycles*, 1998, **48**, 869-873 (*Corchorusoside B*)

3,14,19-Trihydroxycard-20(22)-enolide T-530



$C_{23}H_{34}O_5$ 390.519
Log P 0.5 (uncertain value) (calc).

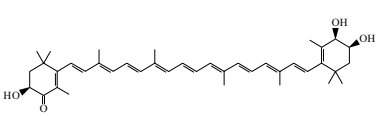
(3β,5β,14β)-*form* [4442-29-9]
Cannogenol. *Erycordigenin*
Amorph. solid.

3-O-*[β-D-Glucopyranosyl-(1→4)-2,6-dideoxy-β-D*-xylo-*hexopyranoside]:* [220710-05-4]
$C_{35}H_{54}O_{13}$ 682.804
Constit. of *Corchorus olitorius* (Jew's mallow). Amorph. powder. $[\alpha]_D^{22}$ -18.3 (c, 0.3 in MeOH).

Nakamura, T. *et al., Phytochemistry*, 1998, **49**, 2097-2101 (*Corchorus olitorius saponin*)

3,3′,4′-Trihydroxy-β,β-caroten-4-one, 9CI T-531

[25510-19-4]

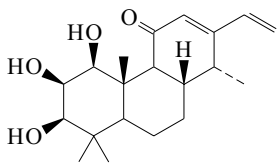


$C_{40}H_{54}O_4$ 598.864

(3*S*,3′*S*,4′*R*)-*form* [97169-13-6]
Idoxanthin
Isol. from Japanese sandfish and marine fish-eggs. Postulated metab. prod. of Astaxanthin, A-474 in mackerel eggs. Cryst. (Me_2CO/hexane). λ_{max} 457 (hexane).

Hodler, M. *et al., Chimia*, 1974, **28**, 723 (*synth*)
Matsuno, T. *et al., Nippon Suisan Gakkaishi*, 1983, **49**, 1475 (*isol*)
Matsuno, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 779; 1995, **111**, 597-605 (*occur, biosynth*)

1,2,3-Trihydroxy-12,15-cassadien-11-one T-532



$C_{20}H_{30}O_4$ 334.455

(1β,2β,3β)-*form* [166547-22-4]
Phytocassane B
Phytoalexin from *Oryza sativa* (rice). Gum. λ_{max} 274 (MeOH) (Berdy).

Koga, J. *et al., Tetrahedron*, 1995, **51**, 7907 (*isol, pmr, cmr*)

2,4,4′-Trihydroxychalcone T-533

3-(2,4-Dihydroxyphenyl)-1-(4-hydroxyphenyl)-2-propen-1-one
$C_{15}H_{12}O_4$ 256.257

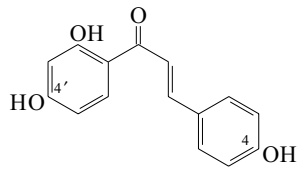
(*E*)-*form*
Constit. of *Glycyrrhiza glabra* (licorice) roots.

2-Me ether: [34221-41-5] *4,4′-Dihydroxy-2-methoxychalcone.* ***Echinatin***†
$C_{16}H_{14}O_4$ 270.284
Yellow needles (EtOH aq.). Mp 209.5-212° dec. A 'retrochalcone' of anomalous subn. pattern λ_{max} 235 (ε 5500); 312 (ε 7400); 367 (ε 12300) (MeOH) (Berdy). λ_{max} 248 (ε 7980); 433 (ε 23500) (MeOH-NaOH) (Berdy).

2,4′-Di-Me ether: [146763-58-8] *4-Hydroxy-2,4′-dimethoxychalcone.* ***Glypallichalcone***
$C_{17}H_{16}O_4$ 284.311
Yellow cryst. Mp 140-142°.

Litvinenko, V.I. *et al., Zh. Obshch. Khim.*, 1963, **33**, 296; *CA*, **59**, 1744b (*isol*)
Furuya, T. *et al., Tet. Lett.*, 1971, 2567 (*isol*)
Saitoh, T. *et al., Tet. Lett.*, 1975, 4463 (*biosynth*)
Shibata, S. *et al., J. Indian Chem. Soc.*, 1978, **55**, 1184 (*isol*)
Ayabe, S.-I. *et al., Phytochemistry*, 1986, **25**, 2803 (*biosynth*)
Cai, L.N. *et al., Yaoxue Xuebao*, 1992, **27**, 748-751 (*Glypallichalcone*)
Nielsen, S.F. *et al., Bioorg. Med. Chem. Lett.*, 1995, **5**, 449 (*Echinatin, synth, activity*)
Barrero, A.F. *et al., J. Nat. Prod.*, 1997, **60**, 65 (*cmr*)

2′,4,4′-Trihydroxychalcone T-534



[961-29-5]
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one. ***Isoliquiritigenin***

$C_{15}H_{12}O_4$ 256.257
Isol. from *Medicago* spp.. Pale yellow needles (EtOAc/petrol or EtOH aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 200-204° (198-200°). Log P 2.25 (calc). λ_{max} 285 ; 328 ; 368 (MeOH) (Berdy). λ_{max} 428 (MeOH-NaOH) (Berdy).

► FL7080000

4-O-*β-D-Glucopyranoside:* [5041-81-6] ***Isoliquiritin***. *Isoliquiritoside*
$C_{21}H_{22}O_9$ 418.399
Isol. from *Glycyrrhiza* spp.. Mp 187-189°. $[\alpha]_D$ -60.8. Log P -0.57 (calc).

4′-O-*β-D-Glucopyranoside:* [59122-93-9] ***Neoisoliquiritin***
$C_{21}H_{22}O_9$ 418.399
Isol. from *Glycyrrhiza glabra* (licorice), *Cicer arietinum* (chickpea) and *Glycine max* (soybean). Yellow needles (EtOH). Mp 230-232°. $[\alpha]_D$ -61.5 (c, 0.5 in EtOH). Log P -0.59 (calc).

4-O-*[α-L-Rhamnopyranosyl-(1→?)-β-D-glucopyranoside]:* [36543-93-8] ***Rhamnoisoliquiritin***
$C_{27}H_{32}O_{13}$ 564.542
Isol. from *Glycyrrhiza glabra* var. *typica* (licorice). Mp 127°.

4-O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [120926-46-7] ***Neolicuroside***
$C_{26}H_{30}O_{13}$ 550.515
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Yellow plates ($CHCl_3$/MeOH). Mp 140°. $[\alpha]_D$ -92.9 (c, 0.6 in EtOH).

4-O-*[4-Hydroxycinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Licorice glycoside B***
$C_{35}H_{36}O_{15}$ 696.66
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. yellow powder. $[\alpha]_D$ -39.8 (c, 1 in MeOH). λ_{max} 206 (log ε 4.61); 228 (log ε 4.42); 318 (log ε 4.59); 359 (log ε 4.45) (MeOH).

4-O-*[4-Hydroxy-3-methoxycinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Licorice glycoside A***
$C_{36}H_{38}O_{16}$ 726.687
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. yellow powder + $2H_2O$. $[\alpha]_D$ -27.4 (c, 1 in MeOH). λ_{max} 205 (log ε 4.59); 219 (sh) (log ε 4.45); 234 (log ε 4.37); 315 (sh) (log ε 4.4); 330 (log ε 4.56); 368 (sh) (log ε 4.4) (MeOH).

2′-Me ether: [51828-10-5] *3-(4-Hydroxyphenyl)-1-(4-hydroxy-2-methoxyphenyl)-2-propen-1-one.* ***4,4′-Dihydroxy-2′-methoxychalcone***
$C_{16}H_{14}O_4$ 270.284
Stress metab. of *Pisum sativum* (pea). Orange cryst. (EtOH aq.). Mp 210-212°.

[2198-19-8, 13745-20-5, 23141-04-0, 27233-96-1, 30925-62-3, 32274-67-2]

Harborne, J. *et al., Phytochemistry*, 1962, **1**, 203 (*glycosides*)
Litvinenko, V.I. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **155**, 600; 1966, **169**, 349 (*Neoisoliquiritin, Licuroside*)
Wong, E. *et al., Phytochemistry*, 1966, **5**, 463; 1968, **7**, 2123; 2131; 2139 (*Isoliquiritin*)
Van Hulle, C. *et al., Planta Med.*, 1971, **20**, 278 (*Rhamnoisoliquiritin*)
Namikoshi, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3568 (*4,4′-Dihydroxy-2′-methoxychalcone*)
Miething, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1989, **322**, 141 (*Neolicuroside*)
Hatano, T. *et al., Phytochemistry*, 1998, **47**, 287-293 (*Licorice glycosides*)

2′,4′,6′-Trihydroxychalcone T-535

[4197-97-1]
3-Phenyl-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one. Pinocembrin chalcone

$C_{15}H_{12}O_4$ 256.257
Yellow needles (C_6H_6). Mp 176-178°.

2′-Me ether: [19309-14-9] *2′,4′-Dihydroxy-6′-methoxychalcone.* ***Cardamonin****. Alpinetin chalcone*
$C_{16}H_{14}O_4$ 270.284
Yellow needles ($CHCl_3$/hexane). Mp 199-200°. λ_{max} 349 (ϵ 21000) (EtOH) (Derep).

4′-Me ether: [18956-15-5] *2′,6′-Dihydroxy-4′-methoxychalcone.* ***Pinostrobin chalcone***
$C_{16}H_{14}O_4$ 270.284
Isol. from *Cajanus cajan* (pigeon pea). Orange needles ($CHCl_3$/hexane). Mp 163.5-164.5°.

2′,4′-Di-Me ether: [1775-97-9] *2′-Hydroxy-4′,6′-dimethoxychalcone.* ***Flavokawain B***
$C_{17}H_{16}O_4$ 284.311
Found in kava (*Piper methysticum*), FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Cryst. (MeOH aq.). Mp 91°.

Tri-Me ether: [1159-58-6] *2′,4′,6′-Trimethoxychalcone*
$C_{18}H_{18}O_4$ 298.338
Yellow needles. Mp 82-84°.

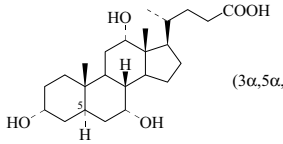
4′-O-(3-Methyl-2-butenyl): [83905-72-0] ***2′,6-Dihydroxy-4′-prenyloxychalcone***
$C_{20}H_{20}O_4$ 324.376
Yellow gum.

2′-Me ether, 4′-O-(3-methyl-2-butenyl): [96386-70-8] ***2′-Hydroxy-6′-methoxy-4′-prenyloxychalcone***
$C_{21}H_{22}O_4$ 338.402
Yellow oil.

[18956-16-6, 82451-30-7]

Nilsson, M. *et al., Acta Chem. Scand.*, 1961, **15**, 211 (*isol*)
Haensel, R. *et al., Z. Naturforsch., B*, 1963, **18**, 370 (*Flavokawain B*)
Kimura, Y. *et al., Yakugaku Zasshi*, 1968, **88**, 239 (*isol*)
Hayashi, N. *et al., Chem. Ind. (London)*, 1969, 1779 (*isol*)
Onodera, J. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 240 (*synth*)
Jaipetch, T. *et al., Aust. J. Chem.*, 1982, **35**, 351 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1982, **21**, 1434; 1984, **23**, 1338 (*isol*)
Wollenweber, E. *et al., Phytochemistry*, 1982, **21**, 1462 (*isol*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 271 (*isol*)
Singh, A.K. *et al., Tet. Lett.*, 1985, **26**, 4125 (*synth*)
Jakupovic, J. *et al., Phytochemistry*, 1986, **25**, 1133 (*isol*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988, 330 (*occur*)
Bremner, P.D. *et al., Planta Med.*, 1998, **64**, 777 (*isol, cmr, nmr, activity*)

3,7,12-Trihydroxycholan-24-oic acid T-536



(3α,5α,7α,12α)-*form*

$C_{24}H_{40}O_5$ 408.577

(3α,5α,7α,12α)-*form* [2464-18-8]
Allocholic acid
Isol. from many animal sources. Bile acid in sturgeon (*Acipenser sturio*). Cryst. (Me_2CO aq.). Mp 250-251°. $[\alpha]_D^{25}$ +27.8 (c, 0.75 in MeOH).

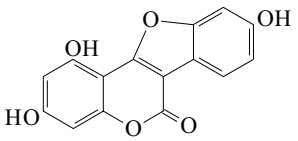
(3α,5β,7α,12α)-*form* [81-25-4]
Cholic acid*. Cholalic acid. Cholagit. Colalin. Hypocholate. NSC 6135*
Emulsifying agent in foods. Cryst. + 1 H_2O (H_2O or Et_2O aq.). Cryst. + 1EtOH (EtOH). Mp 197° (anhyd.). $[\alpha]_D^{20}$ +37 (EtOH). pK_{a1} 4.98 (20°). Log P 2.39 (uncertain value) (calc).
► LD_{50} (mus, orl) 4950 mg/kg. FZ9350000

[361-09-1, 71781-34-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1057C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 594B (*nmr*)
Anderson, I.G. *et al., Biochem. J.*, 1957, **67**, 323-328; 1962, **85**, 236-242 (*isol, 3α,5β,7α,12α-form, 3α,5α,7α,12α-form, synth, bibl*)
Eneroch, P. *et al., J. Lipid Res.*, 1966, **7**, 524-530 (*ms*)
Mitra, M.N. *et al., J.O.C.*, 1968, **33**, 175-181 (*3α,5α,7α,12α-form, 3α,5β,7α,12α-form, synth*)
Leibfritz, D. *et al., J.A.C.S.*, 1973, **95**, 4996-5003 (*cmr*)
Percy-Robb, I.W. *et al., Scott. Med. J.*, 1973, **18**, 166 (*biosynth, rev*)
Paternostre, M.T. *et al., Biochemistry*, 1988, **27**, 2668-2677 (*use*)
Kirk, D.N. *et al., J.C.S. Perkin 2*, 1990, 1567-1594 (*pmr*)
Iida, T. *et al., Chem. Pharm. Bull.*, 1993, **41**, 763-765 (*3α,5α,7α,12α-form, synth, pmr*)
Wahle, M.-C. *et al., Acta Cryst. C*, 1996, **52**, 325-328; 2500-2502 (*3α,5β,7α,12α-form, cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 581-582

1,3,9-Trihydroxycoumestan T-537

[88478-03-9]
*1,3,9-Trihydroxy-6*H*-benzofuro[3,2-*c*]benzopyran-6-one, 9CI.* ***Aureol***†



$C_{15}H_8O_6$ 284.225
Isol. from *Phaseolus aureus* (mung bean) and other *Phaseolus* spp.. No phys. props. reported. Sol. MeOH. λ_{max} 212 ; 257 ; 337 (EtOH) (Berdy). λ_{max} 220 ; 272 ; 305 ; 362 (EtOH-NaOH) (Berdy).

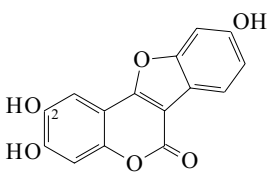
1-Me ether:3,9-Dihydroxy-1-methoxycoumestan. ***Isotrifoliol***
$C_{16}H_{10}O_6$ 298.251
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow needles. Mp >300° λ_{max} 208 (log ϵ 4.42); 227 (sh) ; 249 (log ϵ 4.18); 348 (log ϵ 4.24); 361 (sh) (EtOH).

[88478-00-6]

O'Neill, M.J. *et al., Z. Naturforsch., C*, 1983, **38**, 698 (*isol*)
O'Neill, M.J. *et al., Phytochemistry*, 1984, **23**, 2704 (*isol*)
Adesanya, S.A. *et al., Z. Naturforsch., C*, 1984, **39**, 888 (*isol*)
Hatano, T. *et al., Phytochemistry*, 2000, **55**, 959-963 (*Isotrifoliol*)

2,3,9-Trihydroxycoumestan T-538

[15402-22-9]
*2,3,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 9CI. 6,7,12-Trihydroxycoumestan.* ***Lucernol***



$C_{15}H_8O_6$ 284.225
Constit. of alfalfa (*Medicago sativa*). Cryst. (DMSO). Mp 350°. λ_{max} 232 ; 310 ; 355 ; 372 (sh) (no solvent reported).

2-Me ether: [114216-99-8] *3,9-Dihydroxy-2-methoxycoumestan.* ***2-O-Methyllucernol***
$C_{16}H_{10}O_6$ 298.251
Needles (C_6H_6/EtOAc). Mp 318-320°.

9-Me ether:2,3-Dihydroxy-9-methoxycoumestan. ***Melimessanol A***
$C_{16}H_{10}O_6$ 298.251
Amorph. solid. λ_{max} 230 ; 314 ; 353 ; 366 (sh) (MeOH).

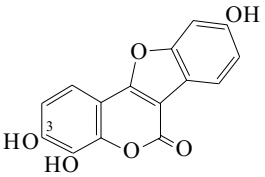
Tri-Me ether:
Cryst. (MeOH). Mp 255°.

Spencer, R.R. *et al., J. Agric. Food Chem.*, 1966, **14**, 162 (*isol, struct*)
Kalna, V.K. *et al., Tet. Lett.*, 1967, 2153 (*synth*)
Rajani, P. *et al., Phytochemistry*, 1988, **27**, 648 (*2-O-Methyllucernol*)
Macias, F.A. *et al., Phytochemistry*, 1999, **50**, 35-46 (*Melimessanol A*)

3,4,9-Trihydroxycoumestan T-539

[7204-24-2]
*3,4,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 9CI. 4-Hydroxy-*

coumestrol



$C_{15}H_8O_6$ 284.225
Green prisms ($CHCl_3$). Mp 287°.

3-Me ether: [7331-58-0] *4,9-Dihydroxy-3-methoxycoumestan*. ***Sativol***. *8,12-Dihydroxy-7-methoxycoumestan*
$C_{16}H_{10}O_6$ 298.251
Constit. of alfalfa (*Medicago sativa*). Cryst. (MeOH). Mp 303° dec.

3-Me ether, di-Ac:
Cryst. (Me_2CO). Mp 256-257°.

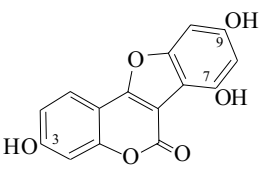
4,9-Di-Me ether:3-Hydroxy-4,9-dimethoxycoumestan
$C_{17}H_{12}O_6$ 312.278
Yellowish cryst. Mp 265-266°. λ_{max} 247 ; 305 (sh) ; 348 (MeOH).

Tri-Me ether:
Needles (MeOH). Mp 209-210°.

Spencer, R.R. *et al., J. Agric. Food Chem.*, 1966, **14**, 162 (*uv*)
Kalra, V.K. *et al., Tet. Lett.*, 1967, 2153 (*synth*)
Chatterjea, J.N. *et al., J. Indian Chem. Soc.*, 1970, **47**, 541 (*synth*)
Nkengfack, A.E. *et al., Phytochemistry*, 1994, **35**, 521 (*isol, pmr, cmr*)
Abdel-Kader, M.S. *et al., Planta Med.*, 2001, **67**, 388-390 (*3-Hydroxy-4,9-dimethoxycoumestan*)

3,7,9-Trihydroxycoumestan T-540

[33280-69-2]
*3,7,9-Trihydroxy-6*H*-benzofuro[3,2-c][1]benzopyran-6-one, 9CI. 7,10,12-Trihydroxycoumestan*. ***Repensol***



$C_{15}H_8O_6$ 284.225
Isol. from fungus-infected *Trifolium repens* (white clover) leaves. Cream needles (MeOH) (synthetic). Mp 346-348°.

9-Me ether: [1857-26-7] *3,7-Dihydroxy-9-methoxycoumestan*. ***Trifoliol***. *7,10-Dihydroxy-12-methoxycoumestan*
$C_{16}H_{10}O_6$ 298.251
Isol. from *Medicago sativa* (alfalfa) infected with leafspot (*Ascochyta imperfecta*) and *Trifolium repens* (white clover). Rods (DMF). Mp 332° dec.

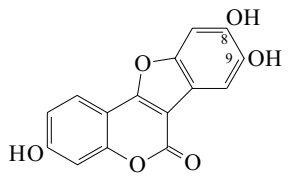
7,9-Di-Me ether: [77331-73-8] *3-Hydroxy-7,9-dimethoxycoumestan*. ***Wairol***. *7-Hydroxy-10,12-dimethoxycoumestan*
$C_{17}H_{12}O_6$ 312.278
Isol. from *Medicago sativa* (alfalfa) infected with leafspot (*Ascochyta imperfecta*). Plates. Mp 292-294°.

Tri-Me ether: [77390-40-0]
Cryst. (DMF). Mp 255-258°.

Bickoff, E.M. *et al., J. Pharm. Sci.*, 1964, **53**, 1496 (*isol*)
Livingston, A.L. *et al., Tetrahedron*, 1964, **20**, 1963 (*isol, struct, uv, synth*)
Wong, E. *et al., Phytochemistry*, 1971, **10**, 466 (*Repensol*)
Shaw, G.J. *et al., Phytochemistry*, 1980, **19**, 2801; 1982, **21**, 249 (*isol, synth*)

3,8,9-Trihydroxycoumestan T-541

[1983-80-8]
*3,8,9-Trihydroxy-6*H*-benzofuro[3,2-c][1]benzopyran-6-one, 9CI. 7,11,12-Trihydroxycoumestan, 8CI. 11-Hydroxycoumestrol*



$C_{15}H_8O_6$ 284.225
Cryst. (Me_2CO). Mp 300°.

Tri-Ac: [2074-56-8] *7,11,12-Triacetoxycoumestan. Stimol 410*
$C_{21}H_{14}O_9$ 410.336
Animal growth stimulant. Needles. Mp 255-257°.

9-Me ether:3,8-Dihydroxy-9-methoxycoumestan. 3′-Methoxycoumestrol (obsol.)
$C_{16}H_{10}O_6$ 298.251
Isol. from alfalfa (*Medicago sativa*). Straw-coloured cryst. (Me_2CO). Mp 329-329.5° dec.

9-Me ether, di-Ac:
Needles. Mp 282-283°.

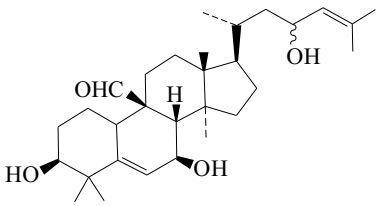
8,9-Di-Me ether: [5252-40-4] *3-Hydroxy-8,9-dimethoxycoumestan. 7-Hydroxy-11,12-dimethoxycoumestan (obsol.)*
$C_{17}H_{12}O_6$ 312.278
Isol. from *Medicago sativa* (alfalfa) and *Myroxylon balsamum* (Tolu balsam). Cryst. (EtOAc). Mp 306°.

8,9-Methylene ether: Medicagol, M-86

Tri-Me ether:3,8,9-Trimethoxycoumestan
$C_{18}H_{14}O_6$ 326.305
Prisms (C_6H_6/petrol). Mp 196-198°.

Livingston, A.L. *et al., J.O.C.*, 1965, **30**, 2353 (*isol, synth, uv, pmr*)
Bickoff, E.M. *et al., J.O.C.*, 1966, **31**, 988 (*isol*)
Spencer, R.R. *et al., J.O.C.*, 1966, **31**, 988 (*isol, synth*)
Malleshwar, D. *et al., Curr. Sci.*, 1969, **38**, 13 (*synth*)
Chatterjea, J.N. *et al., J. Indian Chem. Soc.*, 1970, **47**, 541 (*synth*)
Fukui, K. *et al., Experientia*, 1971, **27**, 361 (*synth*)
Takai, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 2488 (*isol, uv, ir, pmr*)
Simonova, L.L. *et al., Khim. Prir. Soedin.*, 1972, **8**, 436; *Chem. Nat. Compd. (Engl. Transl.)*, 435 (*pmr*)
Donnelly, D.M.X. *et al., J.C.S. Perkin 1*, 1973, **16**, 1737 (*isol, ms*)
Tabakovic, I. *et al., J. Het. Chem.*, 1983, **20**, 635 (*synth*)

3,7,23-Trihydroxycucurbita-5,24-dien-19-al T-542



$C_{30}H_{48}O_4$ 472.707

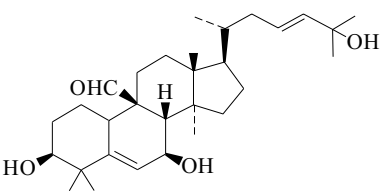
(3β,7β,23ξ)-*form* [91590-76-0]
Momordicin I
Constit. of leaves and vines of *Momordica charantia* (bitter melon). Cryst. ($CHCl_3$). Mp 125-128°. $[\alpha]_D$ +81.3.

23-O-*β*-D-*Glucopyranoside:* [91590-75-9]
Momordicin II
$C_{36}H_{58}O_9$ 634.849
Constit. of *Momordica charantia* (bitter melon). Powder.

Yasuda, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2044

3,7,25-Trihydroxycucurbita-5,23-dien-19-al T-543

19-Oxocucurbita-5,23-diene-3,7,25-triol. 3,7,25-Trihydroxy-19-norlanosta-5,23-diene-9-carboxaldehyde



$C_{30}H_{48}O_4$ 472.707

(3β,7β,23*E*)-*form*
Cryst. Mp 190-193°.

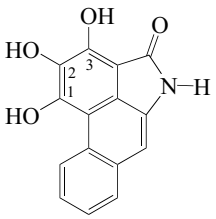
7-O-*β*-D-*Glucopyranoside:* [81348-83-6]
Momordicoside L
$C_{36}H_{58}O_9$ 634.849
Constit. of *Momordica charantia* (bitter melon). Cryst. Mp 227-232°. $[\alpha]_D$ +57.3.

7-O-*β*-D-*Glucopyranoside, 25*-O-*Me:* [81348-84-7] ***Momordicoside K***
$C_{37}H_{60}O_9$ 648.876
Constit. of *Momordica charantia* (bitter melon). Cryst. Mp 236-237°. $[\alpha]_D$ +63.3.

25-Me ether:
$C_{31}H_{50}O_4$ 486.734
Constit. of *Momordica charantia* (bitter melon). Amorph. powder. $[\alpha]_D^{26}$ +48.9 (c, 0.45 in MeOH).

Okabe, H. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4334 (*Momordicoside L*)
Okabe, H. *et al., Tet. Lett.*, 1982, **23**, 77
Fatope, M.O. *et al., J. Nat. Prod.*, 1990, **53**, 1491 (*isol, pmr, cmr*)

1,2,3-Trihydroxydibenz[*cd,f*]indol-4(5*H*)-one, 9CI T-544



$C_{15}H_9NO_4$ 267.24

CAS numbering shown. Alternative (phenanthrene) numbering frequently encountered, in which 1,2,3 are 4,3,2- respectively.

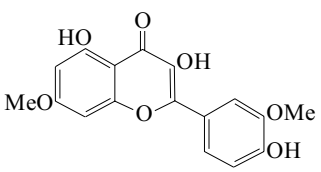
2,3-Di-Me ether: [116084-93-6] *1-Hydroxy-2,3-dimethoxydibenz[*cd,f*]indol-4(5*H*)-one, 9CI. 10-Amino-2,3-dimethoxy-4-hydroxyphenanthrene-1-carboxylic acid lactam.* ***Piperolactam D***
$C_{17}H_{13}NO_4$ 295.294
Alkaloid from the roots of *Piper longum* (long pepper),. Greenish-yellow cryst. (MeOH). Mp 222-224°. This struct. was originally assigned to Piperolactam B by Desai *et al* (1988).

Tri-Me ether: [116064-76-7] *1,2,3-Trimethoxydibenz[*cd,f*]indol-4(5*H*)-one, 9CI.* ***Piperolactam C***
$C_{18}H_{15}NO_4$ 309.321
Alkaloid from the whole plants of *Piper longum* (long pepper),. Yellow cryst. (C_6H_6/MeOH). Mp 187-188°.

Villar, A. *et al., Planta Med.*, 1986, **52**, 556-557 (*activity*)
Desai, S.J. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 775 (*Piperolactam C*)
Olsen, C.E. *et al., Phytochemistry*, 1993, **33**, 518-520 (*Piperolactam B, Piperolactam D*)
Chia, Y.-C. *et al., J. Nat. Prod.*, 2000, **63**, 1160-1163 (*isol, activity*)

3,4′,5-Trihydroxy-3′,7-dimethoxyflavone T-545

[552-54-5]
*3,5-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-4*H*-1-benzopyran-4-one, 9CI. 4′,5-Dihydroxy-3′,7-dimethoxyflavonol.* ***Rhamnazin****. Quercetin 3′,7-dimethyl ether*



$C_{17}H_{14}O_7$ 330.293
Pale yellow needles (toluene). Mp 216-218°. λ_{max} 350 ; 396 (EtOH) (Berdy).

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [64527-08-8] ***Polygalacin****. Rhamnazin 3-rutinoside*
$C_{29}H_{34}O_{16}$ 638.578
Isol. from *Cucurbita pepo*. Cryst. (MeOH). Mp 157-158°. $[\alpha]_D^{35}$ -3.4 (c, 0.12 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [259234-18-9] *Rhamnazin 3-sophoroside*
$C_{29}H_{34}O_{17}$ 654.577
Constit. of *Nasturtium officinale* (water cress). Pale yellow oil. λ_{max} 254 ; 351 (MeOH).

Itokawa, H. *et al., Phytochemistry*, 1981, **20**, 2421 (*3-rutinoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Goda, Y. *et al., Biol. Pharm. Bull.*, 1999, **22**, 1319-1326 (*Alboside, 3-sophoroside*)

3′,4′,7-Trihydroxy-3,5-dimethoxyflavone T-546

[1486-66-4]
*2-(3,4-Dihydroxyphenyl)-7-hydroxy-3,5-dimethoxy-4*H*-1-benzopyran-4-one, 9CI.* ***Caryatin***

$C_{17}H_{14}O_7$ 330.293
Isol. from pecan nuts *Carya pecan*. Cryst. (MeOH). Mp 299-301°.

3′ or 4′-β-D-Glucopyranoside: [63713-69-9] ***Caryatin glucoside***
$C_{23}H_{24}O_{12}$ 492.435
Isol. from pecan nuts *Carya pecan*.

7-O-β-D-Glucopyranoside: [151590-52-2] *Caryatin 7-glucoside*
$C_{23}H_{24}O_{12}$ 492.435
Amorph. powder. Mp 287-291°. $[\alpha]_D$ -16.7 (c, 0.12 in MeOH).

Sasaki, T. *et al., Yakugaku Zasshi*, 1964, **84**, 47; 195 (*isol, synth*)
El-Ansari, M.A. *et al., Bull. Soc. Chim. Fr.*, 1965, 779 (*synth*)
Harborne, J.B. *et al., Phytochemistry*, 1971, **10**, 2727 (*isol*)
El-Ansari, M.A. *et al., Z. Naturforsch., C*, 1977, **32**, 444 (*glucoside*)
Sepulveda-Boza, S. *et al., Phytochemistry*, 1993, **32**, 1301 (*Caryatin 7-glucoside*)

3,5,7-Trihydroxy-3′,4′-dimethoxyflavone T-547

[3306-29-4]
*2-(3,4-Dimethoxyphenyl)-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, 9CI. 5,7-Dihydroxy-3′,4′-dimethoxyflavonol.* ***Dillenetin****. 3′,4′-Di-O-methylquercetin*

$C_{17}H_{14}O_7$ 330.293
Isol. from *Dillenia indica* (elephant apple). Bright yellow cryst. (EtOH aq.). Mp 291-292°.

Pavanasasivam, G. *et al., J.C.S. Perkin 1*, 1975, 612 (*isol, struct*)
Merfort, I. *et al., Planta Med.*, 1985, 136 (*isol*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1986, **41**, 87 (*isol*)

3,5,7-Trihydroxy-4′,8-dimethoxyflavone T-548

[3443-28-5]
*3,5,7-Trihydroxy-8-methoxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one. 5,7-Dihydroxy-4′,8-dimethoxyflavonol.* ***Prudomestin***

$C_{17}H_{14}O_7$ 330.293
Isol. from heartwood of *Prunus domestica* (plum). Yellow needles ($CHCl_3$/petrol). Mp 209-210°.

3-O-β-D-Glucopyranoside: [226952-40-5] *Prudomestin 3-glucoside*
$C_{23}H_{24}O_{12}$ 492.435

7-O-β-D-Glucopyranside: [24568-40-9] *Prudomestin 7-glucoside.* ***Prudomenin***
$C_{23}H_{24}O_{12}$ 492.435

Nagajaran, M. *et al., Phytochemistry*, 1964, **3**, 477 (*isol*)
Krishnamurti, M. *et al., Tetrahedron*, 1966, **22**, 941 (*synth*)
Hasegawa, M. *et al., Shokubutsugaku Zasshi*, 1969, **82**, 148; *CA*, **71**, 67949x (*Prudomenin*)
Goudard, M. *et al., C. R. Hebd. Seances Acad. Sci.*, 1976, **282**, 683 (*synth*)
Goudard, M. *et al., Phytochemistry*, 1978, **17**, 145 (*ms*)
Wollenweber, E. *et al., Phytochemistry*, 1985, **24**, 965 (*isol*)
Parmar, R.K. *et al., Acta Cryst. C*, 1992, **48**, 1090 (*cryst struct*)
Wang, J.-R. *et al., Zhiwu Xuebao*, 1999, **41**, 209-212; *CA*, **131**, 29827j (*3-glucoside*)

4′,5,7-Trihydroxy-3′,5′-dimethoxyflavone T-549

[520-32-1]
*5,7-Dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. Tricetin 3′,5′-dimethyl ether.* ***Tricin****. Phelipeone. Phoelipeone*

$C_{17}H_{14}O_7$ 330.293
Yellow needles (AcOH aq.). Mp 291-292°. Log P 0.6 (calc).

7-O-β-L-Arabinopyranoside: [126394-59-0] ***Setaricin****. Tricin arabinoside*
$C_{22}H_{22}O_{11}$ 462.409
Constit. of the leaves of *Setaria italica* (foxtail millet). Shining yellow needles (MeOH). Mp 300°. Incorrect anomer given in CA.

7-O-β-D-Glucopyranoside: [32769-01-0] ***Glucotricin****. Tricin 7-glucoside*
$C_{23}H_{24}O_{12}$ 492.435
Isol. from rice leaves (*Oryza sativa*). Light yellow powder (butanol/Et_2O); cryst. + $2H_2O$ (MeOH aq.). Mp 260.5-261° (dihydrate) Mp 240-241° (anhyd.).

5,7-Di-O-β-D-glucopyranoside: [74336-88-2] *Tricin 5,7-diglucoside*
$C_{29}H_{34}O_{17}$ 654.577

7-O-(O-Sulfo-β-D-glucopyranoside):
$C_{23}H_{24}O_{15}S$ 572.5
Isol. from sugar cane leaves (*Saccharum officinarum*).

7-O-β-D-Glucuronopyranoside: [32769-02-1] *Tricin 7-glucuronoside*
$C_{23}H_{22}O_{13}$ 506.419
Isol. from alfalfa (*Medicago sativa*).

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [53766-40-8] *Tricin 7-neohesperidoside*
$C_{29}H_{34}O_{16}$ 638.578
Isol. from sugar cane leaves (*Saccharum officinarum*).

7-O-[α-L-Rhamnopyranosyl-(1→?)-β-D-glucopyranoside]:
$C_{29}H_{34}O_{16}$ 638.578
From leaves of *Oryza sativa* (rice). Yellow powder.

7-O-[α-L-Rhamnopyranosyl-(1→2)-α-D-galacturonopyranoside]: [89915-54-8]
$C_{29}H_{32}O_{17}$ 652.562

Isol. from sugar cane mill syrup (*Saccharum* spp.).

5-O-*[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:Tricin 5-(glucosylglucoside)*
$C_{29}H_{34}O_{17}$ 654.577
Isol. from *Triticum dicoccum* (emmer).

7-O-*[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]:* [50867-30-6] *Tricin 7-diglucoside*
$C_{29}H_{34}O_{17}$ 654.577
Isol. from sugar cane leaves (*Saccharum officinarum*).

7-O-*[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [83097-44-3] *Tricin 7-diglucuronoside*
$C_{29}H_{30}O_{19}$ 682.545
Isol. from alfalfa (*Medicago sativa*).

7-O-*[4-Hydroxy*-E-*cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{38}H_{36}O_{21}$ 828.69
Constit. of the aerial parts of alfalfa (*Medicago sativa*). Amorph. yellow powder. Mp 232-233°. $[\alpha]_D^{24}$ -14.7 (c, 0.1 in MeOH/DMSO aq.). λ_{max} 223 (sh) ; 271 ; 323 (MeOH).

7-O-*[4-Hydroxy-3-methoxy*-E-*cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{39}H_{38}O_{22}$ 858.716
Constit. of the aerial parts of alfalfa (*Medicago sativa*). Amorph. yellow powder. Mp 307-308° dec. $[\alpha]_D^{24}$ -70.2 (c, 0.1 in MeOH/DMSO aq.). λ_{max} 247 (sh) ; 269 (sh) ; 338 (MeOH).

7-O-*[4-Hydroxy-3,5-dimethoxy*-E-*cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{40}H_{40}O_{23}$ 888.742
Constit. of the aerial parts of alfalfa (*Medicago sativa*). Amorph. yellow powder. Mp 227-228°. $[\alpha]_D^{24}$ -61.6 (c, 0.1 in MeOH/DMSO aq.). λ_{max} 223 (sh) ; 247 (sh) ; 269 (sh) ; 342 (MeOH).

7-O-*[β-D-Glucuronopyranosyl-(1→?)-β-D-glucuronopyranosyl-(1→?)-β-D-glucuronopyranoside]:* [83097-23-8] *Tricin 7-triglucuronoside*
$C_{35}H_{38}O_{25}$ 858.67
Isol. from alfalfa (*Medicago sativa*).

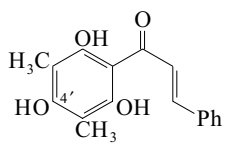
7-O-*[4-Hydroxy-3-methoxy*-E-*cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-[β-D-glucuronopyranosyl-(1→3)]-β-D-glucuronopyranoside]:*
$C_{45}H_{46}O_{28}$ 1034.842
Constit. of the aerial parts of alfalfa (*Medicago sativa*). Amorph. yellow powder. Mp 199-200°. $[\alpha]_D^{24}$ -35.3 (c, 0.1 in MeOH/DMSO aq.). λ_{max} 247 (sh) ; 269 (sh) ; 338 (MeOH).

[50816-55-2]

Gulati, K.L. *et al., J.C.S.*, 1933, 942; 1644 (*synth*)
Minamikawa, T. *et al., Agric. Biol. Chem.*, 1965, **29**, 428 (*Glucotricin*)
Owada, E. *et al., Nippon Kagaku Zasshi*, 1970, **91**, 1002; *CA*, **74**, 76265 (*synth*)
Kaneta, M. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 528 (*isol*)
Williams, C.A. *et al., Phytochemistry*, 1973, **12**, 2417 (*occur*)
Williams, C.A. *et al., Phytochemistry*, 1974, **13**, 1141 (*7-neohesperidoside*)
Desai, H.K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 473 (*isol*)
Bhattacharyya, J. *et al., J. Pharm. Sci.*, 1978, **67**, 1325 (*isol, cmr*)
Saleh, N.A.M. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 33 (*7-triglucuronoside*)
Liu, Y.-L. *et al., Phytochemistry*, 1982, **21**, 209 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Mabry, T.J. *et al., J. Nat. Prod.*, 1984, **47**, 127 (*7-rhamnosylgalacturonoside*)
Harborne, J.B. *et al., Phytochemistry*, 1985, **24**, 751 (*isol*)
Rofi, R.D. *et al., Phytochemistry*, 1985, **24**, 2131 (*isol*)
Hirai, Y. *et al., Chem. Pharm. Bull.*, 1986, **34**, 82 (*deriv*)
Jain, N. *et al., Chem. Ind. (London)*, 1989, 422 (*Setaricin*)
Rettig, J.H. *et al., Biochem. Syst. Ecol.*, 1990, **18**, 393 (*7-glucoside*)
Nagarathnam, D. *et al., J.O.C.*, 1991, **56**, 4884 (*synth*)
Adjei-Afriyie, F. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 443-446 (*5-glucoside*)
Stochmal, A. *et al., J. Agric. Food Chem.*, 2001, **49**, 5310-5314 (*Medicago sativa glucuronides*)

2′,4′,6′-Trihydroxy-3′,5′-dimethylchalcone T-550

3-Phenyl-1-(2,4,6-trihydroxy-3,5-dimethylphenyl)-2-propen-1-one



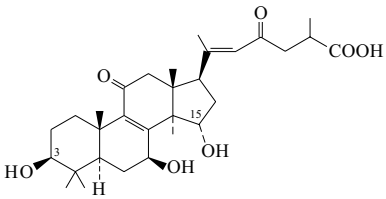
$C_{17}H_{16}O_4$ 284.311

2′-Me ether: [65349-31-7] *1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-2-propen-1-one, 9CI. 2′,4′-Dihydroxy-6′-methoxy-3′,5′-dimethylchalcone*
$C_{18}H_{18}O_4$ 298.338
Isol. from *Myrica gale* (bog myrtle). Yellow needles (MeOH). Mp 125-126°. λ_{max} 212 (ϵ 22907); 336 (ϵ 16596) (MeOH) (Berdy).

4′-Me ether:1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-3-phenyl-2-propen-1-one, 9CI. 2′,6′-Dihydroxy-4-methoxy-3′,5′-dimethylchalcone
$C_{18}H_{18}O_4$ 298.338

Malterud, K.E. *et al., Phytochemistry*, 1977, **16**, 1805
Wollenweber, E. *et al., J. Plant Physiol.*, 1985, **117**, 423
Zhang, F. *et al., Zhiwu Xuebao*, 1990, **32**, 469
Srivastava, R. *et al., Phytochemistry*, 1995, **38**, 687 (*isol, cmr*)

3,7,15-Trihydroxy-11,23-dioxolanosta-8,20(22)-dien-26-oic acid T-551



$C_{30}H_{44}O_7$ 516.673

(3β,7β,15α,20(22)*E*)-*form* [100665-42-7] ***Ganoderenic acid C***
Constit. of fungus *Ganoderma lucidum* (reishi). Amorph. powder. $[\alpha]_D^{22}$ +66.2 (c, 0.15 in $CHCl_3$/MeOH).

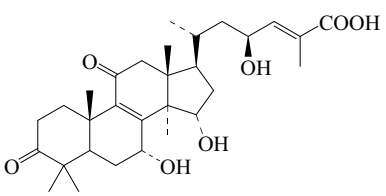
3-Ketone: [100665-40-5] *7β,15α-Dihydroxy-3,11,23-trioxolanosta-8,20(22)*E*-dien-26-oic acid.* ***Ganoderenic acid A***
$C_{30}H_{42}O_7$ 514.658
Constit. of *Ganoderma lucidum* (reishi). Amorph. powder. $[\alpha]_D^{22}$ +127.8 (c, 0.43 in $CHCl_3$).

15-Ketone: [100665-41-6] *3β,7β-Dihydroxy-11,15,23-trioxolanosta-8,20(22)*E*-dien-26-oic acid.* ***Ganoderenic acid B***
$C_{30}H_{42}O_7$ 514.658
Constit. of *Ganoderma lucidum* (reishi). Plates (EtOAc/MeOH). Mp 211-214°. $[\alpha]_D^{22}$ +102.9 (c, 0.30 in $CHCl_3$).

3,15-Diketone: [100665-43-8] *7β-Hydroxy-3,11,15,23-tetraoxolanosta-8,20(22)-dien-26-oic acid.* ***Ganoderenic acid D***
$C_{30}H_{40}O_7$ 512.642
Constit. of *Ganoderma lucidum* (reishi). Needles (EtOH aq.). Mp 214-216°. $[\alpha]_D^{22}$ +163.4 (c, 0.34 in $CHCl_3$).

Komoda, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4829

7,15,23-Trihydroxy-3,11-dioxolanosta-8,24-dien-26-oic acid T-552



(7α,15α,23*S*,24*E*)-*form*

$C_{30}H_{44}O_7$ 516.673

(7α,15α,23*S*,24*E*)-*form* [294674-02-5] ***Ganoderic acid δ***
Constit. of *Ganoderma lucidum* (reishi). Amorph. powder. $[\alpha]_D$ +160 (c, 0.074 in EtOH). λ_{max} 207 (log ϵ 3.95); 252 (log ϵ 3.7) (no solvent reported).

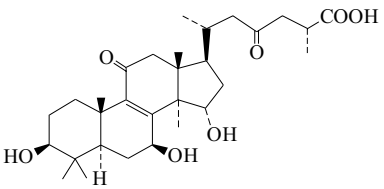
(7β,15α,23*S*,24*E*)-*form* [294674-00-3] ***Ganoderic acid γ***
Constit. of *Ganoderma lucidum* (reishi). Needles (MeOH aq.). Mp 243-245°. $[\alpha]_D$ +155.3 (c, 0.1 in EtOH). λ_{max} 208 (log ϵ 4.05); 252 (log ϵ 3.82) (no solvent reported).

15-Ketone, 3β-alcohol: [294674-05-8] *3,7,23-Trihydroxy-11,15-dioxolanosta-8,24-dien-26-oic acid.* ***Ganoderic acid ϵ***
$C_{30}H_{44}O_7$ 516.673
Constit. of *Ganoderma lucidum* (reishi). Needles (MeOH aq.). Mp 249-251°. $[\alpha]_D$ +153.3 (c, 0.1 in MeOH). λ_{max} 212 (log ϵ 4.13); 253 (log ϵ 4.03) (no solvent reported).

7,15-Diketone, 3β-alcohol: [294674-09-2] *3,23-Dihydroxy-7,11,15-trioxolanosta-8,24-dien-26-oic acid.* ***Ganoderic acid ξ***
$C_{30}H_{42}O_7$ 514.658
Constit. of *Ganoderma lucidum* (reishi). Needles (MeOH aq.). Mp 143-145°. $[\alpha]_D$ +213.5 (c, 0.015 in EtOH). λ_{max} 210 (log ϵ 4.13); 257 (log ϵ 3.81) (no solvent reported).

Min, B.-S. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1026-1033 (*isol, pmr, cmr*)

3,7,15-Trihydroxy-11,23-dioxolanost-8-en-26-oic acid T-553



$C_{30}H_{46}O_7$ 518.689
See note under 3,22-Dihydroxylanosta-7,9(11),24-trien-26-oic acid, D-525.

(3β,7β,15α,25*R*)-*form* [98296-48-1]
Ganoderic acid C†. *Ganoderic acid D*†. *Ganoderic acid E*†. *Ganoderic acid C2*
Constit. of *Ganoderma lucidum* (reishi). Cryst. (MeOH). Mp 231-232° (198-199.5°). $[\alpha]_D^{15}$ +95.5 (c, 0.147 in MeOH).

Me ester:
Prisms. Mp 199-202°. $[\alpha]_D$ +98 ($CHCl_3$).

3,15-Diketone: [95311-97-0] *7-Hydroxy-3,11,15,23-tetraoxolanost-8-en-26-oic acid.* ***Ganoderic acid C1***. *Ganoderic acid D*†
$C_{30}H_{42}O_7$ 514.658
Constit. of *Ganoderma lucidum* (reishi). Cryst. (MeOH). Mp 150-151°. $[\alpha]_D^{15}$ +175.4 (c, 0.057 in $CHCl_3$).

7,15-Diketone:3-Hydroxy-7,11,15,23-tetraoxolanost-8-en-26-oic acid. ***Ganoderic acid AM$_1$***
$C_{30}H_{42}O_7$ 514.658
Cryst. (Me_2CO). Mp 234-236°. $[\alpha]_D^{25}$ +97.5 (c, 0.2 in CH_2Cl_2).

3,7,15-Triketone: [98665-14-6] *3,7,11,15,23-Pentaoxolanost-8-en-26-oic acid. Ganoderic acid E*†. *Ganoderic acid F*†
$C_{30}H_{40}O_7$ 512.642
Constit. of *Ganoderma lucidum* (reishi). Yellow needles (as Me ester). Mp 211-213° (206-208°) (Me ester). $[\alpha]_D$ +167 ($CHCl_3$) (Me ester).

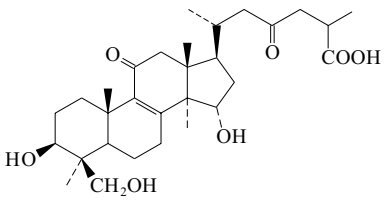
7-Deoxy: [98683-75-1] *3,15-Dihydroxy-11,23-dioxolanost-8-en-26-oic acid.* ***Ganolucidic acid B***
$C_{30}H_{46}O_6$ 502.69
Constit. of *Ganoderma lucidum* (reishi). Needles (as Me ester). Mp 167-169° (Me ester). $[\alpha]_D$ +114 ($CHCl_3$) (Me ester). λ_{max} 255 (ϵ 10000) (EtOH) (Derep).

7-Deoxy, 3-ketone: [98665-21-5] *15-Hydroxy-3,11,23-trioxolanost-8-en-26-oic acid.* ***Ganolucidic acid A***
$C_{30}H_{44}O_6$ 500.674
Constit. of *Ganoderma lucidum* (reishi). λ_{max} 255 (ϵ 10000) (EtOH) (Derep).

[103773-62-2]

Kohda, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1367 (*isol*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2624; 2628 (*isol*)
Hirotani, M. *et al., Phytochemistry*, 1986, **25**, 1189 (*isol*)
Lin, C.N. *et al., Phytochemistry*, 1993, **32**, 1549-1551 (*Ganoderic acid AM1*)

3,15,29-Trihydroxy-11,23-dioxolanost-8-en-26-oic acid T-554



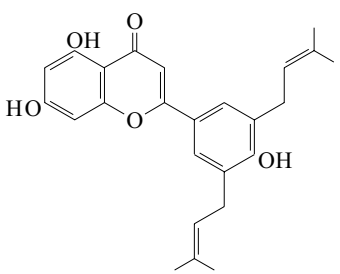
$C_{30}H_{46}O_7$ 518.689

(3β,15α,25ξ)-*form* [100440-27-5]
Ganolucidic acid C
Metab. of *Ganoderma lucidum* (reishi).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 3637 (*isol, pmr, cmr*)

4′,5,7-Trihydroxy-3′,5′-diprenylflavone T-555

[114542-44-8]
*5,7-Dihydroxy-2-[4-hydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, 9CI.* ***Honyucitrin***



$C_{25}H_{26}O_5$ 406.477
Constit. of *Citrus grandis* (pummelo). Pale-yellow powder (diisopropyl ether). Mp 199.5-201°.

Wu, T.-S. *et al., Phytochemistry*, 1988, **27**, 585

4′,5,7-Trihydroxy-3′,6-diprenylflavone T-556

[134958-52-4]
*5,7-Dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Gancaonin Q***

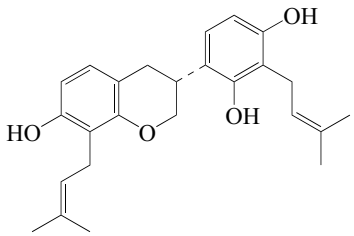
$C_{25}H_{26}O_5$ 406.477
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow needles (Me_2CO/hexane). Mp 212-214°.

$\Delta^{3''}$,$\Delta^{3'''}$-Isomer, 2″,2‴-dihydroxy: [149182-50-3] *4′,5,7-Trihydroxy-3′,6-bis(2-hydroxy-3-methyl-3-butenyl)flavone*
Yellow solid.

Fukai, T. *et al., Phytochemistry*, 1991, **30**, 1245 (*isol, pmr, cmr, struct*)
Iinuma, M. *et al., Heterocycles*, 1993, **35**, 407 (*deriv*)

2′,4′,7-Trihydroxy-3′,8-diprenylisoflavan T-557

Kanzonol X. *Tenuifolin B*

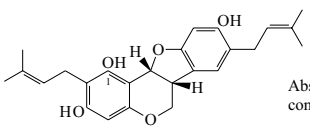


$C_{25}H_{30}O_4$ 394.51

(*R*)-*form* [182745-37-5]
Constit. of *Glycyrrhiza glabra* (licorice). Amorph. powder. $[\alpha]_D^{24}$ +9 (c, 0.2 in MeOH). $[\alpha]_D^{23}$ +1.3 (c, 0.1 in MeOH). λ_{max} 211 (log ϵ 5.02); 230 (sh) (log ϵ 4.59); 282 (log ϵ 3.99); 320 (sh) (log ϵ 3.27) (MeOH).

Fukai, T. *et al., Phytochemistry*, 1996, **43**, 1119-1124 (*isol, uv, cd, pmr, cmr, ms*)

1,3,9-Trihydroxy-2,8-diprenylpterocarpan T-558



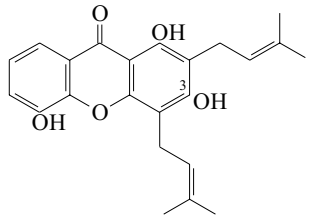
$C_{25}H_{28}O_5$ 408.493

1-Me ether: [129280-35-9] *3,9-Dihydroxy-1-methoxy-2,8-diprenylpterocarpan.* ***1-Methoxyficifolinol***
$C_{26}H_{30}O_5$ 422.52
Isol. from licorice (*Glycyrrhiza* sp.). Needles ($CHCl_3$). Mp 128-132°. $[\alpha]_D$ -173 (c, 3 in $CHCl_3$).

Kiuchi, F. *et al., Heterocycles*, 1990, **31**, 629-636 (*isol, pmr, cmr*)

1,3,5-Trihydroxy-2,4-diprenylxanthone T-559

[33390-41-9]
*1,3,5-Trihydroxy-2,4-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one.* ***8-Desoxygartanin***



$C_{23}H_{24}O_5$ 380.44
Isol. from *Garcinia mangostana* (mangosteen). Yellow needles (C_6H_6/hexane). Sol. H_2O; poorly sol. Me_2CO, hexane. Mp 165.5°. λ_{max} 264 (MeOH) (Berdy). λ_{max} 264 (E1%/1cm 495) (H_2O) (Berdy). λ_{max} 264 (HCl) (Berdy).

3-Me ether: [130774-35-5] *1,5-Dihydroxy-3-methoxy-2,4-diprenylxanthone.* ***Cudraxanthone G***
$C_{24}H_{26}O_5$ 394.466
Yellow prisms (hexane). Mp 129-131°.

3,5-Di-Me ether: [35323-84-3] *1-Hydroxy-3,5-dimethoxy-2,4-diprenylxanthone. 3,5-Di-*O*-methyl-8-deoxygartanin*
$C_{25}H_{28}O_5$ 408.493
Constit. of *Garcinia mangostana* (mangosteen). Yellow needles (MeOH). Mp 117-118° (106-108°).

Tri-Me ether: [54254-64-7] *1,3,5-Trimethoxy-2,4-diprenylxanthone*
$C_{26}H_{30}O_5$ 422.52
128-129.

Govindachari, T.R. *et al., Tetrahedron*, 1971, **27**, 3919
Anand, S.M. *et al., Aust. J. Chem.*, 1974, **27**, 1515 (*synth*)
Bennett, G.J. *et al., J.C.S. Perkin 1*, 1990, 2671 (*isol, deriv*)
Hano, Y. *et al., Planta Med.*, 1990, **56**, 399 (*deriv*)
Ito, C. *et al., Chem. Pharm. Bull.*, 1996, **44**, 441 (*deriv, uv, ir, pmr, cmr, ms*)

1,3,7-Trihydroxy-2,8-diprenylxanthone T-560

[105037-94-3]
*1,3,7-Trihydroxy-2,8-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one, 9CI.* ***6-Deoxy-γ-mangostin***

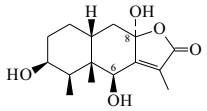
$C_{23}H_{24}O_5$ 380.44
Isol. from *Garcinia mangostana* (mangosteen). Cryst. Mp 171-174°.

7-Me ether: [83133-18-0] *1,3-Dihydroxy-7-methoxy-2,8-diprenylxanthone.* ***Calocalabaxanthone***
$C_{24}H_{26}O_5$ 394.466
Yellow-orange needles (EtOH). Mp 164-166°.

*7-*O*-(1,1-Dimethyl-2-propenoyl):* ***Apetalinone A***
$C_{28}H_{32}O_5$ 448.558
Amorph. orange powder. λ_{max} 241 ; 262 ; 315 ; 365 (MeOH).

Kumar, V. *et al., Phytochemistry*, 1982, **21**, 807 (*Calocalabaxanthone*)
Dharmaratne, H.R.W. *et al., Phytochemistry*, 1986, **25**, 1957 (*6-Deoxymangostin*)
Mahabusarakam, W. *et al., J. Nat. Prod.*, 1987, **50**, 474 (*isol, pmr*)
Iinuma, M. *et al., Phytochemistry*, 1997, **46**, 1423-1429 (*Apetalinone A*)

3,6,8-Trihydroxy-7(11)-eremophilen-12,8-olide T-561



(3β,6β,8α*OH*)-*form*

$C_{15}H_{22}O_5$ 282.336

(3β,6β,8α*OH*)-*form*

6-Angeloyl:
$C_{20}H_{28}O_6$ 364.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (EtOAc/hexane) (as di-Ac). Mp 164.5-165° Mp 174.5-175° (di-Ac). $[\alpha]_D$ +83.6 (c, 0.45 in $CHCl_3$) (di-Ac).

6-Tigloyl: [162613-66-3]
$C_{20}H_{28}O_6$ 364.438
Constit. of *Petasites japonicus* (sweet coltsfoot).

6-Me ether:3,8-Dihydroxy-6-methoxy-7(11)-eremophilen-12,8-olide
$C_{16}H_{24}O_5$ 296.363
Constit. of *Petasites japonicus* (sweet coltsfoot). Amorph. powder. $[\alpha]_D^{19}$ -164.8 (c, 1.1 in MeOH).

8-Me ether, 6-angeloyl: ***Eremopetasitenin C1***
$C_{21}H_{30}O_6$ 378.464
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{22}$ -21.1 (c, 0.94 in $CHCl_3$).

8-Me ether, 3-(3-methylthio-2Z-propenoyl), 6-angeloyl: ***Eremopetasitenin C2***
$C_{25}H_{34}O_7S$ 478.605
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{24}$ -62.5 (c, 0.32 in EtOH).

6,8-Di-Me ether: [162613-65-2] *3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide*
$C_{17}H_{26}O_5$ 310.389
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{26}$ -86.7 (c, 1.1 in $CHCl_3$).

6,8-Di-Me ether, 3-(3-methylthio-2Z-propenoyl): ***Eremopetasitenin C3***
$C_{21}H_{30}O_6S$ 410.53
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{20}$ -142.9 (c, 0.32 in $CHCl_3$).

(3β,6β,8β*OH*)-*form*

6-Angeloyl:
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. (EtOAc/hexane) (as di-Ac). Mp 144.5-146° (di-Ac). $[\alpha]_D$ -92 (c, 0.9 in $CHCl_3$) (di-Ac).

6-Tigloyl: [162613-67-4]
Constit. of *Petasites japonicus* (sweet coltsfoot).

6-(3-Chloro-2-hydroxy-2-methylbutanoyl): [264607-21-8]
$C_{20}H_{29}ClO_7$ 416.898
Constit. of *Petasites japonicus* (sweet coltsfoot). Mixt. of diastereoisomers.

8-Me ether, 6-angeloyl: ***Eremopetasitenin D1***
$C_{21}H_{30}O_6$ 378.464
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{24}$ +116.5 (c, 0.74 in $CHCl_3$).

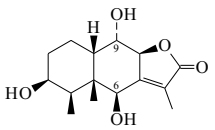
8-Me ether, 3-(3-methylthio-2Z-propenoyl), 6-angeloyl: ***Eremopetasitenin D2***
$C_{25}H_{34}O_7S$ 478.605
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{24}$ +64.8 (c, 0.88 in EtOH).

6,8-Di-Me ether, 3-(3-methylthio-2Z-propenoyl): ***Eremopetasitenin D3***
$C_{21}H_{30}O_6S$ 410.53
Constit. of *Petasites japonicus* (sweet coltsfoot). $[\alpha]_D^{22}$ +97.8 (c, 6.03 in $CHCl_3$).

3-Ketone, 6-angeloyl: [162613-68-5]
$C_{20}H_{26}O_6$ 362.422
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{19}$ +38.1 (c, 0.5 in $CHCl_3$).

Sugama, K. *et al., Phytochemistry*, 1985, **24**, 1531 (*isol, pmr, cmr*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1944; 1996, **44**, 1731 (*isol, pmr, cmr*)
Yaoita, Y. *et al., Annu. Rep. Tohoku Coll. Pharm.*, 1998, **45**, 123-126; *CA*, **132**, 291005a (*3-chloro-2-hydroxy-2-methylbutanoyl*)
Tori, M. *et al., Phytochemistry*, 1998, **47**, 401-409; *CA*, **132**, 291005a (*Eremopetasitenins*)

3,6,9-Trihydroxy-7(11)-eremophilen-12,8-olide T-562



(3β,6β,8β,9α,10β)-*form*

$C_{15}H_{22}O_5$ 282.336

(3β,6β,8β,9α,10β)-*form*

6-Angeloyl: [171422-88-1]
$C_{20}H_{28}O_6$ 364.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{22}$ -32.4 (c, 1.2 in $CHCl_3$).

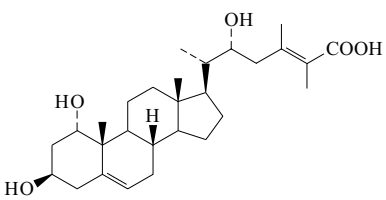
(3β,6β,8β,9β,10β)-*form*

6-Angeloyl: [171595-25-8]
$C_{20}H_{28}O_6$ 364.438
Constit. of *Petasites japonicus* (sweet coltsfoot). Oil. $[\alpha]_D^{22}$ -39.9 (c, 0.6 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1738-1743 (*isol, pmr, cmr*)

1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid T-563

1,3,22-Trihydroxy-24-methylcholesta-5,24-dien-26-oic acid



$C_{28}H_{44}O_5$ 460.653

(1α,3β,22*R*,24*E*)-*form*

*3-*O*-β-D-Glucopyranoside, 26-*O*-β-D-glucopyranosyl ester:* [155510-72-8]
$C_{40}H_{64}O_{15}$ 784.937
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D^{25}$ -21 (c,

0.4 in MeOH).

3-O-*β*-D-*Glucopyranoside, 26*-O-*[β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranosyl] ester:* [155510-73-9]
$C_{46}H_{74}O_{20}$ 947.079
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D^{25}$ -34 (c, 0.5 in MeOH).

3-O-*β*-D-*Glucopyranoside, 26*-O-*[β*-D-*glucopyranosyl-(1→2)-6-acetyl-β*-D-*glucopyranosyl] ester:* [155510-74-0]
$C_{48}H_{76}O_{21}$ 989.116
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D^{25}$ -26 (c, 0.5 in MeOH).

3-O-*β*-D-*Glucopyranoside, 26*-O-*[β*-D-*glucopyranosyl-(1→4)-β*-D-*glucopyranosyl-(1→2)-6-acetyl-β*-D-*glucopyranosyl] ester:* [155520-07-3]
$C_{54}H_{86}O_{26}$ 1151.258
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D^{25}$ -16 (c, 0.5 in MeOH).

3-O-*β*-D-*Glucopyranoside, 26*-O-*[β*-D-*glucopyranosyl-(1→4)-6-acetyl-β*-D-*glucopyranosyl-(1→2)-6-acetyl-β*-D-*glucopyranosyl] ester:* [155520-08-4]
$C_{56}H_{88}O_{27}$ 1193.295
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. solid. $[\alpha]_D^{25}$ -17 (c, 0.5 in MeOH).

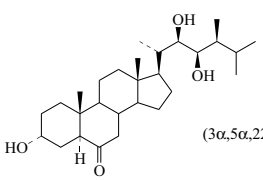
22-Ac, 3-O-*β*-D-*glucopyranoside, 26*-O-*[β*-D-*glucopyranosyl-(1→4)-β*-D-*glucopyranosyl-(1→2)-6-acetyl-β*-D-*glucopyranosyl] ester:* [151194-18-2]
$C_{56}H_{88}O_{27}$ 1193.295
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. powder. $[\alpha]_D^{25}$ -23 (c, 1 in MeOH).

22-Ac, 3-O-*β*-D-*glucopyranoside, 26*-O-*[β*-D-*glucopyranosyl-(1→4)-6-acetyl-β*-D-*glucopyranosyl-(1→2)-6-acetyl-β*-D-*glucopyranosyl] ester:* [151194-19-3]
$C_{58}H_{90}O_{28}$ 1235.332
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. powder. $[\alpha]_D^{25}$ -20 (c, 0.5 in MeOH).

Waiss, A.C. *et al., J. Nat. Prod.*, 1993, **56**, 1365 (*isol, pmr, cmr*)
Elliger, C.A. *et al., J. Nat. Prod.*, 1994, **57**, 348 (*isol, pmr, cmr, cryst struct*)

3,22,23-Trihydroxyergostan-6-one T-564

3,22,23-Trihydroxy-24-methylcholestan-6-one



(3α,5α,22*R*,23*R*,24*S*)-*form*

$C_{28}H_{48}O_4$ 448.685

(3α,5α,22*R*,23*R*,24*S*)-*form* [87734-68-7]
Typhasterol. *2-Deoxycastasterone*
Constit. of green tea (*Thea sinensis*) and wheat grains (*Triticum aestivum*). Cryst. (MeCN aq.). Mp 227-230°.

(3β,5α,22*R*,23*R*,24*S*)-*form* [92751-21-8]
Teasterone
Constit. of green tea (*Thea sinensis*) and wheat grains (*Triticum aestivum*). Cryst. Mp 200-201°.

3-O-*β*-D-*Glucopyranoside:Teasterone 3-glucoside*
$C_{34}H_{58}O_9$ 610.827
Cryst. Mp 275-277°.

3-O-*Dodecanoyl:Teasterone 3-laurate*
$C_{40}H_{70}O_5$ 630.99
Cryst. ($CHCl_3$/MeOH aq.). Mp 179-182°.

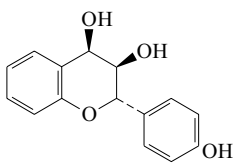
3-O-*Tetradecanoyl:* [154993-52-9] *Teasterone 3-myristate*
$C_{42}H_{74}O_5$ 659.044
Cryst. ($CHCl_3$/MeOH aq.). Mp 173-177°.

3-Ketone: [124853-28-7] *22,23-Dihydroxyergostane-3,6-dione. 22,23-Dihydroxy-24-methylcholestane-3,6-dione.* ***3-Dehydroteasterone***
$C_{28}H_{46}O_4$ 446.669
Constit. of wheat grains *Triticum aestivum*. Cryst. (MeCN aq.). Mp 178°.

Abe, H. *et al., Agric. Biol. Chem.*, 1982, **46**, 2609; 1984, **48**, 2171 (*isol, struct*)
Takastsuto, S. *et al., J.C.S. Perkin 1*, 1984, 139; 1986, 1833 (*synth*)
Aburatani, M. *et al., Agric. Biol. Chem.*, 1987, **51**, 1909 (*synth*)
Ando, T. *et al., Magn. Reson. Chem.*, 1993, **31**, 94 (*pmr, cmr*)
Yokota, T. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1183 (*3-Dehydroteasterone*)
Asakawa, S. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1416 (*isol, synth, esters*)
Voigt, B. *et al., Tetrahedron*, 1996, **52**, 1997 (*synth*)
Soeno, K. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 702-709 (*Teasterone 3-glucoside*)

3,4,4′-Trihydroxyflavan T-565

[72097-76-8]
*3,4-Dihydro-2-(4-hydroxyphenyl)-2*H-*1-benzopyran-3,4-diol, 9CI*



(2*S*,3*R*,4*R*)-*form*

$C_{15}H_{14}O_4$ 258.273

(2*S*,3*R*,4*R*)-*form* [149747-10-4]
Constit. of the seeds of *Musa sapientum* (banana).

(2*RS*,3*SR*,4*RS*)-*form*

4′-Me ether: [18874-01-6] *3,4-Dihydroxy-4′-methoxyflavan. 4′-Methoxy-3,4-flavandiol*
$C_{16}H_{16}O_4$ 272.3
Needles (MeOH). Mp 179°.

4′-Me ether, di-Ac: [18943-76-5]
Prisms (hexane). Mp 96-97° (91-92°).

(2*RS*,3*SR*,4*SR*)-*form*

4′-Me ether: [34811-94-4]
Needles (EtOH). Mp 160-161°.

4′-Me ether, di-Ac: [34811-95-5]
Plates (EtOH). Mp 100-102°.

[60094-50-0]

Clark-Lewis, J.W. *et al., Aust. J. Chem.*, 1971, **24**, 2581; 1973, **26**, 819; 1974, **27**, 865 (*synth, derivs*)
Berge, D.D. *et al., Indian J. Chem., Sect. B*, 1979, **18**, 77 (*synth, deriv*)
Ali, M. *et al., Pharmazie*, 1993, **48**, 455 (*isol*)

4′,5,7-Trihydroxyflavan T-566

[530-82-5]
*3,4-Dihydro-2-(4-hydroxyphenyl)-2*H-*1-benzopyran-5,7-diol*

$C_{15}H_{14}O_4$ 258.273

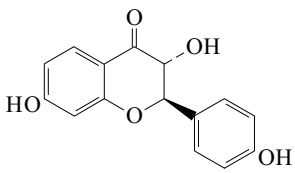
(*S*)-*form*

5,7-Di-Me ether: [103963-45-7] ***4′-Hydroxy-5,7-dimethoxyflavan***
$C_{17}H_{18}O_4$ 286.327
Constit. of the pith of sago palm. Amorph. yellow powder. Mp 134-135° (119-120°). $[\alpha]_D^{21}$ -8.35 (c, 1.16 in MeOH). $[\alpha]_D^{24}$ +10.66 (c, 1.57 in $CHCl_3$).

Okamoto, A. *et al., Agric. Biol. Chem.*, 1986, **50**, 1655 (*4′-Hydroxy-5,7-dimethoxyflavan*)
Diaz, D. *et al., Phytochemistry*, 1986, **25**, 2395 (*4′-Hydroxy-5,7-dimethoxyflavone*)
Gutierrez, A.B. *et al., Phytochemistry*, 1988, **27**, 2225 (*isol*)

3,4′,7-Trihydroxyflavanone T-567

*2,3-Dihydro-3,7-dihydroxy-2-(4-hydroxyphenyl)-4*H-*1-benzopyran-4-one, 9CI. 4′,7-Dihydroxydihydroflavanol.* ***Garbanzol***



$C_{15}H_{12}O_5$ 272.257

(2*R*,3*R*)-*form* [1226-22-8]
Isol. from *Cicer arietinum* (chickpea) and *Capsella bursa-pastoris* (shepherd's purse). Needles (H_2O). Mp 207-208°. λ_{max} 274 ; 310 (MeOH) (Berdy). λ_{max} 250 ; 334 (MeOH/NaOH) (Berdy). λ_{max} 276 ; 311 (EtOH) (Berdy).

3-O-*β*-D-*Glucopyranoside:* [19146-28-2] ***Lecontin***
$C_{21}H_{22}O_{10}$ 434.399
Glass. Mp 125-130°. $[\alpha]_D^{25}$ -16.75 (c, 1.83 in H_2O).

3-Ac: [135607-78-2] *3-Acetoxy-4′,7-dihydroxyflavanone. 3*-O-*Acetylgarbanzol*
$C_{17}H_{14}O_6$ 314.294

4′-Me ether, 7-O-*[β*-D-*xylopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [101236-48-0] ***Kushenol J***
$C_{27}H_{32}O_{14}$ 580.541

[1807-98-3]

Wong, E. *et al., Phytochemistry*, 1965, **4**, 89 (*isol, synth*)
Oyamada, T. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 507 (*synth*)
Markham, K.R. *et al., Tetrahedron*, 1967, **24**, 823 (*Lecontin*)
Wohlfart, R. *et al., Dtsch. Apoth. -Ztg.*, 1972, **112**, 1158 (*isol*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1978, **33**, 146 (*isol*)
Adinarayana, D. *et al., Z. Naturforsch., C*, 1982, **37**, 145 (*isol*)

Wu, L.J. *et al., Yakugaku Zasshi*, 1985, **105**, 1034 (*Kushenol J*)

3,5,7-Trihydroxyflavanone T-568

[96335-75-0]
2,3-Dihydro-3,5,7-trihydroxy-2-phenyl-4H-1-benzopyran-4-one, 9CI. 5,7-Dihydroxydihydroflavonol. ***Pinobanksin***. *Dihydrogalangol*

$C_{15}H_{12}O_5$ 272.257

(2*R*,3*R*)-*form* [548-82-3]
Long yellow prisms (MeOH). Sol. H_2O, Et_2O. Mp 177-178°. $[\alpha]_D$ +15 (c, 2 in MeOH).

5-O-[β-D-Galactopyranosyl-(1→4)-β-D-glucopyranoside]: [91925-95-0]
$C_{27}H_{32}O_{15}$ 596.541
Isol. from the famine food *Adansonia digitata* (baobab). Mp 88-90°.

3-Ac: [52117-69-8] ***3-O-Acetylpinobanksin***
$C_{17}H_{14}O_6$ 314.294
Mp 135°. $[\alpha]_D^{20}$ +17 (Py).

3-Propanoyl: [126394-70-5] *5,7-Dihydroxy-3-propanoyloxyflavanone*. ***3-O-Propanoylpinobanksin***
$C_{18}H_{16}O_6$ 328.321

3-O-(2-Methylpropanoyl):5,7-Dihydroxy-3-isobutanoyloxyflavanone. ***3-O-(2-Methylpropanoyl)pinobanksin***
$C_{19}H_{18}O_6$ 342.348
$[\alpha]_D^{26}$ +12.7 (c, 0.1 in MeOH). λ_{max} 293 (log ε 3.92) (MeOH).

3-O-(2S-Methylbutanoyl): [437717-44-7] ***3-O-(2S-Methylbutanoyl)pinobanksin***
$C_{20}H_{20}O_6$ 356.374
Amorph. yellow solid. $[\alpha]_D^{25}$ +24.5 (c, 0.1 in $CHCl_3$). $[\alpha]_D^{26}$ +62.3 (c, 0.1 in MeOH). λ_{max} 292 (log ε 4.27) (MeOH).

3-Benzoyl: [129693-91-0] *3-Benzoyloxy-5,7-dihydroxyflavanone*. ***3-O-Benzoylpinobanksin***
$C_{22}H_{16}O_6$ 376.365

3-O-E-Cinnamoyl: [110065-73-1] ***3-O-trans-Cinnamoylpinobanksin***
$C_{24}H_{18}O_6$ 402.403

3-Me ether: [129843-35-2] *5,7-Dihydroxy-3-methoxyflavanone*. ***3-O-Methylpinobanksin***
$C_{16}H_{14}O_5$ 286.284

5-Me ether: [87620-04-0] *3,7-Dihydroxy-5-methoxyflavanone*. ***5-O-Methylpinobanksin***
$C_{16}H_{14}O_5$ 286.284
Cryst. (EtOAc/$CHCl_3$). Mp 220°.

5-Me ether, 3-O-β-D-glucopyranoside: [133740-03-1]
$C_{22}H_{24}O_{10}$ 448.426

7-Me ether: [480-13-7] *3,5-Dihydroxy-7-methoxyflavanone*. ***Alpinone***†. *7-O-Methylpinobanksin*
$C_{16}H_{14}O_5$ 286.284
Needles (MeOH). Mp 186-187° (179-181°). $[\alpha]_D^{20}$ -12 ($CHCl_3$). $[\alpha]_D^{20}$ +92 (Py).

7-Me ether, 3-Ac: ***3-Acetylalpinone***. *3-Acetyl-7-O-methylpinobanksin*
$C_{18}H_{16}O_6$ 328.321
Mp 135°. $[\alpha]_D^{20}$ +17 (Py).

5,7-Di-Me ether: [67335-36-8] *3-Hydroxy-5,7-dimethoxyflavanone*. ***5,7-Di-O-methylpinobanksin***
$C_{17}H_{16}O_5$ 300.31

(2*R*,3*S*)-*form*

3-Ac: [102092-27-3]
$[\alpha]_D^{20}$ -198 (c, 1 in MeOH).

5,7-Di-Me ether: Abs. config. not confirmed.

[122585-69-7]

Linstedt, G. *et al., Acta Chem. Scand.*, 1950, **4**, 1042; 1951, 1; 121; 129
Kotake, H. *et al., Chem. Ind. (London)*, 1954, 1562 (*synth*)
Gripenberg, J. *et al., Chem. Ind. (London)*, 1955, 443 (*struct*)
Gripenberg, J. *et al., Acta Chem. Scand.*, 1956, **10**, 393 (*Alpinone, 3-Acetylalpinone*)
Jeffries, P.R. *et al., Aust. J. Chem.*, 1962, **15**, 532 (*isol*)
Fernandes, J.B. *et al., Biochem. Syst. Ecol.*, 1978, **6**, 55 (*5,7-di-Me ether*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 839; 1981, **20**, 1907; 1982, **21**, 371 (*isol*)
Bankova, V. *et al., J. Nat. Prod.*, 1983, **46**, 471 (*5-Me ether*)
Chauhan, J.S. *et al., Planta Med.*, 1984, **50**, 113 (*deriv*)
Wollenweber, E. *et al., J. Plant Physiol.*, 1985, **117**, 423 (*3-Ac*)
Dominguez, X.A. *et al., J. Nat. Prod.*, 1986, **49**, 143 (*3-Ac*)
Jakupovic, J. *et al., Pharmazie*, 1986, **41**, 157 (*3-Ac*)
Nagy, E. *et al., Stud. Org. Chem. (Amsterdam)*, 1986, **23**, 223; 233 (*3-Ac*)
Scheele, C. *et al., J. Nat. Prod.*, 1987, **50**, 181 (*3-cinnamate*)
Greenaway, W. *et al., Z. Naturforsch., C*, 1990, **45**, 587 (*3-benzoyl*)
Shawl, A.S. *et al., Phytochemistry*, 1992, **31**, 1399 (*Alpinone*)
Economides, C. *et al., Phytochemistry*, 1998, **49**, 859-862 (*5,7-di-Me ether*)
Kumazawa, S. *et al., J. Agric. Food Chem.*, 2002, **50**, 4777-4782 (*3-(2-Methylpropanoyl)-, 3-(2-Methylbutanoyl)pinobanksin*)
Usia, T. *et al., J. Nat. Prod.*, 2002, **65**, 673-676 (*3-(2-Methylbutanoyl)pinobanksin*)

4′,5,7-Trihydroxyflavanone T-569

Naringenin. *Floribundigenin*. *Naringetol*. *Salipurpol. BE 14348A*. *Antibiotic BE 14348A*

$C_{15}H_{12}O_5$ 272.257
Nutriceutical with anticancer props.. Log P 1.8 (uncertain value) (calc). λ_{max} 245 (ε 16000); 323 (ε 23100) (MeOH/NaOH) (Derep). λ_{max} 226 (ε 21900); 286 (ε 15600); 330 (sh) (ε 2950) (MeOH) (Derep).

(*S*)-*form* [480-41-1]
Most widely distributed flavanone. Citrus fruits (grapefruit, oranges and pummelos) are especially good sources. Glycosides also widely distributed. Yellowish cryst. Sol. EtOH, alkalis; sl. sol. H_2O. Mp 250-251° (227-228°). $[\alpha]_D^{27}$ -22.5 (MeOH). Originally isol. in 1907 but incorr. descr. as a chalcone.

5-O-α-L-Rhamnopyranoside: [83697-42-1]
$C_{21}H_{22}O_9$ 418.399
Isol. from *Prunus cerasoides* (wild Himalayan cherry). Yellowish plates (MeOH aq.). Mp 135-137°.

O-*Fructoside:*
$C_{21}H_{22}O_{10}$ 434.399
Isol. from *Camellia sinensis* (tea). No phys. props. reported. Rare occurrence of fructose. Posn. of glycosylation not detd..

5-O-β-D-Glucopyranoside: [529-41-9] ***Floribundoside***. *Salipurposide*. *Helichrysin B*
$C_{21}H_{22}O_{10}$ 434.399
Occurs in *Persica vulgaris* (peach). Pale yellow needles (EtOH). Mp 227° dec. (224-226°). $[\alpha]_D^{20}$ -110.2 (EtOH). Fluorescent in soln..

7-O-[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]: [54835-98-2] ***Prunin 6″-O-gallate***. *6″-O-Galloylprunin*
$C_{28}H_{26}O_{14}$ 586.505
Isol. from *Acacia farnesiana* (sweet acacia). Yellowish cryst. + $1H_2O$. Mp 203-206°. $[\alpha]_D^{25}$ -97.2 (c, 1.065 in Py).

7-O-[4,6-Di-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranoside]:Prunin 4″,6″-di-O-gallate. ***4″,6″-Di-O-galloylprunin***
$C_{35}H_{30}O_{18}$ 738.611
Constit. of the pods of *Acacia farnesiana* (sweet acacia). Amorph. powder.

7-O-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside]: [96686-70-3] ***6″-p-Coumaroylprunin***
$C_{30}H_{28}O_{12}$ 580.544
Isol. from *Anacardium occidentale* (cashew). Pale yellow cubes (EtOAc/C_6H_6). Mp 164-166° (153-154°). $[\alpha]_{578}$ -64.6 (MeOH).

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [10236-47-2] ***Naringin***. *Naringenin 7-neohesperidoside. Naringoside. Aurantin*†. *Isohesperidin*
$C_{27}H_{32}O_{14}$ 580.541
Obt. from citrus fruits, *Clymenia polyandra* (clymenia) and *Origanum vulgare* (oregano). Needles + $8H_2O$ (H_2O), losing $6H_2O$ at 110°. Sol. AcOH; fairly sol. H_2O; poorly sol. Et_2O, C_6H_6. Mp 82° (octahydrate) Mp 171° (dihydrate). $[\alpha]_D^{19}$ -82.1 (EtOH). Log P -2.09 (uncertain value) (calc). Bitter taste.
▶ LD_{50} (mus, scu) 1650 mg/kg. QN6340000

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside], 4′-O-β-D-glucopyranoside: [17257-21-5] *Naringin 4′-glucoside. Naringenin 4′-glucoside 7-neohesperidoside*
$C_{33}H_{42}O_{19}$ 742.683
Isol. from grapefruit. Cryst. Mp 239°. $[\alpha]_D^{25}$ -89.3 (c, 1.25 in Py).

7-O-[α-L-Rhamnopyranosyl-(1→2)-6-O-malonyl-β-D-glucopyranoside]: [139934-59-1] ***6″-O-Malonylnaringin***
$C_{30}H_{34}O_{17}$ 666.588
Isol. from grapefruit.

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [14259-46-2] ***Narirutin***. *Naringenin 7-rutinoside. Isonaringin*
$C_{27}H_{32}O_{14}$ 580.541
Obt. from *Camellia sinensis* (tea). Cryst. + H_2O. Mp 160-165°.

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 4′-O-β-D-glucopyranoside: [17257-22-6] *Narirutin 4′-glucoside. Naringenin 4′-glucoside 7-rutinoside*
$C_{33}H_{42}O_{19}$ 742.683
Isol. from grapefruit. Powder + $1H_2O$. Mp 189-200°. $[\alpha]_D$ -62.6 (c, 0.92 in Py).

7-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:

$C_{33}H_{42}O_{18}$ 726.684
Constit. of the fruit of *Citrus junos* (yuzu). Pale yellow powder. Mp 190°. λ_{max} 226 ; 284 ; 334 (MeOH).

5-Me ether, 7-O-β-D-glucopyranoside: [110187-26-3] ***Puddumin A***
$C_{22}H_{24}O_{10}$ 448.426
Constit. of *Prunus cerasoides* (wild Himalayan cherry). Cryst. (MeOH). Mp 210°.

4′-O-(3-Methyl-2-butenyl): [14117-54-5] *5,7-Dihydroxy-4′-prenyloxyflavanone.* ***Selinone***. *4′-O-Prenylnaringenin*. *Archangelone*
$C_{20}H_{20}O_5$ 340.375
Isol. from roots of *Angelica archangelica* (angelica). Cryst. Mp 151-152°. $[\alpha]_D^{29}$ -50 (c, 0.61 in MeOH). λ_{max} 209 (ϵ 18620); 289 (ϵ 11220) (MeOH) (Berdy). λ_{max} 340 (MeOH-NaOH) (Berdy).

[13238-06-7, 17257-04-4, 18196-14-0, 23711-00-4, 26207-67-0, 58001-41-5, 61823-56-1, 66074-95-1, 67604-48-2, 102101-05-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 94D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 915C (*nmr*)
Paris, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1950, **231**, 72-73 (*Floribundoside*)
Paris, R.A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 2112-2114 (*struct, Floribundoside*)
Hänsel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 398; *CA*, **54**, 3854 (*Helichrysins*)
Phillips, D.J. *et al., J. Exp. Bot.*, 1962, **13**, 213 (*use*)
Audier, H. *et al., Bull. Soc. Chim. Fr.*, 1966, 2892 (*ms*)
Seshardri, T.R. *et al., Tet. Lett.*, 1967, 853 (*4′-O-Prenylnaringenin*)
Albach, R.F. *et al., Phytochemistry*, 1969, **8**, 127 (*isol*)
Korkuć, A. *et al., Wiad. Chem.*, 1969, **23**, 345; *CA*, **71**, 56224j (*rev*)
Aurnhammer, G. *et al., Chem. Ber.*, 1970, **103**, 1578; 1971, **104**, 473; 1972, **105**, 3511 (*isol, synth*)
Gaffield, W. *et al., Tetrahedron*, 1970, **26**, 4093 (*ord, abs config*)
Asakawa, Y. *et al., Bull. Chem. Soc. Jpn.*, 1971, **44**, 2761 (*isol*)
Kowalewski, Z. *et al., Planta Med.*, 1971, **19**, 311 (*isol*)
Nevskaya, A.N. *et al., Zh. Anal. Khim.*, 1972, **27**, 1699 (*use*)
Donnelly, D.M.X. *et al., J.C.S. Perkin 1*, 1973, 1737 (*isol*)
El Sissi, H.I. *et al., Phytochemistry*, 1974, **13**, 2843 (*galloylglycoside*)
Gaffield, W. *et al., Bioorg. Chem.*, 1975, **4**, 259 (*biosynth*)
Markham, K.R. *et al., Tetrahedron*, 1976, **32**, 2607 (*cmr*)
Wenkert, E. *et al., Phytochemistry*, 1977, **16**, 1811 (*nmr*)
Rahman, W. *et al., Phytochemistry*, 1978, **17**, 1064 (*coumaroylglycoside*)
Duddeck, H. *et al., Phytochemistry*, 1978, **17**, 1369 (*nmr*)
Rao, M.M. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 178 (*isol*)
Gupta, A.K. *et al., Indian J. Chem., Sect. B*, 1979, **18**, 85 (*rutinoside*)
Srivastava, S.K. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 604 (*deriv*)
Norbedo, C. *et al., J. Nat. Prod.*, 1982, **45**, 635 (*isol*)
Shrivastava, S.P. *et al., Phytochemistry*, 1982, **21**, 1464 (*isol*)
Barros, D.A.D. *et al., Phytochemistry*, 1982, **21**, 2107 (*coumaroylglycosides*)
Shirataki, Y. *et al., Chem. Pharm. Bull.*, 1983, **31**, 2859 (*isol*)
Jaipetch, T. *et al., Phytochemistry*, 1983, **22**, 625 (*isol*)
Shirataki, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 444 (*cmr*)
Shin, W. *et al., Acta Cryst. C*, 1986, **42**, 626 (*cryst struct*)
Bahuguna, R.P. *et al., J. Nat. Prod.*, 1987, **50**, 232 (*Puddumin A*)
Shen, C.-C. *et al., Phytochemistry*, 1993, **34**, 843 (*pmr, cmr*)
Garo, E. *et al., Phytochemistry*, 1998, **48**, 754-763 (*Selinone*)
Barakat, H.H. *et al., Phytochemistry*, 1999, **51**, 139-142 (*4″,6″-Digalloylprunin*)

4′,5,8-Trihydroxyflavanone T-570

[123067-25-4]
$C_{15}H_{12}O_5$ 272.257
Constit. of *Spinacia oleracea* (spinach). Cryst. (MeOH aq.). Mp 262-264°. λ_{max} 295 (log ϵ 4.99); 328 (sh) (log ϵ 4.41) (MeOH).

Rauter, A.P. *et al., Phytochemistry*, 1989, **28**, 2173-2175 (*isol, pmr*)
Edenharder, R. *et al., J. Agric. Food Chem.*, 2001, **49**, 2767-2773 (*isol*)

4′,7,8-Trihydroxyflavanone T-571

[5023-05-2]
2,3-Dihydro-7,8-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one
$C_{15}H_{12}O_5$ 272.257

(*S*)-*form*
8-Me ether:4′,7-Dihydroxy-8-methoxyflavanone. ***Heliannone C***
$C_{16}H_{14}O_5$ 286.284
Constit. of *Helianthus annuus* (sunflower). Gum. $[\alpha]_D^{25}$ +1.2 (c, 0.1 in $CHCl_3$). Tentative abs. config λ_{max} 275 ; 325 (MeOH).

7,8-Di-Me ether:4′-Hydroxy-7,8-dimethoxyflavanone. ***Heliannone B***
$C_{17}H_{16}O_5$ 300.31
Constit. of *Helianthus annuus* (sunflower). Gum. $[\alpha]_D^{25}$ +11.2 (c, 0.1 in $CHCl_3$). Tentative abs. config λ_{max} 282 ; 324 (sh) (MeOH).

(±)-*form*
Needles (H_2O). Mp 104-105°.

Tri-Ac:
Long needles (EtOH). Mp 165-166°. $[\alpha]_D^{26}$ -2.9 (c, 0.3 in EtOH).

Drewes, S.E. *et al., Biochem. J.*, 1966, **98**, 493 (*isol, uv*)
Tindale, M.D. *et al., Phytochemistry*, 1969, **8**, 1713
Clark-Lewis, J.W. *et al., Aust. J. Chem.*, 1972, **25**, 1943 (*isol*)
Macias, F.A. *et al., Phytochemistry*, 1997, **45**, 683 (*Heliannones*)
Rao, Y.K. *et al., J. Nat. Prod.*, 2001, **64**, 368-369 (*Heliannone B,synth*)

5,6,7-Trihydroxyflavanone T-572

[35683-17-1]
Dihydrobaicalein
$C_{15}H_{12}O_5$ 272.257

(*S*)-*form* [117859-32-2]
6-Me ether: [18956-18-8] *5,7-Dihydroxy-6-methoxyflavanone.* ***Dihydrooroxylin***
$C_{16}H_{14}O_5$ 286.284
Isol. from *Prunus avium* (wild cherry) and *Piper* sp.. Mp 177°.

[56226-98-3, 66074-94-0, 89395-31-3, 93344-60-6]

Hansel, A. *et al., Planta Med.*, 1967, **15**, 443 (*Dihydrooroxylin*)

5,7,8-Trihydroxyflavanone T-573

2,3-Dihydro-5,7,8-trihydroxy-2-phenyl-4H-1-benzopyran-4-one. Dihydronorwogonin
$C_{15}H_{12}O_5$ 272.257

(*S*)-*form* [123914-36-3]
8-Me ether: [4431-41-8] *5,7-Dihydroxy-8-methoxyflavanone.* ***Dihydrowogonin***
$C_{16}H_{14}O_5$ 286.284
Isol. from *Prunus avium* (wild cherry). Cryst. (EtOH). Mp 150°. $[\alpha]_D$ -56. λ_{max} 292 (ϵ 14000); 345 (MeOH) (Berdy). λ_{max} 326 (MeOH/NaOH) (Berdy).

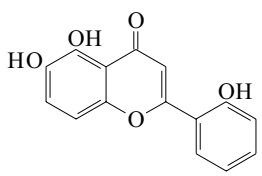
(±)-*form*
7-O-β-D-Glucopyranoside:5,7,8-Trihydroxyflavanone 7-glucoside
$C_{21}H_{22}O_{10}$ 434.399
Isol. from *Prunus avium* (wild cherry).

[24583-19-5, 54377-25-2, 64551-85-5, 75041-39-3]

Chopin, J. *et al., Bull. Soc. Chim. Fr.*, 1957, 192 (*isol*)
Massicot, J. *et al., Bull. Soc. Chim. Fr.*, 1962, 1962 (*pmr*)
Popova, T.P. *et al., Rastit. Resur.*, 1976, **12**, 232
Vieira, P.C. *et al., Planta Med.*, 1980, **39**, 153 (*derivs*)
Gupta, K.K. *et al., Phytochemistry*, 1983, **22**, 314
Rani, I. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 1080 (*synth*)
Scheele, C. *et al., J. Nat. Prod.*, 1987, **50**, 181 (*isol*)

2′,5,6-Trihydroxyflavone T-574

5,6-Dihydroxy-2-(2-hydroxyphenyl)-4H-1-benzopyran-4-one



$C_{15}H_{10}O_5$ 270.241
Yellow needles ($Me_2CO/CHCl_3$). Mp 278-280°.

Tri-Ac:
Needles (MeOH). Mp 144-146°.

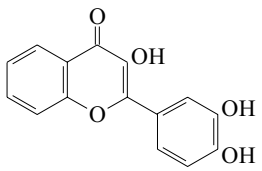
2′,6-Di-Me ether: [16266-96-9] *5-Hydroxy-2′,6-dimethoxyflavone*
$C_{17}H_{14}O_5$ 298.295
Yellow needles (MeOH). Mp 153-154° (150°).

Tri-Me ether: [16266-97-0] ***2′,5,6-Trimethoxyflavone***
$C_{18}H_{16}O_5$ 312.321
Isol. from *Casimiroa edulis* (Mexican apple). Plates (Me_2CO) or prisms. Mp 124-125° (120-121°).

Doporto, M.L. *et al., J.C.S.*, 1955, 4249 (*synth*)
Sondheimer, F. *et al., Tetrahedron*, 1960, **9**, 139 (*isol, synth*)
Dreyer, D.L. *et al., J.O.C.*, 1968, **33**, 3577 (*2′,5,6-Trimethoxyflavone*)
Meyer, B.N. *et al., J. Nat. Prod.*, 1985, **48**, 952 (*2′,5,6-Trimethoxyflavone*)
Wollenweber, E. *et al., Phytochemistry*, 1990, **29**, 633 (*isol, pmr, cmr, ms, synth*)

3,3′,4′-Trihydroxyflavone T-575

[6068-78-6]
*2-(3,4-Dihydroxyphenyl)-3-hydroxy-4*H*-1-benzopyran-4-one. 3′,4′-Dihydroxyflavanol*



$C_{15}H_{10}O_5$ 270.241
Cryst. (EtOH or MeOH). Mp 301-303°.

3-O-*[α-L-Rhamnopyranosyl-(1→2)[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]:* [95880-20-9]
$C_{33}H_{40}O_{18}$ 724.668
Constit. of redcurrant juice.

Tri-Ac:
Mp 199-200°.

3-Me ether: [307521-53-5] *3′,4′-Dihydroxy-3-methoxyflavone*
$C_{16}H_{12}O_5$ 284.268
Cryst. Mp 198.5-199.7°.

3′,4′-Di-Me ether: [6889-80-1] *3-Hydroxy-3′,4′-dimethoxyflavone. 3′,4′-Dimethoxyflavanol*
$C_{17}H_{14}O_5$ 298.295
Yellow needles. Mp 198-200°.

Ozawa, H. *et al., Yakugaku Zasshi*, 1951, **71**, 1178; 1183 (*synth*)
Ternai, B. *et al., Tetrahedron*, 1976, **32**, 565 (*cmr*)
Siewek, F. *et al., Lebensmittelchem. Gerichtl. Chem.*, 1985, **39**, 9 (*isol, deriv*)
Sobottka, A.M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 2000, **333**, 205-210 (*synth, pmr, cmr, ms, 3′,4′-di-Me ether*)
Van Acker, F.A.A. *et al., J. Med. Chem.*, 2000, **43**, 3752-3760 (*synth, pmr*)

3′,4′,5′-Trihydroxyflavone T-576

[126432-36-8]
*2-(3,4,5-Trihydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI*

$C_{15}H_{10}O_5$ 270.241
Mp 302°.

Tri-Me ether: [67858-30-4] *3′,4′,5′-Trimethoxyflavone*
$C_{18}H_{16}O_5$ 312.321
Constit. of the flowers of *Primula veris* (cowslip). Cryst. (MeOH). Mp 175-176°.

Nagarathnam, D. *et al., J.O.C.*, 1991, **56**, 4884-4887 (*synth*)
Nagarathnam, D. *et al., Tetrahedron*, 1991, **47**, 5071-5076 (*synth, deriv*)
Gothelf, K.V. *et al., Acta Chem. Scand.*, 1994, **48**, 61-67 (*synth, deriv*)
Huck, C.W. *et al., Planta Med.*, 1999, **65**, 491 (*isol, deriv*)

3,4′,7-Trihydroxyflavone T-577

[2034-65-3]
*3,7-Dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one. 4′,7-Dihydroxyflavonol.* ***Resokaempferol****. 5-Deoxykaempferol*

$C_{15}H_{10}O_5$ 270.241
Isol. from *Cicer arietinum* (chickpea). Light yellow needles (EtOH or AcOH aq.). Mp 310° (304-306°).

3-O-*β-D-Glucopyranoside:Resokaempferol 3-glucoside*
$C_{21}H_{20}O_{10}$ 432.383

4′-O-*β-D-Glucopyranoside:* [24502-04-3] *Resokaempferol 4′-glucoside*
$C_{21}H_{20}O_{10}$ 432.383

7-O-*β-D-Glucopyranoside:* [16290-10-1] *Resokaempferol 7-glucoside*
$C_{21}H_{20}O_{10}$ 432.383

7-O-*Rutinoside:Resokaempferol 7-rutinoside*
$C_{27}H_{30}O_{14}$ 578.526

3-O-*β-D-Apiofuranoside, 7*-O-*α-L-rhamnopyranoside:* [99208-34-1]
$C_{26}H_{28}O_{13}$ 548.499

7-Me ether: [84638-53-9] *3,4′-Dihydroxy-7-methoxyflavone*
$C_{16}H_{12}O_5$ 284.268
Pale yellow solid. Mp 219-220°.

3,7-Di-Me ether: [111391-83-4] *4′-Hydroxy-3,7-dimethoxyflavone*
$C_{17}H_{14}O_5$ 298.295

Kirby, K.S. *et al., Biochem. J.*, 1955, **60**, 582 (*isol, struct, synth*)
Wong, E. *et al., Phytochemistry*, 1965, **4**, 89 (*isol, synth*)
Hillis, W.E. *et al., Phytochemistry*, 1966, **5**, 483 (*isol*)
Feik, F. *et al., Mikrochim. Acta*, 1967, 900 (*detn, Th*)
Markham, K.R. *et al., Phytochemistry*, 1968, **7**, 791; 1970, **9**, 2359 (*glucosides*)
Wong, E. *et al., Phytochemistry*, 1968, **7**, 2123 (*4′-glucoside*)
Holzbecher, Z. *et al., Handbook of Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976,
Jay, M. *et al., Biochem. Syst. Ecol.*, 1980, **8**, 127 (*isol*)
Camarda, L. *et al., Heterocycles*, 1983, **20**, 39 (*7-Me ether*)
Maurya, R. *et al., J. Nat. Prod.*, 1984, **47**, 179 (*isol*)

3′,4′,7-Trihydroxyflavone T-578

[2150-11-0]
*2-(3,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one*

$C_{15}H_{10}O_5$ 270.241
Yellow needles (MeOH/$CHCl_3$). Mp 331-332° (318-322° dec.).

▶ DJ3010000

4′-Me ether: [54867-60-6] *3′,7-Dihydroxy-4′-methoxyflavone.* ***Farnisin***
$C_{16}H_{12}O_5$ 284.268
Constit. of the seeds of *Acacia farnesiana* (sweet acacia). Pale yellow needles (MeOH). Mp 264-265°. λ_{max} 235 ; 338 (MeOH).

Sahu, N.P. *et al., Phytochemistry*, 1998, **49**, 1425-1426 (*Farnisin*)

3′,5,6-Trihydroxyflavone T-579

*5,6-Dihydroxy-2-(3-hydroxyphenyl)-4*H*-1-benzopyran-4-one*

$C_{15}H_{10}O_5$ 270.241

Tri-Me ether: [17182-55-7] ***3′,5,6-Trimethoxyflavone***
$C_{18}H_{16}O_5$ 312.321
Isol. from *Casimiroa edulis* (Mexican apple). Cryst. (EtOAc/petrol). Mp 126-127°.

Dreyer, D.L. *et al., J.O.C.*, 1968, **33**, 3577 (*isol, synth*)

3,5,7-Trihydroxyflavone, 8CI T-580

[548-83-4]
*3,5,7-Trihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI. 5,7-Dihydroxyflavonol.* ***Galangin****. Norizalpinin*

$C_{15}H_{10}O_5$ 270.241
Constit. of Galanga root (*Alpinia officinarum*). Yellow needles (EtOH). Sol. EtOH, MeOH. Mp 214-215° Mp 217-218°.

▶ LK9275500

Tri-Ac:
Mp 142°.

3-O-*β-D-Glucopyranoside:* [68592-14-3] *Galangin 3-glucoside.* ***Galanginin***
$C_{21}H_{20}O_{10}$ 432.383
Light yellow cryst. Mp 218-220°. $[\alpha]_D^{20}$ -45 (c, 0.2 in MeOH).

7-O-*β-D-Glucopyranoside:* [68592-13-2] *Galangin 7-glucoside*
$C_{21}H_{20}O_{10}$ 432.383

3-O-*α-L-Rhamnopyranoside:Galangin 3-rhamnoside*
$C_{21}H_{20}O_9$ 416.384

7-O-*α-L-Rhamnopyranoside:* [72463-31-1] *Galangin 7-rhamnoside*
$C_{21}H_{20}O_9$ 416.384
Isol. from *Artocarpus lakoocha* (lakoocha).

3-O-*[β-D-Galactopyranosyl-(1→4)-α-L-rhamnopyranoside]:* [73030-72-5]
$C_{27}H_{30}O_{14}$ 578.526
Isol. from *Artocarpus lakoocha* (lakoocha). Mp 85-87°.

3-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [16268-50-1] ***Galanginoside****. Galangin 3-rutinoside*
$C_{27}H_{30}O_{14}$ 578.526

3,7-Di-O-*α-L-rhamnopyranoside:* [120976-46-7] ***Celastroside****. Celastrozide*
$C_{27}H_{30}O_{13}$ 562.526Lit. not accessible.

3-Me ether: [6665-74-3] *5,7-Dihydroxy-3-methoxyflavone*
$C_{16}H_{12}O_5$ 284.268
Occurs in Galanga root. Light yellow cryst. (MeOH). Mp 299°.

3-Me ether, 7-O-*β-D-glucopyranoside:*
$C_{22}H_{22}O_{10}$ 446.41

5-Me ether: [104594-69-6] *3,7-Dihydroxy-5-methoxyflavone. 7-Hydroxy-5-methoxyflavonol*
$C_{16}H_{12}O_5$ 284.268

7-Me ether: [480-14-8] *3,5-Dihydroxy-7-methoxyflavone. 5-Hydroxy-7-methoxyflavonol.* ***Izalpinin***
$C_{16}H_{12}O_5$ 284.268
Mp 195-196°.

*7-Me ether, 3-*O*-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [26260-14-0] ***Cannabin***
$C_{28}H_{32}O_{14}$ 592.552
Mp 232-233°.

5,7-Di-Me ether: [15236-07-4] *3-Hydroxy-5,7-dimethoxyflavone. 5,7-Dimethoxyflavonol*
$C_{17}H_{14}O_5$ 298.295
Pale yellow cryst. (EtOH). Mp 178-180° (174°).

3,7-Di-Me ether: [70786-48-0] *5-Hydroxy-3,7-dimethoxyflavone*
$C_{17}H_{14}O_5$ 298.295
Yellow needles ($CHCl_3$/MeOH). Mp 129-130°.

Tri-Me ether: [26964-29-4] *3,5,7-Trimethoxyflavone*
$C_{18}H_{16}O_5$ 312.321
Cryst. (MeOH). Mp 201-203°. λ_{max} 262 ; 295 ; 325 (MeOH) (Berdy). λ_{max} 262 ; 295 ; 325 (MeOH-NAOH) (Berdy).

[19184-08-8]

Chavan, J.J. *et al., J.C.S.*, 1933, 368 (*synth*)
Khimura, *et al., Yakugaku Zasshi*, 1935, **55**, 229 (*isol*)
Goel, R.N. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1958, **47**, 191 (*Izalpinin*)
Katyal, M. *et al., J. Indian Chem. Soc.*, 1962, **39**, 585; 1963, **40**, 121 (*detn, U, Th*)
Katyal, M. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1963, **57**, 259 (*detn, Zr*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Fukui, K. *et al., Nippon Kagaku Zasshi*, 1965, **86**, 1079 (*Izalpinin*)
Audier, A. *et al., Bull. Soc. Chim. Fr.*, 1966, 2892 (*ms, Izalpinin*)
Grisebach, H. *et al., Phytochemistry*, 1968, **7**, 51 (*3-rutinoside*)
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1969, **5**, 178; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 153 (*Cannabin, Galanginoside*)
Nevskaya, E.M. *et al., Zh. Anal. Khim.*, 1972, **27**, 1899 (*detn, Al, Be, Ti, U, Zr*)
Franca, N.C. *et al., Phytochemistry*, 1976, **15**, 572 (*3,5,7-Trimethoxyflavone*)
Chawla, H.M. *et al., Tet. Lett.*, 1976, 2171 (*synth, uv*)
Gaydou, E.M. *et al., Ann. Chim. (Paris)*, 1977, **2**, 303 (*synth, uv, cmr*)
Wenkert, E. *et al., Phytochemistry*, 1977, **16**, 1811 (*cmr*)
Ulubelen, A. *et al., J. Nat. Prod.*, 1978, **41**, 435 (*glucosides*)
Looker, J.H. *et al., J.O.C.*, 1978, **43**, 2344 (*synth*)
Stepien, W.O. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1978, **52**, 2167 (*3-Me ether, 7-glucoside*)
Wollenweber, E. *et al., Flora (Jena, 1818-1865)*, 1979, **168**, 138 (*5-Hydroxy-3,7-dimethoxyflavone*)
Chauhan, J.S. *et al., Indian J. Chem., Sect. B*, 1979, **18**, 473 (*7-galactosylrhamnoside*)
Chauhan, J.S. *et al., Planta Med.*, 1979, **37**, 86 (*7-rhamnoside*)
Buschi, C.A. *et al., Phytochemistry*, 1980, **19**, 903 (*3,5,7-Trimethoxyflavone*)
Zapesochnaya, G.G. *et al., Khim. Prir. Soedin.*, 1982, **18**, 651; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 618 (*Galanginin*)
Hitz, C. *et al., Z. Naturforsch., C*, 1982, **37**, 337 (*3-Hydroxy-5,7-dimethoxyflavone*)
Bankova, V.S. *et al., J. Nat. Prod.*, 1983, **46**, 471
Jaipetch, T. *et al., Phytochemistry*, 1983, **22**, 625 (*isol*)
Saxena, M. *et al., J. Nat. Prod.*, 1986, **49**, 205 (*3-rhamnoside*)
Wleklik, M. *et al., CA*, 1989, **111**, 173u (*Celastrozide*)
Parmar, S.V. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 244 (*synth, bibl*)
Deng, B.-L. *et al., Liebigs Ann./Recl.*, 1997, 2169-2175 (*3-Me ether*)
Zhang, S.-M. *et al., Youji Huaxue*, 1998, **18**, 259-262 (*activity*)
Kubo, I. *et al., Bioorg. Med. Chem.*, 2000, **8**, 1749-1755 (*isol, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GAZ000

4′,5,7-Trihydroxyflavone T-581

[520-36-5]
*5,7-Dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Apigenin****. Apigenol. Pelargidenone. Versulin*

$C_{15}H_{10}O_5$ 270.241
Flavone found in a wide variety of foodstuffs; buckwheat, cabbage, celeriac, celery, lettuce, oregano, parsley, peppermint, perilla, pummelo juice, thyme, sweet potatoes, green tea and wild carrot. Yellow needles (Py aq.). Sol. EtOH, MeOH. Mp 352°. Log P 0.98 (calc). λ_{max} 269 (ε 18800); 340 (ε 20900) (MeOH) (Berdy).

► LK9276000

7-O-Sulfate: [56857-56-8]
$C_{15}H_{10}O_8S$ 350.305
Isol. from *Bixa orellana* (annatto). No phys. props. reported.

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [17306-46-6] *Apigenin 7-neohesperidoside.* ***Rhoifolin****. Rhoifoloside*
$C_{27}H_{30}O_{14}$ 578.526
Isol. from *Citrus aurantium* (Seville orange). Cryst. + $6H_2O$ (H_2O). Mp 245° (anhyd. 205-208°) Mp 251-253°. $[\alpha]_D^{29}$ -110 (c, 0.21 in MeOH).

5-O-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranoside]: [109232-76-0] ***Camellianin B***
$C_{27}H_{30}O_{14}$ 578.526
Constit. of the folk beverage Baishuica (*Camellia sinensis*). Mp 328-330°.

5-O-[α-L-Rhamnopyranosyl-(1→4)-6-O-acetyl-β-D-glucopyranoside]: [109232-77-1] ***Camellianin A***
$C_{29}H_{32}O_{15}$ 620.563
Constit. of the folk beverage Baishuica (*Camellia sinensis*). Mp 196-197°.

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-galacturonopyranoside]: [124167-97-1]
$C_{27}H_{28}O_{15}$ 592.509
Isol. from flowers of *Silybum marianum* (milk thistle).

7-O-[β-D-Galactopyranosyl-(1→4)-β-D-mannopyranoside]: [84638-36-8]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from seeds of carrot (*Daucus carota*). Cryst. (MeOH). Mp 268-270°.

7-O-[β-D-Galacturonopyranosyl-(1→?)-β-D-galacturonopyranoside]: [126254-75-9] *Apigenin 7-digalacturonoside*
$C_{27}H_{26}O_{17}$ 622.492
Isol. from seeds of *Cuminum cyminum* (cumin).

7-O-[β-D-Galacturonopyranosyl-(1→?)-β-D-galacturonopyranoside], 4′-O-β-D-glucopyranoside: [126207-51-0] *Apigenin 7-digalacuronoside 4′-glucoside*
$C_{33}H_{36}O_{22}$ 784.634
Isol. from *Cuminum cyminum* (cumin).

*4′-O-[4-Hydroxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 7-*O*-β-D-glucuronopyranoside:*
$C_{42}H_{40}O_{25}$ 944.763
Constit. of alfalfa (*Medicago sativa*). Amorph. powder. Mp 197-198°. $[\alpha]_D^{20}$ -52.4 (c, 0.1 in MeOH). λ_{max} 272 (sh) ; 314 (MeOH).

*4′-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{37}H_{34}O_{20}$ 798.664
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 197-198°. $[\alpha]_D^{20}$ -74.2 (c, 0.1 in MeOH). λ_{max} 271 (sh) ; 325 (MeOH).

*4′-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 7-*O*-β-D-glucuronopyranoside:*
$C_{43}H_{42}O_{26}$ 974.789
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 197-198°. $[\alpha]_D^{20}$ -10.2 (c, 0.1 in MeOH). λ_{max} 270 (sh) ; 319 (MeOH).

7-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 4′-O-β-D-glucuronopyranoside:
$C_{33}H_{34}O_{23}$ 798.618
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 182-183° dec. $[\alpha]_D^{20}$ -50.8 (c, 0.05 in MeOH aq.).

*7-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 4′-O-β-D-glucuronopyranoside:*
$C_{43}H_{42}O_{26}$ 974.789
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 205-206°. $[\alpha]_D^{20}$ -13.8 (c, 0.1 in MeOH). λ_{max} 271 ; 323 (MeOH).

*7-O-[4-Hydroxy-*E*-cinnamoyl-(→2)-[β-D-glucuronopyranosyl-(1→3)]-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{42}H_{40}O_{25}$ 944.763
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 203-204°. $[\alpha]_D^{20}$ -61 (c, 0.1 in MeOH). λ_{max} 271 ; 323 (MeOH).

*7-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-[β-D-glucuronopyranosyl-(1→3)]-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{43}H_{42}O_{26}$ 974.789
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 210-211°. $[\alpha]_D^{20}$ -50.8 (c, 0.1 in MeOH). λ_{max} 271 ; 323 (MeOH).

Tri-Me ether: [5631-70-9] *4′,5,7-Trimethoxyflavone*
$C_{18}H_{16}O_5$ 312.321
Occurs in the peel of *Citrus reticulata* (mandarin). Needles (EtOH). Mp 156-157°.

[14134-41-9, 28629-51-8, 41375-89-7, 88083-10-

7]
Seikel, M.J. *et al., J.A.C.S.*, 1955, **77**, 5685 (*derivs*)
Coussio, J.D. *et al., Experientia*, 1964, **20**, 562 (*Rhoifolin*)
Wagner, H. *et al., Chem. Ber.*, 1969, **102**, 2083; 1971, **104**, 1704; 2681 (*isol, synth, derivs, Rhoifolin*)
Harborne, J.B. *et al., Phytochemistry*, 1975, **14**, 1331 (*7-sulfate*)
Matsuura, S. *et al., Chem. Pharm. Bull.*, 1978, **26**, 305 (*synth, 4′,5,7-Trimethoxyflavone*)
Kanao, M. *et al., Yakugaku Zasshi*, 1978, **98**, 366 (*Rhoifolin*)
Gupta, K.R. *et al., Planta Med.*, 1982, **46**, 240 (*7-galactosylmannoside*)
Voigtlaender, H.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 219 (*synth, Rhoifolin*)
Jaipetch, T. *et al., Phytochemistry*, 1983, **22**, 625 (*4′,5,7-Trimethoxyflavone*)
Tamura, H. *et al., Tet. Lett.*, 1983, **24**, 5749
Loo, P.V. *et al., Magn. Reson. Chem.*, 1986, **24**, 879 (*pmr, cmr*)
Cheng, G. *et al., Yaoxue Xuebao*, 1987, **22**, 203-207 (*Camellianins*)
Plant Flavonoids in Biology and Medicine II, (eds. Cody V. *et al*), A.R. Liss, N.Y., 1988, 251
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Ahmed, A.A. *et al., Phytochemistry*, 1989, **28**, 1751 (*7-rhamnosylgalacturonoside*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995,
Manthey, J.A. *et al., Curr. Med. Chem.*, 2001, **8**, 135-153 (*rev, activity*)
Stochmal, A. *et al., J. Agric. Food Chem.*, 2001, **49**, 786-758 (*alfalfa glucuronides*)
Stochmal, A. *et al., Phytochemistry*, 2001, **57**, 1223-1226 (*alfalfa glucuronides*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CDH250

5,6,7-Trihydroxyflavone T-582

[491-67-8]
*5,6,7-Trihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, 9CI.* ***Baicalein****. Noroxylin*

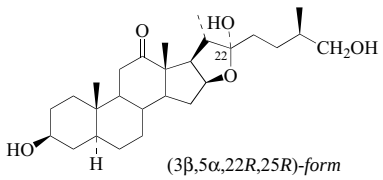
$C_{15}H_{10}O_5$ 270.241
Yellow or brown-yellow prisms (MeOH or EtOH). Sol. MeOH, Et_2O; poorly sol. H_2O, hexane. Mp 223-226° Mp 263-264° dec. Log P 1.05 (calc). λ_{max} 247 (ϵ 58800); 274 (ϵ 42669); 323 (ϵ 17780) (MeOH) (Berdy).

*7-Me ether, 6-*O*-[α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranoside]:* [192224-98-9]
$C_{28}H_{32}O_{13}$ 576.553
Constit. of oregano (*Origanum vulgare*). Yellow cryst. Mp 238-239.3°. λ_{max} 250 ; 279 ; 318 (MeOH).

6,7-Methylene ether: [110204-45-0] *5-Hydroxy-6,7-methylenedioxyflavone.* ***Cochliophilin A***
$C_{16}H_{10}O_5$ 282.252
Isol. as Cochliophilin A from spinach (*Spinacia oleracea*). Yellow cryst. Mp 205° dec.

Horio, T. *et al., Experientia*, 1992, **48**, 410 (*Cochliophilin A*)
Zheng, S. *et al., Indian J. Chem., Sect. B*, 1997, **36**, 104-106 (*6-rhamnosylfucoside*)

3,22,26-Trihydroxyfurostan-12-one T-583



(3β,5α,22*R*,25*R*)-*form*

$C_{27}H_{44}O_5$ 448.642

(3β,5α,22*R*,25*R*)-*form*

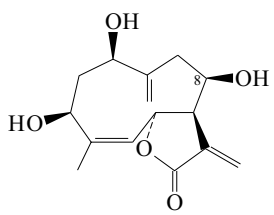
*3-*O*-[α-L-Rhamnopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)-β-D-glucopyranosyl]-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside:* [58546-20-6] ***Agavoside G***
$C_{62}H_{102}O_{33}$ 1375.468
Constit. of the famine food *Agave americana*. Mp 240-245°. $[\alpha]_D^{20}$ -130 (c, 1.0 in MeOH).

*3-*O*-[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)-β-D-glucopyranosyl]-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside:* [58546-21-7] ***Agavasaponin H****. Agavoside H*
$C_{68}H_{112}O_{37}$ 1521.611
Constit. of leaves of the famine food *Agave americana*. Mp 228-230°. $[\alpha]_D^{20}$ -113 (c, 0.62 in MeOH).

► LV2980000

Wilkomirski, B. *et al., Phytochemistry*, 1975, **14**, 2657 (*Agavasaponin H*)
Kintya, P.K. *et al., Khim. Prir. Soedin.*, 1976, **12**, 486; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 427 (*Agavoside G*)

1,3,8-Trihydroxy-4,10(14),11(13)-germacratrien-12,6-olide T-584



(1β,3β,4*Z*,6α,8β)-*form*

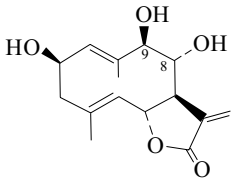
$C_{15}H_{20}O_5$ 280.32

(1ξ,3β,4*Z*,6α,8α)-*form*

8-Angeloyl: ***Hydroxyisonobilin***
$C_{20}H_{26}O_6$ 362.422
Constit. of *Anthemis nobilis* (Roman chamomile). Cryst. (MeOH/Et_2O). Mp 144-146°. $[\alpha]_D^{20}$ +35.4 (c, 0.35 in MeOH).

Ober, A.G. *et al., Phytochemistry*, 1985, **24**, 1743; 1986, **25**, 877
Jakupovic, J. *et al., Phytochemistry*, 1992, **31**, 863-880
De Gutiérrez, A.N. *et al., Phytochemistry*, 1995, **39**, 795-800 (*deriv*)
Samek, Z. *et al., Coll. Czech. Chem. Comm.*, 1997, **42**, 1065-1068 (*Hydroxyisonobilin*)

2,8,9-Trihydroxy-1(10),4,11(13)-germacratrien-12,6-olide T-585



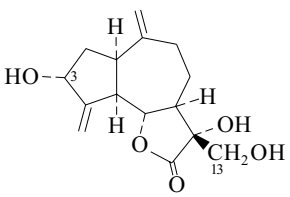
$C_{15}H_{20}O_5$ 280.32

(1(10)*E*,2β,4*E*,6α,8ξ)-*form*

9-Ketone: ***2β,9ξ-Dihydroxy-8-oxo-1(10),4,11(13)-germacratrien-12,6α-olide***
$C_{15}H_{18}O_5$ 278.304
Isol. from *Tanacetum vulgare* (tansy). Oil.

Chandra, A. *et al., Phytochemistry*, 1987, **26**, 1463 (*ketone*)

3,11,13-Trihydroxy-4(15),10(14)-guaiadien-12,6-olide T-586



$C_{15}H_{20}O_5$ 280.32

(1α,3β,5α,6α,11α)-*form* [22738-70-1] ***Solstitialin****. Solstitialin A*
Cryst. Mp 206-207°.

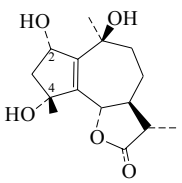
► Neurotoxin.

4β,15-Dihydro: [70894-20-1] *3,11,13-Trihydroxy-10(14)-guaien-12,6-olide.* ***Cynaratriol***
$C_{15}H_{22}O_5$ 282.336
Constit. of *Cynara cardunculus* (cardoon) and *Cynara scolymus* (globe artichoke). Cryst. (EtOAc). Mp 178-179°. $[\alpha]_D^{20}$ +56 (c, 0.6 in $CHCl_3$/MeOH).

*4β,15-Dihydro, 3-*O*-β-D-glucopyranoside:* [117804-06-5] ***Cynaroside A***
$C_{21}H_{32}O_{10}$ 444.478
Constit. of *Cynara cardunculus* (cardoon). Amorph. powder. $[\alpha]_D^{23}$ +38.3 (c, 1.37 in MeOH).

Bernhard, H.O. *et al., Helv. Chim. Acta*, 1979, **62**, 1288 (*Cynaratriol*)
Shimiza, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2466 (*Cynaroside A*)

2,4,10-Trihydroxy-1(5)-guaien-12,6-olide T-587



(2α,4α,6α,10β,11α)-*for*

$C_{15}H_{22}O_5$ 282.336

(2α,4α,6α,10β,11α)-*form* [81907-05-3]
Artabsinolide C
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOAc). Mp 135-137°. $[\alpha]_D$ -22 (c, 0.1 in $CHCl_3$).

2-Ketone: [82078-63-5] *4,10-Dihydroxy-2-oxo-1(5)-guaien-12,6-olide.* ***Artabsinolide A***
$C_{15}H_{20}O_5$ 280.32
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOH). Mp 160-162°. $[\alpha]_D$ +9 (c, 0.1 in $CHCl_3$).

(2β,4β,6α,10β,11α)-*form* [81907-04-2]
Artabsinolide D
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOAc). Mp 143-145°. $[\alpha]_D$ -51 (c, 0.1 in $CHCl_3$).

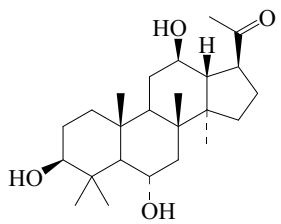
2-Ketone: [76564-29-9] ***Artabsinolide B***. *Artemoline*
$C_{15}H_{20}O_5$ 280.32
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOAc/hexane). Mp 180-182° Mp 205°. $[\alpha]_D$ +20 (c, 0.1 in $CHCl_3$).

Kasymov, S.Z. *et al., Khim. Prir. Soedin.*, 1979, **15**, 658; *Chem. Nat. Compd. (Engl. Transl.)*, 577

Beauhaire, J. *et al., J.C.S. Perkin 1*, 1982, 861

3,6,12-Trihydroxy-22,23,24,25,26,27-hexanordammaran-20-one T-588

3,6,12-Trihydroxy-4,4,8,14-tetramethyl-18-norpregnan-20-one



$C_{24}H_{40}O_4$ 392.578

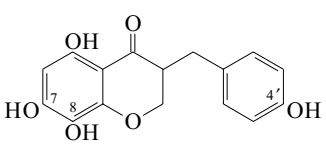
(3β,6α,12β)-*form*

6-O-β-D-Glucopyranoside: [335157-20-5]
Notoginsenoside R$_{10}$
$C_{30}H_{50}O_9$ 554.72
Constit. of *Panax notoginseng* (sanchi) roots. Powder.

Li, H.Z. *et al., Chin. Chem. Lett.*, 2001, **12**, 59-62 (*isol, pmr, cmr*)

5,7,8-Trihydroxy-3-(4-hydroxybenzyl)-4-chromanone T-589

2,3-Dihydro-5,7,8-trihydroxy-3-[(4-hydroxyphenyl)methyl]-4H-1-benzopyran-4-one



$C_{16}H_{14}O_6$ 302.283

7-Me ether: [93078-83-2] *5,8-Dihydroxy-3-(4-hydroxybenzyl)-7-methoxy-4-chromanone. 8-*O*-Demethyl-7-*O*-methyl-3,9-dihydropunctatin*
$C_{17}H_{16}O_6$ 316.31
Isol. from *Muscari comosum* (tassel hyacinth). Cryst. ($CHCl_3$). Mp 172-174°.

7-Me ether, 8-Ac: [99877-75-5]
$C_{19}H_{18}O_7$ 358.347
From *Muscari comosum* (tassel hyacinth). Cryst. ($CHCl_3$/hexane). Mp 155-156°. $[\alpha]_D$ -18 (c, 0.3 in MeOH).

8-Me ether: [27245-79-0] *5,7-Dihydroxy-3-(4-hydroxybenzyl)-8-methoxy-4-chromanone. 3,9-Dihydropunctatin*
$C_{17}H_{16}O_6$ 316.31
Yellow cryst. Mp 204-206°. $[\alpha]_D^{24}$ -37 (dioxan).

4′,8-Di-Me ether: [27245-80-3] *5,7-Dihydroxy-8-methoxy-3-(4-methoxybenzyl)-4-chromanone. 4′-*O*-Methyl-3,9-dihydropunctatin*
$C_{18}H_{18}O_6$ 330.337

7,8-Di-Me ether: [93078-82-1] *5-Hydroxy-3-(4-hydroxybenzyl)-7,8-dimethoxy-4-chromanone. 7-*O*-Methyl-3,9-dihydropunctatin*
$C_{18}H_{18}O_6$ 330.337
Isol. from *Muscari comosum* (tassel hyacinth). Vitreous solid.

4′,5,7-Tri-Me ether:8-Hydroxy-5,7-dimethoxy-3-(4-methoxybenzyl)-4-chromanone
$C_{19}H_{20}O_6$ 344.363
Yellow oil. $[\alpha]_D^{25}$ -109.9 (c, 0.23 in MeOH). λ_{max} 205 (log ε 4.39); 285 (log ε 4.13); 345 (log ε 3.6) (MeOH).

Tetra-Me ether: [27245-82-5]
Mp 99-100°.

(±)-*form*

8-Me ether: [34818-64-9]
Cryst. ($CHCl_3$). Mp 228-231°.

Finckh, R.E. *et al., Experientia*, 1970, **26**, 472 (*isol, struct*)

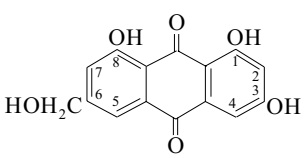
Farkas, L. *et al., Tetrahedron*, 1971, **27**, 5049 (*4′,8-Di-Me ether*)

Adinolfi, M. *et al., Phytochemistry*, 1984, **23**, 2091; 1985, **24**, 2423 (*7-Me ether, 7,8-di-Me ether*)

Silayo, A. *et al., Phytochemistry*, 1999, **52**, 947-955 (*4′,5,7-tri-Me ether*)

1,3,8-Trihydroxy-6-hydroxymethylanthraquinone T-590

[481-73-2]
Citreorosein. *ω-Hydroxyemodin*



$C_{15}H_{10}O_6$ 286.24
Found in roots of *Polygonum cuspidatum* (Japanese knotweed). Yellow-orange needles (EtOH). Mp 282° Mp 288°. λ_{max} 224 (log ε 4.4); 250 (log ε 4.15); 268 (sh) (log ε 4.12); 295 (log ε 3.95); 440 (log ε 3.92); 455 (log ε 3.9) (EtOH). λ_{max} 221 (ε 25700); 252 (ε 15500); 290 (ε 15500); 438 (ε 9000) (EtOH) (Berdy).

1-Me ether: [35688-09-6] *1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthraquinone.* ***Questinol***
$C_{16}H_{12}O_6$ 300.267
Isol. from roots of *Polygonum cuspidatum* (Japanese knotweed). Yellow cryst. (EtOH). Mp 280-282°.

3-Me ether: [569-05-1] *1,8-Dihydroxy-3-hydroxymethyl-6-methoxyanthraquinone.* ***Fallacinol***. *Teloschistin*
$C_{16}H_{12}O_6$ 300.267
Red cryst. Mp 246-247°. λ_{max} 224 ; 250 ; 265 ; 287 ; 433 ; 455 (MeOH) (Berdy).

8-Me ether:1,3-Dihydroxy-6-hydroxymethyl-8-methoxyanthraquinone. ***Carviolin***. *Roseopurpurin*
$C_{16}H_{12}O_6$ 300.267
Yellow needles (AcOH). Mp 286°. λ_{max} 210 ; 248 ; 267 ; 278 ; 284 ; 434 (EtOH) (Berdy).

3-Me ether, 1′-Ac: [20194-61-0] *Fallacinol ω-*O*-acetate. 2-Acetoxymethyl-4,5-dihydroxy-7-methoxyanthraquinone. 3-Acetoxymethyl-1,8-dihydroxy-6-methoxyanthraquinone*
$C_{18}H_{14}O_7$ 342.304
Mp 195-196°.

1,3-Di-Me ether: [33982-71-7] *8-Hydroxy-6-hydroxymethyl-1,3-dimethoxyanthraquinone. Citreosein 6,8-dimethyl ether. 1-Hydroxy-3-hydroxymethyl-6,8-dimethoxyanthraquinone, 8CI*
$C_{17}H_{14}O_6$ 314.294
Orange needles. Mp 237-239°.

*1′,8-Di-Me ether:1,3-Dihydroxy-8-methoxy-6-methoxymethylanthraquinone. 6,8-Di-*O*-methyl-ω-hydroxyemodin*
$C_{17}H_{14}O_6$ 314.294
Orange needles. Mp 238-240°.

Anslow, W.K. *et al., Biochem. J.*, 1940, **34**, 159 (*isol*)

Howard, B.H. *et al., Biochem. J.*, 1955, **59**, 485 (*uv*)

Rajagopalan, T.R. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1956, **44**, 418 (*synth*)

Bloom, H. *et al., J.C.S.*, 1959, 178 (*ir*)

Santesson, J. *et al., Phytochemistry*, 1970, **9**, 2149 (*isol*)

Gottlieb, O.R. *et al., Phytochemistry*, 1971, **10**, 1379 (*isol, deriv*)

Steglich, W. *et al., Chem. Ber.*, 1972, **105**, 2922 (*isol*)

Hirose, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 4186 (*synth, pmr*)

Nikaido, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3075 (*props*)

Benfaremo, N. *et al., J.O.C.*, 1985, **50**, 139 (*synth*)

Kalidhar, S.B. *et al., Phytochemistry*, 1989, **28**, 3459 (*pmr*)

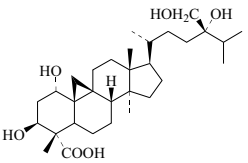
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, pmr*)

Buchanan, M.S. *et al., Aust. J. Chem.*, 1998, **51**, 103-109 (*isol, uv, pmr, cmr*)

Manojlovic, N.T. *et al., J. Serb. Chem. Soc.*, 1998, **67**, 7-11; *CA*, **128**, 203019x (*Fallacinol, activity*)

1,3,24-Trihydroxy-24-(hydroxymethyl)cycloartan-28-oic acid T-591

1,3,24,31-Tetrahydroxy-24-methylcycloartan-28-oic acid



(1α,3β,24S)-*form*

$C_{31}H_{52}O_6$ 520.748

(1α,3β,24*S*)-*form* [292167-35-2]
Cyclopassifloic acid B
Constit. of *Passiflora edulis* (passion fruit). Amorph. powder. $[\alpha]_D^{25}$ +48.7 (c, 2.2 in MeOH).

28-O-*β*-D-*Glucopyranosyl ester:* [292167-39-6] ***Cyclopassifloside II***
$C_{37}H_{62}O_{11}$ 682.89
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{25}$ +46.8 (c, 6.8 in MeOH).

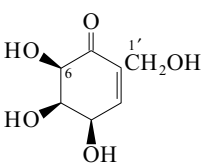
31-O-*β*-D-*Glucopyranoside, 28*-O-*β*-D-*glucopyranosyl ester:* [292167-40-9] ***Cyclopassifloside III***
$C_{43}H_{72}O_{16}$ 845.032
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{25}$ +25.7 (c, 3.5 in MeOH).

(1α,3β,24ξ)-*form* [239794-24-2]
Cyclotricuspidogenin A
$[\alpha]_D^{18}$ +35.1 (c, 2.1 in Py).

31-O-*β*-D-*Glucopyranoside, 28*-O-*β*-D-*glucopyranosyl ester:* [239794-21-9] ***Cyclotricuspidoside A***
$C_{43}H_{72}O_{16}$ 845.032
$[\alpha]_D^{23}$ +24.5 (c, 1 in MeOH).

Kasai, R. *et al., Phytochemistry*, 1999, **51**, 803-808 (*isol, pmr, cmr*)
Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 1229-1234 (*Cyclopassifloic acid B, Cyclopassiflosides*)

4,5,6-Trihydroxy-2-hydroxymethyl-2-cyclohexen-1-one T-592



(4*R*,5*R*,6*R*)-*form*

$C_7H_{10}O_5$ 174.153

(4*R*,5*R*,6*S*)-*form*

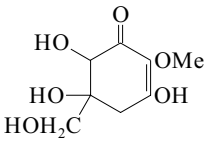
6-O-*(2-Hydroxy-6-methylbenzoyl):*
[146475-71-0]
$C_{15}H_{16}O_7$ 308.287
Prod. by a *Phoma* sp. on leaves and stalks of rhubarb. λ_{max} 211 (ϵ 23000); 240 (ϵ 9500); 309 (ϵ 2800) (MeOH) (Berdy).

[53496-14-3]

Venkatasubbaiah, P. *et al., J. Nat. Prod.*, 1992, **55**, 639 (*deriv*)

3,5,6-Trihydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-one, 9CI T-593

[76663-30-4]
Gadusol



$C_8H_{12}O_6$ 204.179

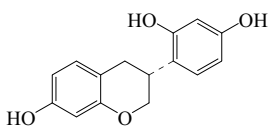
Mycosporine related metabolite. Isol. from the eggs of brine shrimp (*Artemia*), sea urchin, cod and other fish. Amorph. powder (EtOH). Sol. H_2O. Mp 178-179°. Subl.$_{0.03}$ 120. pK_a 4.17 (50% EtOH aq.). λ_{max} 269 (ϵ 12400) (H_2O/HCl) (Derep). λ_{max} 296 (ϵ 22200) (H_2O/NaOH) (Derep). λ_{max} 269 (ϵ 12400) (dil acid) (Derep). λ_{max} 294 (MeOH) (Berdy). λ_{max} 268 (MeOH-HCl) (Berdy).

[105660-63-7]

Chioccara, F. *et al., Bull. Soc. Chim. Belg.*, 1980, **89**, 1101 (*isol, uv, pmr, cmr, ms*)
Grant, P.T. *et al., Tet. Lett.*, 1980, **21**, 4043 (*isol, struct*)
Plack, P.A. *et al., Biochem. J.*, 1981, **199**, 741 (*isol, struct, uv, ir, pmr*)
Grant, P.T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1985, **80**, 755 (*isol*)

2′,4′,7-Trihydroxyisoflavan T-594

[65332-45-8]
*4-(3,4-Dihydro-7-hydroxy-2*H*-1-benzopyran-4-yl)-1,3-benzenediol, 9CI. 3,4-Dihydro-3-(2,4-dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran*. ***Demethylvestitol***



(*R*)-*form*

$C_{15}H_{14}O_4$ 258.273

Compds. in both enantiomeric series appear to occur naturally but in most cases the abs. config.was not detd.. Isol. from *Lablab niger* (hyacinth bean) and *Phaseolus vulgaris* (kidney bean). λ_{max} 209 ; 283 (EtOH) (Berdy). λ_{max} 219 ; 297 (EtOH-NaOH) (Berdy).

2′-Me ether: [63631-42-5] *4′,7-Dihydroxy-2′-methoxyisoflavan*. ***Isovestitol***
$C_{16}H_{16}O_4$ 272.3
Phytoalexin of *Lablab niger* (hyacinth bean). Needles. Mp 95-97°. λ_{max} 209 ; 282 (EtOH) (Berdy). λ_{max} 219 ; 243 ; 295 (EtOH-NaOH) (Berdy).

4′-Me ether: 2′,7-Dihydroxy-4′-methoxyisoflavan, D-540

7-Me ether: [71772-21-9] *2′,4′-Dihydroxy-7-methoxyisoflavan*. ***Neovestitol***
$C_{16}H_{16}O_4$ 272.3
λ_{max} 212 ; 284 ; 289 (EtOH) (Berdy). λ_{max} 215 ; 291 (EtOH-NaOH) (Berdy).

2′,4′-Di-Me ether: [41743-86-6] *7-Hydroxy-2′,4′-dimethoxyisoflavan*. ***Sativan***. *Sativin. 2′-*O*-Methylvestitol*
$C_{17}H_{18}O_4$ 286.327
Phytoalexin of *Medicago* spp., *Trifolium* spp. and *Trigonella* spp.. Cryst. Mp 128-129° (125-127°). $[\alpha]_D^{22}$ -15. Mp. refers to the (*S*)-enantiomer from *D. amazonica* λ_{max} 286 (MeOH) (Berdy).

2′,7-Di-Me ether: [63631-41-4] *4′-Hydroxy-2′,7-dimethoxyisoflavan*. ***Arvensan***
$C_{17}H_{18}O_4$ 286.327
Mp 111-115°. λ_{max} 217 ; 285 ; 290 (MeOH) (Berdy). λ_{max} 205 (ϵ 50000); 225 (ϵ 14800); 281 (ϵ 5900) (EtOH) (Berdy).

4′,7-Di-Me ether: [60102-29-6] *2′-Hydroxy-4′,7-dimethoxyisoflavan*. ***Isosativan***
$C_{17}H_{18}O_4$ 286.327
Phytoalexin of *Trifolium* spp.. λ_{max} 214 ; 281 ; 284 (EtOH) (Berdy). λ_{max} 219 ; 291 (EtOH-NaOH) (Berdy).

(*R*)-*form*

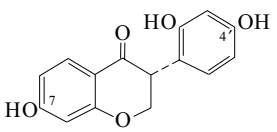
Tri-Me ether: [3722-60-9]
$C_{18}H_{20}O_4$ 300.354
Mp 63°. $[\alpha]_D$ -12 (c, 0.98 in $CHCl_3$).

[64190-84-7, 75556-92-2]

Ingham, J.L. *et al., Nature (London)*, 1973, **242**, 125 (*Sativan*)
Braz Filho, R. *et al., Phytochemistry*, 1975, **14**, 1454 (*isol*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1976, **31**, 331; 1977, **32**, 446,1018; 1979, **34**, 630; 1980, **35**, 384
Ingham, J.L. *et al., Phytochemistry*, 1977, **16**, 1279; 1979, **18**, 1711 (*isol, struct*)
Alves, H.M. *et al., Phytochemistry*, 1978, **17**, 1423 (*synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Herath, H.M.T.B. *et al., Phytochemistry*, 1998, **47**, 117-119 (*isol, pmr, cmr*)
Versteeg, M. *et al., Tetrahedron*, 1999, **55**, 3365-3376 (*R-form, tri-Me ether*)

2′,4′,7-Trihydroxyisoflavanone T-595

[94388-77-9]
*2,3-Dihydro-7-hydroxy-3-(2,4-dihydroxyphenyl)-4*H*-1-benzopyran-4-one. 2′-Hydroxydihydrodaidzein*



(*R*)-*form*

$C_{15}H_{12}O_5$ 272.257
Sol. MeOH.

(*R*)-*form*

2′,4′-Di-Me ether: [70561-31-8] *7-Hydroxy-2′,4′-dimethoxyisoflavanone*. ***Sativanone***
Isol. from *Medicago sativa* (alfalfa) leaves innoculated with the fungus *Helminthosporium cabonum*. $[\alpha]_D$ -35 (c, 0.06 in MeOH).

(±)-*form*
Isol. from pods of *Phaseolus vulgaris* (kidney bean) and also from *Phaseolus coccineus* (scarlet runner bean).

4′-Me ether: [57462-46-1] *2′,7-Dihydroxy-4′-methoxyisoflavanone*. ***Vestitone***
$C_{16}H_{14}O_5$ 286.284
Isol. from *Trifolium repens* (white clo-

ver). λ_{max} 212 ; 277 ; 311 (MeOH) (Berdy). λ_{max} 218 ; 334 (NaOH) (Berdy).

[66211-83-4]

Donnelly, D.M.X. *et al., J.C.S. Perkin 1*, 1973, 1737 (±-*Sativanone*)
Derrick, P.M. *et al., Phytochemistry*, 1977, **16**, 93 (*Vestitone*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1978, **33**, 146 (*Vestitone*)
Woodward, M.D. *et al., Phytochemistry*, 1980, **19**, 921 (*isol, uv, pmr*)
Ingham, J.L. *et al., Planta Med.*, 1982, **45**, 46 (*isol*)
Adesanya, S.A. *et al., Phytochemistry*, 1985, **24**, 2699 (*isol*)
Jain, A.C. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 136 (*synth*)

3′,4′,7-Trihydroxyisoflavanone T-596

*3-(3,4-Dihydroxyphenyl)-2,3-dihydro-7-hydroxy-4*H*-1-benzopyran-4-one*

$C_{15}H_{12}O_5$ 272.257

(±)-*form*

4′-Me ether: [67492-31-3] *3′,7-Dihydroxy-4′-methoxyisoflavanone*
$C_{16}H_{14}O_5$ 286.284
Constit. of *Myroxylon balsamum* (Tolu balsam). Cryst. (MeOH). Mp 185-188°.

3′,4′-Di-Me ether: [83206-83-1] *7-Hydroxy-3′,4′-dimethoxyisoflavanone. 3′-Methoxydihydroformononetin*
$C_{17}H_{16}O_5$ 300.31

Alaide, B. *et al., Phytochemistry*, 1978, **17**, 593 (*isol, struct*)
de Oliveira, A.B. *et al., Phytochemistry*, 1978, **17**, 593
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1
Jain, A.C. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 628 (*synth*)

4′,5,7-Trihydroxyisoflavanone T-597

[21554-71-2]
*2,3-Dihydro-5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one. Dihydrogenistein*

$C_{15}H_{12}O_5$ 272.257

(±)-*form*

Cryst. ($CHCl_3$/MeOH). Mp 221-222°.

7-O-β-D-Glucopyranoside: ***Dihydrogenistin***
$C_{21}H_{22}O_{10}$ 434.399
Constit. of *Glycine max* (soybeans). Amorph. yellow powder. $[\alpha]_D^{25}$ -23.7 (c, 0.5 in MeOH). Stereochem. not confirmed λ_{max} 272 (log ε 4.36); 308 (log ε 3.95) (MeOH).

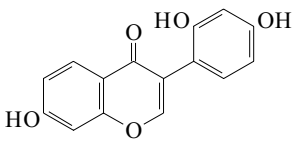
4′-Me ether: [66152-07-6] *5,7-Dihydroxy-4′-methoxyisoflavanone.* ***Dihydrobiochanin A***
$C_{16}H_{14}O_5$ 286.284
Mp 175-177° (167-169°). λ_{max} 214 (ε 26300); 224 (ε 25700); 292 (ε 19050) (EtOH) (Berdy).

[83920-62-1]

Braz Filho, R. *et al., Phytochemistry*, 1973, **12**, 1184 (*isol, ir, ms, pmr, struct*)
Lamberton, J.A. *et al., Aust. J. Chem.*, 1978, **31**, 455 (*synth*)
Jain, A.C. *et al., J.C.S. Perkin 1*, 1986, 215 (*synth*)
Osawa, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2970 (*isol*)
Hosny, M. *et al., J. Nat. Prod.*, 2002, **65**, 805-813 (*Dihydrogenistin*)

2′,4′,7-Trihydroxyisoflavone T-598

[7678-85-5]
*3-(2,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI. 2′-Hydroxydaidzein*



$C_{15}H_{10}O_5$ 270.241
Isol. from pods of *Phaseolus vulgaris* (kidney bean) and *Phaseolus lunatus* (butter bean). Cryst. (MeOH). Mp 275° dec. (synthetic).

4′,7-Di-O-β-D-glucopyranoside: [88048-22-0]
$C_{27}H_{30}O_{15}$ 594.525
Stress metab. from cell suspension cultures of *Vigna angularis* (azuki bean).

4′-Me ether: [1890-99-9] *2′,7-Dihydroxy-4′-methoxyisoflavone.* ***Xenognosin B****. 2′-Hydroxyformononetin*
$C_{16}H_{12}O_5$ 284.268
Isol. from *Trifolium repens* (white clover). Cryst. ($CHCl_3$/MeOH). Mp 215-217°.

Braz Filho, R. *et al., J. Nat. Prod.*, 1977, **40**, 236 (*Xenognosin B*)
Woodward, M.D. *et al., Phytochemistry*, 1980, **19**, 921 (*isol, uv, pmr, ms, struct*)
O'Neill, M.J. *et al., Phytochemistry*, 1986, **25**, 1315 (*isol*)
Brady, W.T. *et al., J.O.C.*, 1988, **53**, 1353 (*synth*)

2′,5,7-Trihydroxyisoflavone T-599

[70943-68-9]
*5,7-Dihydroxy-3-(2-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Isogenistein****. Irilin C*

$C_{15}H_{10}O_5$ 270.241
Dimorphic. Long straw-yellow needles (MeOH) or pale orange needles. Mp 185-187° Mp 222-224° (sinters at 190°). λ_{max} 211 ; 259 ; 328 (MeOH) (Berdy).

7-O-β-D-Glucopyranoside: [70943-69-0]
$C_{21}H_{20}O_{10}$ 432.383
Isol. from rootbark of *Cajanus cajan* (pigeon pea). Needles (EtOH). Mp 200-203°.

Tri-Ac:
$C_{21}H_{16}O_8$ 396.353
Mp 132-134°.

Baker, W. *et al., J.C.S.*, 1963, 1860 (*synth, bibl*)
Bhanumati, S. *et al., Natl. Acad. Sci. Lett. (India)*, 1979, **2**, 53 (*synth*)
Bhanumati, S. *et al., Phytochemistry*, 1979, **18**, 365
Hanawa, F. *et al., Phytochemistry*, 1991, **30**, 157 (*isol*)

3′,4′,7-Trihydroxyisoflavone T-600

[485-63-2]
*3-(3,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, 9CI. 3′-Hydroxydaidzein*

$C_{15}H_{10}O_5$ 270.241
Cryst. (EtOH aq.). Sol. MeOH, HCl; poorly sol. H_2O. Mp 262-265° (252°) Mp 276-280°. All isolations of isoflavonoids from microorganisms are considered suspect λ_{max} 257 (ε); 335 (ε) (MeOH/NaOH) (Derep). λ_{max} 248 (ε); 259 (ε); 292 (ε) (MeOH) (Derep). λ_{max} 259 ; 292 (MeOH/HCl) (Berdy).

4′-Me ether, 7-O-β-D-galactopyranoside: [114272-30-9] *Calycosin 7-galactoside*
$C_{22}H_{22}O_{10}$ 446.41
Isol. from *Trifolium pratense* (red clover).

3′,7-Di-Me ether: [30564-92-2] *4′-Hydroxy-3′,7-dimethoxyflavone.* ***Sayanedin***
$C_{17}H_{14}O_5$ 298.295
Isol. from pods of *Pisum sativum* (pea). Needles (hexane). Mp 165-166°.

Tri-Me ether: [1621-61-0] *3′,4′,7-Trimethoxyisoflavone.* ***Cabreuvin***
$C_{18}H_{16}O_5$ 312.321
Isol. from *Myroxylon balsamum* (Tolu balsam). Cryst. (EtOH). Mp 165° (156-158°).

Dhar, M.L. *et al., J. Sci. Ind. Res., Sect. B*, 1955, **14**, 73 (*isol*)
Gottlieb, O.R. *et al., An. Assoc. Quim. Bras.*, 1959, **18**, 85 (*Cabreuvin*)
Harborne, J.B. *et al., J.O.C.*, 1963, **28**, 881 (*isol*)
Fukui, F. *et al., Nippon Kagaku Kaishi*, 1963, **84**, 189 (*synth*)
Braga de Oliveira, A. *et al., Ann. Acad. Bras. Ci&eenc.*, 1968, **40**, 147 (*isol*)
Markham, K.R. *et al., Phytochemistry*, 1968, **7**, 803 (*glycosides*)
Isogai, Y. *et al., Chem. Pharm. Bull.*, 1970, **18**, 1872 (*Sayanedin*)
Farkas, L. *et al., Acta Chim. Acad. Sci. Hung.*, 1972, **74**, 367 (*synth*)
Kurosawa, K. *et al., Phytochemistry*, 1978, **17**, 1405 (*isol*)
Dewick, P.M. *et al., Phytochemistry*, 1978, **77**, 1751 (*biosynth*)
Kirkiacharian, B.S. *et al., Heterocycles*, 1980, **14**, 1929 (*synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Pathak, V.P. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 778 (*derivs*)
Funayama, S. *et al., J. Antibiot.*, 1989, **42**, 1344; 1350 (*isol, struct, props*)
Nishiyama, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 107 (*synth*)
Ohsaki, A. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 1109-1112 (*Cabreuvin*)

4′,5,7-Trihydroxyisoflavone T-601

[446-72-0]
*5,7-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI.* ***Genistein***†*. Differenol A. Prunetol. Sophoricol. K 254I. Genisteol. NSC 36586*

$C_{15}H_{10}O_5$ 270.241
The major isoflavone in soy beans and isolated soy protein, also found in chick peas *(Cicer arietinum)*, peanuts *(Arachis hypogaea)*, pinto beans, green tea. Nutriceutical with anticancer and bone protective props.. Prisms (EtOH aq.). Mp 301-302° dec. Log P 0.98 (calc). All isolations of isoflavonoids from microorganisms are considered dubious. Methylgenistein, Isogenistin and Methylisogenistin were all

impure Genistein λ_{max} 261 (ϵ 38500) (MeOH) (Derep).

▶ Exp. reprod. effects (large doses). NR2392000

5-O-β-D-Glucopyranoside: [128508-06-5] *Genistein 5-glucoside*
$C_{21}H_{20}O_{10}$ 432.383
Isol. from bark of morello cherry (*Prunus cerasus*).

7-O-β-D-Glucopyranoside: [529-59-9] *Genistein 7-glucoside.* ***Genistin***. *Genistoside*
$C_{21}H_{20}O_{10}$ 432.383
Present in soy foods. Potential nutriceutical. Isol. from *Prunus avium* (wild cherry). Leaflets (EtOH). Mp 254-256° dec. $[\alpha]_D^{21}$ -27.7 (MeOH aq.). λ_{max} 262 (MeOH) (Berdy).

▶ DJ3093000

7-O-(6-O-Acetyl-β-D-glucopyranoside): [73566-30-0] ***6″-O-Acetylgenistin***
$C_{23}H_{22}O_{11}$ 474.42
Isol. from seeds of soybean (*Glycine max*). Present in soy foods. Potential nutriceutical. Needles. Mp 185-186°.

7-O-(6-O-Malonyl-D-glucopyranoside): [51011-05-3] ***Genistein 7-O-glucoside 6″-malonate***. *6″-Malonylgenistin*
$C_{24}H_{22}O_{13}$ 518.43
Present in soy foods. Potential nutriceutical. Glass. Mp 145°.

7-O-[4-Hydroxycinnamoyl-(→2)-β-D-glucopyranoside]: [106915-84-8] *Genistein 7-O-(2-p-coumaroylglucoside)*
$C_{30}H_{26}O_{12}$ 578.528
Isol. from *Trifolium repens* (white clover). Mp 250-252°.

4′-O-α-L-Rhamnopyranoside:Genistein 4′-rhamnoside
$C_{21}H_{20}O_9$ 416.384
Constit. of *Pithecellobium dulce* (manila tamarino). Pale yellow cryst. Mp 301-302°. λ_{max} 264 ; 328 (MeOH).

[52796-14-2]

Rosler, H. *et al., Chem. Ber.*, 1965, **98**, 2193 (*deriv*)
Wagner, H. *et al., Chem. Ber.*, 1967, **100**, 101 (*synth*)
Markham, K.R. *et al., Phytochemistry*, 1968, **7**, 791 (*isol*)
Ganguly, A.K. *et al., Chem. Ind. (London)*, 1970, 201 (*isol*)
Umezawa, H. *et al., J. Antibiot.*, 1975, **28**, 947 (*isol*)
Pelter, A. *et al., Synthesis*, 1976, 326 (*synth, derivs*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799 (*cmr*)
Hazeto, T. *et al., J. Antibiot.*, 1979, **32**, 217 (*isol*)
Ohta, N. *et al., Agric. Biol. Chem.*, 1980, **44**, 469 (*6″-O-Acetylgenistin*)
Asahi, K. *et al., J. Antibiot.*, 1981, **34**, 919 (*uv, ir*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Breytenbach, J.C. *et al., J. Nat. Prod.*, 1986, **49**, 1003 (*isol, deriv*)
Jain, A.C. *et al., J.C.S. Perkin 1*, 1986, 215 (*synth*)
Murthy, M.S.R. *et al., Org. Magn. Reson.*, 1986, **24**, 225 (*cmr*)
Goto, *et al., Agric. Biol. Chem.*, 1987, **51**, 3003 (*isol, props, pmr*)
Sekizaki, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4876 (*synth, derivs*)
Geibel, M. *et al., Phytochemistry*, 1990, **29**, 1351 (*5-glucoside*)
Anyanwutaku, I.O. *et al., J. Nat. Prod.*, 1992, **55**, 1498 (*isol, pmr, cmr, ms*)
Saxena, V.K. *et al., Fitoterapia*, 1998, **69**, 305-306 (*4′-rhamnoside*)
Lewis, P. *et al., J.C.S. Perkin 1*, 1998, 2481-2484 (*Genistin, synth, pmr, cmr*)
Balasubramanian, S. *et al., Synth. Commun.*, 2000, **30**, 469-484 (*synth, pmr*)
Hendrich, S. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press, 2001, 55-75 (*occur, metab*)
Dixon, R.A. *et al., Phytochemistry*, 2002, **60**, 205-211 (*Genistein, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, GCM350

4′,6,7-Trihydroxyisoflavone T-602

[17817-31-1]
6,7-Dihydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. ***Demethyltexasin***. *Soybean factor 2*

$C_{15}H_{10}O_5$ 270.241
Isol. from fermented soybeans (*Glycine max*). Cryst. (MeOH). Mp 322°.

4′-O-β-D-Glucopyranoside:
$C_{21}H_{20}O_{10}$ 432.383
Isol. from seeds of *Glycine max*.

Tri-Ac:
Cryst. (EtOH). Mp 217°.

4′-Me ether: [897-46-1] *6,7-Dihydroxy-4′-methoxyisoflavone.* ***Texasin***
$C_{16}H_{12}O_5$ 284.268
Prisms (EtOH). Mp 291-292.5°.

4′-Me ether, 7-O-β-D-glucopyranoside: [20314-21-0]
$C_{22}H_{22}O_{10}$ 446.41
Cryst. (MeOH aq.). Mp 204-206°.

6-Me ether: [40957-83-3] *4′,7-Dihydroxy-6-methoxyisoflavone.* ***Glycitein***
$C_{16}H_{12}O_5$ 284.268
Isoflavone present in soya foods (inc. tofu, miso); potential nutriceutical. Cryst. (MeOH). Mp 337-339° (311-313°).

6-Me ether, 7-O-β-D-glucopyranoside: [40246-10-4] ***Glycitin***
$C_{22}H_{22}O_{10}$ 446.41
Present in soya foods; potential nutriceutical. Cryst. (EtOH). Mp 192-195°. $[\alpha]_D^{20}$ -13.4 (c, 3.65 in DMF).

6-Me ether, 7-O-(6-O-acetyl-β-D-glucopyranoside): [134859-96-4] *6″-O-Acetylglycitin*
$C_{24}H_{24}O_{11}$ 488.447
Present in soya foods; potential nutriceutical. Needles (MeOH aq.). Mp 155-157°.

6-Me ether, 7-O-(6-O-malonyl-D-glucopyranoside): [137705-39-6] *6″-O-Malonylglycitin*
$C_{25}H_{24}O_{13}$ 532.457
Present in soy foods. Potential nutriceutical. Mp 162°.

6-Me ether, 7-O-(2,4,6-tri-O-acetyl-β-D-glucopyranoside):
$C_{28}H_{28}O_{13}$ 572.521
Constit. of soybean molasses (*Glycine* sp.). Amorph. yellow powder. $[\alpha]_D^{25}$ -23.8 (c, 0.5 in MeOH). λ_{max} 227 (log ϵ 3.9); 275 (log ϵ 4.15) (MeOH).

6-Me ether, 7-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{27}H_{30}O_{14}$ 578.526
Needles (MeOH). $[\alpha]_D^{25}$ -54.3 (c, 0.35 in DMSO). Mp >300° λ_{max} 261 ; 320 (MeOH).

7-Me ether: [57960-04-0] *4′,6-Dihydroxy-7-methoxyisoflavone.* ***Kakkatin***
$C_{16}H_{12}O_5$ 284.268
Needles (MeOH). Mp 290°.

4′,6-Di-Me ether: [550-79-8] *7-Hydroxy-4′,6-dimethoxyisoflavone.* ***Afrormosin***. *Afromosin*. *Castanin*†
$C_{17}H_{14}O_5$ 298.295
Needles (MeOH or EtOH). Mp 236-237° (228-229°).

4′,6-Di-Me ether, 7-O-β-D-glucopyranoside: [19046-26-5] ***Wistin***
$C_{23}H_{24}O_{10}$ 460.437
Present in alfalfa (*Medicago sativa*). Needles (MeOH aq. or Me_2CO aq.). Mp 209-210°. $[\alpha]_D^{12}$ -67.15 (c, 1.43 in AcOH).

4′,6-Di-Me ether, 7-O-(6-O-malonyl-β-D-glucopyranoside): [163310-44-9] ***6″-O-Malonylwistin***
$C_{26}H_{26}O_{13}$ 546.484
Isol. from *Medicago sativa* (alfalfa).

4′,6-Di-Me ether, 7-O-β-D-galactopyranoside: [147023-82-3] *Afrormosin 7-galactoside*
$C_{23}H_{24}O_{10}$ 460.437

4′,6-Di-Me ether, 7-O-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside]: [68862-17-9] *Afrormosin 7-laminaribioside*
$C_{29}H_{34}O_{15}$ 622.579
Tentative identification.

4′,6-Di-Me ether, 7-O-[α-L-rhamnopyranosyl-(1→?)-β-D-glucopyranoside]:
$C_{29}H_{34}O_{14}$ 606.579

4′,6-Di-Me ether, 7-O-[β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:
$C_{28}H_{32}O_{14}$ 592.552
Amorph. powder (MeOH). Mp 146-148°. $[\alpha]_D^{20}$ -97 (c, 0.001 in DMSO). λ_{max} 260 (log ϵ 4.15); 320 (log ϵ 3.6) (MeOH).

4′,6-Di-Me ether, 7-Ac: [4253-19-4] *7-Acetoxy-4′,6-dimethoxyisoflavone.* O-*Acetylafromosin*
$C_{19}H_{16}O_6$ 340.332
Needles (EtOH). Mp 165-167°.

4′,7-Di-Me ether: [970-48-9] *6-Hydroxy-4′,7-dimethoxyisoflavone.* ***Alfalone***
$C_{17}H_{14}O_5$ 298.295
Isol. from alfalfa callus tissue. Needles (EtOH). Mp 246-247°.

Tri-Me ether: [798-61-8] *4′,6,7-Trimethoxyisoflavone*
$C_{18}H_{16}O_5$ 312.321
Cryst. Mp 179-180°.

[11027-11-5]

McMurry, T.B.H. *et al., J.C.S.*, 1960, 1491 (*isol, struct*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1963, **11**, 382 (*deriv*)
Harborne, J. *et al., J.O.C.*, 1963, **28**, 881 (*isol*)
Dyke, S.F. *et al., Tetrahedron*, 1964, **20**, 1331 (*Texasin*)
Bevan, C.W.L. *et al., J.C.S.(C)*, 1966, 509 (*isol, struct*)
Ikehata, H. *et al., Agric. Biol. Chem.*, 1968, **32**, 740 (*isol*)

Markham, K.R. *et al., J.O.C.*, 1968, **33**, 462 (*Texasin*)
Birk, Y. *et al., Phytochemistry*, 1973, **12**, 169 (*Glycitein*)
Antus, S. *et al., Chem. Ber.*, 1975, **108**, 3883 (*synth, Glycitein*)
Kubo, M. *et al., Chem. Pharm. Bull.*, 1975, **23**, 2449 (*Kakkatin*)
Donnelly, D.M.X. *et al., Phytochemistry*, 1975, **14**, 2283 (*synth, Glycitein*)
Ohashi, H. *et al., Mokuzai Gakkaishi*, 1978, **24**, 750-759; *CA*, **90**, 36303y (*Afrormosin 7-laminaribioside*)
Dewick, P.M. *et al., Phytochemistry*, 1978, **17**, 249 (*biosynth*)
Maranduba, A. *et al., Phytochemistry*, 1979, **18**, 815 (*Texasin*)
Jha, H.C. *et al., Can. J. Chem.*, 1980, **58**, 1211 (*cmr*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur, derivs*)
Caballero, P. *et al., J. Nat. Prod.*, 1986, **49**, 1126 (*cryst struct*)
Murthy, M.S.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 225 (*cmr*)
Kobayashi, A. *et al., Agric. Biol. Chem.*, 1988, **52**, 3223 (*Alfalone*)
Kaneko, M. *et al., Phytochemistry*, 1988, **27**, 267 (*Wistin*)
Kessmann, H. *et al., Plant Physiol.*, 1990, **94**, 227 (*Wistin*)
Kudou, S. *et al., Agric. Biol. Chem.*, 1991, **55**, 859 (*7-acetylglucoside*)
Parvez, M. *et al., J. Chem. Soc. Pak.*, 1992, **14**, 221 (*Afrormosin 7-galactoside*)
Nógrádi, M. *et al., Annalen*, 1996, 1651-1652 (*Glycitin, Glycitein, synth, cmr*)
Herath, H.M.T.B. *et al., Phytochemistry*, 1998, **47**, 117-119 (*Afrormosin, pmr, cmr*)
Hosny, M. *et al., J. Nat. Prod.*, 1999, **62**, 853-858 (*6-Me, 7-triacetylglucoside*)
Tostes, J.B.F. *et al., Phytochemistry*, 1999, **50**, 1087-1090 (*Afromosin 7-glycosides*)
Park, H.-J. *et al., Phytochemistry*, 1999, **51**, 147-151 (*6-Me, 7-xylosylglucoside*)
Hendrich, S. *et al., Handbook of Nutraceuticals and Functional Foods*, (ed. Wildman, R.E.C.), CRC Press,, 2001, 55-75 (*Glycitein, occur, metab*)
Lang'at-Thoruwa, C. *et al., J. Nat. Prod.*, 2002, **66**, 149-151 (*Glycitein, synth*)

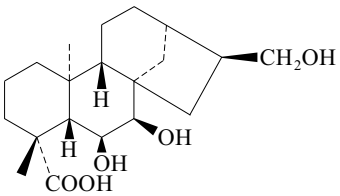
4′,7,8-Trihydroxyisoflavone T-603

[75187-63-2]
*7,8-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 8-Hydroxydaidzein*

$C_{15}H_{10}O_5$ 270.241
Isol. from *Streptomyces* sp. OH-1049 cultured on soybean meal. Cryst. (EtOH aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 210°. All isolations of isoflavonoids from microorganisms are considered dubious. Prob. derived from the culture medium λ_{max} 258 (ϵ 38000) (MeOH/HCl) (Derep). λ_{max} 276 (ϵ) (MeOH/NaOH) (Derep). λ_{max} 260 (ϵ 38000) (MeOH) (Derep).

Karmarkar, S.S. *et al., J. Sci. Ind. Res., Sect. B*, 1961, **20**, 334 (*synth*)
Farkas, L. *et al., Acta Chim. Acad. Sci. Hung.*, 1976, **88**, 173 (*synth*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*rev, occur*)
Murthy, M.S.R. *et al., Magn. Reson. Chem.*, 1986, **24**, 225 (*cmr*)
Jain, A.C. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 1143 (*synth*)
Funayama, S. *et al., J. Antibiot.*, 1989, **42**, 1344; 1350 (*isol, struct, props*)

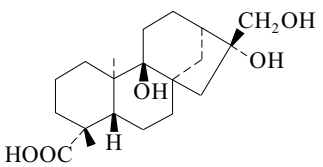
6,7,17-Trihydroxy-19-kauranoic acid T-604



$C_{20}H_{32}O_5$ 352.47
(*ent*-6α,7α,16α*H*)-*form* [56064-72-3]
Isol. from *Phaseolus coccineus* (scarlet runner bean).

MacMillan, J. *et al., Phytochemistry*, 1975, **14**, 779; 1575

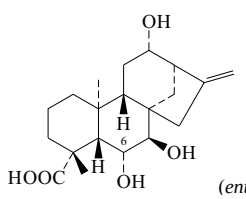
9,16,17-Trihydroxy-19-kauranoic acid T-605



$C_{20}H_{32}O_5$ 352.47
(*ent*-16β*OH*)-*form* [63558-38-3]
Cofarol
Cryst. (MeOH). Mp 179-180°. $[\alpha]_D^{20}$ -46.1 (EtOH).
Me ester:
Cryst. (MeOH). Mp 109-112°.
β-D-Glucopyranosyl ester: [63558-43-0]
Cofaryloside
$C_{26}H_{42}O_{10}$ 514.612
Constit. of green coffee beans. Cryst. (MeOH). Mp 184-187°. $[\alpha]_D^{20}$ -40.1 (EtOH).

Richter, H. *et al., Chem. Ber.*, 1977, **110**, 1963

6,7,12-Trihydroxy-16-kauren-19-oic acid T-606

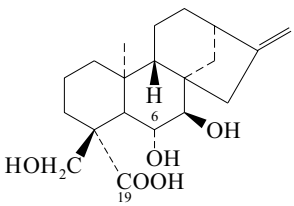


(*ent*-6β,7α,12β)-*form*

$C_{20}H_{30}O_5$ 350.454
(*ent*-6β,7α,12β)-*form*
19→6 Lactone: [62107-03-3] **ent-*7α,12β-Dihydroxy-16-kauren-19,6β-olide***
$C_{20}H_{28}O_4$ 332.439
Constit. of the seeds of *Cucurbita pepo* and *Cucurbita maxima*. Cryst. (EtOAc/hexane). Mp 197-198°.
(*ent*-6α,7α,12α)-*form* [90806-33-0]
Constit. of *Cucurbita maxima*. Gum.

Fukui, H. *et al., Agric. Biol. Chem.*, 1977, **41**, 175; 181
Beale, M.H. *et al., Phytochemistry*, 1984, **23**, 565

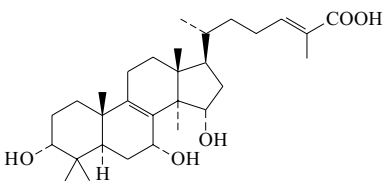
6,7,18-Trihydroxy-16-kauren-19-oic acid T-607



$C_{20}H_{30}O_5$ 350.454
(*ent*-6β,7α)-*form*
19→6 Lactone: [7758-47-6] ent-*7α,18-Dihydroxy-16-kauren-19,6β-olide.* ***7,18-Dihydroxykaurenolide***
$C_{20}H_{28}O_4$ 332.439
Prod. by *Gibberella fujikuroi*, present in barley during germination. Cryst. (EtOAc). Mp 215-217°. $[\alpha]_D^{23}$ -37 (c, 1 in EtOH).
19→6 Lactone, 18-Ac: [52560-10-8]
$C_{22}H_{30}O_5$ 374.476
Gum. $[\alpha]_D^{21}$ -21.7 (c, 2.2 in $CHCl_3$).

Cross, B.E. *et al., J.C.S.*, 1963, 2944; 3783 (*isol*)
Hanson, J.R. *et al., J.C.S. Perkin 1*, 1972, 1892 (*biosynth*)
Hedden, P. *et al., J.C.S. Perkin 1*, 1973, 2773 (*isol*)

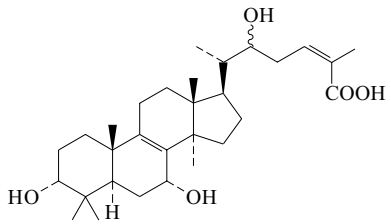
3,7,15-Trihydroxylanosta-8,24-dien-26-oic acid T-608



$C_{30}H_{48}O_5$ 488.706
(3α,5α,7α,15α,24*E*)-*form*
3,7-Di-Ac: ***Ganoderic acid Ma***
$C_{34}H_{52}O_7$ 572.781
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{24}$ -16 (c, 0.3 in MeOH).
3,15-Di-Ac: [86377-49-3] ***Ganoderic acid W***
$C_{34}H_{52}O_7$ 572.781
Constit. of *Ganoderma lucidum* (reishi). Amorph. Mp 114-117°.
7-Me ether, 3-Ac: [110024-16-3] *3-Acetoxy-15-hydroxy-7-methoxylanosta-8,24-dien-26-oic acid.* ***Ganoderic acid Mi***
$C_{33}H_{52}O_6$ 544.77
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ -11 (c, 0.2 in MeOH).
3-Ketone, 15-Ac: [86377-50-6] *15-Acetoxy-7-hydroxy-3-oxolanosta-8,24-dien-26-oic acid.* ***Ganoderic acid V***
$C_{32}H_{48}O_6$ 528.728
Prod. by *Ganoderma lucidum* (reishi).

Toth, J.O. *et al., J. Chem. Res., Miniprint*, 1983, 2733 (*Ganoderic acid W, Ganoderic acid V*)
Nishitoba, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 619; 1149 (*Ganoderic acid Ma, Ganoderic acid Mi*)

3,7,22-Trihydroxylanosta-8,24-dien-26-oic acid T-609



$C_{30}H_{48}O_5$ 488.706

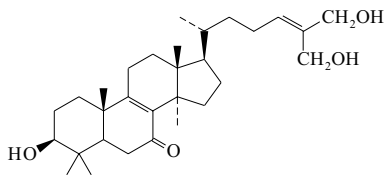
(3α,5α,7α,22ξ,24*E*)-*form*

*3,22-Di-Ac, 7-Me ether:3α,22-Diacetoxy-7α-methoxylanosta-8,24*E*-dien-26-oic acid.* ***Ganoderic acid Md***
$C_{35}H_{54}O_7$ 586.807
Metab. of *Ganoderma lucidum* (reishi). Cryst. Mp 181-182°. $[\alpha]_D^{24}$ -20 (c, 0.33 in MeOH).

22-Ac, 7-Me ether: [110024-15-2] *22-Acetoxy-3α-hydroxy-7α-methoxylanosta-8,24*E*-dien-26-oic acid.* ***Ganoderic acid Mj***
$C_{33}H_{52}O_6$ 544.77
Metab. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ -8 (c, 0.05 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 619; 1149

3,26,27-Trihydroxylanosta-8,24-dien-7-one T-610

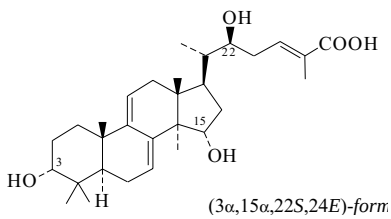


$C_{30}H_{48}O_4$ 472.707

3β-*form* [114567-46-3]
Ganoderiol E
Metab. of *Ganoderma lucidum* (reishi). Syrup (as Tri-Ac). $[\alpha]_D^{21}$ +18 (c, 0.1 in MeOH) (as Tri-Ac).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1988, **52**, 367 (*isol, pmr, cmr*)

3,15,22-Trihydroxylanosta-7,9(11),24-trien-26-oic acid T-611



(3α,15α,22S,24*E*)-*form*

$C_{30}H_{46}O_5$ 486.69

The Ganoderic/Ganodermic synonyms are best avoided as many of them have been duplicated. Use systematic names.

(3α,15α,22*S*,24*E*)-*form*

*3-Ac:3α-Acetoxy-15α,22*S*-dihydroxylanosta-7,9(11),24*E*-trien-26-oic acid*
$C_{32}H_{48}O_6$ 528.728
Constit. of *Ganoderma lucidum* (reishi).

*22-Ac:22*S*-Acetoxy-3α,15α-dihydroxylanosta-7,9(11),24-trien-26-oic acid*
$C_{32}H_{48}O_6$ 528.728
Constit. of *Ganoderma lucidum* (reishi).

15,22-Di-Ac: [112667-14-8] *15α,22*S*-Diacetoxy-3α-hydroxylanosta-7,9(11),24*E*-trien-26-oic acid.* ***Ganoderic acid P***
$C_{34}H_{50}O_7$ 570.765
Constit. of the cultured mycelium of *Ganoderma lucidum* (reishi). Cryst. Mp 211-212.5°.

3,22-Di-Ac: [112790-45-1] *3α,22*S*-Diacetoxy-15α-hydroxylanosta-7,9(11),24*E*-trien-26-oic acid.* ***Ganoderic acid Q****. Ganodermic acid P1*
$C_{34}H_{50}O_7$ 570.765
Constit. of the cultured mycelium of *Ganoderma lucidum* (reishi). Cryst. Mp 131-132°. Also descr. as a resin.

Tri-Ac: [103992-91-2] *3α,15α,22*S*-Triacetoxylanosta-7,9(11),24-trien-26-oic acid.* ***Ganoderic acid T***†
$C_{36}H_{52}O_8$ 612.802
Constit. of the cultured mycelium of *Ganoderma lucidum* (reishi). Cryst. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 200-202°. $[\alpha]_D$ +23 (c, 0.13 in $CHCl_3$). λ_{max} 215 (ε 27000); 216 (ε 10000); 225 (ε 100000); 234 (ε 100000); 241 (ε 28200); 242 ; 250 (ε 17500) (MeOH) (Berdy).

(3α,15α,22ξ,24*E*)-*form*

3,22-Di-Ac:3α,22ξ-Diacetoxy-15α-hydroxylanosta-7,9(11),24-trien-26-oic acid. ***Ganoderic acid Mk***
$C_{34}H_{50}O_7$ 570.765
Constit. of *Ganoderma lucidum* (reishi). Syrup. $[\alpha]_D^{23}$ +23 (c, 0.2 in MeOH). Not clear whether this is identical with Ganoderic acid Q above.

(3β,15α,22*S*,24*E*)-*form*

Constit. of *Ganoderma lucidum* (reishi). Needles ($CHCl_3$/MeOH). Mp 178-180°.

15,22-Di-Ac: [112430-69-0] *15α,22*S*-Diacetoxy-3β-hydroxylanosta-7,9(11),24*E*-trien-26-oic acid.* ***Ganodermic acid P2***
$C_{34}H_{50}O_7$ 570.765
Metab. of *Ganoderma lucidum* (reishi). Resin.

Tri-Ac: [112430-70-3] *3β,15α,22*S*-Triacetoxylanosta-7,9(11),24*E*-trien-26-oic acid*
$C_{36}H_{52}O_8$ 612.802
Metab. of *Ganoderma lucidum* (reishi).

*22-Ac:22*S*-Acetoxy-3β,15α-dihydroxylanosta-7,9(11),24-trien-26-oic acid*
$C_{32}H_{48}O_6$ 528.728
Constit. of *Ganoderma lucidum* (reishi).

(3α,15α,22*R*,24*E*)-*form*

Constit. of *Ganoderma lucidum* (reishi).

*3,15-Di-Ac:3α,15α-Diacetoxy-22*R*-hydroxylanosta-7,9(11),24-trien-26-oic acid*
$C_{34}H_{50}O_7$ 570.765
Constit. of *Ganoderma lucidum* (reishi).

(3β,15α,22*R*,24*E*)-*form*

*3,15-Di-Ac:3β,15α-Diacetoxy-22*R*-hydroxylanosta-7,9(11)24-trien-26-oic acid*
$C_{34}H_{50}O_7$ 570.765
Constit. of *Ganoderma lucidum* (reishi).

Toth, J.O. *et al., Tet. Lett.*, 1983, **24**, 1081 (*isol, deriv*)

Hirotani, M. *et al., Chem. Pharm. Bull.*, 1986, **34**, 2282 (*isol*)

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1987, **51**, 1149 (*isol*)

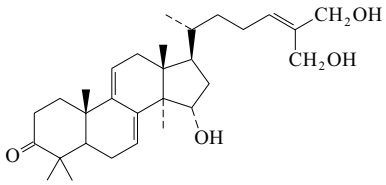
Hirotani, M. *et al., Phytochemistry*, 1987, **26**, 2797 (*isol*)

Lin, L.-J. *et al., J. Nat. Prod.*, 1988, **51**, 918 (*isol*)

Shiao, M.-S. *et al., Phytochemistry*, 1988, **27**, 873; 2911 (*isol*)

Hirotani, M. *et al., J.C.S. Perkin 1*, 1990, 2751 (*biosynth*)

15,26,27-Trihydroxylanosta-7,9(11),24-trien-3-one T-612



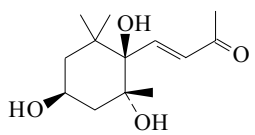
$C_{30}H_{46}O_4$ 470.691

15α-*form* [106518-62-1]
Ganoderiol B
Constit. of *Ganoderma lucidum* (reishi). Amorph. powder.

Sato, H. *et al., Agric. Biol. Chem.*, 1986, **50**, 2887

3,5,6-Trihydroxy-7-megastigmen-9-one T-613

[127643-61-2]
4-(1,2,4-Trihydroxy-2,6,6-trimethylcyclohexyl)-3-buten-2-one



$C_{13}H_{22}O_4$ 242.314

(3*S*,5*R*,6*R*,7*E*)-*form*

Constit. of New Zealand thyme honey (*Thymus vulgaris*). Cryst. (toluene). Mp 68-69°.

(3*S*,5*S*,6*R*,7*E*)-*form*

3-O-β-D-Glucopyranoside: [371113-06-3]
Pisumionoside
$C_{19}H_{32}O_9$ 404.456
Constit. of young seedpods of *Pisum sativum*. Powder. $[\alpha]_D^{26}$ -3.4 (c, 0.2 in MeOH).

[127603-02-5]

Tan, S.T. *et al., Aust. J. Chem.*, 1989, **42**, 1799 (*isol, pmr, cmr, cryst struct*)

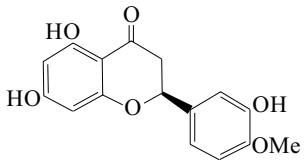
Tan, S.T. *et al., J. Agric. Food Chem.*, 1990, **38**, 1833 (*isol, ms, gc*)

Broom, S.J. *et al., Tet. Lett.*, 1992, **33**, 3197 (*synth*)

Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1003-1008 (*Pisumionoside*)

3′,5,7-Trihydroxy-4′-methoxyflavanone T-614

*2,3-Dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 5,7,3′-Trihydroxy-4′-methoxyflavanone.* ***Hesperetin****. Hesperitin*



$C_{16}H_{14}O_6$ 302.283

(S)-form [520-33-2]
Isol. from *Mentha* (peppermint) and numerous *Citrus* spp., with lemons, tangerines and oranges being especially good sources. Nutriceutical with anticancer props. Glycosides also widely distributed. Plates (EtOH). Sol. EtOH, alkalis. Mp 228-230°. $[\alpha]_D^{27}$ -37.6 (c, 1.8 in EtOH).

5-O-β-D-Glucopyranoside: [69651-80-5]
$C_{22}H_{24}O_{11}$ 464.425
Isol. from peach (*Persica vulgaris*) stem bark. Mp 257-258°. $[\alpha]_D$ -112.8 (EtOH).

7-O-β-D-Glucopyranoside: [2500-68-7] ***Glucohesperetin***
$C_{22}H_{24}O_{11}$ 464.425
Isol. from water mint (*Mentha aquatica*). Cryst. + $1H_2O$. Mp 206°. $[\alpha]_D^{19}$ -53.9 (Py).

7-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]: [13241-33-3] ***Neohesperidin****. Hesperetin 7-neohesperidoside*
$C_{28}H_{34}O_{15}$ 610.568
Constit. of Seville orange peel (*Citrus aurantium*) and other *Citrus* spp. Very bitter flavouring agent. Cryst. (EtOH). Mp 244°. $[\alpha]_D$ -100 (c, 0.5 in Py).

► DJ2981400

7-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [520-26-3] ***Hesperidin****. Citrus-hesperidin. Cirontin. Vitamin B. Cirantin. Hesperidoside. Hesperetin 7-rutinoside*
$C_{28}H_{34}O_{15}$ 610.568
Found in most citrus fruits and other members of the Rutaceae, also in *Mentha longifolia*. Needles. Sol. bases; poorly sol. H_2O. Mp 258-262° (softens at 250°). $[\alpha]_D^{20}$ -47.3 (Py).

► LD_{50} (mus, ipr) 1000 mg/kg. MK6650000

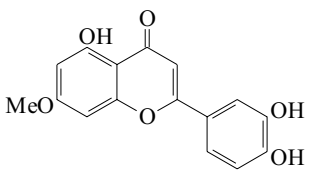
7-O-[α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside]: [97218-30-9]
$C_{34}H_{44}O_{19}$ 756.71
Constit. of *Citrus* spp..

[31712-49-9]

Bognar, R. *et al., Ber.*, 1942, **75**, 1043; 1943, **76**, 773 (*synth*)
Arthur, H.R. *et al., J.C.S.*, 1956, 632 (*isol*)
Arakawa, H. *et al., Annalen*, 1961, **636**, 111 (*struct, abs config*)
Hardegger, E. *et al., Helv. Chim. Acta*, 1961, **44**, 1413 (*Neohesperidin, isol, struct, abs config*)
Horowitz, R.M. *et al., Tetrahedron*, 1963, **19**, 773 (*Neohesperidin*)
Batterham, T.J. *et al., Aust. J. Chem.*, 1964, **17**, 428 (*pmr*)
Boll, P.M. *et al., Tet. Lett.*, 1966, 1293 (*isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1628 (*occur, Hesperidin*)
Chari, V.M. *et al., Tet. Lett.*, 1976, 1799 (*cmr*)
Markham, K.R. *et al., Tetrahedron*, 1976, **32**, 2607 (*cmr*)
Tiwari, K.P. *et al., Planta Med.*, 1979, **36**, 191 (*rhamnoside*)
Plant Flavonoids in Biology and Medicine, (eds. Cody, V. *et al*), A.R. Liss. NY, 1986, (*biol, prop*)
Shin, W. *et al., Acta Cryst. C*, 1987, **43**, 1946 (*Hesperitin, cryst struct*)
Shen, C.-C. *et al., Phytochemistry*, 1993, **34**, 843 (*pmr, cmr*)
Fujii, S. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1143 (*conformn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBU000

3′,4′,5-Trihydroxy-7-methoxyflavone T-615

[20243-59-8]
*2-(3,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-4*H*-1-benzopyran-4-one, 9CI. Luteolin 7-methyl ether*



$C_{16}H_{12}O_6$ 300.267
Isol. from *Salvia officinalis* (sage). Yellow prisms (EtOH). Mp 266-268° Mp 306-308°.

Pankajamani, K.S. *et al., J. Indian Chem. Soc.*, 1954, **31**, 565 (*synth*)
Brieskorn, C.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1971, **304**, 557 (*isol*)

3,5,7-Trihydroxy-4′-methoxyflavone T-616

[491-54-3]
*3,5,7-Trihydroxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 5,7-Dihydroxy-4′-methoxyflavonol.* ***Kaempferide****. Kampheride. Campheride. Kaemferide*

$C_{16}H_{12}O_6$ 300.267
Isol. from roots of *Alpinia officinarum* (lesser galangal). Yellow needles + H_2O (EtOH aq.). Mp 227-229°. Dehydrates at 130-140°.

► LK6915000

3-O-Sulfate: [130827-47-3]
$C_{16}H_{12}O_9S$ 380.331

3-O-α-L-Arabinopyranoside: [123442-27-3] *Kaempferide 3-arabinopyranoside*
$C_{21}H_{20}O_{10}$ 432.383

3-O-L-Arabinopyranoside, 7-O-β-D-glucopyranoside: [108335-09-7]
$C_{27}H_{30}O_{15}$ 594.525

3-O-α-L-Rhamnopyranoside: [148435-12-5] *Kaempferide 3-rhamnoside*
$C_{22}H_{22}O_{10}$ 446.41
Constit. of the aerial parts of *Agrimonia eupatoria* (agrimony). Yellow powder.

3-O-α-L-Rhamnopyranoside, 7-O-β-D-xylopyranoside: [158753-18-5] *Kaempferide 3-rhamnoside 7-xyloside*
$C_{27}H_{30}O_{14}$ 578.526
Pale yellow cryst. solid. Mp 277-278°.

3-O-α-L-Rhamnopyranoside, 7-O-β-D-glucopyranoside: [89764-20-5]
$C_{28}H_{32}O_{15}$ 608.552

3-O-α-L-Rhamnopyranoside, 7-O-(6-O-succinoyl-β-D-glucopyranoside): [107286-94-2] *Kaempferide 3-rhamnoside 7-(6-succinoylglucoside)*
$C_{32}H_{36}O_{18}$ 708.626

7-O-α-L-Rhamnopyranoside: [99208-33-0]
$C_{22}H_{22}O_{10}$ 446.41

3,7-Di-O-α-L-rhamnopyranoside: [111128-11-1]
$C_{28}H_{32}O_{14}$ 592.552

3-O-β-D-Galactopyranoside: [78386-03-5]
$C_{22}H_{22}O_{11}$ 462.409
Yellow needles (EtOAc/petrol). Mp 168°.

3-O-β-D-Glucopyranoside: [70324-47-9]
$C_{22}H_{22}O_{11}$ 462.409

3-O-β-D-Glucopyranoside, 7-O-α-L-rhamnopyranoside: [93078-66-1]
$C_{28}H_{32}O_{15}$ 608.552

5-O-β-D-Glucopyranoside, 7-O-β-D-glucuronopyranoside: [106327-65-5]
$C_{28}H_{30}O_{17}$ 638.535

7-O-β-D-Glucopyranoside: [16290-08-7] ***Mumenin***
$C_{22}H_{22}O_{11}$ 462.409
Isol. from wood of *Prunus mume* (Japanese apricot). Yellow prisms (Py aq.). Mp 312° (278°).

3,7-Di-O-β-D-glucopyranoside: [89764-19-2]
$C_{28}H_{32}O_{16}$ 624.551

3-O-β-D-Glucuronopyranoside: [71926-08-4]
$C_{22}H_{20}O_{12}$ 476.393
Cryst. (MeOH/petrol). Mp 104-105°.

3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:Kaempferide 3-neohesperidoside
$C_{28}H_{32}O_{15}$ 608.552
Amorph. yellow powder (MeOH). Mp 170-180° dec. $[\alpha]_D^{20}$ -85 (c, 0.001 in DMSO). λ_{max} 252 (sh) ; 266 (log ε 3); 353 (log ε 3.5) (MeOH).

3-O-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 7-O-α-L-rhamnopyranoside: [150164-07-1]
$C_{34}H_{42}O_{19}$ 754.694
Constit. of *Actinidia kolomikta* (kiwi-fruit).

3-O-[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside]: [33569-07-2]
$C_{28}H_{32}O_{16}$ 624.551
Isol. from *Dillenia indica* (elephant apple).

3-O-[α-L-Rhamnopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [181270-64-4]
$C_{34}H_{42}O_{19}$ 754.694

3-O-[α-L-Rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: [194657-34-6]
$C_{34}H_{42}O_{19}$ 754.694

Pale yellow cryst. Mp 232-234°.

7-O-*(4-Hydroxy-3,5-dimethoxy*-E-*cinnamoyl):7*-**O-trans-*Sinapoylkaempferide***
$C_{27}H_{22}O_{10}$ 506.465

Brandes, R. *et al., Annalen*, 1839, **32**, 311 (*isol*)
Rao, K.V. *et al., J.C.S.*, 1947, 122
Hasegawa, M. *et al., J.O.C.*, 1959, **24**, 408 (*Mumenin*)
Pacheco, H. *et al., C. R. Hebd. Seances Acad. Sci.*, 1963, **256**, 4927 (*synth, Mumenin*)
Bate-Smith, E.C. *et al., Phytochemistry*, 1971, **10**, 1055 (*3-diglucoside*)
Chauhan, J.S. *et al., Phytochemistry*, 1979, **18**, 691 (*3-glucuronoside*)
Vajpeyi, R.L. *et al., Phytochemistry*, 1981, **20**, 339 (*3-galactoside*)
Imperato, F. *et al., Chem. Ind. (London)*, 1984, 186; 667; 1987, 61; 247; 566 (*glucoside, rhamnosides, 3-arabinoside 7-glucoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Cui, B.L. *et al., Yaoxue Xuebao*, 1989, **24**, 189; *CA*, **111**, 191480 (*3-arabinoside*)
Tomas-Barberan, F.A. *et al., Phytochemistry*, 1990, **29**, 3050 (*3-sulfate*)
Bilia, A.R. *et al., Phytochemistry*, 1993, **32**, 1078 (*Kaempferide 3-rhamnoside*)
Jain, N. *et al., J. Indian Chem. Soc.*, 1994, **71**, 209 (*3-rhamnoside 7-xyloside*)
Khar, S. *et al., J. Indian Chem. Soc.*, 1997, **74**, 506-507 (*rhamnosyl rhamnosyl glucoside*)
Da Silva, B.P. *et al., Phytochemistry*, 2000, **53**, 87-92 (*3-neohesperidoside*)
Bikbulatova, T.N. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2001, **37**, 216-218 (*7-Sinapoylkaempferide*)

3′,5,7-Trihydroxy-4′-methoxyflavone T-617

[520-34-3]
Diosmetin. *Salinigricoflavonol. Vitamin P*

$C_{16}H_{12}O_6$ 300.267
Isol. from peel of lemon (*Citrus limon*) and others. Pale yellow cryst. (EtOH). Sol. MeOH, EtOH. Mp 258-259° (250-253°) Mp 228-230°. λ_{max} 253 (ϵ 19000); 268 (ϵ 17800); 345 (ϵ 21000) (MeOH) (Berdy).

7-O-*β-D-Glucuronopyranoside:* [35110-20-4]
$C_{22}H_{20}O_{12}$ 476.393
Isol. from *Majorana hortensis* (sweet majoram).

7-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [38665-01-9] ***Neodiosmin***. *Diosmetin 7-neohesperidoside*
$C_{28}H_{32}O_{15}$ 608.552
Constit. of bitter orange (*Citrus aurantium*). Pale yellow cryst. + $2H_2O$ (MeOH) or yellow needles. Mp 187-192° (synthetic) Mp 266-268°.

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [520-27-4] *Diosmetin 7-rutinoside.* ***Diosmin, BAN, INN***. *Daflon. Ven-Detrex. Salinigricoflavonoloside. Barosmin*
$C_{28}H_{32}O_{15}$ 608.552
Isol. from parsley. Fine needles + $1H_2O$ (Py aq.). Mp 280° dec. (*in vacuo*). Log P -2.86 (uncertain value) (calc). λ_{max} 255 ; 268 ; 345 (MeOH) (Berdy).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 98C (*ir*)
Lovecy, A. *et al., J.C.S.*, 1930, 817 (*synth*)
Arthur, H.R. *et al., J.C.S.*, 1956, 632 (*Diosmin*)
Horowitz, R.M. *et al., J.O.C.*, 1956, **21**, 1184 (*isol*)
Booth, A.N. *et al., J. Biol. Chem.*, 1958, **230**, 661 (*metab*)
Rösler, H. *et al., J.O.C.*, 1965, **30**, 4346 (*pmr*)
Plouvier, V. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1966, **263**, 439 (*isol, struct*)
Brieskorn, C.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1971, **304**, 557 (*isol*)
Subramanian, S.S. *et al., Phytochemistry*, 1972, **11**, 464 (*7-glucoside, 7-glucuronopyranoside*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799 (*cmr*)
Le Quesne, P.W. *et al., J.C.S. Perkin 1*, 1978, 1572 (*isol, uv, pmr*)
Itokawa, H. *et al., Chem. Lett.*, 1982, **1**, 49 (*ms*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1151 (*cmr*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 12667
Voigtländer, H.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 219 (*synth*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Del Rio, J.A. *et al., Phytochemistry*, 1992, **31**, 723 (*Neodiosmin*)
Rashid, M.A. *et al., Fitoterapia*, 1995, **66**, 471 (*Diosmin, pmr, cmr*)
Bergan, J.J. *et al., Angiology*, 2001, **52**, S43-S47 (*diosmin, rev*)
Garner, R.C. *et al., J. Pharm. Sci.*, 2002, **91**, 32-40 (*diosmin, pharmacol*)

4′,5,7-Trihydroxy-3′-methoxyflavone, 8CI T-618

[491-71-4]
*5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H-*1-benzopyran-4-one, 9CI.* ***Chrysoeriol***. *Scoparol. Luteolin 3′-methyl ether*

$C_{16}H_{12}O_6$ 300.267
Widespread flavone. Yellow needles (EtOH). Sol. Py; fairly sol. EtOH, EtOAc. Mp 330-331°. The identity of Scoparol with Chrysoeriol is not confirmed λ_{max} 252 ; 270 ; 346 (MeOH). λ_{max} 241 ; 249 (sh) ; 269 ; 347 (MeOH).

► LK9278000

7-O-*(Di*-O-*sulfo-β-D-glucopyranoside):*
[121283-88-3]
$C_{22}H_{22}O_{17}S_2$ 622.538
Isol. from *Phoenix dactylifera* (date).

7-O-*(Malonyl-β-D-glucopyranoside):*
$C_{25}H_{24}O_{14}$ 548.456
Isol. from *Petroselinum hortense* (parsley).

4′,7-Di-O-*β-D-glucuronopyranoside:*
[80366-06-9]
$C_{28}H_{28}O_{18}$ 652.518
Constit. of the aerial parts of alfalfa (*Medicago sativa*). Amorph. yellow powder. Mp 207-208°. $[\alpha]_D^{24}$ -47.4 (c, 0.1 in MeOH/DMSO aq.). λ_{max} 247 (sh) ; 271 ; 338 (MeOH).

7-O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [33579-63-4] ***Graveobioside B***
$C_{27}H_{30}O_{15}$ 594.525
Isol. from *Apium graveolens* (celery seeds) and *Petroselinum hortense* (parsley). Pale yellow needles (MeOH). Mp 214-216°. $[\alpha]_D$ -104.4 (Py).

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [32061-83-9] *Chrysoeriol 7-rutinoside*
$C_{28}H_{32}O_{15}$ 608.552
Isol. from *Matricaria chamomilla* (German chamomile).

7-O-*[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [83097-46-5]
$C_{28}H_{28}O_{18}$ 652.518
Isol. from alfalfa (*Medicago sativa*).

7-O-*[4-Hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [380468-53-1]
$C_{38}H_{36}O_{21}$ 828.69
Constit. of the aerial parts of *Medicago sativa* (alfalfa). Amorph. yellow powder. Mp 235-236°. $[\alpha]_D^{24}$ -77.8 (c, 0.1 in DMSO/MeOH aq.). λ_{max} 248 ; 271 (sh) ; 338 (MeOH).

7-O-*[β-D-Glucuronopyranosyl-(→?)-β-D-glucuronopyranosyl-(→?)-β-D-glucuronopyranoside]:* [83077-63-8]
$C_{34}H_{36}O_{24}$ 828.644
Isol. from alfalfa (*Medicago sativa*).

7-O-*[4-Hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranosyl-(1→3)-β-D-glucuronopyranoside]:* [380468-63-3]
$C_{44}H_{44}O_{27}$ 1004.815
Constit. of the aerial parts of alfalfa (*Medicago sativa*). Amorph. yellow powder. Mp 254-255°. $[\alpha]_D^{24}$ -37.6 (c, 0.1 in MeOH/DMSO aq.). λ_{max} 248 ; 269 (sh) ; 338 (MeOH).

[28709-98-0, 38725-01-8, 87861-40-3]

Horowitz, R.M. *et al., J.O.C.*, 1960, **25**, 2183-2187 (*isol, uv*)
Saleh, M. *et al., Indian J. Chem.*, 1964, **2**, 375-376 (*synth*)
Grisebach, H. *et al., Z. Naturforsch., B*, 1967, **22**, 746-751 (*Graveobioside B*)
Harborne, J.B. *et al., Phytochemistry*, 1970, **9**, 2011-2017
Schmid, R.D. *et al., Tetrahedron*, 1972, **28**, 3259-3269 (*Graveobioside B*)
Sakakibara, M. *et al., Phytochemistry*, 1976, **15**, 727-731 (*isol, uv, pmr, ms*)
Wagner, H. *et al., Tet. Lett.*, 1976, 1799-1802 (*cmr*)
Biswas, K.M. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 396-397 (*Graveobioside B*)
Markham, K.R. *et al., Biochem. Syst. Ecol.*, 1980, **8**, 17-36 (*glucosides*)
Saleh, N.A.M. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 33 (*7-glucuronosides*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1151-1156 (*cmr*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107-2145 (*uv*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,
Bucar, F. *et al., Phytochemistry*, 1998, **48**, 573-575 (*7-apiosylglucoside*)
Nakasugi, T. *et al., J. Agric. Food Chem.*, 2000, **48**, 3256-3266 (*activity*)
Stochmal, A. *et al., J. Agric. Food Chem.*, 2001, **49**, 5310-5314 (*Medicago sativa glucuronides*)

5,7,8-Trihydroxy-4′-methoxyflavone T-619

[51876-19-8]
*5,7,8-Trihydroxy-2-(4-methoxyphenyl)-4*H-*1-benzopyran-4-one, 9CI.* ***Takakin***. *Isoscutellarein 4′-methyl ether*

$C_{16}H_{12}O_6$ 300.267
Isol. from aerial parts of *Citrus reticulata* (mandarin). Yellow needles (MeOH). Mp

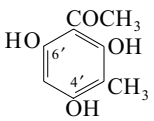
275-277° dec.

8-O-*(2*-O-*Sulfo-β-D-glucopyranoside):*
[136516-95-5]
$C_{22}H_{22}O_{14}S$ 542.473
Isol. from the roots of *Althaea officinalis* (marsh mallow). Pale yellow needles (MeOH) (as K salt). Mp 180° dec. (K salt).

Rao, K.V. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1948, **28**, 210 (*synth*)
Komissarenko, N.F. *et al., Khim. Prir. Soedin.*, 1978, **14**, 521; *Chem. Nat. Compd. (Engl. Transl.)*, 1978, **14**, 445 (*isol, pmr*)
Markham, K.R. *et al., Phytochemistry*, 1979, **18**, 611 (*isol*)
Iinuma, M. *et al., Yakugaku Zasshi*, 1980, **100**, 657 (*isol*)
Chari, M.M. *et al., Phytochemistry*, 1981, **20**, 1977 (*isol*)
Horie, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 3773 (*synth*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Gudej, J. *et al., Planta Med.*, 1991, **57**, 284 (*8-sulfoglucoside*)

2′,4′,6′-Trihydroxy-3′-methylacetophenone T-620

[2657-28-5]
1-(2,4,6-Trihydroxy-3-methylphenyl)ethanone, 9CI. 3-Methylphloracetophenone



$C_9H_{10}O_4$ 182.176

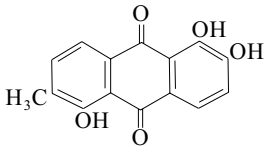
2′,4′-Di-Me ether: [14964-98-8] *6′-Hydroxy-2′,4′-dimethoxy-3′-methylacetophenone.* ***Bancroftinone***
$C_{11}H_{14}O_4$ 210.229
Isol. from clove oil. Mp 44-45°. Bp_2 120-122°.

4′,6′-Di-Me ether: [23121-32-6] *2′-Hydroxy-4′,6′-dimethoxy-3′-methylacetophenone.* ***Methylxanthoxylin***
$C_{11}H_{14}O_4$ 210.229
Isol. from Java plum blossom (*Eugenia jambolana*). Light yellow needles (petrol). Mp 143°.

Whalley, W.B. *et al., J.C.S.*, 1955, 105 (*derivs*)
Baldwin, M.E. *et al., Tetrahedron*, 1961, **16**, 206 (*isol, uv, synth*)
Huneck, S. *et al., Phytochemistry*, 1972, **11**, 3311 (*Bancroftinone*)
Cann, M.R. *et al., Chem. Ind. (London)*, 1982, 779 (*pmr*)
Linde, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 917 (*4′,6′-di-Me ether, isol*)
Hylands, P.J. *et al., Phytochemistry*, 1985, **24**, 127-129 (*pmr, cmr, struct*)
Brophy, J.J. *et al., J. Essent. Oil Res.*, 1995, **7**, 237 (*Bancroftinone*)

1,2,5-Trihydroxy-6-methylanthraquinone, 8CI T-621

[478-29-5]
1,2,5-Trihydroxy-6-methyl-9,10-anthracenedione, 9CI. ***Morindone****. C.I. 75430*



$C_{15}H_{10}O_5$ 270.241
Orange needles. Mp 284°. λ_{max} 232 (ε 31600); 259 (ε 33890); 292 (ε 14450); 301 (ε 15130); 448 (ε 11750) (MeOH) (Berdy).

2-O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [60450-21-7] *Morindone 6-β-primeveroside.* ***Morindin***
$C_{26}H_{28}O_{14}$ 564.499
Yellow cryst. (EtOH aq.). Mp 257-259°. $[\alpha]_D^{25}$ -87.3 (c, 0.6 in dioxan).

2-O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [77587-41-8] *Morindone 6-β-gentiobioside*
$C_{27}H_{30}O_{15}$ 594.525
Orange-red needles (EtOH aq.). Mp 256° (252-253°).

2-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [1400-38-0] *Morindone 6-β-rutinoside*
$C_{27}H_{30}O_{14}$ 578.526
Yellow cryst. (AcOH). Mp 264.5° dec. (darkens > 150°). $[\alpha]_D$ -90.9 (c, 0.054 in dioxan).

1-Me ether: [64809-71-8] *1,6-Dihydroxy-5-methoxy-2-methylanthraquinone.* ***Morindone 5-methyl ether***
$C_{16}H_{12}O_5$ 284.268
Orange-brown cryst. Mp 223°.

1-Me ether, 2-O-*[α-L-arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [163157-76-4]
$C_{27}H_{30}O_{14}$ 578.526
Light pink needles. Mp 180-182°.

2-Me ether: [63965-45-7] *1,5-Dihydroxy-2-methoxy-6-methylanthraquinone*
$C_{16}H_{12}O_5$ 284.268
Isol. from the stem bark of *Aegle marmelos* (baelfruit). Cryst. (C_6H_6/petrol). Mp 252-253° (248°).

1,2-Di-Me ether: [95393-76-3] *1-Hydroxy-5,6-dimethoxy-2-methylanthraquinone*
$C_{17}H_{14}O_5$ 298.295
Mp 238.5-239.5°.

Tri-Me ether: [52541-74-9] *1,2,5-Trimethoxy-6-methylanthraquinone*
$C_{18}H_{16}O_5$ 312.321
Yellow needles (Me_2CO). Mp 237-238°.

Jacobson, R.A. *et al., J.A.C.S.*, 1925, **47**, 283 (*synth*)
Briggs, L.H. *et al., J.C.S.*, 1963, 3471 (*rutinoside*)
Leistner, E. *et al., Phytochemistry*, 1973, **12**, 1669 (*biosynth*)
Leistner, E. *et al., Planta Med.*, (Suppl), 1975, 214 (*biosynth*)
González, A.G. *et al., An. Quim.*, 1977, **73**, 869 (*isol, deriv*)
Roberts, J.L. *et al., Aust. J. Chem.*, 1977, **30**, 1553 (*isol, ir, pmr*)
Rao, P.S. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 497 (*Morindin*)
Vermes, B. *et al., Phytochemistry*, 1980, **19**, 119; 2493 (*deriv*)
Demagos, G.P. *et al., Z. Naturforsch., B*, 1981, **36**, 1180 (*isol, deriv*)
Wijnsma, R. *et al., Phytochemistry*, 1984, **23**, 2307 (*isol, deriv*)
Savard, J. *et al., Tetrahedron*, 1984, **40**, 3455 (*synth, derivs*)
Nema, D. *et al., Proc. Natl. Acad. Sci., India, Sect. A*, 1991, **61**, 465 (*2-Me ether*)
Srivastava, S.K. *et al., Fitoterapia*, 1994, **65**, 517 (*1-Me ether 2-arabinosylglucoside, pmr, cmr*)
Tosa, H. *et al., Biol. Pharm. Bull.*, 1998, **21**, 241-242 (*isol, activity*)
Cameron, D.W. *et al., Aust. J. Chem.*, 1999, **52**, 941-948 (*synth*)

1,2,8-Trihydroxy-3-methylanthraquinone T-622

Norobtusifolin. 2-Hydroxychrysophanol. 1,2,8-Trihydroxy-3-methyl-9,10-anthracenedione, 9CI

$C_{15}H_{10}O_5$ 270.241
Constit. of the roots of *Myrsine africana* (Cape myrtle). Orange-red needles (MeOH). Mp 265° (255°). λ_{max} 208 (log ε 4.19); 235 (log ε 4.05); 258 (log ε 4.11); 426 (log ε 3.73) (EtOH).

1-Me ether: [477-85-0] *2,8-Dihydroxy-1-methoxy-3-methylanthraquinone.* ***Obtusifolin***†
$C_{16}H_{12}O_5$ 284.268
Yellow needles (MeOH). Mp 237-238°. Not the same as Obtusifolin.

1-Me ether, di-Ac:
$C_{20}H_{16}O_7$ 368.342
Light yellow needles. Mp 187-188°.

1-Me ether, 2-O-*β-D-glucopyranoside:* [120163-18-0] ***Glucoobtusifolin***
$C_{22}H_{22}O_{10}$ 446.41
Isol. from seeds of *Cassia tora* (charota). Cryst + $1H_2O$. Mp 205-206°.

1,2-Di-Me ether: [82868-99-3] *8-Hydroxy-1,2-dimethoxy-3-methylanthraquinone*
$C_{17}H_{14}O_5$ 298.295
Orange needles. Mp 214-215°.

Tri-Me ether:1,2,8-Trimethoxy-3-methylanthraquinone
$C_{18}H_{16}O_5$ 312.321
Light yellow needles (petrol). Mp 145-146°.

Takido, M. *et al., Chem. Pharm. Bull.*, 1958, **6**, 397 (*isol, struct*)
Takido, M. *et al., CA*, 1965, **62**, 5326f (*Glucoobtusifolin*)
He, X. *et al., CA*, 1982, **97**, 107044x (*isol, di-Me ether*)
Cameron, D.W. *et al., Tet. Lett.*, 1986, **27**, 4999 (*synth*)
Li, X.-H. *et al., J. Nat. Prod.*, 1989, **52**, 660 (*isol, pmr*)
Wong, S.-M. *et al., Phytochemistry*, 1989, **28**, 211-214 (*Glucoobtusifolin*)
Krohn, K. *et al., Annalen*, 1993, 905-909 (*synth, di-Me ether*)
Cichewicz, R.H. *et al., Tetrahedron*, 2002, **58**, 8597-8606 (*isol, pmr, cmr, Kwanzoquinones*)

1,3,7-Trihydroxy-6-methylanthraquinone T-623

[128885-08-5]
1,3,7-Trihydroxy-6-methyl-9,10-anthracenedione, 9CI. De-O-*methylmacrosporin*

$C_{15}H_{10}O_5$ 270.241
Yellow-orange needles (MeOH). Mp 300°. λ_{max} 284 (ε 23442); 309 (ε 12022); 378 (ε 5250) (MeOH) (Berdy).

1-Me ether: [71241-94-6] *3,7-Dihydroxy-1-methoxy-6-methylanthraquinone.* ***Caja-***

quinone
$C_{16}H_{12}O_5$ 284.268
Isol. from the root of *Cajanus cajan* (pigeon pea). Yellow needles ($CHCl_3$/MeOH). Mp 204°. Struct. incorrectly assigned. CAS name reflects modified struct..

3-Me ether: [22225-67-8] *1,7-Dihydroxy-3-methoxy-6-methylanthraquinone, 8CI. 3,5-Dihydroxy-7-methoxy-2-methylanthraquinone.* ***Macrosporin***
$C_{16}H_{12}O_5$ 284.268
Cryst. (Py). Mp 308-316°. λ_{max} 217 ; 284 ; 307 ; 400 (MeOH) (Berdy). λ_{max} 225 (ϵ 16980); 284 (ϵ 28180); 305 (ϵ 10700); 379 (ϵ 5500) (EtOH) (Berdy).

▶ Mutagen.

3,7-Di-Me ether: [22225-69-0] *1-Hydroxy-3,7-dimethoxy-6-methylanthraquinone, 8CI*
$C_{17}H_{14}O_5$ 298.295
Cryst. ($CHCl_3$/EtOH). Mp 211-214°.

Tri-Me ether: [71241-95-7] *1,3,7-Trimethoxy-6-methylanthraquinone*
$C_{18}H_{16}O_5$ 312.321
Mp 270-271°.

Stoessl, A. *et al., Can. J. Chem.*, 1969, **47**, 767 (*isol, uv*)
Nakajima, S. *et al., Chem. Pharm. Bull.*, 1973, **21**, 2083 (*isol, ir, pmr, ms*)
Wheeler, M.M. *et al., Phytochemistry*, 1975, **14**, 288 (*isol, uv, ms*)
Becker, A.M. *et al., J. Antibiot.*, 1978, **31**, 324 (*isol*)
Bhanumati, S. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 88 (*Cajaquinone*)
Brisson, C. *et al., J.O.C.*, 1981, **46**, 1810 (*synth*)
Stoessl, A. *et al., Can. J. Chem.*, 1982, **61**, 372 (*biosynth*)
Katagiri, N. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2440 (*synth*)
Suemitsu, R. *et al., Phytochemistry*, 1989, **28**, 1621 (*biosynth*)
Hosoe, T. *et al., Phytochemistry*, 1990, **29**, 997 (*isol*)

1,3,8-Trihydroxy-6-methylanthraquinone, 8CI T-624

[518-82-1]
1,3,8-Trihydroxy-6-methyl-9,10-anthracenedione, 9CI. ***Emodin****. Rheum-emodin. Frangula emodin. Archin. Frangulinic acid. Emodol. Alatinone*

$C_{15}H_{10}O_5$ 270.241
Present in Cascara sagrada. Orange or yellow-brown needles (Py aq. or MeOH). Mp 266-268° (264-265°). Log P 1.8 (calc). λ_{max} 222 (ϵ 35500); 252 (ϵ 18200); 265 (ϵ 18600); 289 (ϵ 21900); 437 (ϵ 12600) (EtOH) (Derep).

▶ LD_{50} (mus, ipr) 35 mg/kg. CB7920600

3-O-β-D-Glucopyranoside: [34298-85-6] ***Glucoemodin***
$C_{21}H_{20}O_{10}$ 432.383
Isol. from rhubarb. Mp 176-178°.

3-O-α-L-Rhamnopyranoside: [521-62-0] ***Frangulin A****. Franguloside*
$C_{21}H_{20}O_9$ 416.384
Glycoside present in rhubarb root and Cascara sagrada. Cryst. Mp 228°. Frangulin, Rhamnoxanthin and Cascarin were mixts. of Frangulins A and B λ_{max} 225 (ϵ 33113); 264 (ϵ 19054); 282 (ϵ 14125); 300 (ϵ 9332); 430 (ϵ 11220) (MeOH) (Berdy).

▶ CB0164000

3-Me ether, 1-O-β-D-glucopyranoside: [23451-01-6] ***Physcionin***
$C_{22}H_{22}O_{10}$ 446.41
Constit. of root of *Rheum* spp.. Mp 246-248° (237-239°). λ_{max} 221 (log ϵ 4.57); 254 (log ϵ 4.33); 266 (log ϵ 4.32); 289 (log ϵ 4.36); 436 (log ϵ 4.07) (MeOH). λ_{max} 221 (ϵ 5100); 270 (ϵ 3000); 430 (MeOH) (Berdy).

3-Me ether, O-β-D-glucopyranoside: [29013-18-1] ***Rheochrysin***
$C_{22}H_{22}O_{10}$ 446.41
Occurs in root of *Rheum* spp. Yellow needles (MeOH). Mp 204°. λ_{max} 266 ; 288 ; 430 (MeOH) (Berdy).

3-Me ether, 8-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [84268-38-2] *Physcion 8-gentiobioside*
$C_{28}H_{32}O_{15}$ 608.552
Constit. of seeds of sicklepod (*Cassia torosa*). Yellow powder. Mp 221-223°.

3-Me ether, 1-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Torososide B***
$C_{40}H_{52}O_{25}$ 932.836
Constit. of the seeds of sickle pod *Cassia torosa*. Yellow cryst. (MeOH). Mp 208-209°. $[\alpha]_D$ -71.3 (c, 0.3 in Py). λ_{max} 223 (log ϵ 4.47); 271 (log ϵ 4.38); 418 (log ϵ 3.88) (MeOH).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 91D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 88D (*ir*)
Eder, R. *et al., Helv. Chim. Acta*, 1925, **8**, 140 (*bibl*)
Horhammer, L. *et al., Naturwissenschaften*, 1964, **51**, 310
Romanova, A.S. *et al., Khim. Prir. Soedin.*, 1966, **2**, 83; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 63 (*Glucoemodin*)
Sargent, M.V. *et al., J.C.S.(C)*, 1970, 307
Steglich, W. *et al., Chem. Ber.*, 1972, **105**, 2928
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1265; 1274 (*occur*)
Wagner, H. *et al., Tet. Lett.*, 1972, 5013
Hörhammer, H.P. *et al., Z. Naturforsch., B*, 1972, **27**, 959
Okabe, H. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1254
Hirose, Y. *et al., Chem. Pharm. Bull.*, 1973, **21**, 2790 (*synth*)
Hassall, C.H. *et al., J.C.S. Perkin 1*, 1973, 2853 (*synth, derivs*)
Banville, J. *et al., Can. J. Chem.*, 1974, **52**, 80 (*synth, uv, ir, pmr*)
Banville, J. *et al., J.C.S. Perkin 1*, 1976, 1852
Fairbairn, J.W. *et al., Pharmacology*, Suppl. 1, 1976, **14**, 1 (*rev*)
Kelly, T.R. *et al., J.O.C.*, 1983, **48**, 3573 (*isol*)
Kitanaka, S. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3436; 1985, **33**, 1274 (*3-Me ether diglucoside*)
Ahmed, S.A. *et al., Chem. Comm.*, 1987, 883 (*synth*)
Kalidhar, S.B. *et al., Phytochemistry*, 1989, **28**, 2455; 3459 (*pmr*)
Coskun, M. *et al., Phytochemistry*, 1990, **29**, 2018 (*cd, pmr, cmr*)
Kubo, I. *et al., Phytochemistry*, 1992, **31**, 1063 (*Physcionin*)
Schmidt, R.R. *et al., Synthesis*, 1994, 255 (*synth, pmr*)
Fujimoto, H. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1506-1510 (*isol, activity*)
Francis, G.W. *et al., Magn. Reson. Chem.*, 1998, **36**, 769-772 (*pmr, cmr, Frangulins, Glucofrangulins*)
Kanno, M. *et al., Chem. Pharm. Bull.*, 1999, **47**, 915-918 (*Torososide B*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 684
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MQF250

1,4,6-Trihydroxy-7-methylanthraquinone T-625

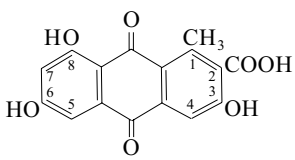
Rhababerone*. Isoemodin*

$C_{15}H_{10}O_5$ 270.241
Identity dubious. Poss. identical with 1,8-Dihydroxy-3-hydroxymethylanthraquinone, D-503. Occurs in rhubarb (*Rheum coreanum*) rhizomes. Yellow leaflets (EtOH). Mp 223-224° (212°). λ_{max} 225 (ϵ 39000); 254 (ϵ 22000); 255 ; 274 ; 276 (ϵ 10200); 285 ; 287 (ϵ 11500); 430 (ϵ 12000) (EtOH) (Berdy).

Keimatsu, H. *et al., CA*, 1931, **25**, 3647 (*isol*)
Uchibayashi, M. *et al., Chem. Pharm. Bull.*, 1961, **9**, 234

3,6,8-Trihydroxy-1-methylanthraquinone-2-carboxylic acid T-626

[18499-84-8]
9,10-Dihydro-3,6,8-trihydroxy-1-methyl-9,10-dioxo-2-anthracenecarboxylic acid, 9CI. ***Laccaic acid D****. Xanthokermesic acid. Flavokermesic acid*



$C_{16}H_{10}O_7$ 314.251
Constit. of rhubarb rhizomes. Yellow needles (H_2O). Dec. >300°.

Me ester: [53254-85-6]
$C_{17}H_{12}O_7$ 328.278
Orange needles (MeOH). Mp 270-275°. λ_{max} 312 (ϵ 7940); 390 (ϵ 1260); 520 (ϵ 1260) (MeOH/KOH) (Derep). λ_{max} 220 (ϵ 100000); 270 (ϵ 79400); 285 (ϵ 100000); 420 (ϵ 7940); 435 (ϵ 7940) (MeOH) (Derep).

3-Me ether: [95796-47-7] *6,8-Dihydroxy-3-methoxy-1-methylanthraquinone-2-carboxylic acid.* ***Rhamnalpinogenin***
$C_{17}H_{12}O_7$ 328.278
Constit. of *Crocus sativus* (saffron).

3-Me ether, 6-O-β-D-apiofuranoside: [95796-48-8] ***Rhamnalpinoside***
$C_{22}H_{20}O_{11}$ 460.393

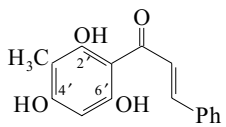
6-Me ether: [120374-28-9] *3,8-Dihydroxy-6-methoxy-1-methylanthraquinone-2-carboxylic acid*
$C_{17}H_{12}O_7$ 328.278
Orange cryst. (MeOH). Mp 238-240°. Diagram incorrect in ref..

Tri-Me ether, Me ester:
Mp 226°.

Gadgil, D.D. *et al., Tet. Lett.*, 1968, 2223 (*synth*)
Mehandale, A.R. *et al., Tet. Lett.*, 1968, 2231 (*isol*)
Yagi, A. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1159 (*ms, ir, pmr*)
Cameron, D.W. *et al., Chem. Comm.*, 1978, 688 (*synth*)
Oshio, H. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2458-2464 (*isol, rhubarb*)
Yagi, A. *et al., Phytochemistry*, 1978, **17**, 895 (*biosynth*)
Rauwald, H.W. *et al., Dtsch. Apoth. -Ztg.*, 1985, **125**, 101 (*Rhamnalpinoside*)
Wouters, J. *et al., Tet. Lett.*, 1987, **28**, 1199 (*isol*)
Ali, A.A. *et al., Phytochemistry*, 1989, **28**, 281 (*6-Me ether*)
Gao, W.-Y. *et al., Zhiwu Xuebao*, 1999, **41**, 531-533 (*3-Me ether, isol*)

2′,4′,6′-Trihydroxy-3′-methylchalcone T-627

3-Phenyl-1-(2,4,6-trihydroxy-3-methylphenyl)-2-propen-1-one



$C_{16}H_{14}O_4$ 270.284

2′-Me ether: [60433-78-5] *1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, 9CI. 4′,6′-Dihydroxy-2′-methoxy-3′-methylchalcone.* ***Aurentiacin A***
$C_{17}H_{16}O_4$ 284.311
Yellow-orange needles. Mp 202°. λ_{max} 210 (ϵ 21877); 324 (ϵ 14790) (MeOH) (Berdy).

4′-Me ether: [67777-33-7] *3-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, 9CI. 2′,6′-Dihydroxy-4′-methoxy-3′-methylchalcone.* ***Triangularin***†
$C_{17}H_{16}O_4$ 284.311
Deep-red prisms (MeOH). Mp 192-196°.

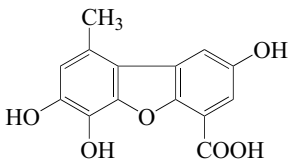
6′-Me ether: [94388-75-7] *1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-3-phenyl-2-propen-1-one. 2′,4′-Dihydroxy-6′-methoxy-3′-methylchalcone.* ***Stercurensin***
$C_{17}H_{16}O_4$ 284.311
Isol. from *Sterculia urens* (karaya gum). Bright yellow needles (MeOH). Mp 210-211°.

4′,6′-Di-Me ether: [58969-62-3] *1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, 9CI. 2′-Hydroxy-4′,6′-dimethoxy-3′-methylchalcone.* ***Aurentiacin***
$C_{18}H_{18}O_4$ 298.338
Orange plates (petrol/C_6H_6). Mp 140-141°.

[80749-77-5]

Cardillo, G. *et al., J.C.S.(C)*, 1971, 3967 (*Aurentiacin A*)
Adityachaudhury, N. *et al., Phytochemistry*, 1976, **15**, 229 (*Aurentiacin*)
Star, A.E. *et al., Phytochemistry*, 1978, **17**, 586 (*Triangularin*)
Dominguez, X.A. *et al., Phytochemistry*, 1980, **19**, 1262 (*Aurentiacin A*)
Wollenweber, E. *et al., Phytochemistry*, 1981, **20**, 1167 (*Aurentiacin*)
Schiemenz, G.P. *et al., Annalen*, 1982, 1509 (*synth*)
Anjaneyulu, A.S.R. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 1010 (*Stercurensin*)
Wollenweber, E. *et al., J. Plant Physiol.*, 1985, **117**, 423 (*Aurentiacin A, Stercurensin*)

2,6,7-Trihydroxy-9-methyl-4-dibenzofurancarboxylic acid T-628



$C_{14}H_{10}O_6$ 274.229

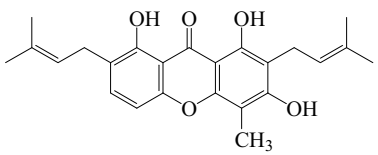
7-Me ether: [207285-02-7] *2,6-Dihydroxy-7-methoxy-9-methyl-4-dibenzofurancarboxylic acid.* ***Porric acid B***
$C_{15}H_{12}O_6$ 288.256
Constit. of the bulbs of *Allium porrum* (leeks). Pale yellow cryst. Mp 217-219°. λ_{max} 210 ; 214 ; 238 ; 258 ; 334 (MeOH).

2,7-Di-Me ether: [207285-00-5] *6-Hydroxy-27-dimethoxy-9-methyl-4-dibenzofurancarboxylic acid.* ***Porric acid A***
$C_{16}H_{14}O_6$ 302.283
Constit. of the bulbs of *Allium porrum* (leeks). Pale yellow cryst. Mp 200-202°. λ_{max} 206 ; 238 ; 260 ; 338 (MeOH).

Carotenuto, A. *et al., Eur. J. Org. Chem.*, 1998, 661-663 (*isol, uv, pmr, cmr*)

1,3,8-Trihydroxy-4-methyl-2,7-diprenylxanthone T-629

*1,3,8-Trihydroxy-4-methyl-2,7-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one, 9CI*

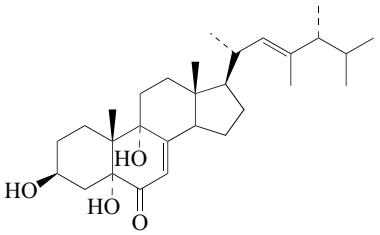


$C_{24}H_{26}O_5$ 394.466
Constit. of the fruit hulls of *Garcinia mangostana* (mangosteen). Mp 174-176°.

Gopalakrishnan, G. *et al., Fitoterapia*, 2000, **71**, 607-609

3,5,9-Trihydroxy-23-methylergosta-7,22-dien-6-one T-630

3,5,9-Trihydroxy-23,24-dimethylcholesta-7,22-dien-6-one



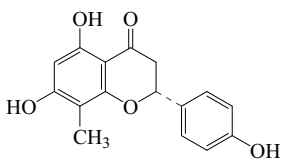
$C_{29}H_{46}O_4$ 458.68

(3β,5α,9α,22E,24R)-form [211486-12-3]
Constit. of *Lentinus edodes* (shiitake). Amorph. powder. $[\alpha]_D^{18}$ -40 (c, 0.05 in $CHCl_3$).

Yaoita, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 944-950 (*isol, pmr, cmr*)

4′,5,7-Trihydroxy-8-methylflavanone T-631

*2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-methyl-4*H*-1-benzopyran-4-one, 9CI. 8-Methylnaringenin*



(*R*)-*form*

$C_{16}H_{14}O_5$ 286.284

(R)-form [78417-15-9]
Mp 195-200°.

(ξ)-form

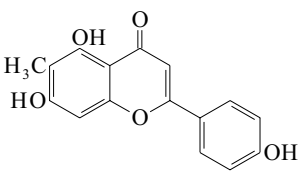
7-Me ether:4′,5-Dihydroxy-7-methoxy-8-methylflavanone
$C_{17}H_{16}O_5$ 300.31
λ_{max} 291 ; 339 (MeOH).

4′-Me ether: [109248-40-0] *5,7-Dihydroxy-4′-methoxy-8-methylflavanone*
$C_{17}H_{16}O_5$ 300.31
Constit. of the flowers of *Amaranthus caudatus* (love-lies-bleeding).

Correa, D. de B. *et al., Phytochemistry*, 1981, **20**, 305-307 (*isol, uv, ir, pmr*)
Srivastava, B.K. *et al., Orient. J. Chem.*, 1994, **10**, 294 (*isol, 4′-Me ether*)
Wollenweber, E. *et al., Phytochemistry*, 2000, **55**, 965-970 (*isol, 7-Me ether*)

4′,5,7-Trihydroxy-6-methylflavone T-632

[5526-57-8]
*5,7-Dihydroxy-2-(4-hydroxyphenyl)-6-methyl-4*H*-1-benzopyran-4-one.* ***6-Methylapigenin***



$C_{16}H_{12}O_5$ 284.268
Yellow cryst.(EtOH aq.). λ_{max} 211 ; 271 ; 318 ; 350 (sh) (MeOH).

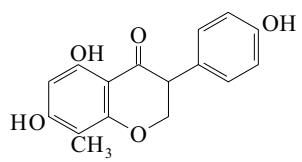
7-Me ether: [80621-54-1] *4′,5-Dihydroxy-7-methoxy-6-methylflavone.* ***8-Demethylsideroxylin***
$C_{17}H_{14}O_5$ 298.295
Isol. from *Gaultheria procumbens* (wintergreen). Yellow needles (MeOH). Mp 284-286°.

4′,5-Di-Me ether: [127324-51-0] *7-Hydroxy-4′,5-dimethoxy-6-methylflavone.* ***Cleroflavone***
$C_{18}H_{16}O_5$ 312.321
Yellow needles ($CHCl_3/C_6H_6$). Mp 260-261°.

4′,7-Di-Me ether: [5689-38-3] *5-Hydroxy-4′,7-dimethoxy-6-methylflavone.* ***8-Demethyleucalyptin***
$C_{18}H_{16}O_5$ 312.321
Isol. from *Gaultheria procumbens* (wintergreen). Cryst. ($CHCl_3$/petrol). Mp 187-188°.

Lamberton, J.A. *et al., Aust. J. Chem.*, 1964, **17**, 692 (*isol, uv, ir, pmr, struct*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 1981, **36**, 913; 1984, **39**, 710 (*derivs*)
Cardona, M.L. *et al., Phytochemistry*, 1982, **21**, 2759 (*8-Demethylsideroxylin*)
Courtney, J.L. *et al., Phytochemistry*, 1983, **22**, 947 (*derivs*)
Zapeschnaya, G.G. *et al., Khim. Prir. Soedin.*, 1984, **20**, 306; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 284 (*uv*)
Inigo, A.C. *et al., An. Quim., Ser. C*, 1985, **81**, 116 (*8-Demethylsideroxylin*)
Ganapaty, S. *et al., Indian J. Chem., Sect. B*, 1990, **29**, 289 (*isol, pmr*)
Huq, F. *et al., Planta Med.*, 1997, **63**, 369-370 (*Demethyleucalyptin, cmr, ms*)
Sarker, S.D. *et al., Biochem. Syst. Ecol.*, 2001, **29**, 759-762 (*isol*)
Wasowski, C. *et al., Planta Med.*, 2002, **68**, 932-934 (*isol, pmr, cmr*)

4′,5,7-Trihydroxy-8-methylisoflavanone T-633



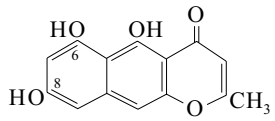
$C_{16}H_{14}O_5$ 286.284

4′-Me ether: [163021-16-7] *5,7-Dihydroxy-4′-methoxy-8-methylisoflavanone*
$C_{17}H_{16}O_5$ 300.31
Constit. of the flowers of *Amaranthus caudatus* (love-lies-bleeding).

Srivastava, B.K. *et al., Orient. J. Chem.*, 1994, **10**, 294 (*isol, uv, ir, pmr, ms*)

5,6,8-Trihydroxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, 9CI T-634

[3566-98-1]
5,6,8-Trihydroxy-2-methylbenzo[g]chromen-4-one. ***Norrubrofusarin***



$C_{14}H_{10}O_5$ 258.23
Isol. from seeds of *Cassia tora* (charota). Orange-red cryst. (dioxan aq.). Mp 298-299° dec.

6-O-β-D-Glucopyranoside, 8-deoxy: [123914-49-8] ***Cassiaside***
$C_{20}H_{20}O_9$ 404.373
Isol. from seeds of *Cassia tora* (charota). Mp 256-257°. $[\alpha]_D$ -1.5 (c, 0.14 in 50% EtOH aq.). Incorrect name in CA.

6-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Norrubrofusarin 6-β-gentiobioside***
$C_{26}H_{30}O_{15}$ 582.514
Constit. of the seeds of *Cassia tora* (charota). Yellow powder. $[\alpha]_D$ -45 (c, 0.1 in Py). λ_{max} 223 (log ϵ 4.13); 254 (log ϵ 4.15); 278 (log ϵ 4.33); 327 (log ϵ 3.26); 399 (log ϵ 3.45) (MeOH).

8-Me ether: [3567-00-8] *5,6-Dihydroxy-8-methoxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, 9CI. 5,6-Dihydroxy-8-methoxy-2-methylbenzo[g]chromen-4-one.* ***Rubrofusarin***
$C_{15}H_{12}O_5$ 272.257
Orange-red cryst. (petrol, C_6H_6 or EtOH). Mp 210-211°. λ_{max} 224 (ϵ 28200); 250 (ϵ); 277 (ϵ 47600); 325 (ϵ 3210); 407 (ϵ 5480) (MeCN) (Derep). λ_{max} 225 (ϵ 28200); 278 (ϵ 49700); 328 (ϵ 3400); 415 (ϵ 5200) (MeOH) (Berdy).

8-Me ether, 6-O-β-D-glucopyranoside: [132922-80-6] ***Rubrofusarin 6-glucoside***
$C_{21}H_{22}O_{10}$ 434.399
Cryst. (MeOH). Mp 194-196°. $[\alpha]_D$ -83 (c, 0.5 in MeOH). λ_{max} 223 (ϵ 17780); 276 (ϵ 29510); 320 (ϵ 2240); 395 (ϵ 5250) (MeOH) (Berdy).

8-Me ether, 6-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [24577-90-0] ***Rubrofusarin 6-gentiobioside***
$C_{27}H_{32}O_{15}$ 596.541
Isol. from seeds of *Cassia tora* (charota). Yellow needles (MeOH). Mp 252.5-254°. $[\alpha]_D^{16}$ -62.5 (c, 0.16 in Py).

8-Me ether, 6-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [119170-51-3] ***Cassiaside B***
$C_{26}H_{30}O_{14}$ 566.515
Isol. from seeds of *Cassia tora* (charota). Orange-yellow needles + $\frac{1}{2}H_2O$ (MeOH aq.). Mp 231-231.5°. $[\alpha]_D^{25}$ -93.3 (c, 0.85 in Py). λ_{max} 221 (ϵ 27542); 274 (ϵ 52480); 320 (ϵ 2820); 392 (ϵ 6456) (MeOH) (Berdy).

8-Me ether, 6-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: ***Cassiaside B$_2$***
$C_{39}H_{52}O_{25}$ 920.825
Constit. of the seeds of *Cassia tora* (charota). Greenish-yellow needles (MeOH aq.). Mp 200-203° Mp 211°. $[\alpha]_D^{25}$ +11.3 (c, 0.4 in H_2O) (*C. obtusifolia*). $[\alpha]_D$ -22.2 (c, 0.1 in H_2O) (*C. tora*). λ_{max} 225 (log ϵ 3.08); 278 (log ϵ 3.39); 394 (log ϵ 2.43) (H_2O).

8-Me ether, 6-O-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:
$C_{33}H_{42}O_{20}$ 758.683
Constit. of the seeds of *Cassia tora* (charota). Needles (MeOH). Mp 198°. $[\alpha]_D$ -16.6 (c, 0.1 in MeOH aq.). λ_{max} 223 (log ϵ 4.49); 258 (sh) (log ϵ 4.51); 276 (log ϵ 4.67); 322 (log ϵ 3.67); 390 (log ϵ 3.79) (MeOH).

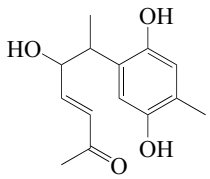
6,8-Di-Me ether: [17276-15-2] *5-Hydroxy-6,8-dimethoxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one.* ***Rubrofusarin B****. Heminigerone. Antibiotic TMC 256A$_2$. TMC 256A$_2$*
$C_{16}H_{14}O_5$ 286.284
Yellow cryst. ($CHCl_3/C_6H_6$). Mp 213°. λ_{max} 224 (ϵ 28200); 250 (ϵ); 277 (ϵ 47600); 325 (ϵ 3210); 407 (ϵ 5480) (MeCN) (Derep). λ_{max} 225 (ϵ 25120); 242 (ϵ 32360); 247 (ϵ 31622); 277 (ϵ 33890); 376 (ϵ 4466) (MeOH) (Berdy). λ_{max} 225 (ϵ 40000); 250 (ϵ 37000); 275 (ϵ 80000); 320 (ϵ 5250); 395 (ϵ 9200) (EtOH) (Berdy).

1′-Hydroxy: [146556-62-9] *5,6,8-Trihydroxy-2-(hydroxymethyl)-4*H*-naphtho[2,3-*b*]pyran-4-one.* ***Parasperone A***
$C_{14}H_{10}O_6$ 274.229
Orange solid. λ_{max} 224 (ϵ 28200); 250 (ϵ); 277 (ϵ 47600); 325 (ϵ 3210); 407 (ϵ 5480) (MeCN) (Derep). λ_{max} 223 ; 250 ; 277 ; 325 ; 408 (MeCN) (Berdy).

Narayana, C.S. *et al., CA*, 1957, **51**, 6740 (*isol, Norrubrofusarin*)
Bycroft, B.W. *et al., J.C.S.*, 1962, 40 (*struct*)
Kimura, Y. *et al., Yakugaku Zasshi*, 1966, **86**, 1087 (*Cassiaside*)
Shoji, S. *et al., Chem. Pharm. Bull.*, 1967, **15**, 1757 (*synth*)
Badawi, M.M. *et al., Indian J. Chem.*, 1967, **5**, 591 (*ms*)
Galmarini, O.L. *et al., Experientia*, 1974, **30**, 586 (*isol*)
Ogura, M. *et al., J. Nat. Prod.*, 1977, **40**, 347 (*isol*)
Gorst-Allman, C.P. *et al., J.C.S. Perkin 1*, 1980, 2474 (*Rubrofusarin B*)
Leeper, F.J. *et al., J.C.S. Perkin 1*, 1984, 1053; 2919 (*cmr, biosynth*)
Abell, C. *et al., Chem. Comm.*, 1986, 15 (*synth*)
Kitanaka, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3980 (*Cassiaside B, 6-gentiobioside*)
Messana, I. *et al., Phytochemistry*, 1991, **30**, 708 (*Rubrofusarin 6-glucoside*)
Brown, D.W. *et al., Tet. Lett.*, 1993, **34**, 419 (*Parasperone A*)
Kitanaka, S. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1650-1652 (*Cassiaside B$_2$*)
Lee, H.J. *et al., Nat. Prod. Sci.*, 1998, **4**, 95-99 (*cmr*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1121-1127 (*Cassiaside B$_2$, Norrubrofusarin 6-gentiobioside*)
Macías, M. *et al., J. Nat. Prod.*, 2000, **63**, 757-761 (*activity*)
Sakurai, M. *et al., J. Antibiot.*, 2002, **55**, 685-692 (*TMC 256A*)

1,4,8-Trihydroxy-13-nor-1,3,5,9-bisabolatetraen-11-one T-635

[201288-95-1]
Helinorbisabone

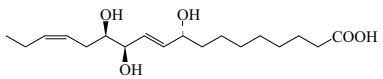


$C_{14}H_{18}O_4$ 250.294
Constit. of *Helianthus annuus* (sunflower). Yellow oil. $[\alpha]_D^{25}$ +3 (c, 0.1 in $CHCl_3$).

Marcás, F.A. *et al., Phytochemistry*, 1998, **48**, 631-636 (*isol, pmr, cmr*)

9,12,13-Trihydroxy-10,15-octadecadienoic acid, 9CI T-636

[51146-90-8]



(9*R*,10*E*,12*R*,13*R*,15*Z*)-*form*

$C_{18}H_{32}O_5$ 328.448

(9*S*,10*E*,12*S*,13*S*,15*Z*)-*form* [95341-44-9]
Corchorifatty acid F
Isol. from rice infected with blast disease and confers activity against rice blast disease. $[\alpha]_D^{24}$ -10.5 (c, 0.7 in MeOH). Unnatural stereoisomers also synthesised.

Kato, T. *et al., Tet. Lett.*, 1985, **26**, 2357 (*isol*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1008-1014 (*Corchorifatty acid F*)

11,12,13-Trihydroxy-9,15-octadecadienoic acid T-637

$C_{18}H_{32}O_5$ 328.448
Stereochem. of nat. prod. not detd.

(9*Z*,11*R*,12*S*,13*S*,15*Z*)-*form* [102735-55-7]
$[\alpha]_D$ -16.6 (c, 1.4 in $CHCl_3$).

Me ester: [130980-39-1]
Oil. $[\alpha]_D$ -16 (c, 0.17 in $CHCl_3$).

[101219-67-4, 102693-71-0]

Kato, T. *et al., Chem. Lett.*, 1986, 577 (*isol*)
Yadav, J.-S. *et al., Tet. Lett.*, 1990, **31**, 4349 (*synth*)
Wu, W.-L. *et al., Tet. Lett.*, 1992, **33**, 3887 (*synth*)
Baudat, A. *et al., Helv. Chim. Acta*, 1994, **77**, 1500 (*synth, bibl*)
Hatakeyama, S. *et al., Chem. Lett.*, 1995, 763 (*synth, bibl*)
Honda, T. *et al., J.C.S. Perkin 1*, 1999, 23-29 (*synth, ir, pmr, cmr*)

9,10,13-Trihydroxyoctadecanoic acid T-638

[50439-74-2]
9,10,13-Trihydroxystearic acid
$H_3C(CH_2)_4CH(OH)CH_2CH_2CH(OH)$-$CH(OH)(CH_2)_7COOH$
$C_{18}H_{36}O_5$ 332.479
Constit. of *Phaseolus vulgaris* (kidney bean) roots. Mp 135-137°.

Me ester: [50439-75-3]
$C_{19}H_{38}O_5$ 346.506
Mp 117.5-119.5°.

Takasugi, M. *et al., Chem. Lett.*, 1973, 445 (*isol, pmr, ms*)

9,10,18-Trihydroxyoctadecanoic acid T-639

[496-86-6]

$C_{18}H_{36}O_5$ 332.479

(9*S*,10*S*)-*form* [17705-68-9]
Phloionolic acid. *Floionolic acid*
Constit. of cork and other plants, e.g. olive (*Olea europaea*), apple wax, the famine food *Agave americana* and also cutins. Cryst. (MeOH). Mp 104-105°. $[\alpha]_D$ +22.75. pK_{a1} 4.95. The (9*R*,10*R*)-(-) form has also been prepared.

Me ester: [36693-05-7]
$C_{19}H_{38}O_5$ 346.506
Mp 79-80.5°. $[\alpha]_D$ +21.52.

(9*RS*,10*RS*)-*form* [583-86-8] (±)-*threo-form*
Cryst. (EtOAc). Mp 104°.

(9*RS*,10*SR*)-*form* [17673-81-3] *erythro-form*. *Isophloionolic acid*
Cryst. (EtOAc). Mp 132-133°. Opt. inactive (*meso*-).

Duhamel, L. *et al., Bull. Soc. Chim. Fr.*, 1965, 399 (*struct*)
Ames, D.E. *et al., J.C.S.(C)*, 1967, 1556 (*synth*)
Eglinton, G. *et al., Phytochemistry*, 1968, **7**, 313 (*ms*)
McGhie, J.F. *et al., Chem. Ind. (London)*, 1972, 463 (*stereochem*)

5,8,12-Trihydroxy-9-octadecenoic acid T-640

$H_3C(CH_2)_5CH(OH)CH_2CH$
$=CHCH(OH)CH_2CH_2CH(OH)(CH_2)_3$-
$COOH$
$C_{18}H_{34}O_5$ 330.464
Constit. of wheat bran.

Albro, P.W. *et al., Phytochemistry*, 1971, **10**, 631 (*isol, pmr, ms*)

9,12,13-Trihydroxy-10-octadecenoic acid T-641

[29907-56-0]
Pinellic acid

$C_{18}H_{34}O_5$ 330.464
Isol. from a rice cultivar. Confers resistance to rice blast disease.

(9*S*,10*E*,12*R*,13*S*)-*form* [102735-58-0]

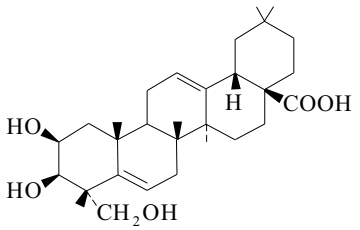
(9*S*,10*E*,12*S*,13*S*)-*form* [97134-11-7]
Found in beer and blast-resistant rice. $[\alpha]_D^{25}$ -8 (c, 0.3 in MeOH).

Me ester: [93380-89-3]
$[\alpha]_D^{25}$ -7.03 (c, 1.28 in $CHCl_3$). Unnatural stereoisomers also synthesised.

[38947-15-8, 95783-98-5, 102735-57-9, 102735-59-1, 135214-42-5, 135214-43-6, 135214-49-2]

Gardner, H.W. *et al., Chem. Phys. Lipids*, 1984, **35**, 87-101 (*synth*)
Herz, W. *et al., Phytochemistry*, 1985, **24**, 89-91; 1986, **25**, 1481-1483 (*isol*)
Suemune, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 3632-3637 (*synth*)
Kato, T. *et al., Agric. Biol. Chem.*, 1991, **55**, 1349-1357 (*synth, abs config*)
Hamberg, M. *et al., J. Agric. Food Chem.*, 1991, **39**, 1568-1572 (*isol*)
Quinton, P. *et al., Tet. Lett.*, 1991, **32**, 4909-4912 (*synth, pmr*)
Sunazuka, T. *et al., Tet. Lett.*, 2002, **43**, 1265-1268 (*synth, abs config*)

2,3,23-Trihydroxy-5,12-oleanadien-28-oic acid T-642



$C_{30}H_{46}O_5$ 486.69

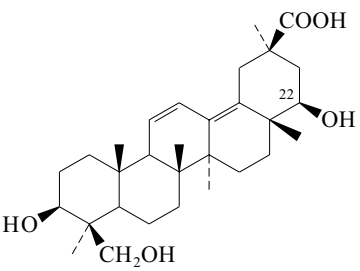
(2β,3β)-*form* [465-01-0]
Bassic acid. *Mimusopssapogenin*. *Bassiaic acid*
Sapogen from the famine food *Madhuca longifolia*. Cryst. (MeOH). Mp 319-324°. $[\alpha]_D$ +82.6 (Py).

2,3-Di-O-*β*-D-*glucopyranoside:* ***Bassiasaponin A***
$C_{42}H_{66}O_{15}$ 810.974
Mp 216-218° dec. $[\alpha]_D$ +35 (c, 0.8 in Py).

2,3-Di-O-*β*-D-*glucopyranoside, [α*-L-*rhamnopyranosyl(1→4)-β*-D-*xylopyranosyl(1→2)-α*-L-*arabinopyranoside]:* ***Bassiasaponin B***
$C_{58}H_{92}O_{27}$ 1221.349
Trihydrate. Mp 212-214°. $[\alpha]_D$ -30 (c, 1.50 in Py).

King, T.J. *et al., J.C.S.*, 1961, 4308 (*struct*)
Cocker, W. *et al., J.C.S.*, 1963, 677 (*isol*)
Gaudemer, A. *et al., Bull. Soc. Chim. Fr.*, 1964, 407 (*pmr*)
Mose, W.P. *et al., J.C.S.(C)*, 1971, 1572 (*struct*)
Hariharan, V. *et al., Phytochemistry*, 1972, **11**, 1791 (*Bassiasaponins*)
Toyota, M. *et al., Phytochemistry*, 1990, **29**, 2849 (*isol, pmr, cmr*)

3,22,24-Trihydroxy-11,13(18)-oleanadien-30-oic acid T-643



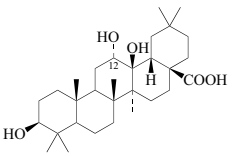
$C_{30}H_{46}O_5$ 486.69

(3β,22β)-*form*

30→22 Lactone: [111150-27-7] *3β,24-Dihydroxy-11,13(18)-oleanadien-30,22β-olide.* ***Uralenolide***
$C_{30}H_{44}O_4$ 468.675
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Cryst. Mp 302-303°.

Shu, Y. *et al., CA*, 1987, **107**, 214819a (*isol*)

3,12,13-Trihydroxy-28-oleananoic acid T-644



(3β,12α,13β)-*form*

$C_{30}H_{50}O_5$ 490.722

(3β,12α,13β)-*form*

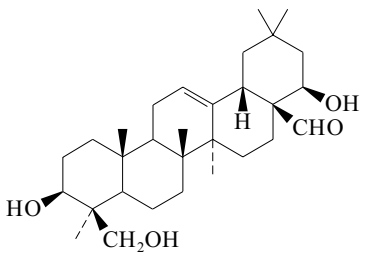
28→13 Lactone, 3-Ac: [62498-83-3]
$C_{32}H_{50}O_5$ 514.744
Constit. of *Rhodomyrtus tomentosa* (hill gooseberry). Cryst. Mp 301-303° (284-286°). $[\alpha]_D$ +39.7 ($CHCl_3$). Initially descr. in CA as an ursane.

12-Ketone, 28→13 lactone, 3-Ac: [35959-11-6] ***3β-Acetoxy-12-oxo-28,13β-oleananolide***
$C_{32}H_{48}O_5$ 512.728
Constit. of *Rhodomyrtus tomentosa* (hill gooseberry). Cryst. Mp 287-289°. $[\alpha]_D$ +38 ($CHCl_3$).

[74048-38-7]

Hui, W.-H. *et al., Phytochemistry*, 1976, **15**, 1741
Poehland, B.L. *et al., J. Nat. Prod.*, 1987, **50**, 706

3,22,24-Trihydroxy-12-oleanen-28-al T-645



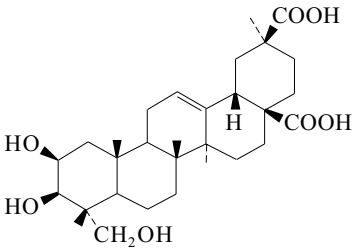
$C_{30}H_{48}O_4$ 472.707

(3β,22β)-*form*

*22-[2,3-Dihydro-5-hydroxy-6-methyl-4-oxo-4*H*-pyran-2-yl], 3-*O*-[α-L-rhamnopyranosyl-(1→2)-β-D-galactopyranosyl-(1→2)-β-D-glucuronopyranoside]:* [161842-85-9] ***Lablabsaponin I***
$C_{54}H_{82}O_{22}$ 1083.229
Constit. of *Dolichos lablab* (hyacinth bean). $[\alpha]_D^{23}$ -92.2 (c, 0.3 in MeOH).

Yoshiki, Y. *et al., Phytochemistry*, 1995, **38**, 229 (*isol, pmr, cmr, ms*)

2,3,23-Trihydroxy-12-oleanene-28,30-dioic acid T-646



$C_{30}H_{46}O_7$ 518.689

(2β,3β)-*form* [51776-39-7]
Jaligonic acid. *Desmethylphytolaccagenin*
Cryst. (MeOH). Mp 315-325° dec. (318-320°). Log P 3.29 (calc).

Glycoside: ***Phytolaccatoxin***
$C_{55}H_{90}O_{22}$ 1103.303
Isol. from seeds of *Phytolacca americana* (pokeberry). Tentative MF. Gives Phytolaccagenin, D-xylose and D-glucose on hydrol..

3-O-β-D-Xylopyranoside: [65649-36-7] ***Esculentoside E***. *Phytolaccoside G*
$C_{35}H_{54}O_{11}$ 650.805
Isol. from *Phytolacca americana* (pokeberry).

3-O-β-D-Xylopyranoside, 30-Me ester: [60820-94-2] ***Phytolaccasaponin G***. *Phytolaccoside B*
$C_{36}H_{56}O_{11}$ 664.832
From *Phytolacca americana* (pokeberry). Needles + $1H_2O$ (MeOH aq.). Sol. MeOH, Py. Mp 266-269°. $[\alpha]_D^{26}$ +67.3 (c, 1.44 in EtOH). λ_{max} 210 (E1%/1cm 285) (MeOH) (Berdy).

▶ RK0177560

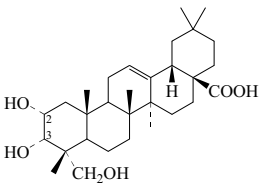
3-O-[β-D-Glucopyranosyl-(1→4)-β-D-xylopyranoside], 20-epimer, 30-Me ester: [65497-07-6] ***Phytolaccasaponin E***. *Phytolaccoside E*
$C_{42}H_{66}O_{16}$ 826.974
Isol. from *Phytolacca americana* (pokeberry). Powder. Mp 257-258°. $[\alpha]_D^{21}$ +51.3 (c, 0.99 in EtOH).

▶ RK0177530

3-O-[β-D-Glucopyranosyl-(1→4)-β-D-xylopyranoside], 28-β-D-glucopyranosyl ester, 30-Me ester: [66656-92-6] ***Phytolaccasaponin B***. *Esculentoside H*
$C_{48}H_{76}O_{21}$ 989.116
Isol. from *Phytolacca americana* (pokeberry). Needles + $3H_2O$. Sol. MeOH, butanol, H_2O. Mp 218-220°. $[\alpha]_D^{29}$ +38.3 (c, 0.93 in EtOH). λ_{max} 213 (MeOH) (Berdy).

Stout, G.H. *et al., J.A.C.S.*, 1964, **86**, 957 (*isol, struct*)
Woo, W.S. *et al., J. Nat. Prod.*, 1973, **36**, 326 (*isol*)
Johnson, A. *et al., Tetrahedron*, 1974, **30**, 2033 (*isol*)
Glombitza, K.W. *et al., Planta Med.*, 1975, **27**, 367 (*isol*)
Woo, W.S. *et al., Phytochemistry*, 1976, **15**, 1315 (*glycoside*)
Harkar, S. *et al., Phytochemistry*, 1984, **23**, 2893 (*deriv*)
Kasai, R. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1486 (*cmr*)
Kobayashi, A. *et al., Z. Naturforsch., C*, 1995, **50**, 398 (*Phytolaccoside B, pmr, cmr*)

2,3,23-Trihydroxy-12-oleanen-28-oic acid T-647



(2α,3α)-*form*

$C_{30}H_{48}O_5$ 488.706

(2α,3β)-*form* [465-00-9]
Arjunolic acid
Constit. of *Psidium guajava* (guava). Cryst. (Me_2CO). Mp 337-340°. $[\alpha]_D^{19}$ +63.5 (c, 0.5 in EtOH).

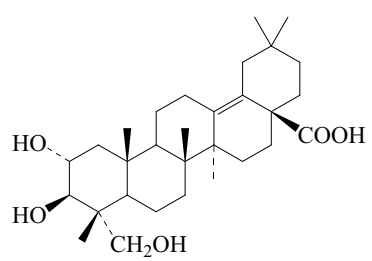
3-O-β-D-Glucopyranoside: [99543-11-0]
$C_{36}H_{58}O_{10}$ 650.848
Constit. of *Luffa cylindrica* (smooth luffa).

(2β,3β)-*form* [6989-24-8]
Bayogenin
Cryst. (dioxan). Mp 328-330°. $[\alpha]_D^{27}$ +98 (c, 0.37 in dioxan).

3-O-[α-L-Rhamnopyranosyl-(1→3)-β-D-glucuronopyranoside], 28-O-β-D-glucopyranosyl ester: [214840-33-2]
$C_{48}H_{76}O_{20}$ 973.116
Constit. of *Amaranthus cruentus* (purple amaranth).

King, F.E. *et al., J.C.S.*, 1954, 3995; 1958, 2830
Eade, R.A. *et al., Aust. J. Chem.*, 1963, **16**, 900; 1969, **22**, 2703 (*isol, struct*)
Cheung, H.T. *et al., J.C.S.(C)*, 1968, 1047 (*isol*)
Bowden, B.F. *et al., Aust. J. Chem.*, 1975, **28**, 91 (*isol*)
Higuchi, R. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1314 (*deriv*)
Ruo, T.-I. *et al., Phytochemistry*, 1976, **15**, 335 (*isol*)
De Pascual Teresa, J. *et al., An. Quim.*, 1979, **75**, 135 (*derivs*)
Kojima, H. *et al., Phytochemistry*, 1986, **25**, 729; 1989, **28**, 1703 (*pmr, struct, Arjunolic acid*)
Araújo, F.W.L. *et al., J. Nat. Prod.*, 1990, **53**, 1436 (*Arjunolic acid*)
Junkuszew, M. *et al., Phytochemistry*, 1998, **49**, 195-198 (*Amaranthus cruentus saponin*)
Ajees, A.A. *et al., Acta Cryst. E*, 2002, **58**, o682-o684 (*Arjunolic acid, cryst struct*)

2,3,23-Trihydroxy-13(18)-oleanen-28-oic acid T-648



$C_{30}H_{48}O_5$ 488.706

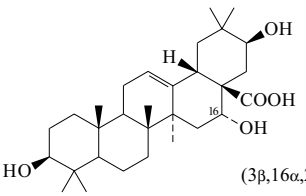
(2α,3β)-*form*
Centellasapogenol A
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. ($CHCl_3$/MeOH). Mp 247-250°. $[\alpha]_D^{28}$ -26.6 (c, 0.1 in MeOH).

28-O-*β*-D-*Glucopyranosyl ester:* [297141-62-9] ***Quadranoside X***
$C_{36}H_{58}O_{10}$ 650.848
Amorph. solid. $[\alpha]_D^{25}$ +15.6 (c, 0.03 in MeOH).

28-O-*[α*-L-*Rhamnopyranosyl-(1→4)-β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranosyl] ester:* ***Centellasaponin A***
$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. ($CHCl_3$/MeOH). Mp 200-201°. $[\alpha]_D^{24}$ -33.4 (c, 0.3 in Py).

Adnyana, I K. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1114-1120 (*Quadranoside X*)
Matsuda, H. *et al., Heterocycles*, 2001, **55**, 1499-1504 (*Centellasapogenol A, Centellasaponin A*)

3,16,21-Trihydroxy-12-oleanen-28-oic acid T-649



(3β,16α,21β)-*form*

$C_{30}H_{48}O_5$ 488.706

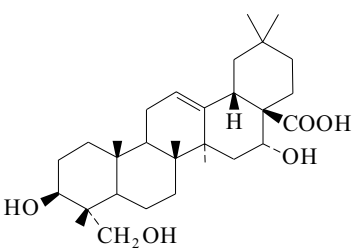
(3β,16α,21β)-*form* [1962-14-7]
Acacic acid. *Acacinoic acid*
Cryst. Mp 280-281° (268-272°).

*21-(6-Hydroxy-2,6-dimethyl-2*E*,7-octadienoyl), 3*-O-*[α*-L-*arabinopyranosyl-(1→2)-α*-L-*arabinopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [248259-55-4] ***Pithecelloside***
$C_{56}H_{88}O_{20}$ 1081.299
Constit. of *Pithecellobium dulce* (manila tamarind). Amorph. powder. $[\alpha]_D^{20}$ +2.85 (c, 0.28 in MeOH).

[68247-77-8]

Sahu, N.P. *et al., J. Chem. Res., Synop.*, 1999, 558-559 (*Pithecelloside*)

3,16,23-Trihydroxy-12-oleanen-28-oic acid T-650



$C_{30}H_{48}O_5$ 488.706

(3β,16α)-*form* [52936-64-8]
Caulophyllogenin. *Collinsogenin*
Cryst. (EtOH). Mp 277-280°. $[\alpha]_D$ +14.3 (Py).

3-O-*α*-L-*Arabinopyranoside:* [12672-43-4] ***Cauloside B***. *Racemoside. Collinsonin*
$C_{35}H_{56}O_9$ 620.822
Needles. Mp 266-267° Mp 313-314° dec. $[\alpha]_D$ +26.5 (c, 0.48 in MeOH). Racemoside was the mono-Na salt.

3-O-*α*-L-*Arabinopyranoside, 28*-O-*[α*-L-*rhamnopyranosyl-(1→4)-β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranosyl] ester:* [188426-48-4] ***Leonticin D***
$C_{53}H_{86}O_{23}$ 1091.249
Needles. Mp 219-220°. $[\alpha]_D^{20}$ -18.9 (c, 0.96 in MeOH).

3-O-*β*-D-*Glucuronopyranoside:* [171828-77-6] ***Elatoside G***
$C_{36}H_{56}O_{11}$ 664.832
Constit. of *Aralia elata* (Japanese angelica tree). Cryst. (MeOH aq.). Mp 247-249°. $[\alpha]_D^{28}$ -5.1 (c, 0.1 in MeOH).

3-O-*β*-D-*Glucuronopyranoside, 28*-O-*[(3,4-dimethoxybenzoyl)-(→2)-β*-D-*glucopyranosyl] ester:* [269055-80-3] ***Ligatoside A***
$C_{51}H_{74}O_{19}$ 991.134
λ_{max} 220 (log ε 4.11); 264 (log ε 3.85); 294 (log ε 3.58) (MeOH).

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-α*-L-*arabinopyranoside]:* [243857-99-0] ***Glycoside L-F$_2$***
$C_{41}H_{66}O_{13}$ 766.965

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-α*-L-*arabinopyranoside], 28*-O-*β*-D-*glucopyranosyl ester:* [158511-58-1] ***Medicagosaponin P$_2$***
$C_{47}H_{76}O_{18}$ 929.107
Amorph. powder. $[\alpha]_D$ -4.1 (c, 0.54 in MeOH).

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-α*-L-*arabinopyranoside], 28*-O-*[β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranosyl] ester:* [158511-57-0] ***Medicagosaponin P$_1$***
$C_{53}H_{86}O_{23}$ 1091.249
Amorph. powder. $[\alpha]_D$ -20.1 (c, 0.3 in Py).

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-α*-L-*arabinopyranoside], 28*-O-*[α*-L-*rhamnopyranosyl-(1→4)-β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranosyl] ester:* [243858-02-8] ***Glycoside L-I$_2$***
$C_{59}H_{96}O_{27}$ 1237.391

3-O-*[β*-D-*Glucopyranosyl-(1→3)-α*-L-*arabinopyranoside], 28*-O-*β*-D-*glucopyranosyl ester:* [289649-65-6] ***Araliasaponin II***
$C_{47}H_{76}O_{19}$ 945.106
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder. $[\alpha]_D$ -39.4 (c, 0.22 in Py).

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucuronopyranoside], 28*-O-*[(3,4-dimethoxybenzoyl)-(→2)-β*-D-*glucopyranosyl] ester:* [269055-81-4] ***Ligatoside B***
$C_{57}H_{84}O_{24}$ 1153.276
λ_{max} 219 (log ε 4.15); 257 (log ε 3.94); 262 (log ε 3.94); 292 (log ε 3.63) (MeOH).

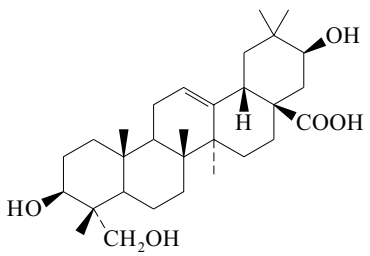
3-O-*[β*-D-*Glucopyranosyl-(1→3)-β*-D-*glucopyranosyl-(1→3)-[β*-D-*glucopyranosyl-(1→2)]-β*-D-*glucopyranoside], 28*-O-*β*-D-*glucopyranosyl ester:* [340982-23-2]
$C_{60}H_{98}O_{30}$ 1299.416
Constit. of *Aralia elata* (Japanese angelica tree). Amorph. powder. $[\alpha]_D$ +23.1 (c, 0.3 in Py).

23-Aldehyde: 3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid, D-598

[90890-76-9]

Strigina, L.I. *et al., Khim. Prir. Soedin.*, 1974, **10**, 733; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **16**, 755 (*Cauloside B*)
Strigina, L.I. *et al., Phytochemistry*, 1974, **13**, 479
Becchi, M. *et al., Eur. J. Biochem.*, 1980, **108**, 271 (*isol, pmr, cmr*)
Joshi, B.S. *et al., J. Nat. Prod.*, 1992, **55**, 1468 (*Collinsonin*)
Kinjo, J. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1339 (*Medicagosaponins*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1878 (*Elatoside G*)
Chen, M. *et al., Phytochemistry*, 1997, **44**, 497 (*Leonticin D*)
Grishkovets, V.I. *et al., Khim. Prir. Soedin.*, 1998, **34**, 777-781; *Chem. Nat. Compd. (Engl. Transl.)*, 1998, **34**, 694-698 (*L-F$_2$, L-I$_2$*)
Song, S.-J. *et al., Chem. Pharm. Bull.*, 2000, **48**, 838-842 (*Araliasaponin II*)
Plasman, V. *et al., J. Nat. Prod.*, 2000, **63**, 646-649 (*Ligatosides*)
Song, S.J. *et al., Phytochemistry*, 2001, **56**, 491-497 (*Araliasaponin VIII*)

3,21,23-Trihydroxy-12-oleanen-28-oic acid T-651



$C_{30}H_{48}O_5$ 488.706

(3β,21β)-*form* [96304-77-7]
21β-Hydroxyhederagenin
Constit. of *Luffa cylindrica* (smooth luffa). Cryst. (as Me ester). Mp 258-261° (Me ester). $[\alpha]_D^{22}$ +47.4 (c, 0.6 in MeOH) (Me ester).

3-O-*β*-D-*Glucopyranoside:* [152845-77-7] ***Lucyoside N***
$C_{36}H_{58}O_{10}$ 650.848
Constit. of *Luffa cylindrica* (smooth luffa). Cryst. Mp 221-223°.

21-O-*β*-D-*Glucopyranoside:* [96304-76-6] ***Anchusoside 4***
$C_{36}H_{58}O_{10}$ 650.848

21-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [103766-07-0] ***Anchusoside 5***
$C_{42}H_{68}O_{15}$ 812.99

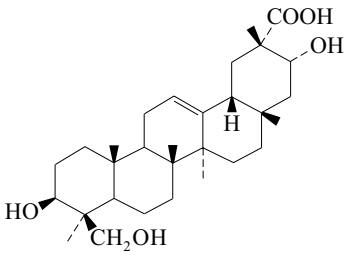
23-Aldehyde: [152845-76-6] *3,21-Dihydroxy-23-oxo-12-oleanen-28-oic acid.* ***Lucyin A***. *21β-Hydroxygypsogenin*
$C_{30}H_{46}O_5$ 486.69
Constit. of *Luffa cylindrica* (smooth luffa). Cryst. Mp 240-242°.

23-Aldehyde, 3-O-*β*-D-*glucopyranoside, 28*-O-*β*-D-*glucopyranosyl ester:* [100156-31-8] ***Lucyoside J***
$C_{42}H_{66}O_{15}$ 810.974

Constit. of *Luffa cylindrica* (smooth luffa). Cryst. Mp 165-167°. $[\alpha]_D$ +29.5 (c, 4.8 in MeOH).

Romussi, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1985, **318**, 219 (*isol, pmr, cmr*)
Takemoto, T. *et al., Yakugaku Zasshi*, 1985, **105**, 834; *CA*, **104**, 95321h (*Lucyoside J*)
Romussi, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1986, **319**, 549 (*Anchusosides*)
Liang, L. *et al., Yaoxue Xuebao*, 1993, **28**, 836-839 (*Lucyin A, Lucyosides N, Q, R*)

3,21,24-Trihydroxy-12-oleanen-29-oic acid T-652



$C_{30}H_{48}O_5$ 488.706

(3β,21α)-*form* [20528-70-5]
Liquiridiolic acid. *Glyyunnansapogenin B*
Constit. of roots of *Glycyrrhiza glabra* (licorice). Cryst. ($CHCl_3$/MeOH). Mp 285-287°. $[\alpha]_D^{20}$ +45 (c, 0.6 in $CHCl_3$/MeOH).

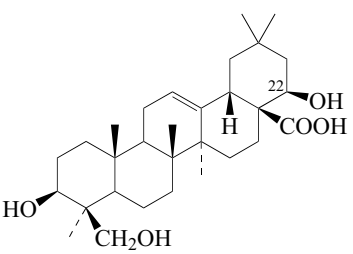
3-O-[α-L-Rhamnopyranosyl-(1→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Yunganoside G1***
$C_{48}H_{74}O_{21}$ 987.1
Amorph. powder. $[\alpha]_D^{23}$ -7.4 (c, 0.75 in MeOH).

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]: ***Yunganoside G2***
$C_{42}H_{64}O_{17}$ 840.957
Amorph. powder. $[\alpha]_D^{20}$ -27.2 (c, 1 in MeOH).

[131177-50-9]

Canonica, L. *et al., Gazz. Chim. Ital.*, 1968, **98**, 712
Zeng, L. *et al., CA*, 1991, **114**, 20975x (*isol, pmr, cmr, ms, cd*)
Ohtani, K. *et al., Phytochemistry*, 1994, **36**, 139 (*Yunganosides*)
Hu, J.F. *et al., Yaoxue Xuebao*, 1995, **30**, 27; *CA*, **123**, 222884p (*Glyyunansaponin B1*)

3,22,24-Trihydroxy-12-oleanen-28-oic acid T-653



$C_{30}H_{48}O_5$ 488.706

(3β,22β)-*form*

22-Angeloyl:
$C_{35}H_{54}O_6$ 570.808
Cryst. ($CHCl_3$/MeOH). Mp 294-298°. $[\alpha]_D$ +73 (c, 1.5 in EtOH).

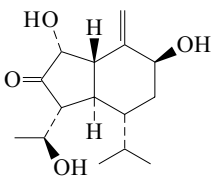
3-Ketone, 22-angeloyl: [561-47-7] ***Icterogenin***. *Icterogenin A*
$C_{35}H_{52}O_6$ 568.792
Cryst. Mp 239-241°. $[\alpha]_D$ +64 (c, 1 in EtOH). Icterogenin C, Mp 155-160° was a hydrate of Icterogenin.

▶ Hepatotoxin.

22-O-(2,3-Dihydro-5-hydroxy-6-methyl-4-oxo-4H-pyran-2-yl) ether, 3-O-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranoside]: ***Az I***
$C_{48}H_{74}O_{18}$ 939.102
Constit. of *Vigna angularis* (azuki bean). $[\alpha]_D^{23}$ -53 (c, 0.5 in Py). λ_{max} 292 (MeCN).

Barton, D.H.R. *et al., J.C.S.*, 1954, 887 (*struct*)
Anderson, L.A.P. *et al., J. S. Afr. Chem. Inst.*, 1961, **14**, 58; *CA*, **57**, 15163 (*angeloyl*)
Hart, N.K. *et al., Aust. J. Chem.*, 1976, **29**, 655 (*isol*)
Iida, T. *et al., Phytochemistry*, 1997, **45**, 1507 (*Az I*)

2,4,9-Trihydroxy-10(14)-oplopen-3-one T-654



$C_{15}H_{24}O_4$ 268.352

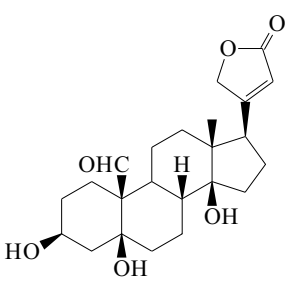
(*ent*-2β,4*S*,9α)-*form*

9-(3-Methyl-2E-pentenoyl), 2-(2-methylbutanoyl): [80489-86-7]
$C_{26}H_{40}O_6$ 448.598
Constit. of *Tussilago farfara* (coltsfoot). Gum. $[\alpha]_D^{24}$ -72 (c, 2.5 in $CHCl_3$).

9-(3-Methyl-2E-pentenoyl), 2-(2-methylbutanoyl), 4-Ac: [80489-87-8]
$C_{28}H_{42}O_7$ 490.636
Gum. $[\alpha]_D^{24}$ -124 (c, 4 in $CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 2024 (*deriv, pmr*)
Kikuchi, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2753 (*deriv, pmr, cmr*)

3,5,14-Trihydroxy-19-oxocard-20(22)-enolide T-655



$C_{23}H_{32}O_6$ 404.502
Log P -0.96 (uncertain value) (calc).

(3β,5β,14β)-*form* [66-28-4]
Strophanthidin. *Corchorin. Corchorigenin. Corchsularin. Corchotoxin*
Cryst. + $2H_2O$ (H_2O). Sol. MeOH, AcOH, C_6H_6; poorly sol. H_2O, Et_2O, hexane. Mp 169-170° Mp 235° (anhyd.). $[\alpha]_D^{25}$ +43.1 (MeOH). Pharmacol. active isomer.

▶ LD_{50} (mus, ivn) 0.33 mg/kg. Very tox. by intravenous route. FH5425000

3-O-(6-Deoxy-β-D-gulopyranoside): [5822-57-1] ***Desglucocheirotoxin***
$C_{29}H_{42}O_{10}$ 550.645
Isol. from *Convallaria majalis*. *Convallaria majalis* has been designated unsafe for inclusion in foods etc. by USA FDA. Cryst. (MeOH aq. or MeOH/Et_2O). Mp 188-189° (181-184°). $[\alpha]_D^{20}$ +1.3 (-8.7) (MeOH).

*3-O-(2,6-Dideoxy-β-D-*ribo*-hexopyranoside):* [630-64-8] ***Helveticoside***. *Alleoside. Erysimotoxin. Erysimine. Allioside A. Strophanthidin digitoxoside*
$C_{29}H_{42}O_9$ 534.645
Constit. of *Hesperis matronalis* (sweet rocket). Cryst. + $2H_2O$ (EtOH aq.). Mp 168-172° dec. $[\alpha]_D^{20}$ +43.5 (EtOH). Log P -1.66 (uncertain value) (calc).

▶ LD_{50} (rat, ivn) 54 mg/kg. MH7440000

*3-O-(2,6-Dideoxy-β-D-*xylo*-hexopyranoside):* [508-76-9] ***Corchoroside A***. *Strophanthidin boivinoside*
$C_{29}H_{42}O_9$ 534.645
Constit. of *Corchorus olitorius* (Jew's mallow) and *Hesperis matronalis* (sweet rocket). Cryst. + $2H_2O$ (EtOH). Mp 188-190° (anhyd.). $[\alpha]_D^{20}$ +19 (MeOH). Log P -1.66 (uncertain value) (calc).

▶ FH4970000

3-O-α-L-Rhamnopyranoside: [508-75-8] ***Convallatoxin***. *Convallaton. Convallopan. Convalpur. Convapur. Corglykon. Korglykon. Corglycone. Convallatoxoside*
$C_{29}H_{42}O_{10}$ 550.645
Constit. of *Convallaria majalis*. *Convallaria majalis* has been designated unsafe for inclusion in foods etc. by USA FDA. Cryst. (MeOH/EtOH). Mp 247° (235-242). $[\alpha]_D^{22}$ -1.7 (c, 0.65 in MeOH). $[\alpha]_D$ 0 ($CHCl_3$). Log P -2.05 (uncertain value) (calc).

▶ LD_{50} (cat, ipr) 0.2 mg/kg. Very toxic by intraperitoneal route. GL4025000

3-O-[β-D-Glucopyranosyl-(1→4)-α-L-fucopyranoside]: [13473-51-3] ***Convalloside***. *Bogoroside*
$C_{35}H_{52}O_{15}$ 712.787
Constit. of seeds of *Convallaria majalis*. *Convallaria majalis* has been designated unsafe for inclusion in foods etc. by USA FDA. Needles (MeOH/Et_2O). Mp 201-204°. $[\alpha]_D^{25}$ -10.4 (80% EtOH aq.).

▶ GL4207500.

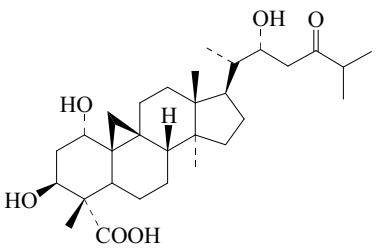
*3-O-[β-D-Glucopyranosyl-(1→4)-2,6-dideoxy-β-D-*xylo*-hexopyranoside]:* [13289-20-8] ***Olitoriside***. *Olitorin*
$C_{35}H_{52}O_{14}$ 696.787
Isol. from *Corchorus olitorius* (Jew's mallow). Mp 204-206°. $[\alpha]_D^{22}$ -4.5.

*3-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→4)-2,6-dideoxy-β-D-*ribo*-hexopyranoside]:* [125708-07-8] ***Olitoriusin***
$C_{41}H_{62}O_{19}$ 858.929
Isol. from the seeds of *Corchorus*

olitorius (Jew's mallow). Solid (MeOH/Et_2O). Mp 185-188°. $[\alpha]_D$ +21.2 (c, 0.45 in MeOH).

Nagata, W. *et al., Helv. Chim. Acta*, 1957, **40**, 41-61 (*Helveticoside, bibl*)
Zorbach, W. *et al., J. Med. Chem.*, 1963, **6**, 298-301 (*Convallatoxin, 6′-Hydroxyconvallatoxin*)
Umarova, R.U. *et al., Khim. Prir. Soedin.*, 1970, **6**, 140; *Chem. Nat. Compd. (Engl. Transl.)*, 1970, **6**, 138 (*Corchoroside A*)
Kubelka, W. *et al., Phytochemistry*, 1974, **13**, 1805-1808 (*Convallatoxin*)
Gonzalez, A.G. *et al., An. Quim.*, 1975, **71**, 97-103 (*Corchoroside A*)
Pal'yants, N.Sh. *et al., CA*, 1976, **85**, 143397a (*Convallatoxin*)
Ricca, G.S. *et al., Gazz. Chim. Ital.*, 1982, **112**, 349-352 (*Glucoolitoriside, Olitoriside*)
Mahato, S.B. *et al., J.C.S. Perkin 1*, 1989, 2065-2068 (*Olitoriusin, isol, pmr*)
Lei, Z.-H. *et al., Phytochemistry*, 1996, **41**, 1187-1189; 1998, **49**, 1801-1803 (*Cheiranthosides III-V, Olitoriside*)
Nakamura, T. *et al., Phytochemistry*, 1998, **49**, 2097-2101 (*Corchoroside A, Helveticoside, pmr, cmr*)

1,3,22-Trihydroxy-24-oxocycloartan-28-oic acid T-656



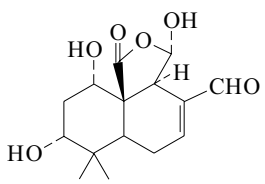
$C_{30}H_{48}O_6$ 504.706

(1α,3β,22*R*)-*form* [292167-37-4] ***Cyclopassifloic acid D***
Constit. of *Passiflora edulis* (passion fruit). Needles. Mp 202-203°. $[\alpha]_D^{25}$ +48.3 (c, 0.4 in MeOH).

28-O-β-D-Glucopyranosyl ester: [292167-43-2] ***Cyclopassifloside VI***
$C_{36}H_{58}O_{11}$ 666.848
Constit. of *Passiflora edulis* (passion fruit). Amorph. solid. $[\alpha]_D^{25}$ +36.2 (c, 2.6 in MeOH).

Yoshikawa, K. *et al., J. Nat. Prod.*, 2000, **63**, 1229-1234 (*isol, pmr, cmr*)

1,3,11-Trihydroxy-12-oxo-7-drimen-15,11-olide T-657

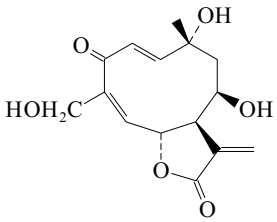


$C_{15}H_{20}O_6$ 296.319

(1α,3α,11α)-*form* [124869-10-9] ***Marasmal***
Metab. of *Marasmius oreades* (fairy ring mushroom). Cryst. ($CHCl_3$). Mp 195-200°. $[\alpha]_D^{24}$ -73.1 (c, 0.32 in MeOH). λ_{max} 228 (ε 18200) (MeOH) (Derep).

Ayer, W.A. *et al., Can. J. Chem.*, 1989, **67**, 1371 (*isol, pmr, cmr*)

8,10,15-Trihydroxy-3-oxo-1,4,11(13)-germacratrien-12,6-olide T-658



$C_{15}H_{18}O_6$ 294.304

(1*E*,4*Z*,6α,8β,10α)-*form*

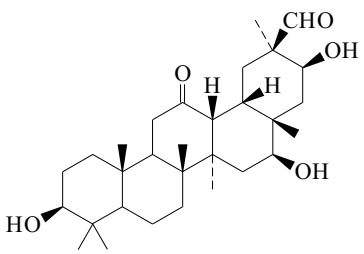
8-(2-Methylbutanoyl): [166528-79-6]
$C_{20}H_{26}O_7$ 378.421
Constit. of *Helianthus* spp.. Stereochem. not clear from ref..

8-Angeloyl: [84588-88-5]

[103188-56-3]
$C_{20}H_{24}O_7$ 376.405
Constit. of *Helianthus annuus* (sunflower). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. λ_{max} 215 (ε 25200); 250 (sh) (ε 14700) (EtOH). λ_{max} 250 (ε 14700) (MeOH) (Berdy).

Spring, O. *et al., Phytochemistry*, 1982, **21**, 2551-2553 (*isol, pmr, cmr, uv*)
Buschmann, H. *et al., Phytochemistry*, 1995, **39**, 367 (*isol, pmr*)

3,16,21-Trihydroxy-12-oxo-30-oleananal T-659



$C_{30}H_{48}O_5$ 488.706

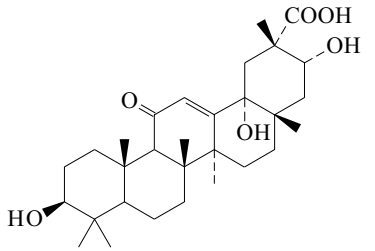
(3β,16β,21β)-*form*

21-Benzoyl: [90578-32-8] ***Avenestergenin B2***
$C_{37}H_{52}O_6$ 592.814
Aglycone from oat root. Fine needles ($CHCl_3$/MeOH). Mp 177-178°.

21-(2-Methylaminobenzoyl): [90578-33-9] ***Avenestergenin B1***
$C_{38}H_{55}NO_6$ 621.856
Fine needles ($CHCl_3$/MeOH). Mp 186-187°.

Begley, M.J. *et al., J.C.S. Perkin 1*, 1986, 1905 (*isol, pmr, cmr, cryst struct*)

3,18,21-Trihydroxy-11-oxo-12-oleanen-29-oic acid T-660



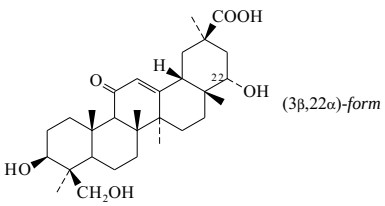
$C_{30}H_{46}O_6$ 502.69

(3β,18α,21α)-*form*

29 → 18 Lactone: [18184-25-3] *3,21-Dihydroxy-11-oxo-12-oleanen-29,18-olide.* ***21-Hydroxyisoglabrolide***
$C_{30}H_{44}O_5$ 484.675
Constit. of *Glycyrrhiza glabra* (licorice). Cryst. ($CHCl_3$/2-propanol). Mp 304-305°. $[\alpha]_D^{20}$ -11 (c, 1 in Py).

Canonica, L. *et al., Gazz. Chim. Ital.*, 1967, **97**, 1347
Zeng, L. *et al., Phytochemistry*, 1990, **29**, 3605 (*pmr, cmr*)
Lin, L.-J. *et al., Phytochemistry*, 1994, **35**, 1549 (*isol, pmr, cmr*)

3,22,24-Trihydroxy-11-oxo-12-oleanen-30-oic acid T-661



(3β,22α)-*form*

$C_{30}H_{46}O_6$ 502.69

(3β,22α)-*form* [102292-11-5]
Mp 300°. $[\alpha]_D^{21}$ +140 (c, 0.57 in EtOH).

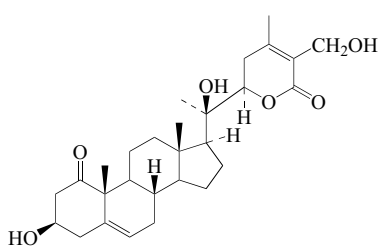
Tri-Ac: [102292-12-6]
Plates (EtOH aq.). Mp 300-306°.

(3β,22β)-*form*

30 → 22 Lactone: [98063-18-4] *3β,24-Dihydroxy-11-oxo-12-oleanen-30,22β-olide.* ***24-Hydroxyglabrolide***
$C_{30}H_{44}O_5$ 484.675
Isol. from *Glycyrrhiza uralensis* (Chinese licorice).

Shu, Y. *et al., CA*, 1985, **103**, 119932r (*isol, pmr*)
Sakano, K. *et al., Agric. Biol. Chem.*, 1986, **50**, 763 (*isol*)

3,20,27-Trihydroxy-1-oxowitha-5,24-dienolide T-662



$C_{28}H_{40}O_6$ 472.62

(3β,20*R*,22*R*)-*form*

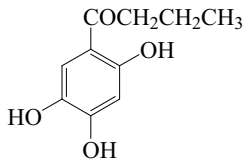
Cryst. Mp 186-188°. $[\alpha]_D^{25}$ +69.4 (c, 0.51 in $CHCl_3$). λ_{max} 218 (log ϵ 3.96) (MeOH).

3-O-β-D-Glucopyranoside: [227179-09-1]
$C_{34}H_{50}O_{11}$ 634.762
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. powder. $[\alpha]_D^{25}$ +73.4 (c, 0.43 in MeOH). λ_{max} 218 (log ϵ 3.91) (MeOH).

Ahmad, S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 477-480 (*isol, pmr, cmr*)

1-(2,4,5-Trihydroxyphenyl)-1-butanone, 9CI T-663

[1421-63-2]
2′,4′,5′-Trihydroxybutyrophenone, 8CI. 5-Butanoyl-1,2,4-benzeneetriol. THBP

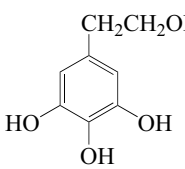


$C_{10}H_{12}O_4$ 196.202
Antioxidant, esp. for fats and oils. Potential food packaging migration residue. Mp 151-153°.

U.S. Pat., 1956, 2 759 828; *CA*, **51**, 4741f (*use, synth*)
Jha, H.C. *et al., Can. J. Chem.*, 1981, **59**, 2266-2282 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2834-2835 (*use*)
Irache, J.M. *et al., Sci. Aliments*, 1997, **17**, 95-105 (*hplc, detn*)
Noguera-Orti, J.F. *et al., Chromatographia*, 2000, **51**, 53-60 (*hplc, detn*)

2-(3,4,5-Trihydroxypheny-l)ethanol T-664

[134695-79-7]
5-(2-Hydroxyethyl)-1,2,3-benzenetriol, 9CI. 3,4,5-Trihydroxyphenethyl alcohol



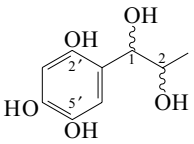
$C_8H_{10}O_4$ 170.165

4′-Me ether:2-(3,5-Dihydroxy-4-methoxyphenyl)ethanol. 3,5-Dihydroxy-4-methoxyphenethyl alcohol. ***Alphitol***
$C_9H_{12}O_4$ 184.191
λ_{max} 270 (no solvent reported).

3′,5′-Di-Me ether, 4′-O-β-D-glucopyranoside:
$C_{16}H_{24}O_9$ 360.36
Constit. of the roots of *Phyllanthus emblica* (emblic). Off-white powder + 1/4 H_2O. $[\alpha]_D^{20}$ +19.3 (c, 0.7 in MeOH).

Dunstan, C.A. *et al., Phytochemistry*, 1998, **48**, 495-497 (*Alphitol*)
Zhang, Y.-J. *et al., J. Nat. Prod.*, 2001, **64**, 870-873 (*3′,5′-di-Me 4′-glucoside*)

1-(2,4,5-Trihydroxyphenyl)-1,2-propanediol T-665



$C_9H_{12}O_5$ 200.191

2′,4′,5′-Tri-Me ether: [146830-05-9] *1-(2,4,5-Trimethoxyphenyl)-1,2-propanediol*
$C_{12}H_{18}O_5$ 242.271
Gum.

2′,4′,5′-Tri-Me ether, 2-Ac: [146830-06-0]
$C_{14}H_{20}O_6$ 284.308
Gum.

2′,4′,5′-Tri-Me ether, 1,2-di-Ac: [146830-07-1]
$C_{16}H_{22}O_7$ 326.346
Gum.

1,2′,4′,5′-Tetra-Me ether: [98205-47-1] *1-Methoxy-1-(2,4,5-trimethoxyphenyl)-2-propanol*
$C_{13}H_{20}O_5$ 256.298
Constit. of *Acorus calamus* (sweet flag). Oil. Racemic.

2,2′,4′,5′-Tetra-Me ether: [146830-08-2] *2-Methoxy-1-(2,4,5-trimethoxyphenyl)-1-propanol*
$C_{13}H_{20}O_5$ 256.298
Gum.

1,2-Diketone, 2′,4′,5′-tri-Me ether: [2020-84-0] *1-(2,4,5-Trimethoxyphenyl)-1,2-propanedione*
$C_{12}H_{14}O_5$ 238.24
Constit. of *Acorus calamus* (sweet flag). Needles (EtOAc/hexane). Mp 129-130°. λ_{max} 237 (log ϵ 4.34); 273 (log ϵ 4.17); 342 (log ϵ 4.12) (MeOH).

Tsuruga, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 3265 (*Trimethoxyphenylpropanedione*)
Koul, S.K. *et al., Phytochemistry*, 1993, **32**, 478

3-(3,4,5-Trihydroxyphenyl)-1,2-propanediol T-666

$C_9H_{12}O_5$ 200.191

3′,4′-Di-Me ether: [120021-92-3] *3-(3-Hydroxy-4,5-dimethoxyphenyl)-1,2-propanediol, 9CI.* ***Todatriol***
$C_{11}H_{16}O_5$ 228.244

3′,4′-Di-Me ether, 1-O-β-D-glucopyranoside:
$C_{17}H_{26}O_{10}$ 390.386
Constit. of the fruit of *Carum ajowan* (ajowan). Amorph. powder. $[\alpha]_D^{23}$ -6 (c, 0.1 in MeOH).

3′,4′,5′-Tri-Me ether: [140385-37-1] *3-(3,4,5-Trimethoxyphenyl)-1,2-propanediol.* ***p-Methoxytodadiol****. Kmeriol*
$C_{12}H_{18}O_5$ 242.271
Oil.

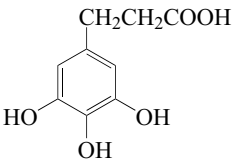
4′,5′-Methylene, 3′-Me ether: [140385-38-2] *3-(3-Methoxy-4,5-methylenedioxyphenyl)-1,2-propanediol.* ***Suavediol***
$C_{11}H_{14}O_5$ 226.229
Oil.

[123199-96-2]

Gonzalez, A.G. *et al., Biochem. Syst. Ecol.*, 1988, **16**, 641 (*Todatriol*)
Dong, X. *et al., Pharm. Res.*, 1989, **6**, 637 (*Kmeriol*)
González, A.G. *et al., Phytochemistry*, 1991, **30**, 4189
Ishikawa, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 840-844 (*3′,4′-di-Me 1-glucoside*)

3-(3,4,5-Trihydroxyphenyl)-propanoic acid T-667

[40284-59-1]
3,4,5-Trihydroxybenzenepropanoic acid, 9CI. 3,4,5-Trihydroxydihydrocinnamic acid



$C_9H_{10}O_5$ 198.175

Tri-Me ether: [25173-72-2] *3-(3,4,5-Trimethoxyphenyl)propanoic acid. 3,4,5-Trimethoxydihydrocinnamic acid*
$C_{12}H_{16}O_5$ 240.255
Constit. of *Piper longum* (long pepper) and *Piper retrofractum* (Javanese long pepper). Cryst. (MeOH). Mp 102-103°.

Tri-Me ether, Et ester: [70311-20-5]
Oil. $Bp_{0.3}$ 142-145°.

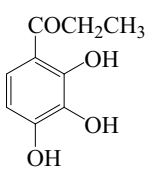
Tri-Me ether, amide:3-(3,4,5-Trimethoxyphenyl)propanamide
$C_{12}H_{17}NO_4$ 239.271
Cryst. (C_6H_6/petrol). Mp 108-109°.

[53560-25-1]

Gutsche, C.D. *et al., J.A.C.S.*, 1950, **72**, 4285 (*synth*)
Koo, J. *et al., J.A.C.S.*, 1953, **75**, 1889 (*synth, ester*)
Benington, F. *et al., J.O.C.*, 1956, **21**, 1545 (*synth*)
Lin, J.-Y. *et al., Agric. Biol. Chem.*, 1972, **36**, 506 (*synth, pmr*)
Kato, M. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1518 (*synth, ester*)
Banerji, A. *et al., Phytochemistry*, 1985, **24**, 279 (*isol, deriv*)
Toth, G. *et al., Synth. Commun.*, 1995, **25**, 3067 (*synth, deriv*)
Das, B. *et al., Planta Med.*, 1996, **62**, 582 (*isol, deriv, pmr, cmr*)

1-(2,3,4-Trihydroxyphenyl)-1-propanone T-668

2′,3′, 4′-Trihydroxypropiophenone



$C_9H_{10}O_4$ 182.176

2′-Me, 3′,4′-methylene ether:1-(2-Methoxy-3,4-methylenedioxyphenyl)-1-propanone
$C_{11}H_{12}O_4$ 208.213
Constit. of *Anethum sowa* (Indian dill). Mp 67°.

Tomar, S.S. *et al., Fitoterapia*, 2001, **72**, 76-77

1-(2,4,5-Trihydroxyphenyl)-1-propanone, 9CI T-669

[79744-62-0]
2′,4′,5′-Trihydroxypropiophenone

$C_9H_{10}O_4$ 182.176
Nearly colourless cryst. Mp 151-153°.

Tri-Me ether: [3904-18-5] *1-(2,4,5-Trimethoxyphenyl)-1-propanone. 2′,4′,5′-Trimethoxypropiophenone.* ***Isoacoramone***
$C_{12}H_{16}O_4$ 224.256
Constit. of *Acorus calamus* (sweet flag). Cryst. (EtOH). Mp 108.5-109.5°.

Mazza, G. *et al., J. Chromatogr.*, 1985, **328**, 179 (*isol, tri-Me ether*)

1-(2,4,5-Trihydroxyphenyl)-2-propanone T-670

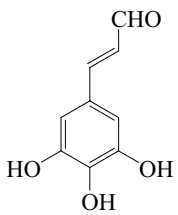
$C_9H_{10}O_4$ 182.176

Tri-Me ether: [2020-90-8] *1-(2,4,5-Trimethoxyphenyl)-2-propanone, 9CI.* ***Acoramone***
$C_{12}H_{16}O_4$ 224.256
Constit. of the oil of *Acorus calamus* (sweet flag). Liq.

Patra, A. *et al., J. Nat. Prod.*, 1981, **44**, 668-669 (*isol, ir, pmr, ms*)

3-(3,4,5-Trihydroxyphenyl)-2-propenal, 9CI T-671

3,4,5-Trihydroxycinnamaldehyde



$C_9H_8O_4$ 180.16
►GD6850000

(E)-form

Tri-Me ether: [71277-13-9] *3-(3,4,5-Trimethoxyphenyl)-2-propenal, 9CI. 3,4,5-Trimethoxycinnamaldehyde*
$C_{12}H_{14}O_4$ 222.24
Mp 109-111°.

3,4-Methylene, 5-Me ether: [74683-19-5] *3-Methoxy-4,5-methylenedioxycinnamaldehyde*
$C_{11}H_{10}O_4$ 206.198
Constit. of *Piper auritum* (Veracruz pepper). Yellow needles (Et_2O/hexane). Mp 136-137°. λ_{max} 243 (ϵ 10800); 337 (ϵ 11000) (MeOH).

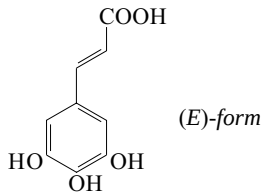
(Z)-form

Tri-Me ether: [71277-12-8]
Cryst. (petrol). Mp 59-60°.

Cook, J.T. *et al., Phytochemistry*, 1978, **17**, 1419 (*isol*)
Olstein, R. *et al., Aust. J. Chem.*, 1979, **32**, 681 (*synth*)
Liptaj, T. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 330 (*pmr, conformn*)
El-Feraly, F.S. *et al., J. Nat. Prod.*, 1980, **43**, 407 (*3-Methoxy-4,5-methylenedioxycinnamaldehyde*)
Boulware, R.T. *et al., J. Nat. Prod.*, 1981, **44**, 200 (*isol*)
Bestmann, H.J. *et al., Chem. Ber.*, 1982, **115**, 161 (*synth, ir, uv*)
Taylor, R.T. *et al., J.O.C.*, 1983, **48**, 5160 (*synth*)
Mohammad, I. *et al., J. Nat. Prod.*, 1985, **48**, 328 (*isol*)
Tachibana, S. *et al., CA*, 1991, **114**, 81152 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLA250

3-(3,4,5-Trihydroxyphenyl)-2-propenoic acid T-672

[6093-59-0]
3-(3,4,5-Trihydroxyphenyl)acrylic acid. 3,4,5-Trihydroxycinnamic acid



(E)-form

$C_9H_8O_5$ 196.159Does not appear to have been found in nature in the free state despite extensive searches.

(E)-form

Needles + $1H_2O$ (H_2O) becoming anhyd. at 120°. Mp 207-208° dec.

3-Me ether: [1782-55-4] *3-(3,4-Dihydroxy-5-methoxy)-2-propenoic acid, 9CI. 3,4-Dihydroxy-5-methoxycinnamoic acid. 5-Hydroxyferulic acid. 3-Methoxycaffeic acid*
$C_{10}H_{10}O_5$ 210.186
Isol. from bamboo (*Phyllostachys edulis*). Cryst. (H_2O). Mp 182° (168-170° dec).

3,5-Di-Me ether: [530-59-6] *4-Hydroxy-3,5-dimethoxycinnamic acid.* ***Sinapic acid****. Sinapinic acid*
$C_{11}H_{12}O_5$ 224.213
A common constit. of plants and fruits. Yellow needles (EtOH). Mp 192°.

3,5-Di-Me ether, β-D-glucopyranosyl ester: [78185-48-5] ***Raphanusol B****. 1-Sinapoylglucose*
$C_{17}H_{22}O_{10}$ 386.355
Isol. from seedlings of *Raphanus sativus* (radish); also identified in *Brassica oleracea* (cabbage). Pale yellow needles. Mp 123-124°.

Tri-Me ether, Me ester: [20329-96-8]

[7560-49-8] ***Methyl 3,4,5-trimethoxycinnamate***
$C_{13}H_{16}O_5$ 252.266
Isol. from *Piper longum* (long pepper) and other plant spp.. Needles (MeOH). Mp 99-100°.

Tri-Me ether, [α-L-arabinofuranosyl-(1→3)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranosyl] ester: [234761-04-7]
$C_{29}H_{42}O_{19}$ 694.639
Constit. of soybean molasses (*Glycine* sp.). Amorph. powder. $[\alpha]_D^{25}$ -19.7 (c, 0.87 in MeOH). λ_{max} 235 (log ϵ 4.18); 283 (log ϵ 4.36) (MeOH).

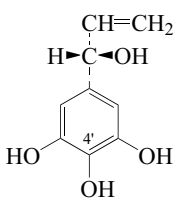
(Z)-form

3,5-Di-Me ether: [7361-90-2]
Constit. of shoots of *Medicago sativa* (alfalfa). Obt. as a mixt. with (*E*)-form by uv irradiation. Occurs only in a bound alkali-labile state.

[54976-67-9]

Späth, E. *et al., Monatsh. Chem.*, 1920, **41**, 271
Shinoda, J. *et al., Yakugaku Zasshi*, 1931, **51**, 249; *CA*, **25**, 3979 (*synth*)
Kung, H.P. *et al., J.A.C.S.*, 1949, **71**, 1836 (*synth, uv, Sinapic acid*)
Freudenberg, K. *et al., Chem. Ber.*, 1952, **85**, 1181
Bate-Smith, E.C. *et al., Sci. Proc. R. Dublin Soc.*, 1956, **27**, 165 (*occur, Sinapic acid*)
Nakamura, T. *et al., Chem. Pharm. Bull.*, 1962, **10**, 281-290 (*synth, 3-Me ether*)
Moffett, R.B. *et al., J. Med. Chem.*, 1964, **7**, 319 (*deriv*)
Horner, L. *et al., Chem. Ber.*, 1965, **98**, 1233-1245 (*synth, 3-Me ether*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 962 (*occur, Sinapic acid*)
Wallace, A.F.A. *et al., Aust. J. Chem.*, 1973, **26**, 1571
Hartley, R.D. *et al., J. Chromatogr.*, 1975, **107**, 213 (*glc, ms*)
Corothie, E. *et al., Planta Med.*, 1975, **27**, 182 (*isol, esters*)
v. Massow, F. *et al., J.C.S. Perkin 2*, 1976, 977 (*cmr*)
Herrmann, K. *et al., Prog. Chem. Org. Nat. Prod.*, 1976, 73 (*rev*)
Dutta, C.P. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 583 (*isol, deriv*)
Ito, H. *et al., Phytochemistry*, 1977, **16**, 1614-1616 (*isol, deriv*)
Bagirov, V.Y. *et al., Khim. Prir. Soedin.*, 1980, 826; *CA*, **94**, 171046 (*isol, Equisetan*)
Newby, V.K. *et al., Phytochemistry*, 1980, **19**, 651 (*occur*)
Hasegawa, K. *et al., Plant Cell Physiol.*, 1980, **21**, 363; 1981, **22**, 303 (*Raphanusol B*)
Fujita, M. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2622 (*cmr*)
Legseir, B. *et al., Phytochemistry*, 1986, **25**, 1735 (*isol*)
Tachibana, S. *et al., Phytochemistry*, 1992, **31**, 3207-3209 (*isol, 3-Me ether*)
Guilhon, G.M.S.P. *et al., Phytochemistry*, 1994, **37**, 1193 (*isol, deriv*)
Hashimoto, K. *et al., Planta Med.*, 1994, **60**, 124 (*Sinapic acid 4-glucoside*)
Pauli, G.F. *et al., Phytochemistry*, 1995, **38**, 1245 (*Raphanusol B*)
Hosny, M. *et al., J. Nat. Prod.*, 1999, **62**, 853-858 (*tri-Me ether arabinosylglucosylglucosyl ester*)
Dall'Acqua, S. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1499-1501 (*Methyl sinapate, isol, pmr, cmr*)

1-(3,4,5-Trihydroxyphenyl)-2-propen-1-ol T-673



(S)-form

$C_9H_{10}O_4$ 182.176

(S)-form

3′-Me, 4′,5′-methylene ether:3-Methoxy-4,5-methylenedioxycinnamyl alcohol. ***Anthriscinol***
$C_{11}H_{12}O_4$ 208.213
Constit. of *Myristica fragrans* (nutmeg). Cryst. (EtOAc/hexane). Mp 83-84°.

3′,5′-Di-Me ether, 4′-O-β-D-glucopyranoside: [117259-33-3] ***Tangshenoside II***
$C_{17}H_{24}O_9$ 372.371
Powder. $[\alpha]_D^{19}$ -29 (c, 1.37 in EtOH).

3′,4′,5′-Tri-Me ether, 1-O-[2-(2-methyl-2-butenoyloxymethyl)-2-butenoyl](Z,Z-):
$C_{22}H_{28}O_7$ 404.459
Oil. $[\alpha]_D^{25}$ -25 (c, 0.09 in $CHCl_3$). Abs. config. of this deriv. not certain.

(±)-form

1-Et, 3′,4′,5′-tri-Me ether:1-(1-Ethoxy-2-propenyl)-3,4,5-trimethoxybenzene
$C_{14}H_{20}O_4$ 252.31
Oil.

Hattori, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 648 (*Anthriscinol*)
Mizutani, K. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2726 (*Tangshenoside*)
Tanoguchi, M. *et al., Chem. Pharm. Bull.*, 1989, **37**, 68 (*Anthriscinol, synth*)
Massanet, G.M. *et al., Phytochemistry*, 1997, **44**, 173 (*tri-Me ether derivs*)

3-(3,4,5-Trihydroxyphenyl)-2-propen-1-ol T-674

3′,4′,5′-Trihydroxycinnamyl alcohol

$C_9H_{10}O_4$ 182.176

(E)-form

Mp 167°. Probable (*E*)-config. assumed here.

3′-Me ether, 4′-O-β-D-glucopyranoside: ***De-O-methylsyringin***
$C_{16}H_{22}O_9$ 358.344
Gum. λ_{max} 222 (log ε 3.31); 264 (log ε 3.81) (MeOH).

3′-Me, 4′,5′-methylene ether: [69618-94-6] *3-(3-Methoxy-4,5-methylenedioxyphenyl)-2-propen-1-ol. 3′-Methoxy-4′,5′-methylenedioxycinnamyl alcohol*
$C_{11}H_{12}O_4$ 208.213
Constit. of *Myristica fragrans* (nutmeg). Needles (EtOAc/hexane). Mp 72-73°.

4′-Me ether, 1-O-(2E-decene-4,6-diynoyl): [79695-03-7] *4′-O-Methylsinapyl lachnophyllate*
$C_{20}H_{20}O_5$ 340.375
Gum.

3′,5′-Di-Me ether: Sinapyl alcohol, S-113

3′,4′,5′-Tri-Me ether: [30273-62-2] *3-(3,4,5-Trimethoxyphenyl)-2-propen-1-ol. 3′,4′,5′-Trimethoxycinnamyl alcohol*
$C_{12}H_{16}O_4$ 224.256
Constit. of *Myristica fragrans* (nutmeg) and other plant spp.. Mp 110°. $Bp_{0.15}$ 145-147°.

3′,4′,5′-Tri-Me ether, Ac: [87200-84-8]
$C_{14}H_{18}O_5$ 266.293
Constit. of oil of bergamot (*Citrus bergamia*). Oil.

3′,4′,5′-Tri-Me ether, O-(3-methylbutanoyl): [105072-20-6] *3,4,5-Trimethoxycinnamyl isovalerate*
$C_{17}H_{24}O_5$ 308.374
Oil.

3′,4′,5′-Tri-Me ether, 1-O-β-D-glucopyranoside: [135743-09-8] ***Icariside H_1***. *Juniperoside*
$C_{18}H_{26}O_9$ 386.398
Amorph. powder. $[\alpha]_D^{23}$ -47.6 (c, 0.62 in MeOH).

3′,4′,5′-Tri-Me ether, 1-O-(2E,6E-decadien-4-ynoyl): [79695-02-6] *4′-O-Methylsinapyl 6,7-dihydrolachnophyllate*
$C_{22}H_{26}O_5$ 370.444
Gum.

3′,4′,5′-Tri-Me ether, 1-O-[2-(2-angeloyloxymethyl)-2Z-butenoyl]:
$C_{22}H_{28}O_7$ 404.459
Oil. λ_{max} 225 ; 270 (EtOH).

1,3′,4′,5′-Tetra-Me ether:3,4,5-Trimethoxy-1-(3-methoxy-1-propenyl)benzene. ***Boropinol B***
$C_{13}H_{18}O_4$ 238.283
Yellow oil. λ_{max} 222 ; 268 (MeOH).

1-Et, 3′,4′,5′-tri-Me ether:1-(3-Ethoxy-1-propenyl)-3,4,5-trimethoxybenzene
$C_{14}H_{20}O_4$ 252.31
Oil. λ_{max} 292 (EtOH).

Aldehyde, 3′-Me, 4′,5′-methylene ether:3-(3-Methoxy-4,5-methylenedioxyphenyl)-propenal. 3′-Methoxy-4′,5′-methylenedioxycinnamaldehyde
$C_{11}H_{10}O_4$ 206.198
Amorph.

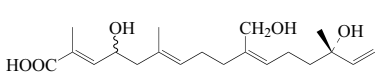
(Z)-form

3′,4′,5′-Tri-Me ether: [30273-66-6]
Pale yellow oil. $Bp_{0.25}$ 138-140°.

[1504-56-9, 30273-66-6, 97094-25-2]

Freudenberg, K. *et al., Chem. Ber.*, 1953, **86**, 190; 1955, **88**, 16 (*synth*)
Cooper, P.D. *et al., Can. J. Chem.*, 1970, **48**, 3882 (*synth*)
Kato, M. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1516 (*deriv, synth*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1335 (*lachnophyllate esters*)
Ehret, C. *et al., Phytochemistry*, 1982, **21**, 2984 (*isol, deriv, Ac*)
Mohammed, I. *et al., J. Nat. Prod.*, 1985, **48**, 328 (*isol, pmr, cmr*)
San Feliciano, A. *et al., J. Nat. Prod.*, 1986, **49**, 677 (*isol, deriv*)
Ponpipom, M.M. *et al., J. Med. Chem.*, 1987, **30**, 136 (*synth*)
Hattori, M. *et al., Chem. Pharm. Bull.*, 1988, **36**, 648 (*isol*)
Matsushita, H. *et al., Phytochemistry*, 1991, **30**, 2025 (*Icariside H_1*)
Comte, G. *et al., Planta Med.*, 1996, **62**, 88 (*Juniperoside*)
Gonzalez, A.G. *et al., Planta Med.*, 1996, **62**, 176 (*Methoxymethylenedioxycinnamaldehyde*)
Massanet, G.M. *et al., Phytochemistry*, 1997, **44**, 173 (*Bupleurum derivs*)
Tan, R.X. *et al., Phytochemistry*, 1998, **48**, 1245-1250 (*Demethylsyringin*)
Ito, C. *et al., J. Nat. Prod.*, 2000, **63**, 1344-1348 (*Boropinol B*)

3,13,19-Trihydroxy-1,6,10,14-phytatetraen-16-oic acid T-675



$C_{20}H_{32}O_5$ 352.47

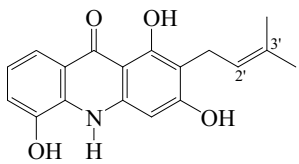
(3S,6Z,10E,14E)-form

3-O-β-D-Glucopyranoside: [121924-06-9] ***Capsianoside V***. *Capsianside V*
$C_{26}H_{42}O_{10}$ 514.612
Constit. of fruits of *Capsicum annuum* var. *grossum*. Powder. $[\alpha]_D$ 0 (MeOH).

Izumitani, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1299-1307 (*isol, ir, pmr, cmr, ms*)

1,3,5-Trihydroxy-2-prenylacridone T-676

1,3,5-Trihydroxy-2-(3-methyl-2-butenyl)-9(10H)-acridinone, 9CI



$C_{18}H_{17}NO_4$ 311.337

N-*Me:* [103956-34-9] *1,3,5-Trihydroxy-10-methyl-2-prenylacridone.* ***Junosine***
$C_{19}H_{19}NO_4$ 325.363
Alkaloid from the bark of *Citrus junos* (yuzu). Light yellow prisms. Mp 210-213°.

3-Me ether:1,5-Dihydroxy-10-methyl-2-prenylacridone. ***Buxifoliadine C***
$C_{19}H_{19}NO_4$ 325.363
Yellow needles (Me_2CO). Mp 275-278° dec. λ_{max} 231 (log ε 3.23); 237 (sh) (log ε 3.19); 262 (log ε 3.66); 273 (log ε 3.55); 275 (sh) (log ε 3.53); 283 (log ε 3.63); 394 (log ε 2.74) (MeOH).

$\Delta^{3'}$-Isomer, 2′ξ-hydroxy, N-*Me:* [176391-58-5] *1,3,5-Trihydroxy-2-(2-hydroxy-3-methyl-3-butenyl)-10-methylacridone.* ***Bosistidine***
$C_{19}H_{19}NO_5$ 341.363
Amorph. $[\alpha]_D$ -15.1 (c, 0.0018 in $CHCl_3$).

Ju-ichi, M. *et al., Heterocycles*, 1986, **24**, 1595 (*Junosine*)
Auzi, A.A. *et al., Phytochemistry*, 1996, **42**, 235 (*Bosistidine*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 2000, **48**, 85-90 (*Buxifoliadine C*)

1,3,5-Trihydroxy-4-prenylacridone T-677

1,3,5-Trihydroxy-4-(3-methyl-2-butenyl)-9(10H)-acridinone, 9CI

$C_{20}H_{21}NO_4$ 339.39

3-Me ether, N-*Me:* [82354-36-7] *1,5-Dihydroxy-3-methoxy-10-methyl-4-prenylacridone.* ***Glycocitrine I***
Orange-yellow needles ($CHCl_3$). Mp 210-212°.

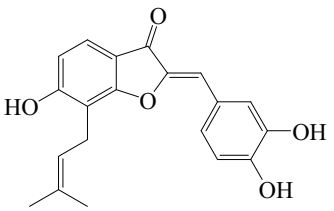
$\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 3-Me ether, N-*Me:* [160927-88-8] *1,5-Dihydroxy-4-(2-hydroxy-3-methyl-3-butenyl)-3-methoxy-10-methylacridone.* ***Marshmine***
$C_{20}H_{21}NO_5$ 355.39
Alkaloid from roots of Marsh grapefruit (*Citrus paradisi*) (Rutaceae). Yellow oil. $[\alpha]_D$ -28 (c, 0.15 in $CHCl_3$).

Wu, T.-S. *et al., J.C.S. Perkin 1*, 1983, 1681 (*uv, ir, pmr, cmr, ms, struct*)
Wu, T.-S. *et al., Phytochemistry*, 1983, **22**, 1493 (*isol*)

Takemura, Y. *et al., Heterocycles*, 1994, **39**, 315 (*Marshmine*)

3′,4′,6-Trihydroxy-7-prenylaurone T-678

Licoagroaurone



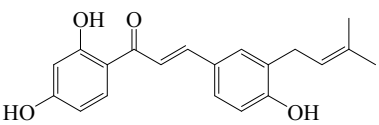
$C_{20}H_{18}O_5$ 338.359

Isol. from hairy root cultures of *Glycyrrhiza glabra* (licorice). Yellow powder. λ_{max} 256 (log ϵ 3.99); 267 (log ϵ 3.98); 396 (log ϵ 4.41) (MeOH).

Li, W. *et al., Phytochemistry*, 2000, **55**, 447-456

2′,4,4′-Trihydroxy-3-prenylchalcone T-679

1-(2,4-Dihydroxyphenyl)-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propen-1-one, 9CI. ***Licoagrochalcone A***



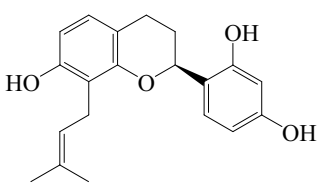
$C_{20}H_{20}O_4$ 324.376

(*E*)-*form* [202815-28-9]

Constit. of hairy root cultures of *Glycyrrhiza glabra* (licorice). Yellow powder. λ_{max} 298 (sh) (log ϵ 3.84); 382 (log ϵ 4.34) (MeOH).

Asada, Y. *et al., Phytochemistry*, 1998, **47**, 389-392 (*isol, uv, pmr, cmr*)

2′,4′,7-Trihydroxy-8-prenylflavan T-680



$C_{20}H_{22}O_4$ 326.391

(*S*)-*form*

4′-Me ether:2′,7-Dihydroxy-4′-methoxy-8-prenylflavan
$C_{21}H_{24}O_4$ 340.418
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D$ -5.5 (c, 1 in MeOH).

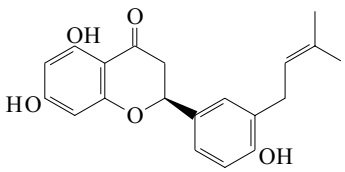
*4′-Me ether, 2′,7-di-*O*-β-*D*-glucopyranoside:*
$C_{33}H_{44}O_{14}$ 664.702
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D$ -91.1 (c, 0.25 in MeOH).

7-Me ether:2′,4′-Dihydroxy-7-methoxy-8-prenylflavan
$C_{21}H_{24}O_4$ 340.418
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D$ -1.6 (c, 1 in MeOH).

Doi, K. *et al., Chem. Pharm. Bull.*, 2001, **49**, 151-153

4′,5,7-Trihydroxy-3′-prenylflavanone T-681

*2,3-Dihydro-5,7-dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, 9CI.* ***Licoflavanone****. 3′-Prenylnaringenin*



$C_{20}H_{20}O_5$ 340.375

(*S*)-*form* [119240-82-3]

Constit. of *Glycyrrhiza glabra* (licorice). Oil. $[\alpha]_D$ -1.1 (c, 2.2 in MeOH).

Fukui, H. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4174 (*isol*)

Nkengfack, A.E. *et al., J. Nat. Prod.*, 1989, **52**, 320 (*isol, pmr, cmr*)

Tahara, S. *et al., Phytochemistry*, 1994, **36**, 1261 (*synth*)

4′,5,7-Trihydroxy-6-prenylflavanone T-682

*2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI. 6-Prenylnaringenin*

$C_{20}H_{20}O_5$ 340.375

Sophoraflavanone B was formerly assigned this struct..

(*S*)-*form* [68236-13-5]

Isol. from *Humulus lupulus* (hops). Cryst. (Et_2O/hexane). Mp 209-209.5°.

7-Me ether: [98621-32-0] *4′,5-Dihydroxy-7-methoxy-6-prenylflavanone*
$C_{21}H_{22}O_5$ 354.402
Yellow needles (EtOAc/petrol). Mp 138°.

(±)-*form* [68682-01-9]

Cryst. (EtOAc/petrol). Mp 214-216°.

Mizobuchi, S. *et al., Agric. Biol. Chem.*, 1984, **48**, 2771 (*isol, bibl*)

Shirataki, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 444 (*cmr*)

Mahmoud, E.N. *et al., J. Nat. Prod.*, 1985, **48**, 648 (*deriv*)

McCormick, S. *et al., Phytochemistry*, 1985, **24**, 1614; 1986, **25**, 1723 (*isol*)

Tahara, S. *et al., Phytochemistry*, 1994, **36**, 1261 (*synth*)

Bu, X. Y. *et al., Synthesis*, 1997, 1246-1248 (*synth, ir, pmr, ms*)

4′,5,7-Trihydroxy-8-prenylflavanone T-683

[72357-32-5]

*2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI. 8-*C*-Prenylnaringenin.* ***Flavaprenin****. Sophoraflavanone B*

$C_{20}H_{20}O_5$ 340.375

Sophoraflavanone B was formerly assigned the 6-*C*-prenyl struct..Sol. MeOH, Et_2O; poorly sol. H_2O. λ_{max} 295 (ϵ 18100) (MeOH) (Berdy). λ_{max} 336 (MeOH-NaOH) (Berdy).

(*S*)-*form* [53846-50-7]

Cryst. (EtOAc/petrol). Mp 202-204° (195.5-196°). $[\alpha]_D^{22}$ -25 (c, 0.1 in EtOH).

5-Me ether: [70872-29-6] *4′,7-Dihydroxy-5-methoxy-8-prenylflavanone.* ***Isoxanthohumol***†*. Humulol*†
$C_{21}H_{22}O_5$ 354.402
Isol. from hop (*Humulus lupulus*). Light yellow needles (AcOH). Sol. MeOH; poorly sol. H_2O. Mp 204-206°. $[\alpha]_D^{15}$ -21.5 (c, 0.9 in MeOH). The name Humulol has historical precedence but Isoxanthohumol has been preferred to avoid confusion with 2,9-Humuladien-7-ol, H-308. However another nat. prod. has since been named Isoxanthohumol (see 2′,4′,6′-Trihydroxy-3′-prenylchalcone).

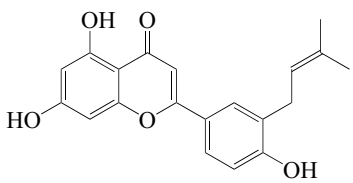
Komatsu, M. *et al., Yakugaku Zasshi*, 1970, **90**, 463 (*Isoxanthohumol*)

Kang, S.S. *et al., Fitoterapia*, 2000, **71**, 511-515 (*Isoxanthohumol*)

4′,5,7-Trihydroxy-3′-prenylflavone T-684

[174286-25-0]

*5,7-Dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one.* ***Yinyanghuo D****. 3′-Prenylapigenin*



$C_{20}H_{18}O_5$ 338.359

Yellow needles. Mp 98-100°.

*7-*O*-[α-*L*-Rhamnopyranosyl-(1→6)-β-*D*-glucopyranoside]:* [245054-57-3]
$C_{32}H_{38}O_{14}$ 646.644
Constit. of *Pithecellobium dulce* (manila tamarind). Cryst. Mp 128°. λ_{max} 270 ; 350 (MeOH).

Chen, C.-C. *et al., J. Nat. Prod.*, 1996, **59**, 412 (*isol, ir, pmr, cmr, ms*)

Saxena, V.K. *et al., Fitoterapia*, 1999, **70**, 98-100 (*7-rutinoside*)

4′,5,7-Trihydroxy-8-prenylflavone T-685

[72357-31-4]

*5,7-Dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI. 8-Prenylapigenin.* ***Licoflavone C***

$C_{20}H_{18}O_5$ 338.359

Pale yellow needles (MeOH). Mp 239°. An isolate from *Marshallia grandiflora* previously given this struct is now assigned as 4′,5,7-Trihydroxy-6-prenylflavone.

*4′-*O*-[α-*L*-Rhamnopyranosyl-(1→6)-β-*D*-glucopyranoside]:*
$C_{32}H_{38}O_{14}$ 646.644

Pale yellow needles (MeOH). Mp 264-265°. λ_{max} 275 (log ϵ 4.26); 305 (log ϵ 4.13); 326 (log ϵ 4.18) (MeOH).

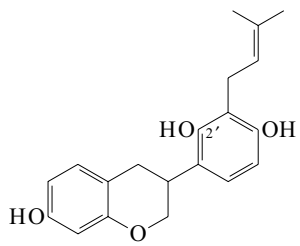
7-Me ether: [123549-17-7] *4′,5-Dihydroxy-7-methoxy-8-prenylflavone.* ***Artonin U***
$C_{21}H_{20}O_5$ 352.386
Constit. of the bark of *Artocarpus heterophyllus* (jackfruit). Yellow needles (MeOH). Mp 238-239°. λ_{max} 205 (ϵ 34670); 272 (ϵ 19950); 324 (ϵ 18200) (MeOH).

Δ³″-Isomer, 2″-hydroxy:4′,5,7-Trihydroxy-8-(2-hydroxy-3-methyl-3-butenyl)flavone. ***Ephedroidin***
$C_{20}H_{18}O_6$ 354.359
$[\alpha]_D$ +16.2 (c, 0.04 in MeOH). λ_{max} 272 ; 310 ; 327 (MeOH).

Kajiyama, K. *et al., J. Nat. Prod.*, 1992, **55**, 1197 (*isol, pmr, cmr*)
Aida, M. *et al., Heterocycles*, 1994, **39**, 847 (*Artonin U*)
Yadava, R.N. *et al., Fitoterapia*, 1998, **69**, 443-444 (*glycoside*)
Pistelli, L. *et al., J. Nat. Prod.*, 1998, **61**, 1404-1406 (*Ephedroidin*)

2′,4′,7-Trihydroxy-3′-prenylisoflavan T-686

3,4-Dihydro-3-[2,4-dihydroxy-3-(3-methyl-2-butenyl)phenyl]-7-hydroxy-2H-1-benzopyran. Phaseollidinisoflavan



$C_{20}H_{22}O_4$ 326.391
Amorph. solid.

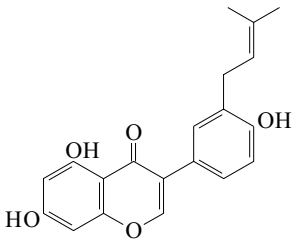
2′-Me ether: [56257-28-4] *4′,7-Dihydroxy-2′-methoxy-3′-prenylisoflavan.* ***2′-O-Methylphaseollidinisoflavan***
$C_{21}H_{24}O_4$ 340.418
Isol. from stems of *Vigna unguiculata* as a phytoalexin.

4′-Me ether: [160825-67-2] ***Gancaonin Z***
$C_{21}H_{24}O_4$ 340.418

Preston, N.W. *et al., Phytochemistry*, 1975, **14**, 1131 (*isol, pmr, struct*)
Biggs, D.R. *et al., J. Nat. Prod.*, 1994, **57**, 663 (*synth, pmr, cmr*)
Fukai, T. *et al., Nat. Med. (Tokyo)*, 1994, **48**, 203 (*Gancaonin Z*)

4′,5,7-Trihydroxy-3′-prenylisoflavone T-687

[68436-47-5]
5,7-Dihydroxy-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4H-1-benzopyran-4-one, 9CI. 3′-(γ,γ-Dimethylallyl)genistein. ***Isowighteone***



$C_{20}H_{18}O_5$ 338.359
Isol. from *Cajanus cajan* (pigeon pea). Needles (1,2-dichloroethane). Mp 171-172°. λ_{max} 262 ; 295 (sh) ; 330 (sh) (MeOH).

4′-Me ether:5,7-Dihydroxy-4′-methoxy-3′-prenylisoflavone. ***4′-O-Methylisowighteone.*** *3′-Prenylbiochanin A*
$C_{21}H_{20}O_5$ 352.386
Cryst. ($CHCl_3$). Mp 196-197°. λ_{max} 208 ; 261 ; 288 (sh) ; 323 (MeOH).

4″-Hydroxy:4′,5,7-Trihydroxy-3′-(4-hydroxy-3-methyl-2-butenyl)isoflavone. ***Vogelin E***
$C_{20}H_{18}O_6$ 354.359
Amorph. yellow powder. λ_{max} 262 (log ϵ 3.7); 325 (sh) (MeOH).

Nakayama, M. *et al., Bull. Chem. Soc. Jpn.*, 1978, **51**, 2398 (*synth*)
Dahiya, J.S. *et al., Phytochemistry*, 1984, **23**, 871-873 (*isol, pmr, ms*)
Tanaka, T. *et al., Phytochemistry*, 1997, **46**, 1431-1437 (*isol, uv, pmr, ms*)
Yenesew, A. *et al., Phytochemistry*, 1998, **49**, 247-249 (*4′-Methylisowighteone*)
Queiroz, E.F. *et al., J. Nat. Prod.*, 2002, **65**, 403-406 (*Vogelin E*)

4′,5,7-Trihydroxy-6-prenylisoflavone T-688

[51225-30-0]
5,7-Dihydroxy-3-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI. ***Wighteone.*** *6-Isopentenylgenistein. Erythrinin B*

$C_{20}H_{18}O_5$ 338.359
Bright yellow plates (Me_2CO/C_6H_6). Mp 220-221°. λ_{max} 215 ; 286 (EtOH) (Berdy). λ_{max} 277 (NaOH) (Berdy).

Tri-Ac:
Cryst. (MeOH). Mp 160-162°.

7-O-β-D-Glucopyranoside: ***Genisteone***
$C_{26}H_{28}O_{10}$ 500.501
$[\alpha]_D^{25}$ -31.6 (c, 0.04 in MeOH). λ_{max} 267 ; 330 (sh) (MeOH).

4′-Me ether: [27762-99-8] *5,7-Dihydroxy-4′-methoxy-6-prenylisoflavone.* ***Gancaonin A***
$C_{21}H_{20}O_5$ 352.386
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow cryst. (C_6H_6/Me_2CO). Mp 213-217°.

7-Me ether: [126716-34-5] *4′,5-Dihydroxy-7-methoxy-6-prenylisoflavone.* ***Gancaonin G***
$C_{21}H_{20}O_5$ 352.386
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Needles (MeOH). Mp 95-98°.

4″-Hydroxy: [104691-87-4] *4′,5,7-Trihydroxy-6-(4-hydroxy-3-methyl-2-butenyl)isoflavone.* ***Hydroxywighteone***
$C_{20}H_{18}O_6$ 354.359
Pale yellow columns. Mp 258-260°. Has (*E*)-config..

Δ³″-Isomer, 2″-hydroxy:4′,5,7-Trihydroxy-6-(2-hydroxy-3-methyl-3-butenyl)isoflavone. ***Laburnetin***
$C_{20}H_{18}O_6$ 354.359
Vitreous solid. Powder. Racemic. Mol. formula incorr. in the lit..

Deshpande, V.H. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 205 (*isol, uv, pmr, struct*)
Ingham, J.L. *et al., Phytochemistry*, 1977, **16**, 1943 (*isol, ir, ms, struct*)
Hashidoko, Y. *et al., Agric. Biol. Chem.*, 1986, **50**, 1797 (*isol, pmr, Hydroxywighteone*)
Fukai, T. *et al., Heterocycles*, 1989, **29**, 1369; 1761 (*Gancaonins*)
Yang, S.S. *et al., Phytochemistry*, 1989, **28**, 1749 (*isol*)
Monache, G.D. *et al., Phytochemistry*, 1994, **37**, 893 (*isol, deriv*)
Sato, H. *et al., Phytochemistry*, 1995, **39**, 673 (*Laburnetin*)
Pistelli, L. *et al., J.O.C.*, 1998, **61**, 1404-1406 (*Genisteone*)
Hou, A.-J. *et al., J. Nat. Prod.*, 2001, **64**, 65-70 (*activity*)

4′,5,7-Trihydroxy-8-prenylisoflavone T-689

[104691-86-3]
5,7-Dihydroxy-3-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one, 9CI. ***Lupiwighteone***

$C_{20}H_{18}O_5$ 338.359
Isol. from *Glycyrrhiza uralensis* (Chinese licorice) and *Vigna angularis* (azuki bean). Amorph. Sol. MeOH; poorly sol. H_2O. λ_{max} 267 (MeOH) (Berdy). λ_{max} 282 ; 324 (MeOH-NaOH) (Berdy).

4′-Me ether: [129145-51-3] *5,7-Dihydroxy-4′-methoxy-8-prenylisoflavone.* ***Gancaonin M***
$C_{21}H_{20}O_5$ 352.386
Isol. from *Glycyrrhiza uralensis* (Chinese licorice). Prisms (Et_2O/hexane). Mp 139-141°.

5-Me ether: [104703-98-2] *4′,7-Dihydroxy-5-methoxy-8-prenylisoflavone.* ***5-Methyllupiwighteone***
$C_{21}H_{20}O_5$ 352.386
Rods. Mp 220-222°.

2″,3″-Dihydro, 3″-hydroxy: [104691-92-1] *4′,5,7-Trihydroxy-8-(3-hydroxy-3-methylbutyl)isoflavone.* ***Lupiwighteone hydrate***
$C_{20}H_{20}O_6$ 356.374
Columns. Mp 244-246°.

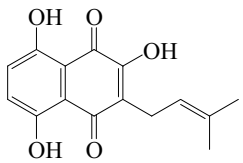
2″,3″-Dihydro, 3″-hydroxy, 7-O-β-D-glucopyranoside:Lupiwighteone hydrate 7-glucoside
$C_{26}H_{30}O_{11}$ 518.516
Constit. of soybean molasses (*Glycine* sp.). Amorph. yellow powder. $[\alpha]_D^{20}$ +5.9 (c, 0.75 in Py aq.). λ_{max} 236 (log ϵ 4.09); 286 (log ϵ 4.28) (MeOH).

Hashidoko, Y. *et al., Agric. Biol. Chem.*, 1986, **50**, 1797 (*isol, pmr*)
Tahara, S. *et al., Agric. Biol. Chem.*, 1986, **50**, 1809 (*5-Methyllupiwighteone*)
Abe, N. *et al., Agric. Biol. Chem.*, 1987, **51**, 349 (*isol, uv, pmr*)

Fukai, T. *et al., Heterocycles*, 1989, **29**, 1369; 1990, **31**, 373 (*Gancaonins*)
Hosny, M. *et al., J. Nat. Prod.*, 1999, **62**, 853-858 (*Lupiwighteone hydrate 7-glucoside*)

2,5,8-Trihydroxy-3-prenyl-1,4-naphthoquinone T-690

2,5,8-Trihydroxy-3-(3-methyl-2-butenyl)-1,4-naphthalenedione. ***Hydroxysesamone***

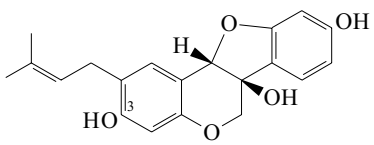


$C_{15}H_{14}O_5$ 274.273
Constit. of the roots of *Sesamum indicum* (sesame). Red needles (hexane/$CHCl_3$). Mp 145-146°. λ_{max} 242 (log ε 4.05); 270 (log ε 3.81); 287 (log ε 3.76); 484 (log ε 3.64); 538 (log ε 3.64) (MeOH).

Feroj Hasan, A.F.M. *et al., Phytochemistry*, 2001, **58**, 1225-1228

3,6*a*,9-Trihydroxy-2-prenylpterocarpan T-691

*2-(3-Methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,6*a*,9(11*a*H)-triol, 9CI.* ***Glyceollidin II****. Glyceocarpin*



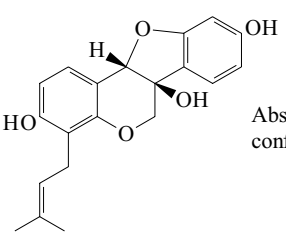
$C_{20}H_{20}O_5$ 340.375
Phytoalexin from *Glycine max* (soybean).

3-Me ether: [69393-94-8] *6a,9-Dihydroxy-3-methoxy-2-prenylpterocarpan.* ***Glyceollin IV***
$C_{21}H_{22}O_5$ 354.402
Phytoalexin from *Glycine max* (soybean) and *Psophocarpus tetragonolobus* (winged bean). Non-cryst. λ_{max} 286 (MeOH) (Berdy).

Lyne, R.L. *et al., Tet. Lett.*, 1978, 3127 (*isol, ms, uv, nmr, cd*)
Ingham, J.L. *et al., Phytochemistry*, 1980, **19**, 1203; 1981, **20**, 795 (*isol, nmr, ms, struct, abs config*)
Zähringer, U. *et al., Z. Naturforsch., C*, 1981, **36**, 234 (*isol*)

3,6*a*,9-Trihydroxy-4-prenylpterocarpan T-692

[77979-21-6]
Glyceollidin I



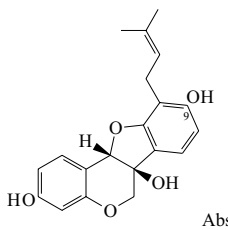
Absolute configuration

$C_{20}H_{20}O_5$ 340.375
Abs. config. by analogy with 3,6*a*,9-Trihydroxy-2-prenylpterocarpan, T-691. No opt. rotn. reported. Phytoalexin from *Glycine max* (soybean). λ_{max} 283 (MeOH) (Berdy). λ_{max} 325 ; 534 (MeOH-NaOH) (Berdy).

Zähringer, U. *et al., Z. Naturforsch., C*, 1981, **36**, 234

3,6*a*,9-Trihydroxy-10-prenylpterocarpan T-693

[74515-45-0]
*10-(3-Methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,6,9(11*a*H)-triol, 9CI.* ***Sandwicarpin****. 6*a*-Hydroxyphaseollidin*



Absolute configuration

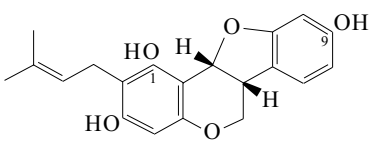
$C_{20}H_{20}O_5$ 340.375
$[\alpha]_D$ -278 (MeOH).

9-Me ether: [74515-47-2] *3,6*a*-Dihydroxy-9-methoxy-10-prenylpterocarpan.* ***Cristacarpin****. Erythrabyssin I*
$C_{21}H_{22}O_5$ 354.402
Isol. from *Psophocarpus tetragonolobus* (winged bean). $[\alpha]_D^{20}$ -250 (c, 0.2 in MeOH).

Ingham, J.L. *et al., Phytochemistry*, 1980, **19**, 1203 (*isol, uv, ms, struct, abs config*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1980, **35**, 384 (*Sandwicarpin*)
Kamat, V.S. *et al., Heterocycles*, 1981, **15**, 1163 (*isol, uv, cd, abs config*)
Fomum, Z.T. *et al., Phytochemistry*, 1986, **25**, 757 (*isol*)
Dagne, E. *et al., J. Nat. Prod.*, 1993, **56**, 1831 (*Cristacarpin*)
Tanaka, H. *et al., Phytochemistry*, 1996, **42**, 1473 (*Cristacarpin*)

1,3,9-Trihydroxy-2-prenylpterocarpan T-694

*6a,11*a*-Dihydro-2-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]-benzopyran-1,3,9-triol, 9CI*



$C_{20}H_{20}O_5$ 340.375

1-Me ether: [63343-94-2] *3,9-Dihydroxy-1-methoxy-2-prenylpterocarpan.* ***Edudiol***
$C_{21}H_{22}O_5$ 354.402
Brown oil. $[\alpha]_D^{21}$ -248 (c, 0.1 in $CHCl_3$).

1-Me ether, di-Ac: [63343-97-5]
Needles (C_6H_6/hexane). Mp 162-164°.

3-Me ether: [205489-25-4] ***1,9-Dihydroxy-3-methoxy-2-prenylpterocarpan***
$C_{21}H_{22}O_5$ 354.402

1,3-Di-Me ether: [156250-72-5] *9-Hydroxy-1,3-dimethoxy-2-prenylpterocarpan.* ***Kanzonol P***
$C_{22}H_{24}O_5$ 368.429
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Amorph. powder. $[\alpha]_D$ -58 (c, 0.01 in MeOH).

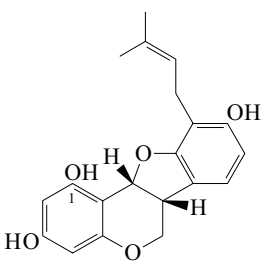
1,9-Di-Me ether: [37706-55-1] *3-Hydroxy-1,9-dimethoxy-2-prenylpterocarpan.* ***Edulenol***
$C_{22}H_{24}O_5$ 368.429
Prisms (MeOH/C_6H_6). Mp 118-120°. $[\alpha]_D^{22}$ -253.1 (c, 1.4 in $CHCl_3$).

*6a,11*a*-Didehydro, 1-Me ether:* [213130-81-5] *3,9-Dihydroxy-1-methoxy-2-prenylpterocarpene.* ***Glyurallin A***
$C_{21}H_{20}O_5$ 352.386
Constit. of *Glycyrrhiza uralensis* (Chinese licorice). Orange-yellow oil. λ_{max} 230 (log ε 4.3); 249 (log ε 4.14); 336 (log ε 4.29); 348 (log ε 4.17); 350 (log ε 4.17) (MeOH).

Rall, G.J. *et al., J. S. Afr. Chem. Inst.*, 1972, **25**, 131-139 (*Edulenol*)
Brink, A.J. *et al., Phytochemistry*, 1977, **16**, 273-276 (*Edudiol*)
Fukai, T. *et al., Heterocycles*, 1994, **38**, 1089-1098 (*Kanzonol P*)
Saxena, V.K. *et al., Fitoterapia*, 1997, **68**, 403-404 (*3-Me ether*)
Shibano, M. *et al., Heterocycles*, 1997, **45**, 2053-2060 (*Glyurallin A*)

1,3,9-Trihydroxy-10-prenylpterocarpan T-695

*6a,11*a*-Dihydro-10-(3-methyl-1-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-1,3,9-triol*



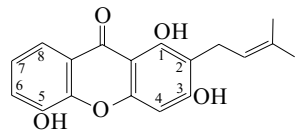
$C_{20}H_{20}O_5$ 340.375

1-Me ether: [65428-13-9] *3,9-Dihydroxy-1-methoxy-10-prenylpterocarpan.* ***1-Methoxyphaseollidin***
$C_{21}H_{22}O_5$ 354.402
Isol. from seeds of *Psophocarpus tetragonolobus* (winged bean). $[\alpha]_D^{18}$ -225 ($CHCl_3$). λ_{max} 287 (ε 1500); 330 (sh) (MeOH).

Preston, N.W. *et al., Phytochemistry*, 1977, **16**, 2044-2045 (*isol*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1511-1517 (*isol, uv, ir, cd, pmr, cmr*)

1,3,5-Trihydroxy-2-prenylxanthone T-696

[20245-38-9]
*1,3,5-Trihydroxy-2-(3-methyl-2-butenyl)-9*H*-xanthene-9-one. 2-(3,3-Dimethylallyl)-1,3,5-trihydroxyxanthone*



$C_{18}H_{16}O_5$ 312.321
Pale yellow needles. Mp 280-282°. λ_{max} 243 (log ϵ 6.82); 312 (log ϵ 3.22) (MeOH).

3-Me ether: [77741-56-1] *1,5-Dihydroxy-3-methoxy-2-prenylxanthone*
$C_{19}H_{18}O_5$ 326.348
Obt. from fruit hulls of *Garcinia mangostana* (mangosteen). Yellow flakes (MeOH). Mp 242-244°.

3-Me ether, di-Ac:
Needles (C_6H_6/petrol). Mp 153-154°.

3,5-Di-Me ether: [35323-89-8] *1-Hydroxy-3,5-dimethoxy-2-prenylxanthone*
$C_{20}H_{20}O_5$ 340.375
Constit. of *Garcinia mangostana* (mangosteen). Yellow needles (MeOH). Mp 168-169°.

Gunasekera, S.P. *et al., J.C.S. Perkin 1*, 1977, 1505 (*isol*)
Sen, A.K. *et al., Phytochemistry*, 1981, **20**, 183 (*deriv*)
Bennett, G.J. *et al., J.C.S. Perkin 1*, 1990, 2671 (*isol, deriv*)
Goh, S.H. *et al., Phytochemistry*, 1991, **30**, 366 (*isol*)
Peres, V. *et al., Phytochemistry*, 1997, **44**, 191 (*rev, occur*)
Cortez, D.A.G. *et al., Phytochemistry*, 1998, **47**, 1367-1374 (*isol*)

1,3,6-Trihydroxy-2-prenylxanthone T-697

*1,3,6-Trihydroxy-2-(3-methyl-2-butenyl)-9*H*-xanthen-9-one*

$C_{18}H_{16}O_5$ 312.321

3-Me ether: [119227-98-4] *1,6-Dihydroxy-3-methoxy-2-prenylxanthone*
$C_{19}H_{18}O_5$ 326.348
Constit. of *Garcinia mangostana* (mangosteen). Cryst. Mp 240°.

Parveen, M. *et al., Phytochemistry*, 1988, **27**, 3694

1,3,7-Trihydroxy-2-prenylxanthone T-698

[20245-39-0]
*1,3,7-Trihydroxy-2-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, 9CI, 8CI. 2-(3,3-Dimethylallyl)-1,3,7-trihydroxyxanthone*

$C_{18}H_{16}O_5$ 312.321
Yellow needles. Mp 227-229° (218-220°). λ_{max} 238 (log ϵ 17.57); 262 (log ϵ 16.08); 316 (log ϵ 8.08); 375 (log ϵ 3) (MeOH).

3-Me ether: [77741-58-3] *1,7-Dihydroxy-3-methoxy-2-prenylxanthone*
$C_{19}H_{18}O_5$ 326.348
Isol. from fruit hulls of *Garcinia mangostana* (mangosteen). Yellow cryst. (C_6H_6/MeOH). Mp 220-222°.

3,7-Di-Me ether: [13179-17-4] *1-Hydroxy-3,7-dimethoxy-2-prenylxanthone*
$C_{20}H_{20}O_5$ 340.375
Pale-cream cryst. (petrol). Mp 147-149°.

2′,3′-Dihydro, 3′-hydroxy:1,3,7-Trihydroxy-2-(3-hydroxy-3-methylbutyl)-xanthone
$C_{18}H_{18}O_6$ 330.337
Yellow cryst. (MeOH). Mp 233-235°. λ_{max} 235 (log ϵ 6.88); 261 (log ϵ 6.07); 312 (log ϵ 3.09); 375 (log ϵ 1.16) (MeOH).

Locksley, H.D. *et al., J.C.S.(C)*, 1966, 2265 (*synth*)
Jackson, B. *et al., J.C.S.(C)*, 1967, 2500 (*isol*)
Carpenter, I. *et al., J.C.S.(C)*, 1969, 486 (*isol*)
Anand, S.M. *et al., Indian J. Chem.*, 1973, **11**, 1233 (*isol*)
Owens, P.J. *et al., J.C.S. Perkin 1*, 1974, 1018 (*isol*)
Sen, A.K. *et al., Phytochemistry*, 1981, **20**, 183 (*3-Me ether*)
Harrison, L.J. *et al., Phytochemistry*, 1993, **33**, 727 (*isol, pmr, cmr*)
Peres, V. *et al., Phytochemistry*, 1997, **44**, 191 (*rev, occur*)
Cortez, D.A.G. *et al., Phytochemistry*, 1998, **47**, 1367-1374 (*isol, uv, pmr, cmr, ms*)

1,4,5-Trihydroxy-3-prenylxanthone T-699

[136364-72-2]
*1,4,5-Trihydroxy-3-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, 9CI*

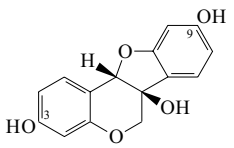
$C_{18}H_{16}O_5$ 312.321
Constit. of the root bark of *Garcinia livingstonei* (imbe). Yellow needles (MeOH). Mp 185-186°.

Tri-Me ether: [139955-61-6] *1,4,5-Trimethoxy-3-prenylxanthone*
$C_{21}H_{22}O_5$ 354.402
Amorph. Mp 141-142°.

Sordat-Diserens, I. *et al., Phytochemistry*, 1992, **31**, 313 (*isol, pmr, cmr*)

3,6*a*,9-Trihydroxypterocarpan T-700

[69393-95-9]
*6*H*-Benzofuro[3,2-*c*][1]benzopyran-3,6*a*,9(11*a*H)-triol, 9CI. **Glycinol***



Absolute configuration

$C_{15}H_{12}O_5$ 272.257
Constit. of soybean seedlings (*Glycine max*) and kudzu (*Pueraria thunbergiana*). λ_{max} 282 ; 287 (no solvent reported).

*3-Me ether:6*a*,9-Dihydroxy-3-methoxypterocarpan.* ***6a-Hydroxyisomedicarpin***
$C_{16}H_{14}O_5$ 286.284
Isol. from fungus-infected leaves of *Melilotus alba* (white melilot).

9-Me ether: [61135-92-0] *3,6*a*-Dihydroxy-9-methoxypterocarpan.* ***6a-Hydroxymedicarpin***
$C_{16}H_{14}O_5$ 286.284
Isol. from fungus-infected leaves of *Melilotus alba* (white melilot). $[\alpha]_D^{25}$ -209 (c, 0.07 in $CHCl_3$).

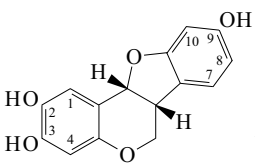
*9-Me ether, 3-*O*-β-D-glucopyranoside:* ***Licoagroside E***
$C_{22}H_{24}O_{10}$ 448.426
Powder. $[\alpha]_D^{22}$ -176.4 (c, 0.66 in MeOH). λ_{max} 224 (log ϵ 4.95); 283 (log ϵ 4.78) (no solvent reported).

3,9-Di-Me ether: [3187-52-8] *6*a*-Hydroxy-3,9-dimethoxypterocarpan.* ***Variabilin†***. *Homopisatin*
$C_{17}H_{16}O_5$ 300.31
Isol. from leaves or cotyledons of *Lens culinaris* (lentil) and *Trifolium pratense* (red clover). λ_{max} 228 (ϵ 10600); 286 (ϵ 4250) (EtOH) (Berdy).

Ingham, J.L. *et al., Phytochemistry*, 1976, **15**, 1489-1495 (*isol*)
Kurosawa, K. *et al., Phytochemistry*, 1978, **17**, 1417-1418 (*Variabilin*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1980, **35**, 384 (*isol*)
Weinstein, L.I. *et al., Plant Physiol.*, 1981, **68**, 358 (*isol*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*occur*)
Macias, F.A. *et al., Phytochemistry*, 1999, **50**, 35-46 (*6a-Hydroxymedicarpin*)
Van Aardt, T.G. *et al., Tetrahedron*, 2001, **57**, 7113-7126 (*Variabilin, synth, cd, pmr, cmr*)
Li, W. *et al., Phytochemistry*, 2002, **60**, 351-355 (*Licoagroside E*)

2,3,9-Trihydroxypterocarpan T-701

*6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-2,3,9-triol*



Absolute configuration

$C_{15}H_{12}O_5$ 272.257

2,3-Di-Me ether: [73793-85-8] *9-Hydroxy-2,3-dimethoxypterocarpan.* ***Sparticarpin***
$C_{17}H_{16}O_5$ 300.31
$[\alpha]_D$ -170 (c, 0.01 in MeOH). λ_{max} 211 ; 294 (EtOH) (Berdy). λ_{max} 215 ; 299 (EtOH-NaOH) (Berdy).

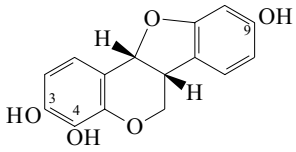
2,9-Di-Me ether: [56752-00-2] *3-Hydroxy-2,9-dimethoxypterocarpan.* ***2-Methoxymedicarpin***
$C_{17}H_{16}O_5$ 300.31
Isol. from root crowns of *Pisum sativum* (pea). Plates (Me_2CO). Mp 146-148°. $[\alpha]_D^{23}$ -297 (EtOH).

Tri-Me ether: [56782-49-1] *2,3,9-Trimethoxypterocarpan.* ***2-Methoxyhomopterocarpin***
$C_{18}H_{18}O_5$ 314.337
Isol. from *Pisum sativum* (pea). Needles (C_6H_6/heptane). Mp 122-124°. $[\alpha]_D^{23}$ -228 (EtOH).

Kalra, V.K. *et al., Indian J. Chem.*, 1967, **5**, 607 (*synth*)
Pueppke, S.G. *et al., J.C.S. Perkin 1*, 1975, 946 (*isol*)
Ingham, J.L. *et al., Z. Naturforsch., C*, 1980, **35**, 197 (*Sparticarpin*)

3,4,9-Trihydroxypterocarpan T-702

[61255-58-1]
*6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,4,9-triol. 4-Hydroxydemethylmedicarpin. 4′,7,8-Trihydroxypterocarpan*



$C_{15}H_{12}O_5$ 272.257
Isol. from fungus-infected leaves of *Melilotus alba* (white melilot). Mp 118-120°.

3-Me ether: [83013-83-6] *4,9-Dihydroxy-3-methoxypterocarpan*. ***Melilotocarpan B***
$C_{16}H_{14}O_5$ 286.284
Isol. from *Melilotus alba* (white melilot). Mp 173-175.5°. $[\alpha]_D^{23}$ -179 (dioxan).

9-Me ether: [53950-54-2] *3,4-Dihydroxy-9-methoxypterocarpan*. ***4-Hydroxymedicarpin***
$C_{16}H_{14}O_5$ 286.284
Isol. from fungus-infected leaves of *Melilotus alba* (white melilot). λ_{max} 230 ; 285 (MeOH) (Berdy).

3,9-Di-Me ether: [61135-95-3] *4-Hydroxy-3,9-dimethoxypterocarpan*. ***Melilotocarpan A***. *4-Hydroxyhomopterocarpin*
$C_{17}H_{16}O_5$ 300.31
Isol. from *Melilotus alba* (white melilot) as fungal metab.. Needles (MeOH). Mp 48-51°. $[\alpha]_D^{23}$ -194 (c, 1.4 in dioxan).

4,9-Di-Me ether:3-Hydroxy-4,9-dimethoxypterocarpan. ***4-Methoxymedicarpin***
$C_{17}H_{16}O_5$ 300.31
Constit. of *Trifolium repens* (white clover). Prisms. Mp 158-160°. $[\alpha]_D$ -161 ($CHCl_3$). λ_{max} 284 (ϵ 11000) (MeOH) (Berdy).

Tri-Me ether: 3,4,9-Trimethoxypterocarpan, T-730

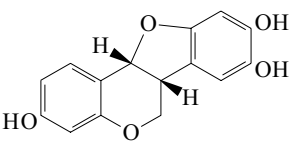
(±)-*form*

4,9-Di-Me ether: [22973-33-7]
Cubes (C_6H_6/petrol). Mp 204-205°.

Tri-Me ether:
Prisms (C_6H_6/petrol). Mp 114-115°.

Kalia, V.K. *et al., Tetrahedron*, 1967, **23**, 3221 (*synth*)
Campbell, R.V.M. *et al., J.C.S.(C)*, 1969, 1109 (*isol*)
Ingham, J.L. *et al., Phytochemistry*, 1976, **15**, 1489 (*isol*)
Miyase, T. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1986 (*Melilotocarpan B*)
Ingham, J.L. *et al., Prog. Chem. Org. Nat. Prod.*, 1983, **43**, 1 (*occur*)

3,8,9-Trihydroxypterocarpan T-703



$C_{15}H_{12}O_5$ 272.257

8-Me ether: [99217-66-0] *3,9-Dihydroxy-8-methoxypterocarpan*. ***Kushenin***. *Lespedezol D_1*
$C_{16}H_{14}O_5$ 286.284
Needles ($CHCl_3$). Sol. MeOH, EtOAc. Mp 230-232°. $[\alpha]_D^{23}$ -97.1 (c, 0.46 in MeOH). λ_{max} 233 (ϵ 2400); 286 (ϵ 18200); 298 (ϵ 2000) (MeOH) (Berdy).

9-Me ether: [108335-33-7] *3,8-Dihydroxy-9-methoxypterocarpan*
$C_{16}H_{14}O_5$ 286.284
Constit. of *Pterocarpus soyauxii*. Brown amorph. solid.

3,9-Di-Me ether: [108335-31-5] *8-Hydroxy-3,9-dimethoxypterocarpan*
$C_{17}H_{16}O_5$ 300.31
From *Pterocarpus soyauxii*. Brown needles (EtOH). Mp 129°.

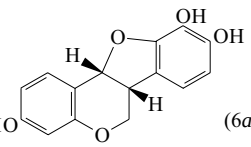
8,9-Di-Me ether:3-Hydroxy-8,9-dimethoxypterocarpan. ***Secundiflorol I***
$C_{17}H_{16}O_5$ 300.31
Solid. λ_{max} 226 ; 275 (sh) ; 287 ; 295 (sh) (MeOH).

8,9-Methylene ether: Maackiain, M-2

Wu, L.J. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3231
Bezuidenhoudt, B.C.B. *et al., Phytochemistry*, 1987, **26**, 531 (*derivs*)
Tanaka, T. *et al., Phytochemistry*, 1998, **48**, 1187-1193 (*Secundiflorol I*)
Miyase, T. *et al., Phytochemistry*, 1999, **52**, 311-319 (*Lespedezol D_1*)

3,9,10-Trihydroxypterocarpan T-704

6a,11a-Dihydro-6H-benzofuro[3,2-c][1]benzopyran-3,9,10-triol, 9CI



(6*aR*,11*aR*)-*form*

$C_{15}H_{12}O_5$ 272.257

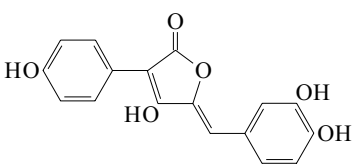
(6*aR*,11*aR*)-*form*

9,10-Di-Me ether: [73340-41-7] *3-Hydroxy-9,10-dimethoxypterocarpan*. ***Methylnissolin***. *10-Methoxymedicarpin. Astrapterocarpan*
$C_{17}H_{16}O_5$ 300.31
Isol. from *Medicago sativa* (alfalfa). λ_{max} 211 ; 284 ; 287 (EtOH) (Berdy). λ_{max} 215 ; 253 ; 287 (EtOH/NaOH) (Berdy).

Al-Ani, H.A.M. *et al., Phytochemistry*, 1985, **24**, 55-61 (*Methylnissolin*)
Spencer, G.F. *et al., Phytochemistry*, 1991, **30**, 4147-4149 (*Methylnissolin*)

3′,4,4′-Trihydroxypulvinone T-705

[51282-12-3]
5-[(3,4-Dihydroxyphenyl)methylene]-4-hydroxy-3-(4-hydroxyphenyl)-2(5H)-furanone, 9CI

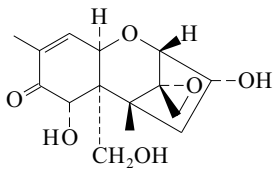


$C_{17}H_{12}O_6$ 312.278
Constit. of *Suillus grevillei* (larch bolete). Yellow needles (EtOH aq.). Mp 291° dec. λ_{max} 243 (log ϵ 4.12); 308 (sh) (log ϵ 3.96); 343 (log ϵ 4.1); 378 (log ϵ 4.14) (EtOH).

Edwards, R.L. *et al., J.C.S. Perkin 1*, 1973, 1921 (*isol, ir, uv, pmr, ms*)

3,7,15-Trihydroxy-8-scirpenone T-706

12,13-Epoxy-3,7,15-trihydroxy-9-trichothecen-8-one



$C_{15}H_{20}O_6$ 296.319

(3α,7α)-*form* [51481-10-8]
Deoxynivalenol. *Rd toxin*. *Vomitoxin*
Prod. by *Fusarium graminearum* and *Fusarium roseum*, responsible for headblight in cereals. Cryst. (EtOAc/petrol). Mp 151-153°. $[\alpha]_D^{26}$ +6.35 (c, 0.07 in EtOH).

▶ Skin irritant. LD_{50} (mus, orl) 46 mg/kg. Exp. reprod. and teratogenic effects. Associated with outbreaks of mycotoxicoses in farm animals. YD0167000

Semicarbazone:
Mp 199-201°.

3-O-β-D-Glucopyranoside: [131180-21-7]
$C_{21}H_{30}O_{11}$ 458.461
Isol. from cultures of sweet corn (*Zea mays*).

3-Ac: [50722-38-8] ***Acetyldeoxynivalenol***
$C_{17}H_{22}O_7$ 338.357
Toxin from infected barley. Cryst. (Et_2O/pentane). Mp 185.5-186°. $[\alpha]_D$ +43 (c, 0.2 in MeOH). λ_{max} 220 (ϵ 7100) (MeOH).

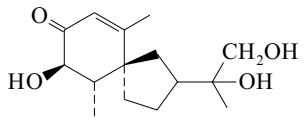
▶ LD_{50} (mus, orl) 34 mg/kg. YD0150000

3,7,15-Tri-Ac:
Needles (EtOAc/petrol). Mp 155-157°.

Yoshizawa, T. *et al., Agric. Biol. Chem.*, 1973, **37**, 2933 (*isol*)
Blight, M.M. *et al., J.C.S. Perkin 1*, 1974, 1691-1693 (*3-Ac*)
Brumley, W.C. *et al., Biomed. Mass Spectrom.*, 1982, **9**, 451 (*ms*)
Miller, J.D. *et al., Can. J. Microbiol.*, 1983, **29**, 1171 (*isol*)
Trichothecenes - Chemical, Biological and Toxicological Aspects, (ed., Ueno, Y.), Elsevier, 1983, (*tox, rev*)
Cameron, S. *et al., J.C.S. Perkin 1*, 1989, 887 (*synth*)
Zamir, L.O. *et al., Tetrahedron*, 1989, **45**, 2277 (*biosynth, deriv*)
Jarvis, B.B. *et al., J.O.C.*, 1990, **55**, 3660 (*cmr*)
Sewald, N. *et al., Tetrahedron: Asymmetry*, 1992, **3**, 953 (*3-glucoside*)
Zamir, L.O. *et al., J. Biol. Chem.*, 1996, **271**, 27353-27359 (*biosynth, deriv*)
Mirocha, C.J. *et al., J. Agric. Food Chem.*, 1998, **46**, 1444-1448 (*occur*)
Zamir, L.O. *et al., J. Biol. Chem.*, 1999, **274**, 12269-12277 (*biosynth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 202
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACH075; VTF500

3,11,12-Trihydroxy-1(10)-spirovetiven-2-one T-707

[84321-96-0]

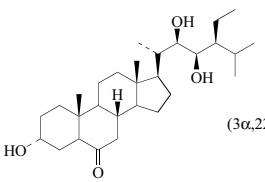


$C_{15}H_{24}O_4$ 268.352
Constit. of potato tubers infected with *Phoma exigua*. Amorph. $[\alpha]_D^{23}$ +88.7 (c, 0.15 in MeOH).

Malmberg, A.G. *et al., Phytochemistry*, 1982, **21**, 1818

3,22,23-Trihydroxystigmastan-6-one T-708

3,22,23-Trihydroxy-24-ethylcholestan-6-one



(3α,22*R*,23*R*,24*S*)-*form*

$C_{29}H_{50}O_4$ 462.712

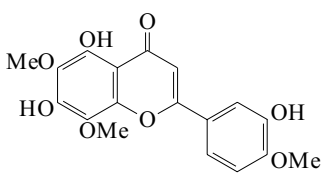
(3α,22*R*,23*R*,24*S*)-*form*
28-Homotyphasterol
Constit. of ricebran (*Oryza sativa*).

(3β,22*R*,23*R*,24*S*)-*form* [90524-90-6]
28-Homoteasterone
Constit. of radish (*Raphanus sativus*) seeds. Cryst. (EtOAc/hexane). Mp 206-209°.

Takatsuto, S. *et al., J.C.S. Perkin 1*, 1984, 439 (*synth, pmr*)
Schmidt, J. *et al., Phytochemistry*, 1993, **34**, 391 (*isol, 28-Homoteasterone*)
Abe, H. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 176 (*28-Homotyphasterol, ms*)

3′,5,7-Trihydroxy-4′,6,8-trimethoxyflavone, 8CI T-709

[15835-74-2]
*5,7-Dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-6,8-dimethoxy-4*H*-1-benzopyran-4-one, 9CI*. ***Acerosin***



$C_{18}H_{16}O_8$ 360.32
Isol. from fruit peel of mandarin orange (*Citrus reticulata*). Cryst. ($CHCl_3$/Et_2O/hexane). Mp 239-241°.

5-O-(6-O-Acetyl-β-D-glucopyranoside):
[72209-43-9]
$C_{26}H_{28}O_{14}$ 564.499
Green cryst. Mp 226-227° dec.

Tri-Ac: [15835-80-0]
Needles (C_6H_6/EtOAc). Mp 131-133°.

Farkas, L. *et al., Tetrahedron*, 1967, **23**, 3557 (*isol, uv, synth*)
Gupta, S.R. *et al., Indian J. Chem.*, 1975, **13**, 785 (*isol*)
Subramanian, P.M. *et al., J. Nat. Prod.*, 1979, **42**, 540 (*glycoside*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 717 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Herz, W. *et al., Phytochemistry*, 1984, **23**, 1453 (*isol*)
Bhargava, S.K. *et al., Plant. Med. Phytother.*, 1984, **18**, 74 (*isol, props*)

4′,5,6-Trihydroxy-3′,7,8-trimethoxyflavone T-710

[76844-67-2]
*5,6-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7,8-dimethoxy-4*H*-1-benzopyran-4-one.* ***Majoranin****. Thymonin*

$C_{18}H_{16}O_8$ 360.32
Isol. from *Majorana hortensis* (sweet majoram), and *Thymus vulgaris* (thyme). Mp 225-226°. Majoranin formerly given struct. of Sudachitin.

Tri-Ac:
$C_{24}H_{22}O_{11}$ 486.431
Mp 186-187°.

Horie, T. *et al., Nippon Kagaku Zasshi*, 1980, 1397 (*synth*)
Van den Brouke, C.O. *et al., Phytochemistry*, 1982, **21**, 2581 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107; 1984, **23**, 2973 (*isol, uv*)
Voirin, B. *et al., Planta Med.*, 1985, 523 (*isol*)
Barberan, F.A.T. *et al., Tetrahedron*, 1985, **41**, 5733 (*uv, tlc*)
Bosabalidis, A.M. *et al., Phytochemistry*, 1998, **49**, 1549-1553 (*isol, uv, pmr, ms*)

4′,5,7-Trihydroxy-3,3′,6-trimethoxyflavone, 8CI T-711

[10173-01-0]
*5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,6-dimethoxy-4*H*-1-benzopyran-4-one, 9CI. Quercetagetin 3,3′,6-trimethyl ether.* ***Jaceidin****. Polycladin*

$C_{18}H_{16}O_8$ 360.32
Polycladin and Jaceidin both prev. given incorrect structs.. Found in buds of *Prunus avium* (wild cherry). Pale yellow needles (MeOH aq.). Mp 130-135° (203°).

4′-O-β-D-Glucuronopyranoside:Jaceidin 4′-glucuronide
$C_{24}H_{24}O_{14}$ 536.445
Constit. of *Spinacia oleracea* (spinach).

Bowie, J.H. *et al., Aust. J. Chem.*, 1966, **19**, 1627 (*ms*)
Fukui, H. *et al., Bull. Chem. Soc. Jpn.*, 1968, **41**, 1413 (*synth, uv, pmr*)
Fukui, H. *et al., Experientia*, 1968, **24**, 108 (*synth*)
Wollenweber, E. *et al., Z. Naturforsch., B*, 1972, **27**, 567 (*isol*)
Goudard, M. *et al., Phytochemistry*, 1978, **17**, 145 (*ms*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Roitman, J.N. *et al., Phytochemistry*, 1985, **24**, 835-848 (*isol, pmr, cmr*)
Singh, M. *et al., Planta Med.*, 1985, 525 (*7-neohesperidoside*)
The Flavonoids: Advances in Research since 1980, (Ed. Harborne, J.B.), Chapman and Hall, London, 1988,

4′,5,7-Trihydroxy-3′,6,8-trimethoxyflavone T-712

[4281-28-1]
*5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6,8-dimethoxy-4*H*-1-benzopyran-4-one.* ***Sudachitin****. Menthocubanone*

$C_{18}H_{16}O_8$ 360.32
Isol. from *Citrus* spp. and peppermint *Mentha piperita*. Yellow needles (EtOAc/MeOH). Mp 241-243°. Formerly thought to be Majoranin.

4′-O-β-D-Glucopyranoside: [70575-17-6]
Sudachiin A
$C_{24}H_{26}O_{13}$ 522.462
Isol. from *Citrus sudachi* peel. Yellow needles (MeOH). Mp 211-213°. $[\alpha]_D$ -37.4 (c, 0.31 in 0.5% NaOH aq.).

7-O-β-D-Glucopyranoside: [70575-23-4]
Sudachitin 7-glucoside
$C_{24}H_{26}O_{13}$ 522.462
Yellow needles (MeOH). Mp 187-188°. $[\alpha]_D$ +58.9 (c, 0.26 in 0.5% NaOH aq.).

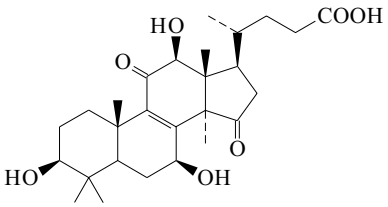
4′-O-β-D-Glucopyranoside, 7-O-(4-carboxy-3-hydroxy-3-methylbutanoyl):
[101899-84-7]
$C_{30}H_{34}O_{17}$ 666.588
Isol. from peel of *Citrus sudachi*. Yellow needles. Mp 150-152°.

4′-O-[6-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl)-β-D-glucopyranoside]:
[98891-96-4] ***Sudachiin B***
$C_{30}H_{34}O_{17}$ 666.588
Isol. from the green peel of *Citrus sudachi*. Yellow needles (2-butanone). Mp 190-192°. $[\alpha]_D$ -82.1 (MeOH aq.).

6-O-[6-O-(4-Carboxy-3-hydroxy-3-methylbutanoyl)-β-D-glucopyranoside]:
[101339-35-9] ***Sudachiin C***
$C_{30}H_{34}O_{17}$ 666.588
Isol. from the green peel of *Citrus sudachi*. Yellow needles (MeOH aq.). Mp 144-146°. $[\alpha]_D$ +61.1 (MeOH aq.).

Horie, T. *et al., Bull. Chem. Soc. Jpn.*, 1961, **34**, 1547 (*isol*)
Lee, H.H. *et al., J.C.S.*, 1964, 6255 (*synth, uv*)
Iinuma, M. *et al., Chem. Pharm. Bull.*, 1980, **28**, 708 (*cmr*)
Tomas, F. *et al., Phytochemistry*, 1980, **19**, 2039 (*7-glucoside*)
Horie, T. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2928 (*Sudachiin A*)
Zakharova, O.I. *et al., Khim. Prir. Soedin.*, 1982, **18**, 652; *Chem. Nat. Compd. (Engl. Transl.)*, 1982, **18**, 619 (*isol*)
Salmenkallis, M. *et al., Phytochemistry*, 1982, **21**, 2990 (*isol*)
Voirin, B. *et al., Phytochemistry*, 1983, **22**, 2107 (*uv*)
Herz, W. *et al., Phytochemistry*, 1984, **23**, 1453 (*isol*)
Kumamoto, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 2797 (*glycoside*)
Mata, R. *et al., Phytochemistry*, 1985, **24**, 1515 (*isol*)
Horie, T. *et al., Phytochemistry*, 1986, **25**, 2621 (*Sudachiins*)
Hradetzky, D. *et al., Z. Naturforsch., C*, 1986, **42**, 73 (*isol*)

3,7,12-Trihydroxy-25,26,27-trinor-11,15-dioxolanost-8-en-24-oic acid T-713



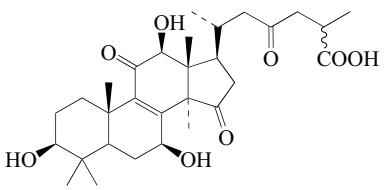
$C_{27}H_{40}O_7$ 476.609

(3β,7β,12β)-*form* [95311-96-9]
Lucidenic acid C
Metab. of *Ganoderma lucidum* (reishi). Pale yellow needles ($CHCl_3$/hexane). Mp 199-200°. $[\alpha]_D^{24}$ +140 (c, 0.2 in MeOH).

3-Ketone: [95311-95-8] *7,12-Dihydroxy-3,11,15-trioxo-25,26,27-trinor-8-lanosten-24-oic acid*. ***Lucidenic acid B***
$C_{27}H_{38}O_7$ 474.593
Metab. of *Ganoderma lucidum* (reishi). Needles (EtOAc). Mp 179-181°. $[\alpha]_D^{24}$ +169 (c, 0.22 in MeOH).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1984, **48**, 2905; 1985, **49**, 1793 (*isol, pmr, cmr*)

3,7,12-Trihydroxy-11,15,23-trioxolanost-8-en-26-oic acid T-714



$C_{30}H_{44}O_8$ 532.673

See note under 3,22-Dihydroxylanosta-7,9(11),24-trien-26-oic acid, D-525 concerning confusion in Ganoderic acid names. C-25-config. need not necessarily be the same in all compds..

(3β,7β,12β,25ξ)-*form* [98665-22-6]
Ganoderic acid G
Constit. of *Ganoderma lucidum* (reishi). Plates (EtOAc/MeOH). Mp 218-220°. $[\alpha]_D^{22}$ +105.7 (c, 0.48 in $CHCl_3$). λ_{max} 252 (ε 10023) (EtOH) (Derep).

Me ester:
Prisms. Mp 134-135°. $[\alpha]_D$ +64 ($CHCl_3$).

12-Ac: [104700-95-0] *Ganoderic acid K*
$C_{32}H_{46}O_9$ 574.71
Constit. of *Ganoderma lucidum* (reishi). Amorph. powder. $[\alpha]_D^{25}$ +48 (c, 0.29 in $CHCl_3$). λ_{max} 251 (ε 13800) (MeOH) (Berdy).

3-Ketone: [97653-94-6] *7,12-Dihydroxy-3,11,15,23-tetraoxolanost-8-en-26-oic acid. Ganoderic acid D*†
$C_{30}H_{42}O_8$ 530.657
Constit. of *Ganoderma lucidum* (reishi). Cryst. (EtOAc). Mp 201-203°. $[\alpha]_D^{22}$ +185 (c, 0.1 in EtOH).

7-Ketone, 12-Ac:12-Acetoxy-3-hydroxy-7,11,15,23-tetraoxolanost-8-en-26-oic acid. Ganoderic acid H. Ganoderic acid C†
$C_{32}H_{44}O_9$ 572.694
From *Ganoderma lucidum* (reishi). Ganoderic acids C and H appear to be identical but the Mps of the Me esters differ.

7-Ketone, 12-Ac, Me ester: [98665-19-1]
Yellow needles. Mp 155-156° (91-93°). $[\alpha]_D$ +167 ($CHCl_3$).

7-Ketone, 15β-alcohol, 12-Ac: [220181-81-7] ***Ganoderic acid α***
$C_{32}H_{46}O_9$ 574.71
Constit. of *Ganoderma lucidum* (reishi). Amorph. powder. $[\alpha]_D$ +55 (c, 1 in $CHCl_3$). λ_{max} 254 (ε 6310) (MeOH) (Berdy).

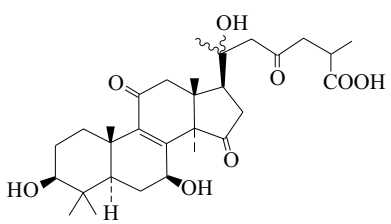
3,7-Diketone, 12-Ac: [98665-15-7] *12-Acetoxy-3,7,11,15,23-pentaoxolanost-8-en-26-oic acid. Ganoderic acid F*†
$C_{32}H_{42}O_9$ 570.678
From *Ganoderma lucidum* (reishi). See also under 3,7,12-Trihydroxy-11,15,23-trioxolanost-8-en-26-oic acid, T-714.

3,7-Diketone, 12-Ac, Me ester:
Amorph. $[\alpha]_D$ +111 ($CHCl_3$).

3,7,12-Triketone: [135357-25-4] *3,7,11,12,15,13-Hexaoxolanost-8-en-26-oic acid*. ***Ganosporeric acid A***
$C_{30}H_{38}O_8$ 526.625
Constit. of *Ganoderma lucidum* (reishi). Yellow cryst. Mp 115-118°. $[\alpha]_D^{28}$ +48 (c,0.1 in $CHCl_3$).

Nishitoba, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 1547 (*Ganoderic acid D*)
Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2624; 2628
Komoda, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 4829 (*isol*)
Hirotani, M. *et al., Phytochemistry*, 1985, **24**, 2055
Morigawa, A. *et al., Chem. Pharm. Bull.*, 1986, **34**, 3025
Chen, R.Y. *et al., CA*, 1991, **115**, 89138q (*Ganosporeric acid A*)
Chen, R.Y. *et al., J. Chin. Pharm. Sci.*, 1993, **2**, 91 (*Ganosporeric acid A*)
El-Mekkawy, S. *et al., Phytochemistry*, 1998, **49**, 1651-1657 (*Ganoderic acid α*)

3,7,20-Trihydroxy-11,15,23-trioxolanost-8-en-26-oic acid T-715



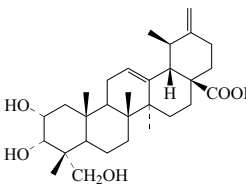
$C_{30}H_{44}O_8$ 532.673

(3β,7β,20ξ)-*form* [98665-20-4]
Ganoderic acid I
Constit. of *Ganoderma lucidum* (reishi).

Me ester:
Prisms. Mp 279-281°. $[\alpha]_D$ +132 ($CHCl_3$).

Kikuchi, T. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2628

2,3,23-Trihydroxy-12,20(30)-ursadien-28-oic acid T-716



(2α,3α)-*form*

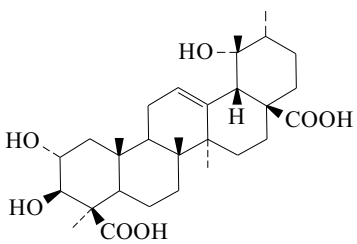
$C_{30}H_{46}O_5$ 486.69

(2α,3α)-*form* [143839-01-4]
Solid. $[\alpha]_D^{21}$ +64.4 (c, 0.2 in Py).

(2α,3β)-*form* [341971-45-7]
Actinidic acid
Constit. of the peel of the unripe fruit of *Actinidia deliciosa* cv. Golden King (kiwi fruit). Powder. $[\alpha]_D^{27}$ +104 (c, 0.14 in MeOH).

Sashida, Y. *et al., Phytochemistry*, 1992, **31**, 2801-2804 (*isol, pmr, cmr*)
Lahlou, E.H. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 480-483 (*isol, pmr, cmr, ms*)

2,3,19-Trihydroxy-12-ursene-24,28-dioic acid T-717



$C_{30}H_{46}O_7$ 518.689

(2α,3β,19α)-*form* [53527-49-4]
Corosin. *Vismiaefolic acid. Trachelosperogenin A. Capsularone*
Constit. of *Corchorus olitorius* (Jew's mallow). Cryst. (EtOH). Mp 292-293° dec Mp 300°. $[\alpha]_D^{26}$ +39 (c, 0.5 in MeOH).

28-O-β-D-Glucopyranosyl ester: [109750-36-9] ***Trachelosperogenin A1***
$C_{36}H_{56}O_{12}$ 680.831
Amorph. solid. $[\alpha]_D^{30}$ +12.6 (c, 0.35 in MeOH).

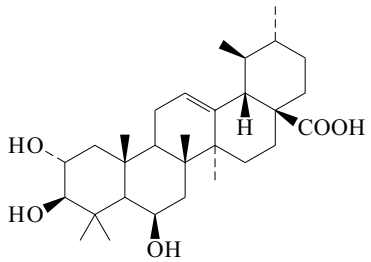
28-O-(3-O-Methyl-β-D-glucopyranosyl) ester: [198129-55-4]
$C_{37}H_{58}O_{12}$ 694.858
Amorph. powder (as Me ester). Mp 180-182° (Me ester). $[\alpha]_D^{20}$ +13 (c, 0.3 in MeOH) (Me ester).

28-O-(6-O-Methyl-β-D-glucopyranosyl) ester: [198129-54-3]
$C_{37}H_{58}O_{12}$ 694.858
Amorph. powder (as Me ester). Mp 193-195° (Me ester). $[\alpha]_D^{20}$ +24 (c, 0.32 in MeOH).

Manzoor-i-Khuda, M. *et al., Pak. J. Sci. Ind. Res.*, 1971, **14**, 49 (*isol*)
Manzoor-i-Khuda, M. *et al., Z. Naturforsch., C*, 1974, **29**, 209 (*struct*)
Abe, F. *et al., Chem. Pharm. Bull.*, 1987, **35**, 1748 (*Trachelosperogenin A1*)

Araújo, F.W.L. *et al., J. Nat. Prod.*, 1990, **53**, 1436 (*isol, pmr, cmr*)
Wang, B.G. *et al., Phytochemistry*, 1997, **46**, 559-563 (*Rubus pileatus saponins*)
Zhang, Q.-Y *et al., J. Asian Nat. Prod. Res.*, 2000, **2**, 81-86; *CA*, **133**, 101980q (*isol*)

2,3,6-Trihydroxy-12-ursen-28-oic acid T-718



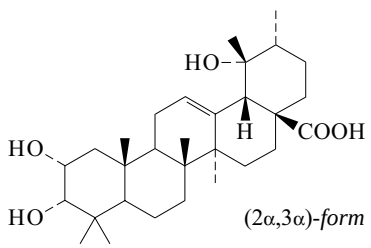
$C_{30}H_{48}O_5$ 488.706

(2α,3β,6β)-*form* [26532-66-1]
Madasiatic acid
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. Mp 248-250° dec.

*28-*O*-[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester:* [386223-76-3] ***Centellasaponin C***
$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. ($CHCl_3$/MeOH). Mp 209-210°. $[\alpha]_D^{25}$ -9 (c, 0.6 in MeOH).

Pinhas, H. *et al., Bull. Soc. Chim. Fr.*, 1969, 3592-3595
Matsuda, H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1368-1371 (*Centellasaponin C*)

2,3,19-Trihydroxy-12-ursen-28-oic acid T-719



$C_{30}H_{48}O_5$ 488.706

(2α,3α,19α)-*form* [53155-25-2]
Euscaphic acid. *Jacarandic acid. Acuminatic acid*
Constit. of *Coleus amboinicus* (Cuban oregano). Powder or cryst. (MeOH). Mp 270-271° (264°). $[\alpha]_D^{23}$ +12 (c, 1 in MeOH).

*3-*O*-(4-Hydroxy-3-methoxy-*E*-cinnamoyl):3-*O*-trans-Feruloyleuscaphic acid*
$C_{40}H_{56}O_8$ 664.878
Constit. of *Eriobotrya japonica* (loquat). Amorph. solid. Mp 185-190° dec. λ_{max} 290 ; 320 (MeOH).

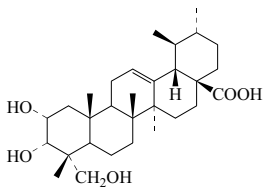
(2α,3β,19α)-*form* [13850-16-3]
Tormentic acid
Cryst. Mp 273°. $[\alpha]_D$ -20 (Py).

*3-*O*-(3,4-Dihydroxy-E-cinnamoyl):* [144604-16-0] ***3-trans-Caffeoyltormentic acid***
$C_{39}H_{54}O_8$ 650.851
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ +1.2 (c, 1 in MeOH). λ_{max} 217 (ε); 380 (ε) (EtOH/NaOH) (Derep). λ_{max} 221 (ε 20900); 235 (ε); 246 (ε); 302 (ε); 333 (ε) (EtOH) (Derep).

[54963-57-4, 77820-51-0]

De Tommasi, N. *et al., J. Nat. Prod.*, 1992, **55**, 1067 (*caffeoyl ester*)
Lontsi, D. *et al., Phytochemistry*, 1992, **31**, 4285 (*Euscaphic acid, pmr, cmr*)
Shimizu, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2181 (*Feruloyleuscaphic acid*)

2,3,23-Trihydroxy-12-ursen-28-oic acid T-720



(2α,3α)-*form*

$C_{30}H_{48}O_5$ 488.706

(2α,3α)-*form* [76964-07-3]
Esculentic acid†
Constit. of the edible fern *Diplazium esculentum*. Cryst. (MeOH). Mp 270°. $[\alpha]_D$ +51 (EtOH). The sample from *N. hindostana* was originally assigned the (2β,3α)-config..

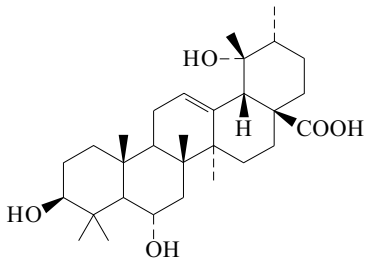
(2α,3β)-*form* [464-92-6]
Asiatic acid. *Dammarolic acid*
Cryst. by subl. Mp 300-305°. Log P 5.37 (calc).
▶ Causes exp. neoplasms.

[α-L-Rhamnopyranosyl-(1→4)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester: [16830-15-2] ***Asiaticoside***. *Blastostimulina. Centelase. Emdecassol. Madecassol. Marticassol. FK 1080*
$C_{48}H_{78}O_{19}$ 959.133
Constit. of *Centella asiatica* (Asiatic pennywort). Cryst. Sol. EtOH aq., Py; fairly sol. MeOH, EtOH; poorly sol. H_2O. Mp 235-238° (230-233°). $[\alpha]_D^{20}$ -14 (EtOH). Log P -0.48 (uncertain value) (calc).
▶ YU9625000

[103974-74-9]

Polonsky, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 880-887; 1961, 1586-1591 (*Asiatic acid, Asiaticoside, isol, struct*)
Shamma, M. *et al., J.O.C.*, 1962, **27**, 4512-4517 (*pmr*)
Chasseaud, L.F. *et al., Arzneim.-Forsch.*, 1971, **21**, 1379-1384 (*metab, Asiaticoside*)
Velasco, M. *et al., Curr. Ther. Res., Clin. Exp.*, 1976, **19**, 121-125 (*Asiaticoside, rev*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 1600
Kojima, H. *et al., Phytochemistry*, 1986, **25**, 729-733 (*cmr*)
Mahato, S.B. *et al., J.C.S. Perkin 2*, 1987, 1509-1515 (*Asiaticoside, cryst struct*)
Kojima, H. *et al., Phytochemistry*, 1989, **28**, 1703-1710 (*pmr, cmr, struct*)
Maeda, C. *et al., Phytochemistry*, 1994, **37**, 1131-1137 (*Asiaticoside, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN500

3,6,19-Trihydroxy-12-ursen-28-oic acid T-721



$C_{30}H_{48}O_5$ 488.706

(3β,6α,19α)-*form* [130289-31-5]
Isol. from leaves of *Eriobotrya japonica* (loquat). Mp 270°. $[\alpha]_D^{25}$ +69 (c, 1 in MeOH).

(3β,6β,19α)-*form*
Uncaric acid
Cryst. (MeOH aq.). Mp 226-227°. $[\alpha]_D^{25}$ +52.7 (c, 1 in MeOH). Mp and opt. rotns. refer to different specimens. Struct. of Uncaric acid revised in 1995.

Me ester:
Mp 220-221°.

3,6-Di-Ac:
$C_{34}H_{52}O_7$ 572.781
Cryst. (MeOH). Mp 220°. Struct. revised in 1995.

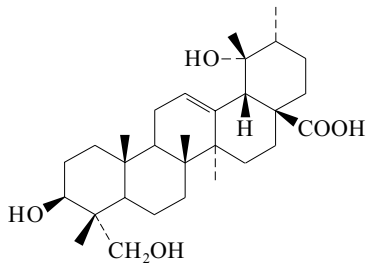
3-Ketone:6,19-Dihydroxy-3-oxo-12-ursen-28-oic acid
$C_{30}H_{46}O_5$ 486.69
$[\alpha]_D^{25}$ +28 (c, 1 in MeOH).

3,6-Diketone: [70237-81-9] *19-Hydroxy-3,6-dioxo-12-ursen-28-oic acid*. ***Diketouncaric acid***
$C_{30}H_{44}O_5$ 484.675
Cryst. (EtOH). Mp 265°. $[\alpha]_D^{27}$ +82 ($CHCl_3$). Struct. revised in 1995.

[70237-76-2]

Herath, W.H.M.W. *et al., Phytochemistry*, 1978, **17**, 1978 (*isol*)
Aimi, N. *et al., Tetrahedron*, 1989, **45**, 4125 (*isol*)
Aquino, R. *et al., J. Nat. Prod.*, 1990, **53**, 559 (*isol, pmr, cmr*)
Liang, Z. *et al., Planta Med.*, 1990, **56**, 330 (*isol, pmr, cmr, ms*)
Diyabalanage, T.K.K. *et al., Phytochemistry*, 1995, **40**, 1311 (*Uncaric acid, struct*)
Aquino, R. *et al., Phytochemistry*, 1997, **45**, 1035-1040 (*3-ketone*)

3,19,23-Trihydroxy-12-ursen-28-oic acid T-722



$C_{30}H_{48}O_5$ 488.706

(3β,19α)-*form* [20137-37-5]
Rotundic acid

Me ester:
Cryst. Mp 257°. $[\alpha]_D^{24}$ +38.

β-D-Glucopyranosyl ester: [42719-32-4]
Pedunculoside
$C_{36}H_{58}O_{10}$ 650.848
Prisms (EtOAc). Mp 213-214°. $[\alpha]_D^{25}$ +22 (c, 0.05 in MeOH).

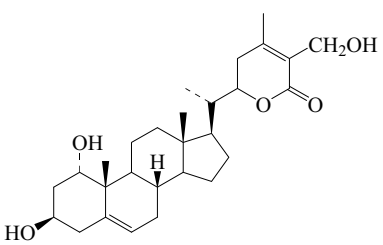
3-O-α-L-Arabinopyranoside, 28-O-β-D-glucopyranosyl ester: [147235-21-0] ***Ilekudinoside D***
$C_{41}H_{66}O_{14}$ 782.964
Amorph. powder. $[\alpha]_D^{23}$ +11.5 (c, 2.16 in MeOH).

3-O-[β-D-Glucopyranosyl-(1→3)-α-L-arabinopyranoside]: [284684-43-1] ***Randiasaponin II***
$C_{41}H_{66}O_{14}$ 782.964
Powder. $[\alpha]_D^{20}$ +10.9 (c, 0.12 in MeOH).

*3-O-(4-Hydroxy-*E*-cinnamoyl):* [144624-03-3] ***3-trans-p-Coumaroylrotundic acid***
$C_{39}H_{54}O_7$ 634.851
Constit. of *Eriobotrya japonica* (loquat). $[\alpha]_D^{25}$ +5.2 (c, 1 in MeOH).

Oyama, T. *et al., Tet. Lett.*, 1968, 4639
Nakatani, M. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 469 (*Pedunculoside*)
Nakatani, M. *et al., Phytochemistry*, 1989, **28**, 1479 (*isol, pmr, cmr*)
De Tommasi, N. *et al., J. Nat. Prod.*, 1992, **55**, 1067 (*p-coumaroyl ester*)
Soares, F.P. *et al., Magn. Reson. Chem.*, 1998, **36**, 608-614 (*pmr, cmr*)
Nishimura, K. *et al., J. Nat. Prod.*, 1999, **62**, 1128-1133 (*Ilekudinoside D*)
Sahpaz, S. *et al., Phytochemistry*, 2000, **54**, 77-84 (*Randiasaponin II*)

1,3,27-Trihydroxywitha-5,24-dienolide T-723



$C_{28}H_{42}O_5$ 458.637

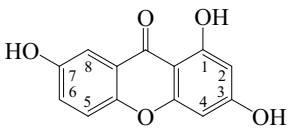
(1α,3β)-*form* [98569-64-3]
Pubesenolide. *Sominone*
Constit. of *Physalis pubescens* (ground cherry). Cryst. (MeOH). Mp 145-146°. $[\alpha]_D$ +28.5 (c, 1.8 in $CHCl_3$).

1-Ac, 3-O-β-D-glucopyranoside: [227179-08-0]
$C_{36}H_{54}O_{11}$ 662.816
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. powder. $[\alpha]_D^{25}$ +29.3 (c, 0.89 in MeOH). λ_{max} 218 (log ϵ 3.89) (MeOH).

Sahai, M. *et al., J. Nat. Prod.*, 1985, **48**, 474
Atta-ur-Rahman, *et al., Heterocycles*, 1992, **34**, 689 (*isol, pmr, cmr*)
Ahmad, S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 477-480 (*1-Ac-3-glucoside*)

1,3,7-Trihydroxyxanthone T-724

[529-49-7]
*1,3,7-Trihydroxy-9*H*-xanthen-9-one, 9CI.*
Gentisein



$C_{13}H_8O_5$ 244.203
Isol. from *Gentiana lutea* (yellow gentian). Orange-yellow needles (MeOH). Mp 321-323°. λ_{max} 204 (ϵ 8912); 237 (ϵ 19500); 260 (ϵ 24550); 310 (ϵ 7580); 374 (ϵ 2450) (MeOH) (Berdy).

▶ ZD6122400

3-O-β-D-Glucopyranoside: ***Xanthohypericoside***
$C_{19}H_{18}O_{10}$ 406.345
Yellow needles. Mp 233-234°. λ_{max} 205 ; 236 ; 260 ; 302 ; 376 (MeOH).

Tri-Ac:
Mp 229-230°.

1-Me ether: [16850-68-3] *3,7-Dihydroxy-1-methoxyxanthone*
$C_{14}H_{10}O_5$ 258.23
Yellow needles (MeOH aq.). Mp 178°.

3-Me ether: [437-50-3] *1,7-Dihydroxy-3-methoxyxanthone*. ***Gentisin***. *Gentianin*†. *Gentianic acid*
$C_{14}H_{10}O_5$ 258.23
Pigment from root of *Gentiana lutea* (yellow gentian). Yellow needles. Mp 273-275° (266-267°).

▶ ZD6034600

3-Me ether, 7-O-β-D-glucopyranoside:
$C_{20}H_{20}O_{10}$ 420.372
Mp 219-222° dec.

3-Me ether, 1-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [85754-76-3] *7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone*
$C_{25}H_{28}O_{14}$ 552.488
Constit. of *Gentiana lutea* (yellow gentian). Needles. Mp 259-260° dec. $[\alpha]_D^{20}$ -81.5 (c, 0.4 in Py).

3-Me ether, 7-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [85761-72-4] *1-Hydroxy-3-methoxy-7-primeverosyloxyxanthone*
$C_{25}H_{28}O_{14}$ 552.488
Constit. of *Gentiana lutea* (yellow gentian). Needles. Mp 293-294° dec. $[\alpha]_D^{20}$ -69.4 (c, 0.36 in Py).

7-Me ether: [491-64-5] *1,3-Dihydroxy-7-methoxyxanthone*. ***Isogentisin***
$C_{14}H_{10}O_5$ 258.23
Isol. from roots of *Gentiana lutea* (yellow gentian). Yellow platelets (EtOH). Mp 241°.

▶ ZD6034500

7-Me ether, 3-O-[β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside]: [529-48-6] ***Gentioside*** †. *Gentiin*
$C_{25}H_{28}O_{14}$ 552.488
Constit. of *Gentiana lutea* roots (yellow gentian). Needles. Mp 278-279° dec. $[\alpha]_D^{25}$ -107 (60% EtOH aq.). $[\alpha]_D^{20}$ -50 (c, 0.3 in Py).

3,7-Di-Me ether: [13379-35-6] *1-Hydroxy-3,7-dimethoxyxanthone*
$C_{15}H_{12}O_5$ 272.257
Isol. from *Gentiana lutea* (yellow gentian). Cryst. (MeOH), yellow needles (CH_2Cl_2/hexane). Mp 169-170°.

▶ ZD6035500

Tri-Me ether: [3722-54-1] *1,3,7-Trimethoxyxanthone*
$C_{16}H_{14}O_5$ 286.284
Cryst. (EtOAc). Mp 173-174°.

▶ ZD6122450

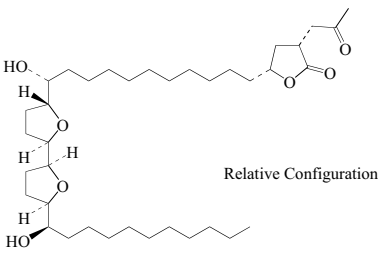
*7-O-(3,7-Dimethyl-2,6-octadienyl)(*E*-):* ***7-Geranyloxy-1,3-dihydroxyxanthone***
$C_{23}H_{24}O_5$ 380.44
Yellow needles (CH_2Cl_2/hexane). Mp 138-140°. λ_{max} 206 (log ϵ 4.25); 236 (log ϵ 4.48); 260 (log ϵ 4.39); 316 (log ϵ 3.89); 364 (log ϵ 3.94) (EtOH).

Shinoda, J. *et al., J.C.S.*, 1927, 1985 (*synth*)
Atkinson, J.E. *et al., Tetrahedron*, 1969, **25**, 1507 (*isol, synth*)
Stout, G.H. *et al., Tetrahedron*, 1969, **25**, 1961 (*isol, synth*)
Chawla, H.M. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1973, **78**, 141 (*ir*)
Hostettmann, K. *et al., Helv. Chim. Acta*, 1974, **57**, 1155 (*isol*)
Ellis, R.C. *et al., J.C.S. Perkin 1*, 1976, 1377 (*synth*)
Chadha, R. *et al., Indian J. Chem., Sect. A*, 1979, **18**, 505 (*cmr*)
Fram, A.W. *et al., Tetrahedron*, 1979, **35**, 2035 (*cmr*)
Hayashi, T. *et al., Phytochemistry*, 1988, **27**, 3696 (*derivs*)
Patel, G.N. *et al., Synth. Commun.*, 1989, **19**, 1641 (*synth, pmr*)
Peres, V. *et al., Phytochemistry*, 1997, **44**, 191 (*rev, occur*)
Nguyen, L.H.D. *et al., Phytochemistry*, 1999, **50**, 471-476 (*7-Geranyloxy-1,3-dihydroxyxanthone*)
Kitanov, G.M. *et al., Pharmazie*, 2000, **55**, 397-398 (*Xanthohypericoside*)

2,4-*cis*-Trilobacinone T-725

[189686-30-4]

[189157-73-1]



$C_{37}H_{66}O_7$ 622.924

Stereoisomer of Rollinone. Constit. of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D^{22}$ +17.3 (c, 0.2 in $CHCl_3$).

2-Epimer: [189686-32-6] ***2,4*-trans-*Trilobacinone***

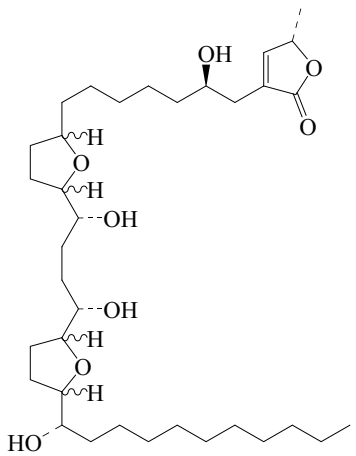
$C_{37}H_{66}O_7$ 622.924

Constit. of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D^{22}$ +9.2 (c, 0.2 in $CHCl_3$).

He, K. *et al., Bioorg. Med. Chem.*, 1997, **5**, 501-506 (*isol, ir, pmr, cmr, ms*)

Trilobalicin T-726

[189747-98-6]



$C_{35}H_{62}O_8$ 610.87

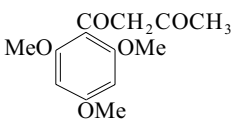
Constit. of *Asimina triloba* (pawpaw). Wax. $[\alpha]_D^{22}$ +13.6 (c, 0.1 in $CHCl_3$).

He, K. *et al., Bioorg. Med. Chem.*, 1997, **5**, 501-506 (*isol, ir, pmr, cmr, ms*)

1-(2,4,6-Trimethoxyphenyl)-1,3-butanedione, 9CI T-727

[480-27-3]

2,4,6-Trimethoxybenzoylacetone. Eugenone



$C_{13}H_{16}O_5$ 252.266

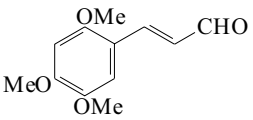
Constit. of *Eugenia caryophyllata* (clove) oil. Cryst. (MeOH). Mp 97-98°.

Schmid, H. *et al., Helv. Chim. Acta*, 1948, **31**, 748

3-(2,4,5-Trimethoxyphenyl)-2-propenal, 9CI T-728

[106128-88-5]

2,4,5-Trimethoxycinnamaldehyde



$C_{12}H_{14}O_4$ 222.24

(E)-form [99217-06-8]

Yellow cryst. Mp 140-142°.

(Z)-form [99217-07-9]

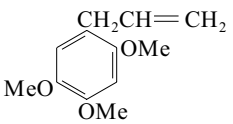
Isol. from the rhizomes of *Acorus calamus* (sweet flag). Fine needles (Et_2O/petrol). Mp 85°.

Saxena, D.B. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 683 (*synth*)
Kulkarni, M.M. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 981
Saxena, D.B. *et al., Phytochemistry*, 1986, **25**, 553 (*isol*)
Sinha, A.K. *et al., J. Nat. Prod.*, 2002, **65**, 764-765 (*synth, pmr, cmr*)

1,2,4-Trimethoxy-5-(2-propenyl)benzene T-729

[5353-15-1]

*1-Allyl-2,4,5-trimethoxybenzene. **γ-Asarone**. Euasarone. Isoasarone. Sekishon*



$C_{12}H_{16}O_3$ 208.257

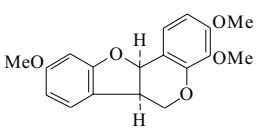
Constit. of *Acorus calamus* (sweet flag). Oil. Mp 25°. Bp_2 145-147°. λ_{max} 291 ; 350 (no solvent reported).

Devgan, O.N. *et al., Aust. J. Chem.*, 1968, **21**, 3001 (*isol, struct*)
Matsui, K. *et al., Agric. Biol. Chem.*, 1976, **40**, 1045 (*isol*)
Kulkarni, M.M. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 981 (*isol, bibl*)
Santos, B.V. de O. *et al., Phytochemistry*, 1998, **49**, 1381-1384 (*isol, uv, pmr, cmr*)

3,4,9-Trimethoxypterocarpan T-730

[22973-36-0]

*6a,11a-Dihydro-3,4,9-trimethoxy-6H-benzofuro[3,2-c][1]benzopyran, 8CI. **4-Methoxyhomopterocarpin***



Probable absolute configuration

$C_{18}H_{18}O_5$ 314.337

(-)-form

Constit. of *Melilotus alba* (white melilot). Needles (EtOH or C_6H_6). Mp 118-120°. $[\alpha]_D^{26}$ -163 (c, 0.9 in MeOH). λ_{max} 284 (log ε 3.84) and 290 sh nm (MeOH).

(±)-form [10528-09-3]

Prisms (C_6H_6/petrol). Mp 114-115°.

Harper, S.H. *et al., Chem. Comm.*, 1965, 309 (*isol, ir, uv*)
Kalra, V.K. *et al., Tetrahedron*, 1967, **23**, 3221 (*synth, ir, uv*)
Harper, S.H. *et al., J.C.S.(C)*, 1969, 1109 (*isol, pmr, abs config*)
Abdel-Kader, M.S. *et al., Planta Med.*, 2001, **67**, 388-390 (*isol, cmr*)

Trimethylamine, 8CI T-731

[75-50-3]

N,N-*Dimethylmethanamine, 9CI. FEMA 3241*

Me_3N

C_3H_9N 59.111

Flavouring ingredient. Present in cheese, caviar, fish, beer, whisky, cocoa and coffee. Volatile liq. with fishy odour. Misc. H_2O, EtOH; sol. Et_2O, C_6H_6, $CHCl_3$. d_4^0 0.67. Mp -117.2°. $Bp_{746.6}$ 3.2-3.8°. pK_a 9.81. Crit. pt. 160.5°/41 atm..

▶ Extremely flammable. Eye, skin and respiratory tract irritant. High vapour conc. may affect CNS. LD_{50} (mus, ivn) 90 mg/kg. LC_{50} (mus, ihl) 19000 mg m^{-3}. OES: long-term 10 ppm; short-term 15 ppm. PA0350000

Hydrochloride: [593-81-7]

Needles (EtOH). Sol. EtOH; insol. Et_2O. Mp 277-278° dec. Sublimes at 200°.

▶ LD_{50} (mus, ivn) 325 mg/kg. YH2700000

Hydrobromide: [2840-24-6]

Prisms (EtOH). Mp 243-245°.

Hydroiodide: [20230-89-1]

Prisms (EtOH). Sol. H_2O, insol. Et_2O. Mp 263°.

SO_3 complex: [3162-58-1]

$C_3H_9NO_3S$ 139.175

Moisture-sensitive solid. Mp 232° dec Mp 240°.

N-*Oxide:* See Trimethylamine oxide in *The Combined Chemical Dictionary.*

N-*Me:* See Tetramethylammonium(1+) in *The Combined Chemical Dictionary.*

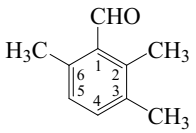
[16962-53-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 298D; 299A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 479C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 383B (*ir*)
Koeppen, A. *et al., Ber.*, 1905, **38**, 882 (*synth*)
Org. Synth., Coll. Vol., 1, 1932, 531 (*synth, props*)
Moede, J.A. *et al., J.A.C.S.*, 1949, **71**, 852 (*SO_3 complex*)
Ger. Pat., 1969, 2 053 709; *CA*, **75**, 35113q (*synth*)
Hvistendahl, G. *et al., Org. Mass Spectrom.*, 1970, **3**, 821 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2446 (*occur*)
Price, C.C. *et al., J.O.C.*, 1973, **38**, 615 (*pmr*)
Sarneski, J.E. *et al., Anal. Chem.*, 1975, **47**, 2116 (*cmr*)
Preti, G. *et al., J. Chem. Ecol.*, 1976, **2**, 177
Blake, A.J. *et al., Acta Cryst. C*, 1984, **40**, 413 (*cryst struct*)
Halpern, A.M. *et al., J.A.C.S.*, 1986, **108**, 3907 (*uv*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1990, **A16**, 535 (*rev*)

Murphy, W.F. *et al., J. Phys. Chem.*, 1993, **97**, 581 (*ir, Raman*)
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **7**, 5195-5197 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 767
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2835; 2836
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1280
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLD500; TLE000; TLD750; TLF750

2,3,6-Trimethylbenzaldehyde T-732

[34341-29-2]



$C_{10}H_{12}O$ 148.204
Constit. of *Eryngium foetidum* (culantro). Liq. Bp_{10} 113-114°.

Oxime:
$C_{10}H_{13}NO$ 163.219
Cryst. (EtOH aq.). Mp 124-126°.

Semicarbazone:
Cryst. (EtOH). Mp 167-169°.

Smith, L. *et al., J.O.C.*, 1941, **6**, 489 (*synth*)
Schwarz, H. *et al., Org. Mass Spectrom.*, 1972, **6**, 815 (*ms*)
Kubeczka, K.-H. *et al., Phytochemistry*, 1981, **20**, 828 (*isol, pmr, cmr*)
Sudalai, A. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 110 (*synth*)
Wong, K.C. *et al., J. Essent. Oil Res.*, 1994, **6**, 369 (*isol*)

2,4,5-Trimethylbenzaldehyde T-733

[5779-72-6]
Duryl aldehyde

$C_{10}H_{12}O$ 148.204
Constit. of *Eryngium foetidum* (culantro) and *Foeniculum vulgare* (fennel). Plates (EtOH). Mp 43.5°. Bp 243°. Turns yellow in air.

Oxime: [60368-00-5]
$C_{10}H_{13}NO$ 163.219
Needles (EtOH aq.). Mp 111-112°.

Semicarbazone:
Prisms (EtOH). Mp 243-244°.

Phenylhydrazone:
Leaflets (AcOH). Mp 127°.

Smith, L. *et al., J.O.C.*, 1941, **6**, 489 (*synth*)
Niedzielski, E. *et al., J.O.C.*, 1943, **8**, 147 (*synth*)
Schwarz, H. *et al., Org. Mass Spectrom.*, 1972, **6**, 815 (*ms*)
Fischer, A. *et al., Can. J. Chem.*, 1976, **54**, 1804 (*synth, nmr*)
Ma, X. *et al., CA*, 1990, **113**, 74832w (*isol*)
Fang, H.J. *et al., CA*, 1990, **113**, 208414x (*isol*)

2,4,6-Trimethylbenzaldehyde T-734

[487-68-3]
β-Isoduryl aldehyde. Mesityl aldehyde. Aldehydomesitylene. β-Isodural. Mesitaldehyde. Isodural

$C_{10}H_{12}O$ 148.204
Constit. of false coriander (*Eryngium foetidum*) and saffron. Liq. Bp 237-240° Bp_{11} 113-115°.
▶ CU8500000

(E)-Oxime: [54130-63-1] syn-*Mesityl oxime*
$C_{10}H_{13}NO$ 163.219
Prisms (Et_2O). Spar. sol. most org. solvs. Mp 124°.

(Z)-Oxime: [54130-62-0] anti-*Mesityl oxime*
$C_{10}H_{13}NO$ 163.219
Needles (Et_2O). More sol. than (*E*)-form. Mp 180-181°.

Semicarbazone: [14066-63-8]
Cryst. (EtOH). Mp 185-188°.

Phenylhydrazone:
Cryst. (EtOH). Mp 74°.

[40188-34-9]

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 964A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 125A (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1303D (*ir*)
Hantzsch, A. *et al., Ber.*, 1895, **28**, 744 (*synth*)
Hinkel, L.E. *et al., J.C.S.*, 1931, 1170; 1932, 2793
Org. Synth., Coll. Vol., 3, 1955, 549; 551 (*synth*)
Schwarz, H. *et al., Org. Mass Spectrom.*, 1972, 815 (*ms*)
Org. Synth., Coll. Vol., 5, 1973, 49 (*synth*)
Haefelinger, G. *et al., Chem. Ber.*, 1976, **109**, 833 (*pmr*)
Zadel, G. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1035 (*synth*)

3,4,5-Trimethylbenzaldehyde T-735

[5779-74-8]
5-Aldehydohemimellitene

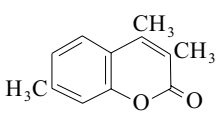
$C_{10}H_{12}O$ 148.204
Constit. of hop oil (*Humulus lupulus*). Needles (EtOH aq.). Mp 52°.

Oxime: [60367-96-6]
$C_{10}H_{13}NO$ 163.219
Mp 135-136°.

Kromer, H. *et al., Ber.*, 1891, **24**, 2407 (*synth*)
Schwarz, H. *et al., Org. Mass Spectrom.*, 1972, 815 (*ms*)
Fischer, A. *et al., Can. J. Chem.*, 1976, **54**, 1795 (*synth, pmr*)
Liu, G. *et al., CA*, 1987, **107**, 64624s (*isol*)

3,4,7-Trimethyl-2*H*-1-benzopyran-2-one T-736

[14002-93-8]
3,4,7-Trimethylcoumarin. ***Trigoforin***

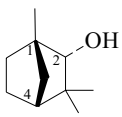


$C_{12}H_{12}O_2$ 188.226
Constit. of *Trigonella foenum-graecum* (fenugreek). Cryst. (MeOH). Mp 112-113°.

Fries, K. *et al., Ber.*, 1906, **39**, 871 (*synth*)
Mangini, A. *et al., Gazz. Chim. Ital.*, 1957, **87**, 243 (*uv*)
Grigg, R. *et al., Tetrahedron*, 1966, **22**, 3301 (*pmr*)
Mali, R.S. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 759 (*synth*)
Khurana, S.K. *et al., Phytochemistry*, 1982, **21**, 2145 (*isol*)
Mali, R.S. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 1271 (*synth*)

1,3,3-Trimethylbicyclo[2.2.1]-heptan-2-ol T-737

[1632-73-1]
Fenchol. *Fenchyl alcohol. 2-Fenchanol. FEMA 2480*



(1*S*,2*S*,4*R*)-*form*

$C_{10}H_{18}O$ 154.252
Flavouring ingredient with a bitter, lime-like flavour.

(1*S*,2*S*,4*R*)-*form* [512-13-0]
(-)-endo-*form. (-)-α-Fenchol*
Cryst. Mp 43.7-48.5°. Bp_{20} 94°. $[\alpha]_D^{20}$ -11 (EtOH).

Hydrogen phthalate:
Mp 146°.

Ac: [20347-65-3] *Fenchyl acetate. FEMA 3390*
$C_{12}H_{20}O_2$ 196.289
Flavouring ingredient, together with stereoisomers. $[\alpha]_D$ -68.7. The FEMA number refers to unspecified stereoisomer mixture.

4-Hydroxy-3-methoxybenzoyl: [77369-06-3] ***Stylosin***†
$C_{18}H_{24}O_4$ 304.385
Cryst. (petrol). Mp 108-109°.

3,4-Dimethoxybenzoyl: [78162-92-2] ***Stylosidin***
$C_{19}H_{26}O_4$ 318.412

4-Nitrobenzoyl:
Mp 108°.

(1*R*,2*R*,4*S*)-*form* [2217-02-9] *(+)*-endo-*form. (+)-α-Fenchol*
Cryst. Mp 47-47.5°. $[\alpha]_D^{20}$ +12.5.
▶ Skin irritant. RB7650000

Hydrogen phthalate:
Mp 145°.

4-Nitrobenzoyl:
Mp 107°.

(1*R*,2*S*,4*S*)-*form* [64439-31-2] *(+)*-exo-*form. (+)-β-Fenchol*
Mp 26-27°. $[\alpha]_D^{22}$ +33.2 (EtOH).

Hydrogen phthalate:
Mp 151°.

Phenylurethane:
Mp 89°.

Ac:
$[\alpha]_D^{20}$ +23 (c, 4.3 in EtOH). Opt. rotn. is for sample contg. 16% *endo* isomer.

(1*S*,2*R*,4*R*)-*form* [470-08-6] *(-)*-exo-*form. (-)-β-Fenchol*
Oil. Mp 7-8° (3-4°). Bp_{18} 91°. $[\alpha]_D^{20}$ -31.

Hydrogen phthalate:
Mp 154°.

4-Nitrobenzoyl:

Mp 82°.

Phenylurethane:
Mp 89°.

(1*RS*,2*RS*,4*SR*)-*form* [36386-49-9]

[14575-74-7] *(±)*-endo-*form. (±)-α-Fenchol*
Mp 38°. Bp 200°.

Hydrogen phthalate:
Mp 169°.

Phenylurethane:
Mp 104°.

(1*RS*,2*SR*,4*SR*)-*form* [36386-50-2]

[22627-95-8] *(±)*-exo-*form. (±)-β-Fenchol*
Mp 6°. Bp 201°.

Hydrogen phthalate:
Mp 153°.

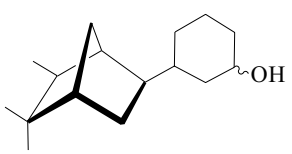
Phenylurethane:
Mp 90°.

[4057-31-2, 36386-52-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 169D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 250B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 246C (*ir*)
Rodd's Chem. Carbon Compd. (2nd edn.), 1969, **2C**, 238 (*bibl*)
Bosworth, N. *et al., J.C.S. Perkin 1*, 1972, 943-948 (*1R,2S,4S-form, synth*)
Teisseire, P. *et al., Recherches*, 1974, **19**, 232-240 (*rev*)
Stothers, J.B. *et al., Can. J. Chem.*, 1976, **54**, 1211-1221 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 775 (*rev, tox*)
Bagirov, V.Y. *et al., Khim. Prir. Soedin.*, 1980, 789-791; 1981, 99-100; *Chem. Nat. Compd. (Engl. Transl.)*, 1980, **16**, 562-563 (*Stylosidin, Stylosin*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 278-279
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1091-1092; 2844-2845
Hückel, W. *et al., Annalen*, 1840, **664**, 31-75 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMD100; FAO000; TLW000

3-(5,6,6-Trimethylbicyclo[2.2.1]hept-1-yl)cyclohexanol, 9CI T-738

[3407-42-9]
1-(5,5,6-Trimethyl-2-norbornyl)cyclohexanol, 8CI. 3-Isocamphylcyclohexanol

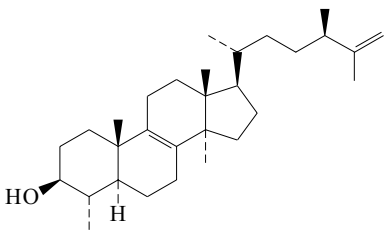


$C_{16}H_{28}O$ 236.397
Flavouring ingredient. Component of sandalwood oil. $Bp_{0.01}$ 122-127°. Several stereoisomers have been individually characterised.

Netherlands Pat., 1965, 6 410 291; *CA*, **63**, 14924t (*use*)
Demole, E. *et al., Helv. Chim. Acta*, 1969, **52**, 2065-2085 (*synth, struct, rev*)
Dahill, R.T. *et al., J.O.C.*, 1970, **35**, 251-253 (*synth, ir, pmr, ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 801 (*rev, tox*)

4,14,24-Trimethylcholesta-8,25-dien-3-ol T-739

[89956-92-3]
4,14-Dimethylergosta-8,25-dien-3-ol, 9CI

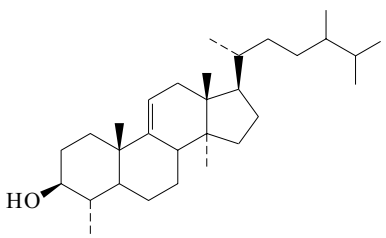


$C_{30}H_{50}O$ 426.724
(3β,4α,5α,14α,24*R*)-*form*
Constit. of *Musa paradisiaca* (banana). Needles ($CHCl_3$/MeOH). Mp 135°. $[\alpha]_D$ +72 ($CHCl_3$).

Dutta, P.K. *et al., Phytochemistry*, 1983, **22**, 2563

4,14,24-Trimethylcholest-9(11)-en-3-ol T-740

24-Methyl-31-norlanost-9(11)-en-3-ol



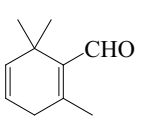
$C_{30}H_{52}O$ 428.74
(3β,4α,5α,14α,24ξ)-*form* [68520-27-4]
Constit. of *Lycopersicon esculentum* (tomato) seeds.

3-Ketone:4α,14α,24-Trimethylcholest-9(11)-en-3-one
$C_{30}H_{50}O$ 426.724
Cryst. (Et_2O/MeOH). Mp 143-144°. $[\alpha]_D^{23}$ +76 (c, 0.54 in EtOH).

Itoh, T. *et al., Phytochemistry*, 1978, **17**, 971 (*isol*)
Naora, M. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 1767 (*isol*)
Yamashita, M. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 1383 (*synth*)

2,6,6-Trimethyl-1,4-cyclohexadiene-1-carboxaldehyde, 9CI T-741

[162376-82-1]

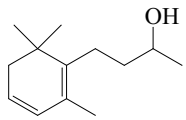


$C_{10}H_{14}O$ 150.22
Steam volatile constit. (ca.3%) of saffron (*Crocus sativus*) essential oil. Liq.

Bennani, Y.L. *et al., J.O.C.*, 1995, **60**, 1195-1200 (*synth, nmr*)
Tarantilis, P.A. *et al., J. Agric. Food Chem.*, 1997, **45**, 459-462 (*isol, glc, ms*)

4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanol T-742

[57069-86-0]
α,2,6,6-Tetramethyl-1,3-cyclohexadiene-1-propanol, 9CI. 7,8-Dehydro-3,4-dihydro-β-ionol. FEMA 3446

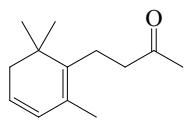


$C_{13}H_{22}O$ 194.316
Flavouring ingredient used in artificial raspberry flavours. Liq. Bp_1 80°.

U.S. Pat., 1975, 3 899 597; *CA*, **83**, 204964 (*use*)
Christen, P. *et al., Pharm. Acta Helv.*, 1987, **62**, 158-162 (*isol*)
Andersson, P.G. *et al., Tetrahedron*, 1994, **50**, 559-572 (*synth, pmr, cmr, ms*)

4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanone, 9CI, 8CI T-743

[20483-36-7]
7,8-Dihydro-3,4-dehydro-β-ionone. Dehydrodihydroionone. FEMA 3447



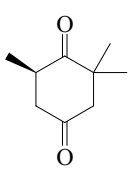
$C_{13}H_{20}O$ 192.3
Flavouring ingredient. Present in cooked raspberries. $Bp_{0.06}$ 90° (bulb).

Winterhalter, P. *et al., J. Agric. Food Chem.*, 1991, **39**, 1825-1829 (*ms*)
Andersson, P.G. *et al., Tetrahedron*, 1994, **50**, 559-572 (*synth, pmr, cmr, ir*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 152 (*props, use*)
Khanina, M.A. *et al., CA*, 2000, **134**, 136427n (*isol*)

2,2,6-Trimethyl-1,4-cyclohexanedione, 9CI T-744

[20547-99-3]

[1125-20-8, 60686-83-1]
Dihydro-4-oxoisophorone



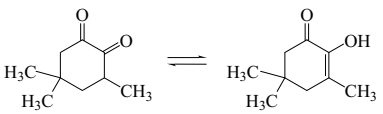
(*R*)-*form*

$C_9H_{14}O_2$ 154.208
(*R*)-*form* [60046-49-3]
Needles (hexane/petrol). Mp 93-94°. $[\alpha]_D$ -270 (c, 0.4 in MeOH).
(ξ)-*form*
Present in saffron and other plants.

Zarghami, N.S. *et al., Phytochemistry*, 1971, **10**, 2755-2761
Leuenberger, H.G.W. *et al., Helv. Chim. Acta*, 1976, **59**, 1832-1849 (*synth, cd, ord, pmr*)
Sode, K. *et al., Appl. Biochem. Biotechnol.*, 1988, **19**, 209-220 (*prodn*)
Lamb, N. *et al., Can. J. Chem.*, 1990, **68**, 1151-1162 (*synth, pmr*)

3,5,5-Trimethyl-1,2-cyclohexanedione, 9CI T-745

[57696-89-6]
2-Hydroxy-3,5,5-trimethyl-2-cyclohexen-1-one, 9CI



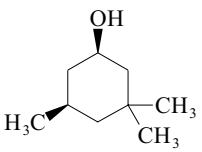
$C_9H_{14}O_2$ 154.208
Flavouring ingredient. Present in alfalfa extract, red clover extract and burley tobacco. Mp 89-91°.

Enol-*form* [4883-60-7]
Ac: [17304-81-3]
$C_{11}H_{16}O_3$ 196.246
Leaflets (petrol). Mp 60-62°.

Tomoeda, M. *et al., Tetrahedron*, 1968, **24**, 959-974 (*synth, Ac, pmr, uv*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1970, **18**, 929-933 (*organoleptic props*)
Srinivas, S.R. *et al., Dev. Food Sci.*, 1988, **18**, 343-353 (*occur*)
Horiuchi, C.A. *et al., Synthesis*, 1989, 785-786 (*synth*)

3,3,5-Trimethylcyclohexanol, 9CI T-746

[116-02-9]
Dihydroisophorol. Homomenthol. Cyclonol. FEMA 3962



(1*R*,5*R*)-*form*

$C_9H_{18}O$ 142.241
The name homomenthol is misleading. Flavouring ingredient. Freq. encountered as a stereoisomeric mixt. obt. by hydrogenation of 3,5,5-Trimethyl-2-cyclohexen-1-ol.
▶ Skin and severe eye irritant. LD_{50} (rat, orl) 3250 mg/kg. GW0875000Never marketed

O-*(2-Hydroxypropanoyl):* [15145-14-9] ***Ciclactate, INN***
$C_{12}H_{22}O_3$ 214.304
Bp_{18} 140°. n_D^{20} 1.4520. Log P 3.39 (calc). Stereochem. not indicated, prob. a mixt..

O-*(2-Hydroxybenzoyl):* [118-56-9] ***Homosalate, INN, USAN***. *Filtrosol A. Heliophan. Lipcote*
$C_{16}H_{22}O_3$ 262.348
Bp_4 161-165°. Stereochem. not indicated.

(1*R*,5*R*)-*form* [54352-39-5]
(-)-cis-*form*
Mp 34-34.5°. Bp_{10} 80°. $[\alpha]_D^{24.5}$ -2.99 (c, 1 in $CHCl_3$).

(1*S*,5*S*)-*form* [54352-41-9]
(+)-cis-*form*
Mp 37.5°. $[\alpha]_D^{24.5}$ +9.43 (c, 1 in $CHCl_3$).

(1*RS*,5*RS*)-*form* [54307-79-8]
(±)-cis-*form*
d_4^{16} 0.9. Mp 12°. Bp_{750} 201-203° Bp_{12} 92°.

Ac: [24691-16-5]
$C_{11}H_{20}O_2$ 184.278
Bp 209-210° approx..

(1*RS*,5*SR*)-*form* [64840-01-3]
[767-54-4] *(±)*-trans-*form*
Needles (petrol). Mp 37° Mp 58.5° (dimorph.).

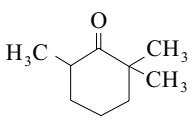
3-Pyridinecarbonyl: [53449-58-4] *3,3,5-Trimethylcyclohexyl nicotinate. Ciclonicate.* ***Ciclonicate, INN***. *Bled. Cortofludan. Elastan. Euronicato. Rolil. Vasargil. Vasocidate*
$C_{15}H_{21}NO_2$ 247.336
$Bp_{0.6}$ 127-128°. Log P 4.36 (calc).
▶ US5942000

[933-48-2, 54110-24-6, 67859-96-5]

U.S. Pat., 1945, 2 369 084; *CA*, **39**, 3886 (*Homosalate*)
Eliel, E.L. *et al., J.O.C.*, 1961, **26**, 3504 (*synth*)
Netherlands Pat., 1967, 6 610 889; *CA*, **67**, 63925j (*Ciclactate*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)
Ger. Pat., 1974, 2 406 849; *CA*, **82**, 4129q (*synth, Ciclonicate*)
Allinger, N.L. *et al., J.O.C.*, 1975, **40**, 1316 (*synth*)
Sekules, G. *et al., Boll. Chim. Farm.*, 1980, **119**, 521 (*hplc, Ciclonicate*)
Faini, D. *et al., Farmaco, Ed. Prat.*, 1981, **36**, 478 (*pharmacol, Ciclonicate*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1309
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1730 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLO500

2,2,6-Trimethylcyclohexanone, 9CI, 8CI T-747

[2408-37-9]



$C_9H_{16}O$ 140.225

(±)-*form* [62861-88-5]
Flavouring ingredient. Fp -31.8. Bp 176.5-178° Bp_{10} 66-67°.

Oxime: [7063-80-1]
$C_9H_{17}NO$ 155.239
Cryst. (EtOH). Mp 106°. Bp_{17} 126-127°.

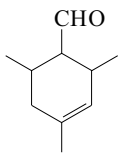
Semicarbazone:
Mp 220-221°.

(ξ)-*form*
Present in bilberries, passion fruit, carob and tea.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 435B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 672B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 520D (*ir*)
Masson, H. *et al., C. R. Hebd. Seances Acad. Sci.*, 1912, **154**, 517 (*isol*)
Stothers, J.B. *et al., Can. J. Chem.*, 1974, **52**, 308 (*cmr*)
Ehrenfreund, J. *et al., Helv. Chim. Acta*, 1974, **57**, 1098 (*synth, ms, ir, pmr*)
Kutney, J.P. *et al., Can. J. Chem.*, 1992, **70**, 2094 (*synth*)
MacLeod, G. *et al., Phytochemistry*, 1992, **31**, 3113 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 770
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2839-2840

2,4,6-Trimethyl-3-cyclohexene-1-carboxaldehyde T-748

[1335-66-6]
2,4,6-Trimethyl-Δ^3-tetrahydrobenzaldehyde. Isocyclocitral



$C_{10}H_{16}O$ 152.236
Listed in the EAFUS Food Additive Database (Jan 2001). Bp_{16} 85-90°. Mixt. of stereoisomers.

Semicarbazone:
Mp 182-183°.

[1423-46-7]

Diels, O. *et al., Annalen*, 1929, **470**, 62 (*synth*)
Dupont, G. *et al., Bull. Soc. Chim. Fr.*, 1939, **6**, 1208 (*synth*)
Nazarov, I.N. *et al., Zh. Obshch. Khim.*, 1958, **28**, 3061; *CA*, **53**, 10069h (*synth*)

2,6,6-Trimethyl-1-cyclohexene-1-carboxaldehyde, 9CI, 8CI T-749

[432-25-7]
β-Cyclocitral

$C_{10}H_{16}O$ 152.236
Constit. of saffron and many other plant materials. Prod. by *Microcystis* spp. A 50:50 mixt. with 2,6,6-Trimethyl-2-cyclohexene-1-carboxaldehyde, T-750 is used as a flavouring ingredient. Bp_{25} 105° Bp_{15} 94-97°.

2,4-Dinitrophenylhydrazone: [14186-18-6]
Mp 172°.

Zarghami, N.S. *et al., Phytochemistry*, 1971, **10**, 2755 (*isol*)
Juettner, F. *et al., Z. Naturforsch., C*, 1976, **31**, 491-495 (*isol*)
Das, P.K. *et al., J. Phys. Chem.*, 1978, **82**, 2081-2093 (*uv*)
Cainelli, G. *et al., J.C.S. Perkin 1*, 1979, 1597-1599 (*synth, ir, pmr*)
Jalali-Naini, M. *et al., Tetrahedron*, 1983, **39**, 749-758 (*synth, ir, pmr*)
Picard, J.-P. *et al., Synth. Commun.*, 1989, **19**, 135-140 (*synth*)
Albeck, A. *et al., J.A.C.S.*, 1992, **114**, 2400-2411 (*cmr*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 771
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2836-2837
Crombie, B.S. *et al., J.C.S. Perkin 1*, 2001, 206-215 (*synth, ir, pmr, ms*)

2,6,6-Trimethyl-2-cyclohexene-1-carboxaldehyde T-750

[432-24-6]

[59462-59-8]
α-Cyclocitral

$C_{10}H_{16}O$ 152.236
A 50:50 mixt. with 2,6,6-Trimethyl-1-cyclohexene-1-carboxaldehyde, T-749 is used as a flavouring ingredient (FEMA 3639).

(*R*)-*form*
Oil. Bp_{10} 75-77°. $[\alpha]_D^{20}$ +618.

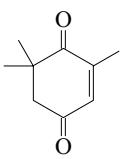
Semicarbazone:
Cryst. Mp 206°.

(*S*)-*form* [14505-74-9]
Bp_{12} 77°. $[\alpha]_D^{25}$ -743 (c, 0.05 in $CHCl_3$) (98% ee).

Buchecker, R. *et al., Helv. Chim. Acta*, 1973, **56**, 2548 (*abs config*)
Mikhailov, B.M. *et al., J. Organomet. Chem.*, 1978, **154**, 131 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 771
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2836-2837
Gan, Y. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 781-787 (*S-form, synth, pmr*)

2,6,6-Trimethyl-2-cyclohexene-1,4-dione T-751

[1125-21-9]
6-Oxoisophorone. Oxopholone. FEMA 3421

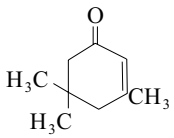


$C_9H_{12}O_2$ 152.193
Present in saffron (*Crocus sativus*) and tea; flavouring ingredient. Cryst. (hexane). Mp 21°. Bp_{20} 99-101° $Bp_{0.2}$ 50-52°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 712A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 542D (*ir*)
Marx, J.N. *et al., Tetrahedron, Suppl. No.* 8, 1966, 1 (*synth*)
Torrance, S.J. *et al., J.O.C.*, 1974, **39**, 1068 (*synth*)
Costantini, M. *et al., J. Mol. Catal.*, 1980, **7**, 89 (*synth*)
Yates, P. *et al., Can. J. Chem.*, 1987, **65**, 69 (*synth, pmr*)
Martin, H.-D. *et al., Chem. Ber.*, 1987, **120**, 1133 (*synth, ir, pe, pmr, cmr*)
Paust, J. *et al., Pure Appl. Chem.*, 1991, **63**, 45 (*rev, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 771
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2841

3,5,5-Trimethyl-2-cyclohexen-1-one, 9CI, 8CI T-752

[78-59-1]
α-Isophorone. FEMA 3553



$C_9H_{14}O$ 138.209
Flavouring ingredient. Present in cranberries (*Vaccinium microcarpa*) and saffron (*Crocus sativus*). Liq. with a sl. minty odour. Insol. H_2O. d_{20}^{20} 0.92. . Bp 214-215° Bp_{10} 89°. n_D^{20} 1.4759. Vp 0.2 mmHg (20°).

▶ Fl. p. 84/96°, autoignition temp. 460/462°. Skin, eye and respiratory tract irritant. Prolonged or repeated exposure can damage eyes and cause olfactory and respiratory changes. LD_{50} (rat, orl) 2330 mg/kg. LD_{50} (rbt, skn) 1500 mg/kg. Exp. nephrotoxic. OES: short-term 5 ppm. GW7700000

2,4-Dinitrophenylhydrazone: [3261-55-0]
Scarlet cryst. Mp 191°.

Semicarbazone: [6293-60-3]
Mp 216°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 448C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 693A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 537D (*ir*)
Wolff, L. *et al., Annalen*, 1902, **322**, 351 (*bibl*)
Surmatis, J.D. *et al., J.O.C.*, 1970, **35**, 1053 (*synth*)
Magnusson, G. *et al., J.O.C.*, 1973, **38**, 1380 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 407
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1478-1479
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 755
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, IMF400

3,5,5-Trimethyl-3-cyclohexen-1-one T-753

[471-01-2]
β-Phorone. β-Isophorone

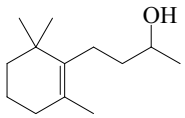
$C_9H_{14}O$ 138.209
Present in oil of saffron and kiwi fruit. Oil. Bp_{10} 70° approx.. Unstable at r.t..

Meinwald, J. *et al., J.O.C.*, 1971, **36**, 1446 (*synth*)
Marx, J.N. *et al., Org. Prep. Proced. Int.*, 1973, **5**, 45 (*synth*)
Bagnell, L. *et al., Aust. J. Chem.*, 1975, **28**, 801 (*synth*)
Meislich, H. *et al., J.O.C.*, 1975, **40**, 2662 (*synth, pmr*)
Birgersson, G. *et al., J. Chem. Educ.*, 1984, **10**, 1029 (*occur*)
Tatsuka, K. *et al., J. Agric. Food Chem.*, 1990, **38**, 2176 (*occur*)

4-(2,6,6-Trimethyl-1-cyclohexenyl)-2-butanol T-754

[3293-47-8]

[160222-97-9]
α,2,6,6-Tetramethyl-1-cyclohexene-1-propanol, 9CI. 7,8-Dihydro-β-ionol. FEMA 3627



$C_{13}H_{24}O$ 196.332
Present in loganberry, Chinese quince oil, yellow passion fruit, Chinese scented green tea. Flavouring ingredient.. Solid with woody-flowery and camphorous odour.

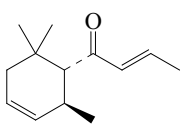
(±)-*form* [98353-28-7]
Bp 234° Bp_{12} 105°.

Schmidt, C. *et al., Synthesis*, 1982, 391-393 (*synth*)
Masuda, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 861-862 (*synth, pmr, ms*)
Yamanishi, T. *et al., Dev. Food Sci.*, 1988, **17**, 181-190 (*occur*)
Takeoka, G.R. *et al., J. Agric. Food Chem.*, 1990, **38**, 471-477 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 166 (*use*)
Werkhoff, P. *et al., J. Agric. Food Chem.*, 1998, **46**, 1076-1093 (*occur*)

1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one, 9CI T-755

[57378-68-4]

[41436-42-4]
δ-Damascone. FEMA 3622



$C_{13}H_{20}O$ 192.3

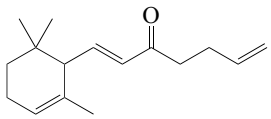
(2*E*,1′*RS*,2′*SR*)-*form* [71048-82-3]
(±)-trans,trans-*form*
Food flavouring and perfumery ingredient. Liq. with intense sweet odour. d_4^{23} 0.92. $Bp_{0.6}$ 65-67°. n_D^{23} 1.4890.

[71048-83-4]

Ayyar, K.S. *et al., J.C.S. Perkin 1*, 1975, 1727-1736 (*synth, ir, uv, pmr, ms*)
Dauben, W.G. *et al., Tet. Lett.*, 1975, 515-517 (*synth*)
Ger. Pat., 1979, 2 840 823; *CA*, **91**, 162898e (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 143 (*props, use*)

1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1,6-heptadien-3-one, 9CI T-756

[79-78-7]
Allyl-α-ionone. Cetone V. Hexalon. Polyone. FEMA 2033



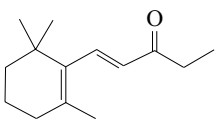
$C_{16}H_{24}O$ 232.365
Flavouring ingredient. Yellow liq., with fruity, woody odour. d_4^{20} 0.93. Bp 265° $Bp_{0.15}$ 102-104°. n_D^{20} 1.5040.

[95470-33-0]

Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1956, 1713 (*synth*)
U.S. Pat., 1984, 4 481 372; *CA*, **102**, 132303k (*synth*)
U.S. Pat., 1990, 4 933 320; *CA*, **113**, 197692h (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 26
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 91-92

1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one, 9CI T-757

[127-43-5]
1-Methyl-β-ionone. β-Methylionone. FEMA 2712



$C_{14}H_{22}O$ 206.327
Flavouring ingredient. d^{25} 0.93. Bp 242° $Bp_{2.7}$ 102-103°. n_D^{25} 1.5140.

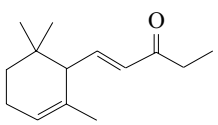
[1322-70-9]

Köster, H. *et al., Chem. Ber.*, 1947, **80**, 248 (*synth*)
Lusskin, R.M. *et al., J.A.C.S.*, 1949, **71**, 2412 (*uv*)
Beets, M.G.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1950, **69**, 236 (*struct, uv*)
Naves, Y.R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1954, **238**, 308 (*ir*)
Lemcote, J. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1956, **53**, 462; *CA*, **50**, 11824h (*ir*)
Ger. Pat., 1978, 2 820 928; *CA*, **90**, 187178h (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 726
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1784-1785

1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one T-758

[127-42-4]

[1322-70-9]
1-Methyl-α-ionone. n-*Methyl-α-ionone. FEMA 2711*

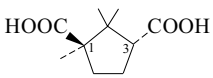


$C_{14}H_{22}O$ 206.327
Flavouring ingredient. d^{25} 0.92. Bp 238° $Bp_{2.6}$ 97°. n_D^{25} 1.4938.

Semicarbazone:
Mp 161°.

Lusskin, R.M. *et al., J.A.C.S.*, 1949, **71**, 2412 (*uv*)
Beets, M.G.J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1950, **69**, 236 (*props, struct, uv*)
Naves, Y.R. *et al., Bull. Soc. Chim. Fr.*, 1951, 639 (*synth*)
Ernest, T. *et al., Am. Perfum. Cosmet.*, 1963, **78**, 27; *CA*, **59**, 12300d (*ir*)
Orishi, T. *et al., Chem. Comm.*, 1978, 651 (*synth*)
Ger. Pat., 1978, 2 820 928; *CA*, **90**, 187178h (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 515
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1783-1784

1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid, 9CI T-759



(1*R*,3*R*)-*form*

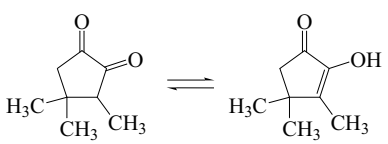
$C_{10}H_{16}O_4$ 200.234
(1*RS*,3*SR*)-*form* [5394-83-2]
(±)-Camphoric acid
Constit. of red tea. Prisms (EtOH aq.). Sol. cold H_2O (1%), hot H_2O (10%), EtOH, Et_2O; spar. sol. $CHCl_3$. Mp 202-203°. pK_{a2} 6.14 (100°). Liq. cryst. polyesters containing acid fragments have been synth..
► EX1319000

[560-05-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 540D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 842A (*nmr*)
Goebel, W.F. *et al., J.A.C.S.*, 1923, **45**, 3064 (*synth*)
Baker, K.M. *et al., Tetrahedron*, 1968, **24**, 1663 (*pmr*)
Brienne, M.-J. *et al., Tetrahedron*, 1970, **26**, 5087 (*abs config*)
Filippo, J.S. *et al., J.O.C.*, 1976, **41**, 1077 (*synth*)
Holzbecher, J. *et al., Organic Reagents in Inorganic Analysis*, Horwood, Chichester, 1976, (*use*)
Barnes, J.C. *et al., Acta Cryst. C*, 1991, **47**, 1888 (*cryst struct*)
Zhao, H. *et al., CA*, 1993, **118**, 167989w (*isol*)
Nie, J.-J. *et al., Acta Cryst. C*, 2000, **58**, o106-o107 (*synth, cryst struct*)
Acta Cryst. C, 2000, **58**, o106-o107 (*synth, cryst struct*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 466

3,4,4-Trimethyl-1,2-cyclopentanedione T-760

[86702-81-0]
2-Hydroxy-3,4,4-trimethyl-2-cyclopenten-1-one



$C_8H_{12}O_2$ 140.182
Aroma constit. of roasted Arabica coffee beans with sweet, burnt odour. Characterised spectroscopically.

Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*occur, ms, synth*)

3,5,5-Trimethyl-1,2-cyclopentanedione T-761

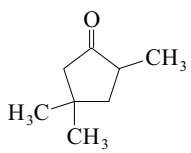
[53263-56-2]
2-Hydroxy-3,5,5-trimethyl-2-cyclopenten-1-one, 9CI

$C_8H_{12}O_2$ 140.182
Enol-form predominates. Aroma constit. of roasted Arabica coffee beans. Cryst. with sweet caramel-like odour. Mp 87-88°.

Gianturco, M.A. *et al., Tetrahedron*, 1963, **19**, 2039-2049 (*synth, ir*)
Naoshima, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1393-1397 (*synth*)
Nishimura, O. *et al., J. Agric. Food Chem.*, 1990, **38**, 1038-1041 (*occur, ms, coffee*)

2,4,4-Trimethylcyclopentanone, 9CI, 8CI T-762

[4694-12-6]

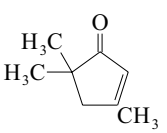


$C_8H_{14}O$ 126.198
Isol. from oil of *Mentha pulegium* (European pennyroyal).
(±)-*form*
Bp 160-161° Bp_{21} 61-62°.
2,4-Dinitrophenylhydrazone:
Mp 160.5°.
Semicarbazone:
Cryst. (EtOH). Mp 171-173°.

Naves, Y.R. *et al., Helv. Chim. Acta*, 1944, **27**, 51 (*isol*)
Org. Synth., Coll. Vol., 4, 1963, 957 (*synth*)
Stothers, J.B. *et al., Can. J. Chem.*, 1974, **52**, 308 (*cmr*)

3,5,5-Trimethyl-2-cyclopenten-1-one, 9CI T-763

[24156-95-4]



$C_8H_{12}O$ 124.182
Top note of *Osmanthus fragrans* (sweet osmanthus). Liq. Bp_{40} 98-100° $Bp_{9.5}$ 47-48°. n_D^{20} 1.4670.
Oxime:
$C_8H_{13}NO$ 139.197
Solid. Mp 99°.
Semicarbazone:
Leaflets. Mp 201°.
2,4-Dinitrophenylhydrazone: [59534-50-8]

Orange needles (EtOAc/EtOH). Mp 227.5-228.5°.

Conia, J.M. *et al., Bull. Soc. Chim. Fr.*, 1959, 493 (*synth, uv*)
Burke, P.M. *et al., Can. J. Chem.*, 1976, **54**, 1449 (*synth, pmr, ir, uv, gc*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1976, **59**, 439 (*synth, pmr, ir*)
Denis, J.M. *et al., Tetrahedron*, 1977, **33**, 399 (*synth, pmr, ir, gc*)
Hayashi, Y. *et al., Tetrahedron*, 1977, **33**, 2513 (*synth, pmr, ir, uv*)
Yates, P. *et al., Can. J. Chem.*, 1987, **65**, 1695 (*synth, pmr, gc*)
Weyerstahl, P. *et al., Annalen*, 1996, 799 (*synth, pmr, cmr*)

2,2,4-Trimethyldecane T-764

[62237-98-3]

$H_3C(CH_2)_5CH(CH_3)CH_2C(CH_3)_3$

$C_{13}H_{28}$ 184.364

Constit. of the essential oil of hops (*Humulus lupulus*).

Chen, J. *et al., CA*, 1993, **118**, 165188k (*isol*)

2,2,8-Trimethyldecane T-765

[62238-01-1]

$H_3CCH_2CH(CH_3)(CH_2)_5C(CH_3)_3$

$C_{13}H_{28}$ 184.364

Constit. of the flowers of *Prunus armeniaca* (apricot) and *Prunus salicina* (Japanese plum).

Gomez, E. *et al., J. Agric. Food Chem.*, 1993, **41**, 1669 (*isol*)

2,2,9-Trimethyldecane T-766

[62238-00-0]

$(H_3C)_2CH(CH_2)_6C(CH_3)_3$

$C_{13}H_{28}$ 184.364

Constit. of the fruit of *Prunus domestica* (plum).

Etievant, P.X. *et al., Sci. Aliments*, 1986, **6**, 417 (*isol*)

2,3,4-Trimethyldecane T-767

[62238-15-7]

$H_3C(CH_2)_5CH(CH_3)CH(CH_3)CH(CH_3)_2$

$C_{13}H_{28}$ 184.364

Constit. of the volatile oil of ginseng.

Zhang, H. *et al., CA*, 1987, **107**, 183403d (*isol*)

2,6,7-Trimethyldecane T-768

[62108-25-2]

$H_3CCH_2CH_2CH(CH_3)CH(CH_3)(CH_2)_3CH(CH_3)_2$

$C_{13}H_{28}$ 184.364

Constit. of *Medicago sativa* (alfalfa).

Zeringue, H.J. *et al., Appl. Environ. Microbiol.*, 1994, **60**, 3543 (*isol*)
Core, R.J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2932 (*isol*)

2,6,8-Trimethyldecane T-769

[62108-26-3]

$H_3CCH_2CH(CH_3)CH_2CH(CH_3)(CH_2)_3CH(CH_3)_2$

$C_{13}H_{28}$ 184.364

Constit. of the flowers of *Osmanthus fragrans* (sweet osmanthus).

Zhang, X. *et al., CA*, 1987, **106**, 47203r (*isol*)
Chen, Y. *et al., Chromatographia*, 1987, **23**, 502 (*isol*)

3,3,4-Trimethyldecane T-770

[49622-18-6]

$H_3C(CH_2)_5CH(CH_3)C(CH_3)_2CH_2CH_3$

$C_{13}H_{28}$ 184.364

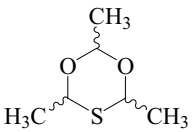
Constit. of the fruit of *Prunus domestica* (plum).

Etievant, P.X. *et al., Sci. Aliments*, 1986, **6**, 417 (*isol*)

2,4,6-Trimethyl-1,3,5-dioxathiane, 9CI T-771

[53897-55-5]

Monothiotriacetaldehyde



$C_6H_{12}O_2S$ 148.226

Component of an onion-like flavouring. Cryst. with dusty, earthy, nutty odour. Mp 53.5-54°. Bp >160° dec..

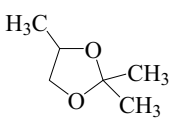
S,S-*Dioxide:* [54061-47-1]
$C_6H_{12}O_4S$ 180.224
Mp 150-152°.

Lebedev, S.V. *et al., Ber.*, 1926, **59**, 762-767 (*dioxide*)
Arbuzov, B.A. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1974, 2346-2348; *CA*, **82**, 57430n (*dioxide, pmr, conformn*)
Boelens, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071-1076 (*isol, ms, pmr*)

2,2,4-Trimethyl-1,3-dioxolane, 9CI, 8CI T-772

[1193-11-9]

1,2-Propanediol acetonide. Propylene glycol acetonide. 1,2-Isopropylidenepropanediol. Acetone propylene glycol acetal. FEMA 3441



$C_6H_{12}O_2$ 116.16

(±)-*form* [99676-60-5]

Detected in commercial beef flavours, believed to be formed from 1,2-propanediol additive. Present in tomato aroma. Flavouring ingredient. Liq. $d_4^{18.5}$ 0.91. Bp 98-100°. n_D^{25} 1.3921. $n_D^{18.5}$ 1.4019. Enantiomers known but characterised only by glc.

[116944-24-2, 116944-25-3]

Boeseken, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1923, **42**, 1104-1110 (*synth*)
Barker, S.A. *et al., J.C.S.*, 1959, 807-813 (*synth, ir, Raman*)
Rondestvedt, C.S. *et al., J.O.C.*, 1961, **26**, 2247-2253 (*synth*)
Anteunis, M. *et al., Bull. Soc. Chim. Belg.*, 1964, **73**, 889-897 (*synth, pmr*)
Schormueller, J. *et al., Z. Lebensm.-Unters. -Forsch.*, 1969, **141**, 1-9 (*occur*)
Eliel, E.L. *et al., Org. Magn. Reson.*, 1979, **12**, 461-466 (*cmr*)
MacLeod, G. *et al., J. Agric. Food Chem.*, 1980, **28**, 441-446 (*occur*)
Schurig, V. *et al., J. Chromatogr.*, 1988, **441**, 135-153 (*(+)-form, (-)-form*)
Lee, S.B. *et al., Chem. Lett.*, 1990, 2019-2022 (*synth*)
Cabrera, A. *et al., J. Mol. Catal.*, 1992, **75**, 101-107 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 774 (*props, use*)
Tateo, F. *et al., J. High Resol. Chromatogr.*, 1998, **21**, 658-660 (*glc, occur*)

2,4,5-Trimethyl-1,3-dioxolane T-773

[3299-32-9]

$C_6H_{12}O_2$ 116.16

Flavour constit. of various wines. Also found in carob (*Ceratonia siliqua*).

(4*R*,5*R*)-*form* [122045-47-0]
Bp 107°.

(4*RS*,5*RS*)-*form* [17226-26-5]
(±)-trans-*form*
Bp 103.2°.

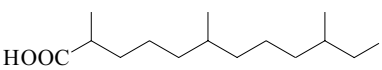
[17226-25-4, 17226-26-5, 29923-83-9, 122045-48-1]

Salomaa, P. *et al., Acta Chem. Scand.*, 1962, **16**, 1532 (*synth*)
Senda, Y. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 2813 (*cmr*)
Burczyk, B. *et al., J. Prakt. Chem.*, 1980, **322**, 173 (*synth*)
Richter, W.J. *et al., J.O.C.*, 1981, **46**, 5119 (*synth*)
Normant, J.F. *et al., Tetrahedron*, 1989, **45**, 507 (*synth, pmr, cmr*)

2,6,10-Trimethyldodecanoic acid T-774

[168254-98-6]

12-Farnesanoic acid. Mangfarnasoic acid



$C_{15}H_{30}O_2$ 242.401

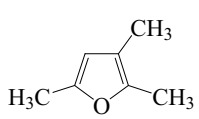
Constit. of the stem bark of *Mangifera indica* (mango).

[177472-22-9, 177472-23-0]

Sharma, S.K. *et al., J. Indian Chem. Soc.*, 1995, **72**, 339-342 (*isol*)
Ferreira, J.T.B. *et al., Bioorg. Med. Chem.*, 1996, **4**, 381-388 (*synth*)

2,3,5-Trimethylfuran T-775

[10504-04-8]



$C_7H_{10}O$ 110.155

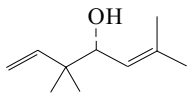
Organoleptic compd. occurring in coffee aroma. Liq. Bp 120-121° Bp_{62} 51.5°.

Reichstein, T.H. *et al., Helv. Chim. Acta*, 1932, **15**, 1115 (*synth*)

Heyns, K.R. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)
Noichi, Y. *et al., Nippon Kagaku Zasshi*, 1967, **88**, 1196 (*synth*)

3,3,6-Trimethyl-1,5-heptadien-4-ol T-776

Artemisia alcohol



(*R*)-*form*

$C_{10}H_{18}O$ 154.252

(*R*)-*form* [77363-66-7]
Oil. $[\alpha]_D^{23}$ +32.1 (neat).

(*S*)-*form* [29887-38-5]
Oil. Bp_9 92-95°. $[\alpha]_D^{23}$ -32.12 (neat).

Ac: [3465-88-1] *Artemisia alcohol acetate*
$C_{12}H_{20}O_2$ 196.289
From *Artemisia* spp.. Oil. Bp_6 74-76°. $[\alpha]_D^{21}$ -33.9.

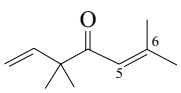
(ξ)-*form*

Propanoyl: [79507-84-9] ***Artemisyl propionate***
$C_{13}H_{22}O_2$ 210.316
Constit. of *Artemisia vulgaris* (mugwort).

Epstein, W.W. *et al., Phytochemistry*, 1973, **12**, 737 (*isol*)
Ruppert, J.F. *et al., J.O.C.*, 1976, **41**, 550 (*synth*)
Grandi, R. *et al., Phytochemistry*, 1976, **15**, 1770 (*isol*)
Poulter, C.D. *et al., J.A.C.S.*, 1977, **99**, 3816 (*synth*)
Segal, R. *et al., Phytochemistry*, 1980, **19**, 2761 (*isol, bibl*)
Näf-Müller, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1424 (*propionate, isol*)
Brown, H.C. *et al., Tet. Lett.*, 1986, **25**, 1215 (*synth*)

3,3,6-Trimethyl-1,5-heptadien-4-one T-777

[546-49-6]
Artemisia ketone

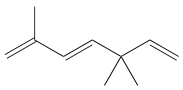


$C_{10}H_{16}O$ 152.236

5,6-Epoxide: [79507-83-8] *5,6-Epoxy-3,3,6-trimethyl-1-hepten-4-one. 1-(3,3-Dimethyloxiranyl)-2,2-dimethyl-3-buten-1-one, 9CI.* ***Epoxyartemisia ketone***
$C_{10}H_{16}O_2$ 168.235
Constit. of *Artemisia vulgaris* (mugwort). Oil. Bp_{10} 75°.

Zalkow, L.H. *et al., J.O.C.*, 1964, **29**, 2786 (*isol, struct*)
Pillot, J.-P. *et al., Tet. Lett.*, 1976, 1871 (*synth*)
Banthorpe, D.V. *et al., Phytochemistry*, 1977, **16**, 1387 (*biosynth*)
Michelot, D. *et al., Synth. Commun.*, 1977, **7**, 95 (*synth*)
Risinger, G.E. *et al., Experientia*, 1978, **34**, 1121 (*synth*)
Gosselin, P. *et al., Tet. Lett.*, 1978, 2717 (*synth*)
Näf-Müller, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1424 (*epoxide*)
Fehr, C. *et al., Helv. Chim. Acta*, 1987, **70**, 1745 (*synth*)

2,5,5-Trimethyl-1,3,6-heptatriene T-778



$C_{10}H_{16}$ 136.236

(*E*)-*form* [18383-70-5]
Artemisiatriene
Constit. of *Artemisia vulgaris* (mugwort).

[29548-02-5]

Thomas, A.F. *et al., Helv. Chim. Acta*, 1971, **54**, 1822-1845 (*synth*)
Näf-Müller, R. *et al., Helv. Chim. Acta*, 1981, **64**, 1424-1430 (*isol, pmr*)

3,5,5-Trimethylhexanal, 9CI, 8CI T-779

[5435-64-3]
FEMA 3524
$(H_3C)_3CCH_2CH(CH_3)CH_2CHO$
$C_9H_{18}O$ 142.241
► MN7820000

(±)-*form*
Flavouring ingredient. Liq. with camphoraceous odour. d_4^{25} 0.82. Bp 170-171° $Bp_{2.5}$ 67-68°. n_D^{23} 1.4205.

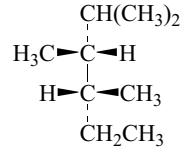
2,4-Dinitrophenylhydrazone:
Mp 94-95°.

Semicarbazone:
Cryst. (MeOH). Mp 115°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 731A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 554C (*ir*)
Bruner, W.M. *et al., Ind. Eng. Chem.*, 1949, **21**, 2860; *CA*, **44**, 2912d (*synth*)
Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1951, 658 (*synth, deriv*)
Bacon, R.G.R. *et al., J.C.S.(C)*, 1966, 1384 (*synth*)
Bergwein, K. *et al., Seifen, Oele, Fette, Wachse*, 1969, **42**, 812; *CA*, **74**, 6015s (*rev*)
Ger. Pat., 1979, 2 804 167; *CA*, **91**, 192845c (*use*)
Opdyke, D.L.J. *et al., Food Chem. Toxicol.*, 1982, **20**, 841 (*rev, tox*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 773
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2843

2,3,4-Trimethylhexane T-780

[921-47-1]



(3*RS*,4*RS*)-*form*

C_9H_{20} 128.257
Isol. from the flowers of *Helianthus annuus* (sunflower).

(3*RS*,4*RS*)-*form* [52896-83-0]
(±)-threo-*form*
Bp 139°.

(3*RS*,4*SR*)-*form* [52896-75-0]
(±)-erythro-*form*
Bp 140°.

[24418-02-8, 24418-03-9]

Levina, R.Y. *et al., CA*, 1952, **46**, 7985c (*synth*)
Pecque, M. *et al., Bull. Soc. Chim. Fr.*, 1969, 1333 (*synth*)
Crowder, G.A. *et al., J. Mol. Struct.*, 1984, **118**, 135 (*ir*)
Pham-Delegue, M.H. *et al., J. Chem. Ecol.*, 1989, **15**, 329 (*isol*)
Yaws, C.L. *et al., Hydrocarbon Process. Int. Ed.*, 1990, **69**, 87

3,5,5-Trimethyl-1-hexanol, 9CI, 8CI T-781

[3452-97-9]
Inonanol. FEMA 3324
$(H_3C)_3CCH_2CH(CH_3)CH_2CH_2OH$
$C_9H_{20}O$ 144.256

(±)-*form*
Flavouring ingredient. Liq. with a strong oily-herbaceous odour. Sol. EtOH, Me_2CO, Et_2O. d^{20} 0.83. Bp 193-194° Bp_{150} 142°. n_D^{20} 1.4352.
► Fl. p. 93° (oc).

Ac: [58430-94-7] *3,5,5-Trimethylhexyl acetate. Inonyl acetate. Isononyl acetate*
$C_{11}H_{22}O_2$ 186.294
Liq. with woody/fruity odour. Bp 209°.
► LD_{50} (rat, orl) 4250 mg/kg. AK0840000

2-Propenoyl: [2664-55-3]
$C_{12}H_{22}O_2$ 198.305
Mp -34°. $Bp_{0.4}$ 55°. n_D^{20} 1.4370.

3,5-Dinitrobenzoyl:
Mp 62°.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 174B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 165A (*ir*)
U.S. Pat., 1950, 2 517 350; *CA*, **44**, 11173 (*synth*)
Bell, H.M. *et al., Org. Magn. Reson.*, 1975, **7**, 240 (*pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 773
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2844
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLT500

2,2,5-Trimethyl-4-hexenal, 9CI T-782

[1000-30-2]
$(H_3C)_2C{=}CHCH_2C(CH_3)_2CHO$
$C_9H_{16}O$ 140.225
Liq. Bp_{71} 89-92°.

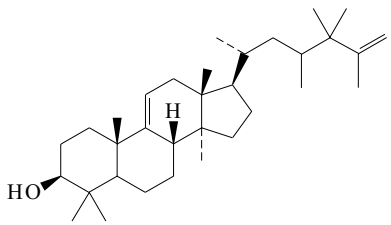
2,4-Dinitrophenylhydrazone:
Mp 125°.

Di-Me acetal: [67674-46-8] *6,6-Dimethoxy-2,5,5-trimethyl-2-hexene, 9CI. Methyl pamplemousse*
$C_{11}H_{22}O_2$ 186.294
Fragrance ingredient with a grapefruit-like aroma.

Cresson, P. *et al., Bull. Soc. Chim. Fr.*, 1964, 2618-2628 (*synth*)
Dillenberger, Z. *et al., Helv. Chim. Acta*, 1978, **61**, 1856-1902 (*synth, ir, pmr*)
Ger. Pat., 1985, 3 341 605; *CA*, **104**, 19341z (*di-Me acetal*)

Mayr, H. *et al., Chem. Ber.*, 1991, **124**, 203-206 (*synth*)

23,24,24-Trimethyllanosta-9(11),25-dien-3-ol T-783



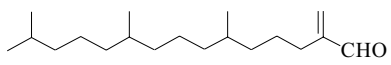
$C_{33}H_{56}O$ 468.805

3β-*form* [62462-35-5]
Lansiol
Constit. of *Clausena lansium* (wampee). Cryst. ($CHCl_3$/MeOH). Mp 197-198°. $[\alpha]_D^{25}$ +83 (c, 1 in $CHCl_3$).

Lakshmi, V. *et al., Phytochemistry*, 1989, **28**, 943

6,10,14-Trimethyl-2-methylenepentadecanal T-784

[83725-57-9]

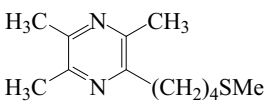


$C_{19}H_{36}O$ 280.493
Constit. of *Tetragonia tetragonoides* (New Zealand spinach). Oil.

Aoki, T. *et al., Phytochemistry*, 1982, **21**, 1361

2,3,5-Trimethyl-6-[4-(methylthio)butyl]pyrazine, 9CI T-785

[92233-83-5]

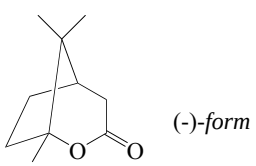


$C_{12}H_{20}N_2S$ 224.369
Strecker degradation product formed from 2,3-butanedione and methionine. Characterised spectroscopically.

Hartman, G.J. *et al., Lebensm.-Wiss. Technol.*, 1984, **17**, 171-174 (*occur, ms*)

1,8,8-Trimethyl-2-oxabicyclo[3.2.1]octan-3-one, 9CI T-786

[1126-91-6]
1,2-Campholide



(-)-*form*

$C_{10}H_{16}O_2$ 168.235

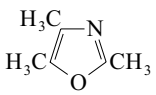
(-)-*form* [28973-92-4]
Cryst. (petrol). Mp 172-174°. $[\alpha]_D^{25}$ -43 (c, 3.0 in EtOH).

(ξ)-*form*
Intermed. metab. of camphor in mature sage.

Sauers, R.R. *et al., J.A.C.S.*, 1959, **81**, 925 (*synth*)
Hirata, T. *et al., Bull. Chem. Soc. Jpn.*, 1970, **43**, 2588 (*synth, abs config, pmr*)
Suga, T. *et al., J.C.S. Perkin 1*, 1972, 258 (*synth*)
Croteau, R. *et al., Arch. Biochem. Biophys.*, 1984, **228**, 667 (*synth, metab, ms*)
Deslongchamps, P. *et al., Can. J. Chem.*, 1990, **68**, 153 (*synth, ir, pmr*)
Ye, S. *et al., Tetrahedron*, 1991, **47**, 5463 (*synth, pmr*)

Trimethyloxazole, 9CI T-787

[20662-84-4]



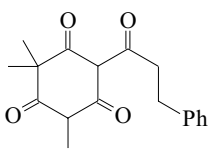
C_6H_9NO 111.143
Constit. of roast peanuts, French fries and roast beef volatiles. Oil. d_{25}^{25} 0.96. Bp 132-133°. n_D^{25} 1.4413.

Picrate:
Large cryst. (EtOH aq.). Mp 110.5-112.5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 638A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 101C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1489D (*ir*)
Wiley, R.H. *et al., J.O.C.*, 1947, **12**, 43 (*synth*)
Brown, D.J. *et al., J.C.S.(B)*, 1969, 270 (*pmr*)
Hartman, G.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1030-1033 (*occur, beef*)
Cunico, R.F. *et al., J.O.C.*, 1992, **57**, 3331 (*synth, pmr*)

2,2,4-Trimethyl-6-(1-oxo-3-phenylpropyl)-1,3,5-cyclohexanetrione, 9CI T-788

[34328-57-9]
Myrigalone A

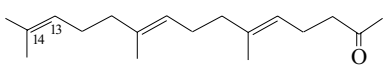


$C_{18}H_{20}O_4$ 300.354
Dihydrochalcone blocked by biomethylation. Several tautomers possible. Isol. from *Myrica gale* (bog myrtle). Pale yellow cubes (Et_2O/cyclohexane). Mp 138-139°.

Uyar, T. *et al., Phytochemistry*, 1978, **17**, 2011 (*isol*)
Misirlioglu, H. *et al., Phytochemistry*, 1978, **17**, 2015 (*synth*)

6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one, 9CI T-789

[762-29-8]



$C_{18}H_{30}O$ 262.434

(5*E*,9*E*)-*form* [1117-52-8]
Farnesylacetone
Present in tomatoes. n_D^{20} 1.4816. Other stereoisomers also prepd..

Semicarbazone:
Mp 81-82°.

13R,14-Epoxide: [66067-35-4] *12-(3,3-Dimethyloxiranyl)-5,9-dodecadien-2-one, 9CI.* ***Farnesylacetone epoxide***
$C_{18}H_{30}O_2$ 278.434
Oil. $[\alpha]_D$ -3.2 (c, 1 in $CHCl_3$).
▶JR1782000

Isler, O. *et al., Helv. Chim. Acta*, 1958, **41**, 786 (*synth*)
Laats, K. *et al., CA*, 1969, **70**, 106666g; 1975, **83**, 97600v (*synth*)
Kazlauskas, R. *et al., Experientia*, 1978, **34**, 156 (*epoxide*)
Ferezou, J.-P. *et al., Helv. Chim. Acta*, 1978, **61**, 669 (*biosynth*)
Enzell, C.R. *et al., Mass Spectrom. Rev.*, 1986, **5**, 39 (*ms*)

2,3,4-Trimethyl-3-pentanol, 9CI, 8CI T-790

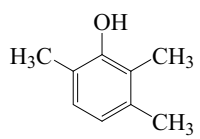
[3054-92-0]
Diisopropylmethylcarbinol. FEMA 3903
$[(H_3C)_2CH]_2C(OH)CH_3$
$C_8H_{18}O$ 130.23
Flavouring agent for foods. Present in muscadine grapes, wines and chinese jujube fruit (*Zizyphus jujuba*). Liq. d_4^{20} 0.85. Bp 156-157° Bp_{125} 101°. n_D^{20} 1.4353.

Stas, J. *et al., Bull. Soc. Chim. Belg.*, 1926, **35**, 379-386 (*synth*)
Whitmore, F.C. *et al., J.A.C.S.*, 1942, **64**, 1239-1242 (*synth*)
Lamikara, O. *et al., J. Food Qual.*, 1987, **10**, 57-66 (*occur*)
Wang, H. *et al., CA*, 1988, **109**, 226695m (*isol*)
Fukuzawa, S. *et al., Chem. Lett.*, 1994, 1981-1984 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1739 (*use*)

2,3,6-Trimethylphenol, 9CI, 8CI T-791

[2416-94-6]

[26998-80-1]
FEMA 3963



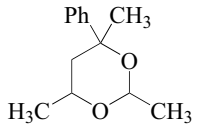
$C_9H_{12}O$ 136.193
Flavouring ingredient. Cryst. (heptane). Mp 63.5-64°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 280B (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1092C (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1029B (*ir*)
Wehrli, P.A. *et al., J.O.C.*, 1972, **37**, 2340 (*synth*)

2,4,6-Trimethyl-4-phenyl-1,3-dioxane, 9CI T-792

[5182-36-5]
Floralate. Vertacetal



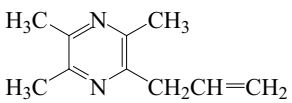
$C_{13}H_{18}O_2$ 206.284
Mixt. of stereoisomers. Fragrance ingredient with a grapefruit-like aroma. $Bp_{0.2}$ 69°.

[78779-38-1, 78779-39-2, 249740-88-3, 249741-12-6]

El Gharbi, R. *et al., Tetrahedron*, 1983, **39**, 2953-2963 (*synth, pmr, cmr*)
Ger. Pat., 1999, 19 822 232; *CA*, **131**, 341795k (*stereoisomers*)

Trimethyl-2-propenylpyrazine, 9CI T-793

[55138-71-1]
2-Allyl-3,5,6-trimethylpyrazine

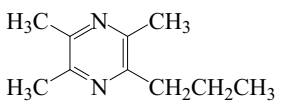


$C_{10}H_{14}N_2$ 162.234
Constit. of roasted green tea aroma.

Tas, A.C. *et al., Riechst., Aromen, Koerperpflegem.*, 1974, **24**, 326; 328; 331-332; *CA*, **82**, 57645m (*synth, ms, ir, pmr*)
Kawakami, M. *et al., CA*, 1999, **132**, 63467x (*occur, tea*)

Trimethylpropylpyrazine T-794

[92233-82-4]

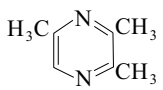


$C_{10}H_{16}N_2$ 164.25
Maillard product. Constit. of cocoa volatiles.

Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur, cocoa*)
Ames, J.M. *et al., J. Agric. Food Chem.*, 2001, **49**, 4315-4323 (*occur*)

Trimethylpyrazine, 9CI T-795

[14667-55-1]
FEMA 3244



$C_7H_{10}N_2$ 122.169
Found in many foodstuffs e.g. asparagus, baked potato, wheat bread, Swiss cheese, coffee, black tea, roasted filbert and peanut, soybean etc. Flavouring ingredient. Liq. with roast coffee odour. Bp_{735} 171-172°. pK_{a1} 2.65; pK_{a2} -3.6 (25°, H_2O). Steam-volatile. Odour threshold 9000ppb in H_2O.
► LD_{50} (rat, orl) 806 mg/kg. UQ3907000
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 401A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 841B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1558B (*ir*)
Das, B.K. *et al., J. Indian Chem. Soc.*, 1968, **45**, 1075 (*uv*)
Bus, J. *et al., Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1973, **92**, 123 (*ir*)
Calabretta, P.J. *et al., Cosmet. Perfum.*, 1975, **90**, 74 (*synth*)
Gumbley, S.J. *et al., J. Het. Chem.*, 1985, **22**, 1143 (*props*)
von Stralendorff, F. *et al., J. Chem. Ecol.*, 1987, **13**, 655
Boyer, M.L. *et al., J. Chem. Ecol.*, 1989, **15**, 649
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TME270

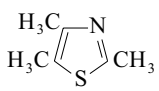
3,6,10-Trimethyltetradecane T-796

[146367-86-4]
$H_3C(CH_2)_3CH(CH_3)(CH_2)_3CH(CH_3)CH_2CH_2CH(CH_3)CH_2CH_3$
$C_{17}H_{36}$ 240.471
Constit. of the oil of *Humulus lupulus* (hops).

Chen, J. *et al., CA*, 1993, **118**, 165188k (*isol*)

Trimethylthiazole T-797

[13623-11-5]
FEMA 3325



C_6H_9NS 127.21
Present in coffee, cooked meats and cooked potatoes. Flavouring ingredient. Bp 167° Bp_{24} 71°. pK_a 4.55 (25°).

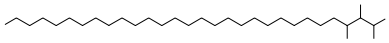
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 110C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1493B (*ir*)
Roussel, C. *et al., Bull. Soc. Chim. Fr.*, 1971, 1087
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 776
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2848-2849

2,3,4-Trimethyltriacontane T-798

[87538-96-3]
$H_3C(CH_2)_{25}CH(CH_3)CH(CH_3)CH(CH_3)_2$
$C_{33}H_{68}$ 464.9
Constit. of the leaves of *Solanum torvum* (pea eggplant). Mp 58°.

Mahmood, U. *et al., Phytochemistry*, 1983, **22**, 167 (*isol, ir, pmr, ms*)

2,3,4-Trimethyltriacontane T-799

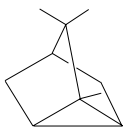


$C_{33}H_{68}$ 464.9
Constit. of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Cryst. (hexane). Mp 58°.

Mahmood, U. *et al., Phytochemistry*, 1983, **22**, 167

1,7,7-Trimethyltricyclo[2.2.1.0^{2,6}]heptane, 9CI T-800

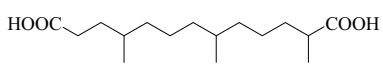
[508-32-7]
Tricyclene. Cyclene



$C_{10}H_{16}$ 136.236
Found in essential oils, e.g. *Juniperus communis* (Juniper), *Ferula galbaniflua* (galbanum) and *Picea* spp.. Cryst. (EtOH). Mp 67-68°. Bp 152-153°. Content in *Pinus* turpentine stated to be 0.2-0.8%.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 56C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 57D (*ir*)
Lipp, P. *et al., Ber.*, 1920, **53**, 779 (*synth*)
Komppa, G. *et al., Ber.*, 1929, **62**, 1366 (*synth*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1964, **47**, 475 (*ms*)
Bardyshev, I.I. *et al., Khim. Prir. Soedin.*, 1968, **4**, 191; *Chem. Nat. Compd. (Engl. Transl.)*, 1968, **4**, 165 (*occur, ir*)

2,6,10-Trimethyltridecane-dioic acid T-801

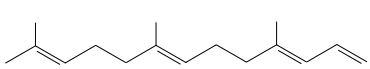


$C_{16}H_{30}O_4$ 286.411

1-(6-Heptenyl) ester: [255833-57-9] ***Lepidiumterpenyl ester***
$C_{23}H_{42}O_4$ 382.582
Constit. of *Lepidium sativum* (garden cress). Cryst. Mp 100-101°. λ_{max} 205 (log ε 1.6) (MeOH).

Pande, S.D. *et al., Pharmazie*, 1999, **54**, 851-853 (*isol, pmr, cmr*)

4,8,12-Trimethyl-1,3,7,11-tridecatetraene T-802



$C_{16}H_{26}$ 218.381
(3E,7E)-form [62235-06-7]
Constit. of essential oil of *Elettaria cardamomum* (cardamom). Oil.

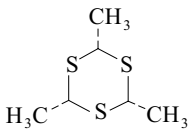
[107554-13-2, 107554-14-3, 107554-15-4]

Maurer, B. *et al., Tet. Lett.*, 1986, **27**, 2111

Boland, W. *et al., Helv. Chim. Acta*, 1989, **72**, 247 (*biosynth, bibl*)

2,4,6-Trimethyl-1,3,5-trithiane T-803

[2765-04-0]
Trithioacetaldehyde. Thioacetaldehyde trimer



(2α,4α,6α)-*form*

$C_6H_{12}S_3$ 180.359
Modifier for blackcurrant flavour.

(2α,4α,6α)-*form* [23769-39-3]
α-form
Monoclinic plates. Mp 101°.

(2α,4α,6β)-*form* [23769-40-6]
β-form
Needles (Me_2CO). Mp 126°.

S^1-*Oxide:* [39058-34-9]
$C_6H_{12}OS_3$ 196.358
Prisms (EtOH aq.).

[6342-28-5]

Fromm, E. *et al., Ber.*, 1925, **58**, 1916 (*synth*)
Hassel, O. *et al., Acta Chem. Scand.*, 1947, **1**, 164 (*struct*)
Schöuberg, A. *et al., J.C.S.*, 1947, 693 (*stereochem*)
Boelans, M. *et al., J. Agric. Food Chem.*, 1974, **22**, 1071
Arai, K. *et al., Tet. Lett.*, 1976, 1685 (*cmr*)
U.S. Pat., 1976, 560 717; *CA*, **84**, 149561a (*use*)
Sekido, K. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 3149 (*cryst struct*)
Andrzejewska, E. *et al., Tet. Lett.*, 1977, 451
Wolkoff, P. *et al., Org. Mass Spectrom.*, 1978, **13**, 338 (*ms*)
Saito, Y. *et al., Acta Cryst. B*, 1980, **36**, 2333 (*oxide, cryst struct*)

Trimethylvinylammonium(1+), 8CI T-804

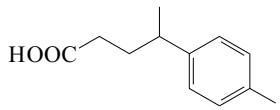
[13448-18-5]
N,N,N-*Trimethylethenaminium, 9CI. Ethenyltrimethylammonium. Neurine*
$H_2C{=}CHN^{\oplus}Me_3$
$C_5H_{12}N^{\oplus}$ 86.156

Hydroxide: [463-88-7]
$C_5H_{13}NO$ 103.164
Occurs free and combined in many animal and vegetable products, formed during putrefaction by dehydration of choline. Syrupy liq. with fishy odour. Sol. H_2O, EtOH. Reacts alkaline and readily absorbs CO_2 from air. Forms hygroscopic cryst. hydrate with $3H_2O$. Easily dec. → Me_3N.
► Highyl toxic. BT3850000

Meyer, K.H. *et al., Ber.*, 1921, **54**, 2265 (*synth, hydroxide*)
Gardner, C. *et al., J.C.S.*, 1949, 789 (*synth, hydroxide, chloride, picrate*)
Grabowska, M. *et al., Diss. Pharm. Pharmacol.*, 1967, **19**, 43 (*synth, pharmacol*)
Kroeller, E. *et al., CA*, 1973, **79**, 16990 (*isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VQR300

11,12,13-Trinor-1,3,5-bisabolatrien-10-oic acid T-805

γ,4-Dimethylbenzenebutanoic acid. 4-(4-Methylphenyl)pentanoic acid. 4-p-Tolylpentanoic acid. Dihydro-α-norcurcumenic acid

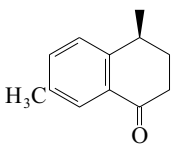


$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient. Constit. of East Indian sandalwood oil.

Nikiforov, A. *et al., Annalen*, 1990, 119 (*isol, pmr*)

11,12,13-Trinor-7-calamenone T-806

[28449-86-7]
3,4-Dihydro-4,7-dimethyl-1(2H)naphthalenone. 4,7-Dimethyltetralone



(*S*)-*form*

$C_{12}H_{14}O$ 174.242

(*S*)-*form* [155748-76-8]
Constit. of lavender oil.

(±)-*form* [85867-62-5]
Liq. Bp_6 129° $Bp_{0.8}$ 106.5-108°.

2,4-Dinitrophenylhydrazone: [74285-39-5]
Red cryst. (EtOAc/$CHCl_3$). Mp 244-244.3°.

Semicarbazone:
Needles (EtOH). Mp 196-197°.

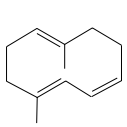
(ξ)-*form*
Constit. of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{20}$ +5.6 (c, 0.3 in $CHCl_3$).

[74285-39-5]

Johnson, W.S. *et al., J.A.C.S.*, 1947, **69**, 792 (*synth*)
Phillips, D.D. *et al., J.A.C.S.*, 1955, **77**, 3658 (*synth*)
Kaiser, R. *et al., Helv. Chim. Acta*, 1983, **66**, 1843 (*isol*)
El-Seedi, H. *et al., Phytochemistry*, 1994, **35**, 1495 (*isol, pmr, cmr*)
Thebtaranonth, C. *et al., Phytochemistry*, 1995, **40**, 125 (*isol, pmr, cmr*)

11,12,13-Trinor-1(10),4,6-germacratriene T-807

[20082-17-1]
1,5-Dimethyl-1,5,7-cyclodecatriene



$C_{12}H_{18}$ 162.274

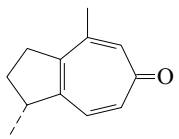
(1(10)*E*,4*E*,6*Z*)-*form*
Pregeijerene
Constit. of *Ruta graveolens* (rue) and *Rubus rosifolius* (Mauritius raspberry). Oil. Bp_5 82°.

$AgNO_3$ adduct: [21687-41-2]
Cryst. (EtOH). Mp 121-123°.

Jones, R.V.H. *et al., Aust. J. Chem.*, 1968, **21**, 2255
Coggon, P. *et al., J.C.S.(B)*, 1970, 1024 (*cryst struct*)
Kubeczka, K.H. *et al., Phytochemistry*, 1974, **13**, 2017

11,12,13-Trinor-1(5),6,9-guaiatrien-8-one T-808

2,3-Dihydro-1,4-dimethyl-6(1H)-azulenone, 9CI



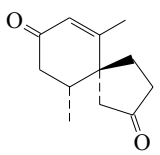
$C_{12}H_{14}O$ 174.242

(*R*)-*form* [71305-89-0]
Isol. from *Acorus calamus* (sweet flag). Cryst. (Et_2O/hexane). Mp 98-99°. $[\alpha]_D^{22}$ -12.8 (c, 0.125 in $CHCl_3$).

Rohr, M. *et al., Phytochemistry*, 1979, **18**, 279 (*isol*)
Afzal, M. *et al., Heterocycles*, 1986, **24**, 2943 (*pmr, cmr*)

11,12,13-Trinor-1(10)-spirovetivene-2,7-dione T-809

[84413-75-2]
6,10-Dimethylspiro[4.5]dec-6-ene-2,8-dione

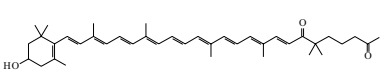


$C_{12}H_{16}O_2$ 192.257
Constit. of potato tubers infected with *Phoma exigua*. Amorph. $[\alpha]_D^{23}$ -11 (c, 0.14 in MeOH).

Malmberg, A.G. *et al., Phytochemistry*, 1982, **21**, 1818

Triphasiaxanthin T-810

[23939-69-7]
3′-Hydroxy-5,6-seco-β,β-carotene-5,6-dione. 3-Hydroxysemi-β-carotenone

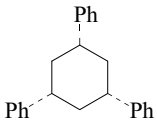


$C_{40}H_{56}O_3$ 584.881
Constit. of fruit of *Triphasia trifolia* (limeberry). Cryst. (Et_2O/petrol). Mp 95-97°. λ_{max} 480 (ε, 96 600) and 510 nm (84 900) ($CHCl_3$).

Yokoyama, H. *et al., J.O.C.*, 1970, **35**, 2080 (*isol, ir, uv, ms, pmr*)
Szabolcs, J. *et al., Acta Chim. Acad. Sci. Hung.*, 1973, **78**, 315 (*synth, uv, ord*)

1,3,5-Triphenylcyclohexane, 8CI T-811

[17342-60-8]
1,1′,1″-(1,3,5-Cyclohexanetriyl)trisbenzene, 9CI



(1α,2α,5α)-*form*

$C_{24}H_{24}$ 312.454
Packaging migration residue. Present as an impurity in polystyrene food containers and other products; liberated on heating.

(1α,3α,5α)-*form* [234079-32-4]
cis-*form*. *ST-7*
Cryst. (EtOH). Mp 97-98°.

(1α,3α,5β)-*form* [28336-57-4]
trans-*form*. *ST-6*

Kurze, J. *et al., Angew. Makromol. Chem.*, 1970, **12**, 25-41 (*synth, pmr*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; 390-398; *CA*, **129**, 4008w; **130**, 251409n (*anal*)
Moriguchi, K. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1999, **48**, 623-629; *CA*, **131**, 129609h (*isol, pmr, cmr*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox*)

2,4,6-Triphenyl-1-hexene, 8CI T-812

[18964-53-9]
1,1′,1″-(1-Methylene-1,3,5-pentanetriyl)-trisbenzene, 9CI. ST-1
$H_2C{=}CPhCH_2CHPhCH_2CH_2Ph$
$C_{24}H_{24}$ 312.454

(±)-*form*
Styrene trimer. Present as an impurity in polystyrene food containers and other products - liberated on heating. Yellow viscous oil.

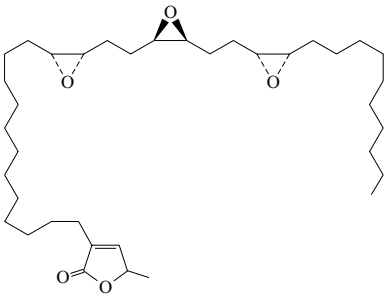
(ξ)-*form*

Staudinger, H. *et al., Annalen*, 1935, **517**, 35-53 (*synth*)
Mayo, F.R. *et al., J.A.C.S.*, 1968, **90**, 1289-1295 (*synth, ir*)
Saido, K. *et al., Eur. Polym. J.*, 1984, **20**, 1061-1065 (*synth*)
Yayli, N. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 556-561 (*isol*)
Ayer, W.A. *et al., Phytochemistry*, 1996, **42**, 1321-1324 (*isol, pmr, cmr*)
Kawamura, Y. *et al., Shokuhin Eisegaku Zasshi*, 1998, **39**, 110-119; 390-398; *CA*, **129**, 4008w; **130**, 251409n (*detn*)
Ohyama, K. *et al., Environ. Health Perspect.*, 2001, **109**, 699-703 (*tox*)

Tripoxyrollin T-813

[155606-59-0]

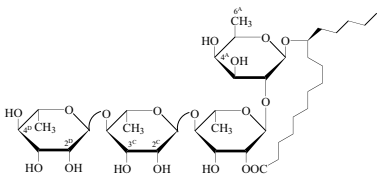
[160637-35-4]
Trieporeticanin



$C_{37}H_{64}O_5$ 588.91
Constit. of *Annona reticulata* (custard apple). $[\alpha]_D$ +13 (c, 1 in $CHCl_3$). Identity of Trieporeticanin and Tripoxyrollin not certain; possible stereoisomers λ_{max} 205 (ϵ 11220) (MeOH) (Berdy).

Sahpaz, S. *et al., Nat. Prod. Lett.*, 1993, **2**, 301-308 (*isol, uv, pmr, cmr*)
Tam, V.T. *et al., Nat. Prod. Lett.*, 1994, **4**, 255-262 (*isol, uv, pmr, cmr*)

Trisdeacylsimonin I T-814



$C_{40}H_{70}O_{18}$ 838.982

2^D-Cinnamoyl, 2^C,4^D-didecanoyl: [151310-50-8] ***Simonin I***
$C_{69}H_{112}O_{21}$ 1277.631
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 114-116°. $[\alpha]_D$ -9.3 (c, 0.2 in MeOH).

3^C-(α-L-Rhamnopyranosyl), 2^C-octanoyl, 4^D-dodecanoyl: [151310-54-2] ***Simonin V***
$C_{66}H_{116}O_{24}$ 1293.628
Constit. of *Ipomoea batatas* (sweet potato). Powder. Mp 115-116°. $[\alpha]_D$ -35.2 (c, 1 in MeOH).

4^A-Epimer, 6^A-hydroxy, 3^C-(α-L-rhamnopyranosyl), 4^D-dodecanoyl, 2^C-(2-methylbutanoyl(S)): [151310-51-9] ***Simonin II***
$C_{63}H_{110}O_{25}$ 1267.547
Constit. of *Ipomoea batatas* (sweet potato). Powder. Mp 121-123.5°. $[\alpha]_D$ -27.8 (c, 1 in MeOH).

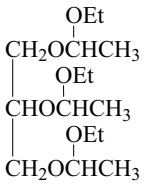
3^C-(α-L-Rhamnopyranosyl), 2^C-(2-methylbutanoyl(S)), 4^D-dodecanoyl: [151310-52-0] *Simonin III*
$C_{63}H_{110}O_{24}$ 1251.548
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 127-132°. $[\alpha]_D$ -37.5 (c, 1 in MeOH).

3^C-(α-L-Rhamnopyranosyl), 4^D-dodecanoyl, 2^C-decanoyl: [151310-53-1] ***Simonin IV***
$C_{68}H_{120}O_{24}$ 1321.682
Constit of *Ipomoea batatas* (sweet potato). Powder. Mp 123-125°. $[\alpha]_D$ -43.3 (c, 1 in MeOH).

Noda, N. *et al., Chem. Pharm. Bull.*, 1992, **40**, 3163-3168 (*isol, pmr, cmr, ms*)

1,2,3-Tris(1-ethoxyethoxy)-propane T-815

[67715-82-6]
7-(1-Ethoxyethoxy)-4,10-dimethyl-3,5,9,11-tetraoxatridecane, 9CI. FEMA 3593

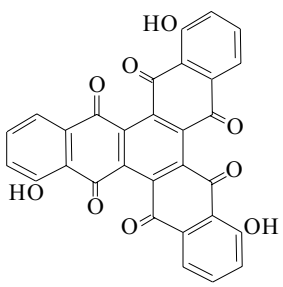


$C_{15}H_{32}O_6$ 308.414
Flavouring ingredient. Aldehyde generator, useful for enhancing the fresh flavour of orange drinks. Liq. d_4^{25} 0.96. Bp_1 117°. n_D^{20} 1.4222. Hydrolysed to acetaldehyde under aq. acidic conditions.

Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-62; 64-66; 68-70 (*use*)
U.S. Pat., 1981, 4 280 011; *CA*, **95**, 219773z (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 777 (*use*)

Trisjuglone T-816

[50838-55-6]
1,7,13-Trihydroxy-5,6,11,12,17,18-trinaphthylenehexone, 9CI. Cyclotrijuglone

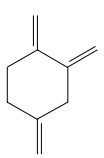


$C_{30}H_{12}O_9$ 516.419
Constit. of *Juglans regia* (walnut) roots. Dark yellow cryst. or prisms (dioxan). Mp 360°. λ_{max} 280 (log ϵ 4.48); 420 (log ϵ 4.04) (dioxan).

Brockmann, H. *et al., Tet. Lett.*, 1973, 3695 (*synth*)
Sidhu, G.S. *et al., Indian J. Chem.*, 1975, **13**, 749 (*isol, ir, uv, ms*)

1,2,4-Tris(methylene)cyclohexane, 9CI T-817

[14296-81-2]
1,2,4-Tri(methylidene)cyclohexane. 1,2,4-Trimethylenecyclohexane



C_9H_{12} 120.194
Minor component of blackcurrant (*Ribes*

nigrum) dormant buds. Liq. Bp_{60} 68-69°. Undergoes acid catalysed rearrangement to 1,2,4-Trimethylbenzene. Readily undergoes Diels-Alder reactions with dienophiles. Poss. artifact.

Benson, R.E. *et al., J.A.C.S.*, 1959, **81**, 4247 (*synth, pmr, glc, uv, ir*)
Weinstein, B. *et al., J.C.S.(C)*, 1967, 368 (*synth, pmr, ir, uv*)
De Pasquale, R.J. *et al., J. Organomet. Chem.*, 1971, **32**, 381 (*pmr, cmr*)
Cermak, J. *et al., Coll. Czech. Chem. Comm.*, 1988, **53**, 1274 (*synth, pmr, ir, ms*)
Hopf, H. *et al., Chem. Ber.*, 1990, **123**, 1169 (*synth*)

Trisodium hydrogen carbonate dihydrate T-818

[6106-20-3]

[533-96-0]

Carbonic acid sodium salt (2:3) dihydrate, 8CI. Sodium sesquicarbonate dihydrate. E500

$Na_3H(CO_3)_2.2H_2O$

$C_2H_5Na_3O_8$ 226.026

Colourless monoclinic cryst. V. sol. H_2O (13 g per 100 cm^3 at 0°; 42 g per 100 cm^3 at 100°). ΔH_f° -2682 kJ mol^{-1}; ΔG_f° -2381 kJ mol^{-1}; S° 301 J K^{-1} mol^{-1}. Dec. on heating by CO_2 and H_2O loss forming Na_2CO_3. The name E500 is also used for Sodium carbonate (Na_2CO_3), S-122 and Sodium hydrogen carbonate, S-130.

▶ FG2099000

Mineral-*form* [15243-87-5]

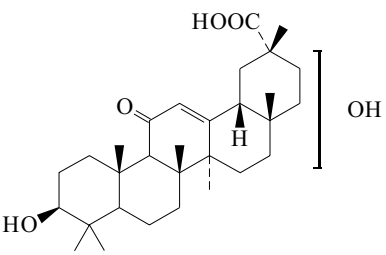
Trona

pH control agent in milk processing. Colourless or off-white needles.

Novak, A. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1963, **60**, 1385 (*ir*)
Rupert, J.P. *et al., J. Phys. Chem.*, 1965, **69**, 3059 (*thermodyn*)
Tomaszewski, E.P. *et al., Przem. Chem.*, 1965, **44**, 334; *CA*, **63**, 7869h (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 21, 1966, **3**, 1363 (*rev, bibl*)
Eugster, H.P. *et al., Contrib. Geol.*, 1971, **10**, 49 (*rev, synth*)
Chois, C.S. *et al., Acta Cryst. B*, 1982, **38**, 2874 (*struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2605-2606

Glycyrrhiza Triterpene T-819

3,x-Dihydroxy-11-oxo-12-oleanen-29-oic acid



$C_{30}H_{46}O_5$ 486.69

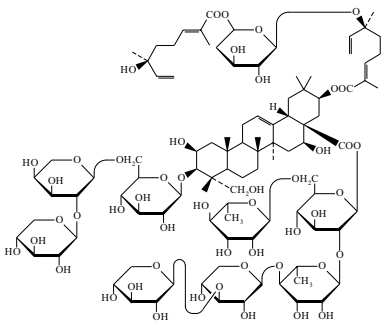
Isol. from roots of *Glycyrrhiza glabra* (licorice).

Di-Ac, Me ester:

Mp 288-290°. $[\alpha]_D$ +25.5 ($CHCl_3$).

Elgamal, M.H.A. *et al., Naturwissenschaften*, 1975, **62**, 183

Triterpenoid-monoterpenoid saponins T-820



A class of oligomeric-type saponins consisting of a pentacyclic triterpenoid sapogenin linked to one or more linear C_{10} monoterpenoid (linalooyl type) residues and a number of glycoside residues. The triterpenoid residues in all saponins so far characterised are oleanenecarboxylic acids but these vary in degree of hydroxylation. The points of attachment and order of assembly of the monoterpenoid groups and the sugar residues varies. Gymnocladussaponin F_1, illus., is typical..

Pitheduloside H [200127-48-6]

$C_{100}H_{158}O_{49}$ 2144.319

Constit. of *Pithecellobium dulce* (manila tamarind). Needles. Mp 196-198°. $[\alpha]_D^{25}$ -23.6 (c, 3.1 in MeOH). Glycoside of, with 2 x C_{10} units plus 1 sugar at C-21, 4 sugars at C-3 and 4 sugars esterifying at C-28.

Pitheduloside I [200127-56-6]

$C_{100}H_{158}O_{50}$ 2160.318

Constit. of *Pithecellobium dulce* (manila tamarind). Needles. Mp 222-224°. $[\alpha]_D^{25}$ -16.2 (c, 2 in MeOH). Glycoside of, with 2 x C_{10} units plus 1 sugar at C-21, 3 sugars at C-3 and 4 sugars esterifying at C-28.

Pitheduloside J [200127-64-6]

$C_{85}H_{136}O_{43}$ 1845.984

Constit. of *Pithecellobium dulce* (manila tamarind). Needles. Mp 199-201°. $[\alpha]_D^{25}$ -28 (c, 2.2 in MeOH). Glycoside of, with 1 x C_{10} unit at C-21, 4 sugars at C-3 and 4 sugars esterifying at C-28.

Yoshikawa, K. *et al., J. Nat. Prod.*, 1997, **60**, 1269-1274 (*Pithedulosides*)

1,2,3-Trithiane T-821

[3325-33-5]

v-Trithiane, 8CI. 1,2,3-Trithiacyclohexane



$C_3H_6S_3$ 138.278

Constit. of garlic (*Allium* spp.). Cryst. (EtOH). Mp 46°.

Yamazaki, N. *et al., Chem. Lett.*, 1980, 1355 (*synth*)
Morel, G. *et al., Synthesis*, 1980, 918 (*synth*)
Pant, N. *et al., Fitoterapia*, 1986, **57**, 302-304 (*isol*)
Nash, C.P. *et al., Appl. Spectrosc.*, 1988, **42**, 494 (*ir, Raman*)
Sato, R. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 1647 (*synth*)
Teuber, L. *et al., Sulfur Rep.*, 1990, **9**, 257 (*rev, derivs, occur*)

1,3,5-Trithiane, 9CI T-822

[291-21-4]

s-*Trithiane, 8CI. Trithioformaldehyde. Tris(methylene sulfide). 1,3,5-Trithiacyclohexane*

$C_3H_6S_3$ 138.278

Trimer of Methanethial. Isol. from various marine organisms; and as a food flavour component. Needles (AcOH). Mp 220°.

▶ Eye and skin irritant. LD_{50} (mus, ipr) 250 mg/kg. YL8225000

S,S,S′,S′,S″,S″-Hexaoxide: [2125-34-0]

$C_3H_6O_6S_3$ 234.275

Cryst. powder. Insol. H_2O, org. solvs.; sol. alkalis. Mp 340°.

▶ YL8400000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 273B (*ir*)
Richtzenhain, H. *et al., Chem. Ber.*, 1953, **86**, 142 (*synth*)
El-Hewehi, Z. *et al., J. Prakt. Chem.*, 1963, **21**, 286 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 564
Asai, M. *et al., Spectrochim. Acta A*, 1978, **34**, 695 (*ir*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)
Cervellati, R. *et al., J. Mol. Struct.*, 1984, **117**, 247 (*microwave*)
Arens, G. *et al., Chem. Ber.*, 1986, **119**, 3631 (*hexaoxide*)
Bencze, Z. *et al., Acta Chem. Scand.*, 1989, **43**, 953 (*struct*)
Blunt, J.W. *et al., New J. Chem.*, 1990, **14**, 761 (*rev, occur*)
Edema, J.J.H. *et al., Inorg. Chim. Acta*, 1993, **207**, 263 (*conformn*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TLS500

1,2,4-Trithiolane, 9CI T-823

[289-16-7]

1,2,4-Trithiacyclopentane



$C_2H_4S_3$ 124.252

Present in patai beans (*Parkia speciosa*) and the shiitake mushroom (*Lentinus edodes*). Component of mushroom flavour. Pale yellow liq. Poorly sol. hexane. Bp_{10} 102-103° Bp_3 78-79°.

1-Oxide: [58966-91-9]

$C_2H_4OS_3$ 140.251

Oil.

4-Oxide: [58966-90-8]

$C_2H_4OS_3$ 140.251

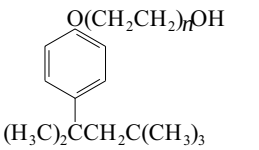
Needles (hexane/$CHCl_3$). Mp 76-77°.

Morita, K. *et al., Chem. Pharm. Bull.*, 1967, **15**, 988 (*synth*)

Tjan, S.B. *et al., Tetrahedron*, 1972, **28**, 3489 (*synth, ms*)
Wratten, S.J. *et al., J.O.C.*, 1976, **41**, 2465 (*isol oxides*)
Gmelin, R. *et al., Phytochemistry*, 1981, **20**, 2521 (*isol*)
Holzmann, G. *et al., Org. Mass Spectrom.*, 1982, **17**, 165 (*ms*)
Juettner, F. *et al., Phytochemistry*, 1982, **21**, 2185 (*isol*)
Borseth, D.G. *et al., J.A.C.S.*, 1984, **106**, 841 (*struct*)
Chen, C.C. *et al., J. Agric. Food Chem.*, 1986, **34**, 830 (*isol*)

Triton X 100 T-824

[9002-93-1]
Polyethylene glycol tert-*octylphenyl ether*



$n \sim 10$

Non-ionic detergent. CAS number also refers to Triton X 305 below. Listed in the EAFUS Food Additive Database (Jan. 2001) but with no reported uses. n_D^{20} 1.4900.

▶ MD0907700

Hexahydro: [101013-07-4]
Non-ionic detergent. n_D^{20} 1.4720.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1163C; 1163D (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 972C (*nmr*)
Okawa, S. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1982, **31**, 373 (*detn, Co*)
Tiller, G.E. *et al., Anal. Biochem.*, 1984, **141**, 262 (*sepn, proteins*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PKF500

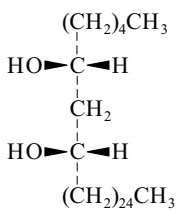
Triton X 305 T-825

α-[4-(1,1,3,3-Tetramethylbutyl)phenyl]-ω-hydroxypoly(oxy-1,2-ethanediyl), 9CI
Non-ionic surfactant. Pesticide diluent in foods. Sol. H_2O.

[9002-93-1]

Wu, Q. *et al., Talanta*, 1983, **30**, 275
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2766-2767

6,8-Tritriacontanediol T-826



$C_{33}H_{68}O_2$ 496.899
(6*R,8*S**)-*form*** [155800-90-1]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 82-84°. $[\alpha]_D$ +0.3 (c, 0.11 in $CHCl_3$).

Akihisa, T. *et al., Phytochemistry*, 1994, **36**, 105 (*isol, ms*)

8,10-Tritriacontanediol T-827

$C_{33}H_{68}O_2$ 496.899
(8*R,10*S**)-*form*** [193419-79-3]
erythro-*form*
Constit. of the dried flowers of *Carthamus tinctorius* (safflower). Cryst. (Me_2CO/MeOH). Mp 79-82°.

Akihisa, T. *et al., Phytochemistry*, 1997, **45**, 725-728 (*isol, ms*)

10,12-Tritriacontanedione T-828

$H_3C(CH_2)_{20}COCH_2CO(CH_2)_8CH_3$
$C_{33}H_{64}O_2$ 492.867
Constit. of the pollen of *Helianthus annuus* (sunflower).

Schultz, S. *et al., Phytochemistry*, 2000, **54**, 325-336

1-Tritriacontanol T-829

[71353-61-2]
$H_3C(CH_2)_{31}CH_2OH$
$C_{33}H_{68}O$ 480.9
Constit. of *Amaranthus* spp. and *Citrus aurantium* (Seville orange). Cryst. (C_6H_6 or hexane). Mp 88.6°.

Octacosanoyl: [105419-00-9] *Tritriacontyl octacosanoate*
$C_{61}H_{122}O_2$ 887.634
Constit. of *Panax pseudoginseng* ssp. *himalaicus* var. *angustifolius*. Cryst. ($CHCl_3$/MeOH). Mp 75°.

[103215-67-4]

Jones, R.G. *et al., J.A.C.S.*, 1947, **69**, 2350 (*synth*)
Tasumi, M. *et al., Spectrochim. Acta*, 1964, **20**, 629 (*synth, ir, cryst struct*)
Sakakibara, J. *et al., Phytochemistry*, 1983, **22**, 2553 (*isol*)
Shukla, Y.N. *et al., Phytochemistry*, 1986, **25**, 2201 (*isol, deriv*)
Misra, T.N. *et al., Phytochemistry*, 1991, **30**, 2076 (*isol*)
Brown, H.C. *et al., Tetrahedron*, 1992, **48**, 9187 (*synth*)

3-Tritriacontanone T-830

[79097-23-7]
$H_3C(CH_2)_{29}COCH_2CH_3$
$C_{33}H_{66}O$ 478.884
Constit. of *Solanum torvum* (pea eggplant). Cryst. (Me_2CO/MeOH). Mp 83°.

Goswami, A. *et al., Phytochemistry*, 1981, **20**, 1315 (*isol*)
Mahmood, U. *et al., Phytochemistry*, 1983, **22**, 167 (*isol*)

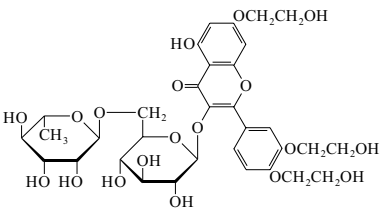
24-Tritriacontene-2,4-dione T-831

$H_3C(CH_2)_7CH$
$=CH(CH_2)_{19}COCH_2COCH_3$
$C_{33}H_{62}O_2$ 490.852
(*Z*)-*form*
Lumequoylacetone
Constit. of the epicuticular waxes of *Vanilla fragrans* (vanilla) and *Vanilla tahitensis* (Tahitian vanilla).

Ramaroson-Raonizafinimanana, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 4739-4743 (*isol*)

Troxerutin, BAN, INN T-832

[7085-55-4]
2-[3,4-Bis(2-hydroxyethoxy)phenyl]-3-[[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-5-hydroxy-7-(2-hydroxyethoxy)-4H-1-benzopyran-4-one, 9CI. 3,5-Dihydroxy-3′,4′,7-tris(2-hydroxyethoxy)flavone 3-[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranoside], 8CI. Vitamin P_4. Posorutin. Ruven. Veinamitol. Many other names



$C_{33}H_{42}O_{19}$ 742.683
Principal component of a mixt. which contains about 40% mono, di and tetrakis(hydroxyethyl)rutins. Bioflavonoid. Yellow powder. Insol. EtOH. Mp 181°.

▶ LK8331500

Mixture: ***Oxerutins****. Factor P-Zyma. Paravan. Relvene. Venoruten. Verutil*
Yellow powder. Mp 156°.

U.K. Pat., 1960, 833 174; *CA*, **54**, 21135i
Courbat, P. *et al., Helv. Chim. Acta*, 1966, **49**, 1203; 1420 (*isol, struct*)
Mucharska, A. *et al., Farm. Pol.*, 1971, **27**, 149; *CA*, **75**, 80315t (*chromatog*)
Tomas, F. *et al., An. Quim.*, 1973, **69**, 357; *CA*, **79**, 57730y (*uv*)
Ger. Pat., 1973, 2 320 858; *CA*, **80**, 30699d
Hackett, A.M. *et al., Arzneim.-Forsch.*, 1976, **26**, 925 (*metab*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7996 (*synonyms*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1342

Trypsin, BAN, JAN T-833

[9002-07-7]
Parenzyme. Parenzymol. Tryptar. Trypure. E.C. 3.4.21.4
Used in baking, meat tenderising, and production of protein hydrolysates. Yellowish cryst. Component of Chymoral.

▶ LD_{50} (rat, orl) >5000 mg/kg. LD_{50} (rat, ivn) 36 mg/kg. YN5075000

U.S. Pat., 1953, 2 637 680, (*Danske Andelsslagteriers Konserv*); *CA*, **47**, 8972h (*isol*)
Walsh, K.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1964, **51**, 301 (*struct, function*)
Tamburro, A.M. *et al., Gazz. Chim. Ital.*, 1968, **98**, 1256 (*conformn*)
Markley, J.L. *et al., Dev. Biochem.*, 1980, **10**, 31 (*rev, props*)
Marquart, M. *et al., Acta Cryst. B*, 1983, **39**, 480 (*cryst struct*)
Bohe, M. *et al., Digestion*, 1986, **34**, 127 (*metab*)
Gerlt, J.A. *et al., Chem. Rev.*, 1987, **87**, 1079 (*struct*)
Tsarbopoulos, A. *et al., Anal. Chim. Acta*, 1990, **241**, 315 (*ms*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1424
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2852-2853 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TNW000

Citrullus vulgaris Trypsin inhibitor I T-834

[113464-76-9]
CVTI I

H-Gly-Arg-Arg-Cys-Pro-Arg-Ile-Tyr-Met-Glu-Cys-Lys-Arg-Asp-Ala-Asp-Cys-Leu-Ala-Asp-Cys-Val-Cys-Leu-Gln-His-Gly-Ile-Cys-Gly-OH

$C_{136}H_{214}N_{46}O_{41}S_7$ 3373.932

Struct. of reduced form shown. Constit. of the seeds of *Citrullus vulgaris* (watermelon).

Otlewski, J. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1987, **368**, 1505-1507 (*isol, struct*)

Cucurbita maxima Trypsin inhibitor I T-835

[84795-93-7]
CMTI-I

H-Arg-Val-Cys-Pro-Arg-Ile-Leu-Met-Glu-Cys-Lys-Lys-Asp-Ser-Asp-Cys-Leu-Ala-Glu-Cys-Val-Cys-Leu-Glu-His-Gly-Tyr-Cys-Gly-OH

Struct. of reduced form shown. Isol. from squash (*Cucurbita maxima*) seeds.

9-L-Lysine analogue: [79044-57-8] Cucurbita maxima *Trysin inhibitor III. CMTI-III*
Isol. from squash seeds.

9-L-Lysine analogue, 1-(histidylglutamyl-glutamyl): [95535-87-8] Curcurbita maxima *Trypsin inhibitor IV. CMTI-IV*
Constit. of *Cucurbita maxima*.

Wilusz, T. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1983, **364**, 93 (*isol, struct*)
Wieczorek, M. *et al., Biochem. Biophys. Res. Commun.*, 1985, **126**, 646 (*CMTI-IV*)
Kupryszewski, G. *et al., Int. J. Pept. Protein Res.*, 1986, **27**, 245 (*synth, deriv*)
Bode, W. *et al., FEBS Lett.*, 1989, **242**, 285 (*struct*)

Linum usitatissimum Trypsin inhibitor T-836

LUTI

Primary struct. contains 69 amino acid residues. For struct. see ref.. Isol. from the seeds of flax, *Linum usitatissimum*.

Lorenc-Kubis, I. *et al., ChemBioChem*, 2001, **1**, 45-51

Momordica charantia Trypsin inhibitor I T-837

MCTI I

H-5-Oxo-Pro-Arg-Arg-Cys-Pro-Arg-Ile-Leu-Lys-Gln-Cys-Lys-Arg-Asp-Ser-Asp-Cys-Pro-Gly-Glu-Cys-Ile-Cys-Met-Ala-His-Gly-Phe-Cys-Gly-OH

Reduced form shown. Constit. of the seeds of *Momordica charantia* (bitter melon).

Hara, S. *et al., J. Biochem. (Tokyo)*, 1989, **105**, 88-92 (*isol, struct*)

Cucumis sativus Trypsin inhibitor III T-838

CSTI III

H-His-Glu-Glu-Arg-Val-Cys-Pro-Lys-Ile-Leu-Met-Lys-Cys-Lys-His-Asp-Ser-Asp-Cys-Leu-Ala-Glu-Cys-Ile-Cys-Leu-Glu-Asp-Ile-Gly-Tyr-Cys-Gly-Val-Ser-OH

Struct. of reduced form shown. Constit. of *Cucumis sativus* (cucumber).

Polanowski, A. *et al., Biol. Zentralbl.*, 1988, **107**, 45-49 (*isol, struct*)

Cucurbita pepo Trypsin inhibitor II T-839

CPTI II

H-Arg-Val-Cys-Pro-Lys-Ile-Leu-Met-Glu-Cys-Lys-Lys-Asp-Ser-Asp-Cys-Leu-Ala-Glu-Cys-Ile-Cys-Leu-Glu-His-Gly-Tyr-Cys-Gly-OH

Struct. of reduced form shown. Constit. of *Cucurbita pepo*.

*1-Histidylglutamylglutamyl:***Cucurbita pepo *Trypsin inhibitor III*.** *CPTI III*
Constit. of *Cucurbita pepo*.

Wieczorek, M. *et al., Biochem. Biophys. Res. Commun.*, 1985, **126**, 646-652 (*isol, struct*)

Momordica charantia Trypsin inhibitor II T-840

MCTI II

H-Arg-Ile-Cys-Pro-Arg-Ile-Trp-Met-Glu-Cys-Lys-Arg-Asp-Ser-Asp-Cys-Met-Ala-Gln-Cys-Ile-Cys-Val-Asp-Gly-His-Cys-Gly-OH

Reduced form shown. Constit. of the seeds of *Momordica charantia* (bitter melon).

Hara, S. *et al., J. Biochem. (Tokyo)*, 1989, **105**, 88-92 (*isol, struct*)

Momordica charantia Trypsin inhibitor III T-841

MCTI III

H-5-Oxo-Pro-Arg-Gly-Cys-Pro-Arg-Ile-Leu-Lys-Gln-Cys-Lys-Gln-Asp-Ser-Asp-Cys-Pro-Gly-Glu-Cys-Ile-Cys-Met-Ala-His-Gly-Phe-Cys-Gly-OH

Constit. of the seeds of *Momordica charantia* (bitter melon).

Hamato, N. *et al., J. Biochem. (Tokyo)*, 1995, **117**, 432-437 (*isol*)

Cucumis sativus Trypsin inhibitor IIb T-842

CSTI IIb

H-Met-Val-Cys-Pro-Lys-Ile-Leu-Met-Lys-Cys-Lys-His-Asp-Ser-Asp-Cys-Leu-Leu-Asp-Cys-Val-Cys-Leu-Glu-Asp-Ile-Gly-Tyr-Cys-Gly-Val-Ser-OH

Struct. of reduced form shown. Constit. of *Cucumis sativus* (cucumber).

Wieczorek, M. *et al., Biochem. Biophys. Res. Commun.*, 1985, **126**, 646-652 (*isol, struct*)

Cucumis sativus Trypsin inhibitor IV T-843

CSTI IV

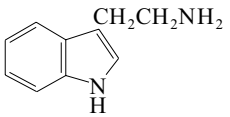
H-Met-Met-Cys-Pro-Arg-Ile-Leu-Met-Lys-Cys-Lys-His-Asp-Ser-Asp-Cys-Leu-Pro-Gly-Cys-Val-Cys-Leu-Glu-His-Ile-Glu-Tyr-Cys-Gly-OH

Struct. of reduced form shown. Constit. of *Cucumis sativus* (cucumber).

Wieczorek, M. *et al., Biochem. Biophys. Res. Commun.*, 1985, **126**, 646-652 (*isol, struct*)

Tryptamine T-844

[61-54-1]
1H-Indole-3-ethanamine, 9CI. 3-(2-Aminoethyl)indole. 2-(3-Indolyl)ethylamine



$C_{10}H_{12}N_2$ 160.218

Occurs widely in plants, esp. *Lens esculenta* (lentil) and the fungi *Coprinus micaceus* (glistening ink cap). Needles (petrol). V. spar. sol. Et_2O, $CHCl_3$, C_6H_6. Mp 118°. $Bp_{0.15}$ 137°. pK_{a1} -6.31; pK_{a2} 10.2 (25°). Log P 1.27 (calc).

▶ LD_{50} (rat, ipr) *ca*. 223 mg/kg. NL4020000

N^b-*Hexadecanoyl:* [21469-15-8] **N^b-*Hexadecanoyltryptamine*.** N^b-*Palmitoyltryptamine*
$C_{26}H_{42}N_2O$ 398.631
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa* (biriba).

N^b-*Octadecanoyl:* [21469-14-7] **N^b-*Octadecanoyltryptamine*.** N^b-*Stearoyltryptamine*
$C_{28}H_{46}N_2O$ 426.684
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa* (biriba).

N^b-*Eicosanoyl:* [152766-92-2] **N^b-*Eicosanoyltryptamine*.** N^b-*Arachidoyltryptamine*
$C_{30}H_{50}N_2O$ 454.738
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa* (biriba).

N^b-*Docosanoyl:* [7367-79-5] N-*[2-(1H-Indol-3-yl)ethyl]docosanamide. 3-[2-(Docosanoylaminoethyl)]indole. Behenic acid tryptamide.* N^b-*Behenoyltryptamine.* N^b-*Docosanoyltryptamine*
$C_{32}H_{54}N_2O$ 482.791
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa* (biriba). Also isol. from cocoa butter and shell. Cryst. (Me_2CO/Me_2CO). Mp 121-123° (116-117°).

N^b-*Tricosanoyl:* [152766-93-3] **N^b-*Tricosanoyltryptamine***
$C_{33}H_{56}N_2O$ 496.818
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa* (biriba).

N^b-*Tetracosanoyl:* [152766-94-4] **N^b-*Tetracosanoyltryptamine*.** N^b-*Lignoceroyltryptamine*
$C_{34}H_{58}N_2O$ 510.845
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa* (biriba). Mp 120-123°.

N^b-*Pentacosanoyl:* [152766-95-5] **N^b-*Pentacosanoyltryptamine***
$C_{35}H_{60}N_2O$ 524.872
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa*

(biriba).

N^b-*Hexacosanoyl:* [152766-96-6] **N^b-*Hexacosanoyltryptamine***. N^b-*Cerotoyltryptamine*
$C_{36}H_{62}N_2O$ 538.899
Alkaloid from seeds of *Annona reticulata* (custard apple) and *Rollina mucosa* (biriba).

N^b-*(25-Triacontenoyl)(Z-):* [223696-37-5] N^b-*(25-Triacontenoyl)tryptamine.* ***Cheritamine***
$C_{40}H_{68}N_2O$ 592.99
Alkaloid from *Annona cherimola* (cherimoya). Powder (MeOH). Mp 121-123°. λ_{max} 222 ; 280 (EtOH).

N^b-*(4-Hydroxycinnamoyl):* [53905-12-7] **N^b-p-*Coumaroyltryptamine***
$C_{19}H_{18}N_2O_2$ 306.363
Found in kernels of sweet corn (*Zea mays*).

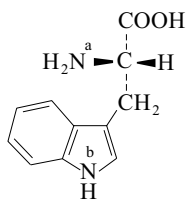
N^b-*(4-Hydroxy-3-methoxycinnamoyl):* [53905-13-8] **N^b-*Feruloyltryptamine***
$C_{20}H_{20}N_2O_3$ 336.39
Found in kernels of sweet corn (*Zea mays*).

[54268-28-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 660C; 660D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 131C (*nmr*)
Ewins, A.J. *et al., J.C.S.*, 1911, **99**, 270 (*synth*)
White, E.P. *et al., N.Z. J. Sci. Technol., Sect. B*, 1944, **25**, 157; 1951, **33**, 54; 1957, **38**, 718 (*isol*)
Cohen, L.A. *et al., J.A.C.S.*, 1960, **82**, 2184 (*pmr*)
Jackson, A.H. *et al., J.C.S.*, 1965, 3498 (*synth*)
Sacher, H. *et al., Z. Lebensm.-Unters. -Forsch.*, 1965, **128**, 264 (*docosanoyl*)
Kametani, T. *et al., Synthesis*, 1972, 475 (*synth*)
Wakahara, A. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2487 (*cryst struct*)
Ehmann, A. *et al., Phytochemistry*, 1974, **13**, 1979 (*N^b-p-Coumaroyltryptamine, N^b-Feruloyltryptamine*)
Cimino, G. *et al., Comp. Biochem. Physiol., C: Comp. Pharmacol.*, 1978, **61**, 361 (*isol*)
Morales-Rios, M.S. *et al., Magn. Reson. Chem.*, 1987, **25**, 377 (*cmr*)
Szelag, H. *et al., Nahrung*, 1988, **32**, 285 (*N-docosanoyl*)
Maeda, U. *et al., Phytochemistry*, 1993, **34**, 1633-1635 (*N-Acyltryptamines*)
Chavez, D. *et al., J. Nat. Prod.*, 1999, **62**, 1119-1122 (*N-Acyltryptamines*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJX000; AJX250

Tryptophan, 9CI, 8CI, USAN T-845

*2-Amino-3-(3-indolyl)propanoic acid. α-Amino-1*H*-indole-3-propanoic acid. Indole-3-alanine. 3-Indolylalanine. Trp*



(S)-form

$C_{11}H_{12}N_2O_2$ 204.228

In CAS the N atoms labelled a and b are referred to as *N*- and 1- respectively.

(*S*)-*form* [73-22-3]
L-*form*
Constit. of many plants. Enzymatic hydrol. prod. of most plant and animal proteins. Dietary supplement, nutrient. Plates (EtOH aq.). Sol. boiling H_2O, hot EtOH; spar. sol. cold H_2O, EtOH; insol. $CHCl_3$. Soly. 1.14 g/100 g in H_2O at 25°. Mp *ca.* ° 282 dec. $[\alpha]_D^{25}$ -68.8 (H_2O). $[\alpha]_D^{20}$ -32.5 (c, 1.1 in H_2O). $[\alpha]_D^{21}$ -5.7 (5*M* HCl). pK_{a3} 16.82 (25°,NH, KOH aq.). pK_a 2.38 (COOH, α-$NH_3^{\oplus}$). Log P -1.57 (uncertain value) (calc). Isoelectric point 5.89. Bitter taste.

▶ LD_{50} (rat, ipr) 1634 mg/kg. Exp. reprod. and teratogenic effects (large dose). Adverse effects when used therapeutically.
YN6130000

N^a-*Hexanoyl,* N^b-*inositol:* [124772-47-0]
$C_{23}H_{32}N_2O_8$ 464.514
Constit. of green gram flowers (*Phaseolus aureus*). Exact struct. not indicated.

N^a-*(Carboxyacetyl):* [29399-11-9] **N-*Malonyltryptophan***
$C_{14}H_{14}N_2O_5$ 290.275
Constit. of various plants incl. *Lycopersicon esculentum* (tomato), *Medicago sativa* (alfalfa) and *Melilotus albus* (white melilot). Originally assigned to the D-form.

N^a-*(4-Hydroxycinnamoyl):* **N^a-p-*Hydroxycoumaroyltryptophan***
$C_{20}H_{18}N_2O_4$ 350.373
Constit. of green coffee beans (*Coffea canephora* var. *robusta*) (Rubiaceae). Amorph. powder. Mp 208° dec.

N^a-*(3,4-Dihydroxycinnamoyl):* [109163-69-1] **N-*Caffeoyltryptophan***
$C_{20}H_{18}N_2O_5$ 366.373
Constit. of green coffee beans. Amorph. powder.

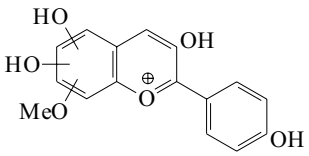
(±)-*form* [54-12-6]
Dietary supplement, nutrient. Plates (EtOH aq.). Mp 275-282° Mp 293°.

▶ YN6129200

[3184-74-5, 7401-26-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 671B; 671C; 671D; 672B; 674B; 674C; 675A (*ir, deriv*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 143C; 144A; 144B; 147A; 147B; 148A; 152B; 152C (*nmr*)
Org. Synth., 1930, **10**, 100 (*synth*)
Boyd, W.J. *et al., Biochem. J.*, 1935, **29**, 2256 (*synth*)
Albertson, N.F. *et al., J.A.C.S.*, 1945, **67**, 36 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 39), Wiley, N.Y., 1961,
Biemann, K. *et al., J.A.C.S.*, 1961, **83**, 3795-3804 (*synth, ms, Et ester*)
Fitzgerald, J.S. *et al., Aust. J. Chem.*, 1963, **16**, 246 (*isol, deriv*)
Masumi, F. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3831 (*synth*)
Morales-Rós, M.S. *et al., J. Het. Chem.*, 1986, **23**, 1617 (*cmr*)
Kulik, W. *et al., Biomed. Mass Spectrom.*, 1988, **15**, 419 (*ms*)
Kinjo, J. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4171 (*PF-P*)
Eto, H. *et al., Bull. Chem. Soc. Jpn.*, 1989, **62**, 961 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TNW500; TNX000
Rzesztarska, B. *et al., Org. Prep. Proced. Int.*, 1990, **22**, 655 (*rev, peptides*)
Gamburg, K.Z. *et al., Plant Sci. (Limerick, Irel.)*, 1991, **77**, 149 (*N-Malonyltryptophan*)
Nagarathnam, D. *et al., J. Het. Chem.*, 1992, **29**, 953 (*synth*)
Phillips, R.S. *et al., J. Het. Chem.*, 1992, **29**, 1181 (*cmr, pmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 664
Sakagami, Y. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1362 (*N-Malonyltryptophan, abs config*)
Murata, M. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1887 (*cinnamoyltryptophans*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADE075; TNX000; TNW250; TNW500

Tuberidin T-846



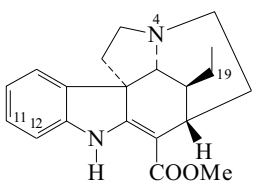
$C_{16}H_{13}O_7^{\oplus}$ 317.274
Amorph. brown-red solid (as chloride).

3-O-*Glucoside:* ***Tuberin*** †
$C_{22}H_{23}O_{12}^{\oplus}$ 479.416
Isol. from violet potatoes.

Chimielewska, I. *et al., Chem. Zentralbl.*, 1936, 2361

Tubotaiwine T-847

[6711-69-9]
14,19-Dihydrocondylocarpine



$C_{20}H_{24}N_2O_2$ 324.422
Cryst. (Et_2O) (difficult to cryst.). Mp 101-103°. $[\alpha]_D^{22}$ +628 (c, 0.8 in $CHCl_3$). λ_{max} 230 (ε 11500); 289 (ε 6310); 324 (ε 7410) (EtOH) (Derep).

Picrate:
Cryst. (Me_2CO aq.). Mp 171-172° dec.

N^4-*Oxide:* [40169-69-5] ***Tubotaiwine* N^4-*oxide***
$C_{20}H_{24}N_2O_3$ 340.421
Cryst. (Me_2CO). Mp 170° Mp 224° dec. (double Mp). Sinters at 130°, melts at 170°, resolidifies at 200° and remelts at 224° λ_{max} 230 (ε 11500); 289 (ε 6310); 324 (ε 7410) (EtOH) (Derep). λ_{max} 230 (ε 11500); 289 (ε 6320); 329 (ε 7400) (MeOH) (Berdy). λ_{max} 208 ; 224 ; 293 ; 327 (EtOH) (Berdy).

11-Methoxy: ***11-Methoxytubotaiwine.*** *14,19-Dihydro-11-methoxycondylocar-*

pine
$C_{21}H_{26}N_2O_3$ 354.448
Amorph. Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. $[\alpha]_D^{29}$ +213 (c, 0.49 in $CHCl_3$). Blue fluor. in soln. λ_{max} 225 ; 250 ; 327 (MeOH) (Berdy).

19-Hydroxy: [126721-42-4] *19-Hydroxytubotaiwine.* ***Lagunamine***
$C_{20}H_{24}N_2O_3$ 340.421
Prisms (MeOH). Mp 230-235°. $[\alpha]_D^{26}$ +578.7 (c, 0.9 in MeOH).

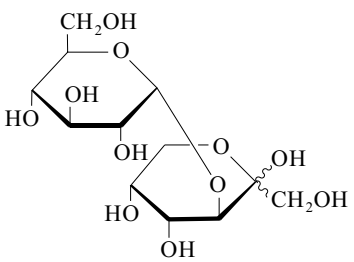
12-Methoxy: ***12-Methoxytubotaiwine***
$C_{21}H_{26}N_2O_3$ 354.448
$[\alpha]_D$ +305 (c, 0.15 in $CHCl_3$).

11-Hydroxy: ***11-Hydroxytubotaiwine***
$C_{20}H_{24}N_2O_3$ 340.421
Alkaloid from cultured cells of *Aspidosperma quebracho-blanco* (quebracho). Amorph. powder. $[\alpha]_D$ +207 (c, 0.04 in EtOH).

Kump, W.E. *et al., Helv. Chim. Acta*, 1964, **47**, 1497 (*isol*)
Gilbert, B. *et al., Tetrahedron*, 1965, **21**, 1141 (*deriv*)
Pinar, M. *et al., Helv. Chim. Acta*, 1972, **55**, 2972 (*oxide, isol, uv, ord, ir, ms*)
Kingston, D.G.I. *et al., J. Nat. Prod.*, 1977, **40**, 215 (*isol, oxide*)
Baassou, S. *et al., Phytochemistry*, 1978, **17**, 1449 (*isol, oxide*)
Caron, C. *et al., Phytochemistry*, 1989, **28**, 1241 (*12-Methoxytubotaiwine*)
Yamauchi, T. *et al., Phytochemistry*, 1990, **29**, 3321 (*Lagunamine*)
Gracia, J. *et al., Chem. Comm.*, 1991, 614 (*synth*)
Kuehne, M.E. *et al., J.O.C.*, 1991, **56**, 2696 (*synth, uv, ir, pmr, cmr, ms*)
Nkiliza, J. *et al., Tet. Lett.*, 1991, **32**, 1787 (*synth, 19-Hydroxytubotaiwine*)
Aimi, N. *et al., Heterocycles*, 1994, **38**, 2411 (*11-Hydroxytubotaiwine*)
Gràcia, J. *et al., J.O.C.*, 1994, **59**, 3939 (*synth*)

Turanose, 9CI, 8CI T-848

[547-25-1]
3-O-*α*-*D*-*Glucopyranosyl*-*D*-*fructose*



$C_{12}H_{22}O_{11}$ 342.299
An aq. soln. at 36° contains < 4% α-pyr, 39% β-pyr, 20% α-fur and 41% β-fur. Isol. from honey. Mp 157° (168°). $[\alpha]_D^{22}$ +22 → +75.3 (c, 3.9 in H_2O).

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 308C (*nmr*)
Hudson, C.S. *et al., Adv. Carbohydr. Chem.*, 1946, **2**, 1; 2 (*rev*)
Pacsu, E. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 353 (*synth*)
de Bruyn, A. *et al., Bull. Soc. Chim. Belg.*, 1975, **84**, 799 (*pmr*)
Neuman, A. *et al., Acta Cryst. B*, 1978, **34**, 242 (*cryst struct*)
Bradbury, J.H. *et al., Carbohydr. Res.*, 1979, **71**, 15 (*pmr*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)
Lichtenthaler, F.W. *et al., J.C.S. Perkin 2*, 1990, 1489 (*equilib*)

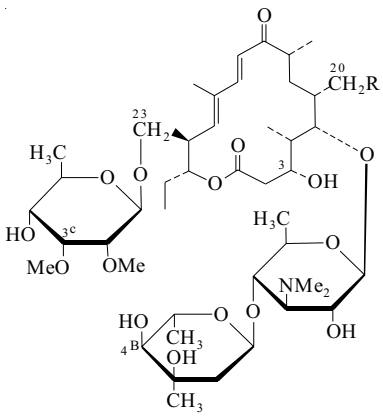
Turmerin T-849

Noncyclic polypeptide containing 40 amino acid residues. Constit. of turmeric (*Curcuma longa*). Cryst.

Srinivas, L. *et al., Arch. Biochem. Biophys.*, 1992, **292**, 617-623

Tylosin, 9CI, 8CI, BAN, INN T-850

[1401-69-0]
Dehydrorelomycin. Corvel-Tylocine. Elanco-M. Norco T-2. Parkenova. Tylan. Tylon. Frazidine

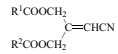


R = CHO

$C_{46}H_{77}NO_{17}$ 916.111
Macrolide antibiotic. Used in treatment of cattle, swine and mycoplasmas in poultry. Amorph. (Me_2CO/hexane) or cryst. (H_2O). Sol. MeOH, Et_2O; fairly sol. H_2O; poorly sol. hexane. Mp 131°. $[\alpha]_D$ -55. Log P -0.79 (uncertain value) (calc). λ_{max} 282 (ϵ 22400) (MeOH) (Derep). λ_{max} 282 (E1%/1cm 245) (MeOH) (Berdy). λ_{max} 284 (E1%/1cm 245) (EtOH) (Berdy). λ_{max} 288 (E1%/1cm 241) (H_2O) (Berdy).
▶ LD_{50} (mus, orl) 10000 mg/kg; LD_{50} (mus, ivn) 400 mg/kg. YP0350000

Morin, R.B. *et al., Tet. Lett.*, 1964, 2339; 1970, 4737 (*uv, struct, ir, ms, nmr*)
Achenbach, H. *et al., Chem. Ber.*, 1975, **108**, 2481 (*struct, nmr*)
Omura, S. *et al., J.A.C.S.*, 1975, **97**, 4001; 4503 (*cmr, biosynth*)
Seno, E.T. *et al., Antimicrob. Agents Chemother.*, 1977, **11**, 455; 1982, **21**, 758 (*biosynth*)
Baltz, R.H. *et al., Antimicrob. Agents Chemother.*, 1981, **20**, 214 (*isol, derivs*)
U.S. Pat., 1981, 4 304 856; *CA*, **96**, 120889
Matsubara, H. *et al., Chem. Pharm. Bull.*, 1982, **30**, 97 (*props*)
Okamoto, R. *et al., J. Antibiot.*, 1982, **35**, 921 (*isol, derivs*)
Kirst, H.A. *et al., J. Antibiot.*, 1982, **35**, 1675; 1983, **36**, 376; 1675 (*props, deriv, rev*)
Tatsuta, K. *et al., Tet. Lett.*, 1982, 3375 (*synth*)
Gray, P.P. *et al., Drugs Pharm. Sci.*, 1984, **22**, 743 (*rev*)
Kirst, H.A. *et al., J. Med. Chem.*, 1988, **31**, 1631 (*sar, activity*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TOE600; TOE750
Shepherd, M.J. *et al., Food Contaminants: Sources and Surveillance*, Royal Society of Chemistry, 1991, 146 (*anal*)
Rossi, C. *et al., Magn. Reson. Chem.*, 1992, **30**, 954 (*pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 220
Shida, Y. *et al., Tetrahedron*, 1993, **49**, 9221 (*ms*)
Simova, S. *et al., Magn. Reson. Chem.*, 1996, **34**, 255 (*pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TOE600; TOE750

Nephelium lappaceum Type II cyanolipids T-851



N-IIb $R^1 = R^2 = -(CH_2)_7CH{=}CH(CH_2)_7CH_3(Z)$
N-IIc $R^1 = -(CH_2)_7CH{=}CH(CH_2)_7CH_3(Z)$-, $R^2 = -(CH_2)_8CH{=}CH(CH_2)_7CH_3(Z)$
N-IId $R^1 = -(CH_2)_7CH{=}CH(CH_2)_7CH_3(Z)$-, $R^2 = -(CH_2)_{18}CH_3$

Constit. of the seeds of *Nephelium lappaceum* (rambutan).

N-IIb [88400-46-8]
$C_{41}H_{71}NO_4$ 642.016

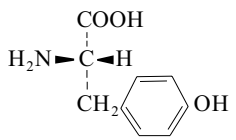
N-IIc [89200-12-4]
[88400-47-9, 88400-48-0]
$C_{43}H_{75}NO_4$ 670.07

N-IId [89946-16-7]
[88400-49-1, 88400-50-4]
$C_{43}H_{77}NO_4$ 672.086

Nishizawa, M. *et al., Phytochemistry*, 1983, **22**, 2853-2855 (*isol, pmr, ms*)
Nishizawa, M. *et al., Tet. Lett.*, 1983, **24**, 4447-4450 (*synth*)

Tyrosine, 9CI, 8CI T-852

[55520-40-6]
α-Amino-4-hydroxybenzenepropanoic acid. 2-Amino-3-(4-hydroxyphenyl)propanoic acid. 4-Hydroxy-α-aminohydrocinnamic acid. p-*Tyrosine. 3*-p-*Hydroxyphenyl-α-alanine. Tyr*



(*S*)-*form*

$C_9H_{11}NO_3$ 181.191

(*S*)-*form* [60-18-4]
L-form. FEMA 3736
Dietary supplement, nutrient. Flavouring ingredient. Needles (H_2O). Almost insol. H_2O (0.05 g/100 g at 25°). Mp 290-295° dec. (slow heat) Mp 314-318° dec. approx. (rapid heat). $[\alpha]_D^{20}$ -11.8 (c, 4.0 in 5*M* HCl) (opt. pure). $[\alpha]_D$ -9.01 (11.6% KOH). pK_{a3} 10.07 (phenolic OH). Isoelectric point 5.66. Bitter taste.
▶ Exp. reprod. and teratogenic effects (large doses). YP2275600

N-*(4-Hydroxycinnamoyl)(*E-*):* [77201-66-2] **N-trans-p-*Coumaroyltyrosine*.** N-*(4-*

Hydroxycinnamoyl)tyrosine. N-*(4-Hydroxycinnamoyl)-3-(4-hydroxyphenyl)alanine*
$C_{18}H_{17}NO_5$ 327.336
Natural food antioxidant. Isol. from cocoa liquor (*Theobroma cacao*).

N-*Jasmonoyl:* [105801-18-1] **N-*Jasmonoyltyrosine***
$C_{21}H_{27}NO_5$ 373.448
Constit. of the flowers of *Vicia faba*. For Jasmonoyl struct., see Jasmonic acid, J-8.

[16978-66-8, 36546-50-6, 81158-85-2, 126060-58-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 255B; 255C; 255D; 258C; 268A; 270C; 284C; 383C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **2**, 1187C; 1188A; 1188B; 1228A; 1228B; 1415A (*nmr*)
Sadtler Standard C-13 NMR Spectra, 12328 (*cmr*)
Sadtler Standard Proton NMR Spectra, 27604 (*pmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, (*rev*)
Parasarathy, R. *et al., Acta Cryst.*, 1962, **15**, 41 (*cryst struct*)
Hooker, T.M. *et al., J.A.C.S.*, 1964, **86**, 4989 (*ord*)
Voellmin, J. *et al., Microchem. J.*, 1966, **11**, 73 (*ms*)
Mostad, A. *et al., Acta Chem. Scand.*, 1971, **25**, 1145; 1972, **26**, 3819; 1973, **27**, 401 (*cryst struct*)
Fries, D.C. *et al., Acta Cryst. B*, 1971, **27**, 401-410 (*cryst struct, O-sulfate*)
Van Heerden, F.R. *et al., Phytochemistry*, 1980, **19**, 2125 (*N-Coumaroyltyrosine*)
Ullmann's Encycl. Ind. Chem., 1985, **A2**, 57 (*rev*)
Brueckner, C. *et al., Phytochemistry*, 1986, **25**, 2236 (*N-Jasmonyltyrosine*)
Lubman, D.M. *et al., Anal. Chem.*, 1987, **59**, 2538 (*uv*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TOG300
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 665
Hare, J.D. *et al., Naturwissenschaften*, 1993, **80**, 92 (*O-Caffeoyltyrosine*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 778
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2862-2863
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TOG300

Ukonans U-1

Neutral polysaccharides. Constits. of the rhizomes of *Curcuma longa* (turmeric).

Ukonan A [128606-57-5]
Powder. $[\alpha]_D^{24}$ -16.7 (c, 0.1 in H_2O).

Ukonan B [128606-58-6]
Powder. $[\alpha]_D^{24}$ -40 (c, 0.1 in H_2O).

Ukonan C [128606-59-7]
Powder. $[\alpha]_D^{24}$ +37.3 (c, 0.1 in H_2O).

Ukonan D [141490-48-4]
Powder. $[\alpha]_D^{23}$ +81.7 (c, 0.1 in H_2O). Also contains a small amount of a peptide moiety.

Gonda, R. *et al., Chem. Pharm. Bull.*, 1990, **38**, 482-486; 1991, **39**, 441-444; 1992, **40**, 185-188; 990-993 (*isol, struct, props*)

Ulceracin 378 U-2

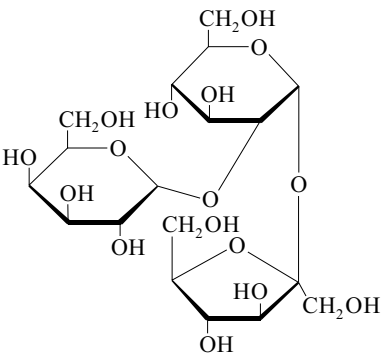
[87347-95-3]

Protein. MW 900 kDa. Bacteriocin prod. by *Corynebacterium ulcerans* 378.

Abrehem, K. *et al., Antimicrob. Agents Chemother.*, 1983, **24**, 262-267 (*isol*)
Abrehem, K. *et al., J. Gen. Microbiol.*, 1985, **131**, 707-713 (*isol*)

Umbelliferose U-3

[546-60-1]
β-D-Fructofuranosyl O-*α-D-galactopyranosyl-(1→2)-α-D-glucopyranoside, 9CI*

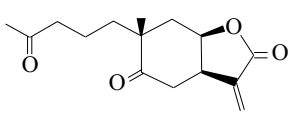


$C_{18}H_{32}O_{16}$ 504.441
Isol. from roots of *Angelica archangelica* (angelica) and other spp. in the Umbelliferae. Powder. $[\alpha]_D$ +125.3 (H_2O).

Wickstrom, A. *et al., Acta Chem. Scand.*, 1956, **10**, 1199; 1957, **11**, 1473 (*isol*)
Svendsen, A.B. *et al., Acta Chem. Scand.*, 1956, **10**, 1500
Hiller, K. *et al., Planta Med.*, 1969, **17**, 79; *CA*, **70**, 112394h (*isol*)
Hopf, H. *et al., Plant Physiol.*, 1974, **54**, 13; *CA*, **81**, 166424p (*biosynth*)
Hopf, W. *et al., Biochem. Physiol. Pflanz.*, 1976, **169**, 5; *CA*, **84**, 118600h

Umbellifolide U-4

[89026-40-4]
*Tetrahydro-6-methyl-3-methylene-6-(4-oxopentyl)-2,5-(3*H,4H*)-benzofurandione, 9CI. 4,5-Dioxo-4,5-seco-11(13)-eudesmen-12,8β-olide*

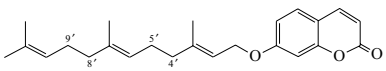


$C_{15}H_{20}O_4$ 264.321
Constit. of *Artemisia umbelliformis* (alpine wormwood). Cryst. (EtOAc/Et_2O). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 113°. $[\alpha]_D^{25}$ +60.8 (c, 0.5 in $CHCl_3$). λ_{max} 220 (ε 19952) (EtOH) (Berdy).

Appendino, G. *et al., J.C.S. Perkin 1*, 1983, 2705 (*isol, cryst struct*)
Bohlmann, F. *et al., Annalen*, 1983, 2227 (*isol*)
Marco, J.A. *et al., Tetrahedron*, 1987, **43**, 2523 (*synth*)

Umbelliprenin U-5

[23838-17-7]
Umbelliferone farnesyl ether



$C_{24}H_{30}O_3$ 366.499
Isol. from *Angelica archangelica* (angelica). Cryst. (Et_2O/petrol). Mp 61-63°.

9′-Hydroxy: [62023-94-3] ***Tadshiferin***
Cryst. Mp 68-70°. $[\alpha]_D^{23}$ +8 ($CHCl_3$).

4′,9′-Dihydroxy: ***Deacetyltadshikorin***
$C_{24}H_{30}O_5$ 398.498
Cryst. Mp 64-66°.

4′-Acetoxy, 9′-hydroxy: [62023-95-4] ***Tadshikorin***
$C_{26}H_{32}O_6$ 440.535
Oil. $[\alpha]_D^{23}$ +15.

5′,8′-Dihydroxy: [122617-02-1] ***Asacoumarin A***
$C_{24}H_{30}O_5$ 398.498
Isol. from *Ferula assa-foetida* (asafoetida). $[\alpha]_D$ +7 (c, 0.7 in $CHCl_3$).

10,11-Dihydro, 10,11-dihydroxy: See Karatavicinol in *The Combined Chemical Dictionary.*

*10′,11′-Dihydro, 9′*R*,10′*S*,11′-trihydroxy:* [146099-78-7] ***9,10,11-Trihydroxyumbelliprenin***
$C_{24}H_{32}O_6$ 416.513
Oil. $[\alpha]_D^{25}$ -14.3 (c, 1.6 in CH_2Cl_2).

Chatterjee, A. *et al., J.C.S.*, 1961, 2246 (*isol*)
Chatterjee, A. *et al., J. Indian Chem. Soc.*, 1967, **44**, 110 (*isol*)
Nikonov, G.K. *et al., Khim. Prir. Soedin.*, 1971, **7**, 115; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 103 (*isol*)
Kutney, J.P. *et al., Tetrahedron*, 1972, **28**, 5091; 1973, **29**, 2645; 2661 (*isol, biosynth*)
Perel'son, M.E. *et al., Khim. Prir. Soedin.*, 1976, **12**, 593; *Chem. Nat. Compd. (Engl. Transl.)*, 1976, **12**, 533 (*Tadshiferin*)
González, A.G. *et al., An. Quim.*, 1977, **73**, 858; 1978, **74**, 637 (*isol*)
Pinar, M. *et al., Phytochemistry*, 1977, **16**, 1987 (*isol*)
Beselovskaya, N.V. *et al., Khim. Prir. Soedin.*, 1984, **20**, 386; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 363 (*Tadshikorin, Deacetyltadshikorin*)
Kajimoto, T. *et al., Phytochemistry*, 1989, **28**, 1761 (*Asacoumarin A*)
Appendino, G. *et al., Phytochemistry*, 1992, **31**, 4223-4226 (*Trihydroxyumbelliprenins, Tetrahydroxyumbelliprenin*)

2,4-Undecadienal, 9CI U-6

[13162-46-4]
FEMA 3422
$H_3C(CH_2)_5CH{=}CHCH{=}CHCHO$
$C_{11}H_{18}O$ 166.263
Present in cooked beef and roasted peanuts. Flavouring ingredient. Oil. d^{26} 0.86. Bp_{17} 110-120°. n_D^{26} 1.5102. Props. refer to an undefined mixt. of isomers.

(2E,4E)-form [30361-29-6]
Nitrosohydrazone: See Triacsin B in *The Combined Chemical Dictionary.*

(2E,4Z)-form [53434-76-7]
2,4-Dinitrophenylhydrazone: [42022-71-9] Red blades. Mp 119-120°.

Forss, D.A. *et al., Aust. J. Chem.*, 1956, **9**, 420-424 (*synth*)
Bohlmann, F. *et al., Chem. Ber.*, 1956, **89**, 1307-1315 (*synth*)
Pippen, E.L. *et al., J.O.C.*, 1958, **23**, 1580-1582 (*synth*)
Stitt, F. *et al., Spectrochim. Acta*, 1961, **17**, 51-63 (*uv*)
Ficini, J. *et al., Bull. Soc. Chim. Fr.*, 1964, 1294-1301 (*synth*)
Näf, F. *et al., Helv. Chim. Acta*, 1974, **57**, 1309-1317 (*synth, E,E-form, E,Z-form*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 779
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2866

2,5-Undecadienal, 9CI U-7

$H_3C(CH_2)_4CH{=}CHCH_2CH{=}CHCHO$
$C_{11}H_{18}O$ 166.263

(2E,5Z)-form [13553-02-1]
Component of cooked chicken flavour. Also by oxidation of *n*-6 polyene lipid chains.

Harkes, P.D. *et al., J. Am. Oil Chem. Soc.*, 1974, **51**, 356

1,4-Undecadiene, 9CI U-8

[53786-93-9]
$H_3C(CH_2)_5CH{=}CHCH_2CH{=}CH_2$
$C_{11}H_{20}$ 152.279
Constituent of ginseng oil (*Panax ginseng*).

(E)-form [55976-13-1]
$Bp_{0.2}$ 37-38°. n_D^{20} 1.4385.

(Z)-form [55976-14-2]
Used in synthetic flavour components. Bp_{10} 66-67°.

Lynd, R.A. *et al., Synthesis*, 1974, 658 (*synth*)
Eisch, J.J. *et al., J.O.C.*, 1976, **41**, 2214 (*synth, ir, pmr*)
Uchida, K. *et al., J.O.C.*, 1976, **41**, 2215 (*synth, ir, pmr, ms*)
Bosshardt, H. *et al., Helv. Chim. Acta*, 1980, **63**, 2393 (*synth, use, ir, pmr, ms*)
Kim, K.R. *et al., Chromatographia*, 1982, **15**, 559 (*ms*)
Hoshi, M. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 2855 (*synth, pmr, ms, ir*)
Arase, A. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 209 (*synth, use, pmr, ir*)

1,5-Undecadiene, 9CI U-9

$H_3C(CH_2)_4CH{=}CHCH_2CH_2CH{=}CH_2$
$C_{11}H_{20}$ 152.279
Liq. d_4^{20} 0.76. Bp_{10} 67°. n_D^{20} 1.4318. Mixt. of *E*- and *Z*-forms.

(Z)-form [106051-44-9]
Constit. of the essential oil of *Tussilago farfara* (coltsfoot).

[106051-45-0]

Prevost, C. *et al., Bull. Soc. Chim. Fr.*, 1964, 2485 (*synth*)
Rossi, R. *et al., Tet. Lett.*, 1986, **27**, 2529 (*synth*)
Suzuki, N. *et al., Yakugaku Zasshi*, 1992, **112**, 571 (*isol*)

2,4-Undecadiene-7,9-diynoic acid U-10

$H_3CC{\equiv}CC{\equiv}CCH_2CH{=}CHCH{=}CHCOOH$

$C_{11}H_{10}O_2$ 174.199

(2E,4Z)-form

2-Methylpropylamide: 2,4-Undecadiene-7,9-diynoic acid isobutylamide. ***Neopellitorine A***
$C_{15}H_{19}NO$ 229.321
Alkaloid from *Artemisia dracunculus* (tarragon). Yellow oil. λ_{max} 257 (MeOH).

Saadali, B. *et al., Phytochemistry*, 2001, **58**, 1083-1086

2,4-Undecadiene-8,10-diynoic acid U-11

$HC{\equiv}CC{\equiv}CCH_2CH_2CH{=}CHCH{=}CHCOOH$

$C_{11}H_{10}O_2$ 174.199

(2E,4E)-form

trans,trans-*form*

4,6-Heptadiynyl ester: [55309-64-3]
$C_{18}H_{16}O_2$ 264.323
Mp 35°.

2-Methylpropylamide: [13891-74-2] 2,4-Undecadiene-8,10-diynoic acid isobutylamide. N-(2-Methylpropyl)-2,4-undecadiene-8,10-diynamide
$C_{15}H_{19}NO$ 229.321
Isol. from *Achillea millefolium* (yarrow). Cryst. (Et_2O/petrol). Mp 99-100°. λ_{max} 252 (Et_2O).

2-Methylbutylamide: [99615-78-8] N-(2-Methylbutyl)-2,4-undecadiene-8,10-diynamide
$C_{16}H_{21}NO$ 243.348

3-Methylbutylamide: [112663-71-5] ***2,4-Undecadiene-8,10-diynoic acid isopentylamide***. 2,4-Undecadiene-8,10-diynecarboxy-N-isopentylamide
$C_{16}H_{21}NO$ 243.348
Noncryst.

2-Phenylethylamide: [37064-11-2] ***N-(2-Phenylethyl)-2,4-undecadiene-8,10-diynamide***
$C_{19}H_{19}NO$ 277.365
Cryst. (Et_2O/petrol). Mp 117°. λ_{max} 250 (no solvent reported).

Piperidide: ***2,4-Undecadien-8,10-diynoic acid piperidide***
$C_{16}H_{19}NO$ 241.332
Oil. Not obt. completely pure.

2,3-Didehydropiperidide: [52704-38-8] ***2,4-Undecadiene-8,10-diynoic acid 2,3-dehydropiperidide***
$C_{16}H_{17}NO$ 239.316
Isol. from Achillea millefolium (yarrow). Oil.

(2E,4Z)-form

2-Methylpropylamide: [113817-70-2]
Cryst. (hexane). Mp 61°. λ_{max} 259 (no solvent reported).

2-Methylbutylamide: [99615-79-9]
Oil. λ_{max} 261 (no solvent reported).

2-Phenylethylamide: [37064-15-6]
Cryst. (Et_2O/petrol). Mp 78°.

(2Z,4E)-form

2-Methylpropylamide: [13894-69-4]
Cryst. (petrol). Mp 60-61°.

2-Phenylethylamide: [99615-80-2]

[52997-51-0, 92264-88-5]

Bohlmann, F. *et al., Chem. Ber.*, 1966, **99**, 3197; 1967, **100**, 104; 3861; 1972, **105**, 1694; 1973, **103**, 1328; 1974, **107**, 1038; 1975, **108**, 739 (*isol, synth, uv, ir, pmr*)
Jente, R. *et al., Chem. Ber.*, 1972, **105**, 1694 (*synth, isol, ms, struct, pmr, ir, uv*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 1535 (*isol*)
Greger, H. *et al., Phytochemistry*, 1984, **23**, 1503; 1989, **28**, 2363 (*isol*)
Martin, R. *et al., Phytochemistry*, 1985, **24**, 2295 (*isol, ms, pmr*)
Kuropka, G. *et al., Planta Med.*, 1986, **52**, 244; 1987, **53**, 440 (*isol, uv, ir, pmr, ms, struct*)
Hofer, O. *et al., Tetrahedron*, 1986, **42**, 2707 (*cmr*)
Jakupovic, J. *et al., Phytochemistry*, 1988, **27**, 1135 (*isol*)
Bauer, R. *et al., Phytochemistry*, 1988, **27**, 2339; 1989, **28**, 505 (*isol, pmr, ms, ir, uv*)
Bauer, R. *et al., Planta Med.*, 1989, **55**, 367 (*hplc*)
Binns, S.E. *et al., Planta Med.*, 2000, **66**, 241-242 (*activity, 2-methylpropylamide*)

Undecanal U-12

[112-44-7]
Undecyl aldehyde. Undecylic aldehyde. FEMA 3092

$H_3C(CH_2)_9CHO$

$C_{11}H_{22}O$ 170.294
Found in many essential oils, e.g. *Citrus* spp. and oval kumquat *Fortunella margarita*. Flavouring ingredient. d_4^{23} 0.83. Mp -4°. Bp_{18} 116-117°. n_D^{23} 1.4322. Readily polymerises.
▶ Skin irritant. LD_{50} (rat, orl) >5000 mg/kg. YQ1500000

Oxime:
$C_{11}H_{23}NO$ 185.309
Cryst. (MeOH). Mp 72°.

Semicarbazone:
Cryst. (MeOH). Mp 103°.

2,4-Dinitrophenylhydrazone:
Yellow cryst. (EtOH). Mp 104°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 732C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 469B (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 555D (*ir*)
Blaise, E.E. *et al., Bull. Soc. Chim. Fr.*, 1904, **31**, 492 (*synth*)
Allen, C.F.H. *et al., J.O.C.*, 1941, **6**, 596 (*synth*)
Davies, R.R. *et al., J. Soc. Chem. Ind., London*, 1943, **62**, 128 (*synth*)
Org. Synth., 1971, **51**, 39 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 481 (*rev, tox*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, UJJ000
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

1,11-Undecanediol, 9CI U-13

[765-04-8]

$HOCH_2(CH_2)_9CH_2OH$

$C_{11}H_{24}O_2$ 188.309
Cryst. (C_6H_6). Mp 61° (57-59°).

Bisphenylurethane:
Mp 132-133°.

Mono-Ac: [78782-06-6] *11-Acetoxy-1-undecanol*
$C_{13}H_{26}O_3$ 230.347
Cryst. (C_6H_6/MeOH). Mp 81°.

Di-Ph ether: [141620-04-4] *1,1′-[1,11-Undecanediylbis(oxy)]bisbenzene, 9CI. 1,11-Diphenoxyundecane*
$C_{23}H_{32}O_2$ 340.505
Isol. from the leaves of *Arachis hypogaea* (peanuts) infected with *Puccinia arachidis*.

Colonge, J. *et al., Bull. Soc. Chim. Fr.*, 1959, 1248 (*synth*)
Dulou, R. *et al., Bull. Soc. Chim. Fr.*, 1959, 1362 (*synth*)
Tolyanova, S.G. *et al., Zh. Obshch. Khim.*, 1963, **34**, 565 (*synth*)
Reinheckel, H. *et al., CA*, 1965, **62**, 8990 (*synth*)
Rao, P.V.S. *et al., Oleagineux*, 1991, **46**, 501; *CA*, **116**, 252152 (*di-Ph ether*)
Gawarikar, R. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 877 (*isol, deriv*)
Narasimhan, S. *et al., Synth. Commun.*, 1997, **27**, 385-390 (*synth*)
Nakamura, N. *et al., Acta Cryst. C*, 1999, **55**, 789-791 (*cryst struct*)

2,3-Undecanedione U-14

[7493-59-6]
FEMA 3090

$H_3C(CH_2)_7COCOCH_3$

$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient. Oily yellow liq., with a sweet-cream and coconut-milk taste. Bp_{10} 109-111°.

Bis(thiosemicarbazone):
Mp 231°.

Ger. Pat., 1933, 573 722; *CA*, **27**, 4446 (*synth*)
U.K. Pat., 1964, 966 849; *CA*, **61**, 14533 (*synth*)

Undecanoic acid, 9CI, 8CI U-15

[112-37-8]
Decane-1-carboxylic acid. Hendecanoic acid. Undecylic acid. FEMA 3245

$H_3C(CH_2)_9COOH$

$C_{11}H_{22}O_2$ 186.294
Flavouring ingredient. Present in butter and coconut. Cryst. (AcOH aq.). Insol. H_2O; sol. EtOH, $CHCl_3$, Me_2CO, C_6H_6. Mp 28.2-28.6°. Bp_{100} 212.5° Bp_{15} 164°.
▶ Skin irritant. LD_{50} (mus, ivn) 140 mg/kg. YQ2275000

Me ester: [1731-86-8] *Methyl undecanoate*
$C_{12}H_{24}O_2$ 200.32
Liq. $Bp_{9.5}$ 123° (lit. gives a pressure range) Bp_1 70-72°.
▶ YQ2573000

Et ester: [627-90-7] *Ethyl undecanoate. FEMA 3492*
$C_{13}H_{26}O_2$ 214.347
Flavouring ingredient. Present in rum, whisky and wine. Liq. Bp_{20} 140°.

Vinyl ester: [20690-63-5]
$C_{13}H_{24}O_2$ 212.331

Liq. d^{20} 0.88. Bp_{10} 125°. n_D^{20} 1.4355. Q/e values for radical polym., Q 0.056, e -0.84.

Chloride: [17746-05-3]
$C_{11}H_{21}ClO$ 204.739
Liq. Bp_{20} 135-136°.

Amide: [2244-06-6] *Undecanamide, 9CI*
$C_{11}H_{23}NO$ 185.309
Cryst. (EtOH). Mp 103° (98°).

Nitrile: [2244-07-7] *Undecanenitrile, 9CI. 1-Cyanodecane*
$C_{11}H_{21}N$ 167.294
Liq. Bp 253-254°.

Anhydride: [2082-77-1]
$C_{22}H_{42}O_3$ 354.572
Cryst. (Me_2CO). Mp 35°. $Bp_{17.5}$ 210-245° (lit. gives a pressure range).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 483D; 608B; 730D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 754C; 924A; 924B; 1196B; 1355A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 576A; 627A; 627B; 799A (*ir*)
Aldrich Library of NMR Spectra, **2**, 147C (*pmr*)
Levene, P.A. *et al., J. Biol. Chem.*, 1914, **18**, 464 (*synth*)
Cason, J. *et al., J.O.C.*, 1950, **15**, 139 (*synth*)
Asahara, T. *et al., Yushi Kagaku Kyokaishi*, 1952, **1**, 76; 79; *CA*, **47**, 3232e,f (*synth, polym, vinyl ester*)
Hayashi, S. *et al., Bull. Inst. Chem. Res., Kyoto Univ.*, 1968, **46**, 213; *CA*, **70**, 110173 (*ir*)
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1976, **17**, 1 (*cmr*)
Vergoten, G. *et al., C. R. Hebd. Seances Acad. Sci. Ser. B*, 1977, **284**, 21 (*Raman*)
Greenley, R.Z. *et al., J. Macromol. Sci., Part A: Chem.*, 1980, **14**, 427 (*Q/e values, vinyl ester*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 271; 782
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1045-1046; 2870
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, UKA000

1-Undecanol, 9CI U-16

[112-42-5]

[30207-98-8]
Alcohol C11. Undecylic alcohol. FEMA 3097

$H_3C(CH_2)_9CH_2OH$

$C_{11}H_{24}O$ 172.31
Isol. from hop oil (*Humulus lupulus*). Found in butter, boiled eggs, cooked pork, oysters. Also in many fruits, eg. apple, banana, sour cherry. Flavouring agent. Liq. or cryst. with floral citrus-like odour and fatty flavour. d_4^{23} 0.83. Mp 19° (16.5°). Bp_{15} 131° Bp_6 123-125°. n_D^{23} 1.4392.

▶ Skin irritant. LD_{50} (rat, orl) 3000 mg/kg. YQ3155000

Ac: [1731-81-3] *Undecyl acetate. Acetate C11*
$C_{13}H_{26}O_2$ 214.347
Bp_5 119°.

Benzoyl: [6316-30-9]
$C_{18}H_{28}O_2$ 276.418
Liq. n_D^{20} 1.4841.

4-Nitrobenzoyl: [93094-34-9]
Mp 29.2°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 111D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 166B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 158A (*ir*)
Sadtler Standard C-13 NMR Spectra, 1047 (*cmr*)
Sadtler Standard Proton NMR Spectra, 6851 (*pmr*)
Robinson, R. *et al., J.C.S.*, 1924, **125**, 229 (*synth*)
Jahnsen, V.J. *et al., Nature (London)*, 1962, **196**, 474 (*isol*)
Smentouski, F.J. *et al., J. Am. Oil Chem. Soc.*, 1972, **49**, 48 (*nmr*)
Roelofs, W. *et al., Environ. Entomol.*, 1974, **3**, 747
Levina, O.V. *et al., CA*, 1976, **85**, 93918y (*derivs*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 641 (*rev, tox*)
Brophy, J.J. *et al., Org. Mass Spectrom.*, 1988, **23**, 659 (*ms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, UNA000
Ruddick, C.L. *et al., Synthesis*, 1996, 1359 (*synth, pmr, ir*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

2-Undecanol U-17

[1653-30-1]

[30207-98-8]
FEMA 3246

$H_3C(CH_2)_8CH(OH)CH_3$

$C_{11}H_{24}O$ 172.31
Present in apple, banana, papaya, strawberry, chive, roasted onion, cheeses, ginger, cognac, hop oil and other foodstuffs. Flavouring agent with fruity taste at low concentration..

▶ Fl. p. 113° (oc).

(R)-form [85617-06-7]
Isol. from leaf oil of *Litsea odorifera*, rue (*Ruta graveolens*) and a few other sources. Bp 231-233°.

(S)-form [85617-05-6]
Isol. from cocoa butter and coconut. Mp 12°. Bp_{20} 128°. $[\alpha]_D^{20}$ +8.11 (EtOH). $[\alpha]_D^{20}$ +10.29 (C_6H_6).

Ac: [14936-67-5]
$C_{13}H_{26}O_2$ 214.347
Bp_{15} 84°.

Benzoyl:
$C_{18}H_{28}O_2$ 276.418
$Bp_{3.5}$ 159°. $[\alpha]_D^{20}$ +27.55.

Hydrogen phthalate:
Mp 31-32°. $[\alpha]_D$ +37.3 ($CHCl_3$). $[\alpha]_D$ +44.3 (EtOH).

(±)-form [113666-64-1]
Bp 228-229° Bp_{12} 119°.

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 72F (*ir*)
Power, F.B. *et al., J.C.S.*, 1902, **101**, 1593 (*isol*)
v. Romburgh, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1911, 1863 (*isol*)
Pickard, R.H. *et al., J.C.S.*, 1914, **105**, 850 (*synth*)
Keil, W. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1942, **274**, 175
VanderMoss, J.H. *et al., Spectrochim. Acta A*, 1974, **30**, 2005 (*ir*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2871 (*props, occur*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 1077

2-Undecanone U-18

[112-12-9]
Methyl nonyl ketone. Enodyl. Luparone. FEMA 3093

$H_3C(CH_2)_8COCH_3$

$C_{11}H_{22}O$ 170.294
Found in palm kernel oil and soya bean oil. Important constit. of rue oil (*Ruta graveolens*) and found in many other essential oils. Also found in black currant buds, raspberry, black berry peach and other fruits. Used in flavourings. Fp 15. Bp 228° Bp_{12} 105-106°.

▶ LD_{50} (rat, orl) 5000 mg/kg. Fl. p. 89°. YQ2820000

Oxime: [2158-28-3]
$C_{11}H_{23}NO$ 185.309
Mp 44-45°.

2,4-Dinitrophenylhydrazone: [2121-90-6]
Orange-yellow cryst. Mp 63°.

Semicarbazone: [820-35-9]
Cryst. (EtOH). Mp 122-123°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 412A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 641A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 497B (*ir*)
Haller, A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1910, **151**, 698 (*isol*)
Dhont, J.H. *et al., Analyst (London)*, 1969, **94**, 1090 (*chromatog*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 425 (*occur*)
Kuleza, J. *et al., CA*, 1973, **78**, 136186 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1975, **13**, 869 (*rev, tox*)
Bradshaw, J.W.S. *et al., Nature (London)*, 1975, **258**, 230 (*biochem*)
Cainelli, G. *et al., J.A.C.S.*, 1976, **98**, 6737 (*synth*)
Anderson, M.W. *et al., J.C.S. Perkin 1*, 1986, 1995 (*synth, ir, pmr*)
McDowell, P.G. *et al., Phytochemistry*, 1988, **27**, 2519 (*isol*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, UKS000

6-Undecanone U-19

[927-49-1]
Dipentyl ketone. Diamyl ketone. Pentyl ketone. Amyl ketone

$H_3C(CH_2)_4CO(CH_2)_4CH_3$

$C_{11}H_{22}O$ 170.294
Constit. of *Osmanthus fragrans* (sweet osmanthus). Mp 14-15°. Bp 226° Bp_9 100-104°.

▶ LD_{50} (mus, ivn) 117 mg/kg. YQ2828000

Oxime: [32504-26-0]
$C_{11}H_{23}NO$ 185.309

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 412B (*ir*)

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 641B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 497D (*ir*)
Sabatier, E.E. *et al., C. R. Hebd. Seances Acad. Sci.* , 1914, **158**, 832 (*synth*)
Lippmaa, E. *et al., CA* , 1968, **69**, 111930 (*cmr*)
Di Paolo, T. *et al., J. Pharm. Sci.* , 1978, **67**, 566 (*pharmacol, tox*)
Mistryukov, E.A. *et al., Synthesis*, 1984, 947 (*synth, pmr*)
Slobodkin, G. *et al., Synth. Commun.* , 1990, **20**, 247 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ULA000

1,3,5-Undecatriene U-20

[16356-11-9]
Cystophorene
$H_3C(CH_2)_4CH{=}CHCH{=}CHCH{=}CH_2$
$C_{11}H_{18}$ 150.263
Food additive listed in the EAFUS Food Additive Database (Jan. 2001). Occurs in Galbanum extract (*Ferula galbaniflua*).

(3*E*,5*E*)-*form* [19883-29-5]
Bp_{10} 100-105°.

(3*E*,5*Z*)-*form* [51447-08-6]
Galbanolene
Bp_{10} 100-105°.

(3*Z*,5*Z*)-*form* [19883-26-2]
Oil. Bp_6 100°. Thermally unstable.

Chretien-Bessiere, Y. *et al., Bull. Soc. Chim. Fr.* , 1967, 97 (*isol*)
Teisseire, P. *et al., Recherches*, 1967, **16**, 5 (*synth*)
Cowie, J.S. *et al., J.C.S. Perkin 1* , 1972, 2197-2201 (*synth*)
Moore, R.E. *et al., J.O.C.* , 1974, **39**, 2201 (*isol*)
Naef, F. *et al., Helv. Chim. Acta* , 1975, **58**, 1016 (*synth*)
Giraudi, E. *et al., Tet. Lett.* , 1983, **24**, 489 (*synth, pmr*)
Hayashi, T. *et al., Tet. Lett.* , 1983, **24**, 2665 (*synth*)
Block, E. *et al., J.A.C.S.* , 1986, **108**, 4568 (*synth, bibl*)
Ratovelomanana, V. *et al., Bull. Soc. Chim. Fr.* , 1987, 174 (*synth, ir, cmr, ms, bibl*)
Andreini, B.P. *et al., Tetrahedron*, 1987, **43**, 4591 (*synth, pmr, ir, ms*)
Ford, R.A. *et al., Food Chem. Toxicol.* , 1988, **26**, 415 (*rev, tox*)
Tsuboi, S. *et al., Bull. Chem. Soc. Jpn.* , 1990, **63**, 1888 (*synth*)
Tellier, F. *et al., Tetrahedron* , 1991, **47**, 7767 (*synth*)
Alexakis, A. *et al., Synth. Commun.* , 1992, **22**, 1839 (*synth*)
Solladie, G. *et al., Synlett* , 1993, 548 (*synth*)
Huynh, C. *et al., Synth. Commun.* , 1994, **24**, 2273 (*Galbanolene, synth, ir, pmr, cmr, ms*)
Alami, M. *et al., Tetrahedron*, 1995, **51**, 1209 (*synth*)

2-Undecenal, 9CI U-21

[2463-77-6]

[1337-83-3]
FEMA 3423
$H_3C(CH_2)_7CH{=}CHCHO$
$C_{11}H_{20}O$ 168.278

(*E*)-*form* [53448-07-0]
Component of dried/smoked fish aroma. Present in leaf and flower essential oils, and fruit (orange peel and blackberries), butter, cooked chicken, beef, mutton, pork and roasted nuts. Flavouring ingredient. Liq. Bp_2 88-90°.

2,4-Dinitrophenylhydrazone:
Solid. Mp 122.6°. Assignment to (*E*)-form is not certain.

Semicarbazone:
Solid. Mp 161.5-162.5°. Assignment to (*E*)-form is not certain.

(*Z*)-*form* [71277-05-9]
Component of roasted chicken/guinea hen meat and mango aroma. Liq. Bp_{18} 129-131°.

Swift, C.E. *et al., J.A.C.S.* , 1949, **71**, 1512 (*synth*)
Bestmann, H.J. *et al., Tet. Lett.* , 1977, 121 (*synth, pmr*)
Bestmann, H.J. *et al., Chem. Ber.* , 1982, **115**, 161 (*synth, pmr, ir, ms, uv*)
Huang, Y.Z. *et al., J.O.C.* , 1987, **52**, 3558 (***synth, pmr, ms, ir, gc***)
Boelens, M.H. *et al., Perfum. Flavor.* , 1987, **12**, 31; *CA* , **107**, 115390x (*props*)
Richardson, S.D. *et al., Environ. Toxicol. Chem.* , 1991, **10**, 991; *CA* , **115**, 141892x (*isol, gc, ms*)
Fortes, C.C. *et al., Synth. Commun.* , 1997, **27**, 3917-3941 (*synth, ir, pmr, cmr, ms*)

9-Undecenal, 9CI, 8CI U-22

[143-14-6]
FEMA 3094
$H_3CCH{=}CH(CH_2)_7CHO$
$C_{11}H_{20}O$ 168.278
Present in juniper leaf oil. Flavouring ingredient. Liq. with orange peel-like odour and sweet citrus flavour.

Von Sydon, E. *et al., Arch. Mass Spectral Data* , 1971, **2**, 52-63 (*ms*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 785 (*use, props*)
Adams, R.P. *et al., J. Essent. Oil Res.* , 1996, **8**, 367-371 (*isol*)

10-Undecenal, 9CI U-23

[112-45-8]

[1337-83-3]
10-Undecylenic aldehyde. FEMA 3095
$H_2C{=}CH(CH_2)_8CHO$
$C_{11}H_{20}O$ 168.278
Found in coriander leaf (*Coriandrum sativum*). Perfumery and flavouring ingredient. Liq. with heavy flowery odour. Bp_{10} 101-103°. n_D^{21} 1.4464.
▶ Skin irritant. YQ2835000

2,4-Dinitrophenylhydrazone:
Mp 91°.

Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **1**, 474B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 740B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 563A (*ir*)
Nigam, S.S. *et al., J.C.S.* , 1957, 3320-3321 (*synth*)
Gringas, B.A. *et al., Can. J. Chem.* , 1960, **38**, 712-719 (*ir*)
Hideg, K. *et al., J.C.S. Perkin 1* , 1986, 1431-1438 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook* , Van Nostrand Reinhold International, New York, 1989, ULJ000
Sasaerila, Y. *et al., J. Chem. Ecol.* , 1997, **23**, 2187-2196 (*isol*)
Clark, G.S. *et al., Perfum. Flavor.* , 1997, **22**, 29-32 (*rev, synth, props*)
Kabalka, G.W. *et al., Can. J. Chem.* , 1998, **76**, 800-805 (*synth, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

1-Undecene U-24

[821-95-4]

[28761-27-5]
$H_3C(CH_2)_8CH{=}CH_2$
$C_{11}H_{22}$ 154.295
Oil from flower stalk of *Petasites japonicus* (sweet coltsfoot). d_4^{20} 0.76. Fp -49.1. Bp 192.7° Bp_{10} 73°. n_D^{20} 1.4284.

Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra , 1992, **1**, 19C (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn. , 1985, **1**, 14D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 19D (*ir*)
Asinger, F. *et al., Chem. Ber.* , 1964, **97**, 1555
Kikuchi, M. *et al., Yakugaku Zasshi*, 1973, **93**, 123 (*isol*)
Bongini, A. *et al., J. Organomet. Chem.* , C4, 1974, **72**, (*synth*)
Tschinkel, W.R. *et al., J. Insect Physiol.* , 1975, **21**, 753 (*isol*)

4-Undecene, 9CI, 8CI U-25

[20810-21-3]

[28761-27-5]
$H_3CCH_2CH_2CH{=}CH(CH_2)_5CH_3$
$C_{11}H_{22}$ 154.295

(*E*)-*form* [693-62-9]
Found in beef. Oil. Fp -63.7. Bp_{10} 73.3°.

Asinger, F. *et al., Chem. Ber.* , 1964, **97**, 1555 (*synth*)
Fuqua, S.M. *et al., J.O.C.* , 1965, **30**, 2543
Rienaecker, R. *et al., Annalen*, 1970, **737**, 182 (*synth*)
Rang, S. *et al., CA* , 1977, **87**, 67504 (*ms*)
Van Horn, D.E. *et al., J.A.C.S.* , 1978, **100**, 2252 (*synth*)

9-Undecenoic acid U-26

[593-25-9]

[1333-28-4]
$H_3CCH{=}CH(CH_2)_7COOH$
$C_{11}H_{20}O_2$ 184.278

(*E*)-*form* [37973-84-5]
Mp 17-18°. $Bp_{0.7}$ 121-123°.

Me ester: [37973-85-6]

[5760-50-9, 54299-07-9] *FEMA 2750*
$C_{12}H_{22}O_2$ 198.305
Flavouring ingredient with a brandy-like flavour. Bp_1 137-140°.

Et ester:
$C_{13}H_{24}O_2$ 212.331
$Bp_{0.5}$ 87-89°.

(*Z*)-*form*
Mp 1-2°. $Bp_{0.8}$ 118-120°.

Et ester:
$Bp_{0.6}$ 88-90°.

Ames, D.E. *et al., J.C.S.* , 1952, 677 (*synth*)
Cowie, J.S. *et al., J.C.S. Perkin 1* , 1972, 2197-2201 (*synth*)
Davies, J.E.D. *et al., Chem. Phys. Lipids*, 1975, **15**, 157 (*ir*)

Lam, C.H. *et al., Chem. Phys. Lipids*, 1976, **16**, 181 (*synth*)
Kabara, J.J. *et al., Lipids*, 1977, **12**, 753
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 580 (*Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1879-1880 (*Me ester*)

10-Undecenoic acid, 9CI U-27

[112-38-9]
Undecylenic acid, USAN. *FEMA 3247*
$H_2C{=}CH(CH_2)_8COOH$
$C_{11}H_{20}O_2$ 184.278
Flavouring ingredient. Insol. H_2O; misc. EtOH, $CHCl_3$, Et_2O, C_6H_6. Mp 24.5°. Bp 275° Bp_{15} 165°. n_D^{25} 1.4480. Log P 4.04 (calc). Component of Cruex, Desenex, Fulvidex and Ting..
▶ Severe skin irritant. LD_{50} (rat, orl) 2500 mg/kg. YQ2975000

Na salt: [3398-33-2]
Solid.

Zn salt (2:1): [557-08-4] *Zinc undecylenate, USAN*
Mp 116-121°.

Me ester: [111-81-9]
$C_{12}H_{22}O_2$ 198.305
Fp -27.5. Bp 248° Bp_{10} 124°.

Et ester: [692-86-4] *FEMA 2461*
$C_{13}H_{24}O_2$ 212.331
Flavouring ingredient. Found in rum and cognac. Oil with wine-like odour. Bp 263.5-265.5° Bp_{16} 131.5°.
▶ LD_{50} (rat, orl) >5000 mg/kg. YQ2978400

Propyl ester:
$C_{14}H_{26}O_2$ 226.358
d_4^{20} 0.88. Bp 268°.

Isopropyl ester: [5459-98-3]
$C_{14}H_{26}O_2$ 226.358
d^{15} 0.87. Bp 260°.

2-Propenyl ester: [7493-76-7] *Allyl undecylenate. FEMA 2044*
$C_{14}H_{24}O_2$ 224.342
Flavouring ingredient with a fruity odour suggestive of pineapple. Liq. d 0.93. Bp 230° Bp_{30} 180°. n_D^{23} 1.4479.

Butyl ester: [109-42-2] *Butyl undecylenate. FEMA 2216*
$C_{15}H_{28}O_2$ 240.385
Flavouring ingredient. d_4^{20} 0.88. Bp 252°. n_D^{20} 1.4426.

3-Methylbutyl ester:3-Methylbutyl 10-undecenoate. Isoamyl undecylenate
$C_{16}H_{30}O_2$ 254.412
Bp_3 160°.

Chloride: [38460-95-6]
$C_{11}H_{19}ClO$ 202.723
Liq. d 0.94. Bp_{10} 120-122° Bp_2 102°. n_D^{20} 1.4540. n_D^{21} 1.4552.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 501A (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 781C; 852B; 986B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 587B; 684C (*ir*)
Krafft, F. *et al., Ber.*, 1884, **17**, 2985 (*synth*)
English, J. *et al., J.A.C.S.*, 1945, **67**, 1413-1414 (*chloride*)
Nimgirawath, S. *et al., Aust. J. Chem.*, 1973, **26**, 183 (*chloride*)
Osman, S.M. *et al., Fette, Seifen, Anstrichm.*, 1975, **77**, 473
McGrattan, C.J. *et al., J. Phycol.*, 1976, **12**, 129
Gunstone, F.D. *et al., Chem. Phys. Lipids*, 1977, **18**, 115 (*cmr*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1978, **16**, 883 (*rev, tox*)
Tamao, K. *et al., J.A.C.S.*, 1978, **100**, 2268 (*synth*)
Hunting, A.L.L. *et al., Cosmet. Toiletries*, 1981, **96**, 29 (*rev, uses*)
Dalavoy, V.S. *et al., J. Sci. Ind. Res.*, 1981, **40**, 520 (*rev*)
Brauner, A. *et al., Org. Mass Spectrom.*, 1985, **20**, 578 (*ms*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2165
Purgett, M.D. *et al., J. Polym. Sci., Part A: Polym. Chem.*, 1988, **26**, 677 (*polym, esters*)
Denton, J.M. *et al., J. Phys. Chem.*, 1993, **97**, 756 (*oligomers, Na salt*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 332
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 33; 96 (*esters*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 102-103; 357-358; 1046; 2876 (*esters*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ULS000

2-Undecen-1-ol U-28

[37617-03-1]
$H_3C(CH_2)_7CH{=}CHCH_2OH$
$C_{11}H_{22}O$ 170.294

(E)-form [75039-84-8]
Liq. Bp_1 98°.

(Z)-form [75039-83-7]
Liq. Bp_1 78-80°. n_D^{20} 1.4529.

Me ether: [100924-61-6] *1-Methoxy-2-undecene, 9CI*
$C_{12}H_{24}O$ 184.321
Liq. Bp_4 60-62°. n_D^{20} 1.4391.

Spur, B. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1985, **318**, 225-228 (*Z-form, synth*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 771-772 (*Z-form, synth, ir, pmr*)
Andreeva, N.I. *et al., Zh. Obshch. Khim.*, 1985, **55**, 1316-1323; *J. Gen. Chem. USSR (Engl. Transl.)*, 1985, **55**, 1176-1182 (*Z-form, synth, Me ether, ir, pmr*)
Aerssens, M.H.P.J. *et al., Synth. Commun.*, 1990, **20**, 3421-3425 (*Z-form, synth*)
Zhang, Z.-B. *et al., J.C.S. Perkin 1*, 2000, 53-57 (*E-form, synth, ir, pmr*)
Kobayashi, Y. *et al., Eur. J. Org. Chem.*, 2001, 1873-1881 (*E-form, synth, cmr*)

10-Undecen-1-ol U-29

[112-43-6]
Undecylenic alcohol
$H_2C{=}CH(CH_2)_8CH_2OH$
$C_{11}H_{22}O$ 170.294
Flavouring ingredient. Liq. Fp -2. Bp_{14} 133° Bp_6 123-125°.
▶ Skin irritant. YQ2985000

Ac: [112-19-6] *FEMA 3096*
$C_{13}H_{24}O_2$ 212.331
Flavouring ingredient. d^{20} 0.88. Bp 272° Bp_7 125-127°.
▶ YQ2990000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 145D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 218A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 214A (*ir*)
Bestmann, H.J. *et al., Tet. Lett.*, 1977, 121 (*synth*)
Miyaura, N. *et al., Tetrahedron*, 1982, **39**, 3271 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 717
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2876-2877; 2878
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, UMA000; UMS000

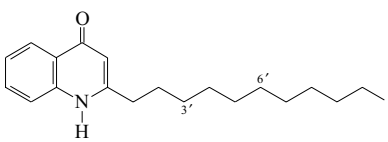
10-Undecen-2-one, 9CI U-30

[36219-73-5]
$H_2C{=}CH(CH_2)_7COCH_3$
$C_{11}H_{20}O$ 168.278
Constit. of dwarf mountain pine (*Pinus mugo*) essential oil. Bp 235° Bp_{30} 135°.

Cottier, L. *et al., Bull. Soc. Chim. Fr.*, 1972, 1072 (*synth*)
Bambagiotti, A.M. *et al., Planta Med.*, 1981, **43**, 39 (*isol*)
Ashby, E.C. *et al., Organometallics*, 1984, **3**, 1718 (*synth, pmr*)
Arbain, D. *et al., Aust. J. Chem.*, 1990, **43**, 1949 (*isol, ir, pmr, cmr, ms*)

2-Undecyl-4(1*H*)-quinolinone, 9CI U-31

[56183-46-1]
4-Hydroxy-2-undecylquinoline



$C_{20}H_{29}NO$ 299.455
Alkaloid from and roots of *Ruta graveolens* (rue) (as the main component of an inseparable mixt. of 2-alkylquinolones contg. the 2-dodecyl, 2-tridecyl and 2-tetradecyl homologues) (Rutaceae). Cryst. (Me_2CO). Mp 130-132°.

N-*Oxide:* [2503-86-8] ***2-Undecyl-4(1H)-quinolinone* N-*oxide***
$C_{20}H_{29}NO_2$ 315.455
Isol. from roots of *Ruta graveolens* (rue). Leaflets. Mp 148.5-149.5°.

N-*Me:* [59443-02-6] ***1-Methyl-2-undecyl-4(1H)-quinolinone, 9CI***
$C_{21}H_{31}NO$ 313.482
Needles (EtOAc/Et_2O). Mp 68.5-70°.

3′,4′-Didehydro: [71932-11-1] *2-(3-Undecenyl)-4(1H)-quinolinone.* ***Pyo V***
$C_{20}H_{27}NO$ 297.439
Mp 114°. λ_{max} 213 (ϵ 37300); 236 (ϵ 37000); 316 (ϵ 12200); 327 (ϵ 12900) (MeOH) (Berdy).

5′,6′-Didehydro, N-*Me (Z-):* ***1-Methyl-2-(5-undecenyl)-4(1H)-quinolinone***
$C_{21}H_{29}NO$ 311.466
Oil. Isol. as an inseparable mixt. with the $\Delta^{6'}$-isomer.

6′,7′-Didehydro, N-*Me (Z-):* ***1-Methyl-2-(6-undecenyl)-4(1H)-quinolinone***

$C_{21}H_{29}NO$ 311.466
Oil.

10′-Acetoxy, N-*(acetoxymethyl):* ***1-Acetoxymethyl-2-(10-acetoxyundecyl)-4(1H)-quinolinone***
$C_{25}H_{35}NO_5$ 429.555
Dark yellow oil. $[\alpha]_D$ -1 (c, 0.45 in MeOH).

10′-Oxo: [29479-53-6] ***2-(10-Oxoundecyl)-4(1H)-quinolinone***
$C_{20}H_{27}NO_2$ 313.439
Cryst. (Me_2CO). Mp 126°.

Cornforth, J.W. *et al., Biochem. J.*, 1956, **63**, 124 (*isol*)
Kan-Fan, C. *et al., Phytochemistry*, 1970, **9**, 1283 (*10′-oxo*)
Reisch, T. *et al., Phytochemistry*, 1975, **14**, 840 (*isol, ir, pmr*)
Kamikado, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 605 (*deriv*)
Budzikiewicz, H. *et al., Monatsh. Chem.*, 1979, **110**, 947 (*deriv*)
Sugimoto, T. *et al., Chem. Pharm. Bull.*, 1988, **36**, 4453 (*isol, uv, ir, pmr, cmr, ms, deriv*)
Tang, Y.-Q. *et al., Phytochemistry*, 1996, **43**, 719 (*deriv*)
Gibbons, S. *et al., Phytochemistry*, 1997, **44**, 1109 (*deriv*)

2-Undecynoic acid U-32

[54299-08-0]
$H_3C(CH_2)_7C{\equiv}CCOOH$
$C_{11}H_{18}O_2$ 182.262
$Bp_{0.03}$ 103°.

S-*Benzylisothiouronium salt:*
Mp 174-175°.

Me ester: [10522-18-6] *FEMA 2751*
$C_{12}H_{20}O_2$ 196.289
Flavouring ingredient. Liq. Insol. H_2O; sol. EtOH. d^{20} 0.92. Bp 230° $Bp_{0.2}$ 116-120°. n_D^{20} 1.4465.

Et ester: [10519-17-2]
$C_{13}H_{22}O_2$ 210.316
Bp_{10} 128°.

Barker, S.A. *et al., Tetrahedron*, 1962, **18**, 177 (*synth*)
Lie Ken Jie, M.S.F. *et al., J. Chromatogr.*, 1974, **97**, 165 (*synth*)
Davies, J.E.D. *et al., Chem. Phys. Lipids*, 1975, **15**, 157 (*ir, uv*)
Bus, J.D. *et al., Chem. Phys. Lipids*, 1976, **17**, 501 (*cmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 581 (*Me ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1880 (*Me ester*)
Fortes, C.C. *et al., Synth. Commun.*, 1997, **27**, 2993-3026 (*synth, Me ester, ir, pmr, cmr, ms*)

Urea, 9CI, 8CI, USAN U-33

[57-13-6]
Carbamide. Ureaphil. E927b
H_2NCONH_2
CH_4N_2O 60.055
Formulation aid. Cattle feed supplement. Tetragonal needles or prisms with faint salty taste (H_2O or EtOH). V. sol. H_2O; sol. MeOH, EtOH; insol. $CHCl_3$, C_6H_6. Mp 133-135°. pK_a 0.1 (21°). Log P -2.11 (calc). Aq. solns hydrol. v. slowly to ammonium carbamate then to NH_3 and CO_2. Weak base. Polymer with formaldehyde (Polynoxylin, BAN, INN) used as a topical antibacterial and antifungal agent.
▶ Irritant to skin, eyes, respiratory tract and mucous membranes. Human reprod. effects (abortifacient), exp. reprod. effects. LD_{50} (rat, orl) 8471 mg/kg. YR6250000

Phosphate salt: [4861-19-2]

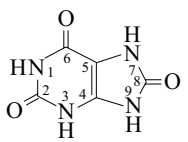
[4401-74-5]
Used in animal feeds. Hygroscopic cryst. (H_2O). Mp 118-121°.

[1433-11-0, 17687-37-5, 21351-39-3]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 670B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 799C (*ir*)
Reifer, J. *et al., J. Biol. Chem.*, 1949, **178**, 715 (*occur*)
Mootz, D. *et al., Acta Cryst. B*, 1972, **28**, 2459-2463 (*cryst struct, phosphate*)
Witanowski, M. *et al., Tetrahedron*, 1976, **32**, 2127 (*nmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 548 (*rev, bibl*)
Swawinathan, S. *et al., Acta Cryst. B*, 1984, **40**, 300 (*cryst struct*)
Gorecki, H. *et al., Przem. Chem.*, 1984, **63**, 411-413; *CA*, **102**, 77486v (*rev, phosphate*)
Horsch, W. *et al., Pharmazie*, 1985, **40**, 665 (*rev, use, props*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, USS000
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HIB500; USS000

Uric acid, 8CI U-34

[69-93-2]
7,9-Dihydro-1H-purine-2,6,8(3H)-trione, 9CI. 2,6,8-Trihydroxypurine. 2,6,8(1H,3H,9H)-Purinetrione



$C_5H_4N_4O_3$ 168.112
Exists in several tautomeric forms. Occurs as phosphate in yeast and meat products. Odourless, tasteless, rhombic prisms or plates. Sol. alkalis, glycerol; spar. sol. min. acids; v. spar. sol. H_2O; insol. EtOH, Et_2O. pK_a 5.75; pK_{a2} 10.6. Dec. without melting.
▶ Exp. reprod. effects (male). May evolve HCN when heated. YU7050080

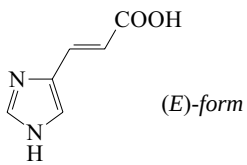
1,3,9-Tri-Me: [7464-93-9] *1,3,9-Trimethyluric acid. 8-Oxocaffeine*
$C_8H_{10}N_4O_3$ 210.192
Present in roasted coffee beans and instant coffee, but not green coffee beans. Needles or plates (H_2O). Insol. H_2O; spar. sol. EtOH, $CHCl_3$. Mp 335° dec.

1,3,7,9-Tetra-Me: [2309-49-1] *Tetramethyluric acid*
$C_9H_{12}N_4O_3$ 224.219
Isol. from tea. Needles (H_2O). Spar. sol. Et_2O; sol. hot $CHCl_3$. Mp 228°. Distils without dec..

[1198-77-2]
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 710A; 710C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 214C; 215A (*nmr*)
Johnson, T.B. *et al., J.A.C.S.*, 1937, **59**, 1261 (*tetra-Me, isol*)
Sutor, D.J. *et al., Acta Cryst.*, 1963, **16**, 97 (*tetra-Me, cryst struct*)
Lifschitz, C. *et al., Isr. J. Chem.*, 1968, **6**, 827 (*ms*)
Pfleiderer, W. *et al., Annalen*, 1974, 2030 (*uv, ms, Me derivs*)
Bryant, W.F. *et al., Anal. Biochem.*, 1975, **65**, 73 (*tetra-Me*)
Weiner, I.M. *et al., CA*, 1975, **82**, 28926 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **23**, 608 (*rev, bibl*)
Stadler, R.H. *et al., J. Agric. Food Chem.*, 1995, **43**, 1332-1338 (*1,3,9-tri-Me, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, UVA400

Urocanic acid U-35

[104-98-3]
3-(1H-Imidazol-4-yl)-2-propenoic acid, 9CI. 4-Imidazoleacrylic acid, 8CI. Urocaninic acid



(*E*)-*form*

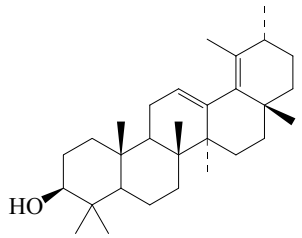
$C_6H_6N_2O_2$ 138.126
Zwitterionic.Mp 243-245°.
▶ NI3425200

(*E*)-*form* [3465-72-3]
Isol from fungi, e.g. *Coprinus atramentarius* (common ink cap) and *Phallus impudicus* (common stinkhorn). Cryst. (dihydrate). Sol. Py, bases; fairly sol. H_2O, butanol, EtOH; poorly sol. EtOAc, hexane. Mp 225° (218-224°). λ_{max} 260 (H_2O) (Berdy).
▶ LD_{50} (mus, ivn) 200 - 400 mg/kg.

[6198-55-6]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 492A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 621A (*ir*)
Edlbacher, S. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1942, **276**, 126; 1943, **279**, 63 (*isol, biosynth*)
Biochem. Prep., 1955, **4**, 50 (*synth*)
Gregoire, J. *et al., Bull. Soc. Chim. Belg.*, 1958, **40**, 767 (*isol*)
List, F.H. *et al., Hoppe Seyler's Z. Physiol. Chem.*, 1960, **319**, 17 (*isol*)
Japan. Pat., 1961, 61 23 094; *CA*, **60**, 2302 (*isol*)
Baden, H. *et al., Nature (London)*, 1966, **210**, 732 (*pmr*)
Shibatari, T. *et al., Appl. Microbiol.*, 1974, **27**, 688 (*biosynth*)
Svinning, T. *et al., Acta Cryst. B*, 1979, **35**, 2813 (*cryst struct*)
Shukla, M.K. *et al., Spectrochim. Acta A*, 1995, **51**, 831 (*uv, fluorescence, photochem*)
Hanson, K.M. *et al., J.A.C.S.*, 1997, **119**, 2715 (*spectra*)
Mohammad, T. *et al., Org. Prep. Proced. Int.*, 2000, **32**, 581-584 (*Z-form, synth, ir, uv, pmr, cmr*)

12,18-Ursadien-3-ol U-36



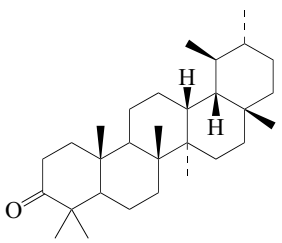
$C_{30}H_{48}O$ 424.709

3β-*form* [239116-64-4]
Momodicaursenol. *Momordicaursenol*
Constit. of the seeds of the famine food *Momordica dioica*. The name Momodicaursenol was prob. an error: Momordicaursenol was prob. meant.

Ali, M. *et al., Indian J. Pharm. Sci.*, 1998, **60**, 287-289 (*isol, pmr, cmr*)

3-Ursanone U-37

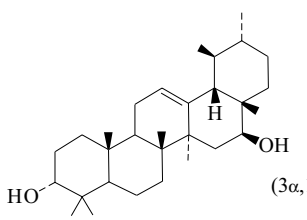
[114717-95-2]
Mangiferursanone



$C_{30}H_{50}O$ 426.724
Constit. of the root bark of *Mangifera indica* (mango). Cryst. ($CHCl_3$/MeOH). Mp 236-238°. λ_{max} 222 (log ϵ 5.4) (MeOH).

Gupta, J. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 1093-1098

12-Ursene-3,16-diol U-38



(3α,16β)-*form*

$C_{30}H_{50}O_2$ 442.724

(3α,16β)-*form* [122475-43-8]
Isol. from *Canarium album* (Chinese white olive). Cryst. Mp 127-128°. $[\alpha]_D^{23}$ +43 (c, 1 in $CHCl_3$).

(3β,16β)-*form* [31575-82-3]
Brein
Cryst. (MeOH aq.). Mp 221-222°. $[\alpha]_D^{26}$ +63.5 ($CHCl_3$). Incorr. descr. in CA as the (3β,16α)-isomer.

3-Dodecanoyl: [357419-18-2] *Brein laurate*
$C_{42}H_{72}O_3$ 625.029
Amorph. solid.

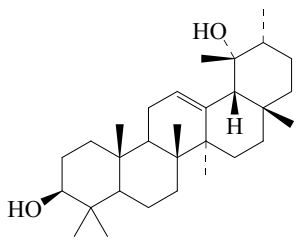
3-Tetradecanoyl: [357419-19-3] *Brein myristate*
$C_{44}H_{76}O_3$ 653.083
Cryst. Mp 90-91°.

3-Hexadecanoyl: [357419-20-6] *Brein palmitate*
$C_{46}H_{80}O_3$ 681.136
Amorph. solid.

[465-08-7]

Laird, W. *et al., J.A.C.S.*, 1960, **82**, 4108 (*struct*)
Kasprzyk, Z. *et al., Phytochemistry*, 1968, **7**, 1631 (*isol*)
Strüby, K. *et al., Phytochemistry*, 1972, **11**, 1733 (*biosynth*)
Tamai, M. *et al., Planta Med.*, 1989, **55**, 44 (*isol*)
Ukiya, M. *et al., J. Agric. Food Chem.*, 2001, **49**, 3187-3197 (*Chrysanthemum morifolium esters*)

12-Ursene-3,19-diol U-39



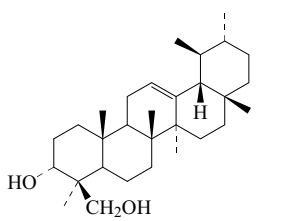
$C_{30}H_{50}O_2$ 442.724

(3β,19α)-*form*

3-Ac: [273223-68-0]
$C_{32}H_{52}O_3$ 484.761
Constit. of *Pyrus communis* (pear).

Younes, M.E. *et al., Egypt. J. Chem.*, 1999, **42**, 573-586; *CA*, **133**, 28459v (*isol, pmr, cmr*)

12-Ursene-3,24-diol U-40



3α-*form*

$C_{30}H_{50}O_2$ 442.724

3α-*form*
Constit. of *Boswellia serrata* (Indian olibanum). Cryst. (EtOAc/petrol). Mp 180°.

24-Carboxylic acid: [631-69-6] *3-Hydroxy-12-ursen-24-oic acid*. ***β-Boswellic acid***
Constit. of frankincense (*Boswellia* spp.) and olibanum oil. Cryst. (MeOH). Mp 238-240° (228-232°). $[\alpha]_D$ +119 (+107) ($CHCl_3$).

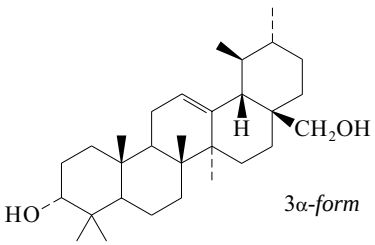
24-Carboxylic acid, Me ester: [17019-94-2]
Cryst. ($CHCl_3$/MeOH). Mp 195-196°. $[\alpha]_D^{14}$ +161 ($CHCl_3$).

24-Carboxylic acid, 3-Ac: [5968-70-7]
$C_{32}H_{50}O_4$ 498.745
Constit. of frankincense and hops. Cryst. (MeOH). Mp 273-275°. $[\alpha]_D$ +149 (c, 2.1 in $CHCl_3$).

3β-*form* [20475-88-1]
Cryst. Mp 227-229°.

Beton, J.L. *et al., J.C.S.*, 1956, 2904 (*isol, struct*)
Budzikiewicz, H. *et al., J.A.C.S.*, 1963, **85**, 3688 (*ms*)
Allan, G.G. *et al., Phytochemistry*, 1968, **7**, 963 (*stereochem*)
Mahajan, B. *et al., Phytochemistry*, 1995, **39**, 453 (*isol, pmr, cmr, struct*)
Van Bergen, P.F. *et al., Tet. Lett.*, 1997, **38**, 8409-8412 (*archaeology*)
Susunaga, G.S. *et al., Fitoterapia*, 2001, **72**, 709-711 (*3β-form, isol, pmr, cmr*)

12-Ursene-3,28-diol U-41



3α-*form*

$C_{30}H_{50}O_2$ 442.724
Log P 8.68 (uncertain value) (calc).

3α-*form* [987-94-0]
Epiuvaol
Mp 212-214° (205-207°). $[\alpha]_D$ +49.7. $[\alpha]_D^{20}$ +65 ($CHCl_3$).

3β-*form* [545-46-0]
Uvaol
Constit. of olive oil and *Osmanthus fragrans* (sweet osmanthus). Cryst. (CH_2Cl_2/MeOH). Mp 232-233°. $[\alpha]_D$ +70 (c, 0.93 in $CHCl_3$). Pharmacol. active isomer λ_{max} 205 (MeOH) (Berdy).

3-Ac: [25089-86-5]
$C_{32}H_{52}O_3$ 484.761
Needles. Mp 264-267°.

28-Aldehyde: [19132-81-1] *3β-Hydroxy-12-ursen-28-al*. ***Ursolic aldehyde***
$C_{30}H_{48}O_2$ 440.708

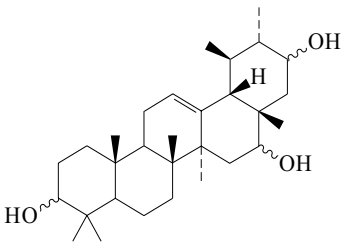
28-Aldehyde, 3-Ac: [86996-88-5] *3β-Acetoxy-12-ursen-28-al*
$C_{32}H_{50}O_3$ 482.745
Needles. Mp 244° (209-210°). $[\alpha]_D$ +73 (C_6H_6).

28-Aldehyde, 3-ketone: [35936-63-1] *3-Oxo-12-ursen-28-al*. ***Ursonic aldehyde***
$C_{30}H_{46}O_2$ 438.692
Cryst. (MeOH). Mp 130°.

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 569C (*nmr*)
Zürcher, A. *et al., Helv. Chim. Acta*, 1954, **37**, 2145 (*synth*)
Shamma, M. *et al., J.O.C.*, 1962, **27**, 4512 (*pmr*)
Yamada, S. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 2313 (*isol*)
Constantine, G.H. *et al., J. Pharm. Sci.*, 1966, **55**, 1378 (*isol*)
Bisset, N.G. *et al., Phytochemistry*, 1967, **6**, 1395 (*occur, derivs*)
Dutta, P.K. *et al., Phytochemistry*, 1972, **11**, 1180 (*Epiuvaol*)
Doddrell, D.M. *et al., Tet. Lett.*, 1974, 2381 (*cmr*)
Romeo, G. *et al., Org. Magn. Reson.*, 1977, **9**, 29 (*pmr*)
Nasini, G. *et al., Phytochemistry*, 1981, **20**, 514 (*Ursonic aldehyde*)

Katai, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 1567 (*isol, derivs*)
Siddiqui, S. *et al., J. Nat. Prod.*, 1986, **49**, 1086 (*cmr*)
Chatterjee, K.S. *et al., J. Indian Chem. Soc.*, 1988, **65**, 458 (*isol*)
Dehmlow, E.V. *et al., J. Chem. Res., Synop.*, 1998, 252-253 (*Uvaol, pmr, cmr*)
Byung, S.-M. *et al., Planta Med.*, 1999, **65**, 374-375 (*Uvaol, activity*)

12-Ursene-3,16,21-triol U-42



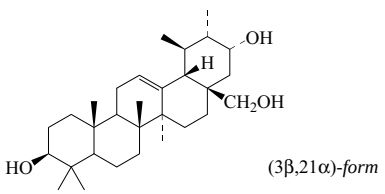
$C_{30}H_{50}O_3$ 458.723

(3ξ,16ξ,21ξ)-*form* [52084-05-6]
Constit. of the flowers of *Calendula officinalis* (pot marigold). Cryst. Mp 244-250°.

[98168-61-7]

Kasprzyk, Z. *et al., Phytochemistry*, 1973, **12**, 2299
Wilkomirski, B. *et al., Phytochemistry*, 1985, **24**, 3066 (*isol*)

12-Ursene-3,21,28-triol U-43



(3β,21α)-*form*

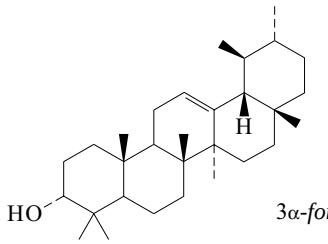
$C_{30}H_{50}O_3$ 458.723

(3β,21β)-*form*
28-Carboxylic acid, 3-O-[α-L-arabinopyranosyl-(1→2)-β-D-glucuronopyranoside]: [117804-12-3] ***Cynarasaponin F***
$C_{41}H_{64}O_{14}$ 780.948
Constit. of *Cynara cardunculus* (cardoon). Powder + $1\frac{1}{2}H_2O$ (as di-Me ester). $[\alpha]_D^{25}$ +23.4 (c, 0.47 in MeOH) (di-Me ester).

[117804-19-0, 117804-21-4]

Shimizu, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 2466 (*Cynarasaponins*)

12-Ursen-3-ol U-44



3α-*form*

$C_{30}H_{50}O$ 426.724Log P 10.66 (uncertain value) (calc).

3α-*form* [5937-48-4]
Epi-α-amyrin
Isol. from leaves of *Rosmarinus officinalis* (rosemary) and *Dacryodes edulis* (African pear). Mp 110-111° Mp 138°.

3β-*form* [638-95-9]
α-Amyrin. *α-Amyrenol. Viminalol*
Constit. of *Artemisia vulgaris* (mugwort). Cryst. (EtOH). Mp 186°. $[\alpha]_D^{17}$ +83.5 ($CHCl_3$). Pharmacol. active isomer.

Ac: [863-76-3]
$C_{32}H_{52}O_2$ 468.762
Constit. of *Artemisia vulgaris* (mugwort). Cryst. (petrol). Mp 225-226°. $[\alpha]_D^{18}$ +77 (C_6H_6).

Hexadecanoyl: [22255-10-3] *α-Amyrin palmitate*
$C_{46}H_{80}O_2$ 665.137
Isol. from *Santalum album* (sandalwood). Flavouring ingredient. Prisms or needles ($EtOH/Et_2O$). Mp 73-74°. $[\alpha]_D^{23}$ +52.5 (c, 1.0 in C_6H_6).

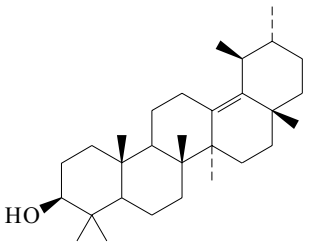
Hexacosanoyl: [307319-21-7]
$C_{56}H_{100}O_2$ 805.405
Constit. of *Rosmarinus officinalis* (rosemary).

Tetratriacontanoyl: [124693-68-1]
$C_{64}H_{116}O_2$ 917.619
Constit. of the root bark of *Scolymus hispanicus* (Spanish salsify).

3-Ketone: [638-96-0] *12-Ursen-3-one.* ***α-Amyrone***. *α-Amyrenone*
$C_{30}H_{48}O$ 424.709
Found in *Sambucus nigra* (elderberry). Cryst. (MeOH). Mp 125-126°. $[\alpha]_D$ +106.5 (c, 1.6 in $CHCl_3$).

Melera, A. *et al., Helv. Chim. Acta*, 1956, **39**, 441 (*struct*)
Shannon, J.S. *et al., Aust. J. Chem.*, 1963, **16**, 683 (*ms*)
Witz, P. *et al., Bull. Soc. Chim. Fr.*, 1963, 1101 (*cd, ketone*)
Laurie, W. *et al., Phytochemistry*, 1964, **3**, 267 (*isol, ketone*)
Bryce, T.A. *et al., Phytochemistry*, 1967, **6**, 727 (*isol*)
Inoue, T. *et al., Chem. Pharm. Bull.*, 1969, **17**, 124 (*palmitate*)
Wahlberg, I. *et al., Acta Chem. Scand.*, 1972, **26**, 1383 (*isol*)
v. Tamelen, E.E. *et al., J.A.C.S.*, 1972, **94**, 8229 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, No. 2011 (*occur*)
Lou-Cam, C.A. *et al., Phytochemistry*, 1973, **12**, 475 (*isol*)
Knight, S.A. *et al., Org. Magn. Reson.*, 1974, **6**, 603 (*cmr*)
Romeo, G. *et al., Org. Magn. Reson.*, 1977, **9**, 29 (*pmr*)
Seo, S. *et al., J.A.C.S.*, 1981, **103**, 2075 (*cmr*)
Erciyas, E. *et al., Pharmazie*, 1989, **44**, 580 (*tetratriacontanoyl*)
Zhou, Q. *et al., J. Chin. Pharm. Sci.*, 2000, **9**, 131-133; *CA*, **134**, 83483u (*hexacosanoyl*)

13(18)-Ursen-3-ol U-45



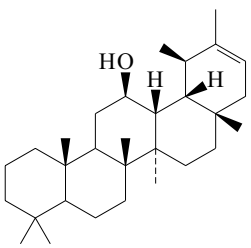
$C_{30}H_{50}O$ 426.724

3β-*form*
Cryst. Mp 200-202°.

Ac: [90745-23-6]
$C_{32}H_{52}O_2$ 468.762
Isol. from mulberry bark. Cryst. ($CHCl_3$/MeOH). Mp 208-210°. $[\alpha]_D^{19}$ -22 ($CHCl_3$).

Misra, T.N. *et al., J. Nat. Prod.*, 1984, **47**, 368

20-Ursen-12-ol U-46



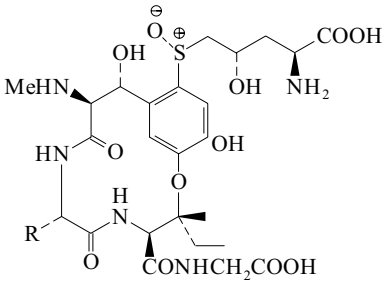
$C_{30}H_{50}O$ 426.724

12β-*form* [20545-50-0]
Isol. from flowers of *Calendula officinalis* (pot marigold). Mp 185-186°. $[\alpha]_D^{25}$ +39 ($CHCl_3$). Poorly descr. in the paper; not clear that it is a nat. prod..

Kasprzyk, Z. *et al., Phytochemistry*, 1968, **7**, 1631

Ustiloxin A U-47

[141044-51-1]



R = $CH(CH_3)_2$

$C_{28}H_{43}N_5O_{12}S$ 673.74

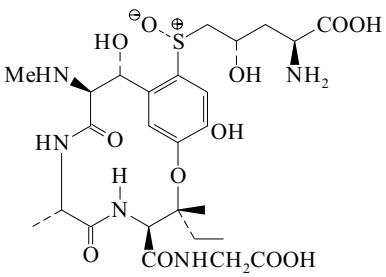
Cyclic peptide. Isol. from the false smut balls caused by *Ustilaginoidea virens* on rice. Needles + 2½ H_2O (MeOH aq.). Sol. MeOH, H_2O. Mp 195° dec. $[\alpha]_D$ +14.5 (c, 0.55 in H_2O). λ_{max} 207 (ϵ 15000); 253 (ϵ 7300); 290 (ϵ 3800) (H_2O) (Derep). λ_{max} 207 (ϵ 21300); 249 (ϵ 6000); 287 (ϵ 3200) (H_2O) (Berdy).

Koiso, Y. *et al., Tet. Lett.*, 1992, **33**, 4157 (*isol, pmr, cmr, struct*)

Koiso, Y. *et al., J. Antibiot.*, 1994, **47**, 765 (*isol, pmr, cmr, props*)

Ustiloxin B U-48

[151841-41-7]



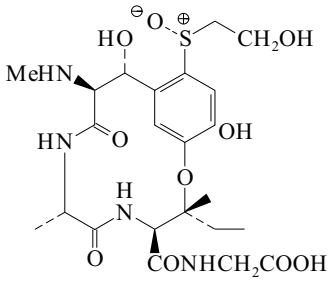
$C_{26}H_{39}N_5O_{12}S$ 645.686

Cyclic peptide. Isol. from the false smut balls caused by *Ustilaginoidea virens* on rice. Powder. Sol. MeOH, H_2O. $[\alpha]_D$ +14.1 (c, 0.5 in H_2O). λ_{max} 207 (ϵ 15000); 253 (ϵ 7300); 290 (ϵ 3800) (H_2O) (Derep). λ_{max} 213 (ϵ 13900); 252 (ϵ 5000); 290 (ϵ 2500) (H_2O) (Berdy).

Koiso, Y. *et al., J. Antibiot.*, 1994, **47**, 765 (*isol, pmr, cmr*)

Ustiloxin C U-49

[158274-98-7]



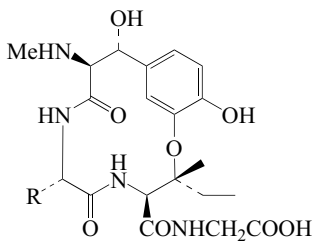
$C_{23}H_{34}N_4O_{10}S$ 558.608

Cyclic peptide. Isol. from the false smut balls caused by *Ustilaginoidea virens* on rice. Powder. Sol. MeOH, H_2O. λ_{max} 216 (ϵ 12400); 253 (ϵ 5000); 290 (ϵ 2900) (H_2O) (Derep).

Koiso, Y. *et al., J. Antibiot.*, 1994, **47**, 765 (*isol, pmr, cmr, props*)

Ustiloxin D U-50

[158243-18-6]



R = $-CH(CH_3)_2$

$C_{23}H_{34}N_4O_8$ 494.544

Cyclic peptide. Isol. from the false smut balls caused by *Ustilaginoidea virens* on rice. Powder. Sol. MeOH, H_2O. $[\alpha]_D$ -48.8 (c, 0.5 in H_2O). λ_{max} 208 (ϵ 10100); 227 (ϵ 8700); 287 (ϵ 2800) (H_2O) (Derep). λ_{max} 227 (ϵ 6200); 280 (ϵ 1600) (MeOH) (Berdy).

Koiso, Y. *et al., J. Antibiot.*, 1994, **47**, 765; 1998, **51**, 418-422; 423-427 (*isol, pmr, cmr, synth, uv, activity*)

Li, Y. *et al., Biochem. Pharmacol.*, 1995, **49**, 1367-1372 (*activity*)

Morisaki, N. *et al., J. Antibiot.*, 1998, **51**, 423-427 (*synth*)

Cao, B. *et al., J.A.C.S.*, 2002, **124**, 520-521 (*Ustiloxin D, synth*)

Ustiloxin E U-51

[158253-87-3]

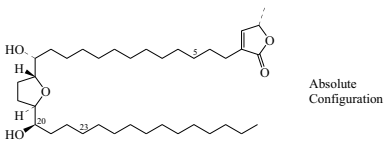
$C_{28}H_{41}N_5O_{11}S$ 655.725

Isol. from the false smut balls caused by *Ustilaginoidea virens* on rice. Powder. Sol. MeOH, H_2O. Struct. not detd. due to lack of material. Poss. metab. of Ustiloxin A, U-47 λ_{max} 207 (ϵ 15000); 253 (ϵ 7300); 290 (ϵ 3800) (H_2O) (Derep). λ_{max} 213 (ϵ 13900); 252 (ϵ 5000); 290 (ϵ 4900) (H_2O) (Berdy).

Koiso, Y. *et al., J. Antibiot.*, 1994, **47**, 765 (*isol, pmr*)

Uvariamicin I U-52

[132309-09-2]



$C_{37}H_{68}O_5$ 592.941

λ_{max} 212 (ϵ 8368) (MeOH) (Berdy).

23,24-Didehydro(Z-): [160964-96-5]

[145066-19-9] ***Bullatenin***. *Bullatencin*

$C_{37}H_{66}O_5$ 590.925

$[\alpha]_D$ +12.7 (c, 0.4 in $CHCl_3$).

19,20-Diepimer: **cis-*Uvariamicin I***

$C_{37}H_{68}O_5$ 592.941

Constit. of *Annona muricata* (soursop). Relative config. only known λ_{max} 220 (ϵ 4265) (MeOH) (Berdy).

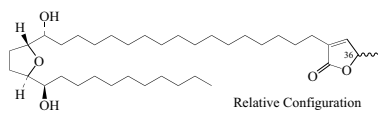
Hisham, A. *et al., Tet. Lett.*, 1990, **31**, 4649-4652 (*isol*)

Hui, Y.-H. *et al., Nat. Toxins*, 1992, **1**, 4-14 (*isol*)

Gleye, C. *et al., J. Nat. Prod.*, 1998, **61**, 576-579 (*cis-Uvariamicin I*)

Uvariamicin III U-53

[132309-11-6]



$C_{37}H_{68}O_5$ 592.941

Acetogenin. C-36 possesses *S*-config.. Isol. from *Annona* spp.. Amorph. solid. $[\alpha]_D$ +19 (c, 1 in $CHCl_3$).

24-Epimer: [166022-36-2] ***Reticulatain 2***

$C_{37}H_{68}O_5$ 592.941

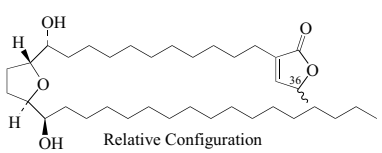
Constit. of *Annona reticulata* (custard apple). $[\alpha]_D$ +28 (c, 1 in $CHCl_3$). The C-36 config. could differ from that of Uvariamicin III.

Hisham, A. *et al., Tet. Lett.*, 1990, **31**, 4649 (*isol*)

Tam, V.T. *et al., Bull. Soc. Chim. Fr.*, 1995, **132**, 324-329 (*isol, uv, ir, pmr, cmr, ms*)

Uvariamicin IV U-54

[145066-20-2]



$C_{37}H_{68}O_5$ 592.941

C-36 possesses *S*-config..$[\alpha]_D$ +13.7 (c, 0.4 in $CHCl_3$).

17,18-Diepimer: [205439-37-8] **cis-*Uvariamicin IV***

$C_{37}H_{68}O_5$ 592.941

Constit. of the roots of *Annona mur-*

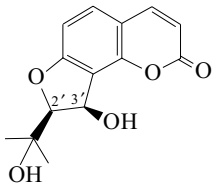
icata (soursop). Powder. Mp 60-62°. $[\alpha]_D$ +20 (c, 0.15 in MeOH). λ_{max} 221 (log ϵ 3.58) (MeOH).

Hisham, A. *et al., Tet. Lett.*, 1990, **31**, 4649-4652
Hui, Y.-H. *et al., Nat. Toxins*, 1992, **1**, 4-14 (*isol*)
Gleye, C. *et al., J. Nat. Prod.*, 1998, **61**, 576-579 (*cis-Uvariamicin IV*)

Vaginidiol V-1

[62624-87-7]

*8,9-Dihydro-9-hydroxy-8-(1-hydroxy-1-methylethyl)-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, 9CI. 2′-Hydroxyisopropyl-3′-hydroxy-2′,3′-dihydroangelicin*



$C_{14}H_{14}O_5$ 262.262
Mp 174°. $[\alpha]_D^{25}$ +234.6 (c, 1.02 in EtOH). λ_{max} 325 (EtOH) (Berdy).

Bis-O-*(3-methyl-2-butenoyl):* [96608-83-2] ***Edulisin II***
$C_{24}H_{26}O_7$ 426.465
Constit. of *Angelica edulis*. Cryst. Mp 119-120°. $[\alpha]_D^{25}$ +13.6 (c, 3.45 in $CHCl_3$).

3′-O-*(3-Methyl-2-butenoyl), 1′′*-O-*(4-hydroxycinnamoyl):* [96608-82-1] ***Edulisin I***
$C_{28}H_{26}O_8$ 490.509
Constit. of *Angelica edulis*. Cryst. Mp 103-104°. $[\alpha]_D^{25}$ -24.3 (c, 2 in $CHCl_3$).

3′-O-*Angeloyl, 1′′*-O-*Ac:* [15591-75-0] ***Edultin***. *Cnidimin*. *Libanotin*
$C_{21}H_{22}O_7$ 386.401
Constit. of *Angelica edulis*. Cryst. Mp 160-161°. $[\alpha]_D$ +79.5 (c, 0.8 in $CHCl_3$).

O,O-*Diangeloyl:* [2607-56-9] ***Archangelicin***
$C_{24}H_{26}O_7$ 426.465
Constit. of the roots of *Angelica archangelica* (anglica). Cryst. (EtOAc/petrol or cyclohexane). Mp 107-108° (100.5-102°). $[\alpha]_D^{26}$ +112.7 (c, 4.5 in MeOH).

1′′-O-*(3-Methylbutanoyl), 3′*-O-*angeloyl:* [143061-67-0]
$C_{24}H_{28}O_7$ 428.481
Constit. of the roots of *Angelica archangelica* (angelica). Amorph. powder. Mp 67-70°.

3′-O-*Propanoyl, 1′′-Ac:* [158446-38-9] ***Edulisin IV***
$C_{19}H_{20}O_7$ 360.363
Constit. of *Angelica edulis*. Needles (hexane/EtOAc). Mp 119-120° dec. $[\alpha]_D^{25}$ +71.2 (c, 0.4 in $CHCl_3$).

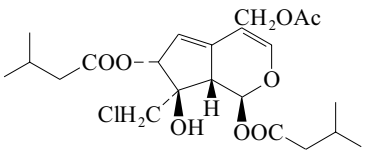
3′-O-*(2-Methylbutanoyl), 1′′-Ac:* [158515-39-0] ***Edulisin III***
$C_{21}H_{24}O_7$ 388.416
Constit. of *Angelica edulis*. Needles (hexane/EtOAc). Mp 143-144° dec. $[\alpha]_D^{25}$ +166 (c, 0.3 in $CHCl_3$).

1′′-O-*Angeloyl, 3′*-O-*(2-methylbutanoyl):* [158446-39-0] ***Edulisin V***
$C_{24}H_{28}O_7$ 428.481
Constit. of *Angelica edulis*. Needles (hexane/EtOAc). Mp 113.5-115° dec. $[\alpha]_D^{25}$ +63.4 (c, 0.3 in $CHCl_3$). Stereochem. not confirmed.

Neilsen, B.E. *et al., Acta Chem. Scand.*, 1964, **18**, 932 (*Archangelicin*)
Prokopenko, A.P. *et al., Khim. Prir. Soedin.*, 1965, **1**, 215; *Chem. Nat. Compd. (Engl. Transl.)*, 1965, **1**, 165 (*Libanotin, isol*)
Bohlmann, F. *et al., Chem. Ber.*, 1969, **102**, 1673 (*derivs*)
Lemmich, J.E. *et al., Acta Chem. Scand.*, 1970, **24**, 2893 (*isol, struct, derivs*)
Perel'son, M.E. *et al., Khim. Prir. Soedin.*, 1971, **7**, 712; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 692 (*pmr, Edultin, Athamantin*)
Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 1047 (*deriv*)
Hata, K. *et al., Chem. Pharm. Bull.*, 1973, **21**, 518 (*derivs*)
Kozawa, M. *et al., Yakugaku Zasshi*, 1978, **98**, 636; *CA*, **89**, 129431 (*deriv*)
Kawasaki, C. *et al., Planta Med.*, 1984, **50**, 492 (*Edulisins, Isopeucenidin*)
Harmala, P. *et al., Planta Med.*, 1992, **58**, 287 (*deriv*)
Mizuno, A. *et al., Planta Med.*, 1994, **60**, 333 (*Edulisins*)

Valechlorin V-2

[51771-49-4]



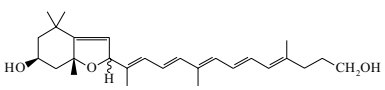
$C_{22}H_{31}ClO_8$ 458.935
Constit. of *Valeriana officinalis* (valerian). Cryst. (EtOH). Mp 79-80°. $[\alpha]_D^{16}$ +104 ($CHCl_3$).

Popov, S.S. *et al., Dokl. Bolg. Akad. Nauk*, 1973, **26**, 913; 1974, **27**, 1007 (*isol, pmr*)
Finner, E. *et al., Planta Med.*, 1984, **50**, 4 (*cmr*)

Valenciachrome V-3

[88853-51-4]

5,8-Epoxy-5,8-dihydro-3-hydroxy-12′-apo-β,ψ-carotenol, 9CI

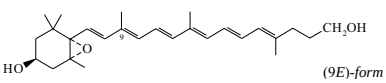


$C_{27}H_{40}O_3$ 412.611
Constit. of Californian Valencia orange juice (*Citrus* sp.).

Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1990, **73**, 468 (*isol, pmr, uv, cd*)

Valenciaxanthin V-4

[129566-99-0]



(9*E*)-*form*

$C_{27}H_{40}O_3$ 412.611

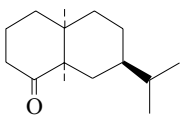
(9*E*)-*form*
Constit. of Californian Valencia orange juice (*Citrus* sp.).

(9*Z*)-*form*
Constit. of Californian Valencia orange juice.

Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1990, **73**, 468 (*isol, pmr, uv, cd*)

Valeranone V-5

Jatamansone



(−)-*form*

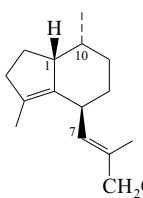
$C_{15}H_{26}O$ 222.37
Log P 4.78 (calc).

(+)-*form* [1803-39-0]
Oil. $Bp_{0.1}$ 95-98°. $[\alpha]_D$ +76 ($CHCl_3$).
▶ QK5075000

(-)-*form* [5090-54-0]
Constit. of the roots of *Valeriana officinalis* (valerian). Oil. $[\alpha]_D^{20}$ -51.9 (c, 0.3 in $CHCl_3$). Log P 4.78 (calc). Pharmacol. active isomer.
▶ LD_{50} (mus, ipr) 350 mg/kg. QK5075000

Klyne, W. *et al., Tet. Lett.*, 1964, 1443 (*abs config*)
Marshall, J.A. *et al., Tet. Lett.*, 1965, 4807 (*synth*)
Banerjee, D.K. *et al., J. Indian Chem. Soc.*, 1972, **49**, 1 (*rev*)
Talvitie, A. *et al., Finn. Chem. Lett.*, 1977, 197 (*pmr*)
Wenkert, E. *et al., J.A.C.S.*, 1978, **100**, 1263 (*synth*)
Sammes, P.G. *et al., J.C.S. Perkin 1*, 1986, 281 (*synth*)
Vite, G.D. *et al., J.O.C.*, 1988, **53**, 2560 (*synth*)
Takeshita, H. *et al., Bull. Chem. Soc. Jpn.*, 1993, **66**, 2694 (*synth*)
Dativani, G. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 716 (*synth*)
Srikrishna, A. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 521 (*synth*)
Srikrishna, A. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 323-325 (*synth*)

4,7(11)-Valerenadien-12-ol V-6



(1β,10α,7(11)E)-*form*

$C_{15}H_{24}O$ 220.354

(1β,10α,7(11)*E*)-*form* [101628-22-2]
Valerenol. *α-Valerenol*
Found as the free alcohol and as esters in *Valeriana officinalis* (valerian). Oil.

12-Aldehyde: [4176-16-3] *4,7(11)-Valeradien-12-al*. ***Valerenal***
$C_{15}H_{22}O$ 218.338
Constit. of *Valeriana officinalis* (valerian). Oil.

12-Aldehyde, semicarbazone:
Mp 176-177°.

(1β,10β,7(11)*E*)-*form* *10*-epi-α-*Valerenol*. *10-Epivalerenol*

12-Aldehyde: ***10*-epi-α-*Valerenal***. *10-Epivalerenal*
$C_{15}H_{22}O$ 218.338
Oil. $[\alpha]_D^{24}$ +5.2 (c, 1.1 in $CHCl_3$).

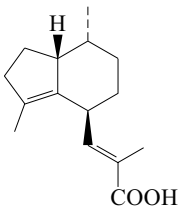
(1β,10α,7(11)*Z*)-*form*

12-Aldehyde:
Oil.

Stoll, A. *et al., Helv. Chim. Acta*, 1957, **40**, 1205 (*Valerenal*)
Bates, R.B. *et al., Chem. Ind. (London)*, 1965, 1731 (*struct, synth, Valerenal*)
Bohlmann, F. *et al., Chem. Ber.*, 1980, **113**, 2410
Bos, R. *et al., Phytochemistry*, 1986, **25**, 133 (*Valerenol*)

Valerenic acid V-7

[3569-10-6]

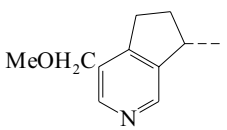


$C_{15}H_{22}O_2$ 234.338
Constit. of *Valeriana officinalis* (valerian). Cryst. (Et_2O/petrol). Mp 140-142°. $[\alpha]_D^{20}$ -120.4 (c, 0.97 in EtOH). Log P 4.74 (calc).

Stoll, A. *et al., Annalen*, 1957, **603**, 158 (*isol*)
Buchi, G. *et al., J.A.C.S.*, 1960, **82**, 2962 (*struct*)
Birnbaum, G.I. *et al., J.O.C.*, 1978, **43**, 272 (*abs config*)
Hendriks, H. *et al., Planta Med.*, 1985, **51**, 28 (*pharmacol*)

Valerianine V-8

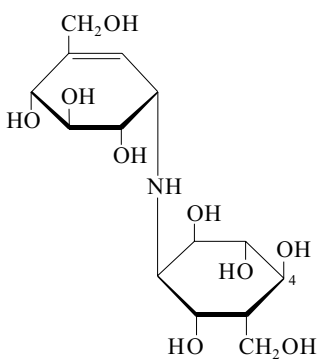
6,7-Dihydro-4-(methoxymethyl)-7-methyl-5H-2-pyrindine, 9CI



$C_{11}H_{15}NO$ 177.246
(*S*)-*form* [30634-66-3]
Alkaloid from roots of *Valeriana officinalis* (valerian).
Hydrochloride:
Mp 134°. $[\alpha]_D^{20}$ -10.5 (c, 0.37 in MeOH).
(±)-*form* [30769-38-1]
Synthetic.
Hydrochloride:
Mp 143°.
Franck, B. *et al., Angew. Chem., Int. Ed.*, 1970, **9**, 891 (*uv, ir, pmr, struct, synth*)

Validoxylamine B V-9

[39318-73-5]



$C_{14}H_{25}NO_9$ 351.353
Thin needles (MeOH) (as nona-Ac). Sol. H_2O, MeOH, DMSO; poorly sol. EtOH, EtOAc, $CHCl_3$. Mp 175-176° (nona-Ac).

4-O-β-D-Glucopyranoside: [102583-47-1]
Validamycin B
$C_{20}H_{35}NO_{14}$ 513.495
Active against rice sheath blight disease and *Pellicularia sasakii*. Sol. H_2O, MeOH, Py; fairly sol. Me_2CO, EtOH; poorly sol. EtOAc, hexane. Mp 132-142° dec. $[\alpha]_D^{24}$ +102 (c, 1 in H_2O).
▶ LD_{50} (mus, ivn) 2000 - 4000 mg/kg.
YV9350200

6-Deoxy: [38665-10-0] ***Validoxylamine A***
$C_{14}H_{25}NO_8$ 335.353
Sol. H_2O. $[\alpha]_D$ +170 (c, 1 in H_2O).
▶ LD_{50} (mus, ivn) 2000-4000 mg/kg.

6-Deoxy, 4-O-β-D-glucopyranoside: [37248-47-8] ***Validamycin A***. *T 7545A. Antibiotic T 7545A. Validamycin, JMAF. Validacin. Mycin. Rhizocin. Solacol*
$C_{20}H_{35}NO_{13}$ 497.495
Used in control of fungal infection in rice, potatoes, strawberries and other crops. Amorph. powder. Sol. H_2O, MeOH, DMSO, DMF; fairly sol. EtOH, Me_2CO; poorly sol. EtOAc, hexane, Et_2O. Mp 95° dec Mp 130-135° dec. $[\alpha]_D^{24}$ +112 (c, 1 in H_2O). pK_a 6.
▶ LD_{50} (mus, ivn) 2000-4000 mg/kg.
NM7540000

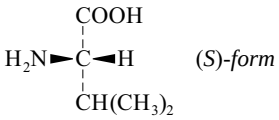
6-Deoxy, 4-O-[β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside]: [12650-71-4] ***Validamycin E***
$C_{26}H_{45}NO_{18}$ 659.637
Sol. H_2O, DMSO, DMF; poorly sol. butanol, hexane. Mp 265-268° dec. $[\alpha]_D$ +148.2 (c, 1 in H_2O).
▶ LD_{50} (mus, ivn) 2000 - 4000 mg/kg.
NM7524800

6-Deoxy, 4-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [130812-69-0] ***Validamycin H***
$C_{26}H_{45}NO_{18}$ 659.637
Amorph. $[\alpha]_D^{25}$ +74.9 (c, 1 in H_2O).

Horii, S. *et al., Chem. Comm.*, 1972, 746
Horii, S. *et al., J. Antibiot.*, 1972, **25**, 48 (*isol*)
Ogawa, S. *et al., Chem. Lett.*, 1982, 279 (*deriv*)
Toyokumi, T. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 2999 (*synth*)
Asano, N. *et al., J. Antibiot.*, 1984, **37**, 859
Kameda, Y. *et al., J. Antibiot.*, 1986, **39**, 1491 (*deriv*)
Ogawa, S. *et al., J.C.S. Perkin 1*, 1988, 2675 (*synth, bibl*)
Asano, N. *et al., J. Antibiot.*, 1990, **43**, 1039 (*Validamycin H*)
Miyamoto, Y. *et al., Carbohydr. Res.*, 1992, **223**, 299 (*Validamycin H, synth*)
Fukase, H. *et al., J.O.C.*, 1992, **57**, 3651 (*synth*)
Pesticide Manual, 11th edn., 1997, No. 747 (*use*)
Pesticide Manual, 12th edn., 2000, No. 800 (*Validamycin*)

Valine V-10

[7004-03-7]
2-Amino-3-methylbutanoic acid, 9CI. 2-Aminoisovaleric acid. Val



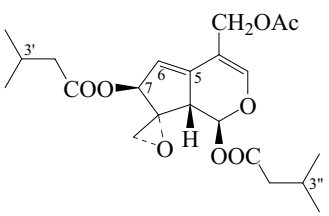
(*S*)-*form*

$C_5H_{11}NO_2$ 117.147
▶ YV9355500
(*S*)-*form* [72-18-4]
L-form
Widely distributed in nature as one of the principal protein amino acids. Dietary supplement. Plates (EtOH aq.). Sol. H_2O (8.85 g per 100 cm^3 at 25°); spar. sol. EtOH. Mp 315° dec. (sealed tube). $[\alpha]_D^{20}$ +6.3 (H_2O). $[\alpha]_D^{20}$ +23.4 (1*M* HCl). $[\alpha]_D^{20}$ +27.6 (6*M* HCl). pK_{a2} 9.62 (NH_2). Isoelectric point 5.96. Bitter taste.
▶ YV9361000
(±)-*form* [516-06-3]
FEMA 3444
Flavouring ingredient. Plates (EtOH). Sol. H_2O; insol. EtOH, Et_2O. Mp 298° dec. (sealed tube). pK_{a2} 9.62 (25°). Sublimes.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 573B; 573C; 573D; 674A; 674B (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 872B; 872C; 1071B; 1071C (*nmr*)
Sadtler Standard C-13 NMR Spectra, 4424 (*cmr*)
Adams, R. *et al., J.A.C.S.*, 1934, **56**, 2093 (*resoln*)
Barrow, F. *et al., J.C.S.*, 1935, 410 (*abs config*)
Org. Synth., Coll. Vol., 3, 1955, 848 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, (Chapter 41), Wiley, N.Y., 1961, **3**, (*rev*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Aruldhas, G. *et al., Spectrochim. Acta A*, 1967, **23**, 1345 (*pmr*)
Pachler, K.G.R. *et al., Spectrochim. Acta A*, 1968, **24**, 1311 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 2348 (*occur*)
Armstrong, F.B. *et al., Chem. Comm.*, 1974, 351 (*biosynth*)
Oguri, T. *et al., Chem. Pharm. Bull.*, 1975, **23**, 167 (*synth*)
Shiraiwa, T. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 2234 (*resoln*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH, Weinheim, 1985, **A2**, 57 (*rev*)
Kulik, W. *et al., Biomed. Mass Spectrom.*, 1988, **15**, 419 (*ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VBP000; VBU000

Valtrate V-11

[18296-44-1]
Valepotriate. Valepotriatum. Valtratum. Baldrisedon. Halazuchrome B



$C_{22}H_{30}O_8$ 422.474

There is some confusion in the older lit. over the nomenclature and structs. of some of these compds.. Constit. of *Valeriana* spp.. Oil. $[\alpha]_D^{21}$ +172.7 (MeOH). Log P 1.48 (calc). λ_{max} 204 (ϵ 4000); 256 (ϵ 16050) (EtOH) (Berdy).

▶ LD_{50} (mus, ipr) 60 mg/kg. EK7902000

11-De-Ac, 11-O-(3-hydroxy-3-methylbutanoyl): [96681-66-2]
$C_{25}H_{36}O_9$ 480.554
Constit. of *Valeriana* sp..

7,11-Bisdeacyl, 11-O-(3-methylbutanoyl): [53773-14-1] ***Deacetylisovaltrate***. *Valepotriate A1*. *Deacetylisovaltratum*
$C_{20}H_{28}O_7$ 380.437
Constit. of *Valeriana officinalis* (valerian). Oil. $[\alpha]_D^{20}$ +35 (MeOH).

7,11-Bisdeacyl, 7-O-(3-methylpentanoyl), 11-O-(3-hydroxy-3-methylbutanoyl): [137088-15-4]
$C_{26}H_{38}O_9$ 494.581
Constit. of *Valeriana* sp.. Incorrect struct. in CA.

3′-Acetoxy: [25161-41-5] ***Acevaltrate, INN***. *Acevaltratum*. *Acetoxyvalepotriate*
$C_{24}H_{32}O_{10}$ 480.511
Prod. by *Valeriana* spp.. Needles (hexane). Mp 83-84°. $[\alpha]_D^{24}$ +163.7 (MeOH). Log P 0.97 (calc).

▶ EK7713300

2″-Acetoxy: [78700-02-4] ***1-α-Acevaltrate***
$C_{24}H_{32}O_{10}$ 480.511
Constit. of *Valeriana* sp..

5β,6-Dihydro, 7,11-bisdeacyl, 11-(3-methylbutanoyl), 7-Ac: [18296-45-2] ***Dihydrovaltrate***. *Dihydrovaltratum*. *Dihydrovalepotriate*. *Didrovaltrate*. *Didrovaltratum*
$C_{22}H_{32}O_8$ 424.49
Isol. from *Valeriana* spp.. Cryst. (Et_2O/hexane). Mp 63-64°. $[\alpha]_D^{20}$ -80. Log P 1.9 (calc).

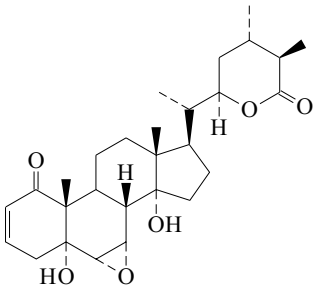
▶ EK7902800

[78779-16-5]

Thies, P.W. *et al., Tetrahedron*, 1968, **24**, 313; 1973, **29**, 3213 (*struct*)
Verzar-Petri, G. *et al., Acta Pharm. Hung.*, (Suppl.), 1974, **44**, 54; *CA*, **81**, 166441s (*biosynth*)
Popov, S. *et al., Phytochemistry*, 1974, **13**, 2815 (*isol, struct*)
Hoelzl, J. *et al., Planta Med.*, 1975, **28**, 301 (*biosynth*)
Tittel, G. *et al., J. Chromatogr.*, 1978, **148**, 459 (*hplc, deriv*)
Bock, K. *et al., Phytochemistry*, 1978, **17**, 753 (*cmr*)
Thies, P.W. *et al., Planta Med.*, 1981, **41**, 15 (*cmr, struct*)
Khandzhieva, N. *et al., Int. J. Mass Spectrom. Ion Phys.*, 1983, **48**, 181 (*ms*)
Becher, H. *et al., Planta Med.*, 1984, **50**, 245 (*struct*)
Cordell, G.A. *et al., Tetrahedron*, 1991, **47**, 3521-3534 (*derivs*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1426

Vamonolide V-12

[114332-66-0]
6,7-Epoxy-5,14-dihydroxy-1-oxo-2-withenolide



$C_{28}H_{40}O_6$ 472.62
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH). Mp 243-247°. $[\alpha]_D^{23}$ +24.9 (c, 0.97 in MeOH).

Vasina, O.E. *et al., Khim. Prir. Soedin.*, 1987, **23**, 856; *Chem. Nat. Compd. (Engl. Transl.)*, 712 (*isol, pmr*)

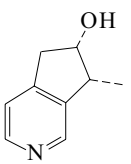
Variacin V-13

Lantibiotic peptide. Prod. by *Micrococcus varians* isol. from meat fermentations. Bacteriocin.

Pridmore, D. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 1799-1802 (*isol*)

Venoterpine V-14

[17948-42-4]
Gentialutine. Alkaloid RW47



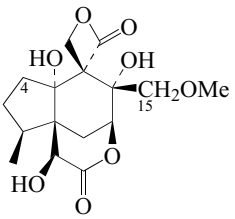
$C_9H_{11}NO$ 149.192
Config. revised in 1985. Alkaloid from *Gentiana lutea* (yellow gentian). Mp 130-132°. $[\alpha]_D$ +27 ($CHCl_3$).

O-*Ac:* [189322-84-7] **O-*Acetylvenoterpine***
$C_{11}H_{13}NO_2$ 191.229
$[\alpha]_D$ +45 (c, 1.5 in $CHCl_3$).

Arthur, H.R. *et al., Phytochemistry*, 1966, **5**, 977-983 (*isol*)
Arthur, H.R. *et al., Aust. J. Chem.*, 1967, **20**, 2505-2508 (*uv, ir, pmr, ms, struct*)
Ray, A.B. *et al., Tet. Lett.*, 1968, 2763-2765 (*uv, ir, pmr, struct*)
Mitscher, L.A. *et al., Experientia*, 1971, **27**, 16-17 (*config*)
Michel, S. *et al., J. Nat. Prod.*, 1982, **45**, 489-494 (*isol*)
Ravao, T. *et al., Tet. Lett.*, 1985, **26**, 837-838 (*config, cmr*)
Thépenier, P. *et al., Bull. Soc. R. Sci. Liege*, 1996, **65**, 379-382 (*Ac*)

Veranisatin A V-15

[153445-92-2]



$C_{16}H_{22}O_8$ 342.345
Constit. of *Illicium verum* (Chinese star anise). Prisms (EtOAc). Mp 181-182°. $[\alpha]_D^{22}$ -14.8 (c, 1 in MeOH).

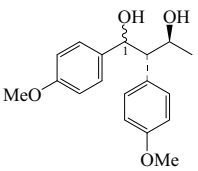
15-Carboxylic acid, Me ester: [153445-93-3] ***Veranisatin B***
$C_{16}H_{20}O_9$ 356.329
Constit. of *Illicium verum* (Chinese star anise). Prisms (EtOAc). Mp 212-213°. $[\alpha]_D^{22}$ -14.5 (c, 1 in MeOH).

4β-Hydroxy, 15-carboxylic acid, Me ester: [182876-51-3] ***Veranisatin C***
$C_{16}H_{20}O_{10}$ 372.328
Constit. of *Illicium verum* (Chinese star anise). Needles (EtOH). Mp 228-229.5°.

Nakamura, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1908 (*isol, pmr, cmr*)

Verimol D V-16

[212516-37-5]
1,2-Bis(4-methoxyphenyl)-1,3-butanediol, 9CI



Relative Configuration

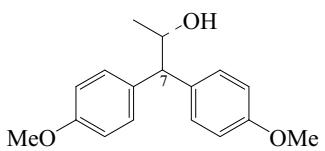
$C_{18}H_{22}O_4$ 302.369
Constit. of *Illicium verum* (Chinese star anise). Oil. $[\alpha]_D$ -1.5 (c, 0.58 in $CHCl_3$).

1-Epimer: [212516-38-6] ***Verimol E***
$C_{18}H_{22}O_4$ 302.369
Constit. of *Illicium verum* (Chinese star anise). Oil. $[\alpha]_D$ +7 (c, 0.43 in $CHCl_3$).

Sy, L.K. *et al., J. Nat. Prod.*, 1998, **61**, 987-992

Verimol F V-17

1,1-Bis(4-methoxyphenyl)-2-propanol

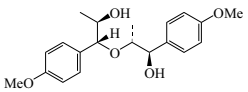


$C_{17}H_{20}O_3$ 272.343
(S)-form [212516-39-7]
Constit. of *Illicium verum* (Chinese star anise). Oil. $[\alpha]_D$ +5.5 (c, 0.52 in $CHCl_3$).

Sy, L.-K. *et al., J. Nat. Prod.*, 1998, **61**, 987-992

Verimol G V-18

[212516-40-0]



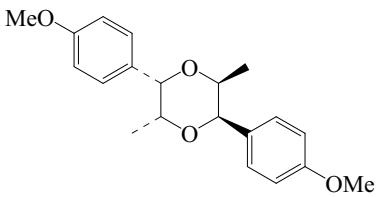
Relative Configuration

$C_{20}H_{26}O_5$ 346.422
Constit. of *Illicium verum* (Chinese star anise). Oil. $[\alpha]_D$ +1.6 (c, 1.67 in $CHCl_3$).

Sy, L.-K. *et al., J. Nat. Prod.*, 1998, **61**, 987-992

Verimol H V-19

[212516-42-2]
2,5-Bis(4-methoxyphenyl)-3,6-dimethyl-1,4-dioxane, 9CI

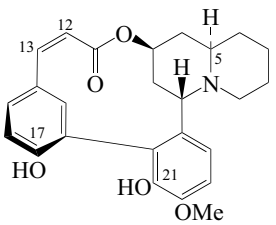


$C_{20}H_{24}O_4$ 328.407
Constit. of *Illicium verum* (Chinese star anise). Oil. Some confusion over stereochem. The text states that each phenylpropanoid residue is *threo*-, but they are drawn as *erythro*-. The struct. shown agrees with the text and also with CAS (*meso*-stereoisomer).

Sy, L.-K. *et al., J. Nat. Prod.*, 1998, **61**, 987-992

Verticillatine V-20

[10247-54-8]
2′,6″-Dihydroxy-5″-methoxylythran-12-one, 9CI



$C_{25}H_{27}NO_5$ 421.492
CAS numbering differs from that shown.Mp 312°.

12,13-Dihydro, O^{21}*-Me:* [10247-53-7] ***Lagerstroemine***. *Indicamine*†. *Lagerstremine*
$C_{26}H_{31}NO_5$ 437.535
Alkaloid from *Plantago psyllium* seeds (African plantain). Cryst. (EtOH). Mp 240°. $[\alpha]_D$ -137 ($CHCl_3$). pK_a 7.7 (EtOH).

Ferris, J.P. *et al., J.A.C.S.*, 1971, **93**, 2942; 2958 (*Lagerstroemine, Dihydroverticillatine, Nesodine, Decodine*)
Balbaa, S.I. *et al., U. A. R. J. Pharm. Sci.*, 1971, **12**, 35; *CA*, **77**, 156311c (*Lagerstroemine, occur*)
Karawya, M.S. *et al., U. A. R. J. Pharm. Sci.*, 1971, **12**, 53; *CA*, **78**, 13729e (*Lagerstroemine, occur*)

Vetiverol V-21

[68129-81-7]

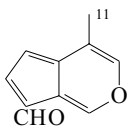
$C_{15}H_{24}O$ 220.354
A mixt. of sesquiterpene alcohols isol. from vetiver oil (*Vetiveria zizanioides* root oil). Limited use in foods. Mainly to reinforce the flavour of asparagus. See 3-Cedren-15-ol, 7-Cedren-14-ol, 12-Cyclocopacamphanol and for specific components.

O-*Ac:* [62563-80-8] *Vetiveryl acetate*
$C_{17}H_{26}O_2$ 262.391
Food flavouring.

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 1011-1012; 1979, **17**, 923 (*rev, tox, use*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 284-285 (*Ac, use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2909-2911 (*Ac, use*)
Fukayama, M.Y. *et al., Toxicol. Lett.*, 1999, **111**, 175-187 (*tox*)

Viburtinal V-22

[63661-79-0]
4-Methylcyclopenta[c]pyran-7-carboxaldehyde, 9CI



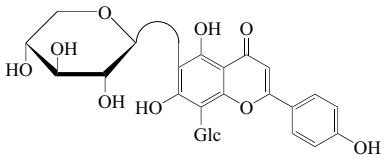
$C_{10}H_8O_2$ 160.172
Prod. from the hydrol. of esters present in *Viburnum opulus* (cranberry bush). Yellow cryst. (H_2O). Mp 90-92°.

11-Acetoxy: [18234-46-3] *Baldrinal*
$C_{12}H_{10}O_4$ 218.209
Yellow-brown cryst. (Et_2O/petrol). Mp 112-113°.
▶ GY5825000

Thies, P.W. *et al., Tetrahedron*, 1968, **24**, 313 (*Baldrinal*)
Godeau, R.-P. *et al., Phytochemistry*, 1977, **16**, 604 (*isol, struct, uv*)
Godeau, R.-P. *et al., CA*, 1979, **90**, 183192q (*occur*)
Brayer, J.-L. *et al., Chem. Comm.*, 1983, 257 (*synth*)

Vicenin 1 V-23

[35927-38-9]
8-β-D-Glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-6-β-D-xylopyranosyl-4H-1-benzopyran-4-one, 9CI. 8-Glucopyranosyl-6-xylopyranosylapigenin. 8-Glucosyl-6-xylosylapigenin



$C_{26}H_{28}O_{14}$ 564.499
Yellow cryst. (MeOH aq.). Mp 234-236° (229-230° dec.).

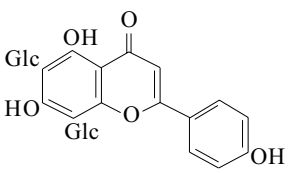
6″-O-*Ac:* [163345-99-1] ***6″-O-Acetylvicenin 1***
$C_{28}H_{30}O_{15}$ 606.536
Constit. of *Prosopis chilensis* (algarrobo blanco).

[51012-98-7]

McClure, J.W. *et al., Am. J. Bot.*, 1966, **53**, 849 (*occur*)
Seikel, M.K. *et al., Phytochemistry*, 1966, **5**, 439 (*isol*)
Bouillant, M.L. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1971, **273**, 1759 (*synth*)
Ohashi, H. *et al., Phytochemistry*, 1977, **16**, 1106 (*isol, pmr*)
Gaffield, W. *et al., Tetrahedron*, 1978, **34**, 3089 (*cd*)
Elrady, H. *et al., CA*, 1995, **122**, 310643u (*6″-Acetylvicenin 1*)

Vicenin 2 V-24

[23666-13-9]
6,8-Di-β-D-glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one, 9CI. 6,8-Di-C-glucosyl-4′,5,7-trihydroxyflavone. 6,8-Di-C-glucopyranosylapigenin. 6,8-Di-C-glucosylapigenin



$C_{27}H_{30}O_{15}$ 594.525
Constit. of lemons (*Citrus limon*). Cryst. (H_2O). Mp 233-236° (214-216° dec.). $[\alpha]_D$ +25 (c, 0.21 in Py). $[\alpha]_D$ +71 (c, 0.36 in H_2O).

Mono-Ac: [50875-08-6]
$C_{29}H_{32}O_{16}$ 636.562

7-Me ether: [128397-01-3] *6,8-Di-C-glucopyranosyl-4′,5-dihydroxy-7-methoxyflavone.* ***6,8-Di-C-glucosylgenkwanin***
$C_{28}H_{32}O_{15}$ 608.552

2‴-O-Xylosyl, 7-Me ether: [128197-78-4] ***6,8-Di-C-glucosyl-2‴-xylosylgenkwanin***
$C_{33}H_{40}O_{19}$ 740.668

6″-O-β-D-Glucopyranosyl: [94530-40-2] *6-Gentiobiosyl-8-glucopyranosyl-4′,5,7-trihydroxyflavone*
$C_{33}H_{40}O_{20}$ 756.667

2″,2‴-Di-O-β-D-glucopyranosyl:2″,2‴-Di-O-β-D-glucopyranosylvicenin 2. 6,8-Di-C-sophorosylapigenin
$C_{39}H_{50}O_{25}$ 918.809
Light yellow powder. λ_{max} 272 ; 332 (MeOH).

4″,4‴-Di-O-β-D-glucopyranosyl:4″,4‴-Di-O-β-D-glucopyranosylvicenin 2. 6,8-

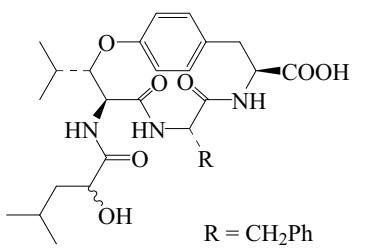
Di-C-*β*-*cellobiosylapigenin*
$C_{39}H_{50}O_{25}$ 918.809
Pale yellow powder.

6″,6‴-Di-O-*β*-D-*glucopyranosyl:* [201417-00-7] *6,8-Digentiobiosyl-4′,5,7-trihydroxyflavone.* ***6,8-Di-C-gentiobiosylapigenin***
$C_{39}H_{50}O_{25}$ 918.809

Seikel, M.K. *et al., Phytochemistry*, 1966, **5**, 439 (*isol*)
Gentili, B. *et al., J.O.C.*, 1968, **33**, 1571 (*isol, struct, pmr*)
Seshardri, T.R. *et al., Curr. Sci.*, 1973, **42**, 421 (*deriv*)
Bacon, J.D. *et al., Rev. Latinoam. Quim.*, 1976, **7**, 83; *CA*, **86**, 15873 (*uv*)
Osterdahl, B.G. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 93 (*isol, cmr*)
Gaffield, W. *et al., Tetrahedron*, 1978, **34**, 3089 (*cd*)
Husein, S.Z. *et al., Phytochemistry*, 1981, **20**, 1171 (*occur*)
Bouillant, M.L. *et al., Phytochemistry*, 1984, **23**, 2653 (*6″-glucoside*)
Baktiar, A. *et al., Phytochemistry*, 1990, **29**, 1339 (*6,8-Diglucosylgenkwanin*)
El-Sayed, N.H. *et al., Asian J. Chem.*, 1997, **9**, 738-741 (*Digentiobiosylapigenin*)
Hussein, S.A.M. *et al., Phytochemistry*, 1997, **45**, 1529 (*diglucosyl*)
El-Mousallamy, A.M.D. *et al., Phytochemistry*, 2000, **53**, 699-704 (*4″,4‴-Diglucosylvicenin 2*)

Vignatic acid A V-25

[181485-19-8]



$C_{30}H_{39}N_3O_7$ 553.654
Constit. of *Vigna radiata* (mung bean).
Powder. $[\alpha]_D$ -99 (c, 0.11 in MeOH).

Sugawara, F. *et al., J. Agric. Food Chem.*, 1996, **44**, 3360-3364 (*isol, pmr, cmr, hplc*)

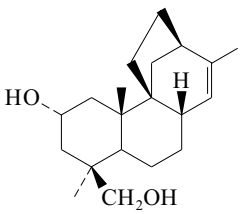
Vignatic acid B V-26

[181485-20-1]
As Vignatic acid A, V-25 with
R = $-CH_2CH(CH_3)_2$
$C_{27}H_{41}N_3O_7$ 519.637
Constit. of *Vigna radiata* (mung bean).
Powder. $[\alpha]_D$ -79 (c, 0.16 in MeOH).

Sugawara, F. *et al., J. Agric. Food Chem.*, 1996, **44**, 3360-3364 (*isol, pmr, cmr, hplc*)

13-Villanovene-2,19-diol V-27

13-Stemarene-2,19-diol



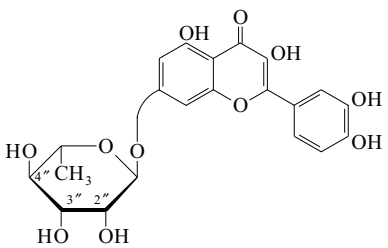
$C_{20}H_{32}O_2$ 304.472

3α-*form* [143437-61-0]
Oryzalexin S
Constit. of rice plants infected with *Pyricularia oryzae*. Cryst. Mp 173°. $[\alpha]_D^{26.5}$ +32 (c, 1 in $CHCl_3$).

Kodama, O. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1002 (*isol, pmr, cmr*)
Tomogami, S. *et al., Tetrahedron*, 1993, **49**, 2025 (*isol, pmr, cmr*)

Vincetoxicoside B V-28

[22007-72-3]
3,3′,4′,5-Tetrahydroxy-7-O-*α*-L-*rhamnopyranosyloxyflavone. Quercetin 7-rhamnoside*



$C_{21}H_{20}O_{11}$ 448.382
Mp 269° (264-267°, 256-257°).

3-O-*Arabinoside:* [38784-82-6] *Quercetin 3-arabinoside 7-rhamnoside*
$C_{26}H_{28}O_{15}$ 580.498

3-O-*β*-D-*Galactopyranoside:* Hyperin, H-837

3-O-*α*-L-*Rhamnopyranoside:* Quercitrin, Q-7

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [64828-40-6] ***Oxymyrioside***
$C_{33}H_{40}O_{21}$ 772.666

3-O-*[Acetyl-(→?)-[β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranoside]]:* [65026-65-5] ***Acetyloxymyrioside***
$C_{35}H_{42}O_{22}$ 814.704

3-O-*[3*-O-*Benzoyl-β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [88064-46-4]
$C_{40}H_{44}O_{22}$ 876.774

3-O-*[4-Hydroxycinnamoyl-(→?)-[β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranoside]]:* [64828-41-7] ***Coumaroyloxymyrioside***
$C_{42}H_{46}O_{23}$ 918.812

3-O-*[4-Hydroxycinnamoyl-(→4)-β*-D-*glucopyranosyl-(1→6)-β*-D-*glucopyranoside]:*
$C_{42}H_{46}O_{23}$ 918.812

3-O-*[4-Hydroxy*-E-*cinnamoyl-(→6)-β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:*
$C_{42}H_{46}O_{23}$ 918.812
Orange-yellow powder. Mp 170-173°. $[\alpha]_D^{25}$ -27.6 (c, 0.1 in MeOH). λ_{max} 247 (log ε 0.53); 340 (log ε 0.74) (MeOH).

3-O-*[3,4-Dihydroxy*-E-*cinnamoyl-(→6)-β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:*
$C_{42}H_{46}O_{24}$ 934.811
Orange-yellow powder. Mp 223-225°. $[\alpha]_D^{25}$ -55 (c, 0.1 in MeOH). λ_{max} 255 (log ε 0.89); 336 (log ε 0.75) (MeOH).

3-O-*[α*-L-*Rhamnopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [161993-01-7]
$C_{33}H_{40}O_{20}$ 756.667

3-O-*[α*-L-*Rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [81970-00-5] ***Clovin***
$C_{33}H_{40}O_{20}$ 756.667
Isol. from *Melilotus alba* (white melilot).

3-O-*[α*-L-*Rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* Rutin, R-74

3-O-*[4-Hydroxycinnamoyl-(→4)-α*-L-*rhamnopyranosyl-(1→6)-β*-D-*glucopyranoside]:* [111545-15-4]
$C_{42}H_{46}O_{22}$ 902.812
Yellow powder. Mp 214-216°.

3-O-*[β*-L-*Rhamnofuranosyl-(1→6)-β*-D-*glucopyranoside]:* [54707-52-7] ***Flavantaside***
$C_{33}H_{40}O_{20}$ 756.667

3-O-*[β*-D-*Glucopyranosyl-(1→2)-β*-D-*glucopyranosyl-(1→2)-β*-D-*glucopyranoside]:* [72089-32-8]
$C_{39}H_{50}O_{26}$ 934.808
Constit. of *Solanum* spp..

3-O-*[4-Hydroxy*-E-*cinnamoyl-(→3)-[α*-L-*rhamnopyranosyl-(1→2)]-[α*-L-*rhamnopyranosyl-(1→6)]-β*-D-*galactopyranoside]:*
$C_{48}H_{56}O_{26}$ 1048.955
Yellow powder. $[\alpha]_D^{21}$ -160 (c, 1 in MeOH). λ_{max} 228 (sh) (log ε 4.42); 255 (log ε 4.4); 270 (sh) (log ε 4.34); 300 (sh) (log ε 4.42); 317 (log ε 4.49); 361 (sh) (log ε 4.24) (MeOH).

3-O-*[4-Hydroxy*-E-*cinnamoyl-(→4)-[α*-L-*rhamnopyranosyl-(1→2)]-[α*-L-*rhamnopyranosyl-(1→6)]-β*-D-*galactopyranoside]:*
$C_{48}H_{56}O_{26}$ 1048.955
Yellow powder. $[\alpha]_D^{24}$ -193 (c, 1 in MeOH). λ_{max} 227 (sh) (log ε 4.35); 256 (log ε 4.31); 270 (sh) (log ε 4.27); 299 (sh) (log ε 4.33); 315 (log ε 4.4); 364 (sh) (log ε 4.14) (MeOH).

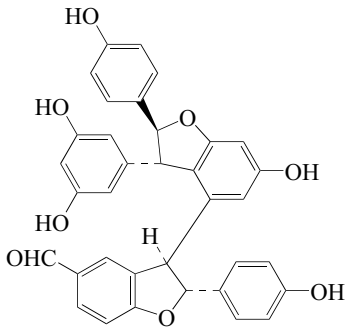
O″-*β*-D-*Glucopyranosyl:*
$C_{27}H_{30}O_{16}$ 610.524
Isol. from *Capparis spinosa* (caper).
Complete struct. not detd. Ref. inaccessible.

Kozjek, F. *et al., C. R. Hebd. Seances Acad. Sci. Ser. D*, 1967, **264**, 2409 (*isol*)
Kommissarenko, N.F. *et al., Rastit. Resur.*, 1974, **10**, 567; 1977, **13**, 342 (*Flavantaside*)
Blinova, K.F. *et al., Rastit. Resur.*, 1977, **13**, 466 (*Oxymyriosides*)
Nicollier, G.F. *et al., J. Agric. Food Chem.*, 1982, **30**, 760 (*Clovin*)
Zaitsev, V.G. *et al., Khim. Prir. Soedin.*, 1983, **19**, 527; *Chem. Nat. Compd. (Engl. Transl.)*, 1983, **19**, 499 (*isol*)

Warnock, M.J. *et al., Phytochemistry*, 1983, **22**, 1834 (*3-Benzoylsophoroside*)
Schaufelberger, D. *et al., Phytochemistry*, 1987, **26**, 2377 (*3-coumaroylrobinobioside*)
Barakat, H.H. *et al., Phytochemistry*, 1991, **30**, 3777 (*3-coumaroylgentiobioside*)
Nunez-Alarcon, J. *et al., Bol. Soc. Chil. Quim.*, 1994, **39**, 269 (*3-arabinoside*)
Mulinacci, N. *et al., Phytochemistry*, 1995, **38**, 531 (*3-neohesperidoside*)
Fico, G. *et al., Planta Med.*, 2001, **67**, 287-290 (*Aconitum napellus glycosides*)
Itoh, A. *et al., J. Nat. Prod.*, 2002, **65**, 352-357 (*Rhazya orientalis glycosides*)

Viniferal V-29

[180413-42-7]

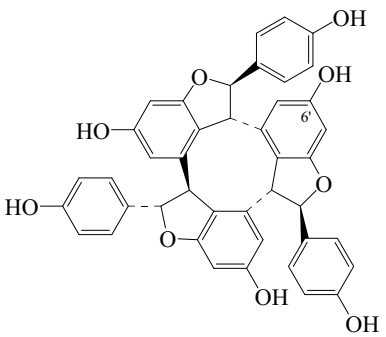


$C_{35}H_{26}O_8$ 574.586
Constit. of *Vitis vinifera* (wine grape). $[\alpha]_D$ -131.7 (c, 1.6 in MeOH).

Ito, J. *et al., Tetrahedron*, 1996, **52**, 9991-9998 (*isol, ir, pmr, cmr*)

α-Viniferin V-30

[62218-13-7]

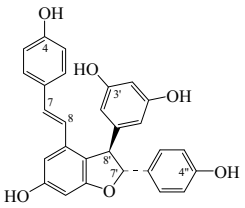


$C_{42}H_{30}O_9$ 678.694
Constit. of *Vitis vinifera* (wine grape). Pale yellow cryst. $[\alpha]_D$ +51.4 (c, 1 in EtOH). λ_{max} 225 (sh) (log ϵ 4.68); 281 (sh) (log ϵ 3.92); 286 (log ϵ 4); 293 (sh) (log ϵ 3.93) (no solvent reported). λ_{max} 286 (ϵ 10000) (EtOH) (Berdy).

6′-O-β-D-Glucopyranoside:
$C_{48}H_{40}O_{14}$ 840.836
Amorph. pale yellow solid. $[\alpha]_D^{24}$ +32 (c, 0.1 in MeOH). λ_{max} 228 ; 285 (MeOH).

Langcake, P. *et al., Experientia*, 1977, **33**, 151 (*isol*)
Langcake, P. *et al., Phytochemistry*, 1977, **16**, 1193 (*biosynth*)
Pryce, R.J. *et al., Phytochemistry*, 1977, **16**, 1452 (*isol*)
Lee, S.-H. *et al., Planta Med.*, 1998, **64**, 204-207 (*isol, pmr, cmr, activity*)
Ito, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1001-1005 (*6′-glucoside*)

ϵ-Viniferin V-31



(7*E*,7′*R*,8′*R*)-*form*

$C_{28}H_{22}O_6$ 454.478
(7*E*,7′*R*,8′*R*)-*form*
Isol. from leaves of wine grape (*Vitis vinifera*) infected with *Botrytis cinerea*. Amorph. solid. Mp 155-156°. λ_{max} 224 (ϵ 54200); 286 (sh) (ϵ 15100); 310 (ϵ 22800); 324 (ϵ 24300); 345 (sh) (ϵ 13000) (EtOH).

3′,5′-Di-O-β-D-glucopyranoside:
$C_{40}H_{42}O_{16}$ 778.762
Isol. from Riesling wine.

7′,8′-Didehydro: [223591-26-2] ***Viniferifuran***. *Amurensin H*
$C_{28}H_{20}O_6$ 452.462
Isol. from Riesling wine. Constit. of wine grapes (*Vitis vinifera* 'Kyohou') and amur grape (*Vitis amurensis*). Amorph. pale yellow powder. λ_{max} 209 (log ϵ 4.79); 227 (sh) (log ϵ 4.62); 258 (log ϵ 4.33); 289 (sh) (log ϵ 4.44); 308 (log ϵ 4.53); 317 (log ϵ 4.54); 337 (log ϵ 4.53); 350 (sh) (log ϵ 4.52) (MeOH).

2″-Hydroxy: [256415-38-0] ***Gnetuhainin A***
$C_{28}H_{22}O_7$ 470.478
Amorph. powder. $[\alpha]_D^{25}$ +13.2 (c, 0.1 in MeOH). λ_{max} 284 (log ϵ 4.2); 307 (log ϵ 4.3); 320 (log ϵ 4.3) (MeOH).

2″-Hydroxy, 7′,8′-didehydro: [256415-39-1] ***Gnetuhainin B***
$C_{28}H_{20}O_7$ 468.462
Amorph. greenish powder. λ_{max} 284 (log ϵ 4.5); 320 (log ϵ 4.6); 356 (log ϵ 4.3) (MeOH).

*7,8-Dihydro, 7*R*,8*R*-dihydroxy:* [142449-88-5] ***ϵ-Viniferin diol***. *Betulifol B*
$C_{28}H_{24}O_8$ 488.493
Amorph. powder. $[\alpha]_D$ +136 (c, 0.2 in MeOH).

(7*E*,7′*S*,8′*R*)-*form* [174023-03-1]
(7*E*,7′*S*,8′*S*)-*form* [129170-22-5]
Constit. of wine grapes *Vitis vinifera*. Brown solid. $[\alpha]_D$ +49.1 (c, 1.9 in MeOH).

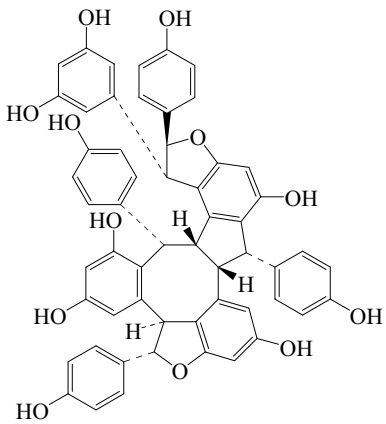
4,4″-Di-O-β-D-glucopyranoside: ***Gnemonoside E***
$C_{40}H_{42}O_{16}$ 778.762
Amorph. brown powder. $[\alpha]_D$ -75 (c, 0.1 in MeOH). λ_{max} 213 ; 318 (MeOH).

(7*Z*,7′*R*,8′*R*)-*form* [62250-12-8] **cis-ϵ-Viniferin**
Isol. from wine grapes.

3′,5′-Di-O-β-D-glucopyranoside:
$C_{40}H_{42}O_{16}$ 778.762
Isol. from Riesling wine.

Langcake, P. *et al., Phytochemistry*, 1977, **16**, 1193-1196 (*biosynth*)
Sotheeswaran, S. *et al., J.C.S. Perkin 1*, 1985, 159-162 (*cmr, struct*)
Sotheeswaran, S. *et al., Phytochemistry*, 1993, **32**, 1083-1092 (*rev, bibl*)
Iinuma, M. *et al., Phytochemistry*, 1994, **37**, 1157-1159 (*isol*)
Engler, T.A. *et al., Tet. Lett.*, 1994, **35**, 1661-1664 (*synth*)
Oshima, Y. *et al., Tetrahedron*, 1995, **51**, 11979-11986 (*ϵ-Viniferin diol*)
Li, W.-W. *et al., Phytochemistry*, 1996, **42**, 1163 (*(+)-Viniferin, Betulifol B*)
Huang, K.S. *et al., Chin. Chem. Lett.*, 1999, **10**, 817-820 (*Amurensin H*)
Ito, J. *et al., Tetrahedron*, 1999, **55**, 2529-2544 (*Viniferifuran*)
Baderschneider, B. *et al., J. Agric. Food Chem.*, 2000, **48**, 2681-2686 (*isol, diglucosides*)
Huang, K.-S. *et al., J. Nat. Prod.*, 2000, **63**, 86-89 (*Gnetuhainins*)
Bala, A.E.A. *et al., J. Phytopathol.*, 2000, **148**, 29-32 (*cis-Viniferin*)
Iliya, I. *et al., Chem. Pharm. Bull.*, 2002, **50**, 796-801 (*Gnemonoside E*)

Viniferol A V-32

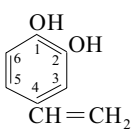


$C_{56}H_{42}O_{12}$ 906.941
Constit. of wine grape *Vitis vinifera* 'Kyohou'. Amorph. solid. $[\alpha]_D$ +136.6 (c, 0.6 in MeOH). λ_{max} 227 (sh) (log ϵ 4.8); 284 (log ϵ 3.99) (MeOH).

Yan, K.-X. *et al., Tetrahedron*, 2001, **57**, 2711-2715

4-Vinyl-1,2-benzenediol V-33

[6053-02-7]
4-Ethenyl-1,2-benzenediol, 9CI. 4-Vinylpyrocatechol, 8CI. (3,4-Dihydroxyphenyl)ethylene. 3,4-Dihydroxystyrene. 3,4-Styrenediol



$C_8H_8O_2$ 136.15
Needles.

Dibenzoyl: [13594-97-3]
$C_{22}H_{16}O_4$ 344.366
Mp 98-99°.

1-Me ether: [621-58-9] *5-Ethenyl-2-meth-*

oxyphenol, 9CI. 3-Hydroxy-4-methoxystyrene. 2-Methoxy-5-vinylphenol
$C_9H_{10}O_2$ 150.177
Mp 55-56°.

2-Me ether: [7786-61-0] *2-Methoxy-4-vinylphenol. Hesperetol. 4-Vinylguaiacol*
$C_9H_{10}O_2$ 150.177
Responsible for off-flavour of 'old fruit' in stored orange juice. Mp 57°. Undergoes radical polym. λ_{max} 211 (ϵ 17780); 287 (ϵ 10300); 312 (ϵ 8900) (MeOH) (Berdy).

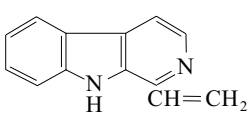
Di-Me ether: [6380-23-0] *1,2-Dimethoxy-4-vinylbenzene. 3,4-Dimethoxystyrene. 4-Vinylveratrole. FEMA 3138*
$C_{10}H_{12}O_2$ 164.204
Flavouring ingredient. Constit. of roasted coffee aroma and boiled buckwheat flour flavour. Bp_{10} 120-125°. n_D^{20} 1.5710. Undergoes radical and cationic polym..

1-Benzyl, 2-Me ether: [55708-65-1]
$C_{16}H_{16}O_2$ 240.301
Needles (hexane). Mp 55-56°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1053D (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 208C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 986B (*ir, di-Me ether*)
Karchmarchik, O.S. *et al., Zh. Org. Khim.*, 1966, **2**, 1528; *CA*, **66**, 65213 (*synth*)
Kametani, T. *et al., Tetrahedron*, 1975, **31**, 235 (*1-benzyl ether 2-Me ether, synth, ir*)
Yajima, I. *et al., Agric. Biol. Chem.*, 1983, **47**, 729-738 (*di-Me ether, occur, buckwheat*)
Iwabuchi, S. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1983, **21**, 1877 (*polym, derivs*)
Rooney, J.M. *et al., Polym. Bull. (Berlin)*, 1983, **10**, 414 (*cationic polym, deriv*)
Koizumi, S. *et al., Biochim. Biophys. Acta*, 1984, **789**, 111 (*isol, props*)
Silwar, R. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1987, **10**, 176-187 (*di-Me ether, occur, coffee*)
Castedo, L. *et al., Synth. Commun.*, 1995, **25**, 1717 (*1-Me ether*)
Walsh, M. *et al., J. Agric. Food Chem.*, 1997, **45**, 1320-1324 (*2-Me ether, occur*)
Fisher, A. *et al., Synth. Commun.*, 1998, **28**, 2959-2968 (*1-Me ether*)
Nagashima, F. *et al., Phytochemistry*, 1999, **51**, 1101-1104 (*di-Me ether, uv, ir, pmr, cmr, ms*)

1-Vinyl-β-carboline V-34

[20127-60-0]
*1-Ethenyl-9*H*-pyrido[3,4-*b*]indole, 9CI. **Pavettine***



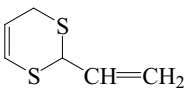
$C_{13}H_{10}N_2$ 194.235
Yellowish cryst. Mp 167-169°.

N-*Methoxy:* [69355-01-7] **N-*Methoxy-1-vinyl-β-carboline***
$C_{14}H_{12}N_2O$ 224.262
Alkaloid from *Picrasma excelsa* (Jamaican quassiawood). Mp 185-190° dec.

Jordaan, A. *et al., J. S. Afr. Chem. Inst.*, 1968, **21**, 22 (*isol, uv, ir, pmr, ms, synth*)
Wagner, H. *et al., Tet. Lett.*, 1978, 2777 (*deriv*)
Bracher, F. *et al., Annalen*, 1992, 1315 (*synth, ir, pmr, cmr, ms*)
Rocca, P. *et al., Tetrahedron*, 1993, **49**, 3325 (*synth, ir, pmr, cmr*)

2-Vinyl-4*H*-1,3-dithiine V-35

[80028-57-5]
*2-Ethenyl-4*H*-1,3-dithiine, 9CI*

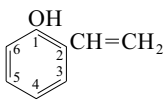


$C_6H_8S_2$ 144.261
Present in garlic (*Allium sativum*) and caucas (*Allium victorialis*) but not in onion or rakkyo. Oil.

Vedejs, E. *et al., J.A.C.S.*, 1982, **104**, 1445-1447 (*synth, pmr*)
Beslin, P. *et al., J. Het. Chem.*, 1983, **20**, 1753-1754 (*synth*)
Nishimura, H. *et al., J. Agric. Food Chem.*, 1988, **36**, 563-566 (*isol, pmr, ms*)
Mochizuki, E. *et al., J. Agric. Food Chem.*, 1998, **46**, 5170-5176 (*occur, glc*)

2-Vinylphenol, 8CI V-36

[695-84-1]
2-Ethenylphenol, 9CI. (2-Hydroxyphenyl)ethylene. 2-Hydroxystyrene



C_8H_8O 120.151
Sol. H_2O, Et_2O, EtOH. d^{18} 1.06. Fp 26. Bp_{15} 165°. n_D^{20} 1.5851. Undergoes radical and cationic polym..

Ac: [63600-35-1]
$C_{10}H_{10}O_2$ 162.188
Bp_1 85°.

Me ether: [612-15-7] *1-Ethenyl-2-methoxybenzene, 9CI. 1-Methoxy-2-vinylbenzene.* o-*Vinylanisole.* o-*Methoxystyrene*
$C_9H_{10}O$ 134.177
Flavouring ingredient. Bp_{10} 73-75°. n_D^{20} 1.5530.

Marvel, C.S. *et al., J.A.C.S.*, 1948, **70**, 1895-1898 (*Me ether*)
Corson, B.B. *et al., J.O.C.*, 1958, **23**, 544-549 (*synth*)
Dale, W.J. *et al., J.A.C.S.*, 1959, **81**, 2143-2146 (*Me ether*)
Kato, M. *et al., J. Polym. Sci., Part A-1*, 1966, **4**, 1773-1782; 2771-2780; 1969, **7**, 2405-2410 (*polym*)
Morlyan, N.M. *et al., CA*, 1973, **78**, 3864 (*synth*)
Dhekne, V.V. *et al., Synthesis*, 1980, 58-60 (*Ac*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **1**, 796 (*Me ether*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2916-2917 (*Me ether*)

4-Vinylphenol, 8CI V-37

[2628-17-3]
(4-Hydroxyphenyl)ethylene. 4-Ethenylphenol, 9CI. 4-Hydroxystyrene. FEMA 3739

C_8H_8O 120.151
Flavour component of tea; flavouring ingredient. Needles by subl. with vanilla odour. Mp 68-69°. Undergoes radical and cationic polym..

▶ Severe eye irritant. SN3800000

O-*[α-L-Arabinopyranosyl-(1→6)-β-D-glucopyranoside]:* [98755-18-1] ***Ptelatoside C***
$C_{19}H_{26}O_{10}$ 414.408
Isol. from *Pteridium aquilinum* (bracken fern). Amorph. powder. $[\alpha]_D$ -70 (c, 1 in H_2O).

O-*[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]:* [90899-20-0] ***Ptelatoside A***
$C_{19}H_{26}O_{10}$ 414.408
Constit. of bracken fern *Pteridium aquilinum*. Cryst. (Me_2CO aq.). Mp 183-185°. $[\alpha]_D^{22}$ -104 (c, 0.68 in H_2O). λ_{max} 202 (MeOH) (Berdy).

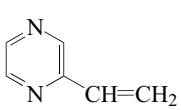
O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [90852-99-6] ***Ptelatoside B***
$C_{20}H_{28}O_{10}$ 428.435
Constit. of *Pteridium aquilinum* (bracken fern). Amorph. $[\alpha]_D^{23}$ -94.8 (c, 1 in H_2O).

[95418-58-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1052C (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 207C; 1287C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 984B; 985B (*ir*)
Schmid, H. *et al., Helv. Chim. Acta*, 1945, **28**, 722 (*isol*)
Corson, B.B. *et al., J.O.C.*, 1958, **23**, 544 (*synth*)
Arshady, R. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1974, **12**, 2017 (*synth*)
Hatakeyama, H. *et al., Polymer*, 1978, **19**, 593 (*synth*)
Ojika, M. *et al., J. Nat. Prod.*, 1985, **48**, 634 (*Ptelatoside C*)
Ojika, M. *et al., Tetrahedron*, 1987, **43**, 5275 (*Ptelatosides*)
Everhart, E.T. *et al., J.C.S. Perkin 1*, 1991, 1701 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 798
Ayer, W.A. *et al., Phytochemistry*, 1996, **42**, 1321 (*isol, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2918
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VQA200

Vinylpyrazine V-38

[4177-16-6]
Ethenylpyrazine, 9CI, 8CI



$C_6H_6N_2$ 106.127
Liq. d^{20} 1.05. Bp_{21} 63-64°. n_D^{25} 1.5533.

Methiodide:
Yellow cryst. (Me_2CO). Mp 126°.

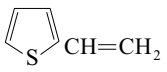
Picrate:
Cryst. (EtOH). Mp 99-100°.

Kitchen, L.J. *et al., J.A.C.S.*, 1957, **73**, 1838-1839 (*synth*)

Kamal, M.R. *et al., J.O.C.*, 1962, **27**, 1363-1366 (*synth*)
Bondarovich, H.A. *et al., J. Agric. Food Chem.*, 1967, **15**, 1093 (*ir, uv, ms*)
Oertel, R.P. *et al., Anal. Chem.*, 1972, **44**, 1589-1593 (*Raman*)
Rezanka, T. *et al., Biotechnol. Lett.*, 1994, **16**, 75-78 (*glc, ms*)

2-Vinylthiophene V-39

[1918-82-7]
2-Ethenylthiophene, 9CI

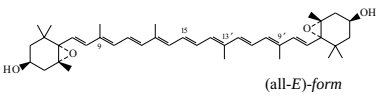


C_6H_6S 110.179
Maillard product. Liq. Bp_{50} 65-67°.

v. Reuendam, J. *et al., Tetrahedron*, 1970, **26**, 1291 (*synth, uv*)
Matsumoto, M. *et al., Tet. Lett.*, 1975, **50**, 4471

Violaxanthin V-40

5,6:5′,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3,3′-diol. Zeaxanthin diepoxide. Violeaxanthin



(all-*E*)-*form*

$C_{40}H_{56}O_4$ 600.88

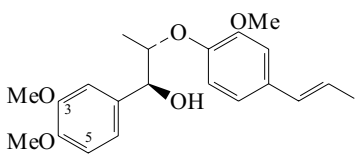
(all-*E*)-*form* [126-29-4]
Red cryst. (MeOH). Mp 208°. $[\alpha]_D^{20}$ +38 ($CHCl_3$).

Monodeoxy: [2086-87-5] *5,5′,6,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-caroten-3-ol, 9CI. Cryptoxanthin diepoxide*
$C_{40}H_{56}O_3$ 584.881
Isol. from *Eriobotrya japonica* (loquat) fruit and *Prunus persica* fruit (peach mesocarp during ripening). Cryst. (C_6H_6/petrol). Mp 194°. λ_{max} 473 ; 503 (CS_2). λ_{max} 415 ; 438 ; 468 (no solvent reported). λ_{max} 442 ; 472 (EtOH).

Stransky, H. *et al., Arch. Microbiol.*, 1970, **71**, 164 (*isol, deoxy*)
Sapozhnikov, D.I. *et al., Pure Appl. Chem.*, 1973, **35**, 47 (*rev*)
Lessertois, D. *et al., Phytochemistry*, 1978, **17**, 411 (*isol, deoxy*)

Virolin V-41

[68143-83-9]



$C_{21}H_{26}O_5$ 358.433
Neolignan numbering shown. Stereochemical information for the compounds covered by this entry is incomplete.Oil.

7-Ketone: [139343-57-0] ***Bennettinone***
$C_{21}H_{24}O_5$ 356.418
Needles (petrol). Mp 85-87°. Racemic λ_{max} 231 (ε 23440); 279 (ε 12300); 309 (ε 8510) (EtOH).

O^4-De-Me: [110269-53-9] ***Machilin D***
$C_{20}H_{24}O_5$ 344.407
Oil. $[\alpha]_D^{25}$ +38.1 (c, 0.07 in $CHCl_3$).

O^4-De-Me, diastereoisomer: [110269-51-7] ***Machilin C***
$C_{20}H_{24}O_5$ 344.407
Oil. $[\alpha]_D^{25}$ -16.5 (c, 0.27 in $CHCl_3$).

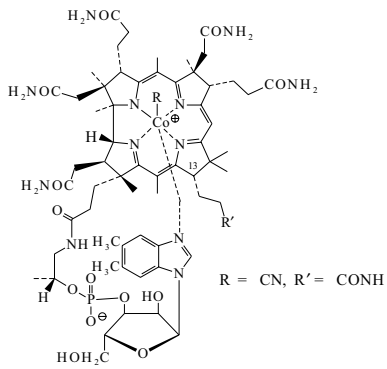
5-Methoxy: [68143-82-8] ***Surinamensin***
$C_{22}H_{28}O_6$ 388.46
Oil. $[\alpha]_D$ +52 (c, 1 in $CHCl_3$).

5-Methoxy, O^4-de-Me: [108907-56-8] ***1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[2-methoxy-4-(1-propenyl)phenoxy]-1-propanol***
$C_{21}H_{26}O_6$ 374.433
Constit. of *Myristica fragrans* (nutmeg) oil. Oil. No stereochem. indicated.

Barata, L.E.S. *et al., Phytochemistry*, 1978, **17**, 783 (*isol*)
Zacchino, S.A. *et al., J. Nat. Prod.*, 1985, **48**, 830 (*synth*)
Calvacante, S.H. *et al., Phytochemistry*, 1985, **24**, 1051
Hattori, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 668
Shimomura, H. *et al., Phytochemistry*, 1987, **26**, 1513
Santos, L. da S. *et al., J. Braz. Chem. Soc.*, 1990, **1**, 47-49 (*Surinamensin, abs config*)
Carroll, A.R. *et al., Aust. J. Chem.*, 1991, **44**, 1627 (*Bennettinone*)
Zacchino, S.A. *et al., J. Nat. Prod.*, 1994, **57**, 446 (*synth*)
Sung, S.H. *et al., Chem. Pharm. Bull.*, 2001, **49**, 1192-1194 (*isol, pmr, cmr*)

Vitamin B_{12} V-42

[68-19-9]
Cyanocobalamin, BAN, INN, USAN. *α-(5,6-Dimethylbenzimidazoyl)cobamide cyanide. Cobamin. Cykobemin. Factor II*



R = CN, R′ = CONH

$C_{63}H_{88}CoN_{14}O_{14}P$ 1355.38
Antipernicious anaemia factor isol. from liver extracts; now obt. comly. from fermentation liquors of *Streptomyces griseus* and other microorganisms, e.g. *Propionibacterium shermanii*, *Pseudomonas denitrificans*. Nutrient, dietary supplement, stabiliser. Haematopoietic vitamin. Red needles. Sol. H_2O, alcohols, AcOH. Mp 300° Mp 210-220° darkens. Isotopic variants contg. ^{57}Co ($t_{1/2}$ 270d), ^{58}Co ($t_{1/2}$ 71.3d) and ^{60}Co ($t_{1/2}$ 5.26y) are prepd. by fermentation in the presence of radiocobalt and are used for diagnostic purposes λ_{max} 279 ; 306 ; 322 ; 361 ; 520 ; 550 (no solvent reported).

▶ Exp. reprod. and teratogenic effects. GG3750000

13-Epimer: [32627-64-8] *Cyanoneocobalamin. Neovitamin B_{12}*
Red cryst. (Me_2CO aq.). CD; λ 330 nm, Δε + 8.4 (0.1*M* KCN). Dec. at *ca.* 200° without melting.

Decyano: [13408-78-1] *Cobalamin*
$C_{62}H_{88}CoN_{13}O_{14}P^{\oplus}$ 1329.363

Decyano, Co(II) complex: [14463-33-3] *Vitamin B_{12r}. Cob(II)-alamin*
$C_{62}H_{88}CoN_{13}O_{14}P$ 1329.363

[13115-03-2, 13422-53-2, 18195-32-9]

Bonnett, R. *et al., Chem. Rev.*, 1963, **63**, 573 (*rev*)
Nockolds, C.K. *et al., Nature (London)*, 1967, **214**, 129 (*cryst struct*)
Pratt, J.M. *et al., Inorg. Chem. of Vit. B_{12}*, Academic Press, 1972, (*rev*)
Stöckli-Evans, H. *et al., J.C.S. Perkin 2*, 1972, 605 (*cryst struct*)
Woodward, R.B. *et al., Pure Appl. Chem.*, 1973, **33**, 145 (*synth*)
Bonnett, R. *et al., Philos. Trans. R. Soc. London*, 1976, **273**, 295 (*epimer*)
Schrauzer, G.N. *et al., Angew. Chem.*, 1977, **89**, 239
Rajoria, D.S. *et al., J. Inorg. Nucl. Chem.*, 1977, **39**, 1291 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **24**, 158 (*rev*)
Florent, J. *et al., Microb. Technol.*, 2nd edn., (eds. Peppler, H.J. *et al*), Academic Press, 1979, **1**, 497 (*rev, manuf*)
Zagalak, B. *et al., Vitamin B_{12}*, Walter de Gruyter, New York, 1979,
Kirschbaum, J. *et al., Anal. Profiles Drug Subst.*, 1981, **10**, 183 (*rev*)
B_{12} [Twelve], (ed. Dolphin, D.), Wiley, New York, 1982, **1**, ; **2**,
Anton, D.L. *et al., Biochemistry*, 1982, **21**, 2372 (*cmr*)
Ellenbogen, L. *et al., Food Sci. Technol.*, 1984, **13**, 497 (*rev*)
Brown, K.L. *et al., J.A.C.S.*, 1984, **106**, 7894 (*P-31 nmr*)
Leeper, F.J. *et al., Nat. Prod. Rep.*, 1985, **2**, 19; 561; 1987, **4**, 441; 1989, **6**, 171 (*revs, biosynth*)
Battersby, A.R. *et al., Acc. Chem. Res.*, 1986, **19**, 147 (*rev, biosynth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 8358
Eschenmoser, A. *et al., Angew. Chem., Int. Ed.*, 1988, **27**, 6 (*rev*)
Halpern, J. *et al., Bull. Soc. Chim. Fr.*, 1988, 187 (*rev, chem*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, VSZ000
Briois, V. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1989, **86**, 1623 (*x-ray absorption*)
Kraeutler, B. *et al., J.A.C.S.*, 1989, **111**, 8936 (*Vitamin B_{12r}*)
Kurumaya, K. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1058 (*biosynth, N-15 nmr*)
Sagi, I. *et al., J.A.C.S.*, 1990, **112**, 8639 (*Vitamin B_{12r} exafs*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1055
Scott, A.I. *et al., Tetrahedron*, 1994, **50**, 13315 (*rev, biosynth*)
Blanche, F. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 383 (*rev, biosynth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 99 (*bibl, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2926-2929 (*props*)

Kräutler, B. *et al., Vitamin B12 and B12-proteins*, Wiley-VCH, 1997,
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VSZ000

Vitamin B_{12a} V-43

[13422-51-0]

*Cobinamide dihydroxide dihydrogen phosphate (ester) mono (inner salt) 3′-ester with 5,6-dimethyl -1-α-D-ribofuranosyl-1*H*-benzimidazole, 9CI.* ***Hydroxycobalamin, BAN, INN, USAN****. Hydroxocobalamin. AlphaRedisol. Codroxomin. Lipflavonoid. Neo-Betalin 12. Sytobex H. Vibeden*

As Vitamin B_{12}, with

R = OH, R′ = $CONH_2$

$C_{62}H_{89}CoN_{13}O_{15}P$ 1346.37

Exists in aq. soln. as an equilibrium mixture with the ionic aquo isomer Vitamin B_{12b}. Vitamin (haematopoietic). Red cryst. (Me_2CO aq.).

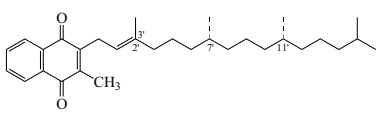
▶ GG3820000

Bonnett, R. *et al., Chem. Rev.*, 1963, **63**, 573
Rajoria, D.S. *et al., J. Inorg. Nucl. Chem.*, 1977, **39**, 1291 (*ir*)
Bratt, G.T. *et al., Biochemistry*, 1984, **23**, 5653 (*cmr*)
Brown, K.L. *et al., J.A.C.S.*, 1984, **106**, 7894; 1986, **108**, 496 (*pmr, P-31 nmr, cmr*)
Brouard, A. *et al., J. Toxicol. Clin. Exp.*, 1987, **7**, 155 (*rev, use*)

Vitamin K_1 V-44

[84-80-0]

2-Methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-naphthalenedione, 9CI. 2-Methyl-3-phytyl-1,4-naphthoquinone. ***Phytomenadione, BAN, INN****. Phytonadione, USAN. Combinal K_1. Kativ N. Kaywan. Konakim. Phylloquinone. α-Phyllostin. Many other names*



$C_{31}H_{46}O_2$ 450.703

Widely distributed in green leaves and vegetables, esp. cabbage and spinach. Infant formula fortifier. Pale yellow oil, yellow cryst. (Me_2CO at -20°). Mp -4°. Log P 11.76 (uncertain value) (calc). All 4 stereoisomers have been synthesised λ_{max} 248 ; 261 ; 270 ; 328 (MeOH) (Berdy).

▶ Local effects in humans following intramuscular or subcutaneous administration. LD_{50} (mus, orl) 25000 mg/kg. QJ5800000

2′,3′-Dihydro: [64236-23-3]

[86784-49-8] *2-Methyl-3-(3,7,11,15-tetramethylhexadecyl)-1,4-naphthalenedione, 9CI. 2′,3′-Dihydrovitamin K_1*

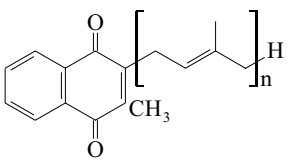
$C_{31}H_{48}O_2$ 452.719

Present in hydrogenated vegetable oils and a wide range of foods prepared from them. Readily absorbed by humans from dietary sources. About 15-fold less potent than natural vitamin K_1 in chick blood coagulation assay. Golden yellow oil. Individual diastereomers at C-3′ have not been well described.

[16033-41-3, 132487-93-5, 132487-94-6, 132487-95-7]

Fieser, L.F. *et al., J.A.C.S.*, 1939, **61**, 3467
Tishler, M. *et al., J.A.C.S.*, 1940, **62**, 2866-2871 (*dihydro, synth*)
Doisy, E.A. *et al., Chem. Rev.*, 1941, **28**, 477 (*rev, bibl*)
Jacobsen, B.K. *et al., Biochim. Biophys. Acta*, 1960, **40**, 211 (*isol, purifn*)
Mayer, H. *et al., Helv. Chim. Acta*, 1964, **47**, 221 (*abs config*)
Jackman, L.M. *et al., Helv. Chim. Acta*, 1965, **48**, 1332 (*config*)
Barkhan, P. *et al., Proc. R. Soc. Med.*, 1977, **70**, 93 (*rev, metab*)
Chenard, B.L. *et al., J.O.C.*, 1980, **45**, 378 (*synth*)
Naruta, Y. *et al., J.O.C.*, 1980, **45**, 4097 (*synth*)
Doetz, K.H. *et al., J. Organomet. Chem.*, 1981, **209**, C4 (*synth*)
Schmid, M. *et al., Helv. Chim. Acta*, 1982, **65**, 684 (*synth*)
Weiser, H. *et al., Int. J. Vitam. Nutr. Res.*, 1983, **53**, 143-155 (*dihydro, biochem*)
Bentley, R. *et al., J. Nat. Prod.*, 1983, **46**, 44 (*biosynth*)
Masaki, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3959 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 7926
Hassan, M.M.A. *et al., Anal. Profiles Drug Subst.*, 1988, **17**, 449 (*rev*)
Schmid, R. *et al., Helv. Chim. Acta*, 1990, **73**, 1276 (*synth, ord, hplc, bibl*)
Ryall, R.P. *et al., J. Med. Chem.*, 1990, **33**, 1790-1797 (*dihydro, occur, hplc, synth, pmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1062
Booth, S.L. *et al., J. Agric. Food Chem.*, 1994, **42**, 295-300; 1995, **43**, 1574-1579; 1996, **44**, 980-983 (*occur, hplc, dihydro*)
Tso, H.-H. *et al., J. Chem. Res., Synop.*, 1995, 104 (*synth*)
Booth, S.L. *et al., Lipids*, 1996, **31**, 709-713; 715-720 (*dihydro, !occur, pharmacol, props*)
Koivu, T. *et al., Food Chem.*, 1999, **64**, 411-414 (*dihydro, occur, hplc*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, VTA000

Vitamin K_2 V-45



Consists of a mixt. of homologues. The figure in brackets after the name indicates the number of carbon atoms in the sidechain. The name vitamin K_2 is sometimes applied to vitamin K_2(30). Widely distributed in green leaves and vegetables. Fat sol. dietary factor effective in controlling blood coagulation. Various partially hydrogenated derivatives Dihydromenaquinones, Tetrahydromenaquinones, Hexahydromenaquinone 9 and Octahydromenaquinone 9 with partly saturated side-chains occur, e.g. in cultures of *Oerskovia turbata, Breisbacterium lipopolyticum* and *Actinomadura madurae*.

Vitamin K_2(25) [1182-68-9]

Menaquinone 5

$C_{36}H_{48}O_2$ 512.774

Yellow cryst. (EtOH). Mp 39°. λ_{max} 248 (petrol).

Vitamin K_2(30) [84-81-1]

Menaquinone 6. Menaquinone K_6. Farnoquinone. β-Phylloquinone

$C_{41}H_{56}O_2$ 580.892

Yellow cryst. (Me_2CO/EtOH or petrol). Mp 50°.

Vitamin K_2(35) [2124-57-4]

Menaquinone 7. Menaquinone K_7

$C_{46}H_{64}O_2$ 649.01

Cryst. (Me_2CO/EtOH or MeOH/$CHCl_3$). Mp 54°.

Vitamin K_2(40) [523-38-6]

Menaquinone 8. Menaquinone K_8

$C_{51}H_{72}O_2$ 717.129

Vitamin K_2(45) [523-39-7]

Menaquinone 9. Menaquinone K_9

$C_{56}H_{80}O_2$ 785.247

Cryst. Mp 58-59°.

Vitamin K_2(50) [523-40-0]

Menaquinone 10. Menaquinone K_{10}

$C_{61}H_{88}O_2$ 853.365

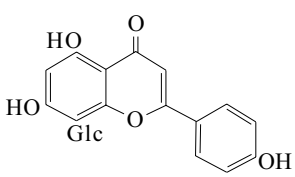
Cryst. Mp 62°.

Isler, O. *et al., Helv. Chim. Acta*, 1958, **41**, 786-803 (*synth, uv*)
Isler, O. *et al., Vitam. Horm. (N.Y.)*, 1959, **17**, 53 (*rev*)
Noll, H. *et al., Helv. Chim. Acta*, 1960, **43**, 433 (*isol*)
Noll, H. *et al., J. Biol. Chem.*, 1960, **235**, 2207 (*isol*)
Osnitskaya, L.K. *et al., Nature (London)*, 1964, **204**, 80
Sato, K. *et al., J.C.S. Perkin 1*, 1973, 2289 (*synth*)
Snyder, C.D. *et al., J.A.C.S.*, 1974, **96**, 8046 (*synth*)
Yamada, Y. *et al., Biochim. Biophys. Acta*, 1977, **486**, 195 (*isol, derivs*)
Yamada, Y. *et al., Agric. Biol. Chem.*, 1980, **44**, 1693; 1982, **46**, 1105 (*isol, derivs*)
Haroon, Y. *et al., J. Chromatogr.*, 1981, **206**, 333-342 (*hplc*)
Kroppenstedt, R.M. *et al., J. Liq. Chromatogr.*, 1982, **5**, 2359-2367 (*hplc*)
Tso, H.-H. *et al., J. Chem. Res., Synop.*, 1995, 104 (*synth*)
Seto, H. *et al., Tet. Lett.*, 1996, **37**, 7979 (*biosynth*)
Duvold, T. *et al., Tet. Lett.*, 1997, **38**, 6181-6184 (*biosynth*)

Vitexin V-46

[3681-93-4]

*8-β-D-Glucopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 8-Glucopyranosyl-4′,5,7-trihydroxyflavone. 8-Glucopyranosylapigenin. 8-Glucosylapigenin. Orientoside*



$C_{21}H_{20}O_{10}$ 432.383

Yellow cryst. Mp 269-270° dec. $[\alpha]_D^{20}$ -14.5 (c, 2.79 in Py). λ_{max} 270 ; 302 (sh) ; 336

(MeOH).

▶ DJ2984000

4′-O-α-L-Rhamnopyranoside: [32426-34-9]
$C_{27}H_{30}O_{14}$ 578.526
Constit. of *Passiflora incarnata* (maypops).

6″-O-(3-Hydroxy-3-methylglutaroyl):
[154639-29-9]
$C_{27}H_{28}O_{14}$ 576.51
Constit. of finger millet *Eleusine coracana*.

2″-O-(4-Hydroxycinnamoyl): [59282-55-2]
2″-O-p-Coumaroylvitexin
$C_{30}H_{26}O_{12}$ 578.528
Isol. from fenugreek seeds *Trigonella foenum-graecum*. Yellow needles. Mp 195-198°.

2″-O-(4-Hydroxycinnamoyl), 7-O-β-D-glucopyranoside: [93446-17-4]
$C_{36}H_{36}O_{17}$ 740.67
Isol. from *Mollugo oppositifolia* (wheat).

7-Me ether, 4′-O-β-D-glucopyranoside:
[35480-14-9]
$C_{28}H_{32}O_{15}$ 608.552
Isol. from wheat (*Triticum aestivum*).

2″-α-L-Rhamnopyranosyl, 4′-Me ether:
[64271-10-9] ***Margaritene***
$C_{28}H_{32}O_{14}$ 592.552
Isol. from *Fortunella margarita* (oval kumquat) and *Fortunella japonica* (round kumquat). Yellow needles. Mp 192-193°.

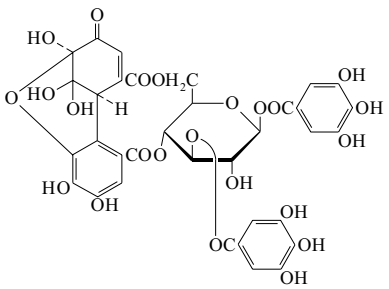
2″-α-L-Rhamnopyranosyl, 7-Me ether:
[64821-00-7] *Isowertin 2″-rhamnoside*
$C_{28}H_{32}O_{14}$ 592.552
Isol. from *Avena sativa* (coats) and *Gnetum africanum*.

[11044-10-3, 58578-65-7, 89613-12-7]

Evans, W.H. *et al., J.C.S.*, 1957, 3510 (*isol*)
Hillis, W.E. *et al., Aust. J. Chem.*, 1965, **18**, 531 (*pmr*)
Chopin, J. *et al., Tet. Lett.*, 1966, 3657 (*synth*)
Gentili, B. *et al., J.O.C.*, 1968, **33**, 1571 (*pmr, derivs*)
Julian, E.A. *et al., Phytochemistry*, 1971, **10**, 3185 (*Isoswertisin 4′-glucoside*)
Wagner, H. *et al., Phytochemistry*, 1972, **11**, 1518 (*isol*)
Soeder, R.W. *et al., Phytochemistry*, 1972, **11**, 3079 (*isol*)
Jurnak, F.A. *et al., Acta Cryst. B*, 1975, **31**, 1304 (*cryst struct*)
Giaminetto, I.B. *et al., J. Nat. Prod.*, 1975, **38**, 265 (*isol*)
Niemann, G.J. *et al., Phytochemistry*, 1975, **14**, 1436 (*isol*)
Sood, A.R. *et al., Phytochemistry*, 1976, **15**, 351 (*2″-4-hydroxycinnamoyl*)
Chopin, J. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 1007 (*Margaritene*)
Davoust, D. *et al., Org. Magn. Reson.*, 1980, **13**, 218 (*cmr*)
Chopin, J. *et al., Phytochemistry*, 1984, **23**, 2106 (*2″-4-hydroxycinnamoyl 7-glucoside*)
Kumamoto, H. *et al., Agric. Biol. Chem.*, 1985, **49**, 2613; 1986, **50**, 781 (*2″-rhamnoside, 2″-xyloside, Margaritene*)
Kim, C.-S. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 380 (*3-hydroxy-3-methylglutarate*)

Vitilagin V-47

[85200-63-1]

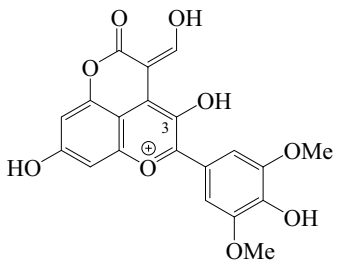


$C_{34}H_{26}O_{23}$ 802.566

Tautomeric with the alternate (dibenzofuranoid) ketal struct.. Constit. of the leaves of *Vitis vinifera* (wine grape). Mp 220-228° dec. $[\alpha]_D^{20}$ +122 (c, 0.33 in MeOH).

Karl, C. *et al., Z. Naturforsch., C*, 1983, **38**, 13 (*isol*)

Vitisidin A V-48



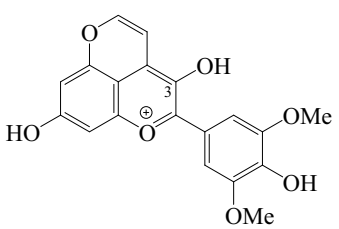
$C_{20}H_{15}O_9^{\oplus}$ 399.333

3-O-β-D-Glucopyranoside: [184362-09-2]
Vitisin A
$C_{26}H_{25}O_{14}^{\oplus}$ 561.475
Constit. of some red wines.

3-O-(O-Acetyl-β-D-glucopyranoside): ***Acetylvitisin A***
$C_{28}H_{27}O_{15}^{\oplus}$ 603.512
Constit. of some red wines. Position of Ac on Glc not determined.

Bakker, J. *et al., J. Agric. Food Chem.*, 1997, **45**, 35-43 (*isol, uv, pmr*)
Bakker, J. *et al., Phytochemistry*, 1997, **44**, 1375-1382 (*isol, uv*)

Vitisidin B V-49



$C_{19}H_{15}O_7^{\oplus}$ 355.323

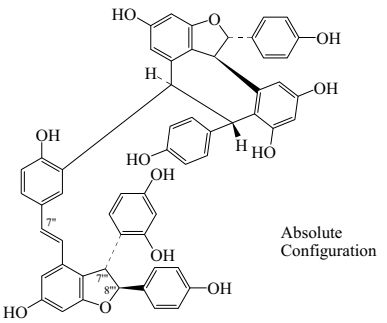
A cyclised pyranoflavonoid. Flavonoid numbering shown.

3-O-β-D-Glucopyranoside: ***Vitisin B***†
$C_{25}H_{25}O_{12}^{\oplus}$ 517.465
Constit. of some red wines.

3-O-(O-Acetyl-β-D-glucopyranoside): ***Acetylvitisin B***
$C_{27}H_{27}O_{13}^{\oplus}$ 559.503
Constit. of some red wines.

Bakker, J. *et al., J. Agric. Food Chem.*, 1997, **45**, 35-43 (*isol, uv, pmr*)

Vitisin A V-50



$C_{56}H_{42}O_{12}$ 906.941

Oligostilbene.Isol. as a mixt. with its (*Z*)-isomer λ_{max} 283 (ϵ 25100); 320 (ϵ 16600) (MeOH) (Derep).

(7″Z)-Isomer: cis-*Vitisin A*
$C_{56}H_{42}O_{12}$ 906.941
λ_{max} 283 (ϵ 25100); 320 (ϵ 16600) (MeOH) (Derep).

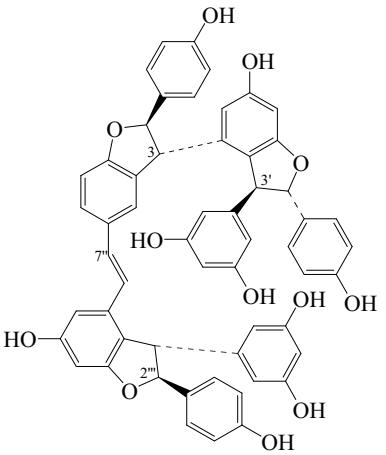
7‴,8‴-Didehydro: ***Vitisifuran A***
$C_{56}H_{40}O_{12}$ 904.925
Constit. of wine grape *Vitis vinifera* 'Kyohou'. Amorph. powder. $[\alpha]_D$ +236.1 (c, 0.44 in MeOH). λ_{max} 208 (log ϵ 5.07); 232 (sh) (log ϵ 4.82); 296 (log ϵ 4.41); 313 (log ϵ 4.39); 322 (log ϵ 4.39); 340 (sh) (log ϵ 4.45); 356 (log ϵ 4.5) (MeOH).

[142449-89-6, 142507-85-5]

Oshima, Y. *et al., J.O.C.*, 1993, **58**, 850
Ito, J. *et al., Tetrahedron*, 1998, **54**, 6651-6660 (*pmr, cmr, abs config*)
Ito, J. *et al., Tetrahedron*, 1999, **55**, 2529-2544 (*Vitisifuran A*)
Takaya, Y. *et al., Tetrahedron*, 2002, **58**, 9265-9271 (*abs config*)

Vitisin B V-51

[142449-90-9]



$C_{56}H_{42}O_{12}$ 906.941
Amorph. powder. $[\alpha]_D$ -90 (c, 2.3 in MeOH). λ_{max} 285 (ϵ 12590); 320 (ϵ 10960) (MeOH).

2‴,3‴-Didehydro: [223558-40-5] ***Vitisifuran B***
$C_{56}H_{40}O_{12}$ 904.925
Constit. of wine grape *Vitis vinifera* 'Kyohou'. Amorph. powder. $[\alpha]_D$ -133.7 (c, 0.12 in MeOH). λ_{max} 204 (log ϵ 4.99); 228 (sh) (log ϵ 4.75); 287 (log ϵ 4.29); 297 (log ϵ 4.28); 324 (log ϵ 4.31); 357 (sh) (log ϵ 4.25) (MeOH).

7″Z-Isomer: [142507-86-6] **cis-*Vitisin B***
$C_{56}H_{42}O_{12}$ 906.941
$[\alpha]_D$ -42 (c, 0.7 in MeOH).

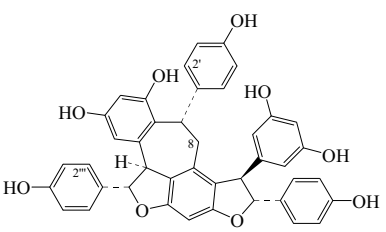
3-Epimer: [180580-73-8] ***Vitisin C***
$C_{56}H_{42}O_{12}$ 906.941
Isol. from the stems of *Vitis vinifera* (wine grape). $[\alpha]_D$ +239.9 (c, 0.5 in MeOH).

2,3-Diepimer: [165883-77-2] **r-*Viniferin***
$C_{56}H_{42}O_{12}$ 906.941
Oligostilbene. Isol. from the roots of *Vitis vinifera* (wine grape).

Korhammer, S. *et al., Phytochemistry*, 1995, **38**, 1501-1504 (*r-Viniferin*)
Oshima, Y. *et al., Tetrahedron*, 1995, **51**, 11979-11986 (*isol, uv, ir, pmr, cmr, ms*)
Ito, J. *et al., Tetrahedron*, 1996, **52**, 9991-9998; 1999, **55**, 2529 (*Vitisin C, Vitisifuran B*)
Takaya, Y. *et al., Tetrahedron*, 2002, **58**, 9265-9271 (*abs config*)

Vitisin E V-52

[206192-30-5]



$C_{42}H_{32}O_9$ 680.709
$[\alpha]_D$ +94.5 (c, 0.2 in MeOH). Incorrect MF given in ref..

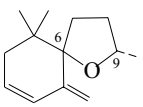
8α-Hydroxy: [290296-37-6] ***Hemsleyanol B***
$C_{42}H_{32}O_{10}$ 696.709
Amorph. yellow solid. $[\alpha]_D^{24}$ -205 (c, 0.1 in MeOH). Relative config. only known λ_{max} 230 ; 284 ; 301 (MeOH).

Stereoisomer, 2′-hydroxy: ***Gnemonol A***
$C_{42}H_{32}O_{10}$ 696.709
Constit. of the roots of *Gnetum gnemon* (bago). Amorph. powder. $[\alpha]_D$ -205 (c, 0.1 in MeOH). λ_{max} 218 ; 284 ; 323 (MeOH).

Shinoda, K. *et al., Heterocycles*, 1997, **46**, 169-172 (*isol, pmr, cmr*)
Ito, T. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1001-1005 (*Hemsleyanol B*)
Iliya, I. *et al., Chem. Pharm. Bull.*, 2002, **50**, 796-801 (*Gnemonol A*)

Vitispirane V-53

[65416-59-3]
6,9-Epoxy-3,5(13)-megastigmadiene

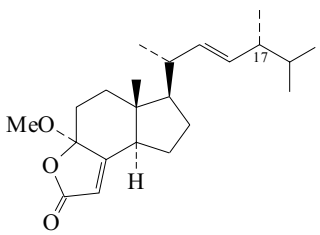


$C_{13}H_{20}O$ 192.3
Natural vitispirane is a mixture of the (6*R*) and (6*S*) epimers. Constit. of the juice of wine grape (*Vitis vinifera*). Oil. $Bp_{0.2}$ 57-59°.

Simpson, R.F. *et al., Chem. Ind. (London)*, 1977, 663 (*isol*)
Schulte-Elte, K.H. *et al., Helv. Chim. Acta*, 1978, **61**, 1125 (*synth, struct*)
Marschall, H. *et al., Annalen*, 1982, 68 (*synth*)
Nilsson, Y.I.M. *et al., J.O.C.*, 1996, **61**, 1825 (*synth*)

Volemolide V-54

[125974-96-1]
17*R-*Methylincisterol



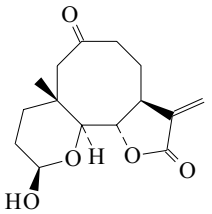
$C_{22}H_{34}O_3$ 346.509
Constit. of the edible chichitake mushroom (*Lactarius volemus*). Needles. Mp 61-62°. $[\alpha]_D^{23}$ +215 (c, 0.1 in $CHCl_3$).

17-Epimer: [126060-08-0] ***17*S-*Methylincisterol***
$C_{22}H_{34}O_3$ 346.509

Ciminiello, P. *et al., J.A.C.S.*, 1990, **112**, 3505-3509 (*isol, uv, ir, pmr, cmr, ms, 17epimer*)
Kobata, K. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1542-1544 (*isol, pmr, cmr*)

Vulgarolide V-55

[120674-40-0]

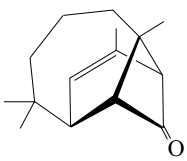


$C_{15}H_{20}O_5$ 280.32
Constit. of *Tanacetum vulgare* (tansy). Oil. $[\alpha]_D^{25}$ -45 (c, 1 in $CHCl_3$).

Appendino, G. *et al., Gazz. Chim. Ital.*, 1988, **118**, 55 (*isol, pmr, cmr*)
Paquette, L.A. *et al., Tet. Lett.*, 1995, **36**, 673 (*synth*)

Vulgarone A V-56

[62065-10-5]

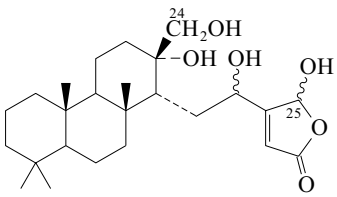


$C_{15}H_{22}O$ 218.338
Constit. of *Chrysanthemum vulgare* (tansy). Oil. $[\alpha]_D^{25}$ +113.7 (c, 0.95 in $CHCl_3$).

Uchio, Y. *et al., Tetrahedron*, 1978, **34**, 2893

Vulgaroside V-57

[172705-29-2]



$C_{25}H_{40}O_6$ 436.587

25-Ac: [172616-88-5] ***25-Acetylvulgaroside***
$C_{27}H_{42}O_7$ 478.625
Constit. of *Cydonia vulgaris* (quince). $[\alpha]_D^{25}$ +63 (c, 1 in $CHCl_3$).

24,25-Di-Ac: [172616-87-4] ***24,25-Diacetylvulgaroside***
$C_{29}H_{44}O_8$ 520.662
Constit. of *Cydonia vulgaris* (quince). $[\alpha]_D^{25}$ +30 (c, 1 in $CHCl_3$).

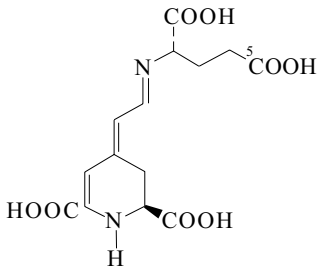
25-Cinnamoyl: [172616-90-9]
$C_{34}H_{46}O_7$ 566.733
Constit. of *Cydonia vulgaris* (quince). $[\alpha]_D^{25}$ +17 (c, 1 in $CHCl_3$).

25-Cinnamoyl, 24-Ac: [172616-89-6]
$C_{36}H_{48}O_8$ 608.77
Constit. of *Cydonia vulgaris* (quince). $[\alpha]_D^{25}$ +17 (c, 1 in $CHCl_3$).

De Tommasi, N. *et al., J. Nat. Prod.*, 1996, **59**, 267 (*isol, pmr, cmr*)

Vulgaxanthin II V-58

[1047-87-6]
4-[[(1,3-Dicarboxypropyl)imino]ethylidene]-1,2,3,4-tetrahydro-2,6-pyridinedicarboxylic acid, 9CI



$C_{14}H_{16}N_2O_8$ 340.289
Yellow pigment from beetroot (*Beta vulgaris*).

5-Amide: [904-62-1] ***Vulgaxanthin I***
$C_{14}H_{17}N_3O_7$ 339.304
Yellow pigment from *Beta* spp. Food colourant.

5-Alcohol: [111534-70-4] ***Humilixanthin***
$C_{14}H_{18}N_2O_7$ 326.305
Iso. from the yellow-coloured root of beetroot *Beta vulgaris*.

Piattelli, M. *et al., Phytochemistry*, 1965, **4**, 121 (*isol, ir, uv, struct*)
Singer, J.W. *et al., J. Food Sci.*, 1980, **45**, 489 (*isol, use*)
Strack, D. *et al., Phytochemistry*, 1987, **26**, 2285 (*isol, uv, pmr, ms, struct, Humilixanthin*)

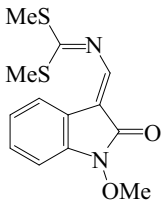
Vulracine V-59

$C_{18}H_{19}NO_3$ 297.353

Struct. unknown. Alkaloid from *Berberis vulgaris* (barberry). Fine needles (Me_2CO). Mp 164°. $[\alpha]_D^{24}$ -114 (c, 0.2 in $CHCl_3$).

Döpke, W. *et al., Naturwissenschaften*, 1963, **50**, 595

Wasalexin A W-1



$C_{13}H_{14}N_2O_2S_2$ 294.398
Constit. of *Wasabia japonica* (Japanese horseradish). Yellow solid.

(Z)-Isomer: ***Wasalexin B***
$C_{13}H_{14}N_2O_2S_2$ 294.398
Constit. of *Wasabia japonica* (Japanese horseradish). Yellow solid.

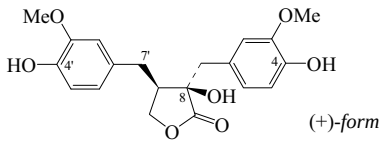
Pedras, M.S.C. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3015-3020 (*isol, synth, pmr, cmr, ms*)

Water, 11CI W-2

[7732-18-5]
Oxidane. Aqua. Hydrogen oxide (H_2O)
H_2O (C_{2v})
H_2O 18.015
Essential component of all forms of life. 76% of earth's water occurs as oceanic and fresh water;1% as ice, 21% in sedimentary rocks and sediments. Bond length: H–O 96 pm; angle: HOH 104.5°. Solvent, vehicle. Colourless, odourless, tasteless liq. Misc. with many polar org. liqs. $d^{3.98}$ 1. Mp 0°. Bp 100°. pK_a 14 (25°). ΔH_f° -285.89 kJ mol^{-1}; ΔH_{fus}° 6.01 kJmol^{-1}; ΔH_{vap}° 40.66 kJ mol^{-1}; ΔH_{sub}° 51.06 kJ mol^{-1}.
▶ ZC0110000
[13670-17-2, 13768-40-6, 14314-42-2]
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 109A (*ir*)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 620B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 155A; 1604B (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1922, **1**, 122; 405 (*rev*)
Eisenberg, D. *et al., The Structure and Properties of Water*, OUP, 1969,
Gmelin Handbook Inorg. Chem., Syst. No. 3, *Appended Vol.*, 1974, ; *Supplement Vol.*, 1979, 119 (*water desalting*)
Cook, R.L. *et al., J. Mol. Spectrosc.*, 1974, **53**, 62
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 133
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, 257
Franks, F. *et al., Water*, RSC Monograph, 1983, (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 546-549
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1767
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HAK000; WAT259

Wikstromol W-3

4,4′,8-Trihydroxy-3,3′-dimethoxylignan-9,9′-olide. Pinopalustrin. Nortrachelogenin



(+)-form

$C_{20}H_{22}O_7$ 374.39
Lignan numbering shown.
(+)-*form* [61521-74-2]
Yellow powder. $[\alpha]_D$ +15.4 ($CHCl_3$). Inactive as antileukaemic agent λ_{max} 230 ; 282 (no solvent reported).

8′-Epimer: [125072-69-7] ***Epinortrachelogenin***
$C_{20}H_{22}O_7$ 374.39
Powder. Mp 171-172° (166-168°). $[\alpha]_D^{25}$ -21.1 (c, 0.4 in MeOH). $[\alpha]_D^{20}$ -5 (c, 0.5 in $CHCl_3$).

(-)-*form* [34444-37-6]
Obt. from *Pinus palustris* (pitch pine) and *Carissa edulis* (agam). Amorph. $[\alpha]_D^{17}$ -16.8 (c, 0.178 in EtOH).
▶ LU3560500

4-O-β-D-Glucopyranoside: [33464-78-7] ***Nortracheloside***
$C_{26}H_{32}O_{12}$ 536.532
Cryst. + H_2O. $[\alpha]_D^{19}$ -47.9 (c, 1.02 in EtOH).

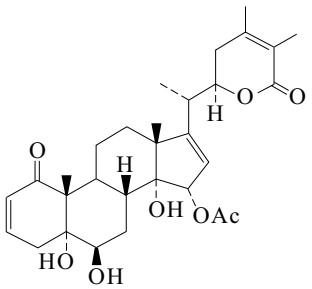
4,4′-Di-O-β-D-glucopyranoside: [38976-09-9]
$C_{32}H_{42}O_{17}$ 698.674
Powder. Mp 137-140°. $[\alpha]_D^{14}$ -15.9 (c, 0.8 in EtOH).

7′-Oxo: ***8-Hydroxyoxomatairesinol***
$C_{20}H_{20}O_8$ 388.373
Pale yellow powder. $[\alpha]_D^{25}$ +97.3 (c, 0.38 in MeOH). λ_{max} 201 (log ε 4.62); 232 (log ε 4.29); 281 (log ε 4.08); 309 (log ε 3.94) (MeOH).

[63902-22-7, 116261-31-5, 116261-33-7, 124988-62-1]
Vanhaelen, M. *et al., Phytochemistry*, 1925, **14**, 2709 (*isol*)
Nishibe, S. *et al., Phytochemistry*, 1971, **10**, 2231 (*isol*)
Nishibe, S. *et al., Chem. Pharm. Bull.*, 1973, **21**, 1108; 1114 (*isol, 4,4′-diglucoside*)
Tandon, S. *et al., Phytochemistry*, 1976, **15**, 1789 (*isol, synth*)
Carnmalm, B. *et al., Acta Chem. Scand., Ser. B*, 1977, **31**, 433 (*struct*)
Kato, A. *et al., J. Nat. Prod.*, 1979, **42**, 159 (*isol, cmr, cd*)
Torrance, S.J. *et al., J. Pharm. Sci.*, 1979, **68**, 664 (*isol*)
Achenbach, H. *et al., Phytochemistry*, 1983, **22**, 749 (*isol, nmr*)
Belletire, J.L. *et al., J.O.C.*, 1988, **53**, 4724 (*synth*)
Belletire, J.L. *et al., J. Nat. Prod.*, 1990, **53**, 1587 (*synth, cryst struct, bibl*)
Khamlach, K. *et al., Tetrahedron*, 1992, **48**, 10115 (*synth*)
Appendino, G. *et al., J. Nat. Prod.*, 1994, **57**, 607 (*Epinortrachelogenin*)
Esterez-Braun, A. *et al., Tetrahedron*, 1994, **50**, 5203 (*Epinortrachelogenin*)
Kawamura, F. *et al., Phytochemistry*, 2000, **54**, 439-444 (*8-Hydroxyoxomatairesinol*)
Hu, K. *et al., Planta Med.*, 2000, **66**, 564-567 (*isol, pmr, cmr, activity*)
Sefkow, M. *et al., J.O.C.*, 2001, **66**, 2343-2349 (*synth*)

Withaminimin W-4

*15α-Acetoxy-5,6β,14-trihydroxy-1-oxo-5α,20*S*,22*R*-witha-2,16,24-trienolide*



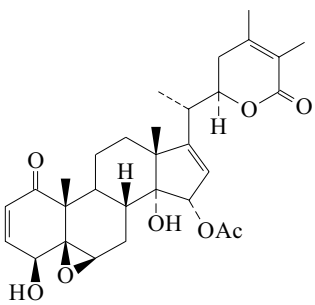
$C_{30}H_{40}O_8$ 528.641
Amorph. powder. Mp 208°.

16β,17β-Epoxide: ***Physagulin F***
$C_{30}H_{40}O_9$ 544.641
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Powder. $[\alpha]_D$ +70.7 (c, 1.1 in MeOH).

Gottlieb, H.E. *et al., Phytochemistry*, 1987, **26**, 1801
Shingu, K. *et al., Chem. Pharm. Bull.*, 1992, **40**, 2448

Withangulatin A W-5

[120824-03-5]

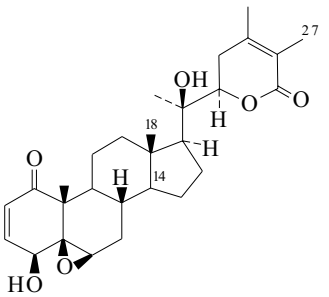


$C_{30}H_{38}O_8$ 526.625
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Amorph. powder. Mp 152-153°. $[\alpha]_D^{20}$ +23.9 (c, 0.018 in $CHCl_3$). λ_{max} 215 (ε 16500) (MeOH) (Berdy).

Chen, C.-M. *et al., Heterocycles*, 1990, **31**, 1371 (*isol, pmr, cmr*)

Withanolide D W-6

[30655-48-2]
*5β,6β-Epoxy-4β,20*R*-dihydroxy-1-oxo-22*R*-witha-2,24-dienolide*



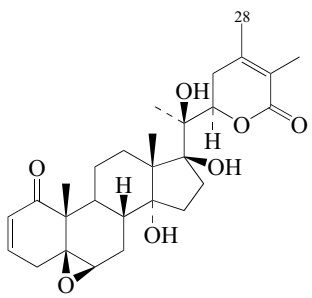
$C_{28}H_{38}O_6$ 470.605
Cryst. ($CHCl_3$/EtOAc). Mp 253-255°. $[\alpha]_D$ +80 ($CHCl_3$).

24S,25S-Epoxide:24,25-Epoxywithanolide D
$C_{28}H_{38}O_7$ 486.604
Constit. of the famine food *Physalis angulata* (cutleaf ground cherry). Cryst. (MeOH). Mp 257-261°. $[\alpha]_D^{20}$ +23 (c, 1.18 in $CHCl_3$).

Lavie, D. *et al., Isr. J. Chem.*, 1968, **6**, 671 (*isol*)
Kirson, I. *et al., Tetrahedron*, 1970, **26**, 2209 (*struct*)
Abraham, A. *et al., Phytochemistry*, 1975, **14**, 189
Lockley, W.J.S. *et al., Phytochemistry*, 1976, **15**, 937 (*biosynth*)
Gamoh, K. *et al., J.C.S. Perkin 1*, 1984, 449 (*synth*)
Vasina, O.E. *et al., Khim. Prir. Soedin.*, 1986, **22**, 596; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 560 (*deriv*)
Raffauf, R.F. *et al., J. Nat. Prod.*, 1991, **54**, 1601 (*derivs*)

Withanolide E W-7

[38254-15-8]
5,6β-Epoxy-14α,17β,20S-trihydroxy-1-oxo-5β,22R-witha-2,24-dienolide



$C_{28}H_{38}O_7$ 486.604
Cryst. + $2H_2O$ (Me_2CO). Mp 167-168°. $[\alpha]_D$ +103.5 (c, 0.7 in $CHCl_3$). Log P -0.03 (uncertain value) (calc).

17-Epimer: [76109-42-7] ***17-Isowithanolide E****. 5,6β-Epoxy-14α,17α,20S-trihydroxy-1-oxo-5β,22R-witha-2,24-dienolide*
$C_{28}H_{38}O_7$ 486.604
Cryst. (EtOAc). Mp 262°. $[\alpha]_D$ +21.3 (c, 0.2 in MeCN).

4β-Hydroxy: [54334-04-2] *5,6β-Epoxy-4β,14α,17β,20S-tetrahydroxy-1-oxo-5β,22R-witha-2,24-dienolide.* ***4β-Hydroxywithanolide E***
$C_{28}H_{38}O_8$ 502.603
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. (EtOAc). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 205-214° (197-198°). $[\alpha]_D$ +95.8 (c, 0.5 in $CHCl_3$). λ_{max} 219 (ε 14700) (EtOH) (Berdy).

▶ KE7283000

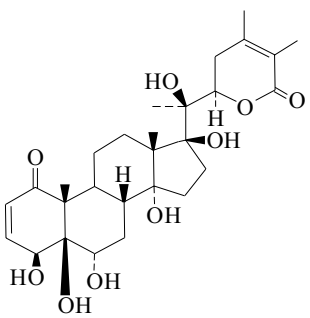
2,3-Dihydro: [38253-76-8] ***2,3-Dihydrowithanolide E****. 5β,6β-Epoxy-14α,17β,20S-trihydroxy-1-oxo-22R-with-24-enolide*
$C_{28}H_{40}O_7$ 488.62
Isol. from *Physalis peruviana* (Cape gooseberry). Cryst. Mp 273-275°.

28-Hydroxy: [188346-67-0] ***28-Hydroxywithanolide E***
$C_{28}H_{38}O_8$ 502.603
Constit. of *Physalis peruviana* (Cape gooseberry). Amorph. λ_{max} 222 (log ε 4.2) (no solvent reported).

Sakurai, K. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1403 (*deriv*)
Kirson, I. *et al., Phytochemistry*, 1976, **15**, 340 (*isol*)
Glotter, E. *et al., J.C.S. Perkin 1*, 1977, 341 (*isol, struct*)
Hunter, I.R. *et al., J. Chromatogr.*, 1979, **170**, 437 (*hplc*)
Kirson, I. *et al., J. Chem. Res., Synop.*, 1980, 338; *J. Chem. Res., Miniprint*, 1980, 4275 (*isol*)
Gottlieb, H.E. *et al., Org. Magn. Reson.*, 1981, **16**, 20 (*cmr*)
Dinan, L.N. *et al., Phytochemistry*, 1997, **44**, 509 (*28-Hydroxywithanolide E, activity*)

Withaperuvin W-8

[78285-97-9]
4β,5β,6α,14α,17β,20R-Hexahydroxy-1-oxowitha-2,24-dienolide



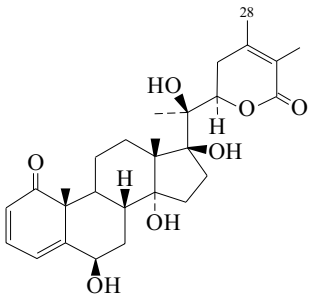
$C_{28}H_{40}O_9$ 520.619
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. + $1H_2O$ (MeOH). Mp 225-227°. $[\alpha]_D$ +156.8 (c, 0.15 in $CHCl_3$).

20-Epimer: [81644-35-1] ***Withaperuvin B***
From *Physalis peruviana* (Cape gooseberry). Cryst. Mp 269-270°. $[\alpha]_D$ +215 (Py).

Frolow, F. *et al., J.C.S. Perkin 1*, 1981, 1029
Sahai, M. *et al., Heterocycles*, 1982, **19**, 37

Withaperuvin C W-9

[81644-34-0]
(20S,22R)-6β,14,17β,20-Tetrahydroxy-1-oxowitha-2,4,24-trienolide



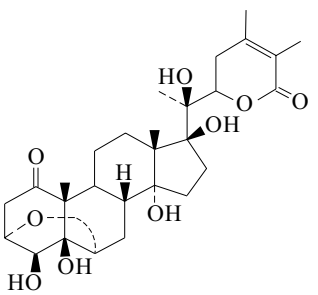
$C_{28}H_{38}O_7$ 486.604
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. Mp 190°. $[\alpha]_D$ -4.5 (Py).

28-Hydroxy: [100668-02-8] *(20S,22R)-6β,14α,17β,20,28-Pentahydroxy-1-oxo-2,4,24-withatrienolide. 28-Hydroxywithaperuvin C*
$C_{28}H_{38}O_8$ 502.603
Cryst. (MeOH). Mp 185-186°. $[\alpha]_D^{20}$ +152 (MeOH).

Sahai, M. *et al., Heterocycles*, 1982, **19**, 37 (*isol, struct*)
Abdullaev, N.D. *et al., Khim. Prir. Soedin.*, 1985, **21**, 657; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 616 (*deriv*)

Withaperuvin D W-10

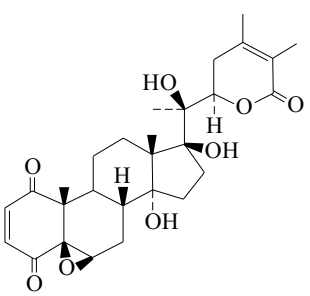
[87749-17-5]
4β,5α,14α,17β,20S-Pentahydroxy-3α,6α-oxido-1-oxo-24-ergosten-26,22R-olide



$C_{28}H_{40}O_9$ 520.619
Constit. of leaves of *Physalis peruviana* (Cape gooseberry). Cryst. (Me_2CO). Mp 209-211°. $[\alpha]_D$ +12 (c, 0.51 in Me_2CO).

Sahai, M. *et al., J. Chem. Res., Synop.*, 1983, 152

Withaperuvin E W-11



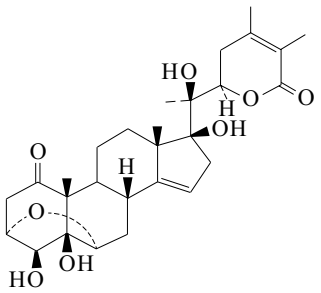
$C_{28}H_{36}O_8$ 500.588
Constit. of *Physalis peruviana* (Cape

gooseberry). Pale yellow cryst. (Me_2CO). Mp 248-250°. $[\alpha]_D$ -72.7 (c, 0.715 in MeCN). λ_{max} 226 (ϵ 10700) (MeOH) (Derep).

Bagchi, A. *et al., Phytochemistry*, 1984, **23**, 853

Withaperuvin F W-12

*3α,6α-Epoxy-4β,5,17β,20*R-*tetrahydroxy-1-oxo-5β,22*R-*witha-14,24-dienolide*

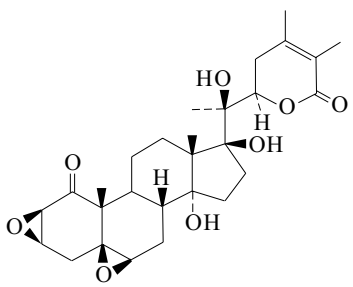


$C_{28}H_{38}O_8$ 502.603
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. ($CHCl_3$). Mp 174-175°. $[\alpha]_D$ +39.7 (c, 0.26 in $CHCl_3$).

Neogi, P. *et al., Phytochemistry*, 1987, **26**, 243

Withaperuvin G W-13

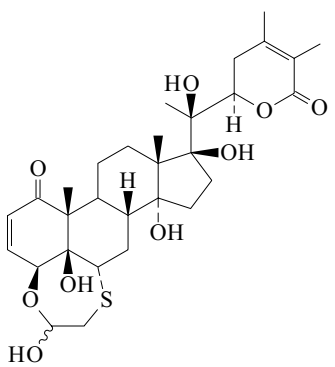
*2β,3β;5,6β-Diepoxy-14,17β,20*R-*trihydroxy-1-oxo-5β,22*R-*with-24-enolide*



$C_{28}H_{38}O_8$ 502.603
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. ($CHCl_3$). Mp 163°.

Neogi, P. *et al., Phytochemistry*, 1987, **26**, 243

Withaperuvin H W-14

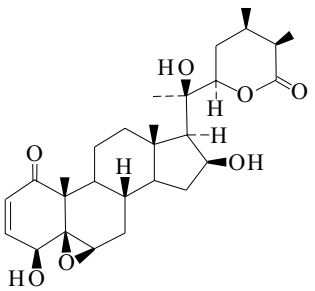


$C_{30}H_{42}O_9S$ 578.722
Constit. of *Physalis peruviana* (Cape gooseberry). Cryst. Mp 213-214°. $[\alpha]_D$ +84.3 (c, 0.51 in Py). λ_{max} 222 (ϵ 12100) (MeOH) (Derep).

Oshima, Y. *et al., Chem. Comm.*, 1989, 628 (*isol, pmr, cmr*)

Withaphysacarpin W-15

[41929-21-9]
*5,6β-Epoxy-4β,16β,20*R-*trihydroxy-1-oxo-5β,22*R,*24*R,*25*R-*with-2-enolide*

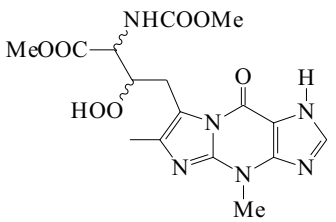


$C_{28}H_{40}O_7$ 488.62
Constit. of *Physalis ixocarpa* (tomatillo). Cryst. Mp 275-278°. $[\alpha]_D$ +20 ($CHCl_3$).

Subramanian, S.S. *et al., Indian J. Pharm.*, 1973, **35**, 36

Wybutoxine W-16

[36238-44-5]
*Methyl 4,9-dihydro-β-hydroperoxy-α-[(methoxycarbonyl)amino]-4,6-dimethyl-9-oxo-1*H-*imidazo[1,2-*a*]purine-7-butanoate, 9CI. Peroxywybutine*

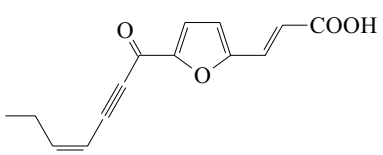


$C_{16}H_{20}N_6O_7$ 408.37
Constit. of phenylalanine tRNA of beef, chicken, calf and rat livers. Fluorescent.

Feinberg, A.M. *et al., J.A.C.S.*, 1974, **96**, 7797 (*isol, struct*)
Mochizaki, A. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 813 (*isol, pmr*)

Wyerone acid W-17

[54954-14-2]
3-[5-(1-Oxo-4-hepten-2-ynyl)-2-furanyl]-2-propenoic acid, 9CI. 4,7-Epoxy-8-oxo-2,4,6,11-tetradecatetraen-9-ynoic acid



$C_{14}H_{12}O_4$ 244.246
(2E,11Z)-form
Isol. from broad bean leaves (*Vicia faba*) infected with *Botrytis* spp..

Me ester: [20079-30-5] ***Wyerone***
$C_{15}H_{14}O_4$ 258.273
Constit. of broad bean seedlings (*Vicia faba*) infected with *Botrytis* spp.. Cryst. (hexane or cyclohexane). Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 63.5-64°. λ_{max} 226 (ϵ 13300); 291 (ϵ 9100); 351 (ϵ 27000) (EtOH) (Derep). λ_{max} 224 ; 292 ; 351 (EtOH) (Berdy).

11,12-Epoxide, Me ester: [60375-16-8] ***Wyerone epoxide***
$C_{15}H_{14}O_5$ 274.273
Constit. of broad bean *Vicia faba* seedlings infected with *Botrytis* spp.. Cryst. (Et_2O/hexane). Mp 74-76°.

8-Alcohol, Me ester: [20450-52-6] *Methyl 3-[5-(1-hydroxy-4-hepten-2-ynyl)-2-furanyl]-2-propenoate.* ***Wyerol***
$C_{15}H_{16}O_4$ 260.289
Isol. from seedlings of broad bean *Vicia faba* infected with *Botrytis* spp.. Needles (hexane). Mp 55-56°. λ_{max} 312 (EtOH) (Berdy).

11,12-Dihydro: [70711-57-8] ***Dihydrowyerone acid***
$C_{14}H_{14}O_4$ 246.262
Constit. of broad bean *Vicia faba* infected with *Botrytis* spp..

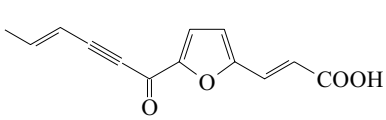
11,12-Dihydro, Me ester: ***Dihydrowyerone***
$C_{15}H_{16}O_4$ 260.289
Minor constit. of broad bean *Vicia faba* infected with *Botrytis* spp.. Small prisms. Mp 79-80°.

11,12-Dihydro, 8-alcohol, Me ester: [70711-58-9] ***Dihydrowyerol***
$C_{15}H_{18}O_4$ 262.305
Constit. of broad bean *Vicia faba* infected with *Botrytis* spp..

Fawcett, C.H. *et al., J.C.S.(C)*, 1968, 2455-2462 (*isol, struct, alcohol*)
Letcher, R.M. *et al., Phytochemistry*, 1970, **9**, 249-252 (*isol*)
Mansfield, J.W. *et al., Nature (London)*, 1974, **252**, 316 (*isol*)
Hargreaves, J.A. *et al., Ann. Appl. Biol.*, 1975, **81**, 271 (*isol, epoxide*)
Hearn, M.T.W. *et al., Aust. J. Chem.*, 1976, **29**, 107-113 (*cmr*)
Hargreaves, J.A. *et al., Phytochemistry*, 1976, **15**, 651-653; 1119 (*isol, epoxide*)
Knight, D.W. *et al., J.C.S. Perkin 1*, 1982, 623-626 (*synth, alcohol, bibl*)

Wyeronic acid W-18

[117783-52-5]
3-[5-(1-Oxo-4-hexen-2-ynyl)-2-furanyl]-2-propenoic acid, 9CI

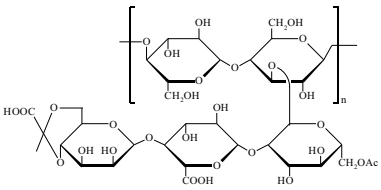


$C_{13}H_{10}O_4$ 230.22
Isol. from *Vicia faba*.

Thynn, M. *et al., Z. Naturforsch., C*, 1988, **43**, 636; 1989, **44**, 237 (*isol*)

Xanthan X-1

[11138-66-2]
Xanthan gum. Biozan R. E415

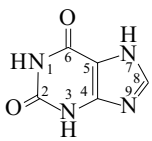


High molecular weight in range 10^6-10^7 with rodlike ordered struct.. An emulsion stabilizing and gelling agent.

Dea, I.C.M. *et al., Carbohydr. Res.*, 1977, **57**, 249
Southwick, J.G. *et al., Carbohydr. Res.*, 1980, **84**, 287
Norton, I.T. *et al., Coll. Czech. Chem. Comm.*, 1980, 545
Horton, D. *et al., Carbohydr. Res.*, 1985, **141**, 340 (*cmr*)
Gravanis, G. *et al., Carbohydr. Res.*, 1987, **160**, 259 (*props*)
Gamini, A. *et al., Carbohydr. Res.*, 1991, **220**, 33 (*cmr, O-17 nmr, struct*)
Bezemer, L. *et al., Carbohydr. Res.*, 1994, **263**, 197 (*conformn*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2961-2965 (*props, use*)

Xanthine, 8CI X-2

[69-89-6]
*3,7-Dihydro-1*H*-purine-2,6-dione, 9CI. 2,6-Dihydroxypurine. 2,6-Purinediol*



7H-form

$C_5H_4N_4O_2$ 152.112
Found in potatoes, coffee beans, etc.. Cryst. Mp 350°. pK_{a1} 7.7; pK_{a2} 11.94 (20°). pK_{a1} 0.8; pK_{a2} 7.45; pK_{a3} 11.13 (20°).

▶ LD_{50} (mus, ipr) 500 mg/kg. ZD7700000

7H-form

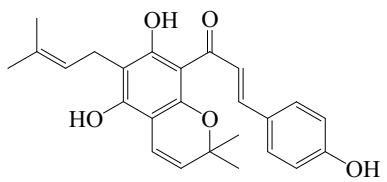
7-Me: [552-62-5]

[28109-92-4] *3,7-Dihydro-7-methyl-1*H*-purine-2,6-dione, 9CI. Heteroxanthine. 7-Methylxanthine*
$C_6H_6N_4O_2$ 166.139
Found in sugar cane and other biol. sources, a urinary metab. of caffeine in man. Needles (H_2O). Mp 380° dec.

▶ ZD8925000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 709C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 213C; 214A (*nmr*)
Sarasin, E. *et al., Helv. Chim. Acta*, 1924, **7**, 713 (*7-Me*)
Birkofer, L. *et al., Chem. Ber.*, 1964, **97**, 934 (*7-Me*)
Mizuno, H. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 3099 (*cryst struct*)
Kwiatkowski, J.S. *et al., Theor. Chim. Acta*, 1969, **13**, 149 (*uv*)
Lister, J.H. *et al., Chem. Heterocycl. Compd.*, (Weissberger, A. *et al*, Ed.), 1971, (*rev*)
Twanmoh, L.-M. *et al., J. Het. Chem.*, 1973, **10**, 187 (*pmr*)
Takayama, S. *et al., Chem. Pharm. Bull.*, 1974, **22**, 1200 (*synth*)
Kistenmacher, T.J. *et al., Acta Cryst. B*, 1975, **31**, 489 (*7-Me*)
Marzilli, L.G. *et al., J.A.C.S.*, 1975, **97**, 3351 (*7-Me*)
Sekiya, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1331 (*synth*)
Coxon, B. *et al., J.O.C.*, 1977, **42**, 3132 (*cmr*)
Saha, S.K. *et al., Indian J. Chem.*, 1980, **19**, 325 (*ms*)
Sponer, J. *et al., Struct. Chem.*, 1995, **6**, 281 (*tautom*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PAK300; XCA000

Xanthohumol E X-3

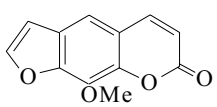


$C_{25}H_{26}O_5$ 406.477
Constit. of *Humulus lupulus* (hops). λ_{max} 369 (MeOH).

Stevens, J.F. *et al., Phytochemistry*, 2000, **53**, 759-775

Xanthotoxin X-4

[298-81-7]
*9-Methoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI, 8CI. 9-Methoxyfuro[3,2-*g*]chromen-7-one. 8-Methoxy-4′,5′:6,7-furocoumarin. 9-Methoxypsoralen. 8-Methoxypsoralen. **Methoxsalen, BAN**. Zanthotoxin. Ammoidin. Meloxine. Methoxa-Dome. Geroxalen. Oxsoralen*



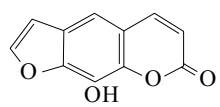
$C_{12}H_8O_4$ 216.193
Present in celery, esp. the outer leaves, and other common grocery vegetables. Implicated in photodermatitis among grocery workers. Isol. from *Aegle marmelos* (bael). Cryst. (EtOH aq.). Sol. EtOH. Mp 148°. Log P 2.3 (calc). Bitter tasting with tingling sensation λ_{max} 218 (ϵ 25300); 248 (ϵ 24600); 299 (ϵ 12400) (MeOH). λ_{max} 219 (ϵ 30000); 249 (ϵ 28800); 301 (ϵ 14400) (EtOH) (Berdy).

▶ Human carcinogen (IARC) in combination with UV light. LD_{50} (rat, orl) 791 mg/kg. LV1400000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 684D (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **3**, 173B (*nmr*)
Späth, E. *et al., Ber.*, 1936, **69**, 769 (*isol*)
Schonberg, J.R. *et al., Nature (London)*, 1947, **168**, 468 (*isol*)
Sommers, A.H. *et al., J.A.C.S.*, 1957, **79**, 3491 (*synth*)
Scheel, W. *et al., Biochemistry*, 1963, **12**, 1127 (*isol*)
Barnes, C.S. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
Sheinker, Yu.N. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 1382 (*pmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1375 (*occur*)
Chatterjee, A. *et al., Tetrahedron*, 1972, **28**, 5175 (*synth*)
Austin, D.J. *et al., Phytochemistry*, 1973, **12**, 1657 (*biosynth*)
Miyakado, M. *et al., Phytochemistry*, 1978, **17**, 143 (*synth*)
Lin, Y.-Y. *et al., J. Het. Chem.*, 1979, **16**, 799 (*synth*)
Loutfy, M.A. *et al., Anal. Profiles Drug Subst.*, 1980, **9**, 427 (*rev*)
Anderson, T.F. *et al., Annu. Rev. Pharmacol. Toxicol.*, 1980, **20**, 235 (*rev, pharmacol*)
Nore, P. *et al., J. Het. Chem.*, 1980, **17**, 985 (*synth, bibl*)
Dall'Acqua, F. *et al., Cryst. Struct. Commun.*, 1981, **10**, 505 (*cryst struct*)
IARC Monog., 1981, **24**, 101; *Suppl.* 7, 243; *Suppl*. 6, 380 (*rev, tox*)
Mays, D.C. *et al., J. Pharmacol. Exp. Ther.*, 1986, **236**, 364 (*metab*)
Stolk, L.M.L. *et al., Pharm. Int.*, 1986, **7**, 259 (*rev, pharmacol*)
Duddeck, H. *et al., Magn. Reson. Chem.*, 1987, **25**, 489 (*O-17 nmr*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2202
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 763
Diawara, M.M. *et al., J. Agric. Food Chem.*, 1995, **43**, 723-727 (*occur*)
Masuda, T. *et al., Phytochemistry*, 1998, **47**, 13-16 (*isol, uv, pmr, cmr*)
Fujioka, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 96-100 (*isol, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, XDJ000

Xanthotoxol X-5

[2009-24-7]
*9-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI*



$C_{11}H_6O_4$ 202.166
Isol. from *Aegle marmelos* (bael fruit), *Angelica archangelica* (angelica) and the seeds of *Pastinaca sativa* (parsnip). Cryst. (EtOH aq.). Mp 251-252°.

▶ LD_{50} (rat, orl) 480 mg/kg. LV1069000

O-*β-L-Arabinopyranoside:* [160845-06-7] *Xanthotoxol arabinoside*
$C_{16}H_{14}O_8$ 334.282
Constit. of *Ruta graveolens* (rue). Needles. Mp 180-182°. $[\alpha]_D^{25}$ +12 (MeOH). λ_{max} 220 ; 250 ; 260 ; 300 (no solvent reported).

O-*β-D-Glucopyranoside:*
$C_{17}H_{16}O_9$ 364.308
Constit. of *Aegle marmelos* (bael fruit). Cryst. Mp 219-220°.

Me ether: Xanthotoxin, X-4

O-*(3-Methyl-2-butenyl):* Imperatorin, I-14

O-*(3-Methyl-3-butenyl):* [55747-78-9] ***Ferulidene***
$C_{16}H_{14}O_4$ 270.284
Cryst. Mp 119-120°.

O-*(2,3-Epoxy-3-methylbutyl):* See Heraclenin in *The Combined Chemical Dictionary.*

O-*(3-Methyl-2-oxobutyl):* See Pabularinone in *The Combined Chemical Dictionary.*

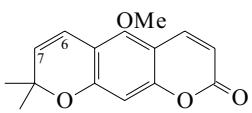
O-*(2,3-Dihydroxy-3-methylbutyl):* Heraclenol, H-125

O-*(3,7-Dimethyl-2,6-octadienyl):* 9-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, D-837

Späth, E. *et al., Ber.*, 1937, **70**, 248
Späth, E. *et al., Monatsh. Chem.*, 1938, **72**, 179 (*isol, synth*)
Kommissarenko, N.F. *et al., Khim. Prir. Soedin.*, 1966, **2**, 375; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 307
Nikonov, G.K. *et al., Khim. Prir. Soedin.*, 1971, **7**, 115; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 103
Perel'son, M.E. *et al., Khim. Prir. Soedin.*, 1971, **7**, 576; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 557 (*pmr*)
Stemple, N.R. *et al., Acta Cryst. B*, 1972, **28**, 2485 (*cryst struct*)
Gellert, M. *et al., Phytochemistry*, 1972, **11**, 2894 (*isol*)
Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1974, **10**, 83; 568; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 79; 581 (*Isogosferol, Ferulidene*)
Sharma, B.R. *et al., Indian J. Chem., Sect. B*, 1980, **19**, 162 (*isol*)
Murray, R.D.H. *et al., The Natural Coumarins*, J. Wiley, 1982, (*occur*)
Ceska, O. *et al., Experientia*, 1986, **42**, 1302 (*occur, tox*)
Jain, A.K. *et al., J. Indian Chem. Soc.*, 1991, **68**, 452 (*glycoside*)
Srivastava, S.K. *et al., Fitoterapia*, 1994, **65**, 301-303 (*arabinoside*)
Adebajo, A.C. *et al., Fitoterapia*, 2000, **71**, 334-337 (*pmr, cmr*)

Xanthoxyletin X-6

[84-99-1]
*5-Methoxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one,9CI. Xanthoxylin N. Xanthoxyloin*



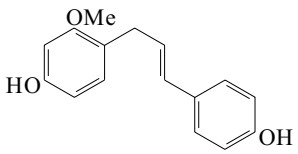
$C_{15}H_{14}O_4$ 258.273
Isol. from *Zanthoxylum americanum* (prickly ash). Cryst. (petrol). Mp 133°. Log P 3.04 (calc).

6,7-Dihydro: [17053-75-7] ***Kanzonol Q***
$C_{15}H_{16}O_4$ 260.289
Constit. of the roots of *Glycyrrhiza uralensis* (Chinese licorice). Pale yellow needles (C_6H_6). Mp 108.5-114°.

Vrkov, J. *et al., Phytochemistry*, 1972, **11**, 2647 (*isol*)
Mujumdar, R.B. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 200 (*isol*)
Gray, A.J. *et al., J.C.S. Perkin 2*, 1978, 391 (*pmr*)
Murray, R.D.H. *et al., Tetrahedron*, 1984, **40**, 3129 (*synth, bibl*)
Fukai, T. *et al., Heterocycles*, 1994, **38**, 1089 (*Kanzonol Q*)

Xenognosin A X-7

[76907-79-4]
4-[3-(4-Hydroxyphenyl)-2-propenyl]-3-methoxyphenol, 9CI. 1-(4-Hydroxyphenyl)-3-(4-hydroxy-2-methoxyphenyl)propene



$C_{16}H_{16}O_3$ 256.301
Isol. from gum tragacanth. Stress metab. of pea (*Pisum sativum*). Thick pale-yellow oil.

Lynn, D.G. *et al., J.A.C.S.*, 1981, **103**, 1868 (*isol*)
El-Feraly, F.S. *et al., J.O.C.*, 1982, **47**, 1527 (*synth, cmr*)
Carlson, R.E. *et al., Phytochemistry*, 1982, **21**, 1733 (*isol*)
Kamat, V.S. *et al., Tet. Lett.*, 1982, **23**, 1541 (*synth*)

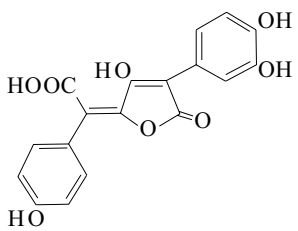
Xenorhabdicin X-8

[164003-58-1]
Peptide comprising 2 major subunits of 43 and 20 kDa. Bacteriocin prod. by *Xenorhabdus naematophilus*.

Thaler, J.O. *et al., Appl. Environ. Microbiol.*, 1995, **61**, 2049-2052 (*isol*)

Xerocomic acid X-9

[25287-88-1]



$C_{18}H_{12}O_8$ 356.288
Isol. from *Boletus erythropus* (dotted-stem bolete) and *Gomphidius glutinosus* (spike cap). Cryst. (H_2O). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 295°. λ_{max} 261 ; 411 (EtOH) (Berdy). λ_{max} 256 ; 378 (H_2O) (Berdy). λ_{max} 230 ; 360 ; 620 (pH 10 buffer) (Berdy).

Steglich, W. *et al., Z. Naturforsch., B*, 1968, **23**, 1044; 1969, **24**, 941
Edwards, R.L. *et al., J.C.S.(C)*, 1971, 2582 (*isol*)
Edwards, R.L. *et al., J.C.S. Perkin 1*, 1973, 1529
Ramage, R. *et al., J.C.S. Perkin 1*, 1984, 1547 (*synth*)

Xylan, 9CI, 8CI X-10

[9014-63-5]
$C_5H_8O_4$ 132.116
A typical hemicellulose pentosan formed by chains of (1→4) linked β-D-xylopyranosyl residues. True xylans, composed exclusively of D-xylose residues, are extremely rare. Esparto grass D-xylan is an example. Polymeric. Minimum formula given. Occurs in all land plants, component of dietary roughage. $[\alpha]_D^{21}$ -92 (c, 0.5 in 0.5*N* NaOH). Approved by FDA (1996) (as sodium salt)

Poly(hydrogen sulfate): [37300-21-3] *Pentosan polysulfate. Xylan hydrogen sulfate, 9CI. Xylan polysulfate. Fibrase. Hemoclar. Thrombocid. CB 8061. SP 54. Fibrezym. Cartrophen vet. PZ 68*
$[\alpha]_D^{20}$ -57 (Na salt). Used as sodium salt (Pentosan polysulfate sodium, BAN, INN, USAN).

[37319-17-8, 116001-96-8]

Whistler, R.L. *et al., Adv. Carbohydr. Chem.*, 1950, **5**, 269 (*rev*)
Chanda, S.K. *et al., J.C.S.*, 1950, 1289 (*isol*)
Swiss Pat., 1953, 293 566; *CA*, **49**, 1787h (*synth, polysulfate*)
Paramelle, B. *et al., Therapie*, 1962, **17**, 719 (*activity, polysulfate*)
Adams, G.A. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 170 (*synth*)
Mizuno, T. *et al., CA*, 1968, **68**, 3140k (*synth*)
Zelenev, Yu.V. *et al., CA*, 1968, **68**, 44624g (*pmr*)
Frandoli, G. *et al., Arzneim.-Forsch.*, 1972, **22**, 759 (*use*)
Marchessault, R.M. *et al., Adv. Carbohydr. Chem. Biochem.*, 1976, **33**, 397 (*cryst struct*)
Wilkie, K.C.B. *et al., Adv. Carbohydr. Chem. Biochem.*, 1979, **36**, 215
Kindness, G. *et al., Biochem. Biophys. Res. Commun.*, 1979, **88**, 1062 (*pharmacol, polysulfate*)
Esquivel, C.O. *et al., Thromb. Res.*, 1982, **28**, 389 (*activity, polysulfate*)
Doctor, V.M. *et al., Thromb. Res.*, 1983, **30**, 573 (*isol, props, polysulfate*)
MacGregor, I.R. *et al., Thromb. Haemostasis*, 1984, **51**, 321 (*metab, polysulfate*)
Willuweit, B. *et al., Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1988, **337**, 354 (*activity*)
Kiesel, J. *et al., Thromb. Res.*, 1991, **64**, 301 (*pharmacol*)
Zugmaier, G. *et al., J. Natl. Cancer Inst.*, 1992, **84**, 1716 (*pharmacol*)
Labrouche, S. *et al., Thromb. Haemostasis*, 1992, **68**, 556 (*pharmacol*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 233
Priola, S.A. *et al., Infect. Agents Dis.*, 1994, **3**, 54 (*activity*)

endo-1,4-β-Xylanase, 9CI X-11

[9025-57-4]
1,4-β-D-Xylan xylanohydrolase. Xylanase. Pentosanase. Endoxylanase. E.C. 3.2.1.8
Used in baked goods and brewing to treat whole grain, grain mashes and doughs to reduce viscosity for processing. Hydrolyses 1,4-β-D-xylosidic linkages in xylans.

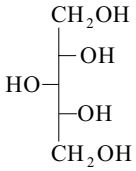
Howard, B.H. *et al., Biochem. J.*, 1960, **74**, 173-180 (*isol*)
Wong, K.K. *et al., Microbiol. Rev.*, 1988, **52**, 305-317 (*rev*)
Torronen, A. *et al., J. Biotechnol.*, 1997, **57**, 137-149 (*rev, struct*)

Xylitol, 9CI X-12

[87-99-0]

[16277-71-7]

Xylite. Xyliton. E967. Klinit. Kylit



$C_5H_{12}O_5$ 152.147

Occurs in a variety of plants, berries and fruits including plums, raspberries, cauliflower and endive; sweetening agent used in sugar free sweets and chewing gum. Two forms: metastable, rhombic cryst. and stable, monoclinic cryst. Poorly sol. hexane. Mp 61-61.5° (metastable) Mp 93-94.5° (stable). Opt. inactive (*meso*-).

► LD_{50} (mus, orl) 22000 mg/kg; adverse gastrointestinal effects (large dose). ZF0800000

Penta-Ac: [13437-68-8]
$C_{15}H_{22}O_{10}$ 362.333
Mp 62.5-63°.

Pentabenzoyl: [36030-82-7]
$C_{40}H_{32}O_{10}$ 672.687
Mp 106-107°.

2,3,4-Tri-Me:2,3,4-Tri-O-*methylxylitol*
$C_8H_{18}O_5$ 194.227
Syrup.

2,3,4-Tri-Me, 1,5-ditosyl:2,3,4-Tri-O-*methyl-1,5-ditosylxylitol*
$C_{22}H_{30}O_9S_2$ 502.606
Cryst. (EtOAc/hexane). Mp 121-123°. 1,5-Dimesyl analogue also prepd..

1,2:3,4-Di-O-*isopropylidene:*
$C_{11}H_{20}O_5$ 232.276
Mp 36°.

1,2:4,5-Di-O-*isopropylidene, 3-benzoyl:*
$C_{18}H_{24}O_6$ 336.384
Mp 114-116°.

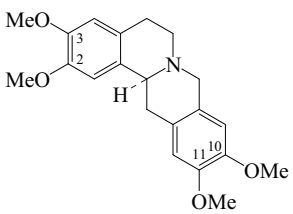
1,3:2,4-Di-O-*benzylidene, 5-benzoyl:*
$C_{26}H_{24}O_6$ 432.472
Mp 173-175°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 185B (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 289A (*nmr*)
Wolfrom, M.L. *et al., J.A.C.S.*, 1942, **64**, 1739
Carson, J.F. *et al., J.A.C.S.*, 1943, **65**, 1777
Kratzl, K. *et al., Naturwissenschaften*, 1963, **50**, 154 (*occur*)
Baggett, N. *et al., J.C.S.*, 1965, 3382
Begbie, R. *et al., Carbohydr. Res.*, 1966, **2**, 272 (*occur*)
Barton, D.H.R. *et al., J.C.S. Perkin 1*, 1972, 542
Brimacombe, J.S. *et al., The Carbohydrates*, 1972, **1A**, 479
Chautemps, P. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1977, **284**, 807 (*synth*)
Xylitol, Int. Symp., (Ed. Counsell, J.N.), Applied Science Publishers, London, 1978, (*book*)
Angyal, S.J. *et al., Carbohydr. Res.*, 1980, **84**, 201 (*cmr*)
Minami, N. *et al., J.A.C.S.*, 1982, **104**, 1109 (*total synth*)
Holland, D. *et al., J.C.S. Perkin 1*, 1983, 1553 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, XPJ000
Kopf, J. *et al., Carbohydr. Res.*, 1992, **233**, 35 (*cryst struct, penta-Ac*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1063
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 564-567
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1395
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2967-2970
Rozenberg, M. *et al., Carbohydr. Res.*, 2000, **328**, 307-319 (*ir*)
Garcia-Martin, M.G. *et al., Carbohydr. Res.*, 2001, **333**, 95-103 (*2,3,4-tri-Me, 2,3,4-tri-Me ditosyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, XPJ000

Xylopinine X-13

[4216-86-8]

5,8,13,13a-Tetrahydro-2,3,10,11-tetramethoxy-6H-dibenzo[a,g]quinolizine, 9CI. Norcoralydine. O,O-*Dimethylcoreximine.* O,O-*Dimethylgovanine*



(*S*)-*form*

$C_{21}H_{25}NO_4$ 355.433

(*S*)-*form* [523-02-4]
Light-yellow prismatic cryst. ($CHCl_3$/Me_2CO). Mp 182-183° (177°). $[\alpha]_D$ -297 (c, 1 in $CHCl_3$).

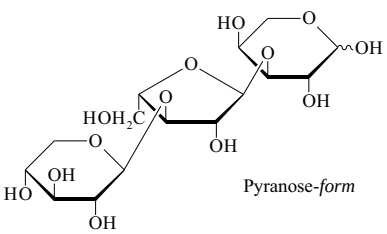
► HQ1793000

O^2,O^{11}-*Di-de-Me:* [483-45-4] ***Coreximine.*** *Coramine. Alkaloid F29*
$C_{19}H_{21}NO_4$ 327.379
Alkaloid from *Papaver somniferum* (opium poppy). Prisms ($CHCl_3$). Mp 254-256°. $[\alpha]_D^{25}$ -420 (c, 0.69 in Py).

Manske, R.H.F. *et al., Can. J. Res., Sect. B*, 1938, **16**, 81 (*Coreximine*)
Battersby, A.R. *et al., Tetrahedron*, 1961, **14**, 46 (*Coreximine, synth, uv*)
Brockmann-Hanssen, E. *et al., J.O.C.*, 1977, **42**, 3588 (*Coreximine, pmr*)

β-D-Xylopyranosyl-(1→3)-α-L-arabinofuranosyl-(1→3)-L-arabinose, 9CI X-14

[79409-35-1]



Pyranose-*form*

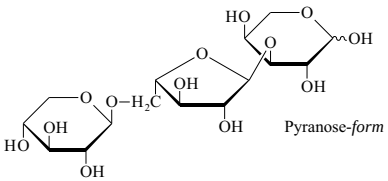
$C_{15}H_{26}O_{13}$ 414.363

Isol. from the mucilage of *Opuntia ficus-indica* (Indian fig). $[\alpha]_D$ -21 (c, 0.57 in H_2O).

McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol*)

β-D-Xylopyranosyl-(1→5)-α-L-arabinofuranosyl-(1→3)-L-arabinose, 9CI X-15

[7268-42-0]



Pyranose-*form*

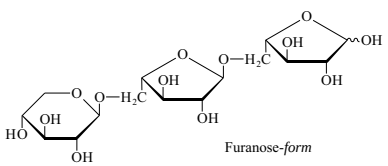
$C_{15}H_{26}O_{13}$ 414.363

Isol. from the mucilage of *Opuntia ficus-indica* (Indian fig). Amorph. solid (Me_2CO/MeOH). Mp 131-140°. $[\alpha]_D$ -32 (c, 0.47 in H_2O). $[\alpha]_D$ -74.2 (c, 1.1 in H_2O).

Parikh, V.M. *et al., Can. J. Chem.*, 1966, **44**, 1531 (*isol*)
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol*)

β-D-Xylopyranosyl-(1→5)-α-L-arabinofuranosyl-(1→5)-L-arabinose, 9CI X-16

[79403-08-0]



Furanose-*form*

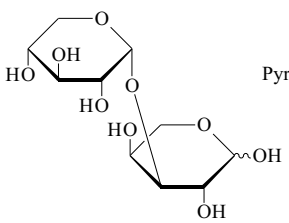
$C_{15}H_{26}O_{13}$ 414.363

Isol. from the mucilage of *Opuntia ficus-indica* (Indian fig). $[\alpha]_D$ -56.5 (c, 0.52 in H_2O).

McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol*)

3-*O*-α-D-Xylopyranosyl-L-arabinose, 9CI X-17

[4119-17-9]



Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247

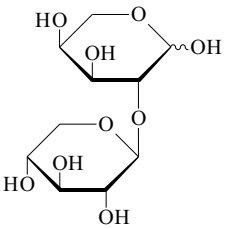
Isol. from the autohydrolysate of golden apple (*Spondias cytherea*), gum, garden cress mucilage and the partial acid hydrolysates of corn hemicelluloses. Cryst. + $1H_2O$ (EtOH aq.). Mp 117-119°. $[\alpha]_D^{25}$ +175 → +183 (c, 1.0 in H_2O, 1h).

Phenylosazone:
Mp 226°.

Hexa-Ac:
$C_{22}H_{30}O_{15}$ 534.47
Cryst. (MeOH). Mp 168-170°. $[\alpha]_D^{28}$ +106 (c, 1.0 in $CHCl_3$).

Andrews, P. *et al., J.C.S.*, 1954, 4134 (*isol*)
Whistler, R.L. *et al., J.A.C.S.*, 1955, **77**, 6328 (*isol*)
Montgomery, R. *et al., J.A.C.S.*, 1957, **79**, 698 (*isol*)
Tyler, J.M. *et al., J.C.S.*, 1965, 5288

2-*O*-β-D-Xylopyranosyl-L-arabinose X-18



Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247
Isol. from barley husk and corn-cob hemicelluloses. Mp 167-168° (anhyd.) Mp 80-81° (monohydrate) Mp 98-99° (trihydrate). $[\alpha]_D$ +33 (H_2O).

α-L-Pyranose-*form*

Me glycoside: [89734-27-0] *Methyl 2-O-β-D-xylopyranosyl-α-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
Needles (MeOH/EtOAc). Mp 187.5-189°. $[\alpha]_D^{20}$ -48.5 (c, 0.92 in H_2O).

β-L-Pyranose-*form*

Me glycoside: [89734-31-6] *Methyl 2-O-β-D-xylopyranosyl-β-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
Cryst. (EtOH/EtOAc). Mp 182-184°. $[\alpha]_D^{26}$ +95.3 (c, 0.6 in H_2O).

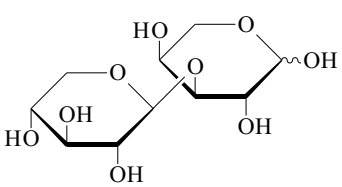
L-Furanose-*form*

5-O-(4-Hydroxy-3-methoxycinnamoyl)(E-): [169697-21-6] *2-O-β-D-Xylopyranosyl-5-O-feruloyl-L-arabinofuranose*
$C_{20}H_{26}O_{12}$ 458.418Anomeric mixture.

Whistler, R.L. *et al., J.A.C.S.*, 1955, **77**, 1884; 3822 (*isol*)
Aspinall, G.O. *et al., J.C.S.*, 1957, 4188
Mizutani, K. *et al., Carbohydr. Res.*, 1984, **126**, 177 (*synth, Me gly, cmr*)
Wende, G. *et al., Phytochemistry*, 1997, **44**, 1011-1019 (*feruloyl deriv*)

3-*O*-β-D-Xylopyranosyl-L-arabinose X-19

[78248-68-7]

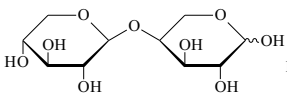


$C_{10}H_{18}O_9$ 282.247
Hydrolysate product from the stem mucilage of *Opuntia ficus-indica* (Indian fig). Syrup. $[\alpha]_D$ +15 (c, 0.76 in H_2O).

McGarvie, D.M. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol, struct*)
Komori, T. *et al., Annalen*, 1981, 683 (*ms*)
Anjaneyalu, Y.V. *et al., Phytochemistry*, 1983, **22**, 1961 (*isol, glc, ms*)

4-*O*-β-D-Xylopyranosyl-L-arabinose X-20

[51755-05-6]



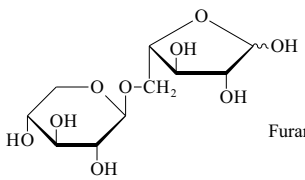
Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247
Isol. from acid hydrolysate of peach gum.

Rosik, J. *et al., Chem. Zvesti*, 1973, **27**, 688; *CA*, **80**, 108782x (*isol*)
Czech. Pat., 1979, 180 902; *CA*, **92**, 215729e (*isol*)
Hrmova, M. *et al., Arch. Microbiol.*, 1984, **138**, 371; *CA*, **101**, 187678w (*isol*)

5-*O*-β-D-Xylopyranosyl-L-arabinose, 9CI X-21

[7268-80-6]



Furanose-*form*

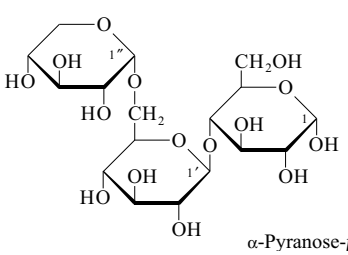
$C_{10}H_{18}O_9$ 282.247
Isol. from partial acid hydrolysates of peach, Cholla (*Opuntia fulgida*), *Opuntia ficus-indica* (Indian fig) and *Virgilia oroboides* gums. $[\alpha]_D$ -53 (c, 1.2 in H_2O). $[\alpha]_D^{23}$ -38 (c, 1.4 in H_2O).

Phenylosazone:
Cryst. (EtOH/Et_2O). Mp 216° (214° dec.). $[\alpha]_D^{23}$ +51 (c, 0.8 in Py/EtOH, 3:2).

Andrews, P. *et al., J.C.S.*, 1953, 4090 (*isol*)
Ball, D.H. *et al., J.C.S.*, 1957, 4871 (*synth*)
Smith, F. *et al., J.C.S.*, 1961, 4892 (*isol*)
Parikh, V.M. *et al., Can. J. Chem.*, 1966, **44**, 1531 (*isol*)
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol*)

α-D-Xylopyranosyl-(1→6)-β-D-glucopyranosyl-(1→4)-D-glucose, 9CI X-22

[69637-98-5]



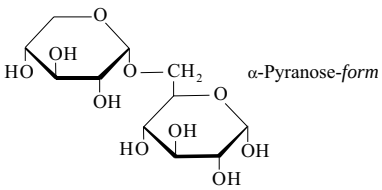
α-Pyranose-*form*

$C_{17}H_{30}O_{15}$ 474.415
Constituent in cell wall polysaccharide of immature barley plants. Isol. from the enzymatic hydrolysates of tamarind polysaccharide. $[\alpha]_D$ +74 (c, 0.5 in H_2O) (+71).

Mori, M. *et al., Agric. Biol. Chem.*, 1979, **43**, 145 (*isol*)
Kato, Y. *et al., Agric. Biol. Chem.*, 1981, **45**, 2745 (*occur*)
Kato, Y. *et al., Carbohydr. Res.*, 1982, **109**, 233
Watanabe, T. *et al., Carbohydr. Res.*, 1984, **129**, 229
Zong, N. *et al., Agric. Biol. Chem.*, 1989, **53**, 2129 (*isol, hplc*)
York, W.S. *et al., Carbohydr. Res.*, 1990, **200**, 9 (*ms, cmr, pmr*)

6-*O*-α-D-Xylopyranosyl-D-glucose, 9CI X-23

[534-98-5]
Isoprimeverose. Serotinose

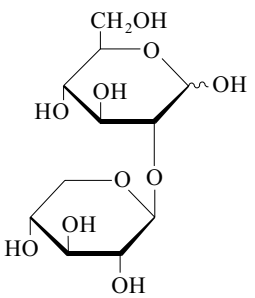


$C_{11}H_{20}O_{10}$ 312.273
From glucomannan of *Tamarindus indica*. Mp 200-201°. $[\alpha]_D^{20}$ +151.3 → +121.3 (H_2O).

Zemplen, G. *et al., Ber.*, 1939, **72**, 1160 (*synth*)
Perila, O. *et al., Can. J. Chem.*, 1961, **39**, 815 (*isol*)
Le Dizet, P. *et al., Carbohydr. Res.*, 1972, **24**, 505 (*isol*)

2-*O*-β-D-Xylopyranosyl-D-glucose, 9CI, 8CI X-24

[26388-68-1]
Sambubiose

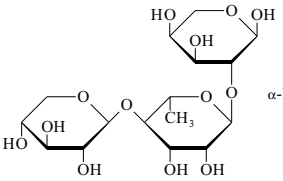


$C_{11}H_{20}O_{10}$ 312.273
Isol. from *Sambucus nigra* (elderberry). Mp 202-203°. $[\alpha]_D$ +32 → +17 (c, 1 in H_2O).

Reichel, L. *et al., Naturwissenschaften*, 1960, **47**, 40
Erbing, B. *et al., Acta Chem. Scand.*, 1969, **23**, 2213 (*synth*)
Erbing, B. *et al., CA*, 1976, **84**, 122160g (*rev*)

β-D-Xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-L-arabinose X-25

β-D-Xylopyranosyl-(1→4)-6-deoxy-α-L-mannopyranosyl-(1→2)-L-arabinose, 9CI



α-Pyranose-*form*

$C_{16}H_{28}O_{13}$ 428.389

Constit. of Acutosides from *Luffa acutangula* (Chinese okra).

α-Pyranose-*form*

Me glycoside: [135545-80-1]
$C_{17}H_{30}O_{13}$ 442.416
Amorph. powder. $[\alpha]_D^{26}$ -50.5 (c, 1.0 in MeOH) (-45.3).

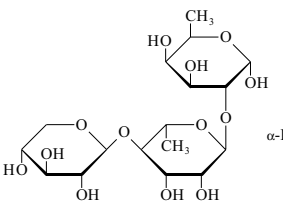
β-Pyranose-*form*

Me glycoside: [135545-81-2]
Amorph. powder. $[\alpha]_D^{26}$ +39.3 (c, 0.90 in MeOH) (+29.3).

Tanaka, R. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1153 (*α-Me pyr, β-Me pyr, pmr, cmr, ms*)
Nagao, T. *et al., Chem. Pharm. Bull.*, 1991, **39**, 599 (*isol, α-Me pyr, β-Me pyr, pmr, cmr, ms*)

β-D-Xylopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-D-fucose X-26

β-D-Xylopyranosyl-(1→4)-6-deoxy-α-L-mannopyranosyl-(1→2)-6-deoxy-D-galactose, 9CI



α-Pyranose-*form*

$C_{17}H_{30}O_{13}$ 442.416

Constit. of desacylsaponins from the bark of *Quillaja saponaria* (soap-bark tree).

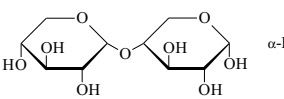
α-Pyranose-*form*

Me glycoside: [107091-14-5]
$C_{18}H_{32}O_{13}$ 456.443
Hygroscopic powder. $[\alpha]_D$ +11.8 (c, 1.0 in MeOH).

Topping, D.L. *et al., Proc. Nutr. Soc. Aust.*, 1980, **5**, 195 (*use*)
Higuchi, R. *et al., Phytochemistry*, 1986, **26**, 229 (*isol, ir, cmr, ms*)

4-*O*-α-D-Xylopyranosyl-D-xylose, 9CI X-27

[82970-38-5]



α-Pyranose-*form*

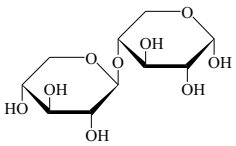
$C_{10}H_{18}O_9$ 282.247

Occurs as side chains in the xylomannan polysaccharide obt. from mycelia of *Armillaria mellea* (honey mushroom). Amorph. $[\alpha]_D^{25}$ +108 (c, 1.5 in H_2O).

Kovac, P. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 892
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1464
Takeo, K. *et al., Carbohydr. Res.*, 1991, **209**, 167 (*synth*)

4-*O*-β-D-Xylopyranosyl-D-xylose, 9CI, 8CI X-28

[6860-47-5]
Xylobiose



α-Pyranose-*form*

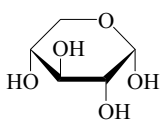
$C_{10}H_{18}O_9$ 282.247

Major or sole repeating unit in the main xylan chains of the plant xylans, arabinoxylans and glucuronoxylans. Isol. from Scotch pine (*Pinus sylvestris*). Mp 185-190°. $[\alpha]_D^{22}$ -32 → -25.5 (H_2O).

Whistler, R.L. *et al., J.A.C.S.*, 1952, **74**, 3059; 3609 (*isol, synth*)
Myhre, D.V. *et al., J.O.C.*, 1961, **26**, 4609 (*synth*)
Tu, C.C. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 357 (*synth*)
Bailey, R.W. *et al., Oligosaccharides*, Pergamon, 1965, 43 (*occur*)
Pazur, J.H. *et al., The Carbohydrates*, 2nd edn., (Eds., Pigman, W. *et al*), Academic Press, New York, 1970, 114 (*rev*)
Gast, J.C. *et al., Carbohydr. Res.*, 1980, **84**, 137 (*cmr*)
Kovac, P. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 892 (*synth*)

Xylose, 9CI, 8CI, USAN X-29

Wood sugar. Losan. Xylomed. Xylo-Pfan. FEMA 3606



α-D-Pyranose-*form*

$C_5H_{10}O_5$ 150.131

An aq. soln. at 31° contains 36.5% α-pyr, 63% β-pyr, < 1% α- and β-fur and 0.02% aldehyde.

D-*form* [58-86-6]
Flavouring ingredient, sweetener. Present in straw, corncobs and pecan shells. Needles (EtOH). Mp 153° (144-145°). $[\alpha]_D^{20}$ +19 (H_2O, equilib.). pK_{a1} 12.29 (25°). Weak sweet taste, sweetness =0.26 × sucrose.

► ZF2285000

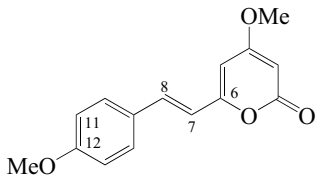
[3154-36-7, 41546-29-6, 41546-30-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 187C; 187D; 188C (*ir*)
Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra, 1992, **1**, 293C; 294A; 294B (*nmr*)
Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 136 (*rev*)
Whistler, R.L. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 88 (*synth, D-form*)
Ness, R.K. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 90 (*synth, D-form*)
Hough, L. *et al., Rodd's Chem. Carbon Compd. (2nd edn.)*, 1967, **1F**, 231 (*occur, isol*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 585 (*occur*)
Bock, K. *et al., Tet. Lett.*, 1973, **13**, 1037 (*cmr*)
Bock, K. *et al., Annu. Rep. NMR Spectrosc.*, (Webb, G.A. ed.), Acad. Press, London and New York, 1982, **13**, 38; 41 (*pmr, cmr*)
Angyal, S.J. *et al., Adv. Carbohydr. Chem. Biochem.*, 1984, **42**, 15 (*equilib*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 780
Benesi, A.J. *et al., Carbohydr. Res.*, 1994, **258**, 27 (*pmr, cmr*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1109

Yangonin Y-1

[500-62-9]

*4-Methoxy-6-[2-(4-methoxyphenyl)ethenyl]-2*H*-pyran-2-one, 9CI. 4-Methoxy-6-(4-methoxystyryl)-α-pyrone*



$C_{15}H_{14}O_4$ 258.273

Found in kava root (*Piper methysticum*). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Greenish-yellow cryst. with blue fluor. (MeOH or Me_2CO). Mp 153-154°. Log P 2.7 (calc).

▶ LD_{50} (mus, orl) >1500 mg/kg. LD_{50} (mus, ivn) 41 mg/kg. UQ1225200

*12-*O*-De-Me:* [39986-86-2] ***Noryangonin***
$C_{14}H_{12}O_4$ 244.246
Greenish-yellow needles (Me_2CO/C_6H_6). Mp 268° dec.

*12-*O*-De-Me, Ac:*
Mp 178°.

*Di-*O*-de-Me:* [13709-27-8] *4-Hydroxy-6-(4-hydroxystyryl)-2-pyrone.* ***Bisnoryangonin***
$C_{13}H_{10}O_4$ 230.22
Cryst. (MeOH). Sol. MeOH. Mp 250-255° (dec.)(240-244° dec.). λ_{max} 217 ; 364 (No solvent reported).

5,6-Dihydro: [3328-60-7]

[3155-49-5, 130464-78-7] ***5,6-Dihydroyangonin***
$C_{15}H_{16}O_4$ 260.289
Constit. of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002).

7,8-Dihydro: [3155-52-0] ***7,8-Dihydroyangonin***
$C_{15}H_{16}O_4$ 260.289
Constit. of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002).

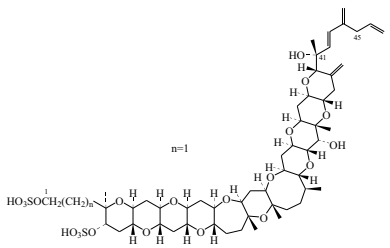
*5,6*S*,7,8-Tetrahydro:* [49776-58-1] *5,6-Dihydro-4-methoxy-6-[2-(4-methoxyphenyl)ethyl]-2*H*-pyran-2-one.* ***5,6,7,8-Tetrahydroyangonin***
$C_{15}H_{18}O_4$ 262.305
Constit. of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Needles (Et_2O). Mp 89-90°. $[\alpha]_D^{20}$ +20 (c, 0.08 in $CHCl_3$).

10-Methoxy: [77900-32-4] ***10-Methoxyyangonin***
$C_{16}H_{16}O_5$ 288.299
Constit. of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002).

Chmielewska, I. *et al., Tetrahedron*, 1958, **4**, 36
Beak, P. *et al., J.O.C.*, 1962, **27**, 3715 (*pmr*)
Werny, F. *et al., Naturwissenschaften*, 1963, **50**, 355 (*tetrahydro, synth*)
Haensel, R. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1966, **299**, 503; 507 (*11-Methoxynoryangonin, 11-Methoxyyangonin*)
Harris, T.M. *et al., J.O.C.*, 1968, **33**, 2399 (*synth*)
Hatfield, G.M. *et al., Lloydia*, 1968, **31**, 225 (*Bisnoryangonin*)
Achenbach, H. *et al., Chem. Ber.*, 1971, **104**, 2688 (*tetrahydro, isol, struct*)
Engel, P. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1971, **134**, 180 (*cryst struct*)
Franca, N.C. *et al., Phytochemistry*, 1973, **12**, 1182 (*tetrahydro, abs config*)
Pradhan, D.K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 300 (*isol*)
Hipolito, E. *et al., Rev. Latinoam. Quim.*, 1977, **8**, 79; *CA*, **87**, 53025q (*isol, synth*)

Yessotoxin Y-2

[112514-54-2]



$C_{55}H_{82}O_{21}S_2$ 1143.372

Toxic constit. of scallops (*Patinopecten yessoensis*). Amorph. solid (as di-Na salt). Sol. MeOH, butanol. $[\alpha]_D^{20}$ +3.01 (c, 0.45 in MeOH). λ_{max} 230 (ε 10600) (MeOH) (Derep).

▶ Toxic. LD_{50} (mus, ipr) 0.1 mg/kg. ZF9109000

1-Desulfo: [255041-59-9] ***1-Desulfoyessotoxin***
$C_{55}H_{82}O_{18}S$ 1063.308
Isol. from mussels.

*45*R*-Hydroxy:* [124863-39-4] ***45-Hydroxyyessotoxin***
$C_{55}H_{82}O_{22}S_2$ 1159.372
Constit. of toxic scallop (*Patinopecten yessoensis*). Amorph. solid. λ_{max} 230 (ε 15600) (MeOH).

▶ LD_{50} (mus, ipr) 0.5 mg/kg.

*44-De(methylene), 44*R*-carboxy:* [262842-91-1] ***Carboxyyessotoxin***
$C_{55}H_{82}O_{23}S_2$ 1175.371
Constit. of the mussel *Mytilus galloprovincialis*. Amorph. (as di-Na salt).

45,46,47-Trinor: [181365-95-7] ***45,46,47-Trinoryessotoxin***
$C_{52}H_{78}O_{21}S_2$ 1103.308
Constit. of toxic scallop (*Patinopecten yessoensis*). Amorph. solid. Lacks the 3 terminal carbons from the C-7 end chain, i.e. terminal group is 1-hydroxy-1-methyl-2,4-pentadienyl λ_{max} 226 (ε 22600) (MeOH).

▶ Toxic ; LD_{50} (mus, ipr) 0.22 mg/kg.

Homologue (n = 2): [196309-94-1] ***Homoyessotoxin***
$C_{56}H_{84}O_{21}S_2$ 1157.399
Isol. from mussels.

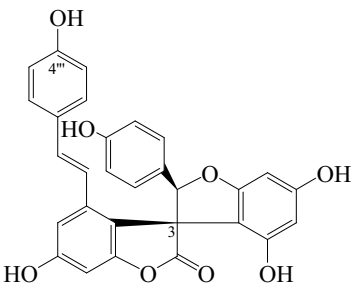
Homologue (n = 2), 45-hydroxy: [196309-97-4] ***45-Hydroxyhomoyessotoxin***
$C_{56}H_{84}O_{22}S_2$ 1173.398
Constit. of mussel *Mytilus* sp..

*Homologue (n = 2), 44-demethylene, 44*R*-carboxy:* [292850-13-6] ***Carboxyhomoyessotoxin***
$C_{56}H_{84}O_{23}S_2$ 1189.398
Isol. from Adriatic mussels.

[112574-50-2]

Murata, M. *et al., Tet. Lett.*, 1987, **28**, 5869-5872 (*isol, struct*)
Kumagai, M. *et al., CA*, 1988, **108**, 70214v (*isol, struct*)
Naoki, H. *et al., Rapid Commun. Mass Spectrom.*, 1993, **7**, 179 (*ms*)
Satake, M. *et al., Tet. Lett.*, 1996, **37**, 5955-5958 (*Trinoryessotoxin, 45-Hydroxyyessotoxin, config*)
Takahashi, H. *et al., Tet. Lett.*, 1996, **37**, 5955-5958; 7087-7090 (*abs config*)
Yasumoto, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1775-1777 (*hplc*)
Satake, M. *et al., Nat. Toxins*, 1997, **5**, 107-110; 1998, **6**, 235-239 (*1-Desulfoyessotoxin, Homoyessotoxin, 45-Hydroxyhomoyessotoxin*)
Morohashi, A. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1761-1763 (*45-Hydroxyyessotoxin, abs config*)
Ciminiello, P. *et al., Chem. Res. Toxicol.*, 2000, **13**, 770-774 (*Carboxyhomoyessotoxin*)
Ciminiello, P. *et al., Eur. J. Org. Chem.*, 2000, 291-295 (*Carboxyyessotoxin*)

Yuccaol A Y-3



$C_{29}H_{20}O_8$ 496.472

Constit. of the bark of *Yucca schidigera* (Mojave yucca). Amorph. powder. Mp 205-206° dec. $[\alpha]_D^{20}$ +78.4 (c, 0.1 in MeOH).

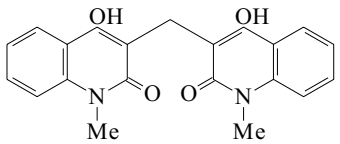
3-Epimer: ***Yuccaol B***
$C_{29}H_{20}O_8$ 496.472
Constit. of the bark of *Yucca schidigera* (Mojave yucca). Amorph. powder. Mp 209-210° dec. $[\alpha]_D^{20}$ +93.8 (c, 0.1 in MeOH).

3-Epimer, 3‴,5‴-dihydroxy, 4‴-Me ether: ***Yuccaol C***
$C_{30}H_{22}O_{10}$ 542.498
Constit. of the bark of *Yucca schidigera* (Mojave yucca). Amorph. powder. Mp 212-213°. $[\alpha]_D^{20}$ +20.8 (c, 0.1 in MeOH).

Oleszek, W. *et al., J. Agric. Food Chem.*, 2001, **49**, 747-752 (*isol, pmr, cmr, ms*)

Zanthobisquinolone Z-1

[57147-67-8]

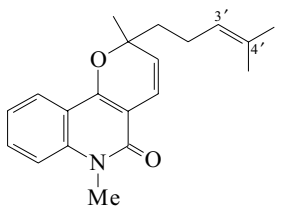


$C_{21}H_{18}N_2O_4$ 362.384
Alkaloid from root wood of *Zanthoxylum simulans* (Szechuan pepper). Needles ($CHCl_3$/MeOH). Mp 295-298°.

Chen, I.-S. *et al., Phytochemistry*, 1994, **36**, 237 (*isol, uv, ir, pmr, cmr, ms, struct*)

Zanthosimuline Z-2

[155416-20-9]



$C_{20}H_{23}NO_2$ 309.407
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Solid. Mp 127-128°. $[\alpha]_D$ +7 (c, 0.1 in $CHCl_3$).

3′,4′-Dihydro, 3′-oxo: [155416-21-0] ***Huajiaosimuline***
$C_{20}H_{23}NO_3$ 325.407
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Oil.

3′,4′-Dihydro, 3′-hydroxy: [176520-66-4] ***Simulansine***
$C_{20}H_{25}NO_3$ 327.422
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Oil.

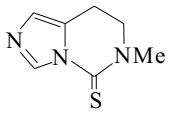
Δ$^{2'}$-Isomer, 4′-hydroxy: [198336-56-0] ***Simulenoline***
$C_{20}H_{23}NO_3$ 325.407
Alkaloid from the bark of *Zanthoxylum simulans* (Szechuan pepper). Oil. $[\alpha]_D^{23}$ +6.9 (c, 0.2 in $CHCl_3$). λ_{max} 228 (log ϵ 4.33); 256 (sh) (log ϵ 3.86); 336 (log ϵ 3.68); 350 (log ϵ 3.73); 367 (log ϵ 3.56) (EtOH).

Δ$^{2'}$-Isomer, 4′-hydroperoxy: [198336-57-1] ***Peroxysimulenoline***
$C_{20}H_{23}NO_4$ 341.406
Alkaloid from the bark of *Zanthoxylum simulans* (Szechuan pepper). Oil. λ_{max} 228 (log ϵ 4.33); 256 (sh) (log ϵ 3.86); 336 (log ϵ 3.68); 350 (log ϵ 3.73); 367 (log ϵ 3.56) (EtOH).

Wu, S.-J. *et al., Phytochemistry*, 1993, **34**, 1659-1661 (*isol, uv, ir, pmr, cmr, ms, struct*)
Chen, I.-S. *et al., Phytochemistry*, 1996, **42**, 217-219 (*Simulansine*)
Chen, I.-S. *et al., Phytochemistry*, 1997, **46**, 525-529 (*Simulenoline, Peroxysimulenoline*)
McLaughlin, M.J. *et al., J.O.C.*, 2001, **66**, 1049-1053 (*Huajiaosimuline,Simulenoline,synth*)
Lee, Y.R. *et al., Synthesis*, 2001, 1851-1855 (*synth, ir, pmr*)

Zapotidine Z-3

[525-84-8]
6-Methylimidazo[1,5-c]tetrahydropyrimidine-5-thione



$C_7H_9N_3S$ 167.234
Minor alkaloid from the seeds of *Casimiroa edulis* (Mexican apple). Plates (Et_2O). Mp 96-98°.

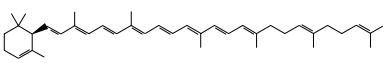
▶ LD_{50} (mus, ipr) 50 mg/kg.

Picrate:
Mp 195-196°.

Kincl, F.A. *et al., J.C.S.*, 1956, 4163 (*isol, uv, ir*)
Mechoulam, R. *et al., J.A.C.S.*, 1961, **83**, 2022 (*pmr, struct*)
Mechoulam, R. *et al., Tetrahedron*, 1967, **23**, 239 (*synth*)
Wróbel, J.T. *et al., Alkaloids (N.Y.)*, 1985, **26**, 56 (*props, synth*)

α-Zeacarotene Z-4

[50657-19-7]
7′,8′-Dihydro-ϵ,ψ-carotene



$C_{40}H_{58}$ 538.898
Constit. of corn gluten. Oil.

Petzold, E.N. *et al., Arch. Biochem. Biophys.*, 1959, **82**, 117 (*isol*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1973, **56**, 1124 (*config*)

Zeamatin Z-5

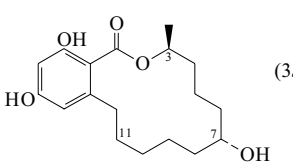
[130590-19-1]
Corn synergstic antifungal protein. Corn SAFP

Protein, MW 22 kDa. Isol. from maize grains.

Pat. Coop. Treaty (WIPO), 1995, 95 18 959; *CA*, **123**, 246800j (*isol*)
Batalia, M.A. *et al., Nature Struct. Biology*, 1996, **3**, 19-23 (*cryst struct*)
Wilson, S. *et al., Biotechnol. Prog.*, 2000, **16**, 38-43 (*isol*)

Zearalanol Z-6

*3,4,5,6,7,8,9,10,11,12-Decahydro-7,14,16-trihydroxy-3-methyl-1*H*-2-benzoxacyclotetradecin-1-one, 9CI*



(3*S*,7*R*)-*form*

$C_{18}H_{26}O_5$ 322.4
Log P 4.37 (calc).

(3*S*,7*R*)-*form* [26538-44-3]
α-Zearalanol. ***Zeranol, BAN, INN, USAN****. Frideron. Ralabol. Ralgro. Ralone. Zerano. MK 188. P 1496*
Isol. from *Fusarium* spp. Anabolic agent, estrogenic agent (mainly vet. use). Used as a growth promoter for food animals. Banned by the EU in 1989, but still permitted in the USA and some other countries. May also arise in livestock by ingestion of *Fusarium* contaminated pasture or feeds.. Cryst. (2-propanol aq.). Mp 182-184°. $[\alpha]_D$ +46.3 (c, 1 in MeOH).

▶ Exp. reprod. and teratogenic effects. Hepatotoxic. Causes hepatic neoplasms in rodents. DM2520000

*11,12*E*-Didehydro:* [36455-72-8] ***α-Zearalenol***
$C_{18}H_{24}O_5$ 320.385
Sol. MeOH, $CHCl_3$; poorly sol. H_2O.

7-Deoxy: [7344-47-0] *Zearalane*
Mp 154-156°.

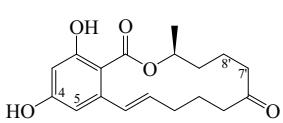
(3*S*,7*S*)-*form* [42422-68-4] *β-Zearalanol.* ***Taleranol, INN, USAN****. P 1560*
Cryst. (2-propanol aq.). Mp 146-148°. $[\alpha]_D^{25}$ +39 (MeOH).

*11,12*E*-Didehydro:* [71030-11-0] ***β-Zearalenol***
$C_{18}H_{24}O_5$ 320.385

Ger. Pat., 1974, 2 328 605; *CA*, **81**, 3788w (*synth*)
Bennett, G. *et al., Vet. Rec.*, 1974, **94**, 235 (*pharmacol*)
Crawley, G.C. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **12**, 658 (*rev, pharmacol, tox*)
Galbraith, H. *et al., Vet. Res. Commun.*, 1983, **7**, 27; 35 (*pharmacol*)
Richardson, K.E. *et al., J. Agric. Food Chem.*, 1985, **33**, 862 (*Zearalenol, isol*)
Snatzke, G. *et al., Helv. Chim. Acta*, 1986, **69**, 734 (*abs config, synth*)
Gimeno, E.J. *et al., Rev. Med. Vet. (Buenos Aires)*, 1986, 32 (*rev*)
Everett, D.J. *et al., J. Toxicol. Environ. Health*, 1987, **20**, 435
Coe, J.E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 1085 (*tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1198
Miles, C.O. *et al., J. Agric. Food Chem.*, 1996, **44**, 3244-3250 (*occur*)
Fuerstner, A. *et al., Tetrahedron*, 1999, **55**, 8215-8230 (*synth*)
Bracher, F. *et al., Eur. J. Org. Chem.*, 2001, 4701-4704 (*Zearalane, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, RBF100

Zearalenone Z-7

*3,4,5,6,9,10-Hexahydro-14,16-dihydroxy-3-methyl-1*H*-2-benzoxacyclotetradecin-1,7(8*H*)-dione, 9CI. Mycotoxin F2. Toxin F2*



(*S*,*E*)-*form*

$C_{18}H_{22}O_5$ 318.369
Sol. MeOH, Et_2O, MeCN; fairly sol. hexane; poorly sol. H_2O. λ_{max} 236 (ϵ 29700); 274 (ϵ 13909); 316 (ϵ 6020) (MeOH) (Berdy).

(*S*,*E*)-*form* [17924-92-4]
Fungal metab. of *Fusarium* spp. and of *Gibberella zeae*. Potential food myco-

toxin. Has weak estrogenic activity and causes physiol. changes when ingested by animals as foodstuffs contaminant.. Mp 164-165° (157-159°). $[\alpha]_D$ -190 ($CHCl_3$). λ_{max} 236 (ε 29700); 274 (ε 13900); 316 (ε 6000) (EtOH).

▶ Severe skin irritant. Exp. neoplastic agent and teratogen. Exp. reprod. effect. DM2550000

4-Sulfate: [132505-04-5] *Zearalenone 4-sulfate*
$C_{18}H_{22}O_8S$ 398.433
Prod. by *Fusarium graminearum* grown on rice. Estrogenic mycotoxin. Yellow powder. Sol. H_2O. λ_{max} 228 ; 260 ; 300 (MeOH).

5-Formyl: [41432-76-2] ***5-Formylzearalenone***
$C_{19}H_{22}O_6$ 346.379
Platelets. Mp 188-190°. $[\alpha]_D^{24}$ -42 ($CHCl_3$).

4-Ac: [119950-10-6] ***4-Acetylzearalenone***
$C_{20}H_{24}O_6$ 360.406
Metab. of *Fusarium graminearum*. λ_{max} 230 ; 264 ; 323 (MeOH).

Di-Ac:
Mp 123-125°.

1′,2′-Dihydro: [21307-27-7] *Zearalanone*
$C_{18}H_{24}O_5$ 320.385
Mp 192-193°.

*7′,8′-Didehydro(*E-*):* [40785-63-5] ***7′-Dehydrozearalenone***
$C_{18}H_{20}O_5$ 316.353
Needles (Me_2CO/Et_2O). Mp 197-200°. $[\alpha]_D^{24}$ -133.8 ($CHCl_3$).

8′-Hydroxy: [40785-64-6] ***8′-Hydroxyzearalenone***. *F-5-3*
$C_{18}H_{22}O_6$ 334.368
Cryst. ($MeOH/CHCl_3$). Mp 210-212° (198-199°). $[\alpha]_D^{24}$ -149.1 (c, 1 in Me_2CO). 8′-Config. unknown.

Epi-8′-hydroxy: [40785-65-7] ***8′-Epihydroxyzearalenone***. *F-5-4*
$C_{18}H_{22}O_6$ 334.368
Cryst. ($MeOH/CHCl_3$). Mp 172-174° (168-169°). $[\alpha]_D^{24}$ -53.1 (c, 1 in Me_2CO).

(*S,Z*)-*form* [36455-70-6] **cis-*Zearalenone***
Metab. of *Fusarium* spp..

4-Ac: [119975-33-6] ***4-Acetyl*-cis-*zearalenone***
$C_{20}H_{24}O_6$ 360.406
Metab. of *Fusarium graminearum*. λ_{max} 219 ; 253 ; 315 (MeOH).

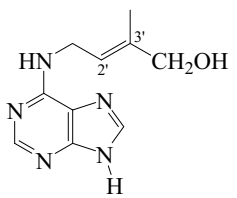
(±)-(*E*)-*form*
Prismatic needles ($MeNO_2$). Mp 188-190°.

[5975-78-0, 42011-78-9, 54933-67-4]

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **2**, 1315B (*nmr*)
Stob, M. *et al., Nature (London)*, 1962, **196**, 1318 (*isol*)
Urry, W.H. *et al., Tet. Lett.*, 1966, 3109-3114 (*uv, pmr, ms, struct*)
Taub, D. *et al., Tetrahedron*, 1968, **24**, 2443-2461 (*synth, resoln, abs config*)
Girotra, N.N. *et al., J.O.C.*, 1969, **34**, 3192-3194 (*synth*)
Bolliger, G. *et al., Helv. Chim. Acta*, 1972, **55**, 3030-3048 (*Gibberella zeae constits*)
Jackson, R.A. *et al., J. Agric. Food Chem.*, 1974, **22**, 1015-1019 (*ms*)
Mirocha, C.J. *et al., Mycotoxins*, Purchase, I.F.H. ed., Elsevier, 1974, 129 (*rev*)
Shipchandler, M.T. *et al., Heterocycles*, 1975, **3**, 471-520 (*rev, bibl*)
Ciegler, A. *et al., J. Nat. Prod.*, 1975, **38**, 21-35 (*rev*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2219-2284 (*rev, uv, ir, pmr, ms*)
Betina, V. *et al., Dev. Food Sci.*, 1984, **8**, 237-257 (*rev, anal, tox*)
Schoental, R. *et al., Adv. Cancer Res.*, 1985, **45**, 217-290 (*rev, props*)
Richardson, K.E. *et al., J. Agric. Food Chem.*, 1985, **33**, 862-866 (*Z-form, isol*)
Wilson, M.E. *et al., CA*, 1986, **104**, 223931 (*rev, metab*)
Rao, A.V.R. *et al., Tetrahedron*, 1987, **43**, 779-784 (*synth*)
Munoz, L. *et al., Phytochemistry*, 1989, **28**, 83-85 (*Fusarium graminearum constits*)
Cordier, C. *et al., Magn. Reson. Chem.*, 1990, **28**, 835-845 (*pmr, cmr, conformn*)
Plasencia, J. *et al., Appl. Environ. Microbiol.*, 1991, **57**, 146-150 (*4-sulfate*)
El-Sharkawy, S.H. *et al., Appl. Environ. Microbiol.*, 1991, **57**, 549-552 (*4-sulfate*)
Keinan, E. *et al., J.C.S. Perkin 1*, 1991, 3333-3339 (*synth, bibl*)
Solladié, G. *et al., J.O.C.*, 1991, **56**, 2317-2322 (*synth*)
Kalivretenos, A.G. *et al., J.O.C.*, 1991, **56**, 2883-2394 (*synth*)
Veldman, A. *et al., Food Addit. Contam.*, 1992, **9**, 647 (*occur*)
Hitchcock, S.A. *et al., J.C.S. Perkin 1*, 1992, 1323-1328 (*synth*)
Panneerselvam, K. *et al., Acta Cryst. C*, 1996, **52**, 3095-3097 (*cryst struct*)
Wang, Z.Q. *et al., Chin. Chem. Lett.*, 1997, **8**, 591-594 (*synth*)
Fuerstner, A. *et al., J.O.C.*, 2000, **65**, 7990-7905 (*synth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, New York, 1981, 902
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ZAT000

Zeatin Z-8

[13114-27-7]
*2-Methyl-4-(1*H*-purin-6-ylamino)-2-buten-1-ol, 9CI. 6-(4-Hydroxy-3-methyl-2-butenylamino)purine.* N^6*-(ω-Hydroxyisopentenyl)adenine*



(*E*)-*form*

$C_{10}H_{13}N_5O$ 219.246

(*E*)-*form* [1637-39-4]
Isol. from sweet corn (*Zea mays*) and numerous other plants. Sol. H_2O. Mp 212-213° (207-208°). λ_{max} 212 (ε 17050); 270 (ε 16150) (H_2O) (Berdy). λ_{max} 207 (ε 14500); 275 (ε 14650) (HCl) (Berdy). λ_{max} 220 (ε 15900); 276 (ε 14650) (NaOH) (Berdy).

▶ EM9506000

Picrate:
Mp 180-190°.

O-*β-D-Glucopyranoside:* [56329-06-7]
$C_{16}H_{23}N_5O_6$ 381.388
Cryst. (1-butanol). Mp 124-128°.

O-*Ac:*
Mp 168-169°.

*7-β-D-Glucopyranosyl (7*H*-form):* [38165-56-9] ***Raphanatin***
$C_{16}H_{23}N_5O_6$ 381.388
Prod. by *Raphanus sativus* (radish). Cryst. (MeOH). Mp 266-271° (dec.). $[\alpha]_D^{26}$ -14.8 (c, 3.5 in DMSO).

9-β-D-Glucopyranosyl: [51255-96-0]
$C_{16}H_{23}N_5O_6$ 381.388
λ_{max} 269 (no solvent reported).

9-β-D-Ribofuranosyl: [6025-53-2] ***9-(β-D-Ribofuranosyl)zeatin***. *Ribosylzeatin*
$C_{15}H_{21}N_5O_5$ 351.361
Isol. from many plants. Sol. H_2O. Mp 180-182°. λ_{max} 265 (ε 19200) (pH 1 H_2O) (Derep). λ_{max} 269 (ε 19400) (pH 13 H_2O) (Derep). λ_{max} 270 (ε 18400) (95% EtOH) (Derep). λ_{max} 270 (ε 18200) (MeOH) (Berdy). λ_{max} 270 (ε 8100) (EtOH) (Berdy). λ_{max} 265 (ε 19100) (pH 1 buffer) (Berdy).

9-β-D-Ribofuranosyl, 5′′-phosphate: [25615-16-1]

[15075-52-2] *Ribosylzeatin phosphate*
$C_{15}H_{22}N_5O_8P$ 431.341
Isol. from *Zea mays* (sweet corn). Solid.

9-β-D-Ribofuranosyl, O-*β-D-glucopyranoside:* [62512-97-4]
$C_{21}H_{31}N_5O_{10}$ 513.503
Cytokinin, widely distributed in plants. No phys. props. accessible.

9-β-D-Ribofuranosyl, O-*[α-L-arabinopyranosyl-(1→4)-[β-D-galactopyranosyl-(1→2)-α-D-galactopyranosyl-(1→3)-α-L-arabinofuranosyl-(1→3)]-β-D-galactopyranoside]:* [171628-14-1] ***Gazer***
$C_{43}H_{67}N_5O_{28}$ 1102.019
Constit. of coconut milk (*Cocos nucifera*). $[\alpha]_D^{25}$ -5.2 (c, 1 in H_2O). λ_{max} 210 (ε 16600); 267 (ε 18200) (H_2O).

9-(2-Deoxy-β-D-ribofuranosyl): [124325-91-3] ***Zeatin 2-deoxyribofuranoside***. *2′-Deoxyzeatin riboside*
$C_{15}H_{21}N_5O_4$ 335.362
Oil. $[\alpha]_D^{25}$ -13.5 (c, 0.35 in EtOH).

Deoxy: [2365-40-4] ***6-(3-Methyl-2-butenylamino)purine***. N^6*-Isopentenyladenine. 6-(γ,γ-Dimethylallylamino)purine*
$C_{10}H_{13}N_5$ 203.246
Fine yellow needles (as picrate). Mp 221-223° (picrate).

2-Hydroxy: [29736-32-1] ***2-Hydroxyzeatin***
$C_{10}H_{13}N_5O_2$ 235.245
Oil. Sol. H_2O. λ_{max} 270 (MeOH).

(*Z*)-*form* [32771-64-5] **cis-*Zeatin***
Mp 206-208°.

9-β-D-Glucopyranosyl: [169565-72-4] cis-*Zeatin 9-glucoside*
$C_{16}H_{23}N_5O_6$ 381.388
Isol. from *Solanum tuberosum* (potatoes).

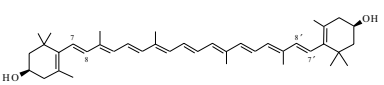
9-β-D-Ribofuranosyl: [15896-46-5]
Cryst. (EtOH). Mp 202-205°. λ_{max} 267 (ε 20280) (no solvent reported).

Shaw, G. *et al., J.C.S.(C)*, 1966, 921 (*synth, uv, ir*)
Letham, D.S. *et al., Life Sci.*, 1966, **5**, 1999-2004 (*isol, ribosylzeatin phosphate*)
Klambt, D. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1966, **56**, 52 (*isol, deriv*)

Helgeson, J.P. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1966, **56**, 60 (*deriv*)
Letham, D.S. *et al., Tetrahedron*, 1967, **23**, 479 (*ms, uv, pmr, struct*)
Hecht, S.M. *et al., Phytochemistry*, 1970, **9**, 1173-1180 (*2-Hydroxyzeatin*)
Playtis, A.J. *et al., Biochem. Biophys. Res. Commun.*, 1971, **45**, 1-5 (*synth, 9-ribosyl*)
Leonard, N.J. *et al., J.A.C.S.*, 1971, **93**, 3056 (*synth, uv, pmr, ms*)
Corse, J. *et al., Synthesis*, 1972, **11**, 618 (*synth, pmr*)
Fujii, T. *et al., Tet. Lett.*, 1972, 3074 (*synth*)
Parker, C.W. *et al., Biochem. Biophys. Res. Commun.*, 1973, **55**, 1370-1376 (*synth, 9-glucoside*)
Scarbrough, E. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1973, **70**, 3825 (*cis-Zeatin*)
Parker, C.W. *et al., Planta*, 1974, **115**, 337-344 (*isol, 9-glucosyl*)
Parker, C.W. *et al., Ann. Bot. (London)*, 1975, **39**, 375-376 (*O-glucoside*)
Letham, D.S. *et al., Ann. Bot. (London)*, 1976, **41**, 261-263 (*9-ribosyl O-glucoside*)
Mackenzie, G. *et al., J.C.S. Perkin 1*, 1976, 1446 (*synth*)
Wang, T.L. *et al., Planta*, 1977, **135**, 285; 1978, **140**, 151 (*glycosides*)
Cowley, D.E. *et al., Aust. J. Chem.*, 1978, **31**, 1095 (*Raphanatin*)
Duke, C.C. *et al., Aust. J. Chem.*, 1978, **31**, 1291-1301 (*glucopyranoside, isol, synth, uv, pmr*)
Chen, S.C. *et al., Agric. Biol. Chem.*, 1982, **46**, 2361 (*cmr*)
Corse, J. *et al., J. Plant Growth Regul.*, 1983, **2**, 47; *CA*, **100**, 34316 (*synth, resoln*)
Evidente, A. *et al., Phytochemistry*, 1989, **28**, 2603 (*2-deoxyribosyl*)
De Napoli, L. *et al., Phytochemistry*, 1990, **29**, 701 (*2-deoxyribosyl*)
Shadid, B. *et al., Tetrahedron*, 1990, **46**, 901-912 (*synth, ribosylzeatin phosphate*)
Evidente, A. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1937 (*synth, 2-deoxyribosyl*)
Nicander, B. *et al., Plant Physiol.*, 1995, **109**, 513 (*9-glucoside*)
Kobayashi, H. *et al., Chem. Pharm. Bull.*, 1997, **45**, 260 (*Gazer*)
Jordis, U. *et al., Org. Prep. Proced. Int.*, 1997, **29**, 549-560 (*synth, pmr*)

Zeaxanthin Z-9

β,β-Carotene-3,3′-diol. Anchovixanthin. Zeaxanthol



$C_{40}H_{56}O_2$ 568.881

(3*R*,3′*R*, *all-E*)-*form* [144-68-3]
Constit. of crustaceans, fish, barley, maize (*Zea mays*), tomatoes, paprika pods, hen egg yolk, fruits and numerous green vegetables. Potential nutriceutical for treatment of age-related macular degeneration of the eye (AMD). Yellow cryst. + ½MeOH (MeOH/C_6H_6). Mp 215.5°. $[\alpha]^{20}_{656.3}$ -44 (c, 0.2 in $CHCl_3$).

3-O-*[11-Methyldodecanoyl-(→6)-β-D-glucopyranoside]:* [165525-68-8] ***Thermozeaxanthin 13***
$C_{59}H_{90}O_8$ 927.355

3-O-*[13-Methyltetradecanoyl-(→6)-β-D-glucopyranoside]:* [165525-69-9] ***Thermozeaxanthin 15***
$C_{61}H_{94}O_8$ 955.409

3-O-*[15-Methylhexadecanoyl-(→6)-β-D-glucopyranoside]:* [165525-70-2] ***Thermozeaxanthin 17***
$C_{63}H_{98}O_8$ 983.462

3-O-*α-L-Rhamnopyanoside:* [55823-76-2] *Zeaxanthin monorhamnoside*
$C_{46}H_{66}O_6$ 715.024
Ppt. (MeOH/C_6H_6/petrol). Mp 149-150°. λ_{max} 428 ; 452 ; 480 (Me_2CO).

Di-O-*β-D-glucopyranoside:* [53762-00-8]
$C_{52}H_{76}O_{12}$ 893.165
λ_{max} 449 ; 477 (no solvent reported).

3,3′-Bis-O-*[11-methyldodecanoyl-(→6)-β-D-glucopyranoside]:* [165525-71-3] ***Thermozeaxanthin 13-13***
$C_{78}H_{124}O_{14}$ 1285.829

3-O-*[11-Methyldodecanoyl-(→6)-β-D-glucopyranoside], 3′*-O-*[13-methyltetradecanoyl-(→6)-β-D-glucopyranoside]:* [165525-72-4] ***Thermozeaxanthin 13-15***
$C_{80}H_{128}O_{14}$ 1313.883

3,3′-Bis[13-methyltetradecanoyl-(→6)-β-D-glucopyranoside]: [165525-73-5] ***Thermozeaxanthin 15-15***
$C_{82}H_{132}O_{14}$ 1341.936

Di-O-*α-L-rhamnopyranoside:* [55823-75-1] *Zeaxanthin dirhamnoside*
$C_{52}H_{76}O_{10}$ 861.166
Red needles. Mp 218-219°. λ_{max} 428 ; 452 ; 480 (Me_2CO).

Dihexadecanoyl: [144-67-2] ***Physalien***. *Zeaxanthin dipalmitate*
$C_{72}H_{116}O_4$ 1045.706
Constit. of *Physalis* spp., asparagus (*Asparagus officinalis*), beans and others. Red cryst. (C_6H_6/MeOH). Mp 98.5-99.5°. $[\alpha]_{Hg}$ -45 ($CHCl_3$).

Mono-Me ether: [54200-44-1] *3-Hydroxy-3′-methoxy-β-carotene. 3′-Methoxy-β,β-caroten-3-ol. Zeaxanthin monomethyl ether*
$C_{41}H_{58}O_2$ 582.908
Cryst. (MeOH). Mp 153°. Isol. not well documented.

Di-Me ether: [58526-52-6] *3,3′-Dimethoxy-β,β-carotene. Zeaxanthin dimethyl ether*
$C_{42}H_{60}O_2$ 596.935
Glistening dark red needles (C_6H_6). Mp 176°. Isol. not well documented λ_{max} 452 ; 480 (C_6H_{11}).

5,6-Epoxide: Antheraxanthin, A-356

5,6:5′,6′-Diepoxide: Violaxanthin, V-40

5,6-Dihydro, 5β,6α-dihydroxy: 5,6-Dihydro-β,β-carotene-3,3′,5,6-tetrol, D-224

(3*R*,3′*R*,9*Z*)-*form*

3-O-*α-L-Rhamnopyranoside:* [186525-05-3]
$C_{46}H_{66}O_6$ 715.024
λ_{max} 335 ; 446 ; 472 (no solvent reported).

Di-O-*α-L-rhamnopyranoside:* [186525-04-2]
$C_{52}H_{76}O_{10}$ 861.166
λ_{max} 442 ; 474 (no solvent reported).

(3*R*,3′*R*,13*Z*)-*form*

3-O-*α-L-Rhamnopyranoside:* [186525-06-4]
$C_{46}H_{66}O_6$ 715.024
λ_{max} 339 ; 444 ; 470 (no solvent reported).

(3*R*,3′*R*,15*Z*)-*form*

3-O-*α-L-Rhamnopyranoside:* [186525-07-5]
$C_{46}H_{66}O_6$ 715.024
λ_{max} 337 ; 448 ; 472 (no solvent reported).

(3*S*,3′*S*,*all-E*)-*form* [72002-36-9]
Isol. from various fishes, including *Paratya compressa compressa* (shrimp) and *Theragra chalcogramma* (pollack). Mp 209-209.5°.

(3*RS*,3′*SR*,*all-E*)-*form* [31272-50-1] *meso-form*
Constit. of shrimp *Paratya compressa compressa* and many fish. Mp 212-213°.

(3ξ,3′ξ,all-*E*)-*form*

7′,8′-Dihydro: [62994-48-3] *7′,8′-Dihydro-β,β-carotene-3,3′-diol.* ***Parasiloxanthin***
$C_{40}H_{58}O_2$ 570.897
Isol. from skin and fin of Japanese catfish (*Parasilurus asotus*). Orange-yellow needles. Mp 202°. Abs. config. not certain.

7,7′,8,8′-Tetrahydro: [62994-71-2] *7,7′,8,8′-Tetrahydro-β,β-carotene-3,3′-diol.* ***7,8-Dihydroparasiloxanthin***
$C_{40}H_{60}O_2$ 572.913
Constit. of skin and fin of Japanese catfish (*Parasilurus asotus*). Orange-yellow cryst. Mp 197°.

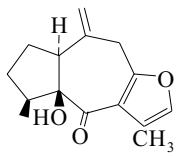
[7756-97-0]

Curl, A.L. *et al., J. Food Sci.*, 1961, **26**, 106-111 (*isol*)
Cholnoky, L. *et al., J.C.S.(C)*, 1969, 1256-1263 (*struct*)
Loeber, D.E. *et al., J.C.S.(C)*, 1971, 404-408 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, nos. 1839; 1840 (*occur*)
McDermott, J.C.B. *et al., Biochem. J.*, 1973, **134**, 1115-1117 (*biosynth*)
Nybraaten, G. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 584-586; 1219-1224 (*isol, rhamnosides, Me ethers*)
Buchecker, R. *et al., Helv. Chim. Acta*, 1974, **57**, 631-656 (*di-Me ether*)
Hlubucek, J.R. *et al., J.C.S. Perkin 1*, 1974, 848-852 (*abs config*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367-2390 (*cmr*)
Hertzberg, S. *et al., Arch. Microbiol.*, 1976, **110**, 95-99 (*abs config, rhamnosides*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97-102 (*cmr*)
Weedon, B.C.L. *et al., Pure Appl. Chem.*, 1976, **47**, 161-171 (*synth*)
Matsuno, T. *et al., Tet. Lett.*, 1976, 4601-4604 (*Parasiloxanthin, Dihydroparasiloxanthin*)
Britton, G. *et al., Chem. Comm.*, 1977, 655-656 (*biosynth*)
Rüttimann, A. *et al., Helv. Chim. Acta*, 1980, **63**, 1456-1462 (*3S,3′S-form, 3R,3′S-form, synth, pmr, cd*)
Widmer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 944-957; 958-967 (*synth*)
Rüttimann, A. *et al., J. High Resol. Chromatogr.*, 1983, **6**, 612-616 (*chiral hplc*)
Maoka, T. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1986, **83**, 121-124 (*stereoisomers, occur*)
Parkes, K.E.B. *et al., Tet. Lett.*, 1986, **27**, 2535-2538 (*epoxide, isol*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 119; 123 (*bibl*)
Widmer, E. *et al., Helv. Chim. Acta*, 1990, **73**, 861-867 (*synth*)
Soukup, M. *et al., Helv. Chim. Acta*, 1990, **73**, 868-873 (*synth*)

Palermo, J.A. *et al., Phytochemistry*, 1991, **30**, 2983-2986 (*isol, pmr, cmr*)
Yokoyama, A. *et al., Tet. Lett.*, 1995, **36**, 4901-4904 (*Thermozeaxanthins*)
Sliwka, H.-R. *et al., Acta Chem. Scand.*, 1996, **50**, 637-639 (*synth*)
Kull, D.R. *et al., J. Nat. Prod.*, 1997, **60**, 371-374 (*glycosides*)
Eisenreich, W. *et al., J.O.C.*, 2002, **67**, 871-875 (*biosynth*)
Humphries, J.M. *et al., J. Agric. Food Chem.*, 2003, **51**, 1322-1327 (*occur, zeaxanthin*)

Zedoarol Z-10

[103994-22-5]



$C_{15}H_{18}O_3$ 246.305
Constit. of *Curcuma zedoaria* (zedoary). Oil. $[\alpha]_D^{28}$ +11.6 (c, 2.0 in $CHCl_3$).

Shiobara, Y. *et al., Phytochemistry*, 1986, **25**, 1351-1353

Zein Z-11

[9010-66-6]

17-aminoacid peptide belonging to the prolamine class, deficient in lysine and tryptophan. Component of corn gluten (*Zea mays*). Obt. comly. by extraction of corn gluten with alkaline aq. 2-propanol. Moisture control agent. Used in edible coatings for nuts and other foods and as a binder in confectionery glazes. GRAS approved. Powder. Insol, H_2O, sol. alcohols, glycols.

Ger. Pat., 1971, 2 002 337; *CA*, **75**, 117 341b (*manuf*)
Peterson, M.S. *et al., Encycl. Food Technol. Food Sci. Ser.*, 1978, **3**, 881-884 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2984-2985 (*props, use, manuf*)

Zinc acetate, USAN Z-12

[557-34-6]
E650

$Zn(OAc)_2$

$C_4H_6O_4Zn$ 183.479

Two cryst. forms. α: distorted ZnO_4 tetrahedra; 3D-network with $OAc^{\ominus}$ groups linking two ZnO_4 tetrahedra. β: 2D polymeric sheet of ZnO_4 tetrahedra connected by AcO bridges in a *syn-anti* arrangement. Nutrient supplement. Sol. H_2O; org. solvs. except EtOH. Mp 242°. Subl.150 200. Dec. at 180° to $Zn_4O(OAc)_6$.

► AK1500000

Dihydrate: [5970-45-6]
Cryst. (AcOH aq.).

► Eye and skin irritant. LD_{50} (rat, orl) 2170 mg/kg. ZG8750000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1275C (*ir*)
Duval, C. *et al., Ann. Phys. (Leipzig)*, 1942, **17**, 5 (*uv*)
McCrone, W.C. *et al., Anal. Chem.*, 1949, **21**, 645 (*powder struct, dihydrate*)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 980 (*rev, bibl*)
Ananthanarayanan, V. *et al., Proc. Indian Acad. Sci., Sect. A*, 1962, **50**, 188 (*Raman, dihydrate*)
McAdie, H.G. *et al., J. Inorg. Nucl. Chem.*, 1966, **28**, 2801 (*thermal anal, dihydrate*)
Djega-Mariadassou, G. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1967, **264**, 1753 (*synth, ir, β-form, powder struct*)
Valero Capilla, A. *et al., Cryst. Struct. Commun.*, 1979, **8**, 795 (*cryst struct*)
Panevchik, V.V. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1981, **26**, 1373 (*powder struct*)
Baraldi, P. *et al., Spectrochim. Acta A*, 1981, **37**, 89 (*ir, salt and dihydrate*)
Johnson, M.K. *et al., Spectrochim. Acta A*, 1981, **37**, 899 (*Raman, ir, salt and dihydrate*)
Brewer, G.J. *et al., Ann. Intern. Med.*, 1983, **99**, 314 (*use*)
Marshall, G.L. *et al., Org. Mass Spectrom.*, 1983, **18**, 168 (*ms*)
Caminiti, R. *et al., J. Chem. Phys.*, 1984, **81**, 543 (*cmr, soln struct*)
Clegg, W. *et al., Acta Cryst. C*, 1986, **42**, 1701 (*cryst struct*)
Kunwar, A.C. *et al., J. Magn. Reson.*, 1986, **69**, 124 (*Zn-67 nmr*)
Meier, B.H. *et al., J.A.C.S.*, 1987, **109**, 7937 (*cmr*)
Prozarovskaya, Z.N. *et al., Koord. Khim.*, 1988, **14**, 435 (*ir, pmr, dihydrate*)
Tackett, J.E. *et al., Appl. Spectrosc.*, 1989, **43**, 483 (*ir, Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1428
Brewer, G.J. *et al., J. Lab. Clin. Med.*, 1994, **123**, 849 (*use*)
Ishioka, T. *et al., Acta Cryst. C*, 1997, **53**, 1029-1031 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2986
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ZBS000; ZCA000

Zinc carbonate ($ZnCO_3$) Z-13

[3486-35-9]

$ZnCO_3$

CO_3Zn 125.399

Calcite struct.. Nutrient supplement. Rhombohedral colourless cryst. Pract. insol. H_2O (5.7×10^{-5} g per 100 cm^3). Dec. at 140°. Forms a basic salt on boiling in H_2O.

► FG3375000

Mineral-*form* [14476-25-6]
Smithsonite
Trigonal cryst., rarely colourless, ranges from bright apple green to deep pink purple.

Hüttig, G.F. *et al., Monatsh. Chem.*, 1939, **72**, 31
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 973
Graf, D.L. *et al., Am. Mineral.*, 1961, **46**, 1283 (*powder struct*)
Kirk-Othmer Encycl. Chem. Technol., 2nd edn., Wiley, 1963, **22**, 604
Cibor, E. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1964, **38**, 1715 (*synth, powder struct*)
Donogline, M. *et al., Spectrochim. Acta A*, 1971, **27**, 1065 (*ir*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 1035 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2986-2987
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ZEJ050

Zinc chloride, JAN, USAN Z-14

[7646-85-7]
Zinctrace

$ZnCl_2$

Cl_2Zn 136.295

Orthorhombic form comprises hcp Cl layers in which Zn occupy some tetrahedral holes. 3 other different cryst. forms (α, β and γ) may contain H_2O. α, β and γ have pseudo close-packed Cl with Zn in tetrahedral sites. In α- and γ-forms, anion layers have a cubic sequence, in β a four layer sequence is present. Linear in gas phase. Structure in molten phase (350-580°) with increase in temp.: Zn-Cl (1st), almost no increase; Cl-Cl (1st shell), increase in width; Zn-Zn (1st shell), decrease in width; order of underlying tetrahedra diminished at 580°. Nutrient supplement. Colourless, hygroscopic cryst. Sol. MeOH, EtOH, Et_2O, Me_2O; v. sol. H_2O (= 367 g per 100 cm^3 at 20°). Mp 290° Mp 300° Mp 318°. Bp 732°. Molten-form: viscosity much large, than many glass-forming compds; can be supercooled into glass by normal methods, with persistance of tetrahedral coord. to well above Mp; model system for studying tetrahedral-network (e.g. SiO_2) glass systems.

► OES: long-term 1 mg m^{-3} (fume); short-term 2 mg m^{-3} (fume). Eye, skin and mucous membrane irritant, can cause pulmonary oedema at high concs. (as fume). ZH1400000

[24359-56-6]

Bruner, H.D. *et al., Fed. Proc.*, 1950, **9**, 260 (*tox*)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 847
Brehler, B. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1961, **115**, 373 (*cryst forms*)
Kiser, R.W. *et al., Adv. Chem. Ser.*, 1968, **72**, 153 (*ms*)
Angell, C.A. *et al., J. Chem. Phys.*, 1969, **51**, 4519 (*ir, solid, glass, melt*)
Beattie, I.R. *et al., J.C.S.(A)*, 1970, 2433 (*Raman, gas phase*)
Selivanov, G.K. *et al., Vestn. Mosk. Univ., Ser. 2: Khim.*, 1972, **13**, 712 (*far ir*)
Holinski, R. *et al., Z. Anorg. Allg. Chem.*, 1974, **406**, 69 (*soln ir*)
Brauer, G. *et al., Handbuch Pr&cap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 1023 (*synth*)
Maciel, G.E. *et al., J. Phys. Chem.*, 1977, **81**, 263 (*soln Zn-67 nmr*)
Loewenschuss, A. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1978, **82**, 69 (*matrix Raman*)
Brynestad, J. *et al., Inorg. Chem.*, 1978, **17**, 1376 (*cryst struct*)
Yakel, H.L. *et al., Inorg. Chem.*, 1978, **17**, 3294 (*cryst struct*)
Fontana, M.P. *et al., J. Chem. Phys.*, 1978, **69**, 676 (*soln Raman*)
James, D.W. *et al., J. Raman Spectrosc.*, 1978, **7**, 70 (*phase trans, Raman*)

Givan, A. *et al., J. Chem. Phys.*, 1980, **72**, 3809 (*ir, Raman, matrix*)
Bastow, T.J. *et al., J. Magn. Reson.*, 1980, **37**, 269 (*Cl-35 nqr*)
Aliotta, F. *et al., J. Chem. Phys.*, 1981, **75**, 613 (*Raman, melt, glass*)
Biggin, S. *et al., J. Phys. C: Solid State Phys.*, 1981, **14**, 3129 (*nd, melt*)
Palinkas, G. *et al., Z. Naturforsch., A*, 1981, **36**, 1367 (*soln struct*)
Desa, J.A.E. *et al., J. Non-Cryst. Solids*, 1982, **51**, 57 (*nd, glass*)
Bristow, D.J. *et al., Chem. Phys.*, 1983, **75**, 213 (*pe*)
Hargittai, M. *et al., Inorg. Chem.*, 1986, **25**, 3163 (*ed*)
Drier, P. *et al., J. Phys., Colloq.*, 1986, **C8**, 809 (*soln, exafs*)
Staples, B.R. *et al., NBS Spec. Publ. (U.S.)*, 1986, 718 (*soln, props*)
Rankin, P.W. *et al., J. Biol. Chem.*, 1989, **264**, 4312 (*activity*)
Yamaguchi, T. *et al., J. Phys. Chem.*, 1989, **93**, 2620 (*ed, Raman, hydrates*)
Dake, L.S. *et al., SIA, Surf. Interface Anal.*, 1989, **14**, 71 (*Auger*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1064
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2987-2988
Neuefeind, J. *et al., J. Non-Cryst. Solids*, 1998, **224**, 205-215 (*nd, photon diffraction, struct*)
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 591
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1330
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ZFA000; ZFJ000
Beliles, R.P. *et al., Patty's Ind. Hyg. Toxicol.*, 4th edn., Vol. 2, Wiley, 1993, 2332 (*tox, rev*)

Zinc dithionite Z-15

[7779-86-4]

Zinc hyposulfite

$Zn(S_2O_4)$

O_4S_2Zn 193.52

Food contaminant arising from its use as a packaging additive. White powder. Sol. H_2O.

▶ JP2105000

Ladhabhoy, M.E. *et al., Indian Chem. J.*, 1970, **5**, 22 (*rev, manuf*)
Brauer, G. *et al., Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 395 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **3**, 946; **22**, 137; 155; **24**, 811 (*props, use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2988

Zinc oxide, JAN, USAN Z-16

[1314-13-2]

Zinc white. Philosopher's wool

ZnO

OZn 81.389

2 Cryst. forms; wurtzite struct. at low temps., zinc blende struct. at higher temps.. Nutrient supplement. Hexagonal white cryst.; yellow above 25°. Spar. sol. H_2O (1.6×10^{-4} g per 100 cm^3 at 29°); sol. dil. AcOH, mineral acids, NH_3. Mp 1975°. Subl. 1720 (normal pressure). Component of Wyanoids and Ziradryl. K_{sp} 2.2×10^{-17} at 25°.

▶ OES: long-term 5 mg m^{-3} (fume); short-term 10 mg m^{-3} (fume). Occupational exposure to fume causes influenza-like illness ('metal fume fever'). Skin and eye irritant. ZH4810000

Mineral-*form* [20431-17-8]

Zincite

Deep yellow to dark red trigonal cryst.

Palache, *et al., Dana's System of Mineralogy*, 7th ed., 1944, **1**, 504 (*mineral*)
U.S. Pat., 1945, 2 372 367, (*American Zinc, Lead and Smelting*); *CA*, **39**, 3405[7] (*purifn*)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 772 (*bibl*)
Abrahams, S.C. *et al., Acta Cryst. B*, 1969, **25**, 1233 (*cryst struct*)
Sabine, T.M. *et al., Acta Cryst. B*, 1969, **25**, 2254 (*nd*)
Shalimova, K.V. *et al., Kristallografiya*, 1972, **17**, 541 (*struct*)
Industrial Chemicals, (Eds. Lowenheim, F.A. *et al*), 4th Ed., Wiley-Interscience, N.Y., 1975, 882 (*synth*)
Mead, D.G. *et al., J. Raman Spectrosc.*, 1977, **6**, 123 (*Raman*)
Lloyd, T.B. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **24**, 854 (*rev*)
Schultz, H. *et al., Solid State Commun.*, 1979, **32**, 783 (*cryst struct*)
Littbarski, R. *et al., Curr. Top. Mater. Sci.*, 1981, **7**, 212 (*elect props*)
Kolb, D.M. *et al., Curr. Top. Mater. Sci.*, 1981, **7**, 226 (*optical props*)
McMurdie, H.F. *et al., Powder Diffr.*, 1986, **1**, 64 (*powder struct*)
Wriedt, H.A. *et al., Bull. Alloy Phase Diagrams*, 1987, **8**, 166 (*struct, props*)
Islam, M.N. *et al., J. Mater. Sci.*, 1987, **22**, 1379 (*elect props, optical props*)
Hussain, G. *et al., Can. J. Spectrosc.*, 1988, **33**, 138 (*ir*)
Andres-Vierges, M. *et al., J. Mater. Sci. Lett.*, 1988, **7**, 970 (*ir, powder struct*)
Bastow, T.J. *et al., Phys. Status Solidi B*, 1988, **145**, 719 (*Zn-67 nmr, O-17 nmr*)
Drapak, T.T. *et al., Izv. Vyssh. Uchebn. Zaved., Fiz.*, 1989, **32**, 101 (*luminescence*)
Ruskov, T. *et al., Nucl. Instrum. Methods Phys. Res.*, Sect. B, 1989, **36**, 82 (*Mössbauer*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 771
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **8**, 5573-5574 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2991
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 592
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1332
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ZKA000
Beliles, *et al., Patty's Ind. Hyg. Toxicol.*, 4th edn., Vol. 2, Wiley, 1993, 2332 (*tox, rev*)

Zinc sulfate, JAN, USAN Z-17

[7733-02-0]

Zincosite. Verazinc. Zincate. Zincomed

$ZnSO_4$

O_4SZn 161.454

α-Form (r.t.) contains edge-sharing ZnO_6 octahedra; β-form (high temps.) has zinc blende struct., transition temp. 700°. Used as a malting/fermenting aid and as a nutrient supplement. Colourless cryst. V. sol. H_2O; sl. sol. EtOH; sol. MeOH. Stable to 850° in presence of SO_3; otherwise dec. to ZnO at *ca.* 680°. Component of Phenylzin and Zincfrin.

▶ Eye irritant. ZH5260000

Monohydrate: [7446-19-7]
Cryst. (H_2O at 60-100°). Dehydrates at 225-235°.

Hexahydrate: [13986-24-8]
Monoclinic cryst. (H_2O at 39-60°). Dehydrates to monohydrate.

Heptahydrate: [7446-20-0]
Orthorhombic cryst. (H_2O at 0-39°). Insol. EtOH. Mp 100°. Dehydrates to hexahydrate at *ca.* 40°. Dec. > 500°.

▶ ZH5300000

[80867-26-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1262A (*ir*)
Lautie, R. *et al., Bull. Soc. Chim. Fr.*, 1947, 508 (*synth*)
Gmelin Handbook Inorg. Chem., Syst. No. 32, 1956, 936 (*rev, bibl*)
Kokkoros, P.A. *et al., Acta Cryst.*, 1958, **11**, 361 (*cryst struct, hexahydrate, α-form*)
Pistorius, C.W.F.-T. *et al., Acta Cryst.*, 1961, **14**, 534 (*struct, monohydrate*)
Steger, E. *et al., Ber. Bunsen-Ges. Phys. Chem.*, 1964, **68**, 102 (*ir, solid*)
Le Fur, Y. *et al., C. R. Hebd. Seances Acad. Sci. Ser. C*, 1966, **262**, 632 (*powder struct, monohydrate*)
Ben-Dor, L. *et al., Inorg. Chim. Acta*, 1967, **1**, 49 (*ir, thermal anal, monohydrate*)
Shokarev, M.M. *et al., Zh. Strukt. Khim.*, 1970, **11**, 151 (*ir*)
Chan, F.L. *et al., Dev. Appl. Spectrosc.*, 1971, **9**, 319 (*powder struct, heptahydrate*)
Michaelsson, G. *et al., Arch. Dermatol.*, 1977, **113**, 31 (*use*)
Tayal, V.P. *et al., Chem. Phys. Lett.*, 1978, **55**, 136 (*ir, monohydrate*)
Spiess, M. *et al., Naturwissenschaften*, 1978, **65**, 594 (*cryst struct, high-temp form*)
Spiess, M. *et al., Z. Anorg. Allg. Chem.*, 1979, **456**, 222 (*dehydration of hydrates*)
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Zosterine, 9CI Z-18

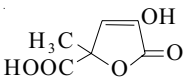
[11113-95-4]

Pectic polysaccharide, mol. wt. *ca*. 40000-45000. Contains galacturonan, apiogalacturonan and heteroglycanogalacturonan, interlinked by residues of galacturonic acid and rhamnose.$[\alpha]_D^{20}$ +230 (c, 0.5 in H_2O).

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Zymonic acid Z-19

[24891-71-2]
2,5-Dihydro-4-hydroxy-2-methyl-5-oxo-2-furancarboxylic acid, 9CI



$C_6H_6O_5$ 158.11
Used as a flavour constit. for confectionery and tobacco. Unstable, resinifying and evolving CO_2 at room temp..

Me ether:2,5-Dihydro-4-methoxy-2-methyl-5-oxo-2-furancarboxylic acid
$C_7H_8O_5$ 172.137
Cryst. + $1H_2O$. Mp 86-90°.

Me ether, Me ester: [15023-85-5]
$C_8H_{10}O_5$ 186.164
Yellow oil. Sol. Et_2O. Bp_1 118-123° ($Bp_{0.05}$ 125-127°). $[\alpha]_D^{27}$ +1.2.

Me ether, amide:
$C_7H_9NO_4$ 171.152
Cryst. (Me_2CO/petrol). Mp 209-210°.

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1,2-Dihydro-1,1,6-trimethylnaphthalene, D-362
2,3-Dihydro-1,2,3-trihydroxy-4-(4-hydroxyphenyl)-1*H*-phenalene, D-279
12,13-Dihydro-1,2-dimethoxy-12-methyl[1,3]benzodioxolo[5,6-*c*]phenanthridine-13-acetaldehyde, D-225
12,13-Dihydro-1,2-dimethoxy-12-methyl[1,3]benzodioxolo[5,6-*c*]phenanthridine-13-methanol, B-165
3,7-Dihydro-1,3,7-trimethyl-1*H*-purine-2,6-dione, C-18
3,7-Dihydro-1,3-dimethyl-1*H*-purine-2,6-dione, T-344
6*a*,13*a*-Dihydro-1,3-dioxolo[6,7][1]benzopyrano[3,4-*b*]furo[3,2-*g*][1]benzopyran-13(6*H*)-one, D-1032
5,7*a*-Dihydro-1,4,4,7*a*-tetramethyl-4*H*-indene, D-356
2,3-Dihydro-1,4-dimethyl-6(1*H*)-azulenone, T-808
6,7-Dihydro-1,5,8-trimethylnaphtho[2,1-*b*]-furan, P-609
7,8-Dihydro-1,5,8-trimethylnaphtho[2,1-*b*]furan-9(6*H*)-one, C-407
1,2-Dihydro-1,6-dimethyl-4-(1-methylethyl)-naphthalene, C-32
5,6-Dihydro-1-(3,4,5-trimethoxycinnamoyl)-2(1*H*)-pyridinone, P-405
4,5-Dihydro-1-benzoxepin-3(2*H*)-one, D-223
1,2-Dihydro-1-isopropyl-4,7-dimethylnaphthalene, C-31
3,4-Dihydro-1-methyl-β-carboline, D-293
4,9-Dihydro-1-methyl-3*H*-pyrido[3,4-*b*]indol-7-ol, H-9
4,9-Dihydro-1-methyl-3*H*-pyrido[3,4-*b*]indole, D-293

N-(4,5-Dihydro-1-methyl-4-oxo-1*H*-imidazol-2-yl)alanine, D-310
2,3-Dihydro-1-phenyl-1*H*-pyrrole, D-349
5,6-Dihydro-1-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-propenyl]-2(1*H*)-pyridinone, P-405
11′,12′-Dihydro-10′-apo-β-carotene-3,10′-diol, M-720
11′,12′-Dihydro-10′-apo-ϵ-carotene-3,10′-diol, M-720
6*a*,11*a*-Dihydro-10-(3-methyl-1-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-1,3,9-triol, T-695
6*a*,11*a*-Dihydro-10-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,9-diol, D-672
2,3-Dihydro-10-hydroxy-3,3-dimethyl-1*H*,7*H*-furo[2,3-*c*:5,4-*f*′]bis[1]benzopyran-7-one, S-150
7,8-Dihydro-11,12-dimethoxykawain, D-631
14,19-Dihydro-11-methoxycondylocarpine, T-847
5,6-Dihydro-11-methoxyyangonin, D-631
14,19-Dihydro-12,13-dihydroxy-20-norcrotalanan-11,15-dione, M-741
11-Dihydro-12-norneoquassin, N-56
6*a*,13*a*-Dihydro-13*a*-hydroxy-2,3-dimethoxy[1]-benzopyrano[3,4-*b*]furo[3,2-*g*][1]benzopyran-13(6*H*)-one, H-447
14,15-Dihydro-14,15-dihydroxygeranyllinalol, P-363
16,17-Dihydro-17-hydroxygibberellin A_4, G-103
2,3-Dihydro-1*H*-pyrrole, D-349
1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-1,4-pentanedione, D-353
1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-1-butanone, D-352
1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-2-propen-1-one, D-354
2,3-Dihydro-1*H*-pyrrolizine-5-carboxaldehyde, D-351
7,9-Dihydro-1*H*-purine-2,6,8(3*H*)-trione, U-34
3,7-Dihydro-1*H*-purine-2,6-dione, X-2
7,9-Dihydro-1*H*-purine-6,8-dione, P-584
1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-1-propanone, D-346
1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)-3-hydroxy-1-propanone, D-280
1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)ethanone, A-45
3,4-Dihydro-2′,2′-dimethyl-8-(3-methyl-2-butenyl)-[3,6′-bi-2*H*-1-benzopyran]-5,7′-diol, P-460
Dihydro-2(3*H*)-furanone, D-253
Dihydro-2(3*H*)-thiophenone, D-358
2,3-Dihydro-2,2,3-trimethyl-5-(1-propenyl)benzofuran, A-338
1,2-Dihydro-2,2,4-trimethyl-6-quinolinol, D-364
3,4-Dihydro-2,2,5,7,8-pentamethyl-2*H*-1-benzopyran-6-ol, D-340
6*a*,11*a*-Dihydro-2,2-dimethyl-2*H*,6*H*-benzofuro[3,2-*c*]pyrano[2,3-*h*][1]benzopyran-9-ol, S-98
2,3-Dihydro-2,2-dimethyl-3,7-benzofurandiol 7-(methylcarbamate), C-89
2,6-Dihydro-2,2-dimethyl-5*H*-pyrano[3,2-*c*]quinolin-5-one, F-47
2,3-Dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate, C-89
3,4-Dihydro-2,2-dimethyl[3,6′-bi-2*H*-1-benzopyran]-5′,7-diol, P-242
6*a*,11*a*-Dihydro-2,3,9-trimethoxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-4-ol, T-286
2,3-Dihydro-2,3-dihydroxy-4-(4-hydroxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-4-(4-methoxyphenyl)-1*H*-phenalen-1-one, D-279
5,8-Dihydro-2,3-dihydroxy-6-methyl-4-(1-methylethyl)-5,8-dioxo-1-naphthalenecarboxaldehyde, H-24
2,3-Dihydro-2,3-dihydroxy-9-(4-hydroxy-3-methoxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-9-phenyl-1*H*-phenalen-1-one, D-279
6,7-Dihydro-2,3-dimethyl-5*H*-cyclopentapyrazine, D-241
4,5-Dihydro-2,3-dimethylthiazolium(1+), D-322
4,5-Dihydro-2,4(5)-dimethyl-1*H*-imidazole, D-245
2,5-Dihydro-2,4,5-trimethyloxazole, D-363
2,5-Dihydro-2,4,5-trimethylthiazole, D-365
2,3-Dihydro-2,4,6-trimethyl-3-oxo-1*H*-indene-5-acetic acid, P-567
Dihydro-2,4,6-trimethyl-4*H*-1,3,5-dithiazine, D-361
Dihydro-2,4-dimethyl-6-(1-methylethyl)-4*H*-1,3,5-dithiazine, D-106
2,5-Dihydro-2,4-dimethyloxazole, D-248
2,5-Dihydro-2,4-dimethylthiazole, D-252
3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2*H*-1-benzopyran-6-ol, T-415
3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, T-406
2,3-Dihydro-2,5,7-trihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-187
2,3-Dihydro-2,5,8-trihydroxy-6-methoxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, F-58
3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-4*H*-1-benzopyran-6-ol, T-416
3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, T-407
6,7-Dihydro-2,5-dimethyl-5*H*-cyclopentapyrazine, D-242
9,10-Dihydro-2,6-dimethoxy-4,5-phenanthrenediol, P-248
6,7-Dihydro-2,6-dimethyl-5*H*-cyclopentapyrazine, D-243
3,4-Dihydro-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, T-409
3,4-Dihydro-2,8-bis(4-hydroxyphenyl)-8,14-methano-2*H*,14*H*-1-benzopyrano-[7,8-*d*][1,3]benzodioxocin-3,5,11,13,15-pentol, T-200
3,4-Dihydro-2,8-dimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2*H*-1-benzopyran-6-ol, T-417
3,4-Dihydro-2,8-dimethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol, T-408
2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, D-270
1,2-Dihydro-2-(1-methylethenyl)-6*H*-benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-6*a*,9(11*aH*)-diol, G-234
3,4-Dihydro-2-(3,4,5-trihydroxyphenyl)-2*H*-1-benzopyran-3,4,5,7-tetrol, H-85
3,4-Dihydro-2-(3,4,5-trihydroxyphenyl)-2*H*-1-benzopyran-3,5,7-triol, H-198
3,4-Dihydro-2-(3,4,5-trihydroxyphenyl)-2*H*-1-benzopyran-7-ol, T-183
2,3-Dihydro-2-(3,4-dihydroxyphenyl)-7-hydroxy-3-methyl-5-(1-propenyl)benzofuran, E-64
2,3-Dihydro-2-(3,4-methylenedioxy)-3-methyl-5-(1-propenyl)benzofuran, D-616
6*a*,11*a*-Dihydro-2-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]-benzopyran-1,3,9-triol, T-694
6*a*,11*a*-Dihydro-2-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,9-diol, D-670
3,4-Dihydro-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2*H*-1-benzopyran-6-ol, D-366
2,3-Dihydro-2-(4-hydroxy-3-methoxyphenyl)-3-methyl-5-(1-propenyl)benzofuran, D-616
3,4-Dihydro-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-3,4,7-triol, T-182
3,4-Dihydro-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-3,4-diol, T-565
3,4-Dihydro-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-3,5,7-triol, T-184
3,4-Dihydro-2-(4-hydroxyphenyl)-2*H*-1-benzopyran-5,7-diol, T-566
2,3-Dihydro-2-(hydroxymethyl)-6-methyl-4*H*-pyran-4-one, D-272
4,9-Dihydro-2-(methylsulfinyl)-1,3-thiazino[6,5-*b*]indole, C-434
1-[4,9-Dihydro-2-(methylthio)-1,3-thiazino[6,5-*b*]indol-4-yl]-2-propanone, D-332
4,9-Dihydro-2-(methylthio)-1,3-thiazino[6,5-*b*]indole, C-434
2,3-Dihydro-2-hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1*H*-inden-1-one, P-568
Dihydro-2-methoxy-2-methyl-3(2*H*)-thiophenone, D-290
3,4-Dihydro-2-methyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2*H*-1-benzopyran-6-ol, D-333
Dihydro-2-methyl-3(2*H*)-furanone, D-298
Dihydro-2-methyl-3(2*H*)-furanthione, D-302
Dihydro-2-methyl-3(2*H*)-thiophenone, D-330
4,5-Dihydro-2-methyl-3-furanthiol, D-302
S-(4,5-Dihydro-2-methyl-3-furanyl) ethanethioate, D-302
4,5-Dihydro-2-methyl-3-thiophenethiol, D-328
6,7-Dihydro-2-methyl-5*H*-cyclopenta[*b*]pyrazine, D-294
4,5-Dihydro-2-methylthiazole, D-322
5,7-Dihydro-2-methylthieno[3,4-*d*]pyrimidine, D-324
2,3-Dihydro-2-methylthiophene, D-325
1,2-Dihydro-2-octadecyl-3*H*-indol-3-one, H-649
2,3-Dihydro-2-oxo-1*H*-indole-3-acetic acid, D-339
3,4-Dihydro-2-phenyl-2*H*-1-benzopyran-5,7-diol, D-469
1-(4,5-Dihydro-2-thiazolyl)ethanone, A-47
1-[2,3-Dihydro-2-[1-(hydroxymethyl)ethenyl]-5-benzofuranyl]ethanone, B-159
3,4-Dihydro-2*H*-1-benzopyran-2-one, D-222
3,4-Dihydro-2*H*-pyran-2-one, D-348
3,4-Dihydro-2*H*-pyrrole, D-350
1-(3,4-Dihydro-2*H*-1,4-thiazin-5-yl)ethanone, A-46
1-(3,4-Dihydro-2*H*-pyrrol-5-yl)-1-propanone, D-345
1-(3,4-Dihydro-2*H*-pyrrol-5-yl)ethanone, A-44
3-(3,4-Dihydro-2*H*-pyrrol-5-yl)pyridine, M-832
Dihydro-3(2*H*)-thiophenone, D-359
3,11-Dihydro-3,3,5-trimethylpyrano[3,2-*a*]carbazol-8-ol, K-41
3,11-Dihydro-3,3,5-trimethylpyrano[3,2-*a*]carbazole, G-130
6*b*,12*b*-Dihydro-3,3-dimethyl-3*H*,7*H*-furo[3,2-*c*:5,4-*f*]bis[1]benzopyran-10-ol, P-241
3,11-Dihydro-3,3-dimethylpyrano[3,2-*a*]carbazole-5-carboxaldehyde, M-814
6*a*,11*a*-Dihydro-3,4,9-trimethoxy-6*H*-benzofuro[3,2-*c*][1]benzopyran, T-730
4,5-Dihydro-3,4-bis(3,4,5-trihydroxybenzyl)-2(3*H*)-furanone, H-216
Dihydro-3,4-bis(3-hydroxyphenyl)methyl-2(3*H*)-furanone, E-48
Dihydro-3,4-bis[(4-hydroxy-3-methoxyphenyl)-methyl]-2(3*H*)-furanone, M-81
7,8-Dihydro-3,4-dehydro-β-ionone, T-743
4,5-Dihydro-3,4-dihydroxy-3-methyl-2(3*H*)-furanone, D-234
Dihydro-3,4-divanillyl-2(3*H*)-furanone, M-81
2,3-Dihydro-3,5,6,7-tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, P-110
2,3-Dihydro-3,5,6,7-tetrahydroxy-2-phenyl-4*H*-1-benzopyran-4-one, T-193
2,3-Dihydro-3,5,7,8-tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, P-112
2,3-Dihydro-3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, H-201
2,3-Dihydro-3,5,7-trihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-190
2,3-Dihydro-3,5,7-trihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, T-568
2,3-Dihydro-3,5-dihydroxy-2-oxo-1*H*-indole-3-acetic acid, D-237
2,3-Dihydro-3,5-dihydroxy-2-oxo-3-indoleacetic acid, D-239
2,3-Dihydro-3,5-dihydroxy-6-methyl-4*H*-pyran-4-one, D-235
3,11-Dihydro-3,5-dimethyl-3-(4-methyl-3-pentenyl)pyrano[3,2-*a*]carbazol-9-ol, M-33
3,11-Dihydro-3,5-dimethyl-3-(4-methyl-3-pentenyl)pyrano[3,2-*a*]carbazole, M-32
7,7*a*-Dihydro-3,6,7-trihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]oxiren-2(1*aH*)-one, D-360
9,10-Dihydro-3,6,8-trihydroxy-1-methyl-9,10-dioxo-2-anthracenecarboxylic acid, T-626
2,3-Dihydro-3,6-dihydroxy-2,2-dimethyl-4*H*-1-benzopyran-4-one, D-228
5,6-Dihydro-3,6-dimethyl-2(4*H*)-benzofuranone, M-133
2,3-Dihydro-3,7-dihydroxy-2-(4-hydroxyphenyl)-

4*H*-1-benzopyran-4-one, T-567
2,3-Dihydro-3,7-dihydroxy-2-oxo-1*H*-indole-3-acetic acid, D-238
2,3-Dihydro-3,7-dimethyl-1*H*-indene-5-carboxylic acid, D-810
3,7-Dihydro-3,7-dimethyl-1*H*-purine-2,6-dione, T-342
9,10-Dihydro-3,8-dihydroxy-1-methyl-9,10-dioxo-2-anthracenecarboxylic acid, D-545
3,11-Dihydro-3,8-dimethyl-3-(4-methyl-3-pentenyl)pyrano[3,2-*a*]carbazole, M-30
1,2-Dihydro-3,8-dimethyl-5-(1-methylethyl)-naphthalene, C-356
Dihydro-3-(1-octenyl)-2,5-furandione, D-335
3,4-Dihydro-3-(2,4-dihydroxyphenyl)-6,7-dihydroxy-2*H*-1-benzopyran, T-219
3,4-Dihydro-3-(2,4-dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran, T-594
3,4-Dihydro-3-(2-hydroxy-4-methoxyphenyl)-2*H*-1-benzopyran-7-ol, D-540
Dihydro-3-(2-octenyl)-2,5-furandione, D-336
4,5-Dihydro-3-(3,4-dihydroxybenzyl)-4-(3,4,5-trihydroxybenzyl)-2(3*H*)-furanone, P-155
3,4-Dihydro-3-(3-hydroxy-2,4-dimethoxyphenyl)-2*H*-1-benzopyran-7-ol, D-429
3,4-Dihydro-3-(3-hydroxy-4-methoxyphenyl)-8-hydroxyisocoumarin, D-614
3*a*,4-Dihydro-3-(3-methylbutylidene)-1(3*H*)-isobenzofuranone, D-292
N-[2,5-Dihydro-3-(hydroxymethyl)-2-furanyl]-4-hydroxyglutamine, O-261
3,4-Dihydro-3-hydroxy-1-methyl-4,5-diphenyl-2(1*H*)-pyridinone, D-268
2,3-Dihydro-3-hydroxy-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, D-260
2,3-Dihydro-3-hydroxy-2-isopropenyl-5-benzofurancarboxylic acid, D-266
2,3-Dihydro-3-hydroxy-2-oxo-1*H*-indole-3-acetic acid, D-277
[(2,3-Dihydro-3-hydroxy-2-oxo-1*H*-indol-3-yl)-methyl]carbamodithioic acid methyl ester, D-937
2,3-Dihydro-3-hydroxy-2-oxo-1*H*-indole-3-acetonitrile, C-411
1,3-Dihydro-3-hydroxy-2*H*-pyrrol-2-one, D-281
2,3-Dihydro-3-hydroxy-3-methylthiazolo[3,2-*a*]indole-9-carboxaldehyde, B-178
Dihydro-3-hydroxy-4,4-dimethyl-2(3*H*)-furanone, D-256
2,3-Dihydro-3-hydroxy-5-methoxy-6-methyl-4*H*-pyran-4-one, D-235
2,3-Dihydro-3-hydroxy-6-(2-hydroxyethyl)-2,2,5,7-tetramethyl-1*H*-inden-1-one, P-562
2,3-Dihydro-3-hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1*H*-inden-1-one, P-561
2,3-Dihydro-3-hydroxy-6-(2-hydroxyethyl)-2-(hydroxymethyl)-2,5,7-trimethyl-1*H*-inden-1-one, P-566
2,3-Dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-4*H*-1-benzopyran-4-one, D-228
ϵ-(1,4-Dihydro-3-hydroxy-6-methyl-4-oxo-1-pyridyl)lysine, P-604
3,4-Dihydro-3-hydroxy-7-oxociguatoxin, C-259
4,5-Dihydro-3-mercapto-2-methylfuran, D-302
2,3-Dihydro-3-methyl-1*H*-pyrrole, D-316
Dihydro-3-methyl-2(3*H*)-furanone, D-299
3,11-Dihydro-3-methyl-3-(4-methyl-3-pentenyl)-pyrano[3,2-*a*]carbazole-5-carboxaldehyde, M-815
4,5-Dihydro-3-methyl-5-(3-methyl-1,3-butadienyl)-2(3*H*)-furanone, D-306
2,3-Dihydro-3-methylfuran, D-296
2,3-Dihydro-3-methylpyrrole, D-317
7,8-Dihydro-3-methylpyrrolo[1,2-*a*]pyrimidin-2(6*H*)-one, D-321
4,5-Dihydro-3-oxo-α-ionone, H-540
2-(1,3-Dihydro-3-oxo-5-sulfo-2*H*-indol-2-ylidene)-2,3-dihydro-3-oxo-1*H*-indole-5-sulfonic acid, I-21
3,4-Dihydro-3-oxoedulan, H-186
7,9-Dihydro-3-ribofuranosyl-1*H*-purine-2,6,8(3*H*)-trione, R-33
3,4-Dihydro-3-[2,4-dihydroxy-3-(3-methyl-2-butenyl)phenyl]-7-hydroxy-2*H*-1-benzopyran, T-686
6*a*,11*a*-Dihydro-4,10-bis(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,9-diol, D-442
9,10-Dihydro-4,5-dihydroxy-10-oxo-2-anthracenecarboxylic acid, D-236
9,10-Dihydro-4,5-dihydroxy-10-oxo-2-anthroic acid, D-236
9,10-Dihydro-4,5-dihydroxy-2,6-dimethoxyphenanthrene, P-248
9,10-Dihydro-4,5-dihydroxy-9,10-dioxo-2-anthracenecarboxylic acid, D-378
2,5-Dihydro-4,5-dimethyl-2-(1-methylpropyl)thiazole, D-246
2,5-Dihydro-4,5-dimethyl-2-(2-methylpropyl)thiazole, D-247
4,5-Dihydro-4,5-dioxo-1*H*-pyrrolo[2,3-*f*]quinoline-2,7,9-tricarboxylic acid, M-247
Dihydro-4,6-dimethyl-2-(1-methylethyl)-4*H*-1,3,5-dithiazine, D-106
Dihydro-4,6-dimethyl-4*H*-1,3,5-dithiazine, D-244
25,27-Dihydro-4,7-didehydro-7-deoxyphysalin A, D-227
3,4-Dihydro-4,7-dimethyl-1(2*H*)naphthalenone, T-806
1,2-Dihydro-4,7-dimethyl-1-(1-methylethyl)-naphthalene, C-31
3,4-Dihydro-4,8-dihydroxy-1(2*H*)-naphthalenone, I-163
3,4-Dihydro-4,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one, D-232
3,4-Dihydro-4,8-dihydroxy-3-methylisocoumarin, D-232
3,4-Dihydro-4,8-dihydroxy-6-methyl-1(2*H*)-naphthalenone, S-97
2,3-Dihydro-4-(4-hydroxyphenyl)-1*H*-phenalene-1,2,3-triol, D-279
2,3-Dihydro-4-(4-methoxyphenyl)-1*H*-phenalene-1,2,3-triol, D-279
3,6-Dihydro-4-(4-methyl-3-pentenyl)-1,2-dithiin, D-311
6,7-Dihydro-4-(hydroxymethyl)-2-(*p*-hydroxyphenethyl)-7-methyl-5*H*-2-pyrindinium, D-271
6,7-Dihydro-4-(methoxymethyl)-7-methyl-5*H*-2-pyrindine, V-8
Dihydro-4-hydroxy-2(3*H*)-furanone, D-258
2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-5-(2-methyl-1-oxobutyl)-9-propyl-7*H*-furo[2,3-*f*][1]benzopyran-7-one, C-489
2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-5-(3-methyl-1-oxobutyl)-9-propyl-7*H*-furo[2,3-*f*][1]benzopyran-7-one, C-483
2,5-Dihydro-4-hydroxy-2-methyl-5-oxo-2-furancarboxylic acid, Z-19
4,5-Dihydro-4-hydroxy-5-(hydroxymethyl)-2(3*H*)-furanone, D-265
Dihydro-4-hydroxy-5-methylene-3-(11-tetradecenylidene)-3(2*H*)-furanone, D-269
Dihydro-4-hydroxy-5-methylene-3-tetradecylidene-2(3*H*)-furanone, D-269
2,3-Dihydro-4-hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1*H*-inden-1-one, P-567
2,3-Dihydro-4-hydroxy-7-(hydroxymethyl)-2-(1-hydroxy-1-methylethyl)-5*H*-furo[3,2-*g*][1]benzopyran-5-one, A-329
3,4-Dihydro-4-hydroxy-7-oxociguatoxin, C-259
1,4-Dihydro-4-imino-1-β-D-ribofuranosyl-3-pyridinecarboxylic acid, C-306
1,2-Dihydro-4-isopropyl-1,6-dimethylnaphthalene, C-32
Dihydro-4-mercapto-3(2*H*)-furanone, D-286
Dihydro-4-mercapto-5-methyl-3(2*H*)-thiophenone, D-287
4,5-Dihydro-4-mercapto-5-methylthiophene-3-ol, D-287
2,3-Dihydro-4-methoxy-α,α-dimethylfuro[2,3-*b*]quinoline-2-methanol, P-411
Dihydro-4-methoxy-2(3*H*)-furanone, D-258
2,5-Dihydro-4-methoxy-2-methyl-5-oxo-2-furancarboxylic acid, Z-19
5,6-Dihydro-4-methoxy-2*H*-pyran-2-one, D-291
5,6-Dihydro-4-methoxy-6-(2-phenylethenyl)-2*H*-pyran-2-one, K-28
6,7-Dihydro-4-methoxy-6-methylfuro-[2,3-*f*]-1,3-benzodioxole, F-140
5,6-Dihydro-4-methoxy-6-[2-(4-methoxyphenyl)ethyl]-2*H*-pyran-2-one, Y-1
1,6-Dihydro-4-methyl-1-methylene-7-(1-methylethenyl)azulene, L-22
Dihydro-4-methyl-2(3*H*)-furanone, D-300
3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2*H*-pyran, D-308
2-[4,5-Dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-4(5)-methylbenzoic acid, I-5
5,6-Dihydro-4-methyl-6-[(1-methyl-2-piperidinyl)-methyl]-2*H*-pyran-2-one, D-1058
2,3-Dihydro-4-methylfuran, D-297
1,1′-(1,4-Dihydro-4-nonyl-3,5-pyridinediyl)bis[1-decanone], D-105
1,1′-(1,4-Dihydro-4-nonyl-3,5-pyridinediyl)bis[1-dodecanone], D-105
1-[1,4-Dihydro-4-nonyl-5-(1-oxodecyl)-3-pyridinyl]-1-dodecanone, D-105
Dihydro-4-oxoisophorone, T-744
3,4-Dihydro-4-[(5-methyl-2-furanyl)methylene]-2*H*-pyrrole, D-303
1,2-Dihydro-5,10-dihydroxy-1,1,2-trimethyl-6*H*-furo[2,3-*c*]xanthen-6-one, P-18
5,10-Dihydro-5,10-dioxonaphtho[2,3-*b*]-1,4-dithiin-2,3-dicarbonitrile, D-989
2,3-Dihydro-5,5′,7,7′-tetrahydroxy-2-(4-hydroxyphenyl)[3,8′-bi-4*H*-1-benzopyran]-4,4′-dione, D-355
2,3-Dihydro-5,6,7,8-tetrahydroxy-3-[(4-hydroxyphenyl)methyl]-4*H*-1-benzopyran-4-one, T-213
2,3-Dihydro-5,6,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, H-202
2,3-Dihydro-5,6,7-trihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-194
2,3-Dihydro-5,6-dihydroxy-1*H*-indole-2-carboxylic acid, C-449
9,10-Dihydro-5,6-dihydroxy-2,4-dimethoxyphenanthrene, P-248
5,6-Dihydro-5,6-dihydroxyzeaxanthin, D-224
2,3-Dihydro-5,6-dimethyl-1*H*-pyrrolizine-7-carboxaldehyde, D-250
1-(2,3-Dihydro-5,6-dimethyl-1*H*-pyrrolizin-7-yl)ethanone, A-37
2,3-Dihydro-5,7,8-trihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, T-573
2,3-Dihydro-5,7,8-trihydroxy-3-[(4-hydroxyphenyl)methyl]-4*H*-1-benzopyran-4-one, T-589
2,3-Dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-1-benzopyran-4-one, T-614
2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-682
2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-683
2,3-Dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-methyl-4*H*-1-benzopyran-4-one, T-631
2,3-Dihydro-5,7-dihydroxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, D-537
2,3-Dihydro-5,7-dihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, D-471
2,3-Dihydro-5,7-dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, T-681
2,3-Dihydro-5,7-dihydroxy-3-(2,4-dihydroxyphenyl)-4*H*-1-benzopyran-4-one, T-220
2,3-Dihydro-5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-597
2,3-Dihydro-5,7-dihydroxy-3-[(4-hydroxyphenyl)-methyl]-4*H*-1-benzopyran-4-one, D-502
2,3-Dihydro-5,7-dihydroxy-6,8-dimethyl-2-phenyl-4*H*-1-benzopyran-4-one, D-432
2,3-Dihydro-5,7-dihydroxy-6-(3-methyl-2-butenyl)-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, P-168
2,3-Dihydro-5,7-dihydroxy-6-(3-methyl-2-butenyl)-2-phenyl-4*H*-1-benzopyran-4-one, D-669
2,3-Dihydro-5,7-dihydroxy-6-methyl-2-phenyl-4*H*-1-benzopyran-4-one, D-553
7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, D-231

7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(2-methyl-1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, D-229
7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(3-methyl-1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, D-230
9,10-Dihydro-5,7-dimethoxy-3,4-phenanthrenediol, P-248
2,8-Dihydro-5,8-dihydroxy-2,2-dimethyl-6*H*-furo[3,4-*g*]-1-benzopyran-6-one, S-14
Dihydro-5-(1-hydroxyethyl)-2(3*H*)-furanone, H-450
Dihydro-5-(2-octenyl)-2(3*H*)-furanone, D-337
2,3-Dihydro-5-(3-hydroxypropanoyl)-1*H*-pyrrolizine, D-280
4,7-Dihydro-5-(4-methyl-3-pentenyl)-1,2,3-trithiepin, D-313
2,3-Dihydro-5-(4-oxopentanoyl)-1*H*-pyrrolizine, D-353
2,3-Dihydro-5-(5-methyl-2-furanyl)-1*H*-pyrrolizine, D-305
3,4-Dihydro-5-(5-methyl-2-furanyl)-2*H*-pyrrole, D-304
1-(2,3-Dihydro-5-ethyl-1*H*-pyrrolizin-7-yl)ethanone, A-38
2,3-Dihydro-5-hydroxy-1,4-naphthoquinone, H-625
2,11-Dihydro-5-hydroxy-10-methoxy-2,2,11-trimethyl-6*H*-pyrano[3,2-*b*]acridin-6-one, J-18
1,11-Dihydro-5-hydroxy-11-methyl-2-(1-methylethenyl)furo[2,3-*c*]acridin-6(2*H*)-one, R-69
2,8-Dihydro-5-hydroxy-2,2-dimethyl-6*H*-furo[3,4-*g*]-1-benzopyran-6-one, S-14
2,3-Dihydro-5-hydroxy-2-methyl-1,4-naphthoquinone, D-274
2,3-Dihydro-5-hydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, E-361
1,5-Dihydro-5-hydroxy-2*H*-pyrrol-2-one, D-282
5,6-Dihydro-5-hydroxy-3-methyl-6-phenyl-3-benzazocin-4(3*H*)-one, C-301
5,6-Dihydro-5-hydroxy-4-methoxy-6-(2-phenylethyl)-2*H*-pyran-2-one, D-267
5,6-Dihydro-5-hydroxy-6-methyl-2*H*-pyran-2-one, D-276
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-263
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(1-oxobutyl)-4-propyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-264
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, M-4
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, M-5
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxopropyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-262
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, C-484
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-261
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-isovaleryl-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, C-484
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-isovaleryl-4-propylfuro[2,3-*h*]coumarin, D-261
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-9-methoxy-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, C-484
8,9-Dihydro-5-hydroxy-8-(1-methylethenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, C-484
2,8-Dihydro-5-hydroxy-8-methoxy-2,2-dimethyl-6*H*-furo[3,4-*g*]-1-benzopyran-6-one, S-14
5,6-Dihydro-5-isopropyl-3,8-dimethyl-2-naphthol, C-31
1,2-Dihydro-5-isopropyl-3,8-dimethylnaphthalene, C-356
1,5-Dihydro-5-methoxy-2*H*-pyrrol-2-one, D-282
4-(3,4-Dihydro-5-methoxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-3-yl)-1,3-benzenediol, N-40
2,3-Dihydro-5-methyl-1*H*-pyrrolizine-7-carboxaldehyde, D-318
1-(2,3-Dihydro-5-methyl-1*H*-pyrrolizin-7-yl)ethanone, A-43
Dihydro-5-methyl-2(3*H*)-furanone, D-301
Dihydro-5-methyl-2(3*H*)-thiophenone, D-331
2,5-Dihydro-5-methyl-2-oxo-3-furantridecanal, D-309
2,3-Dihydro-5-methyl-3-thiophenethiol, D-327
4,5-Dihydro-5-methyl-3-thiophenethiol, D-329
2,3-Dihydro-5-methyl-4-(methylthio)furan, D-302
6,7-Dihydro-5-methyl-5*H*-cyclopenta[*b*]pyrazine, D-295
2,3-Dihydro-5-methylthiophene, D-326
Dihydro-5-octyl-2(3*H*)-furanone, D-338
4,5-Dihydro-5-oxo-1-(4-sulfophenyl)-4-[(4-sulfophenyl)azo]-1*H*-pyrazole-3-carboxylic acid, T-28
N-(2,5-Dihydro-5-oxo-2-furanyl)acetamide, A-254
Dihydro-5-pentyl-2(3*H*)-furanone, D-341
2,3-Dihydro-5-propanoyl-1*H*-pyrrolizine, D-346
3,4-Dihydro-5-propanoyl-2*H*-pyrrole, D-345
Dihydro-5-propyl-2(3*H*)-furanone, D-347
7,8-Dihydro-6α-hydroxy-α-ionol, M-101
8,9-Dihydro-6,10,11,13-tetrahydroxy-3,3-dimethyl-9-(1-methylethenyl)-3*H*,7*H*-benzo[*c*]pyrano[3,2-*h*]xanthen-7-one, A-426
3,12-Dihydro-6,10,11-trihydroxy-3,3,12-trimethyl-7*H*-pyrano[2,3-*c*]acridin-7-one, C-280
3,12-Dihydro-6,11-dihydroxy-10-methoxy-3,3,12-trimethyl-7*H*-pyrano[2,3-*c*]acridin-7-one, C-280
3,4-Dihydro-6,7-dimethoxy-1-methylisoquinoline, D-555
1-(2,3-Dihydro-6,7-dimethyl-1*H*-pyrrolizin-5-yl)-2-hydroxy-1-propanone, D-251
1-(2,3-Dihydro-6,7-dimethyl-1*H*-pyrrolizin-5-yl)ethanone, A-36
2,3-Dihydro-6,7-dimethyl-5-(2-hydroxypropionyl)-1*H*-pyrrolizine, D-251
6,7-Dihydro-6,7-ocimenediol, D-828
3,4-Dihydro-6,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one, D-233
3,4-Dihydro-6,8-dihydroxy-3-methylisocoumarin, D-233
5-[5,6-Dihydro-6-(1-hydroxy-1-methylethyl)benzo[1,2-*b*:5,4-*b*′]difuran-2-yl]-1,3-benzenediol, M-757
2,3-Dihydro-6-(2-hydroxyethyl)-2,2,5,7-tetramethyl-1*H*-inden-1-one, P-570
2,3-Dihydro-6-(2-hydroxyethyl)-2,5,7-trimethyl-1*H*-inden-1-one, P-560
2,3-Dihydro-6-(2-hydroxyethyl)-2-(hydroxymethyl)-2,5,7-trimethyl-1*H*-inden-1-one, P-559
2,3-Dihydro-6-(2-hydroxyethyl)-5-(hydroxymethyl)-2,7-dimethyl-1*H*-inden-1-one, P-569
5,8-Dihydro-6-(4-methyl-3-pentenyl)-1,2,3,4-tetrathiocin, D-312
5,6-Dihydro-6-(6-hydroxyheptyl)-2*H*-pyran-2-one, H-122
6,7-Dihydro-6-(6-methoxy-1,3-benzodioxol-5-yl)-5*H*-furo-[3,2-*g*][1]benzopyran-5-one, N-42
2,3-Dihydro-6-(hydroxymethyl)-2-methyl-4*H*-pyran-4-one, D-273
1,2-Dihydro-6-hydroxy-2,2,4-trimethylquinoline, D-364
3,4-Dihydro-6-hydroxy-2,2,5,7,8-pentamethyl-2*H*-1-benzopyran, D-340
2,3-Dihydro-6-hydroxy-2,2-dimethyl-4*H*-1-benzopyran-4-one, D-255
3,4-Dihydro-6-hydroxy-2,5,7,8-tetramethyl-2*H*-1-benzopyran-2-carboxylic acid, D-283
2,3-Dihydro-6-hydroxy-2-(1-hydroxy-1-methylethyl)-4-methoxy-9-methylfuro[2,3-*b*]quinolinium, R-31
3,9-Dihydro-6-hydroxy-2-(1-hydroxy-1-methylethyl)-9-methylfuro[2,3-*b*]quinolin-4(2*H*)-one, R-30
1-[2,3-Dihydro-6-hydroxy-2-(1-methylethenyl)-5-benzofuranyl]-2-hydroxyethanone, D-259
1,2-Dihydro-6-hydroxy-2-oxo-4-quinolinecarboxylic acid, D-681
1,4-Dihydro-6-hydroxy-4-oxo-2-quinolinecarboxylic acid, D-683
2,3-Dihydro-6-hydroxy-5-(hydroxyacetyl)-2-isopropenylbenzofuran, D-259
5-(6,7-Dihydro-6-hydroxy-7,7-dimethyl-5*H*-furo[3,2-*g*][1]benzopyran-2-yl)-1,3-benzenediol, M-758
N-Dihydro-6-isojasmonoylisoleucine, J-9
3,4-Dihydro-6-methoxy-2,2-dimethyl-2*H*-1-benzopyran-4-ol, D-255
2,3-Dihydro-6-methoxy-2,2-dimethyl-4*H*-1-benzopyran-4-one, D-255
3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7*H*-pyrano[2,3-*c*]acridin-7-one, A-119
3,4-Dihydro-6-methoxy-3,7-dimethyl-1*H*-2-benzopyran-8-ol, D-288
1,4-Dihydro-6-methoxy-4-oxo-2-quinolinecarboxylic acid, D-683
3,4-Dihydro-6-methyl-1,2,3-oxathiazin-4-one 2,2-dioxide, A-18
1-(2,3-Dihydro-6-methyl-1*H*-pyrrolizin-5-yl)-1,4-pentanedione, D-320
2,3-Dihydro-6-methyl-1*H*-pyrrolizine-5-carboxaldehyde, D-319
1-(2,3-Dihydro-6-methyl-1*H*-pyrrolizin-5-yl)-1-propanone, D-314
1-(2,3-Dihydro-6-methyl-1*H*-pyrrolizin-5-yl)ethanone, A-41
2,3-Dihydro-6-methyl-5-(4-oxopentanoyl)-1*H*-pyrrolizine, D-320
2,3-Dihydro-6-methyl-5-(5-methyl-2-furanyl)-1*H*-pyrrolizine, D-307
2,3-Dihydro-6-methyl-5-propanoyl-1*H*-pyrrolizine, D-314
2,3-Dihydro-6-methylthieno[2,3-*c*]furan, D-323
10,11-Dihydro-6-oxoatlantone, B-96
5,6-Dihydro-6-pentyl-2*H*-pyran-2-one, D-342
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-9-ol, N-33
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-2,3,9-triol, T-701
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,4,9-triol, T-702
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,9,10-triol, T-704
6*a*,11*a*-Dihydro-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,9-diol, D-679
6*a*,12*a*-Dihydro-6*H*-[1,3]dioxolo[5,6]benzofuro[3,2-*c*][1]benzopyran-3-ol, M-2
7′,8′-Dihydro-7′-apo-β-caroten-8′-one, S-114
2,3-Dihydro-7,8-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-571
5-(3,4-Dihydro-7,8-dihydroxy-2*H*-1-benzopyran-2-yl)-1,2,3-benzenetriol, P-106
7,8-Dihydro-7,8-dihydroxy-3,5,7-trimethyl-6*H*-2-benzopyran-6-one, D-240
7,8-Dihydro-7,8-dihydroxy-3,7-dimethyl-6-oxo-6*H*-2-benzopyran-5-carboxaldehyde, A-501
2,3-Dihydro-7-*O*-demethylrobustigenin, P-149
3,4-Dihydro-7-hydroxy-1-methyl-β-carboline, H-9
2,3-Dihydro-7-hydroxy-2,2-dimethyl-4-oxo-4*H*-1-benzopyran-6-propanoic acid, D-257
2,3-Dihydro-7-hydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, D-470
2,3-Dihydro-7-hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-acetic acid, D-275
2,3-Dihydro-7-hydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, D-440
4-(3,4-Dihydro-7-hydroxy-2*H*-1-benzopyran-4-yl)-1,3-benzenediol, T-594
3,4-Dihydro-7-hydroxy-3-(2,3,4-trihydroxyphenyl)-2*H*-1-benzopyran, T-217
3,4-Dihydro-7-hydroxy-3-(2,4,5-trihydroxyphenyl)-2*H*-1-benzopyran, T-218
2,3-Dihydro-7-hydroxy-3-(2,4-dihydroxyphenyl)-4*H*-1-benzopyran-4-one, T-595
2,3-Dihydro-7-hydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, D-512

6,9-Dihydro-7-hydroxy-7-methyl-2-(1-methylethylidene)-7*H*-furo[3,2-*h*][2]benzopyran-3(2*H*)-one, P-228
7,8-Dihydro-7-hydroxy-8,8-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, D-254
6,7-Dihydro-7-hydroxyciguatoxin, C-259
1,6-Dihydro-7-isopropenyl-4-methyl-1-methyleneazulene, L-22
3,4-Dihydro-7-methoxy-1-methyl-β-carboline, H-9
4,9-Dihydro-7-methoxy-1-methyl-3*H*-pyrido[3,4-*b*]indole, H-9
2,3-Dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(1-propenyl)benzofuran, D-289
2,3-Dihydro-7-methoxy-2-methyl-5,6-methylenedioxybenzofuran, F-140
3,7-Dihydro-7-methyl-1*H*-purine-2,6-dione, X-2
1-(2,3-Dihydro-7-methyl-1*H*-pyrrolizin-5-yl)-1-propanone, D-315
1-(2,3-Dihydro-7-methyl-1*H*-pyrrolizin-5-yl)ethanone, A-42
2,3-Dihydro-7-methyl-5-propanoyl-1*H*-pyrrolizine, D-315
7′,8′-Dihydro-8′-hydroxy-6′-methyl-6′-apo-β-caroten-6′-one, C-281
7′,8′-Dihydro-8′-hydroxycitraniaxanthin, C-281
8′,9′-Dihydro-8′-hydroxycitraniaxanthin (incorr.), C-281
7′,8′-Dihydro-8′-hydroxyreticulataxanthin, R-9
3,11-Dihydro-8,10-dimethoxy-3,3,5-trimethylpyrano[3,2-*a*]carbazole, M-780
6-(3,4-Dihydro-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-3-yl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, H-285
4-(3,4-Dihydro-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-3-yl)-2-(3-methyl-2-butenyl)-1,3-benzenediol, H-284
4-[3,4-Dihydro-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-3-yl]-1,3-benzenediol, G-135
6,7-Dihydro-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2,6-dione, G-321
3,11-Dihydro-8,9-dimethoxy-3,3,5-trimethylpyrano[3,2-*a*]carbazole, K-39
10,11-Dihydro-8-(1-methylethyl)-11-(2-methylpropylidene)-6*H*-oxepino[2,3-*d*]pyrazino[1,2-*a*]pyrimidine-6,9(8*H*)-dione, C-263
1,2-Dihydro-8-hydroxy-2-oxo-4-quinolinecarboxylic acid, D-682
3,4-Dihydro-8-hydroxy-3-(3-hydroxy-4-methoxyphenyl)-1*H*-2-benzopyran-1-one, D-614
3,4-Dihydro-8-hydroxy-3-(6-pentadecenyl)-1*H*-2-benzopyran-1-one, D-278
3,4-Dihydro-8-hydroxy-3-(6-pentadecenyl)isocoumarin, D-278
3,4-Dihydro-8-hydroxy-3-tridecyl-1*H*-2-benzopyran-1-one, D-284
3,4-Dihydro-8-hydroxy-3-tridecylisocoumarin, D-284
7,8-Dihydro-8-hydroxy-4-methoxy-7-methyl-5*H*-furo[2,3-*g*][2]benzopyran-5-one, C-355
3,4-Dihydro-8-hydroxy-6-methoxy-3-methyl-1*H*-2-benzopyran-1-one, D-233
3*a*,12*c*-Dihydro-8-hydroxy-6-methoxy-7*H*-furo[3′,2′:4,5]furo[2,3-*c*]xanthen-7-one, S-222
7,8-Dihydro-8-hydroxymethylfagaridine, B-165
6*a*,13*a*-Dihydro-8-methoxy-1,3-dioxolo[6,7][1]benzopyrano[3,4-*b*]furo[3,2-*g*]benzopyran-13(16*H*)-one, P-4
1,2-Dihydro-8-methoxy-2-oxo-4-quinolinecarboxylic acid, D-682
3,11-Dihydro-8-methoxy-3,3,5-trimethylpyrano[3,2-*a*]carbazol-9-ol, K-39
3,11-Dihydro-8-methoxy-3,3,5-trimethylpyrano[3,2-*a*]carbazole, K-41
3,4-Dihydro-8-methoxy-3-tridecylisocoumarin, D-284
5-(7,10-Dihydro-8-methylfuro[2,3-*g*][1]benzoxepin-2-yl)-1,3-benzenediol, M-753
3,4-Dihydro-9,10-dihydroxy-7-methoxy-3-methylene-1*H*-naphtho[2,3-*c*]pyran-1-one, T-424
9,10-Dihydro-9,10-dihydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, K-32
5,6-Dihydro-9,10-dimethoxybenzo[*g*]-1,3-benzodioxolo[5,6-*a*]quinolizinium(1+), B-62
6*a*,12*a*-Dihydro-9,12*a*-dihydroxy-3-methoxy[1]-benzopyrano[3,4-*b*][1]benzopyran-12(6*H*)-one, G-146
1,9-Dihydro-9-β-D-ribofuranosyl-6*H*-purin-6-one, I-38
2,3-Dihydro-9-hydroxy-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, R-73
2,3-Dihydro-9-hydroxy-2-(1-methylethenyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, A-375
8,9-Dihydro-9-hydroxy-8-(1-hydroxy-1-methylethyl)-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, V-1
6*a*,11*a*-Dihydro-9-methoxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-3-ol, H-555
Dihydro-*ar*-turmerone, B-102
7,8-Dihydro-*N*-methylberberine, L-36
Dihydro-*O*-methylsterigmatocystin, S-222
Dihydro-*p*-coumaric acid, H-741
Dihydro-*p*-coumaroyl alcohol, H-742
4′-Dihydroabscisic acid, A-11
2,3-Dihydroabscisic alcohol, A-12
9,10-Dihydroabscisic alcohol, A-12
Dihydroactinidiolide, T-130
11α,13-Dihydroalantolactone, E-374
Dihydroalliin, P-527
Dihydroargolide, H-472
Dihydroasparagusic acid, M-212
Dihydroaspidospermatine, A-469
10,11-Dihydroatlantone, B-114
Dihydrobaicalein, T-572
Dihydroberberine, L-36
Dihydrobiochanin A, T-597
Dihydrobrassicasterol, E-223
Dihydrobufothionine, B-197
3,4-Dihydrocadalene, C-31
7,8-Dihydrocadalene, C-31
1,2-Dihydrocadalene, C-32
9,10-Dihydrocadalene, C-32
Dihydrocajanin, T-220
Dihydrocapsaicin, C-75
Dihydrocapsenone, E-194
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(-)-Dihydrocarveol, M-180
Dihydrocarveol acetate, M-180
Dihydrocarvone, M-187
Dihydrochalcone, D-954
Dihydrochelerythrinyl-8-acetaldehyde, D-225
Dihydrochiapagenin, S-183
22-Dihydrochondrillasterol, S-245
(8α,9*R*)-10,11-Dihydrocinchonan-9-ol, C-261
(9*S*)-10,11-Dihydrocinchonan-9-ol, C-262
10,11-Dihydrocinchonidine, C-261
10,11-Dihydrocinchonine, C-262
Dihydrocinnamic acid, P-304
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Dihydrocitronellol, D-845
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14,19-Dihydrocondylocarpine, T-847
Dihydroconiferin, D-649
Dihydrocoriandrin, C-351
11,13-Dihydrocostic acid, E-368
3,4-Dihydrocoumarin, D-222
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1,2-Dihydrodehydroguaiaretic acid, D-71
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Dihydrodeoxy-8-epiaustdiol, D-240
11,13-Dihydrodesoxoachalensolide, G-334
14,15-Dihydrodinophysistoxin 1, O-118
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22,23-Dihydroergosterol, E-205
Dihydroeugenol, P-524
1,2-Dihydrofalcarinone, H-72
N-Dihydroferuloyltyramine, H-712
Dihydroferuperine, C-363
Dihydrofisetin, T-189
Dihydroflavokawin B, P-322
Dihydroformononetin, D-512
Dihydrofukinolide, F-84
Dihydrogalangol, T-568
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Dihydrogenistin, T-597
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Dihydroharman, D-293
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Dihydrohydroxy-*O*-methylsterigmatocystin, S-222
Dihydrohydroxyaflatoxin B_1, A-134
Dihydroisoalantolactone, E-373
Dihydroisocycloartomunin, C-488
Dihydroisojasmonic acid, O-241
Dihydroisophorol, T-746
Dihydroisorhamnetin, P-109
Dihydrojasmone, M-566
Dihydrojasmonic acid, O-241
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11,12-Dihydrolactaroviolin, M-498
7′,8′-Dihydrolutein, L-124
7,8-Dihydrolycopene, D-285
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15,16-Dihydrominquartynoic acid, H-644
5,6-Dihydromocimyin C, M-726
Dihydromorelloflavone, M-760
Dihydromurrayacine, M-814
Dihydromyoporone, M-831
Dihydromyricetin, H-201
Dihydronarigenin, H-752
Dihydronepetalactone, D-334
2′,3′-Dihydroniveusin A, E-181
4,5-Dihydroniveusin A, E-181
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2,3-Dihydroononin, D-512
Dihydrooroxylin, T-572
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7,8-Dihydroparasiloxanthin, Z-9
Dihydropergillin, P-228
2,2-Dihydroperoxypropane, D-343
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25,27-Dihydrophysalin C, P-343
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10,11-Dihydropipercide, R-14
6,7-Dihydropiperettine, P-388
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Dihydroprudomenin, P-112
7,8-Dihydropterin-6-carboxylic acid, A-267
3,9-Dihydropunctatin, T-589
Dihydropyrocurzerenone, P-609
Dihydroquercetin, P-109
5,12-Dihydroquino[2,3-*b*]acridine-7,14-dione, Q-8
Dihydroretrofractamide B, R-14
5,21-Dihydrorhazinilam, R-22
Dihydroroseoside, D-533
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Dihydrosorbinol, T-106
Dihydrosterigmatocystin, S-222
22,23-Dihydrostigmasterol, S-244
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2,3-Dihydrothiophene, D-357
2,3-Dihydrothiophene 1,1-dioxide, D-357

11,12-Dihydrothwaitesixanthone, T-395
2,3-Dihydrotoluene, M-369
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2′,3′-Dihydrovitamin K_1, V-44
4,5-Dihydrovomifoliol, D-533
2,3-Dihydrowithanolide E, W-7
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3,4-Dihydroxy(γ-glutamyl)anilide, A-140
3β,6α-Dihydroxy-α-ionol, M-91
α,3-Dihydroxy-α-toluic acid, H-503
α,4-Dihydroxy-α-toluic acid, H-504
3,3′-Dihydroxy-β,β-carotene-4,4′-dione, A-474
3,3′-Dihydroxy-β,κ-caroten-6′-one, C-76
3,4-Dihydroxy-β-ionone, D-529
3,3′-Dihydroxy-κ,κ-carotene-6,6′-dione, C-80
4,8-Dihydroxy-1(10),2-guaiadien-12,6-olide, D-485
3,8-Dihydroxy-1(10),4,11(13)-germacratrien-12,6-olide, D-484
3,8-Dihydroxy-1(10),4-germacradien-12,6-olide, D-480
3,14-Dihydroxy-1(10),4-germacradien-12,6-olide, D-481
11,12-Dihydroxy-1(10)-spirovetiven-2-one, D-691
11,12-Dihydroxy-1(10)eremophilen-2-one, D-453
6,7-Dihydroxy-1(3*H*)-isobenzofuranone, D-511
3,4-Dihydroxy-1,10-bisaboladien-9-one, D-406
2,9-Dihydroxy-1,10-dimethoxyaporphine, B-166
2,9-Dihydroxy-1,10-dimethoxynoraporphine, B-166
1,2-Dihydroxy-1,2,3-propanetricarboxylic acid, D-675
3,4-Dihydroxy-1,2-benzenedicarboxylic acid, D-383
4,5-Dihydroxy-1,2-benzenedicarboxylic acid, D-384
9,10-Dihydroxy-1,3,11(13)-guaiatrien-12,6-olide, D-490
2,7-Dihydroxy-1,3,4,6-tetramethoxydibenzofuran, D-125
2,6-Dihydroxy-1,3,4-trimethoxydibenzofuran, D-126
2,7-Dihydroxy-1,3,4-trimethoxydibenzofuran, D-127
6,7-Dihydroxy-1,3-dimethoxyxanthone, T-297
2,3-Dihydroxy-1,3-diphenyl-1-propanone, D-439
2,5-Dihydroxy-1,4-benzoquinone, D-397
2,6-Dihydroxy-1,4-benzoquinone, D-398
2,5-Dihydroxy-1,4-dithiane, D-988
8,10-Dihydroxy-1,4-guaiadien-12,6-olide, D-486
5-(3,8-Dihydroxy-1,5-dimethyl-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl-2,4-pentadienoic acid, D-344
3,13-Dihydroxy-1,6,10,14-phytatetraen-16-oic acid, D-662
1,7-Dihydroxy-1,6-dimethyl-4-(1-methylethyl)-2(1*H*)-naphthalenone, L-20
6,8-Dihydroxy-1,7-bis(3-methyl-2-butenyl)-9-oxo-9*H*-xanthene-2-carboxylic acid, D-443
3,6-Dihydroxy-1,7-dimethoxyxanthone, T-297
6,8-Dihydroxy-1,7-diprenylxanthone-2-carboxylic acid, D-443
2,4-Dihydroxy-1,8-cineole, E-156
2,5-Dihydroxy-1,8-cineole, E-157
2,6-Dihydroxy-1,8-cineole, E-158
2,7-Dihydroxy-1,8-cineole, E-159
2,7-Dihydroxy-1-(3-methyl-2-butenyl)-9*H*-carbazole-3-carboxaldehyde, H-100
2,3-Dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone, D-623
6,7-Dihydroxy-1-(4-hydroxybenzyl)isoquinoline, H-364
2-[1,2-Dihydroxy-1-(hydroxymethyl)ethyl]-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one, R-69
5-(3,4-Dihydroxy-1-butynyl)-2,2′-bithiophene, B-160
11,21-Dihydroxy-1-gammaceranone, D-479
3,9-Dihydroxy-1-methoxy-10-prenylpterocarpan, T-695
3,9-Dihydroxy-1-methoxy-2,8-diprenylpterocarpan, T-558
3,9-Dihydroxy-1-methoxy-2-prenylcoumestan, P-558
3,9-Dihydroxy-1-methoxy-2-prenylpterocarpan, T-694
3,9-Dihydroxy-1-methoxy-2-prenylpterocarpene, T-694
2,8-Dihydroxy-1-methoxy-3-methylanthraquinone, T-622
3,7-Dihydroxy-1-methoxy-6-methylanthraquinone, T-623
2,7-Dihydroxy-1-methoxyaporphine, P-2
3,9-Dihydroxy-1-methoxycoumestan, T-537
2,7-Dihydroxy-1-methoxynoraporphine, P-2
3,7-Dihydroxy-1-methoxyxanthone, T-724
3,6-Dihydroxy-1-methyl-4,5-diphenyl-2-piperidinone, D-438
3,8-Dihydroxy-1-methylanthraquinone-2-carboxylic acid, D-545
2-(1,2-Dihydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one, R-69
2-(1,2-Dihydroxy-1-methylethyl)-2,3-dihydro-7*H*-furo[3,2-*g*][1]benzopyran-7-one, D-552
2-(1,2-Dihydroxy-1-methylethyl)-6,10-dimethylspiro[4.5]dec-6-en-8-one, D-691
6,7-Dihydroxy-1-methylisoquinoline, D-555
4α,7α-Dihydroxy-1-oxo-24α,25α-epoxywithanolide, P-575
4,8-Dihydroxy-1-tetralone, I-163
3,8-Dihydroxy-10(14)-guaien-12,6-olide, D-493
4,9-Dihydroxy-10(14)-oplopen-3-one, D-589
3,9-Dihydroxy-10-(2-hydroxy-3-methyl-3-butenyl)pterocarpan, D-1030
3,9-Dihydroxy-10-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, I-167
3,8-Dihydroxy-10-methoxy-9-(3-methyl-1-butenyl)-6-(2-methyl-1-propenyl)-6*H*,7*H*-[1]benzopyrano[4,3-*b*][1]benzopyran-7-one, C-430
1,5-Dihydroxy-10-methyl-2-prenylacridone, T-676
9,13-Dihydroxy-10-oxo-11-octadecenoic acid, D-595
3,9-Dihydroxy-10-prenylcoumestan, I-167
3,9-Dihydroxy-10-prenylpterocarpan, D-672
1,4-Dihydroxy-11(13)-eudesmen-12,6-olide, D-460
3β,24-Dihydroxy-11,13(18)-oleanadien-30,22β-olide, T-643
3,24-Dihydroxy-11,13(18)-oleanadien-30-oic acid, D-569
3,14-Dihydroxy-11,13-dihydrocostunolide, D-481
3,7-Dihydroxy-11,15,23-trioxolanost-8-en-26-oic acid, D-701
3β,7β-Dihydroxy-11,15,23-trioxolanosta-8,20(22)*E*-dien-26-oic acid, T-551
3,7-Dihydroxy-11,15-dioxolanosta-8,24-dien-26-oic acid, D-436
3,15-Dihydroxy-11,23-dioxolanost-8-en-26-oic acid, T-553
3,10-Dihydroxy-11-dodecene-6,8-diynoic acid, D-445
6,12-Dihydroxy-11-methoxy-3,3-dimethyl-8-(2-methyl-1-propenyl)-3*H*,7*H*,8*H*-bis[1]benzopyrano[4,3-*b*:6′,5′-*e*]pyran-7-one, C-431
3,13-Dihydroxy-11-oleanen-28-oic acid, D-577
3,21-Dihydroxy-11-oxo-12-oleanen-29,18-olide, T-660
3,18-Dihydroxy-11-oxo-12-oleanen-29-oic acid, D-599
3,21-Dihydroxy-11-oxo-12-oleanen-29-oic acid, D-601
3,24-Dihydroxy-11-oxo-12-oleanen-29-oic acid, D-603
3,*x*-Dihydroxy-11-oxo-12-oleanen-29-oic acid, T-819
3β,24-Dihydroxy-11-oxo-12-oleanen-30,22β-olide, T-661
3,18-Dihydroxy-11-oxo-12-oleanen-30-oic acid, D-600
3,22-Dihydroxy-11-oxo-12-oleanen-30-oic acid, D-602
3,24-Dihydroxy-11-oxo-12-oleanen-30-oic acid, D-604
3,28-Dihydroxy-11-oxo-12-oleanen-30-oic acid, D-606
3,22-Dihydroxy-11-oxo-12-oleanene-27,29-dioic acid, D-596
2,3-Dihydroxy-11-spirovetiven-14-al, D-690
3,13-Dihydroxy-11-ursen-28-oic acid, D-715
1,3-Dihydroxy-12,15-cassadien-11-one, D-411
1,2-Dihydroxy-12,15-heneicosadien-4-one, D-495
2,3-Dihydroxy-12,18-ursadien-28-oic acid, D-706
3,23-Dihydroxy-12,19(29)-ursadien-28-oic acid, D-707
1,3-Dihydroxy-12,6-eudesmanolide, D-457
1,4-Dihydroxy-12,6-eudesmanolide, D-458
7,10-Dihydroxy-12-methoxycoumestan, T-540
9,10-Dihydroxy-12-octadecenoic acid, D-567
3,30-Dihydroxy-12-oleanen-11-one, H-694
3,24-Dihydroxy-12-oleanen-22-one, O-139
3,22-Dihydroxy-12-oleanen-24-al, O-139
2,3-Dihydroxy-12-oleanen-28-oic acid, D-574
3,6-Dihydroxy-12-oleanen-28-oic acid, D-576
3,16-Dihydroxy-12-oleanen-28-oic acid, D-578
3,19-Dihydroxy-12-oleanen-28-oic acid, D-580
3,21-Dihydroxy-12-oleanen-28-oic acid, D-581
3,23-Dihydroxy-12-oleanen-28-oic acid, D-582
3,24-Dihydroxy-12-oleanen-28-oic acid, D-583
3,30-Dihydroxy-12-oleanen-28-oic acid, D-587
3,24-Dihydroxy-12-oleanen-29-oic acid, D-584
3,24-Dihydroxy-12-oleanen-30-oic acid, D-585
2,3-Dihydroxy-12-oleanene-23,28-dioic acid, D-571
2,3-Dihydroxy-12-oleanene-28,30-dioic acid, D-572
3,23-Dihydroxy-12-oleanene-28,30-dioic acid, D-573
14,18-Dihydroxy-12-oxo-9,13,15-octadecatrienoic acid, D-593
2,3-Dihydroxy-12-ursen-24-oic acid, D-709
3,11-Dihydroxy-12-ursen-24-oic acid, D-713
2,3-Dihydroxy-12-ursen-28-oic acid, D-710
3,6-Dihydroxy-12-ursen-28-oic acid, D-711
3,7-Dihydroxy-12-ursen-28-oic acid, D-712
3,11-Dihydroxy-12-ursen-28-oic acid, D-714
3,19-Dihydroxy-12-ursen-28-oic acid, D-716
3,20-Dihydroxy-12-ursen-28-oic acid, D-717
3,23-Dihydroxy-12-ursen-28-oic acid, D-718
6β,7β-Dihydroxy-12*E*-abienol, L-8
2,3-Dihydroxy-13(18)-oleanen-28-oic acid, D-575
3,16-Dihydroxy-13(18)-oleanen-28-oic acid, D-579
3,16-Dihydroxy-13-atisen-2-one, D-380
3-[2,13-Dihydroxy-13-[octahydro-5′-(1-hydroxyundecyl)[2,2′-bifuran]-5-yl]tridecyl]-5-methyl-2(5*H*)-furanone, A-450
7,8-Dihydroxy-14,15-dinor-11-labden-13-one, D-435
2,3-Dihydroxy-14-taraxeren-28-oic acid, D-693
3-(11,12-Dihydroxy-15,19-dotriacontadienyl)-5-methyl-2(5*H*)-furanone, M-747
ent-2α,3β-Dihydroxy-15-beyeren-12-one, B-74
ent-3β,12α-Dihydroxy-15-beyeren-2-one, B-74
ent-3β,12β-Dihydroxy-15-beyeren-2-one, B-74
1,2-Dihydroxy-16-heptadecen-4-one, D-499
1,2-Dihydroxy-16-heptadecyn-4-one, D-500
ent-7α,12β-Dihydroxy-16-kauren-19,6β-olide, T-606
ent-7α,18-Dihydroxy-16-kauren-19,6β-olide, T-607
6,7-Dihydroxy-16-kauren-19-oic acid, D-516
3,25-Dihydroxy-18-oleanen-30-oic acid, D-586
4,16-Dihydroxy-19-nor-17-kauranoic acid, D-562
3,6-Dihydroxy-1*a*-(3-methyl-2-butenyl)naphth[2,3-*b*]-2,7(1*aH*,7*aH*)-dione, D-360
3,5-Dihydroxy-1*H*-inden-1-one, H-513
2,5-Dihydroxy-1*H*-indole-3-acetic acid, H-685
5′,7-Dihydroxy-2′,3′,4′-trimethoxyisoflavan, P-148
5,7-Dihydroxy-2′,4′,5′,6-tetramethoxyisoflavone, H-214
3′,6′-Dihydroxy-2′,4′,5′,7′-tetraiodospiro[isobenzofuran-1(3*H*),9′(9*H*)-xanthen]-3-one, E-237
5,7-Dihydroxy-2′,4′,5′-trimethoxyisoflavanone, P-149
5,7-Dihydroxy-2′,4′,6′-trimethoxy-8-prenylflavanone, P-167

3′,5′-Dihydroxy-2′,4′,7-trimethoxyisoflavan, P-148
6′,7-Dihydroxy-2′,4′-dimethoxy-3′-prenylflavanone, T-264
3′,7-Dihydroxy-2′,4′-dimethoxyisoflavan, D-429
5,7-Dihydroxy-2′,4′-dimethoxyisoflavanone, T-220
5,7-Dihydroxy-2′,4′-dimethoxyisoflavone, T-222
4′,7-Dihydroxy-2′,5-dimethoxyisoflavanone, T-220
4′,7-Dihydroxy-2′,5-dimethoxyisoflavone, T-222
4,4′-Dihydroxy-2′,6′-dimethoxychalcone, T-147
5,7-Dihydroxy-2′,6-dimethoxy-4′,5-methylenedioxyisoflavone, H-214
4′,5-Dihydroxy-2′,7-dimethoxy-8-prenylflavone, T-268
4′,5-Dihydroxy-2′,7-dimethoxyisoflavanone, T-220
4′,6′-Dihydroxy-2′-methoxy-3′-methylchalcone, T-627
4′,7-Dihydroxy-2′-methoxy-3′-prenylisoflavan, T-686
5,7-Dihydroxy-2′-methoxy-4′,5′-methylenedioxyisoflavanone, P-149
3,5-Dihydroxy-2′-methoxybibenzyl, D-638
4,4′-Dihydroxy-2′-methoxychalcone, T-534
4′,7-Dihydroxy-2′-methoxyisoflavan, T-594
4,8-Dihydroxy-2(1*H*)-quinolinone, Q-14
3,12-Dihydroxy-2(9),7(14)-illudadien-8-one, D-510
3,13-Dihydroxy-2(9),7(14)-illudadien-8-one, D-510
1,11-Dihydroxy-2,10-dimethoxyaporphine, C-361
1,9-Dihydroxy-2,10-dimethoxyaporphine, I-74
1,11-Dihydroxy-2,10-dimethoxynoraporphine, C-361
1,9-Dihydroxy-2,10-dimethoxynoraporphine, I-74
3,9-Dihydroxy-2,10-diprenylpterocarpan, D-441
5,8-Dihydroxy-2,2-dimethyl-2*H*,6*H*-pyrano[3,2-*b*]xanthen-6-one, O-180
3,6-Dihydroxy-2,2-dimethyl-4-chromanone, D-228
6,11-Dihydroxy-2,2-dimethylpyrano[3,2-*c*]xanthen-7(2*H*)-one, D-434
1,5-Dihydroxy-2,3,4-trimethoxy-10-methylacridone, P-89
3′,4′-Dihydroxy-2,4,6-trimethoxybenzophenone, P-91
2,3-Dihydroxy-2,4-cyclopentadien-1-one, D-420
2,5-Dihydroxy-2,5-cyclohexadiene-1,4-dione, D-397
2,6-Dihydroxy-2,5-cyclohexadiene-1,4-dione, D-398
2,5-Dihydroxy-2,5-dimethyl-1,4-dithiane, D-781
2,4-Dihydroxy-2,5-dimethyl-3(2*H*)-thiophenone, T-349
4,8′-Dihydroxy-2,6′-dimethyl[1,2′-binaphthalene]-1′,4′,5,8-tetrone, N-32
4,14-Dihydroxy-2,6,10,14-tetramethyl-2,6,10,15-hexadecatetraenoic acid, D-662
4-(2,4-Dihydroxy-2,6,6-trimethylcyclohexylidene)-3-buten-2-one, D-530
5,7-Dihydroxy-2,6-dimethyl-4*H*-1-benzopyran-4-one, D-430
5,7-Dihydroxy-2,6-dimethylchromone, D-430
10,11-Dihydroxy-2,6-farnesadien-1-oic acid, D-464
8,14-Dihydroxy-2,6-lactaradien-5,14-olide, D-519
5,7-Dihydroxy-2,8-dimethyl-4*H*-1-benzopyran-4-one, D-431
5,7-Dihydroxy-2,8-dimethylchromone, D-431
5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione, D-507
5,6-Dihydroxy-2-(2-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-574
4,6-Dihydroxy-2-(3,4,5-trihydroxybenzylidene)-3(2*H*)-benzofuranone, P-90
5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)-1-benzopyrylium(1+), P-145
5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, P-135
2-[3,5-Dihydroxy-2-(3,7-dimethyl-2,6-octadienyl)-phenyl]-6-hydroxybenzofuran, A-152
5,7-Dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-6,8-dimethoxy-4*H*-1-benzopyran-4-one, T-709
5,6-Dihydroxy-2-(3-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-579
5,7-Dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-4*H*-1-benzopyran-4-one, T-549
5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,6-dimethoxy-4*H*-1-benzopyran-4-one, T-711
5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H*-1-benzopyran-4-one, T-618
5,7-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6,8-dimethoxy-4*H*-1-benzopyran-4-one, T-712
5,6-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7,8-dimethoxy-4*H*-1-benzopyran-4-one, T-710
3,5-Dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-4*H*-1-benzopyran-4-one, T-545
3,7-Dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-577
5,7-Dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-581
5,7-Dihydroxy-2-(4-hydroxyphenyl)-6-methyl-4*H*-1-benzopyran-4-one, T-632
3,5-Dihydroxy-2-(4-hydroxyphenyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, C-299
5,7-Dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-685
5,7-Dihydroxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, D-538
5,7-Dihydroxy-2-(5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, K-48
5,7-Dihydroxy-2-(5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)-3-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, K-47
3,4-Dihydroxy-2-(hydroxymethyl)piperidine, H-603
3,4-Dihydroxy-2-(hydroxymethyl)pyrrolidine, D-508
2′,4′-Dihydroxy-2-biphenylcarboxylic acid, D-405
1,6-Dihydroxy-2-caroten-9-one, D-423
1,4-Dihydroxy-2-cyclopentene-1-carboxylic acid, D-421
9,10-Dihydroxy-2-fenchanone, D-465
3,4-Dihydroxy-2-hydroxymethyl-1-pyrrolidinepropanamide, D-508
3,5-Dihydroxy-2-indolinone-3-acetic acid, D-237
3,7-Dihydroxy-2-indolinone-3-acetic acid, D-238
1,4-Dihydroxy-2-isopropylbenzene, I-120
2-[4,6-Dihydroxy-2-methoxy-3-(3-methyl-2-butenyl)phenyl]-6-hydroxy-3(2*H*)-benzofuranone, L-83
1-(4,6-Dihydroxy-2-methoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, T-627
1,5-Dihydroxy-2-methoxy-6-methylanthraquinone, T-621
3,6*a*-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan, P-174
1,3-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan, P-175
4,4′-Dihydroxy-2-methoxychalcone, T-533
3,9-Dihydroxy-2-methoxycoumestan, T-538
3-(3,4-Dihydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)-2-propen-1-one, T-146
5,7-Dihydroxy-2-methyl-4*H*-1-benzopyran-4-one, D-546
3,5-Dihydroxy-2-methyl-4*H*-pyran-4-one, D-559
6,7-Dihydroxy-2-methyl-5-[[(3-methylbutyl)imino]-methyl]-8-(1-methylethyl)-1,4-naphthalenedione, G-301
5,7-Dihydroxy-2-methyl-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, P-236
5,7-Dihydroxy-2-methyl-6-prenylchromone, P-236
2,3-Dihydroxy-2-methylbutanoic acid, D-547
2,3-Dihydroxy-2-methylbutanolide, D-234
9-(2,3-Dihydroxy-2-methylbutoxy)-4-methoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, B-264
2,3-Dihydroxy-2-methylbutyrolactone, D-234
5,7-Dihydroxy-2-methylchromone, D-546
1,4-Dihydroxy-2-methylnaphthalene, M-506
3,4-Dihydroxy-2-methylpiperidine, M-601
8,15-Dihydroxy-2-oxo-1(10),3,11(13)-guaiatrien-12,6-olide, D-590
4,10-Dihydroxy-2-oxo-1(5)-guaien-12,6-olide, T-587
5,6-Dihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, D-472
5,7-Dihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, D-473
6,7-Dihydroxy-2-phenyl-4*H*-1-benzopyran-4-one, D-474
5,7-Dihydroxy-2-phenylchroman, D-469
4,6-Dihydroxy-2-phenylquinoline, D-658
4,7-Dihydroxy-2-phenylquinoline, D-659
3,4-Dihydroxy-2-piperidinemethanol, H-603
3,9-Dihydroxy-2-prenylcoumestan, P-558
3,9-Dihydroxy-2-prenylpterocarpan, D-670
4,6-Dihydroxy-2-quinolinecarboxylic acid, D-683
3,5-Dihydroxy-2-stilbenecarboxylic acid, D-629
5,7-Dihydroxy-2-tritriacontyl-4*H*-1-benzopyran-4-one, D-703
5,7-Dihydroxy-2-tritriacontylchromone, D-703
4,6-Dihydroxy-2-[(3,4-dihydroxyphenyl)methylene]-3(2*H*)-benzofuranone, T-137
2,3-Dihydroxy-2-[(4-hydroxyphenyl)methyl]butanedioic acid, P-407
5,7-Dihydroxy-2-[4-hydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, T-555
5,7-Dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, T-684
5,7-Dihydroxy-2-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-556
2,3-Dihydroxy-20(29)-lupen-28-oic acid, L-118
3,16-Dihydroxy-20(29)-lupen-28-oic acid, L-119
11,12-Dihydroxy-20-nor-5(10),8,11,13-abietatetraen-1-one, D-561
3β,7β-Dihydroxy-22,23,24,25,26,27-hexanorlanost-8-ene-11,15,20-trione, L-111
3,24-Dihydroxy-22-oxo-12-oleanen-29-oic acid, D-605
3,26-Dihydroxy-23-hydroxymethylfurost-20(22)-en-6-one, D-506
2,3-Dihydroxy-23-oxo-12-oleanen-28-oic acid, D-597
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid, D-598
3,21-Dihydroxy-23-oxo-12-oleanen-28-oic acid, T-651
3,15-Dihydroxy-23-oxo-7,9(11),24-lanostatrien-26-oic acid, D-592
20,26-Dihydroxy-24-dammaren-3-one, D-422
3,22-Dihydroxy-24-methylcholest-5-en-7-one, E-222
3,5-Dihydroxy-24-methylcholesta-7,22-dien-6-one, E-204
22,23-Dihydroxy-24-methylcholestane-3,6-dione, T-564
3,16-Dihydroxy-24-methyllanosta-8,25-dien-21-oic acid, D-556
3,7-Dihydroxy-25,26,27-trinor-11,15-dioxolanost-8-en-24-oic acid, L-110
3,13-Dihydroxy-28-lupanoic acid, D-527
3,17-Dihydroxy-28-nor-12-oleanen-16-one, D-564
3,19-Dihydroxy-28-oleananoic acid, D-570
3,13-Dihydroxy-28-ursanoic acid, D-708
2,7-Dihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-399
4,7-Dihydroxy-2*H*-1-benzopyran-2-one, D-392
5,7-Dihydroxy-2*H*-1-benzopyran-2-one, D-393
6,7-Dihydroxy-2*H*-1-benzopyran-2-one, D-395
7,8-Dihydroxy-2*H*-1-benzopyran-2-one, D-396
4,8-Dihydroxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-477
2,4-Dihydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, H-353
6,7-Dihydroxy-2[(3,4-dihydroxyphenyl)methylene]-3(2*H*)-benzofuranone, T-138
2′,8-Dihydroxy-3′,4′,5′,7-tetramethoxyflavan, H-196
5,7-Dihydroxy-3′,4′,5′,8-tetramethoxyflavone, H-210
5,7-Dihydroxy-3′,4′,5′-trimethoxyflavone, P-135
7,8-Dihydroxy-3′,4′,5′-trimethoxyflavone, P-140
5,7-Dihydroxy-3′,4′,6,8-tetramethoxyflavone, D-695
5,7-Dihydroxy-3′,4′,6-trimethoxyflavone, D-699
5,6-Dihydroxy-3′,4′,7,8-tetramethoxyflavone, H-211
5′,8-Dihydroxy-3′,4′,7-trimethoxyflavan, P-106
2′,5′-Dihydroxy-3′,4′,7-trimethoxyisoflavan, P-148
3,5-Dihydroxy-3′,4′,7-tris(2-hydroxyethoxy)flavone 3-[6-*O*-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranoside], T-832
3′,4′-Dihydroxy-3′,4′-dihydroseselin, K-32

5,7-Dihydroxy-3′,4′-dimethoxy-5′-prenylflavanone, T-265
2′,4-Dihydroxy-3′,4′-dimethoxychalcone, T-145
5,7-Dihydroxy-3′,4′-dimethoxyflavonol, T-547
2′,7-Dihydroxy-3′,4′-dimethoxyisoflavan, T-217
2′,7-Dihydroxy-3′,4′-methylenedioxyisoflavone, T-221
2,4′-Dihydroxy-3′,4,6-trimethoxybenzophenone, P-91
4′,5-Dihydroxy-3′,5′,7,8-tetramethoxyflavone, H-210
4′,5-Dihydroxy-3′,5′,7-trimethoxyflavone, P-135
2,4′-Dihydroxy-3′,5′-dimethoxyacetophenone, T-133
4,4′-Dihydroxy-3′,5-dimethoxy-2,7′-cycloligna-7,7′-diene, D-71
4,4′-Dihydroxy-3′,5-dimethoxy-2,7′-cyclolignan, G-327
5,7-Dihydroxy-3′,6-dimethoxy-4′,5′-methylenedioxyflavanone, H-202
4′,5-Dihydroxy-3′,7-dimethoxydihydroflavonol, P-109
4′,5-Dihydroxy-3′,7-dimethoxyflavonol, T-545
4′,5-Dihydroxy-3′,7-dimethoxyisoflavone, T-224
4′,5-Dihydroxy-3′,8-dimethoxy-7-prenyloxyflavonol, T-157
4′,7-Dihydroxy-3′,8-diprenylflavanone, D-440
5,7-Dihydroxy-3′-methoxy-4′-*O*-isobutanoylflavanone, T-191
4,10-Dihydroxy-3,10-dimethoxypterocarpan, T-287
4,9-Dihydroxy-3,10-dimethoxypterocarpan, T-287
8,10-Dihydroxy-3,11(13)-guaiadien-12,6-olide, D-487
7,20-Dihydroxy-3,11,15,23-tetraoxolanost-8-en-26-oic acid, D-697
7,12-Dihydroxy-3,11,15,23-tetraoxolanost-8-en-26-oic acid, T-714
7,12-Dihydroxy-3,11,15,23-tetraoxolanosta-8,20(22)-dien-26-oic acid, D-696
7,12-Dihydroxy-3,11,15-trioxo-25,26,27-trinor-8-lanosten-24-oic acid, T-713
7β,12α-Dihydroxy-3,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid, L-105
7,15-Dihydroxy-3,11,23-trioxolanost-8-en-26-oic acid, D-702
7β,15α-Dihydroxy-3,11,23-trioxolanosta-8,20(22)*E*-dien-26-oic acid, T-551
15,23-Dihydroxy-3,11-dioxolanosta-8,24-dien-26-oic acid, D-437
5,8-Dihydroxy-3,3′,4′,7-tetramethoxyflavone, H-209
4,4′-Dihydroxy-3,3′,5,5′-tetramethoxy-7,7′-epoxylignan, H-194
4,4′-Dihydroxy-3,3′,5,5′-tetramethoxy-7,9′:7′,9-diepoxylignan, S-292
4,4′-Dihydroxy-3,3′,5-trimethoxy-7,7′-epoxylignan, P-99
4,4′-Dihydroxy-3,3′-dimethoxy-2,7′-cyclolign-7-ene, D-71
4,4′-Dihydroxy-3,3′-dimethoxy-7,7′-epoxylignan, D-427
4,4′-Dihydroxy-3,3′-dimethoxy-7,9′:7′,9-diepoxylignan, P-383
4,4′-Dihydroxy-3,3′-dimethoxy-9,9′-epoxylignan, D-428
4,4′-Dihydroxy-3,3′-dimethoxylignan-9,9′-olide, M-81
4,4′-Dihydroxy-3,3′-dimethoxystilbene, B-124
5,13-Dihydroxy-3,3,10,10-tetramethyl-6-(3-methyl-2-butenyl)-2*H*-dipyrano[2,3-*a*:2′,3′-*i*]xanthen-14-one, T-426
N-(2,4-Dihydroxy-3,3-dimethyl-1-oxobutyl)-β-alanine, P-31
6,11-Dihydroxy-3,3-dimethyl-8-(2-methyl-1-propenyl)-3*H*,7*H*,8*H*-bis[1]benzopyrano[4,3-*b*:6′,5′-*e*]pyran-7-one, C-487
2,4-Dihydroxy-3,3-dimethylbutyric acid γ-lactone, D-256
3′,5-Dihydroxy-3,4′,6,7-tetramethoxyflavone, D-694
5,6-Dihydroxy-3,4′,8-trimethoxyflavone, P-138
9,9′-Dihydroxy-3,4,5-trimethoxy-3′,4′-methylenedioxylignan, H-89
2,6-Dihydroxy-3,4,7-trimethoxydibenzofuran, D-128
1,5-Dihydroxy-3,4-dimethoxy-10-methylacridone, T-135
4′,7-Dihydroxy-3,4-flavandiol, T-182
1,6-Dihydroxy-3,5-dimethoxy-10-methylacridone, T-136
1,8-Dihydroxy-3,5-dimethoxy-2-prenylxanthone, T-282
1,6-Dihydroxy-3,5-dimethoxyacridone, T-136
2,7-Dihydroxy-3,5-dimethoxyphenanthrene, P-247
4′,5-Dihydroxy-3,6,8-trimethoxyflavone, P-138
1,5-Dihydroxy-3,6-dimethoxy-10-methylacridone, T-136
1,7-Dihydroxy-3,6-dimethoxy-2,8-diprenylxanthone, T-173
1,5-Dihydroxy-3,6-dimethoxy-4,8-diprenylxanthone, T-171
4′,7-Dihydroxy-3,6-dimethoxyflavone, T-207
1,7-Dihydroxy-3,6-dimethoxyxanthone, T-297
1,8-Dihydroxy-3,7(11)-eudesmadien-12,8-olide, D-456
10,11-Dihydroxy-3,7,11-trimethyl-2,6-dodecadienoic acid, D-464
1,6-Dihydroxy-3,7-dimethoxy-2,8-diprenylxanthone, T-173
3′,4′-Dihydroxy-3,7-dimethoxyflavanone, T-189
5,8-Dihydroxy-3,7-dimethoxyflavone, T-209
1,6-Dihydroxy-3,7-dimethoxyxanthone, T-297
7-[(6,7-Dihydroxy-3,7-dimethyl-2-octenyl)oxy]-2*H*-1-benzopyran-2-one, M-77
4-[(6,7-Dihydroxy-3,7-dimethyl-2-octenyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, B-66
7-[(6,7-Dihydroxy-3,7-dimethyl-5-oxooctyl)oxy]-2*H*-1-benzopyran-2-one, M-77
5,7-Dihydroxy-3,8-bis(3-methyl-2-butenyl)-2-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, P-98
5,7-Dihydroxy-3,8-dimethoxyflavone, T-209
2,5-Dihydroxy-3-(10-pentadecenyl)-1,4-benzoquinone, D-609
6,7-Dihydroxy-3-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, P-150
5,7-Dihydroxy-3-(2-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-599
2,5-Dihydroxy-3-(3,7,11-trimethyl-2,6,10-dodecatrienyl)cyclohexadiene-1,4-dione, B-176
5,7-Dihydroxy-3-(3-hydroxy-4-methoxybenzyl)-4-chromanone, D-404
4,6-Dihydroxy-3-(3-methyl-2-butenyl)-2-(2-phenylethenyl)benzoic acid, D-674
2,4-Dihydroxy-3-(3-methyl-2-butenyl)-6-(2-phenylethenyl)benzoic acid, D-673
3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-(3,4-dihydroxyphenyl)-2-propen-1-one, T-262
3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-166
1-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-2-(2-hydroxy-4-methoxyphenyl)ethanedione, L-78
1-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-3-(2,4-dihydroxyphenyl)-2-propen-1-one, T-261
[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-5,7-dihydroxy-4*H*-1-benzopyran-4-one, T-275
3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-167
3-[2,4-Dihydroxy-3-(3-methyl-2-butenyl)phenyl]-7-hydroxy-8-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, L-81
5,7-Dihydroxy-3-(4-hydroxybenzyl)-4-chromanone, D-502
5,8-Dihydroxy-3-(4-hydroxybenzyl)-6,7-dimethoxy-4-chromanone, T-213
5,8-Dihydroxy-3-(4-hydroxybenzyl)-7-methoxy-4-chromanone, T-589
5,7-Dihydroxy-3-(4-hydroxybenzyl)-8-methoxy-4-chromanone, T-589
6,7-Dihydroxy-3-(4-hydroxyphenyl)-2*H*-furo[3,2-*b*][1]benzopyran-2-one, A-490
5,7-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-601
6,7-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-602
7,8-Dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-603
5,7-Dihydroxy-3-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-688
5,7-Dihydroxy-3-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-689
5,7-Dihydroxy-3-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, D-542
5,7-Dihydroxy-3-(8-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-4*H*-1-benzopyran-4-one, S-83
2,5-Dihydroxy-3-(8-pentadecenyl)-1,4-benzoquinone, D-609
1,10-Dihydroxy-3-guaien-12,6-olide, D-491
1,8-Dihydroxy-3-hydroxymethyl-6-methoxyanthraquinone, T-590
1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthraquinone, T-590
1,8-Dihydroxy-3-hydroxymethyl-9,10-anthracenedione, D-503
1,8-Dihydroxy-3-hydroxymethylanthraquinone, D-503
3,4-Dihydroxy-3-hydroxymethylbutanoic acid, D-504
5,7-Dihydroxy-3-isobutanoyloxyflavanone, T-568
6,8-Dihydroxy-3-methoxy-1-methylanthraquinone-2-carboxylic acid, T-626
1,5-Dihydroxy-3-methoxy-10-methyl-4-prenylacridone, T-677
1,5-Dihydroxy-3-methoxy-10-methylacridone, T-514
1,6-Dihydroxy-3-methoxy-10-methylacridone, T-515
1,5-Dihydroxy-3-methoxy-2,4-diprenylxanthone, T-559
6*a*,9-Dihydroxy-3-methoxy-2-prenylpterocarpan, T-691
1,9-Dihydroxy-3-methoxy-2-prenylpterocarpan, T-694
1,5-Dihydroxy-3-methoxy-2-prenylxanthone, T-696
1,6-Dihydroxy-3-methoxy-2-prenylxanthone, T-697
1,7-Dihydroxy-3-methoxy-2-prenylxanthone, T-698
4,9-Dihydroxy-3-methoxy-3′,4′-methylenedioxy-7,9′-epoxylignan, P-100
1,7-Dihydroxy-3-methoxy-6-methylanthraquinone, T-623
2,6*a*-Dihydroxy-3-methoxy-8,9-methylenedioxypterocarpan, P-174
4,9-Dihydroxy-3-methoxycoumestan, T-539
5,7-Dihydroxy-3-methoxyflavanone, T-568
3′,4′-Dihydroxy-3-methoxyflavone, T-575
5,7-Dihydroxy-3-methoxyflavone, T-580
6*a*,9-Dihydroxy-3-methoxypterocarpan, T-700
4,9-Dihydroxy-3-methoxypterocarpan, T-702
α,4-Dihydroxy-3-methoxytoluene, D-400
1,7-Dihydroxy-3-methoxyxanthone, T-724
2,4-Dihydroxy-3-methyl-2-hexenoic acid γ-lactone, E-319
1-(1,8-Dihydroxy-3-methyl-2-naphthalenyl)ethanone, A-72
6,11-Dihydroxy-3-methyl-3-(4-methyl-3-pentenyl)-3*H*,7*H*-pyrano[2,3-*c*]xanthen-7-one, D-557
6-(1,2-Dihydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, C-291
1,6-Dihydroxy-3-methyl-9,10-anthracenedione, D-543
1,8-Dihydroxy-3-methyl-9,10-anthracenedione, D-544
1,6-Dihydroxy-3-methylanthraquinone, D-543
1,8-Dihydroxy-3-methylanthraquinone, D-544
9-(2,3-Dihydroxy-3-methylbutoxy)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, H-125
5-(2,3-Dihydroxy-3-methylbutyl)-4-(3,4-epoxy-4-methylpentanoyl)-3,4-dihydroxy-2-isopentanoyl-2-cyclopenten-1-one, D-549
3-(2,3-Dihydroxy-3-methylbutyl)-4-methoxy-1-methyl-2(1*H*)-quinolinone, E-2
6-(2,3-Dihydroxy-3-methylbutyl)-5,7-dimethoxy-2*H*-1-benzopyran-2-one, T-419

3,4-Dihydroxy-3-methyldihydro-2(3*H*)-furanone, M-433
11,13-Dihydroxy-3-oxo-10(14)-guaien-12,6-olide, D-591
2,20-Dihydroxy-3-oxo-12-ursen-28-oic acid, D-607
6,19-Dihydroxy-3-oxo-12-ursen-28-oic acid, T-721
2,5-Dihydroxy-3-pentadecyl-1,4-benzoquinone, D-609
2,5-Dihydroxy-3-pentadecyl-2,5-cyclohexadiene-1,4-dione, D-609
5,7-Dihydroxy-3-phenyl-4*H*-1-benzopyran-4-one, D-514
2,3-Dihydroxy-3-phenylpropanoic acid, D-646
4,6-Dihydroxy-3-prenyl-2-styrylbenzoic acid, D-674
2,4-Dihydroxy-3-prenyl-6-styrylbenzoic acid, D-673
5,7-Dihydroxy-3-propanoyloxyflavanone, T-568
β-(2,4-Dihydroxy-3-pyrimidinyl)alanine, I-196
2,5-Dihydroxy-3-undecyl-1,4-benzoquinone, D-705
2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione, D-705
6,7-Dihydroxy-3-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-2*H*-1-benzopyran-2-one, E-1
5,7-Dihydroxy-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, T-687
2,3-Dihydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, D-563
2,3-Dihydroxy-30-nor-12,20(29)-oleanadiene-23,28-dioic acid, D-565
2,3-Dihydroxy-30-nor-23-oxo-12,20(29)-oleanadien-28-oic acid, D-565
3β,7β-Dihydroxy-4α-hydroxymethyl-4β,14α-dimethyl-11,15-dioxo-5α-chol-8-en-24-oic acid, L-108
3β,12β-Dihydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, L-108
3′,5-Dihydroxy-4′,5′,7,8-tetramethoxyflavone, H-210
3′,5-Dihydroxy-4′,5′,7-trimethoxyflavone, P-135
3′,8-Dihydroxy-4′,5′,7-trimethoxyflavone, P-140
3,3′-Dihydroxy-4′,5,7-trimethoxyflavan, P-104
2′,7-Dihydroxy-4′,5-dimethoxy-3′-prenylisoflavan, T-273
3,7-Dihydroxy-4′,5-dimethoxyflavan, T-184
6,7-Dihydroxy-4′,5-dimethoxyflavone, T-210
2′,4-Dihydroxy-4′,6′-dimethoxy-3′-prenylchalcone, T-263
2′,7-Dihydroxy-4′,6′-dimethoxy-3′-prenylisoflavone, T-278
2′,4-Dihydroxy-4′,6′-dimethoxychalcone, T-147
2′,4-Dihydroxy-4′,6′-dimethoxydihydrochalcone, H-752
2′,4-Dihydroxy-4′,6-dimethoxychalcone 4-glucoside, T-147
2′,7-Dihydroxy-4′,6-dimethoxyisoflavan, T-219
3′,5-Dihydroxy-4′,7-dimethoxydihydroflavonol, P-109
2′,5-Dihydroxy-4′,7-dimethoxyflavanone, T-186
3′,5-Dihydroxy-4′,7-dimethoxyflavanone, T-191
5,8-Dihydroxy-4′,7-dimethoxyflavone, T-211
2′,5-Dihydroxy-4′,7-dimethoxyisoflavone, T-222
5,7-Dihydroxy-4′,8-dimethoxyflavone, T-211
5,7-Dihydroxy-4′,8-dimethoxyflavonol, T-548
3′,7-Dihydroxy-4′,8-dimethoxyisoflavone, T-225
2′,6′-Dihydroxy-4′-methoxy-β-phenylpropiophenone, P-322
2′,6′-Dihydroxy-4′-methoxy-2-methylpropiophenone, M-705
2′,6′-Dihydroxy-4′-methoxy-3′,5′-dimethyldihydrochalcone, P-320
2′,6′-Dihydroxy-4′-methoxy-3′-methylchalcone, T-627
2′,6′-Dihydroxy-4′-methoxy-3′-methyldihydrochalcone, P-321
5,7-Dihydroxy-4′-methoxy-3′-prenylisoflavone, T-687
5,7-Dihydroxy-4′-methoxy-6-prenylisoflavone, T-688
5,7-Dihydroxy-4′-methoxy-8-methylflavanone, T-631
5,7-Dihydroxy-4′-methoxy-8-methylisoflavanone, T-633
2′,7-Dihydroxy-4′-methoxy-8-prenylflavan, T-680
5,7-Dihydroxy-4′-methoxy-8-prenylisoflavone, T-689
2′,6′-Dihydroxy-4′-methoxyacetophenone, T-512
2′,6′-Dihydroxy-4′-methoxychalcone, T-535
2′,6′-Dihydroxy-4′-methoxydihydrochalone, P-322
3,4-Dihydroxy-4′-methoxyflavan, T-565
5,7-Dihydroxy-4′-methoxyflavanone, D-537
5,7-Dihydroxy-4′-methoxyflavone, D-538
3′,7-Dihydroxy-4′-methoxyflavone, T-578
5,7-Dihydroxy-4′-methoxyflavonol, T-616
2′,7-Dihydroxy-4′-methoxyisoflavan, D-540
2′,7-Dihydroxy-4′-methoxyisoflavanone, T-595
3′,7-Dihydroxy-4′-methoxyisoflavanone, T-596
5,7-Dihydroxy-4′-methoxyisoflavanone, T-597
5,7-Dihydroxy-4′-methoxyisoflavone, D-542
2′,7-Dihydroxy-4′-methoxyisoflavone, T-598
6,7-Dihydroxy-4′-methoxyisoflavone, T-602
2′,6-Dihydroxy-4′-prenyloxychalcone, T-535
2′,6′-Dihydroxy-4′-prenyloxydihydrochalcone, P-322
5,7-Dihydroxy-4′-prenyloxyflavanone, T-569
3,8-Dihydroxy-4(15),10(14),11(13)-guaiatrien-12,6-olide, D-489
1,5-Dihydroxy-4(15),11(13)-eudesmadien-12,6-olide, D-455
(11α)-1β,5α-Dihydroxy-4(15)-eudesmen-12,6α-olide, D-455
3,8-Dihydroxy-4(15)-guaien-12,6-olide, D-492
2,8-Dihydroxy-4(6)-lactaren-5,14-olide, D-520
8,12-Dihydroxy-4(6)-lactaren-5,14-olide, H-531
8,14-Dihydroxy-4(6)-lactaren-5-al, H-530
1,6-Dihydroxy-4,10(14),11(13)-germacratrien-12,8-olide, D-483
2,9-Dihydroxy-4,10(14)-oplopadien-3-one, D-588
3,9-Dihydroxy-4,10-diprenylpterocarpan, D-442
1,3-Dihydroxy-4,11(13)-eudesmadien-12,6-olide, D-454
3,10-Dihydroxy-4,11-dodecadiene-6,8-diynoic acid, D-444
3,3′-Dihydroxy-4,4′-diketo-β-carotene, A-474
2′,6′-Dihydroxy-4,4′-dimethoxychalcone, T-147
2′,6′-Dihydroxy-4,4′-dimethoxydihydrochalcone, H-752
3β,12β-Dihydroxy-4,4,14α-trimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, L-109
3,7-Dihydroxy-4,4,14-trimethyl-11,15-dioxochol-8-en-24-oic acid, L-110
7β,12α-Dihydroxy-4,4,14-trimethyl-3,11,15-trioxochol-8-en-24-oic acid, L-105
3β,7β-Dihydroxy-4,4,14-trimethyl-5α-pregn-8-ene-11,15,20-trione, L-111
2,3-Dihydroxy-4,5-dimethoxybibenzyl, P-319
1-(2,3-Dihydroxy-4,5-dimethoxyphenyl)-2-phenylethane, P-319
3,6-Dihydroxy-4,5-diphenyl-2-piperidinone, D-438
2′,4′-Dihydroxy-4,6′-dimethoxychalcone, T-147
2′,4′,-Dihydroxy-4,6′-dimethoxydihydrochalcone, H-752
β,2-Dihydroxy-4,6-dimethoxy-3-methylchalcone, T-247
9,10-Dihydroxy-4,6-heptadecadiyn-3-one, D-498
6,9-Dihydroxy-4,7-megastigmadien-3-one, D-531
6,10-Dihydroxy-4,7-megastigmadiene-3,9-dione, D-528
1,6-Dihydroxy-4,9,11(13)-germacratrien-12,8-olide, D-482
1,5-Dihydroxy-4-(2-hydroxy-3-methyl-3-butenyl)-3-methoxy-10-methylacridone, T-677
2-[3,5-Dihydroxy-4-(3,7-dimethyl-2,6-octadienyl)-phenyl]-6-hydroxybenzofuran, A-153
4-[2-[3,5-Dihydroxy-4-(3-methyl-1-butenyl)phenyl]ethenyl]-1,2-benzenediol, A-398
3,9-Dihydroxy-4-(3-methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, P-238
2,3-Dihydroxy-4-decynoic acid, D-424
1,3-Dihydroxy-4-eudesmen-12,6-olide, D-459
2,11-Dihydroxy-4-eudesmen-3-one, D-462
6,11-Dihydroxy-4-eudesmen-3-one, D-463
1,3-Dihydroxy-4-eudesmen-6-one, D-461
1,7-Dihydroxy-4-isopropyl-1,6-dimethyl-2(1*H*)-naphthalenone, L-20
2,8-Dihydroxy-4-isopropyl-7-methoxy-6-methyl-1-naphthalenecarboxaldehyde, T-527
2,7-Dihydroxy-4-isopropyl-8-methoxy-6-methyl-1-naphthalenecarboxaldehyde, T-527
9,13-Dihydroxy-4-megastigmen-3-one, D-534
2′,6′-Dihydroxy-4-methoxy-3′,5′-dimethylchalcone, T-550
1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone, P-320
1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-3-phenyl-2-propen-1-one, T-550
1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
3-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, T-627
2,3′-Dihydroxy-4-methoxy-5′,6-dimethyldiphenyl ether, D-536
2,6-Dihydroxy-4-methoxybenzophenone, T-521
3,5-Dihydroxy-4-methoxyphenethyl alcohol, T-664
2-(3,5-Dihydroxy-4-methoxyphenyl)-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, P-159
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone, H-752
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one, T-147
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)-1-propanone, H-752
1-(2,6-Dihydroxy-4-methoxyphenyl)-3-phenyl-1-propanone, P-322
2-(3,5-Dihydroxy-4-methoxyphenyl)ethanol, T-664
3,9-Dihydroxy-4-prenylcoumestan, P-238
2-(3,5-Dihydroxy-4-prenylphenyl)-6-hydroxybenzofuran, M-750
3,9-Dihydroxy-4-prenylpterocarpan, D-671
3,5-Dihydroxy-4-prenylstilbene, M-348
2,6-Dihydroxy-4-pyrimidinecarboxylic acid, D-680
2,6-Dihydroxy-4-quinolinecarboxylic acid, D-681
2,8-Dihydroxy-4-quinolinecarboxylic acid, D-682
5,7-Dihydroxy-4*H*-1-benzopyran-4-one, D-394
3β,20*S*-Dihydroxy-5α-pregnane-20,16β-carbolactone, L-129
2′,6′′-Dihydroxy-5′′-methoxylythran-12-one, V-20
2,3′-Dihydroxy-5′-methoxybibenzyl, D-638
1,2-Dihydroxy-5,12,15-heneicosatrien-4-one, D-496
4,4′-Dihydroxy-5,5′-diisopropyl-2,2′-dimethyl-3,6-biphenyldione, D-426
3,6-Dihydroxy-5,6-dihydro-β-ionol, M-104
1,3-Dihydroxy-5,6-dimethoxy-10-methylacridone, T-136
2′,4′-Dihydroxy-5,7-dimethoxy-3′,6-diprenylisoflavan, T-164
2′,4′-Dihydroxy-5,7-dimethoxyisoflavone, T-222
3,4-Dihydroxy-5,7-megastigmadien-9-one, D-529
6,12-Dihydroxy-5,8,11,13-abietatetraen-7-one, H-327
3,7-Dihydroxy-5,8-dimethoxyflavone, T-209
3,4-Dihydroxy-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)benzoic acid, P-400
3,4-Dihydroxy-5-(3-methyl-2-butenoyl)benzoic acid, D-548
3,4-Dihydroxy-5-(3-methyl-2-butenyl)benzoic acid, D-548
2-[3,4-Dihydroxy-5-(3-methyl-2-butenyl)phenyl]-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, T-265
2-[3,4-Dihydroxy-5-(3-methyl-2-butenyl)phenyl]-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-162
3-[3,4-Dihydroxy-5-(3-methyl-2-butenyl)phenyl]-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-168
7-[2,4-Dihydroxy-5-(3-methyl-2-butenyl)phenyl]-7,8-dihydro-5-hydroxy-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, C-28
4,4′-[[2,4-Dihydroxy-5-(hydroxymethyl)-1,3-phenylene]bis(azo)]bis-1-naphthalenesulfonic acid, C-252
3,4-Dihydroxy-5-(hydroxymethyl)-2(5*H*)-furanone, D-505
6,7-Dihydroxy-5-(isobutyliminomethyl)-8-isopropyl-2-methyl-1,4-naphthoquinone, G-301
4,6-Dihydroxy-5-benzofuranpropanoic acid, D-385

1,2-Dihydroxy-5-heneicosen-4-one, D-497
2,7-Dihydroxy-5-isopropyl-3-methyl-1,4-naphthoquinone, D-515
3,4-Dihydroxy-5-megastigmen-9-one, D-532
3-(3,4-Dihydroxy-5-methoxy)-2-propenoic acid, T-672
1,3-Dihydroxy-5-methoxy-10-methylacridone, T-514
1,6-Dihydroxy-5-methoxy-2-methylanthraquinone, T-621
4′,7-Dihydroxy-5-methoxy-8-prenylflavanone, T-683
4′,7-Dihydroxy-5-methoxy-8-prenylisoflavone, T-689
3,4-Dihydroxy-5-methoxybenzoic acid, T-520
3,3′-Dihydroxy-5-methoxybibenzyl, D-639
3,4-Dihydroxy-5-methoxycinnamoic acid, T-672
N-(3,4-Dihydroxy-5-methoxycinnamoyl)-1,4-butanediamine, S-256
3,7-Dihydroxy-5-methoxyflavanone, T-568
3,7-Dihydroxy-5-methoxyflavone, T-580
2-(3,4-Dihydroxy-5-methoxyphenyl)-3,5,7-trihydroxy-1-benzopyrylium(1+), P-161
1,3-Dihydroxy-5-nonadecylbenzene, N-95
3,4-Dihydroxy-5-prenylbenzoic acid, D-548
2,3-Dihydroxy-5-undecyl-1,4-benzoquinone, D-704
2,3-Dihydroxy-5-undecyl-2,5-cyclohexadiene-1,4-dione, D-704
3,4-Dihydroxy-5-[(3,4,5-trihydroxybenzoyl)oxy]-benzoic acid 5-carboxy-2,3-dihydroxyphenyl ester, T-503
2′,4′-Dihydroxy-6′-methoxy-2-methylpropiophenone, M-705
2′,4′-Dihydroxy-6′-methoxy-3′,5′-dimethylchalcone, T-550
2′,4′-Dihydroxy-6′-methoxy-3′,5′-dimethyldihydrochalcone, P-320
2′,4′-Dihydroxy-6′-methoxy-3′-methylchalcone, T-627
2′,4′-Dihydroxy-6′-methoxy-3′-methyldihydrochalcone, P-321
2′,4′-Dihydroxy-6′-methoxyacetophenone, T-512
2′,4′-Dihydroxy-6′-methoxychalcone, T-535
2′,4′-Dihydroxy-6′-methoxydihydrochalcone, P-322
5,5′-Dihydroxy-6,6′,8,8′-tetramethoxy-2,2′-dimethyl-7,10′-bi-4*H*-naphtho[2,3-*b*]pyran-4,4′-dione, A-493
5,5′-Dihydroxy-6,6′,8,8′-tetramethoxy-2,2′-dimethyl[10,10′-bi-4*H*-naphtho[2,3-*b*]pyran]-4,4′-dione, N-61
4′,5-Dihydroxy-6,7,8-trimethoxyflavone, P-143
2,4-Dihydroxy-6,7-dimethoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, T-524
3,4′-Dihydroxy-6,7-dimethoxyflavone, T-207
1,3-Dihydroxy-6,7-dimethoxyxanthone, T-297
3,5-Dihydroxy-6,7-megastigmadien-9-one, D-530
2′,5-Dihydroxy-6,7-methylenedioxyflavanone, T-188
3,5-Dihydroxy-6,7-methylenedioxyflavanone, T-193
4′,5-Dihydroxy-6,7-methylenedioxyisoflavone, D-551
7,7′-Dihydroxy-6,8′-bicoumarin, B-76
5,7-Dihydroxy-6,8-dimethyl-2-phenyl-4*H*-1-benzopyran-4-one, D-433
5,7-Dihydroxy-6,8-dimethylflavanone, D-432
5,7-Dihydroxy-6,8-dimethylflavone, D-433
3,11-Dihydroxy-6,9-eremophiladien-8-one, D-449
2,4-Dihydroxy-6-(2-phenylethenyl)benzoic acid, D-629
7,8-Dihydroxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, D-668
5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, N-153
5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, M-50
5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, N-38
5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methylbutyryl)-4-phenylcoumarin, M-50
5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(2-methylbutyryl)-4-propylcoumarin, N-38
5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, M-49
5,7-Dihydroxy-6-(3-methyl-2-butenyl)-8-(3-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, M-53
2,4-Dihydroxy-6-(8-pentadecenyl)benzoic acid, D-608
1,3-Dihydroxy-6-hydroxymethyl-8-methoxyanthraquinone, T-590
5,7-Dihydroxy-6-isovaleryl-8-(3-methyl-2-butenyl)-4-propylcoumarin, I-99
3,8-Dihydroxy-6-methoxy-1-methylanthraquinone-2-carboxylic acid, T-626
5,7-Dihydroxy-6-methoxy-2-phenyl-4*H*-1-benzopyran-4-one, D-539
1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone, P-320
1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-2-propen-1-one, T-550
5,7-Dihydroxy-6-methoxy-3-(2,4,5-trimethoxyphenyl)-4*H*-1-benzopyran-4-one, H-214
7-[2,4-Dihydroxy-6-methoxy-3-(3-methyl-2-butenyl)phenyl]-5-hydroxy-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, C-27
1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, T-627
3,8-Dihydroxy-6-methoxy-7(11)-eremophilen-12,8-olide, T-561
2,4-Dihydroxy-6-methoxybenzophenone, T-521
5,7-Dihydroxy-6-methoxyflavanone, T-572
5,7-Dihydroxy-6-methoxyflavone, D-539
4′,7-Dihydroxy-6-methoxyisoflavone, T-602
1-(2,4-Dihydroxy-6-methoxyphenyl)-2-methyl-1-propanone, M-705
1-(2,4-Dihydroxy-6-methoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone, H-752
1-(2,4-Dihydroxy-6-methoxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one, T-147
1-(2,4-Dihydroxy-6-methoxyphenyl)-3-(4-methoxyphenyl)-1-propanone, H-752
1-(2,4-Dihydroxy-6-methoxyphenyl)-3-phenyl-1-propanone, P-322
2,8-Dihydroxy-6-methyl-1,4-naphthoquinone, D-558
5,7-Dihydroxy-6-methyl-2-phenyl-4*H*-1-benzopyran-4-one, D-554
2,4-Dihydroxy-6-methyl-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)benzaldehyde, S-60
2,4-Dihydroxy-6-methylbenzoic acid 3-hydroxy-4,5-bis(hydroxymethyl)-2-(3-methyl-2-butenyl)-phenyl ester, M-770
5,7-Dihydroxy-6-methylflavanone, D-553
5,7-Dihydroxy-6-methylflavone, D-554
3,9-Dihydroxy-6-oxopterocarpen (obsol.), C-370
7,8-Dihydroxy-6-prenylcoumarin, D-668
5,7-Dihydroxy-6-prenylflavanone, D-669
2,4-Dihydroxy-6-styrylbenzoic acid, D-629
3,9-Dihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, C-370
4,5-Dihydroxy-7(11),9-guaiadien-8-one, D-488
1,8-Dihydroxy-7(11)-eremophilen-12,8-olide, D-450
3,6-Dihydroxy-7(11)-eremophilen-12,8-olide, D-451
6,8-Dihydroxy-7(11)-eremophilen-12,8-olide, D-452
4,10-Dihydroxy-7(11)-guaien-8-one, D-494
3β,28-Dihydroxy-7,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid, L-108
3β,12β-Dihydroxy-7,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid, L-109
3,20-Dihydroxy-7,11,15-trioxolanosta-8,24-dien-26-oic acid, D-700
3,23-Dihydroxy-7,11,15-trioxolanosta-8,24-dien-26-oic acid, T-552
11,12-Dihydroxy-7,14-dimethoxy-8,11,13-abietatrien-20,6-olide, R-54
2,6-Dihydroxy-7,15-pimaradien-19-oic acid, D-663
3,4-Dihydroxy-7,8-dihydro-β-ionone, D-532
2,4-Dihydroxy-7,8-dimethoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, T-525
3,4′-Dihydroxy-7,8-dimethoxyflavone, T-208
3,5-Dihydroxy-7,8-dimethoxyflavone, T-209
4′,5-Dihydroxy-7,8-dimethoxyflavone, T-211
4,4′-Dihydroxy-7,9′:7′,9-diepoxylignan, L-85
3,14-Dihydroxy-7,9(11),15-pimaratriene-2,12-dione, D-665
5,7-Dihydroxy-7-(3-methyl-2-butenyl)-8-(2-methyl-2-oxopropyl)-3-propyl-2*H*-1-benzopyran-2-one, M-54
O-(3,6-Dihydroxy-7-drimen-11-yl)umbelliferone, D-447
6,9-Dihydroxy-7-megastigmen-3-one, D-533
1,3-Dihydroxy-7-methoxy-2,8-diprenylxanthone, T-560
3,5-Dihydroxy-7-methoxy-2-methylanthraquinone, T-623
2,4-Dihydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-399
9,10-Dihydroxy-7-methoxy-3-methyl-1*H*-naphtho[2,3-*c*]pyran-1-one, T-424
4′,5-Dihydroxy-7-methoxy-6-methylflavone, T-632
4′,5-Dihydroxy-7-methoxy-6-prenylflavanone, T-682
4′,5-Dihydroxy-7-methoxy-6-prenylisoflavone, T-688
4′,5-Dihydroxy-7-methoxy-8-methylflavanone, T-631
2′,4′-Dihydroxy-7-methoxy-8-prenylflavan, T-680
4′,5-Dihydroxy-7-methoxy-8-prenylflavone, T-685
2,6-Dihydroxy-7-methoxy-9-methyl-4-dibenzofurancarboxylic acid, T-628
1,6-Dihydroxy-7-methoxycarbonyl-8-methylanthraquinone, D-545
8,12-Dihydroxy-7-methoxycoumestan, T-539
3,5-Dihydroxy-7-methoxyflavanone, T-568
3,4′-Dihydroxy-7-methoxyflavone, T-577
3,5-Dihydroxy-7-methoxyflavone, T-580
2′,4′-Dihydroxy-7-methoxyisoflavan, T-594
4′,5-Dihydroxy-7-methoxyisoflavone, D-541
4′,6-Dihydroxy-7-methoxyisoflavone, T-602
1,3-Dihydroxy-7-methoxyxanthone, T-724
5,6-Dihydroxy-7-protoilluden-14-al, D-677
5,9-Dihydroxy-7-protoilluden-14-al, D-678
6,14-Dihydroxy-7-protoilluden-5-one, D-677
15,19-Dihydroxy-7-trachylobanone, D-698
4,9-Dihydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, D-476
3,12-Dihydroxy-8(14),15-pimaradien-2-one, D-664
5,11-Dihydroxy-8(14),15-rosadien-7-one, D-684
14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid, D-518
11,12-Dihydroxy-8,11,13-abietatrien-20,7-olide, C-117
11,14-Dihydroxy-8,11,13-abietatrien-20,7-olide, C-117
11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid, A-9
7,12-Dihydroxy-8,11,13-abietatrien-6-one, D-367
11,12-Dihydroxy-8,11,13-icetexatrien-20-one, D-509
6,13-Dihydroxy-8,14-labdadien-7-one, L-6
3,6*a*-Dihydroxy-8,9-methylenedioxypterocarpan, T-285
5,7-Dihydroxy-8-(2-methyl-1-oxopropyl)-7-prenyl-3-propylcoumarin, M-54
5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, M-52
5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, M-48
5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methyl-1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, M-51
5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methylbutryl)-4-propylcoumarin, M-51
5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(2-methylbutyryl)-4-phenylcoumarin, M-48
5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*-1-benzopyran-2-one, M-56
5,7-Dihydroxy-8-(3-methyl-2-butenyl)-6-(3-methyl-

1-oxobutyl)-4-propyl-2*H*-1-benzopyran-2-one, I-99
5,7-Dihydroxy-8-(4-hydroxy-3-methyl-2-butenyl)-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, G-55
5,10-Dihydroxy-8-daucen-2-one, D-423
5,7-Dihydroxy-8-isopentenyl-6-isovaleroyl-4-phenylcoumarin, M-56
5,7-Dihydroxy-8-isovaleryl-6-(3-methyl-2-butenyl)-4-phenylcoumarin, M-49
5,7-Dihydroxy-8-isovaleryl-6-(3-methyl-2-butenyl)-4-propylcoumarin, M-53
5,6-Dihydroxy-8-methoxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, T-634
5,6-Dihydroxy-8-methoxy-2-methylbenzo[*g*]chromen-4-one, T-634
5,7-Dihydroxy-8-methoxy-3-(4-methoxybenzyl)-4-chromanone, T-589
1,3-Dihydroxy-8-methoxy-6-methoxymethylanthraquinone, T-590
4′,7-Dihydroxy-8-methoxyflavanone, T-571
5,7-Dihydroxy-8-methoxyflavanone, T-573
5,7-Dihydroxy-8-methoxyflavonol, T-209
3,9-Dihydroxy-8-methoxypterocarpan, T-703
3,29-Dihydroxy-8-multifloren-7-one, D-560
2β,9ξ-Dihydroxy-8-oxo-1(10),4,11(13)-germacratrien-12,6α-olide, T-585
9,10-Dihydroxy-8-oxo-12-octadecenoic acid, D-594
1,3-Dihydroxy-9(10*H*)-acridinone, D-375
3,24-Dihydroxy-9(11),12-oleanadien-30-oic acid, D-568
16,17-Dihydroxy-9(11)-kauren-19-oic acid, D-517
1,3-Dihydroxy-9,10-anthracenedione, D-376
1,8-Dihydroxy-9,10-anthracenedione, D-377
2,2′-Dihydroxy-9,9′-bis(4-hydroxyphenyl)-[3,3′-bi-1*H*-phenalene]-1,1′-dione, B-140
2,2′-Dihydroxy-9,9′-diphenyl-[3,3′-bi-1*H*-phenalene]-1,1′-dione, B-140
2,3-Dihydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, H-732
2,4-Dihydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, H-732
3,7-Dihydroxy-9-methoxy-1-methyl-6*H*-dibenzo[*b,d*]pyran-6-one, A-192
3,6*a*-Dihydroxy-9-methoxy-10-prenylpterocarpan, T-693
7,12-Dihydroxy-9-methoxy-2,2-dimethyl-2*H*,6*H*-pyrano[3,2-*b*]xanthen-6-one, F-59
2,3-Dihydroxy-9-methoxycoumestan, T-538
3,7-Dihydroxy-9-methoxycoumestan, T-540
3,8-Dihydroxy-9-methoxycoumestan, T-541
3,6*a*-Dihydroxy-9-methoxypterocarpan, T-700
3,4-Dihydroxy-9-methoxypterocarpan, T-702
3,8-Dihydroxy-9-methoxypterocarpan, T-703
2,7-Dihydroxy-9-methyl-4-dibenzofurancarboxylic acid, D-550
2,4-Dihydroxy-9-phenyl-1*H*-phenalen-1-one, H-732
1,6-Dihydroxy-9*H*-carbazole-3-carboxaldehyde, D-407
1,5-Dihydroxy-9*H*-xanthen-9-one, D-719
1,7-Dihydroxy-9*H*-xanthen-9-one, D-720
2,3-Dihydroxy-D-friedoolean-14-en-28-oic acid, D-693
8,9-Dihydroxy-*p*-menth-1(6)-en-2-one, D-535
2,5-Dihydroxy-*m*-xylene, D-757
2,4-Dihydroxy-*N*-(3-hydroxypropyl)-3,3-dimethylbutanamide, P-30
2′,3′-Dihydroxyacetophenone, D-368
2′,4′-Dihydroxyacetophenone, D-369
2,4′-Dihydroxyacetophenone, D-370
2′,5′-Dihydroxyacetophenone, D-371
2′,6′-Dihydroxyacetophenone, D-372
3′,4′-Dihydroxyacetophenone, D-373
3′,5′-Dihydroxyacetophenone, D-374
Dihydroxyacidissiminol, A-105
1,3-Dihydroxyacridone, D-375
3,4-Dihydroxyallylbenzene, P-504
4′,4″-Dihydroxyanigorootin, A-337
Dihydroxyanigorufone, H-732
4,5-Dihydroxyanthranilic acid, A-237
1,3-Dihydroxyanthraquinone, D-376
1,8-Dihydroxyanthraquinone, D-377
4,5-Dihydroxyanthraquinone-2-carboxylic acid, D-378
1,2-Dihydroxyaporphine, D-379
4′,6-Dihydroxyaurone, D-381
2′,4′-Dihydroxyazobenzene-4-sulfonic acid, D-610
3,4-Dihydroxybenzaldehyde, D-382
1,3-Dihydroxybenzene, B-20
1,4-Dihydroxybenzene, B-21
α,3-Dihydroxybenzeneacetic acid, H-503
α,4-Dihydroxybenzeneacetic acid, H-504
3,4-Dihydroxybenzeneethanol, D-627
3,4-Dihydroxybenzenemethanol, D-400
3,5-Dihydroxybenzenemethanol, D-401
α,β-Dihydroxybenzenepropanoic acid, D-646
3,4-Dihydroxybenzenepropanoic acid, D-647
α,2-Dihydroxybenzenepropanoic acid, H-508
α,4-Dihydroxybenzenepropanoic acid, H-509
6′,7-Dihydroxybenzofuro[3′,2′,3,4]coumarin (obsol.), C-370
2,3-Dihydroxybenzoic acid, D-386
2,4-Dihydroxybenzoic acid, D-387
2,5-Dihydroxybenzoic acid, D-388
2,6-Dihydroxybenzoic acid, D-389
3,4-Dihydroxybenzoic acid, D-390
3,5-Dihydroxybenzoic acid, D-391
3,4-Dihydroxybenzoyl β-D-xylopyranoside, D-390
3,4-Dihydroxybenzyl alcohol, D-400
3,5-Dihydroxybenzyl alcohol, D-401
1-(3,4-Dihydroxybenzyl)-1,2,3,4-tetrahydro-6,7-isoquinolinediol, N-152
2-(3,4-Dihydroxybenzyl)-2,6-dihydroxy-3(2*H*)-benzofuranone, D-403
3-(3,4-Dihydroxybenzyl)-5,7-dihydroxy-4-chromanone, D-404
1-(3,4-Dihydroxybenzyl)-6,7-dihydroxyisoquinoline, P-36
3-(3,4-Dihydroxybenzyl)-7-hydroxy-5-methoxy-4-chromanone, D-404
3,4-Dihydroxybenzylamine, D-402
3,4-Dihydroxybenzyltartaric acid, F-82
6′,7′-Dihydroxybergamottin, B-66
2,3-Dihydroxybutanedioic acid, T-27
3,4-Dihydroxybutanoic acid γ-lactone, D-258
3-(1,2-Dihydroxybutyl)-1*H*-2-benzopyran-1-one, B-228
3-(2,3-Dihydroxybutyl)-7-hydroxy-1(3*H*)-isobenzofuranone, B-252
3-(2,3-Dihydroxybutyl)-7-hydroxyphthalide, B-252
1-(1,4-Dihydroxybutyl)-9*H*-pyrido[3,4-*b*]indole, P-603
2,4-Dihydroxybutyrophenone, D-612
7α,8α-Dihydroxycalonectrin, S-56
3,3′-Dihydroxycanthaxanthin, A-474
3,14-Dihydroxycard-20(22)-enolide, D-410
3,15-Dihydroxycarda-16,20(22)-dienolide, D-409
3,14-Dihydroxycarda-4,20(22)-dienolide, D-408
2,4-Dihydroxychalcone, D-412
2′,5′-Dihydroxychalcone, D-413
3′,4′-Dihydroxychalcone, D-414
3,12-Dihydroxycholan-24-oic acid, D-415
3,26-Dihydroxycholest-5-ene-16,22-dione, D-416
22,23-Dihydroxycholestan-3-one, C-231
5,7-Dihydroxychromone, D-394
2,6-Dihydroxycinchoninic acid, D-681
2,8-Dihydroxycinchoninic acid, D-682
2,4-Dihydroxycinnamaldehyde, D-651
2,3-Dihydroxycinnamic acid, D-652
3,4-Dihydroxycinnamic acid, D-653
3,5-Dihydroxycinnamic acid, D-654
N-(3,4-Dihydroxycinnamoyl)-1,4-butanediamine, P-50
N-(3,4-Dihydroxycinnamoyl)-5-hydroxyanthranilic acid, A-260
N-(3,4-Dihydroxycinnamoyl)DOPA, C-309
6-*O*-(3,4-Dihydroxycinnamoyl)glucose, D-417
1-(3,4-Dihydroxycinnamoyl)quinic acid, C-19
3-(3,4-Dihydroxycinnamoyl)quinic acid, C-20
4-(3,4-Dihydroxycinnamoyl)quinic acid, C-21
5-(3,4-Dihydroxycinnamoyl)quinic acid, C-22
3,4-Dihydroxycinnamyl alcohol, D-656
Dihydroxycitracridone I, C-280
3,8-Dihydroxycostunolide, D-484
4,7-Dihydroxycoumarin, D-392
5,7-Dihydroxycoumarin, D-393
6,7-Dihydroxycoumarin, D-395
7,8-Dihydroxycoumarin, D-396
3,9-Dihydroxycoumestan, C-370
7,12-Dihydroxycoumestan (obsol.), C-370
2,5-Dihydroxycumene, I-120
3,22-Dihydroxycycloart-24-en-26-oic acid, C-426
3,23-Dihydroxycycloart-24-en-26-oic acid, D-418
3,27-Dihydroxycycloart-24-en-26-oic acid, D-419
24,25-Dihydroxycycloartan-3-one, C-419
12,20-Dihydroxydammar-24-en-3-one, D-21
1,2-Dihydroxydibenz[*cd,f*]indol-4(5*H*)-one, D-425
p,p′-Dihydroxydicinnamoylmethane, C-397
2,2′-Dihydroxydiethyl ether, O-255
α,β-Dihydroxydihydrochalcone, D-439
4′,7-Dihydroxydihydroflavanol, T-567
5,7-Dihydroxydihydroflavonol, T-568
O-(3,8-Dihydroxydriman-11-yl)umbelliferone, D-446
10,20-Dihydroxyeicosanoic acid, D-448
3,22-Dihydroxyergost-5-en-7-one, E-222
3,5-Dihydroxyergosta-7,22-dien-6-one, E-204
22,23-Dihydroxyergostane-3,6-dione, T-564
4-(1,2-Dihydroxyethyl)-1,2-benzenediol, D-626
4-(1,2-Dihydroxyethyl)phenol, H-722
9,10-Dihydroxyfenchone, D-465
6,9-Dihydroxyfenchone, D-466
8,10-Dihydroxyfenchone, D-467
9,10-Dihydroxyfenchone, D-468
5,7-Dihydroxyflavan, D-469
3′,4′-Dihydroxyflavanol, T-575
4′,7-Dihydroxyflavanone, D-470
5,7-Dihydroxyflavanone, D-471
5,6-Dihydroxyflavone, D-472
5,7-Dihydroxyflavone, D-473
6,7-Dihydroxyflavone, D-474
4′,7-Dihydroxyflavonol, T-577
5,7-Dihydroxyflavonol, T-580
Dihydroxyfumitremorgin C, F-89
1,4-Dihydroxyfuranoeremophilan-6-one, D-475
3,26-Dihydroxyfurost-20(22)-en-6-one, D-478
4,6-Dihydroxyfuro[2,3-*b*]quinoline, F-148
4,8-Dihydroxyfuro[2,3-*b*]quinoline, F-149
3,13-Dihydroxygibberellin A_{15}, G-104
3,4-Dihydroxyglutamic acid, A-239
10,16-Dihydroxyhexadecanoic acid, D-501
α,β-Dihydroxyhydrocinnamic acid, D-646
3,4-Dihydroxyhydrocinnamic acid, D-647
1,5-Dihydroxyiridanyllycopene, C-482
4′,7-Dihydroxyisoflavanone, D-512
4′,7-Dihydroxyisoflavone, D-513
5,7-Dihydroxyisoflavone, D-514
7,18-Dihydroxykaurenolide, T-607
24,25-Dihydroxylanost-7,9(11)-dien-3-one, L-38
3,26-Dihydroxylanost-8,24-dien-7-one, D-521
24,25-Dihydroxylanost-8-ene-3,7-dione, D-526
3,15-Dihydroxylanosta-7,9(11),24-trien-26-oic acid, D-524
3,22-Dihydroxylanosta-7,9(11),24-trien-26-oic acid, D-525
15,26-Dihydroxylanosta-7,9(11),24-trien-3-one, D-524
26,27-Dihydroxylanosta-7,9(11),24-trien-3-one, L-41
3,7-Dihydroxylanosta-8,24-dien-26-oic acid, D-521
3,15-Dihydroxylanosta-8,24-dien-26-oic acid, D-522
3,24-Dihydroxylanosta-8,25-dien-21-oic acid, D-523
6,8-Dihydroxyluteolin, H-211
16,16′-Dihydroxylycopene, L-130
1α,15-Dihydroxymarasmene, M-72
3α,15-Dihydroxymarasmene, M-72
3,4-(3,4-Dihydroxymethylenedioxyphenyl)benzaldehyde, D-611
1,4-Dihydroxynaphthalene, N-7
3β,6β-Dihydroxynortropane, A-517
3,6-Dihydroxynortropane, A-517
15,16-Dihydroxyoctadecanoic acid, D-566
4,6-Dihydroxyorcinol, M-316
10,16-Dihydroxypalmitic acid, D-501
3-(1,4-Dihydroxypentyl)furan, F-127
3,4-Dihydroxyphenacyl alcohol, T-511

3,4-Dihydroxyphenacyl caffeate, T-511
3,4-Dihydroxyphenethyl alcohol, D-627
3,4-Dihydroxyphenethyl glucoside, D-627
3,4-Dihydroxyphenethylamine, D-1035
3,5-Dihydroxyphenyl 1-*O*-(6-*O*-galloyl-β-D-glucopyranoside), B-25
2,5-Dihydroxyphenyl styryl ketone, D-413
3,4-Dihydroxyphenyl styryl ketone, D-414
(3,4-Dihydroxyphenyl)(2,4,6-trihydroxyphenyl)-methanone, P-91
1-(2,5-Dihydroxyphenyl)-1,2-epoxypropane, M-528
1-(3,4-Dihydroxyphenyl)-1,2-ethanediol, D-626
1-(3,4-Dihydroxyphenyl)-1,2-propanediol, D-643
3-(2,4-Dihydroxyphenyl)-1,2-propanediol, D-644
3-(3,4-Dihydroxyphenyl)-1,2-propanediol, D-645
2-(3,4-Dihydroxyphenyl)-1,3-benzodioxole-5-carboxaldehyde, D-611
7-(3,4-Dihydroxyphenyl)-1,5-epoxy-3-hydroxy-1-(3,4,5-trihydroxyphenyl)heptane, D-632
3-(3,4-Dihydroxyphenyl)-1,7,8-trihydroxy-2-methoxydibenzofuran, P-147
3-(3,4-Dihydroxyphenyl)-1,7,8-trihydroxy-4-methoxydibenzofuran, P-147
3-(2,4-Dihydroxyphenyl)-1-(4-hydroxyphenyl)-2-propen-1-one, T-533
1-(2,4-Dihydroxyphenyl)-1-butanone, D-612
N-[3-(3,4-Dihydroxyphenyl)-1-oxo-2-propenyl]-3-hydroxytyrosine, C-309
3-(2,4-Dihydroxyphenyl)-1-phenyl-2-propen-1-one, D-412
3-(3,4-Dihydroxyphenyl)-1-propanol, D-649
4-(3,4-Dihydroxyphenyl)-2,3-dihydro-2,3-dihydroxy-1*H*-phenalen-1-one, D-279
2-(2,5-Dihydroxyphenyl)-2,3-dihydro-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, P-107
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, P-109
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3,7-dihydroxy-4*H*-1-benzopyran-4-one, T-189
3-[2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3-hydroxymethyl-1,4-benzodioxin-6-yl]-2-propenal, A-207
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3-methyl-5-(1-propenyl)benzofuran, D-616
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-5,7,8-trihydroxy-4*H*-1-benzopyran-4-one, P-111
2-(2,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, T-186
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, T-191
2-(3,5-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, T-192
3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-274
3-(2,4-Dihydroxyphenyl)-2,3-dihydro-5-hydroxy-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, C-475
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-7-hydroxy-3-hydroxymethyl-5-benzofuranpropanol, E-144
3-(3,4-Dihydroxyphenyl)-2,3-dihydro-7-hydroxy-4*H*-1-benzopyran-4-one, T-596
1-(3,4-Dihydroxyphenyl)-2,3-dihydroxy-1-propanone, D-623
3-(3,4-Dihydroxyphenyl)-2,7,8-trihydroxydibenzofuran-1,4-dione, D-660
1-(3,5-Dihydroxyphenyl)-2-(2-hydroxyphenyl)ethane, D-638
1-(3,5-Dihydroxyphenyl)-2-(2-methoxyphenyl)ethane, D-638
1-(3,5-Dihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethylene, D-661
1-(2,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene, D-620
1-(3,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene, D-621
1-(3,5-Dihydroxyphenyl)-2-(3-hydroxy-4-methoxyphenyl)ethylene, D-621
1-(3,5-Dihydroxyphenyl)-2-(3-hydroxyphenyl)ethane, D-639
1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene, D-640
4-(3,4-Dihydroxyphenyl)-2-butanone, D-613
4-(3,4-Dihydroxyphenyl)-2-hydroxy-1*H*-phenalen-1-one, H-506
9-(3,4-Dihydroxyphenyl)-2-hydroxy-1*H*-phenalen-1-one, H-732
1-(3,4-Dihydroxyphenyl)-2-hydroxyethanone, T-511
3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid, D-641
3-(3,4-Dihydroxyphenyl)-2-methoxy-1,7,8-dibenzofurantriol, P-147
1-(2,5-Dihydroxyphenyl)-2-methyloxirane, M-528
1-(3,5-Dihydroxyphenyl)-2-nonadecanone, N-95
1-(3,5-Dihydroxyphenyl)-2-pentadecanone, P-85
1-(3,5-Dihydroxyphenyl)-2-phenylethylene, D-692
1-(2,4-Dihydroxyphenyl)-2-propanol, D-648
1-(3,4-Dihydroxyphenyl)-2-propanone, D-650
1-(3,4-Dihydroxyphenyl)-2-propen-1-ol, D-655
3-(3,4-Dihydroxyphenyl)-2-propen-1-ol, D-656
3-(2,4-Dihydroxyphenyl)-2-propenal, D-651
3-(2,3-Dihydroxyphenyl)-2-propenoic acid, D-652
3-(3,4-Dihydroxyphenyl)-2-propenoic acid, D-653
3-(3,5-Dihydroxyphenyl)-2-propenoic acid, D-654
2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-3,5,7-triol, P-104
2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-3,7-diol, T-181
2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-4,5,7-triol, P-105
2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-benzopyran-3,4,5,7-tetrol, H-197
3-(3,4-Dihydroxyphenyl)-3,4-dihydro-8-hydroxy-1*H*-2-benzopyran-1-one, D-614
3-(3,4-Dihydroxyphenyl)-3,4-dihydro-8-hydroxyisocoumarin, D-614
2-(3,4-Dihydroxyphenyl)-3,5,6,7,8-pentahydroxy-4*H*-1-benzopyran-4-one, H-88
2-(3,4-Dihydroxyphenyl)-3,5,6,7-tetrahydroxy-4*H*-1-benzopyran-4-one, H-207
2-(3,4-Dihydroxyphenyl)-3,5,6,8-tetrahydroxy-4*H*-1-benzopyran-4-one, H-208
2-(3,4-Dihydroxyphenyl)-3,5,7,8-tetrahydroxy-4*H*-1-benzopyran-4-one, H-209
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-1-benzopyrylium(1+), P-144
2-(2,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, P-133
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, P-134
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, P-170
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-6-methoxy-4*H*-1-benzopyran-4-one, P-157
2-(3,4-Dihydroxyphenyl)-3,5,8-trihydroxy-7-methoxy-4*H*-1-benzopyran-4-one, P-158
2-(3,4-Dihydroxyphenyl)-3,5-dihydroxy-7-methoxy-4*H*-1-benzopyran-4-one, T-234
6-(3,4-Dihydroxyphenyl)-3,5-hexadien-2-one, D-633
3-(3,4-Dihydroxyphenyl)-3,7,11-trimethyl-1,6,10-dodecatriene, E-247
2-(3,4-Dihydroxyphenyl)-3,7-dihydroxy-4*H*-1-benzopyran-4-one, T-204
2-(3,4-Dihydroxyphenyl)-3,7-dihydroxy-5-methoxy-4*H*-1-benzopyran-4-one, T-235
2-(3,4-Dihydroxyphenyl)-3,8-di-β-D-glucopyranosyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one, D-217
2-(3,4-Dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, I-158
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2-(2,4-Dihydroxyphenyl)-3-(3,7-dimethyl-2,6-octadienyl)-7-hydroxy-4*H*-1-benzopyran-4-one, R-63
1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one, T-534
2-(3,4-Dihydroxyphenyl)-3-glucosyloxy-8-hydroxy-5-methylpyrano[4,3,2-*de*]-1-benzopyrylium(1+), P-590
2-(3,4-Dihydroxyphenyl)-3-hydroxy-4*H*-1-benzopyran-4-one, T-575
1-(2,5-Dihydroxyphenyl)-3-phenyl-2-propen-1-one, D-413
1-(3,4-Dihydroxyphenyl)-3-phenyl-2-propen-1-one, D-414
5-(3,4-Dihydroxyphenyl)-3-[(3,5-dihydroxyphenyl)-methylene]-2(3*H*)-furanone, A-365
1-(2,4-Dihydroxyphenyl)-3-[2-(3,7-dimethyl-2,6-octadienyl)-3,4-dihydroxyphenyl]-1-propanone, D-625
1-(2,4-Dihydroxyphenyl)-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propen-1-one, T-679
1-(2,4-Dihydroxyphenyl)-3-[8-hydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-5-yl]-1-propanone, D-637
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2-(3,4-Dihydroxyphenyl)-4,6-dimethoxy-5-prenylbenzofuran, D-622
6-(3,4-Dihydroxyphenyl)-4-hydroxy-3,5-hexadien-2-one, H-286
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2-(3,4-Dihydroxyphenyl)-4-methyl-1,3-dioxolane, D-642
2-(3,4-Dihydroxyphenyl)-5,6,7,8-tetrahydroxy-4*H*-1-benzopyran-4-one, H-211
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3-(2,4-Dihydroxyphenyl)-5,7,8-trihydroxy-4*H*-1-benzopyran-4-one, P-151
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2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, T-205
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3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, T-224
2-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-267
2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-271
3-(2,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-276
3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-279
2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-6-methoxy-4*H*-1-benzopyran-4-one, T-241
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3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-8-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, T-

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3-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-8-methyl-4*H*-1-benzopyran-4-one, T-250
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3-(2,4-Dihydroxyphenyl)-5,7-dimethoxy-6-prenylcoumarin, G-288
2-(3,4-Dihydroxyphenyl)-5-(1,2-dihydroxypropyl)-2,3-dihydro-6-hydroxy-3-methylbenzofuran, D-624
6-(3,4-Dihydroxyphenyl)-5-hexene-2,4-dione, H-286
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2-(2,4-Dihydroxyphenyl)-5-hydroxy-3-(3-hydroxy-3-methylbutyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, M-766
2-(2,4-Dihydroxyphenyl)-5-hydroxy-6-methoxybenzofuran, D-617
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2-(3,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-4*H*-1-benzopyran-4-one, T-615
2-(2,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-6-(3-methyl-1-butenyl)-3-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, A-427
2-(2,4-Dihydroxyphenyl)-5-hydroxy-8,8-dimethyl-3-(3-methyl-2-butenyl)-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, M-765
3-(2,4-Dihydroxyphenyl)-5-hydroxy-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, P-41
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)-benzofuran, D-619
2-(3,4-Dihydroxyphenyl)-6,8-di-β-D-glucopyranosyl-5,7-dihydroxy-4*H*-1-benzopyran-4-one, L-102
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2-(3,4-Dihydroxyphenyl)-6-β-D-glucopyranosyl-5-hydroxy-7-methoxy-4*H*-1-benzopyran-4-one, S-284
2-(2,4-Dihydroxyphenyl)-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, A-157
2-(2,4-Dihydroxyphenyl)-6-hydroxy-3-benzofurancarboxylic acid, D-636
2-(3,4-Dihydroxyphenyl)-6-hydroxy-4-methoxy-5-prenylbenzofuran, D-622
2-(3,5-Dihydroxyphenyl)-6-hydroxy-5-(3-methyl-1-butenyl)benzofuran, M-756
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2-(2,4-Dihydroxyphenyl)-6-hydroxybenzofuran, D-634
2-(3,5-Dihydroxyphenyl)-6-hydroxybenzofuran, D-635
3-(2,4-Dihydroxyphenyl)-7,8-dihydro-5-methoxy-8,8-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]bipyran-2-one, I-91
3-(3,4-Dihydroxyphenyl)-7,8-dihydroxy-4*H*-1-benzopyran-4-one, T-225
8-(2,4-Dihydroxyphenyl)-7-(3,7-dimethyl-2,6-octadienyl)-5-hydroxy-2,2-dimethyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-6-one, R-64
1-(3,4-Dihydroxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, C-397
2-(3,4-Dihydroxyphenyl)-7-hydroxy-3,5-dimethoxy-4*H*-1-benzopyran-4-one, T-546
2-(3,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, T-578
3-(2,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, T-598
3-(3,4-Dihydroxyphenyl)-7-hydroxy-4*H*-1-benzopyran-4-one, T-600
3-(2,4-Dihydroxyphenyl)-7-hydroxy-5-methoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, G-288
1-(3,4-Dihydroxyphenyl)-7-phenyl-6-hepten-3-ol, H-733
3-(2,4-Dihydroxyphenyl)-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, K-13
3-(2,4-Dihydroxyphenyl)-8,9-dihydro-5-hydroxy-8-(1-methylethenyl)-4*H*-furo[2,3-*h*]-1-benzopyran-5-one, D-615
3-(2,4-Dihydroxyphenyl)-9,10-dihydro-5,9-dihydroxy-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, L-114
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5-[2-(3,5-Dihydroxyphenyl)ethenyl]-1,2,3-benzenetriol, D-661
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6-[2-(3,4-Dihydroxyphenyl)ethenyl]-4-hydroxy-2*H*-pyran-2-one, D-631
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1-(2,4-Dihydroxyphenyl)hexane, H-262
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3-[(3,4-Dihydroxyphenyl)methyl]-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, D-404
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3,4-Dihydroxyphenylglycol, D-626
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3,3′-Dimethoxy-β,β-carotene, Z-9
3,3′-Dimethoxy-β,ε-carotene, L-124
3,4-Dimethoxy-ω-(2-piperidyl)acetophenone, P-413
6,7-Dimethoxy-1(3*H*)-benzoxazolone, D-738
6,7-Dimethoxy-1(3*H*)-isobenzofuranone, D-511
3,4-Dimethoxy-1,2-benzenedicarboxylic acid, D-383
4,5-Dimethoxy-1,2-benzenedicarboxylic acid, D-384
9,10-Dimethoxy-1,2-methylenedioxyaporphine, D-154
2,5-Dimethoxy-1,4-benzoquinone, D-397
2,6-Dimethoxy-1,4-benzoquinone, D-398
2,4-Dimethoxy-1-(2-propenyl)benzene, P-505
6,7-Dimethoxy-1-(3,4-dimethoxybenzoyl)isoquinoline, P-34
6,7-Dimethoxy-1-(3,4-dimethoxybenzyl)isoquinoline, P-35
(2,2-Dimethoxy-1-methylethyl)benzene, P-301
6,7-Dimethoxy-1-methylisoquinoline, D-555
4,4-Dimethoxy-1-pentene, P-207
1,1-Dimethoxy-1-phenylpropane, P-310
1,2-Dimethoxy-13-methyl-[1,3]benzodioxolo[5,6-*c*]phenanthridine, M-514
2,3-Dimethoxy-16-methyl-10,11-[methylenebis(oxy)]rheadan-8-ol, G-143
3,5-Dimethoxy-1*H*-inden-1-one, H-513
4,8-Dimethoxy-2(1*H*)-quinolinone, Q-14
2,3-Dimethoxy-2,4-cyclopentadien-1-one, D-420
6,6-Dimethoxy-2,5,5-trimethyl-2-hexene, T-782
8,8-Dimethoxy-2,6-dimethyl-2-octanol, H-417
1,4-Dimethoxy-2,6-dimethylbenzene, D-757
1,1-Dimethoxy-2,6-dimethyloctane, D-843
3,5-Dimethoxy-2,7-phenanthrenediol, P-247
5,7-Dimethoxy-2,8-dimethyl-4*H*-1-benzopyran-4-one, D-431
1,1-Dimethoxy-2-(methylthio)ethane, M-196
4,4-Dimethoxy-2-butanone, O-197
3,5-Dimethoxy-2-methyl-4*H*-pyran-4-one, D-559
1,4-Dimethoxy-2-methylnaphthalene, M-506
1,1-Dimethoxy-2-phenylethane, P-257
1,1-Dimethoxy-2-phenylpropane, P-301
1,1-Dimethoxy-2-phenylpropane, P-301
4,6-Dimethoxy-2-phenylquinoline, D-658
1-(4,6-Dimethoxy-2-pyrimidinyl)-3-[[1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)pyrazol-5-yl]sulfonyl]urea, A-527
N-[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]-1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)-1*H*-pyrazole-5-sulfonamide, A-527
2-[(4,6-Dimethoxy-2-pyrimidinyl)oxy]-6-[1-(methoxyimino)ethyl]benzoic acid, P-608
2,7-Dimethoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-399
4,7-Dimethoxy-2*H*-1-benzopyran-2-one, D-392
5,7-Dimethoxy-2*H*-1-benzopyran-2-one, D-393
6,7-Dimethoxy-2*H*-1-benzopyran-2-one, D-395
3,6-Dimethoxy-2*H*-furo[2,3-*h*][1]benzopyran-2-one, F-144
3′,4′-Dimethoxy-3′,4′-desmethylenecubebin, P-101
3,4-Dimethoxy-3′,4′-methylenedioxy-7,7′-epoxylignan, H-549
3,4-Dimethoxy-3′,4′-methylenedioxy-7,9′:7′,9-diepoxylignan, S-170
3,7-Dimethoxy-3′,4′-methylenedioxyflavone, T-204
1,1′-Dimethoxy-3,3′-dimethyl-4,9′-bi-9*H*-carbazole, M-813
3,4-Dimethoxy-3,4-desmethylenecubebin, P-101
2,5-Dimethoxy-3,4-methylenedioxycinnamaldehyde, A-373
3-(2,5-Dimethoxy-3,4-methylenedioxyphenyl)-2-propenal, A-373
6,7-Dimethoxy-3,7′-bicoumarin, E-1
1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene, D-822
2,5-Dimethoxy-3-(10-pentadecenyl)-1,4-benzoquinone, D-609
6,7-Dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-*g*]isoquinolin-5-yl)-1(3*H*)-isobenzofuranone, N-17
1,1-Dimethoxy-3-(methylthio)propane, M-688
2,4-Dimethoxy-3-dibenzofuranol, D-130
6,7-Dimethoxy-3-methyl-1*H*-carbazole-1,4(9*H*)-dione, K-40
2,6-Dimethoxy-3-methyl-5-(1-methylethyl)pyrazine, I-128
1,1-Dimethoxy-3-methylbutane, M-325
2,5-Dimethoxy-3-pentadecyl-1,4-benzoquinone, D-609
2,2-Dimethoxy-3-pentanone, P-184
5,5-Dimethoxy-3-phenyl-1-pentene, P-300
1,1-Dimethoxy-3-phenylpropane, P-302
2,3-Dimethoxy-4,5-methylenedioxy-1-propenylbenzene, D-739
2,3-Dimethoxy-4,5-methylenedioxycinnamaldehyde, D-733
3-(2,3-Dimethoxy-4,5-methylenedioxyphenyl)-2-propen-1-al, D-733
1,2-Dimethoxy-4-(1-methoxy-2-propenyl)benzene, D-655
1,2-Dimethoxy-4-(1-methoxyallyl)benzene, D-655
1,2-Dimethoxy-4-(1-propenyl)benzene, P-503
2,6-Dimethoxy-4-(1-propenyl)phenol, P-507
1,2-Dimethoxy-4-(2-propenyl)benzene, P-504
2,6-Dimethoxy-4-(2-propenyl)phenol, P-508
2,5-Dimethoxy-4-(2-propenyl)phenol, P-509
α-[1-[2,6-Dimethoxy-4-(2-propenyl)phenoxy]ethyl]-4-hydroxy-3-methoxybenzenemethanol, A-184
1,2-Dimethoxy-4-(3-methyloxiranyl)benzene, P-503
2,3-Dimethoxy-4-(4-hydroxyphenyl)-1*H*-phenalen-1-one, H-506
1,2-Dimethoxy-4-methylbenzene, M-314
2,6-Dimethoxy-4-methylphenol, M-316
2,6-Dimethoxy-4-phenanthrenol, P-249
3,6-Dimethoxy-4-phenanthrenol, P-250
3,5-Dimethoxy-4-prenylstilbene, M-348
1,2-Dimethoxy-4-propylbenzene, P-524
2,6-Dimethoxy-4-propylphenol, P-525
N′-(2,6-Dimethoxy-4-pyrimidinyl)sulfanilamide, S-270
1,2-Dimethoxy-4-vinylbenzene, V-33
5,7-Dimethoxy-4*H*-1-benzopyran-4-one, D-394
4,7-Dimethoxy-5-(2-propenyl)-1,3-benzodioxole, A-372
4-[4,6-Dimethoxy-5-(3-methyl-2-butenyl)-2-benzofuranyl]-1,3-benzenediol, D-622
2,3-Dimethoxy-5-methylphenol, M-316
1,3-Dimethoxy-5-nonadecylbenzene, N-95
2′,5-Dimethoxy-6,7-methylenedioxyflavanone, T-188
7,7′-Dimethoxy-6,8′-bicoumarin, B-76
4,5-Dimethoxy-6-(1-propenyl)-1,3-benzodioxole, D-739
4,5-Dimethoxy-6-(2-propenyl)-1,3-benzodioxole, D-732
7,8-Dimethoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, D-668
2,8-Dimethoxy-6-methyl-1,4-naphthoquinone, D-558
1,2-Dimethoxy-6-methyl-4*H*-dibenzo[*de,g*]quinoline-4,5(6*H*)-dione, C-179
5,7-Dimethoxy-6-methylflavanone, D-553
5,7-Dimethoxy-6-methylflavone, D-554
3,9-Dimethoxy-6-oxopterocarpen, C-370
7,8-Dimethoxy-6-prenylcoumarin, D-668
4,5-Dimethoxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, N-58
4,5-Dimethoxy-7-(2-propenyl)-1,3-benzodioxole, P-506
6,7-Dimethoxy-7-epirosmanol, T-132
4,9-Dimethoxy-7-oxofuro[3,2-*g*]chromene, I-113
4,9-Dimethoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, I-113
15,15-Dimethoxy-8(17),12-labdadien-16-al, L-1
11,12-Dimethoxy-8,11,13-abietatrien-20,7-olide, C-117
1,2-Dimethoxy-9,10-methylenedioxyaporphine, N-4
1,2-Dimethoxy-9,10-methylenedioxynoraporphine, N-4
1,2-Dimethoxy-9,10-methylenedioxyoxoaporphine, O-244
1,6-Dimethoxy-9*H*-carbazole-3-carboxaldehyde, D-407
2,6-Dimethoxy-9*H*-carbazole-3-carboxaldehyde, L-48
3,4-Dimethoxy-*N*,*N*-dimethyl-1-phenanthreneethanamine, A-484
2,6-Dimethoxy-*p*-cresol, M-316
7,7′-Dimethoxy-[6,8′-bi-2*H*-benzopyran]-2,2′-dione, B-76
2′,3′-Dimethoxyacetophenone, D-368
2′,6′-Dimethoxyacetophenone, D-372
3′,5′-Dimethoxyacetophenone, D-374
3,6-Dimethoxyangelicin, F-144
1,3-Dimethoxyanthraquinone, D-376
1,8-Dimethoxyanthraquinone, D-377
3,4-Dimethoxybenzaldehyde, D-734
1,2-Dimethoxybenzene, D-735
1,3-Dimethoxybenzene, D-736
1,4-Dimethoxybenzene, D-737
3,5-Dimethoxybenzenemethanol, D-401

3,5-Dimethoxybenzyl alcohol, D-401
3-(3,4-Dimethoxybenzyl)-5,7-dihydroxy-4-chromanone, D-404
4,5-Dimethoxycanthin-6-one, N-58
5,8-Dimethoxychalepensin, C-184
5,7-Dimethoxychromone, D-394
2,3-Dimethoxycinnamic acid, D-652
3,4-Dimethoxycinnamic acid, D-653
3,5-Dimethoxycinnamic acid, D-654
3,5-Dimethoxycinnamic acid pyrrolidide, D-654
N^1-(3,4-Dimethoxycinnamoyl)agmatine, A-221
N-(3,5-Dimethoxycinnamoyl)pyrrolidine, D-654
4,7-Dimethoxycoumarin, D-392
5,7-Dimethoxycoumarin, D-393
6,7-Dimethoxycoumarin, D-395
3,9-Dimethoxycoumestan, C-370
2,2-Dimethoxycyclohexanone, C-460
1,1-Dimethoxydecane, D-39
11,12-Dimethoxydihydrokawain, D-631
1,2-Dimethoxydodecane, D-1015
1,1-Dimethoxyethane, A-20
(2,2-Dimethoxyethyl)benzene, P-257
5,7-Dimethoxyflavan, D-469
3′,4′-Dimethoxyflavanol, T-575
4′,7-Dimethoxyflavanone, D-470
5,7-Dimethoxyflavanone, D-471
5,6-Dimethoxyflavone, D-472
5,7-Dimethoxyflavone, D-473
6,7-Dimethoxyflavone, D-474
5,7-Dimethoxyflavonol, T-580
4,6-Dimethoxyfuro[2,3-*b*]quinoline, F-148
4,8-Dimethoxyfuro[2,3-*b*]quinoline, F-149
1,4-Dimethoxyglucobrassicin, I-35
3′,8-Dimethoxygraveoline, G-320
1,1-Dimethoxyheptane, H-90
1,1-Dimethoxyhexadecane, H-156
1,1-Dimethoxyhexane, H-225
4′,7-Dimethoxyisoflavanone, D-512
5,7-Dimethoxyisoflavone, D-514
Dimethoxyisolariciresinol, O-71
3,3′-Dimethoxylarreatricin, D-427
4-(Dimethoxymethyl)-1,2-dimethoxybenzene, D-734
[2-(Dimethoxymethyl)-1-heptenyl]benzene, P-217
2-(Dimethoxymethyl)-1-phenyl-1-heptene, P-217
1-(Dimethoxymethyl)-4-methoxybenzene, M-249
(Dimethoxymethyl)benzene, B-16
1-(Dimethoxymethyl)piperidine, P-390
1-(Dimethoxymethyl)pyrrolidine, P-620
1,1-Dimethoxyoctane, O-73
3,3-Dimethoxyoctane, O-86
5,5-Dimethoxypentanal, P-183
1,1-Dimethoxypentane, P-181
2,6-Dimethoxyphenol, B-24
1-(3,4-Dimethoxyphenyl)-1,2-epoxypropane, P-503
9-(3,4-Dimethoxyphenyl)-2-methoxy-1*H*-phenalen-1-one, H-732
1-(3,4-Dimethoxyphenyl)-2-propanone, D-650
1-(3,4-Dimethoxyphenyl)-2-propen-1-ol, D-655
3-(2,3-Dimethoxyphenyl)-2-propenoic acid, D-652
3-(3,4-Dimethoxyphenyl)-2-propenoic acid, D-653
2-(3,4-Dimethoxyphenyl)-3,5,7-trihydroxy-4*H*-1-benzopyran-4-one, T-547
3-(3,4-Dimethoxyphenyl)-3-methoxy-1-propene, D-655
2-(3,4-Dimethoxyphenyl)-3-methyloxirane, P-503
2-(3,4-Dimethoxyphenyl)-5,6,7,8-tetramethoxy-4*H*-1-benzopyran-4-one, H-223
2-(3,4-Dimethoxyphenyl)-5,7-dihydroxy-6,8-dimethoxy-4*H*-1-benzopyran-4-one, D-695
2-(3,4-Dimethoxyphenyl)-5,7-dihydroxy-6-methoxy-4*H*-1-benzopyran-4-one, D-699
2-(3,4-Dimethoxyphenyl)-5-hydroxy-6-methoxybenzofuran, D-617
2-(3,4-Dimethoxyphenyl)-6-(3,4-methylenedioxyphenyl)3,7-dioxabicyclo[3.3.0]octane, S-170
1-[(2,5-Dimethoxyphenyl)azo]-2-naphthalenol, C-257
7-[2-(2,4-Dimethoxyphenyl)ethenyl]-2,2-dimethyl-2*H*-1-benzopyran, D-630
6-[2-(3,4-Dimethoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one, D-631
6-[(3,4-Dimethoxyphenyl)ethyl]-5,6-dihydro-4-methoxy-2*H*-pyran-2-one, D-631
5-[4-(3,4-Dimethoxyphenyl)tetrahydro-1*H*,3*H*-furo[3,4-*c*]furan-1-yl]-1,3-benzodioxole, S-170
Dimethoxyphenylmethane, B-16
2-[(Dimethoxyphosphinyl)amino]pentanedioic diamide, P-329
(Dimethoxyphosphinyl)formamide, C-85
3,4-Dimethoxyphthalic acid, D-383
4,5-Dimethoxyphthalic acid, D-384
6,7-Dimethoxyphthalide, D-511
3,3-Dimethoxypropanal, P-469
(3,3-Dimethoxypropyl)benzene, P-302
(1,1-Dimethoxypropyl)benzene, P-310
4,9-Dimethoxypsoralen, I-113
4,9-Dimethoxysampangine, S-26
10,11-Dimethoxysterigmatocystin, S-222
5,6-Dimethoxysterigmatocystin, S-222
3,4-Dimethoxystyrene, V-33
6-(3,4-Dimethoxystyryl)-4-methoxy-2-pyrone, D-631
3,4-Dimethoxytoluene, M-314
16,17-Dimethoxytricyclo[12.3.1.1^{2,6}]nonadeca-1(18),2,4,6(19),14,16-hexaene-3,9,15-triol, M-833
1,5-Dimethoxyxanthone, D-719
Dimethulene, D-789
Dimethyl (2-ethenyl-5-hydroxy-4-oxo-4*H*-1-benzopyran-3-yl)propanedioate, M-829
Dimethyl 1-methyl-2-methylcarbamoylvinyl phosphate, M-742
Dimethyl 1-methyl-3-(methylamino)-3-oxo-1-propenyl phosphate, M-742
Dimethyl 2-[(dibenzyloxyphosphinyl)amino]pentanedioate, P-329
Dimethyl *ent*-16α-kaurane-17,19-dioate, K-19
O,*O*-Dimethyl *O*-[(3-methyl-4-methylsulfinyl)phenyl] phosphorothioate, F-29
O,*O*-Dimethyl *O*-[(3-methyl-4-methylsulfonyl)-phenyl] phosphorothioate, F-29
O,O-Dimethyl *O*-[(3-methyl-4-methylthio)phenyl] phosphorothioate, F-29
O,*S*-Dimethyl amidothiophosphate, M-239
Dimethyl aminocarbonylphosphonate, C-85
Dimethyl carbonate, D-740
Dimethyl cyanodithioiminocarbonate, C-410
Dimethyl dicarbonate, D-153
Dimethyl diketone, B-211
Dimethyl diselenide, D-741
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Dimethyl fumarate, F-86
Dimethyl glycol phthalate, B-19
Dimethyl ketone, A-25
Dimethyl oxalate, O-189
Dimethyl peroxide, D-743
Dimethyl phosphate, ester with 3-hydroxy-*N*-methylcrotonamide, 8CI, M-742
O,*S*-Dimethyl phosphoramidothioate, M-239
Dimethyl phthalate, B-19
Dimethyl pyrocarbonate, D-153
Dimethyl selenide, D-744
Dimethyl selenone, D-744
Dimethyl selenoxide, D-744
Dimethyl succinate, S-261
Dimethyl sulfide carboxylic acid, M-665
Dimethyl sulfoxide, D-745
Dimethyl tetrasulfide, D-746
Dimethyl trisulfide, D-747
Dimethyl yellow, D-750
2′,2′-Dimethyl(pyrano-5′,6′:3:4)-1,5-dihydroxy-6-methoxy-10-methylacridone, C-280
γ,δ-Dimethyl-δ-valerolactone, T-83
N,*N*-Dimethyl-(+)-coniine, P-533
3,5-Dimethyl-1,2,4-trithiolane, D-917
1,1′-(3,4-Dimethyl-1,2-cyclobutanediyl)bis[2,4,5-trimethoxybenzene], D-769
3,4-Dimethyl-1,2-cyclopentanedione, D-777
3,5-Dimethyl-1,2-cyclopentanedione, D-778
3,3-Dimethyl-1,2-dithiolane, D-782
4,8-Dimethyl-1,3,7-nonatriene, D-821
3,7-Dimethyl-1,3,7-octatriene, D-847
7-(3,4-Dimethyl-1,3-cyclohexadienyl)-2-methyl-3-heptene, D-820
2,6-Dimethyl-1,4-benzenediol, D-757
2,3-Dimethyl-1,4-butanedithial, D-770
2,5-Dimethyl-1,4-dithiane-2,5-diol, D-781
4-(1,5-Dimethyl-1,4-hexadienyl)-1-methylcyclohexene, B-108
1,5-Dimethyl-1,5,7-cyclodecatriene, T-807
3,7-Dimethyl-1,5,7-octatrien-3-ol, D-849
2-(2,6-Dimethyl-1,5-heptadienyl)-4-methyl-1,3-dioxolane, D-799
3,7-Dimethyl-1,6-octadien-3-ol, D-832
2,6-Dimethyl-1,7-octadien-3-one, D-834
3,7-Dimethyl-1,7-octanediol, D-844
α,4-Dimethyl-1-cyclohexene-1-acetaldehyde, M-157
2,4-Dimethyl-1-hexanol, D-809
N,N-Dimethyl-1-octadecanamine, O-52
3,7-Dimethyl-1-octanol, D-845
3,7-Dimethyl-1-octene-3,7-diol, D-827
2,7-Dimethyl-10-(1-methylethyl)-1-oxaspiro[4.5]deca-3,6-diene, I-132
2,6-Dimethyl-10-methylene-2,6,11-dodecatrienal, F-5
4,8-Dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoic acid, D-865
2,4-Dimethyl-1*H*-indole, D-811
2,5-Dimethyl-1*H*-pyrrole, D-898
1,6-Dimethyl-1*H*-furo[2,3-*b*]imidazo[4,5-*e*]pyridin-2-amine, A-241
N,*N*-Dimethyl-1*H*-imidazole-4-ethanamine, D-752
N,*N*-Dimethyl-1*H*-indole-3-methanamine, D-753
1,2-Dimethyl-1*H*-pyrrole, M-639
3,5-Dimethyl-2(1*H*)-pyrazinone, H-422
3,6-Dimethyl-2(3*H*)-benzofuranone, D-760
3,5-Dimethyl-2(5*H*)-furanone, D-792
5,5-Dimethyl-2(5*H*)-furanone, D-793
2,6-Dimethyl-2,4-heptadiene, D-797
2,7-Dimethyl-2,4-octadiene-1,8-diol, D-829
2,7-Dimethyl-2,4-octadienedioic acid, D-824
2,6-Dimethyl-2,5,7-octatrien-1-ol, D-848
2,6-Dimethyl-2,5-heptadienoic acid, D-798
3,7-Dimethyl-2,6-octadien-1-ol, D-833
3,7-Dimethyl-2,6-octadienal, D-822
2,6-Dimethyl-2,6-octadiene-1,8-diol, D-825
3,7-Dimethyl-2,6-octadiene-1-thiol, D-830
3,7-Dimethyl-2,6-octadienoic acid, D-831
2-(3,7-Dimethyl-2,6-octadienyl)-1,3,5-trihydroxyxanthone, D-841
4-(3,7-Dimethyl-2,6-octadienyl)-1,3,5-trihydroxyxanthone, D-842
3′-(3,7-Dimethyl-2,6-octadienyl)-2′,3,4,4′-tetrahydroxychalcone, D-838
3′-(3,7-Dimethyl-2,6-octadienyl)-2′,4,4′,6′-tetrahydroxychalcone, D-839
4-(3,7-Dimethyl-2,6-octadienyl)-2,3,6,8-tetrahydroxy-1-prenylxanthone, D-840
6-(3,7-Dimethyl-2,6-octadienyl)-2,3-dihydro-7-hydroxy-5-methoxy-2-(2-phenylethyl)-1*H*-isoindol-1-one, H-132
2-[5-(3,7-Dimethyl-2,6-octadienyl)-2,4-dihydroxyphenyl]-2,3-dihydro-5,7-dihydroxy-4*H*-1-benzopyran-4-one, K-50
3-(3,7-Dimethyl-2,6-octadienyl)-2-hydroxy-6-(hydroxymethyl)-4-methoxybenzaldehyde, D-866
1-(3,7-Dimethyl-2,6-octadienyl)-2-hydroxy-9*H*-carbazole-3-carboxaldehyde, M-778
2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone, D-836
1-[2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyphenyl]ethanone, D-836
6-(3,7-Dimethyl-2,6-octadienyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, A-156
4-(3,7-Dimethyl-2,6-octadienyl)-5-(6-hydroxy-2-benzofuranyl)-1,3-benzenediol, A-152
2-(3,7-Dimethyl-2,6-octadienyl)-5-(6-hydroxy-2-benzofuranyl)-1,3-benzenediol, A-153
1-(3,7-Dimethyl-2,6-octadienyl)-6-methyl-9*H*-carbazole-2,7-diol, E-362
2-(3,7-Dimethyl-2,6-octadienyl)cyclopentanone, D-835
7-(3,7-Dimethyl-2,6-octadienyl)oxy-2*H*-1-benzopyran-2-one, A-491
9-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-

g][1]benzopyran-7-one, D-837
4-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, B-66
2,6-Dimethyl-2,7-octadiene-1,6-diol, D-826
2,9-Dimethyl-2,9-diazatricyclo[10.2.2.2^{5,8}]octadeca-5,7,12,14,15,17-hexaene-3,10-diol, D-779
2,3-Dimethyl-2-(1-methylethyl)butanoic acid, I-130
4,5-Dimethyl-2-(1-methylethyl)oxazole, T-444
4,5-Dimethyl-2-(1-methylethyl)thiazole, T-445
3,5-Dimethyl-2-(1-propenyl)pyrazine, D-887
3,4-Dimethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, D-899
4,5-Dimethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, D-900
3,5-Dimethyl-2-(2-propenyl)pyrazine, D-888
2,8-Dimethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-6-chromanol, T-417
1,3-Dimethyl-2-(methylthio)benzene, D-758
1,3-Dimethyl-2-(phenylthio)benzene, D-758
2,4-Dimethyl-2-buten-4-olide, D-792
2,3-Dimethyl-2-butenoic acid, D-771
4,4-Dimethyl-2-butenolide, D-793
2,3-Dimethyl-2-cyclohexen-1-one, D-776
β,5-Dimethyl-2-furanpropanal, M-443
2′-(3,6-Dimethyl-2-heptenyl)-3′,4′,7-trihydroxyflavanone, D-805
8-(3,6-Dimethyl-2-heptenyl)-4′,5,7-trihydroxyflavanone, D-806
2,4-Dimethyl-2-imidazoline, D-245
8,8-Dimethyl-2-methylene-6-oxabicyclo[3.2.1]octan-7-one, D-816
7,7-Dimethyl-2-methylenebicyclo[2.2.1]heptane, D-814
6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptan-3-ol, P-379
6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane, P-376
2,3-Dimethyl-2-norbornene, D-765
6,6-Dimethyl-2-norpinene-2-ethanol, N-142
2,4-Dimethyl-2-pentenoic acid, D-868
1,3-Dimethyl-2-phenoxybenzene, D-875
3,3-Dimethyl-2-phenylbutanoic acid, D-879
1,1-Dimethyl-2-propenyl glucoside, M-343
4-(1,1-Dimethyl-2-propenyl)-1,3,5,6-tetrahydroxy-7-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, D-889
4-(1,1-Dimethyl-2-propenyl)-1,3,5,6-tetrahydroxy-7-prenylxanthone, D-889
7-(1,1-Dimethyl-2-propenyl)-2,3,5,8-tetrahydroxy-1,4-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one, D-1055
7-(1,1-Dimethyl-2-propenyl)-2,3,5,8-tetrahydroxy-1,4-diprenylxanthone, D-1055
6-(1,1-Dimethyl-2-propenyl)-2,3-dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, C-185
3-[5-(1,1-Dimethyl-2-propenyl)-4-hydroxy-2-methoxyphenyl]-1-(4-hydroxyphenyl)-2-propen-1-one, L-80
3-(1,1-Dimethyl-2-propenyl)-6,7-dihydroxy-2*H*-1-benzopyran-2-one, D-880
3-(1,1-Dimethyl-2-propenyl)-6,7-dimethoxy-2*H*-1-benzopyran-2-one, D-880
3-(1,1-Dimethyl-2-propenyl)-6-hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, D-880
3-(1,1-Dimethyl-2-propenyl)-7,8-dihydroxy-2*H*-1-benzopyran-2-one, D-881
3-(1,1-Dimethyl-2-propenyl)-7,8-dimethoxy-2*H*-1-benzopyran-2-one, D-881
3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-2*H*-1-benzopyran-2-one, A-332
3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, G-319
3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, D-880
3-(1,1-Dimethyl-2-propenyl)-7-methoxy-2*H*-1-benzopyran-2-one, A-332
6-(1,1-Dimethyl-2-propenyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one, C-184
3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin, D-882
4-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, C-171
3-(1,1-Dimethyl-2-propenyl)-8-hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, D-881
3,5-Dimethyl-2-propylpyrazine, D-893
3,5-Dimethyl-2-pyrazinol, H-422
4,6-Dimethyl-2-pyrimidinamine, A-245
N-[4-[[(4,6-Dimethyl-2-pyrimidinyl)amino]sulfonyl]phenyl]acetamide, S-271
N′-(4,6-Dimethyl-2-pyrimidinyl)sulfanilamide, S-271
3,5-Dimethyl-2-vinylpyrazine, D-920
4,25-Dimethyl-24-methylenecholest-7-en-3-ol, D-788
4,4-Dimethyl-24-methylenecholest-8-en-3-ol, D-784
4,14-Dimethyl-24-methylenecholest-9(11)-en-3-ol, D-787
2,2-Dimethyl-2*H*-1-benzopyran-6-carboxylic acid, D-763
2,2-Dimethyl-2*H*,6*H*-benzofuro[3,2-*c*]pyrano[2,3-*h*][1]benzopyran-6*a*,9(11*aH*)-diol, G-232
8,8-Dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran, S-92
8,8-Dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, S-92
3-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)-5,7-dihydroxy-6-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, I-78
1-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)ethanone, A-50
3,7-Dimethyl-3(10)-octene-1,2,6,7-tetrol, M-493
1,2-Dimethyl-3,4-bis(2,4,5-trimethoxyphenyl)cyclobutane, D-769
3,7-Dimethyl-3,6-octadienal, D-823
2-(4,8-Dimethyl-3,7-nonadienyl)-2-methyl-2*H*-1-benzopyran-6-carboxylic acid, P-399
2-(4,8-Dimethyl-3,7-nonadienyl)-3,4-dihydro-8-hydroxy-3-methylene-2*H*-1-benzopyran-6-carboxylic acid, P-398
3-(4,8-Dimethyl-3,7-nonadienyl)furan, D-78
2,6-Dimethyl-3,7-octadiene-2,6-diol, D-827
1,2-Dimethyl-3-(1-methylethyl)cyclopentane, I-131
2,5-Dimethyl-3-(1-propenyl)pyrazine, D-885
2,5-Dimethyl-3-(2-propenyl)pyrazine, D-886
2,5-Dimethyl-3-(2-thiofuroyl)furan, D-795
2,5-Dimethyl-3-(methyldithio)furan, D-813
2,5-Dimethyl-3-(methylthio)furan, D-794
2,5-Dimethyl-3-(thioisovaleryl)furan, D-796
β,4-Dimethyl-3-cyclohexene-1-ethanol, M-176
β,4-Dimethyl-3-cyclohexene-1-propanal, M-378
1-(1,4-Dimethyl-3-cyclohexenyl)ethanone, A-51
2,6-Dimethyl-3-formyl-3-heptene, I-145
2,5-Dimethyl-3-furanthiol, D-794
S-2,5-Dimethyl-3-furanyl 3-methylbutanethioate, D-796
2,5-Dimethyl-3-furanyl methyl disulfide, D-813
S-(2,5-Dimethyl-3-furanyl) 2-furancarbothioate, D-795
1-(2,5-Dimethyl-3-furanyl)ethanone, A-52
2,5-Dimethyl-3-furyl methyl ketone, A-52
7,11-Dimethyl-3-methylene-1,6,10-dodecatriene, F-7
6,6-Dimethyl-3-methylenebicyclo[3.1.1]heptan-3-one, P-380
3,7-Dimethyl-3-octanol, D-846
3,7-Dimethyl-3-octene-1,2,6,7-tetrol, D-853
6,10-Dimethyl-3-oxa-9-undecanal, D-860
2,4-Dimethyl-3-oxazoline, D-248
8-(2,2-Dimethyl-3-oxopropyl)-7-methoxy-2*H*-1-benzopyran-2-one, C-294
2,4-Dimethyl-3-pentanone, D-867
2,5-Dimethyl-3-propylpyrazine, D-892
2,4-Dimethyl-3-thiazoline, D-252
2,5-Dimethyl-3-thienyl methyl ketone, A-57
1-(2,5-Dimethyl-3-thienyl)ethanone, A-57
2,5-Dimethyl-3-vinyl-4-hexen-2-ol, S-43
2,5-Dimethyl-3-vinyl-5-hexene-2,4-diol, D-919
2,6-Dimethyl-3-[(2-methyl-3-furanyl)thio]-4-heptanone, D-819
3,3-Dimethyl-3*H*,7*H*-benzofuro[3,2-*c*]pyrano[3,2-*g*][1]benzopyran-7*a*,10(12*aH*)-diol, G-233
3,3-Dimethyl-3*H*,7*H*-furo[3,2-*c*:5,4-*f*′]bis[1]benzopyran-6*b*,10(12*bH*)-diol, H-711
3,8-Dimethyl-3*H*-imidazo[4,5-*f*]quinoxalin-2-amine, A-243
1,1′-Dimethyl-4,4′-bipyridinium(2+), D-768
N,N′-Dimethyl-4,4′-bipyridyl(2+), D-768
2,5-Dimethyl-4-(1-pyrrolidinyl)-3(2*H*)-furanone, D-901
1,2-Dimethyl-4-(6-methyl-4-heptenyl)-1,3-cyclohexadiene, D-820
N,*N*-Dimethyl-4-(phenylazo)benzenamine, D-750
2,6-Dimethyl-4-heptanol, D-801
2,6-Dimethyl-4-heptanone, D-802
5-(1,5-Dimethyl-4-hexenyl)-2-methylphenol, B-101
1-(1,5-Dimethyl-4-hexenyl)-4-methylenebicyclo[3.1.0]hexane, S-94
3-(1,5-Dimethyl-4-hexenyl)-6-methylenecyclohexene, B-105
4-(1,5-Dimethyl-4-hexenylidene)-1-methylcyclohexene, B-107
N,*N*-Dimethyl-4-hydroxytryptamine, D-751
α,α-Dimethyl-4-methylenecyclohexanemethanol, M-174
2,4-Dimethyl-4-phenyltetrahydrofuran, T-82
2,5-Dimethyl-4-vinyl-2,5-hexadien-1-ol, L-131
2,5-Dimethyl-4-vinyl-2,5-hexadienoic acid, L-131
1,4-Dimethyl-4-[4-hydroxy-2-(hydroxymethyl)-1-methyl-2-cyclopentenyl]-2-cyclohexen-1-ol, T-427
2,3-Dimethyl-5,6-dithiabicyclo[2.1.1]hexane, D-780
2,6-Dimethyl-5,7-octadiene-2,3-diol, D-828
6,10-Dimethyl-5,9-undecadien-2-one, D-927
2,2-Dimethyl-5-(1-methyl-1-propenyl)tetrahydrofuran, T-81
2,3-Dimethyl-5-(1-propenyl)pyrazine, D-883
2,3-Dimethyl-5-(2-propenyl)pyrazine, D-884
2,6-Dimethyl-5-heptenal, D-803
2,6-Dimethyl-5-heptenoic acid, D-803
5-(4,4-Dimethyl-5-hexenyl)-1,3-benzodioxole, M-410
1-(1,5-Dimethyl-5-hexenyl)-4-methyl-1,4-cyclohexadiene, B-106
3,7-Dimethyl-5-indanecarboxylic acid, D-810
N,*N*-Dimethyl-5-methoxytryptamine, B-197
1-(1,9-Dimethyl-5-methylene-8-decenyl)-4-methylbenzene, D-815
5,6-Dimethyl-5-norbornen-2-ol, D-766
3,7-Dimethyl-5-octene-1,7-diol, D-852
1-(2,4-Dimethyl-5-oxazolyl)ethanone, A-53
3-(3,7-Dimethyl-5-oxo-2,6-octadienyl)-2-hydroxy-6-(hydroxymethyl)-4-methoxybenzaldehyde, D-866
3,4-Dimethyl-5-pentyl-2-furanheptanoic acid, D-869
3,4-Dimethyl-5-pentyl-2-furanundecanoic acid, D-870
3,4-Dimethyl-5-pentylidene-2(5*H*)-furanone, D-871
2,3-Dimethyl-5-propylpyrazine, D-891
3-[(2,4-Dimethyl-5-sulfophenyl)azo]-4-hydroxy-1-naphthalenesulfonic acid, C-253
2,4-Dimethyl-5-thiazolyl methyl ketone, A-56
1-(2,4-Dimethyl-5-thiazolyl)ethanone, A-56
2,4-Dimethyl-5-vinylthiazole, D-921
1,4-Dimethyl-5*H*-pyrido[4,3-*b*]indol-3-amine, A-244
2,3-Dimethyl-6-(dimethylethylidene)-2-[[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]methyl]cyclohexanepropanoic acid, G-44
2,2-Dimethyl-6-chromenecarboxylic acid, D-763
5-[(3,6-Dimethyl-6-formyl-2-heptenyl)oxy]psoralen, A-489
2,6-Dimethyl-6-hepten-1-ol, D-804
2,10-Dimethyl-6-methylene-1,4-dodecanediol, F-13
2,2-Dimethyl-6-methylene-3-oxabicyclo[3.3.0]octane, H-177
4-(2,2-Dimethyl-6-methylenecyclohexyl)-3-buten-2-one, M-98
2,6-Dimethyl-6-octanol, D-846
3,7-Dimethyl-6-octen-1-ol, D-857
3,7-Dimethyl-6-octenal, D-850
3,7-Dimethyl-6-octene-1,2,3,8-tetrol, D-854
3,7-Dimethyl-6-octenoic acid, D-856
[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde, D-860
8-(3,7-Dimethyl-6-oxo-2-octenyloxy)psoralen, D-

837
1,4-Dimethyl-7-(1-methylethenyl)azulene, D-818
1,4-Dimethyl-7-(1-methylethyl)azulene, I-129
1,4-Dimethyl-7-ethylazulene, D-789
3,7-Dimethyl-7-methoxyoctanal, H-417
3,7-Dimethyl-7-octen-1-ol, D-858
2,6-Dimethyl-7-octen-3-one, D-859
2,6-Dimethyl-7-octene-1,6-diol, D-851
2,6-Dimethyl-7-octene-2,3,6-triol, D-855
2,6-Dimethyl-7-octene-2,6-diol, D-827
2,2-Dimethyl-7-[[(methylamino)carbonyl]oxy]-3(2*H*)-benzofuranone, C-89
1,4*a*-Dimethyl-8-methylenegibbane-1,10-dicarboxylic acid, G-92
4,14-Dimethyl-9,19-cyclocholest-20-en-3-one, D-772
14,24-Dimethyl-9,19-cyclocholest-25-en-3-ol, M-367
4,14-Dimethyl-9,19-cycloergost-23-en-3-ol, D-773
4,14-Dimethyl-9,19-cycloergost-24(28)-en-3-ol, C-450
4,14-Dimethyl-9,19-cycloergost-24-en-3-ol, D-774
4,14-Dimethyl-9,19-cycloergost-25-en-3-ol, D-775
4,14-Dimethyl-9,19-cycloergost-25-en-3-one, D-775
3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraen-1-ol, R-12
1,10-Dimethyl-9-decalol, G-78
6,10-Dimethyl-9-methylene-5-undecen-2-one, D-817
6,10-Dimethyl-9-undecen-2-one, D-918
O,O-Dimethyl-*O*-(4-methylthio-*m*-tolyl) phosphorothioate, F-29
N,N-Dimethyl-*p*-(phenylazo)aniline, D-750
Dimethyl-*p*-tolylcarbinol, M-596
3,3′-Dimethyl-[1,1′-bi-9*H*-carbazole]-2,2′-diol, B-135
3,3′-Dimethyl-[2,2′-bi-1*H*-carbazole]-1,1′,4,4′(9*H*,9′*H*)-tetrone, B-153
2′,4′-Dimethylacetophenone, D-748
2,3-Dimethylacrolein, M-336
3,3-Dimethylacrolein, M-337
3,3-Dimethylacrylic acid, M-341
N,O-Dimethylactinodaphnine, D-154
1,1-Dimethylallyl alcohol, M-343
1,1-Dimethylallyl glucoside, M-343
Dimethylallyl mercaptan, M-339
2-(3,3-Dimethylallyl)-1,3,5-trihydroxyxanthone, T-696
2-(3,3-Dimethylallyl)-1,3,7-trihydroxyxanthone, T-698
1-(3,3-Dimethylallyl)-2,3,6,8-tetrahydroxyxanthone, T-284
5-(1,1-Dimethylallyl)-4,4′-dihydroxy-2-methoxychalcone, L-80
3-(3,3-Dimethylallyl)-4-hydroxybenzoic acid, H-572
3-(1,1-Dimethylallyl)-6,7-dihydroxycoumarin, D-880
3-(1,1-Dimethylallyl)-6,7-dimethoxycoumarin, D-880
3-(1,1-Dimethylallyl)-7,8-dihydroxycoumarin, D-881
3-(1,1-Dimethylallyl)-7,8-dimethoxycoumarin, D-881
3-(1,1-Dimethylallyl)-7-hydroxy-6-(3-methyl-2-butenyl)coumarin, G-319
3-(1,1-Dimethylallyl)-7-hydroxycoumarin, A-332
3-(1,1-Dimethylallyl)-7-methoxycoumarin, A-332
3-(1,1-Dimethylallyl)-8-(3,3-dimethylallyl)xanthyletin, D-882
3-(1,1-Dimethylallyl)-8-hydroxy-7-methoxycoumarin, D-881
3′-(γ,γ-Dimethylallyl)genistein, T-687
O-(3,3-Dimethylallyl)halfordinol, H-3
3-(1,1-Dimethylallyl)herniarin, A-332
3-(1,1-Dimethylallyl)isoscopoletin, D-880
3′-(3,3-Dimethylallyl)kievitone, T-166
3-(γ,γ-Dimethylallyl)luteone, T-167
3-(1,1-Dimethylallyl)psoralen, C-184
3-(1,1-Dimethylallyl)scopoletin, D-880
6-(γ,γ-Dimethylallylamino)purine, Z-8
8-(1,1-Dimethylallyloxy)bergapten, D-476
N-2-[4-(3,3-Dimethylallyloxy)phenyl]ethylcinnamide, H-712
N^5-(*N,N*′-Dimethylamidino)ornithine, D-754
N^5-(*N,N*-Dimethylamidino)ornithine, D-755
Dimethylamine, D-749
2-(Dimethylamino)-3-methyl-*N*-[3-(1-methylethyl)-7-(2-methylpropyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-pentanamide, F-68
2-(Dimethylamino)-4-methyl-*N*-[3-(1-methylethyl)-7-(1-methylpropyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]-hexadeca-10,12,14,15-tetraen-4-yl]-pentanamide, A-130
2-(Dimethylamino)-*N*-[2-methyl-1-[[3,3*a*,12,13,14,15,16,16*a*-octahydro-8-methoxy-13,16-dioxo-14-(phenylmethyl)-5,9-metheno-9*H*-pyrrolo[3,2-*b*][1,5,8]oxadiazacyclopentadecin-1(2*H*)-yl]carbonyl]propyl]propanamide, A-321
α-(Dimethylamino)-*N*-[7-(1-methylpropyl)-5,8-dioxo-3-phenyl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]benzenepropanamide, A-131
α-(Dimethylamino)-*N*-[7-(2-methylpropyl)-5,8-dioxo-3-phenyl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]benzenepropanamide, C-166
4-(Dimethylamino)azobenzene, D-750
2-(Dimethylamino)butanoic acid, A-219
N′-[4-(Dimethylamino)butyl]-*N,N*-dimethyl-1,4-butanediamine, S-153
5-[[6-[2-(Dimethylamino)ethyl]-1,3-benzodioxol-5-yl]acetyl]-1,3-benzodioxole-4-carboxylic acid, A-127
6-[[6-[2-(Dimethylamino)ethyl]-4-methoxy-1,3-benzodioxol-5-yl]acetyl]-2,3-dimethoxybenzoic acid, N-15
3-[[6-[2-(Dimethylamino)ethyl]-4-methoxy-1,3-benzodioxol-5-yl]methylene]-2,3-dihydro-6,7-dimethoxy-1*H*-isoindol-1-one, N-16
1-[2-(Dimethylamino)ethyl]-4-methoxy-3-phenanthrenol, A-484
4-[2-(Dimethylamino)ethyl]imidazole, D-752
N^5-[(Dimethylamino)iminomethyl]ornithine, D-755
(Dimethylamino)oxoacetic acid, O-189
N-[4-[[4-(Dimethylamino)phenyl](2-hydroxy-3,6-disulfo-1-naphthalenyl)methylene]-2,5-cyclohexadien-1-ylidene]-1-methylmethanaminium hydroxide inner salt, C-246
N-[4-[[4-(Dimethylamino)phenyl][4-[ethyl[(3-sulfophenyl)methyl]amino]phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-3-sulfobenzenemethanaminium inner salt, C-247
p-Dimethylamino-*N*-methylphenylalanine, A-216
3-(2-Dimethylaminoethyl)-1*H*-indol-4-ol, D-751
3-(2-Dimethylaminoethyl)-1*H*-indol-5-ol, B-197
1-(2-Dimethylaminoethyl)-3-hydroxy-4-methoxyphenanthrene, A-484
3-(2-Dimethylaminoethyl)-4-hydroxyindole, D-751
3-(2-Dimethylaminoethyl)-5-hydroxyindole, B-197
4-(2-Dimethylaminoethyl)phenol, H-302
1-Dimethylaminoethyl-3,4-dimethoxyphenanthrene, A-484
3-(Dimethylaminomethyl)indole, D-753
3-(4-Dimethylaminophenyl)-2-methylaminopropanoic acid, A-216
Dimethylammonium chloride, D-749
α,α-Dimethylanisalacetone, H-726
2,3-Dimethylanisole, D-872
2,4-Dimethylanisole, D-873
2,5-Dimethylanisole, D-874
2,6-Dimethylanisole, D-875
3,4-Dimethylanisole, D-876
N^G,N'^G-Dimethylarginine, D-754
N^G,N^G-Dimethylarginine, D-755
2,4-Dimethylbenzaldehyde, D-756
α,4-Dimethylbenzeneacetaldehyde, M-593
γ,4-Dimethylbenzenebutanoic acid, T-805
α,α-Dimethylbenzeneethanol, M-594
β,4-Dimethylbenzeneethanol, M-595
α,4-Dimethylbenzenemethanol, M-582
α,α-Dimethylbenzenemethanol, P-308
α,2-Dimethylbenzenepropanal, M-502
α,4-Dimethylbenzenepropanal, M-503
α,α-Dimethylbenzenepropanol, M-578
2,6-Dimethylbenzenethiol, D-758
α-(5,6-Dimethylbenzimidazoyl)cobamide cyanide, V-42
2,3-Dimethylbenzofuran, D-759
2,6-Dimethylbenzoic acid, D-761
3,4-Dimethylbenzoic acid, D-762
2,6-Dimethylbenzonitrile, D-761
3,4-Dimethylbenzonitrile, D-762
α,4-Dimethylbenzyl alcohol, M-582
α,α-Dimethylbenzyl alcohol, P-308
α,α-Dimethylbenzyl isobutyrate, P-308
2,3-Dimethylbicyclo[2.2.1]hept-2-ene, D-765
5,6-Dimethylbicyclo[2.2.1]hept-5-en-2-ol, D-766
2,3-Dimethylbicyclo[2.2.1]heptan-2-ol, D-764
6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-ethanol, N-142
6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-methanol, P-378
1,5-Dimethylbicyclo[3.2.1]octan-8-one, D-767
Dimethylbiochanin B, D-513
Dimethylcaffeic acid, D-653
Dimethylcarbamodithioic acid sodium salt, S-125
4,24-Dimethylcholest-7-en-3-ol, M-432
23,24-Dimethylcholesta-7,22-diene-3,5,6,9-tetrol, M-424
23,24-Dimethylcholesta-7,22-diene-3,5,6-triol, M-425
4,24-Dimethylcholesta-7,23-dien-3-ol, M-426
14,24-Dimethylcholestan-3-one, M-429
O,O-Dimethylcoreximine, X-13
2,3-Dimethylcrotonic acid, D-771
N,O-Dimethylcrotsparine, P-466
4-(2,2-Dimethylcyclobutyl)-3-buten-2-one, J-17
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2-Hydroxy-1,6,7,8-tetramethoxy-3-methylanthraquinone, P-163
7-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-1-heptene-3,5-dione, H-372
5-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-4,6-heptadien-3-one, C-397
2-Hydroxy-1,8-cineole, E-160
3-Hydroxy-1,8-cineole, E-161
3-Hydroxy-1,9-dimethoxy-2-prenylpterocarpan, T-694
8-Hydroxy-1,9-heptadecadien-4,6-diyn-3-one, H-49
2-Hydroxy-1-(1*H*-indol-3-yl)ethanone, H-333
2-Hydroxy-1-(3,4,5-trihydroxyphenyl)ethanone, T-133
2-Hydroxy-1-(3-methyl-2-butenyl)-9*H*-carbazole-3-carboxaldehyde, H-100
5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-decanone, G-120
5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-dodecanone, G-121
5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-hexadecanone, G-123
5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-tetradecanone, G-122
6-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-4-decen-3-one, S-99
7-Hydroxy-1-(4-hydroxybenzyl)-6-methoxyisoquinoline, H-364
3-Hydroxy-1-(4-hydroxyphenyl)-1-propanone, H-510
2-Hydroxy-1-(4-hydroxyphenyl)ethanone, D-370
5-Hydroxy-1-(4-sulfophenyl)-4-[(4-sulfophenyl)azo]pyrazole-3-carboxylic acid, T-28
2-Hydroxy-1-(hydroxymethyl)ethyl decanoate, G-237
2-Hydroxy-1-(hydroxymethyl)ethyl dodecanoate, G-237
2-Hydroxy-1-(hydroxymethyl)ethyl octadecanoate, G-237
2-Hydroxy-1-(hydroxymethyl)ethyl octanoate, G-237
5-(4-Hydroxy-1-butynyl)-2,2′-bithiophene, B-161
1β-Hydroxy-1-desoxotamirin, D-483
2-Hydroxy-1-ethanesulfonic acid, H-449
11-Hydroxy-1-eudesmen-3-one, H-461
2-Hydroxy-1-hydroxymethylpyrrolizidine, H-501

8-Hydroxy-1-methoxy-3-methylanthraquinone, D-544
2-Hydroxy-1-methoxy-4*H*-dibenzo[*de,g*]quinoline-4,5-dione, C-179
2-Hydroxy-1-methoxy-9,10-methylenedioxyaporphine, N-4
2-Hydroxy-1-methoxy-9,10-methylenedioxynoraporphine, N-4
2-Hydroxy-1-methoxyaporphine, D-379
5-Hydroxy-1-methoxyxanthone, D-719
7-Hydroxy-1-methyl-β-carboline, H-576
α-Hydroxy-1-methyl-1*H*-indole-3-propanoic acid, H-518
6-[4-(1-Hydroxy-1-methylethyl)-1-cyclohexene-1-carboxylate] sucrose, O-152
4-(1-Hydroxy-1-methylethyl)-1-cyclohexene-1-carboxylic acid, H-544
4-(1-Hydroxy-1-methylethyl)-1-methyl-1,2-cyclohexanediol, M-143
4-(1-Hydroxy-1-methylethyl)-1-methylcyclohexanol, M-137
5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one, H-546
8-(1-Hydroxy-1-methylethyl)-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, O-171
1-(1-Hydroxy-1-methylethyl)-4-methylcyclohexane, M-151
2-(1-Hydroxy-1-methylethyl)-6*H*-benzofuro[3,2-*c*]furo[3,2-*g*][1]benzopyran-6*a*,9(11*aH*)-diol, G-231
4-[(2-Hydroxy-1-naphthalenyl)azo]benzenesulfonic acid, H-624
4-[(4-Hydroxy-1-naphthalenyl)azo]benzenesulfonic acid, O-163
4-Hydroxy-1-oxo-2-eudesmen-12,6-olide, H-681
ent-8α-Hydroxy-1-oxo-7(11)-eremophilen-12,8-olide, D-450
3-Hydroxy-1-phenyl-1-eicosanone, P-270
3-Hydroxy-1-phenyl-1-heneicosanone, P-280
3-Hydroxy-1-phenyl-1-heptadecanone, P-281
3-Hydroxy-1-phenyl-1-hexadecanone, P-282
3-Hydroxy-1-phenyl-1-octadecanone, P-291
1-Hydroxy-1-phenyl-3-hexadecanone, P-282
1-Hydroxy-1-phenyl-3-octadecanone, P-291
4-(3-Hydroxy-1-propenyl)-1,2-benzenediol, D-656
4-(3-Hydroxy-1-propenyl)-2,6-dimethoxyphenol, S-113
α-[1-[4-(3-Hydroxy-1-propenyl)-2,6-dimethoxyphenoxy]ethyl]-3,4,5-trimethoxybenzenemethanol, M-834
4-(3-Hydroxy-1-propenyl)phenol, H-750
2-Hydroxy-1-[2,4-dihydroxy-5-(3-methyl-2-butenyl)phenyl]-3-[4-hydroxy-3-(3-methyl-2-butenyl)phenyl]-1-propanone, K-14
11-Hydroxy-1-[3-(2-pentenyl)oxiranyl]-9-undecenoic acid, E-133
3-Hydroxy-10′-apo-β,ψ-carotenal, A-384
9-Hydroxy-10(14)-oplopen-4-one, H-668
9-Hydroxy-10,12,15-octadecatrienoic acid, H-646
7-Hydroxy-10,12-dimethoxycoumestan, T-540
9-Hydroxy-10,12-octadecadienoic acid, H-640
11-Hydroxy-10-methoxy-1,2-methylenedioxyaporphine, B-198
9-Hydroxy-10-methoxy-1,2-methylenedioxyaporphine, D-154
11-Hydroxy-10-methoxy-1,2-methylenedioxynoraporphine, B-198
1-Hydroxy-10-methylacridone, H-337
13-Hydroxy-10-oxo-11-octadecenoic acid, H-691
16-Hydroxy-10-oxohexadecanoic acid, D-501
9-Hydroxy-10-undecene-5,7-diynoic acid, H-822
9-Hydroxy-10-undecenoic acid, H-824
1α-Hydroxy-11α,13-dihydroalantolactone, H-459
1β-Hydroxy-11α,13-dihydroalantolactone, H-459
7-Hydroxy-11,12-dimethoxycoumestan (obsol.), T-541
7-Hydroxy-11,12-methylenedioxycoumestan, M-86
3-Hydroxy-11,13(18)-oleanadien-30-oic acid, H-660
7-Hydroxy-11,16-dioxo-8,14-apianadien-22,6-olide, H-425
4-Hydroxy-11-*cis*-retinal, R-11
1β-Hydroxy-11-epicolartin, D-458
3-Hydroxy-11-eremophilen-1-one, E-194
2-Hydroxy-11-eremophilen-9-one, H-443
10-Hydroxy-11-methoxy-1,2-methylenedioxynoraporphine, N-3
12-Hydroxy-11-methoxy-8,11,13-abietatrien-20-oic acid, A-9
5-Hydroxy-11-methylfuro[2,3-*c*]acridin-6(11*H*)-one, F-145
3β-Hydroxy-11-oxo-12-oleanen-29,18α-olide, D-599
3-Hydroxy-11-oxo-12-oleanen-29-oic acid, H-693
3β-Hydroxy-11-oxo-12-oleanen-30,22β-olide, D-602
3-Hydroxy-11-oxo-12-oleanen-30-oic acid, H-694
3-Hydroxy-11-oxo-12-ursen-24-oic acid, D-713
3-Hydroxy-11-oxo-12-ursen-28-oic acid, D-714
3-Hydroxy-11-oxolanosta-8,24-dien-26-al, H-686
2-Hydroxy-11-spirovetiven-14-al, H-784
2-Hydroxy-11-spirovetiven-14-oic acid, H-784
14-Hydroxy-11-spirovetiven-2-one, H-785
3β-Hydroxy-11-ursen-28,13-olide, D-715
18-Hydroxy-12,14-dioxo-9,15-octadecadienoic acid, D-593
3-Hydroxy-12,15-cassadiene-2,11-dione, H-386
1-Hydroxy-12,15-cassadiene-3,11-dione, D-411
2-Hydroxy-12,15-cassadiene-3,11-dione, H-385
3-Hydroxy-12,18-ursadien-28-oic acid, H-825
3-Hydroxy-12,19(29)-ursadien-28-oic acid, H-827
3-Hydroxy-12,19-ursadien-28-oic acid, H-826
3-Hydroxy-12,20(30)-ursadien-28-oic acid, H-828
11-Hydroxy-12-methoxydihydrokawain, D-631
3β-Hydroxy-12-oleanen-28-al, O-127
3-Hydroxy-12-oleanen-28-oic acid, H-663
3-Hydroxy-12-oleanen-29-oic acid, H-664
3β-Hydroxy-12-oleanen-30,22β-olide, O-141
3-Hydroxy-12-oleanen-30-oic acid, H-665
3-Hydroxy-12-oleanene-23,28-dioic acid, H-661
3-Hydroxy-12-oleanene-28,30-dioic acid, H-662
8-Hydroxy-12-oxo-13-abieten-18-oic acid, H-670
11-Hydroxy-12-oxo-7,9(11),13-abietatrien-20,6-olide, H-669
3-Hydroxy-12-taraxasten-28-oic acid, H-794
3-Hydroxy-12-ursen-24-oic acid, U-40
3β-Hydroxy-12-ursen-28-al, U-41
3-Hydroxy-12-ursen-28-oic acid, H-830
20-Hydroxy-12-ursen-3-one, H-831
28-Hydroxy-12-ursene-3,11-dione, D-714
3-Hydroxy-13(18)-oleanen-28-oic acid, H-666
3α-Hydroxy-13,14,15,16-tetranor-12,8-labdanolide, T-315
6α-Hydroxy-13,14,15,16-tetranor-12,8-labdanolide, T-315
12α-Hydroxy-13,18-dehyroparain, N-57
ent-16α-Hydroxy-13-atisen-3-one, A-485
10-Hydroxy-13-deoxypaxilline, P-51
7-Hydroxy-13-deoxypaxilline, P-51
11-Hydroxy-13-nor-6-eremophilen-8-one, H-634
3-Hydroxy-13-nor-6-eremophilene-8,11-dione, H-633
22-Hydroxy-13-tetratriacontanone, H-801
3-[13-Hydroxy-13-[tetrahydro-5-(1-hydroxytridecyl)-2-furanyl]tridecyl]-5-methyl-2(5*H*)-furanone, S-152
1-Hydroxy-14,16-epoxy-20-nor-5(10),6,8,13,15-abietapentaene-11,12-dione, T-13
3α-Hydroxy-14,16-epoxy-20-nor-5(10),6,8,13,15-abietapentaene-11,12-dione, T-13
5-Hydroxy-14,16-hentriacontanedione, H-483
8-Hydroxy-14,16-hentriacontanedione, H-484
25-Hydroxy-14,16-hentriacontanedione, H-485
8-Hydroxy-14-oxo-1(10),4,11(13)-germacratrien-12,6-olide, H-683
3-Hydroxy-14-oxo-1(10),4-germacradien-12,6-olide, D-481
8-Hydroxy-14-oxoacanthospermolide, H-683
3-Hydroxy-14-taraxeren-28-al, H-795
28-Hydroxy-14-taraxeren-3-one, T-25
ent-3β-Hydroxy-15-beyeren-12-one, B-72
ent-3β-Hydroxy-15-beyerene-2,12-dione, B-74
ent-17-Hydroxy-15-kauren-19-oic acid, K-24
ent-18-Hydroxy-15-kauren-7-one, K-23
16-Hydroxy-15-nonacosen-14-one, N-86
6-Hydroxy-15-nor-7(14)-caryophyllen-3-one, I-95
17-Hydroxy-15-octadecene-9,11,13-triynoic acid, H-644
ent-19-Hydroxy-16α-kauran-17-oic acid, K-19
ent-17-Hydroxy-16β-kauran-19-al, K-19
4-Hydroxy-16,18-tritriacontanedione, H-818
10-Hydroxy-16-hentriacontanone, H-486
19-Hydroxy-16-kauren-15-one, H-529
ent-7α-Hydroxy-16-kauren-19,6β-olide, D-516
13-Hydroxy-16-kauren-19-oic acid, H-528
15-Hydroxy-16-kauren-19-oic acid, H-529
9-Hydroxy-16-oxo-10,12,14-octadecatrienoic acid, H-689
18-Hydroxy-16-tritriacontanone, H-819
4-Hydroxy-17-methoxy-2-oxatricyclo[13.2.2.1^{3,7}]eicosa-3,5,7(20),15,17,18-hexaen-10-one, G-45
3-Hydroxy-18-lupen-21-one, H-536
ent-16β-Hydroxy-19-kauranal, K-18
ent-16β-Hydroxy-19-kauranoic acid, K-18
15-Hydroxy-19-trachylobanoic acid, H-806
4-Hydroxy-1*H*-indole-3-acetic acid, H-514
6-Hydroxy-1*H*-indole-3-acetic acid, H-515
6-Hydroxy-1*H*-indole-3-carboxaldehyde, H-516
4-Hydroxy-1*H*-pyrrole-2-carboxylic acid, H-774
3-(7-Hydroxy-1*H*-indol-3-yl)-2-propenoic acid, I-36
6-Hydroxy-1*H*-indole-3-acetamide, H-515
2-Hydroxy-1*H*-indole-3-acetic acid, D-339
4-Hydroxy-1*H*-indole-3-acetonitrile, H-514
α-Hydroxy-1*H*-indole-3-propanoic acid, H-518
7-Hydroxy-2′,3′,4′-trimethoxyisoflavan, T-217
7-Hydroxy-2′,4′,5′-trimethoxyisoflavan, T-218
7-Hydroxy-2′,4′,5-trimethoxyflavanone, T-186
5-Hydroxy-2′,4′,6′,7-tetramethoxy-8-prenylflavanone, P-167
5-Hydroxy-2′,4′,6′,7-tetramethoxyflavone, P-108
5-Hydroxy-2′,4′,7-trimethoxyflavone, T-202
5-Hydroxy-2′,4′,7-trimethoxyisoflavone, T-222
6′-Hydroxy-2′,4′-dimethoxy-3′-methylacetophenone, T-620
7-Hydroxy-2′,4′-dimethoxyisoflavan, T-594
7-Hydroxy-2′,4′-dimethoxyisoflavanone, T-595
4′-Hydroxy-2′,4,6′-trimethoxychalcone, T-147
7-Hydroxy-2′,5,6-trimethoxy-4′,5′-methylenedioxyisoflavone, H-214
5-Hydroxy-2′,6,6′-trimethoxyflavone, T-203
3-Hydroxy-2′,6-dimethoxy-4′-prenyloxyacetophenone, T-134
5-Hydroxy-2′,6-dimethoxyflavone, T-574
4′-Hydroxy-2′,7-dimethoxyisoflavan, T-594
8-Hydroxy-2(1*H*)-quinolinone-4-carboxylic acid, D-682
1-Hydroxy-2,10,11-trimethoxyaporphine, C-359
1-Hydroxy-2,10,11-trimethoxynoraporphine, C-359
7-Hydroxy-2,10-bisaboladien-1-one, H-368
1-Hydroxy-2,12,15-heneicosatrien-4-one, H-482
5-Hydroxy-2,2,6,6-tetrakis(3-methyl-2-butenyl)-4-(2-methyl-1-oxopropyl)-4-cyclohexene-1,3-dione, C-332
3-Hydroxy-2,2,6-trimethyl-6-vinyltetrahydropyran, T-92
1-(5-Hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-3-(4-hydroxyphenyl)-2-propen-1-one, I-72
6-Hydroxy-2,2-dimethyl-4-chromanone, D-255
7-Hydroxy-2,3,4,6-tetramethoxydibenzofuran, D-128
4-Hydroxy-2,3,9-trimethoxypterocarpan, T-286
6*a*-Hydroxy-2,3-dimethoxy-8,9-methylenedioxypterocarpan, P-174
1-Hydroxy-2,3-dimethoxyacridone, T-513
1-Hydroxy-2,3-dimethoxydibenz[*cd,f*]indol-4(5*H*)-one, T-544
9-Hydroxy-2,3-dimethoxypterocarpan, T-701
5-Hydroxy-2,3-dimethyl-1,4-naphthoquinone, H-413
15-Hydroxy-2,3-seco-16-kaurene-2,3-dioic acid, O-177
9-Hydroxy-2,3-seco-4,7,10(14)-oplopatrien-3,2-olide, H-779
9-Hydroxy-2,3-seco-4,7,10(14)-oplopatrien-3,2-olide, H-780
4-Hydroxy-2,4′-dimethoxychalcone, T-533
1-Hydroxy-2,4(18),11(13)-eudesmatrien-12-oic

acid, H-458
8-Hydroxy-2,4,6-octatriynamide, H-656
8-Hydroxy-2,4,6-octatriynoic acid, H-656
1-(13-Hydroxy-2,4,8-tetradecatrienoyl)glycerol, G-236
3-(13-Hydroxy-2,4,8-tetradecatrienoyloxy)-1,2-propanediol, G-236
5-Hydroxy-2,4-decadienoic acid δ-lactone, P-218
3-Hydroxy-2,4-dimethoxydibenzofuran, D-130
1-Hydroxy-2,5,12,15-heneicosatetraen-4-one, H-482
6-Hydroxy-2,5,7,8-tetramethyl-2-chromancarboxylic acid, D-283
3-Hydroxy-2,5,7-trimethoxyphenanthrene, P-247
4-Hydroxy-2,5-bis(4-hydroxyphenyl)-4-cyclopentene-1,3-dione, G-359
8-Hydroxy-2,5-cuparadiene-1,4,10-trione, H-388
2-Hydroxy-2,5-cyclohexadiene-1,4-dione, H-352
4-Hydroxy-2,5-dimethyl-3(2*H*)-furanone, H-407
7-Hydroxy-2,5-dimethyl-4*H*-1-benzopyran-4-one, H-405
7-Hydroxy-2,5-dimethylchromone, H-405
1-Hydroxy-2,6,10-farnesatrien-9-one, H-462
12-Hydroxy-2,6,10-trimethyl-2,6,10-dodecatrien-4-one, H-462
10-Hydroxy-2,6,6,8-tetramethyltricyclo[6.2.1.0^{1,5}]undecan-7-one, C-34
4-Hydroxy-2,6,6-trimethyl-1-cyclohexenecarboxaldehyde, H-811
4-Hydroxy-2,6,6-trimethyl-3-oxo-1,4-cyclohexadiene-1-carboxaldehyde, H-813
5-(1-Hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-2,4-pentadienoic acid, A-11
2-Hydroxy-2,6,6-trimethylcyclohexanone, H-810
2-Hydroxy-2,6,6-trimethylcyclohexylidene-1-acetic acid lactone, T-130
4-Hydroxy-2,6-dimethoxybenzophenone, T-521
4-Hydroxy-2,6-dimethoxyphenanthrene, P-249
4-Hydroxy-2,6-dimethoxyphenyl glucoside, B-22
6-Hydroxy-2,6-dimethyl-1,7-octadien-3-one, H-415
6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one, H-416
6-Hydroxy-2,6-dimethyl-2,7-octadienoic acid, H-414
4-Hydroxy-2,6-dimethyl-7-octen-3-one, H-419
6-Hydroxy-2,6-dimethyl-7-octen-4-one, H-420
10-Hydroxy-2,8-decadiene-4,6-diynoic acid, H-392
3-Hydroxy-2,9-dimethoxypterocarpan, T-701
5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran, H-499
2-Hydroxy-2-(1-methylethyl)butanedioic acid, H-522
4′-Hydroxy-2-(1-methylpiperidin-2-yl)acetophenone, P-413
4-Hydroxy-2-(1-nonenyl)quinoline, N-139
6-Hydroxy-2-(2-hydroxy-4-methoxyphenyl)benzofuran, D-634
7-Hydroxy-2-(2-hydroxypropyl)-5-methyl-4*H*-1-benzopyran-4-one, A-189
7-Hydroxy-2-(2-hydroxypropyl)-5-methylchromone, A-189
3-Hydroxy-2-(2-pentenyl)cyclopentaneacetic acid, C-383
N-[[3-Hydroxy-2-(2-pentenyl)cyclopentyl]acetyl]isoleucine, J-9
7-Hydroxy-2-(3,4,5-trihydroxyphenyl)chroman, T-183
4-Hydroxy-2-(3,6-nonadienyl)quinoline, N-139
5-Hydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6,7-trimethoxy-4*H*-benzopyran-4-one, D-694
6-Hydroxy-2-(3-hydroxy-5-methoxyphenyl)-5-methoxybenzofuran, D-618
2-Hydroxy-2-(3-hydroxyphenyl)acetic acid, H-503
6-Hydroxy-2-(4-hydroxy-2-methoxyphenyl)benzofuran, D-634
5-Hydroxy-2-(4-hydroxyphenyl)-8,8-dimethyl-4*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-4-one, A-479
2-Hydroxy-2-(4-hydroxyphenyl)acetic acid, H-504
2-Hydroxy-2-(4-hydroxyphenyl)ethyl glucosinolate, H-505
N-[2-Hydroxy-2-(4-hydroxyphenyl)ethyl]-3-phenyl-2-propenamide, O-111
N-[2-Hydroxy-2-(4-hydroxyphenyl)ethyl]cinnamide, O-111
N-[2-Hydroxy-2-(4-methoxyphenyl)ethyl]-3-phenyl-2-propenamide, A-132
N-[2-Hydroxy-2-(4-methoxyphenyl)ethyl]benzamide, T-30
3-Hydroxy-2-(4-methylbenzoyl)-4*H*-1-benzopyran-4-one, H-563
3-Hydroxy-2-(4-methylbenzoyl)chromone, H-563
6-Hydroxy-2-(5-hydroxy-3-methoxy-2-prenylphenyl)benzofuran, M-749
5-Hydroxy-2-(5-methyl-1-oxo-4-hexenyl)benzofuran, H-499
6-Hydroxy-2-(*p*-hydroxybenzylidene)-3(2*H*)-benzofuranone, D-381
4-Hydroxy-2-(hydroxymethyl)-2-butenoic acid, H-497
5-Hydroxy-2-(hydroxymethyl)-4*H*-pyran-4-one, H-500
4-(6-Hydroxy-2-benzofuranyl)-1,3-benzenediol, D-634
5-(6-Hydroxy-2-benzofuranyl)-1,3-benzenediol, D-635
6-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, G-292
8-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, K-12
7-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-5-ol, M-751
5-(6-Hydroxy-2-benzofuranyl)-2,2-dimethyl-2*H*-1-benzopyran-7-ol, M-752
5-(6-Hydroxy-2-benzofuranyl)-2-(3-methyl-2-butenyl)-1,3-benzenediol, M-750
1-(5-Hydroxy-2-benzofuranyl)-5-methyl-4-hexen-1-one, H-499
5-Hydroxy-2-benzyl-1,3-dioxane, H-362
4′-Hydroxy-2-biphenylcarboxylic acid, H-366
6-Hydroxy-2-bornanone, H-373
1-Hydroxy-2-butanone, H-375
3-Hydroxy-2-butanone, H-376
7-Hydroxy-2-calamenenone, C-33
8-Hydroxy-2-carbazolecarboxylic acid (obsol.), H-383
2-Hydroxy-2-cyclohexen-1-one, C-460
10-Hydroxy-2-decene-4,6-diynoic acid, H-397
5-Hydroxy-2-decenoic acid δ-lactone, D-342
5-Hydroxy-2-dodecenoic acid lactone, H-122
5-Hydroxy-2-hexen-4-olide, H-450
4-Hydroxy-2-hexen-5-olide, D-276
1-(7-Hydroxy-2-hydroxymethyl-4-oxo-4*H*-1-benzopyran-5-yl)-2-propanone, C-145
7-Hydroxy-2-hydroxymethyl-5-(2-oxopropyl)-4*H*-1-benzopyran-4-one, C-145
2-Hydroxy-2-isopropylbutanedioic acid, H-522
3-Hydroxy-2-isopropylpyrazine, H-526
2-Hydroxy-2-isopropylsuccinamic acid, H-522
2-Hydroxy-2-isopropylsuccinamide, H-522
2-Hydroxy-2-isopropylsuccinic acid, H-522
1-Hydroxy-2-methoxy-10-methyl-3-prenyloxyacridone, T-513
4-Hydroxy-2-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, H-353
2-(6-Hydroxy-2-methoxy-3,4-methylenedioxyphenyl)benzofuran, H-550
8-Hydroxy-2-methoxy-6-methyl-1,4-naphthoquinone, D-558
8-Hydroxy-2-methoxy-6-methylnaphthalene-1,4-dione, D-558
4′-Hydroxy-2-methoxyacetophenone, D-370
4-Hydroxy-2-methoxycinnamaldehyde, D-651
1-Hydroxy-2-methoxydibenz[*cd,f*]indol-4(5*H*)-one, D-425
3-(4-Hydroxy-2-methoxyphenyl)-2-propenal, D-651
2-(4-Hydroxy-2-methoxyphenyl)-6-methoxybenzofuran, D-634
3-Hydroxy-2-methyl-γ-pyrone, H-609
8-Hydroxy-2-methyl-1,4-naphthalenedione, H-594
8-Hydroxy-2-methyl-1,4-naphthoquinone, H-594
4-Hydroxy-2-methyl-2-pentenoic acid γ-lactone, D-792
7-Hydroxy-2-methyl-3-phenyl-4*H*-1-benzopyran-4-one, H-592
7-Hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-carboxylic acid, H-596
7-Hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-acetic acid, D-275
3-Hydroxy-2-methyl-4*H*-pyran-4-one, H-609
3-Hydroxy-2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one, H-542
4-Hydroxy-2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one, H-543
7-Hydroxy-2-methyl-5-(2-oxopropyl)-4*H*-1-benzopyran-4-one, C-145
3-[(2-Hydroxy-2-methyl-5-oxo-3-cyclopenten-1-ylidene)methyl]-2-methylene-6-oxoheptanoic acid, A-103
2-Hydroxy-2-methylbutanedioic acid, H-565
2-Hydroxy-2-methylbutanoic acid, H-567
2-Hydroxy-2-methylbutyl glucosinolate, H-573
3-Hydroxy-2-methylenebutanoic acid, H-582
7-Hydroxy-2-methylisoflavone, H-592
2-Hydroxy-2-methylpropanoic acid, H-605
2-Hydroxy-2-methylpropyl glucosinolate, H-606
2-Hydroxy-2-methylsuccinic acid, H-565
3-Hydroxy-2-methyltetrahydrofuran, T-101
5-Hydroxy-2-methylthiazole, H-618
4-Hydroxy-2-nonenal, H-630
4-Hydroxy-2-nonylquinoline, N-139
3-Hydroxy-2-octadecylindole, H-649
8-Hydroxy-2-octene-4,6-diynoic acid, H-657
α-Hydroxy-2-octyl-1-cyclopropene-1-octanoic acid, H-786
8-Hydroxy-2-oxo-1(10),3,11(13)-guaiatrien-12,6-olide, H-684
5-Hydroxy-2-oxo-1*H*-indole-3-acetic acid, H-685
7-Hydroxy-2-oxo-2*H*-1-benzopyran-6-carboxaldehyde, H-671
7-Hydroxy-2-oxo-2*H*-1-benzopyran-6-carboxylic acid, H-672
5-Hydroxy-2-oxo-3,5-hexadienal, D-942
3-Hydroxy-2-oxobutanoic acid, H-674
4-Hydroxy-2-oxobutanoic acid, H-675
3-Hydroxy-2-oxopropanoic acid, H-698
3-Hydroxy-2-pentanone, H-705
2-(5-Hydroxy-2-pentenyl)-3-oxocyclopentaneacetic acid, H-709
1-Hydroxy-2-phenoxyethane, P-254
5-Hydroxy-2-phenyl-1,3-dioxane, H-721
6-Hydroxy-2-phenyl-4(1*H*)-quinolinone, D-658
7-Hydroxy-2-phenyl-4(1*H*)-quinolinone, D-659
3-Hydroxy-2-phenyl-4*H*-1-benzopyran-4-one, H-466
5-Hydroxy-2-phenyl-4*H*-1-benzopyran-4-one, H-467
2-Hydroxy-2-phenylacetamide, H-715
2-Hydroxy-2-phenylacetic acid, M-57
2-Hydroxy-2-phenylacetonitrile, H-718
2-Hydroxy-2-phenylacetophenone, B-33
3-Hydroxy-2-phenylchromone, H-466
5-Hydroxy-2-phenylchromone, H-467
2-Hydroxy-2-phenylethyl glucosinolate, H-725
5-Hydroxy-2-piperidinecarboxylic acid, H-757
2-(3-Hydroxy-2-piperidinyl)-5-methylfuran, M-447
2-(3-Hydroxy-2-piperidinyl)furan, F-132
1-Hydroxy-2-propanone, H-766
4-(1-Hydroxy-2-propenyl)phenol, H-749
1-Hydroxy-2-propylbenzene, P-531
N-[(5-Hydroxy-2-pyridinyl)methyl]adenosine, H-773
6-(5-Hydroxy-2-pyridinylmethylamino)-9β-ribofuranosylpurine, H-773
3-Hydroxy-2-pyrrolidinecarboxylic acid, H-775
4-Hydroxy-2-pyrrolidinecarboxylic acid, H-776
5-Hydroxy-2-pyrrolidinone, H-777
5-Hydroxy-2-pyrrolidone, H-777
5-Hydroxy-2-styryl-1,3-dioxan, P-274
4-Hydroxy-2-undecylquinoline, U-31
6-Hydroxy-2-[(4-hydroxyphenyl)methylene]-3(2*H*)-benzofuranone, D-381
N-2-Hydroxy-2-[4-(3,3-dimethylallyloxy)phenyl]ethylcinnamide, O-111
N-[2-Hydroxy-2-[4-[(3-methyl-2-butenyl)oxy]phenyl]ethyl]-3-phenyl-2-propenamide, O-111
3α-Hydroxy-20(29)-lupen-27-oic acid, L-116
3β-Hydroxy-20(29)-lupen-27-oic acid, L-116
3-Hydroxy-21,22-seco-8(26),14,22(29)-onocera-

trien-21-oic acid, L-49
3-Hydroxy-21-oxoeupha-8,24-dien-26-oic acid, H-682
3-Hydroxy-21-oxotirucalla-8,24-dien-26-oic acid, H-682
3β-Hydroxy-22(30)-hopen-29-al, H-299
2-Hydroxy-22-methyltetracosanoic acid, H-617
3-Hydroxy-23,24,25,26,27-pentanorcucurbit-5-en-22-al, H-706
3-Hydroxy-23-oxo-12-oleanen-28-oic acid, H-695
6-Hydroxy-24-methyl-4,7,22-cholestatrien-3-one, H-446
3-Hydroxy-24-methylcholesta-5,8,22-trien-7-one, H-445
3-Hydroxy-24-methylcholestan-6-one, E-210
3β-Hydroxy-24-methylene-25*R*-cycloartan-26-oic acid, A-205
26-Hydroxy-24-methylenecycloartan-3-one, H-583
24-Hydroxy-24-vinylcholesterol, S-223
7-Hydroxy-25,26,27-trinor-3,11,15-trioxo-8-lanosten-24,20-olide, H-815
7-Hydroxy-25,26,27-trinor-3,11,15-trioxo-8-lanosten-24-oic acid, H-814
4-Hydroxy-25-desoxyneorollinicin, A-450
3β-Hydroxy-25-oxo-18-oleanen-30-oic acid, D-586
6-Hydroxy-27-dimethoxy-9-methyl-4-dibenzofurancarboxylic acid, T-628
3-Hydroxy-27-norcycloart-23-en-25-one, H-632
3-Hydroxy-27-norcycloartan-25-one, H-632
3-Hydroxy-28,13-lupanolide, D-527
3β-Hydroxy-28,13-ursanolide, D-708
3-Hydroxy-28-nor-12,17-oleanadien-16-one, H-637
3-Hydroxy-28-nor-12-oleanen-16-one, H-637
3-Hydroxy-28-nor-17-oleanen-16-one, H-637
17β-Hydroxy-28-nor-3,16-oleanenedione, D-564
2-Hydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one, H-353
4-Hydroxy-2*H*-1-benzopyran-2-one, H-349
5-Hydroxy-2*H*-1-benzopyran-2-one, H-350
7-Hydroxy-2*H*-1-benzopyran-2-one, H-351
3-Hydroxy-2*H*-pyran-2-one, H-772
4-Hydroxy-2*H*-pyran-3-carboxaldehyde, H-771
11-Hydroxy-2*H*-benzo[*c*]pyrano[2,3-*h*]cinnolin-2-one, N-20
2′-Hydroxy-3′,4′,5′,7,8-pentamethoxyflavan, H-196
5-Hydroxy-3′,4′,5′,7-tetramethoxy-6-prenylflavanone, P-168
8-Hydroxy-3′,4′,5′,7-tetramethoxyflavan, P-106
5-Hydroxy-3′,4′,5′,7-tetramethoxyflavone, P-135
7-Hydroxy-3′,4′,5,6,8-pentamethoxyflavone, H-211
7-Hydroxy-3′,4′,5,6-tetramethoxyflavone, P-137
2′-Hydroxy-3′,4′,6′-trimethoxyacetophenone, T-134
5-Hydroxy-3′,4′,6,7,8-pentamethoxyflavanone, H-203
5-Hydroxy-3′,4′,6,7,8-pentamethoxyflavone, H-211
5′-Hydroxy-3′,4′,7,8-tetramethoxyflavan, P-106
5-Hydroxy-3′,4′,7,8-tetramethoxyflavone, P-141
5-Hydroxy-3′,4′,7-trimethoxy-8-methylisoflavone, T-250
5′-Hydroxy-3′,4′,7-trimethoxyflavan, T-183
3-Hydroxy-3′,4′,7-trimethoxyflavanone, T-189
1′-Hydroxy-3′,4′-didehydro-1′,2′-dihydro-β,ψ-caroten-2′-one, P-412
9-Hydroxy-3′,4′-dimethoxy-3,4-methylenedioxy-9,9′-epoxylignan, P-101
3-Hydroxy-3′,4′-dimethoxyflavone, T-575
7-Hydroxy-3′,4′-dimethoxyisoflavanone, T-596
7-Hydroxy-3′,4′-methylenedioxyisoflavone, H-585
2-Hydroxy-3′,4′:4,5-bis(methylenedioxy)-7,9′:7′,9-diepoxylignan, J-20
5-Hydroxy-3′,5′,7-trimethoxy-4′-prenyloxyflavone, P-135
4′-Hydroxy-3′,5,6,7,8-pentamethoxyflavone, H-211
5-Hydroxy-3′,7-dimethoxy-4′,5′-methylenedioxyflavone, P-135
4′-Hydroxy-3′,7-dimethoxyflavone, T-600
4′-Hydroxy-3′-isovalerylacetophenone, A-65
3-Hydroxy-3′-methoxy-β-carotene, Z-9
4′-Hydroxy-3′-methoxy-2-(2-piperidyl)acetophenone, P-413
4′-Hydroxy-3′-methoxy-3,4-methylenedioxy-7,9′:7′,9-diepoxylignan, P-393
5′-Hydroxy-3′-methoxysativan, P-148
4′-Hydroxy-3′-prenylacetophenone, H-571
15-Hydroxy-3,10(14),11(13)-guaiatrien-12,6-olide, H-478
15-Hydroxy-3,10(14)-guaiadien-12,6-olide, H-478
1-Hydroxy-3,11(13)-eudesmadien-12,8-olide, H-455
7-Hydroxy-3,11,15,23-tetraoxolanost-8-en-26-oic acid, T-553
7β-Hydroxy-3,11,15,23-tetraoxolanosta-8,20(22)-dien-26-oic acid, T-551
15-Hydroxy-3,11,23-trioxolanost-8-en-26-oic acid, T-553
19-Hydroxy-3,11-dioxo-12-ursen-28-oic acid, H-427
15-Hydroxy-3,11-dioxo-8,24-lanostadien-26-oic acid, H-426
10-Hydroxy-3,11-dodecadiene-6,8-diynoic acid, H-430
5-Hydroxy-3,11-eudesmadien-2-one, H-457
7-Hydroxy-3,21,24-trimethylhentriacontan-5-olide, T-86
7-Hydroxy-3,3′,4′,5,6,8-hexamethoxyflavone, H-88
6-Hydroxy-3,3′,4′,5,7,8-hexamethoxyflavone, H-88
5-Hydroxy-3,3′,4′,6,7,8-hexamethoxyflavone, H-88
9-Hydroxy-3,3′,4,4′,5,5′-hexamethoxy-9,9′-epoxylignan, C-381
8-Hydroxy-3,3′,4,4′-tetramethoxylignan-9,9′-olide, P-156
4′-Hydroxy-3,3′,4,5-tetramethoxy-7,7′-epoxylignan, P-99
5-Hydroxy-3,3′,7,8-tetramethoxy-4′,5′-methylenedioxyflavone, H-87
13-Hydroxy-3,3,10,10-tetramethyl-10*H*-dipyrano[3,2-*a*:2′,3′-*i*]xanthen-14(3*H*)-one, T-395
3-Hydroxy-3,3-dimethylpropanoic acid, H-568
2′-Hydroxy-3,4′,5′,7,8-pentamethoxyflavone, H-204
5-Hydroxy-3,4′,6,7,8-pentamethoxyflavone, H-212
7-Hydroxy-3,4′,8-trimethoxyflavone, T-208
2-Hydroxy-3,4,4-trimethyl-2-cyclopenten-1-one, T-760
9-Hydroxy-3,4,5-trimethoxy-3′,4′-methylenedioxy-9,9′-epoxylignan, C-310
2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one, H-812
10-Hydroxy-3,4,9-trimethoxypterocarpan, T-287
3′-Hydroxy-3,4-diketo-β-carotene, D-1037
2-Hydroxy-3,4-dimethyl-2-buten-1,4-olide, H-406
2-Hydroxy-3,4-dimethyl-2-cyclopenten-1-one, D-777
2-(2-Hydroxy-3,4-methylenedioxyphenyl)-6-(3,4-methylenedioxyphenyl)-3,7-dioxabicyclo[3.3.0]octane, J-20
9-Hydroxy-3,4:3′,4′-bis(methylenedioxy)-9,9′-epoxylignan, C-380
8-Hydroxy-3,4:3′,4′-bis(methylenedioxy)lignan-9,9′-olide, P-156
14-Hydroxy-3,5(10),11-cyathatrien-15-al, H-389
2-Hydroxy-3,5,5-trimethyl-2-cyclohexen-1-one, T-745
2-Hydroxy-3,5,5-trimethyl-2-cyclopenten-1-one, T-761
1-Hydroxy-3,5,6-trimethoxy-10-methylacridone, T-136
1-Hydroxy-3,5,6-trimethoxy-4-prenylxanthone, T-281
1-Hydroxy-3,5,6-trimethoxyacridone, T-136
7-Hydroxy-3,5,8-trimethoxyflavone, T-209
1-Hydroxy-3,5-dimethoxy-10-methylacridone, T-514
1-Hydroxy-3,5-dimethoxy-2,4-diprenylxanthone, T-559
1-Hydroxy-3,5-dimethoxy-2-prenylxanthone, T-696
4′-Hydroxy-3,5-dimethoxy-4-prenylstilbene, A-399
4-Hydroxy-3,5-dimethoxybenzoic acid, T-520
4-Hydroxy-3,5-dimethoxycinnamic acid, T-672
1-(4-Hydroxy-3,5-dimethoxyphenyl)-1,2,3-propanetriol, S-294
7-(4-Hydroxy-3,5-dimethoxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one, G-118
2-[[3-(4-Hydroxy-3,5-dimethoxyphenyl)-1-oxo-2-propenyl]oxy]-*N,N,N*-trimethylethanaminium, S-111
1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-propanone, D-650
3-(4-Hydroxy-3,5-dimethoxyphenyl)-2-propen-1-ol, S-113
1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[2-methoxy-4-(1-propenyl)phenoxy]-1-propanol, V-41
1-(4-Hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-3,5-heptanediol, H-403
1-(4-Hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one, G-118
α-(4-Hydroxy-3,5-dimethoxyphenyl)glycerol, S-294
α-Hydroxy-3,5-dimethoxytoluene, D-401
2-Hydroxy-3,5-dimethyl-2-cyclopenten-1-one, D-778
2-Hydroxy-3,5-dimethylpyrazine, H-422
2-Hydroxy-3,5-dinitrobenzoic acid [(5-nitro-2-furanyl)methylene]hydrazide, N-54
1-Hydroxy-3,6,7-trimethoxy-2,8-diprenylxanthone, T-173
1-Hydroxy-3,6,7-trimethoxyxanthone, T-297
19-Hydroxy-3,6-dioxo-12-ursen-28-oic acid, T-721
20ξ-Hydroxy-3,7,11,15,23-pentaoxolanost-8-en-26-oic acid, D-697
12α-Hydroxy-3,7,11,15-tetraoxo-25,26,27-trisnorlanost-8-en-24-oic acid, L-109
15-Hydroxy-3,7,11,23-tetraoxolanost-8-en-26-oic acid, H-800
5-Hydroxy-3,7,8-trimethoxyflavone, T-209
1-Hydroxy-3,7-dimethoxy-2-prenylxanthone, T-698
1-Hydroxy-3,7-dimethoxy-6-methylanthraquinone, T-623
4′-Hydroxy-3,7-dimethoxyflavone, T-577
5-Hydroxy-3,7-dimethoxyflavone, T-580
1-Hydroxy-3,7-dimethoxyxanthone, T-724
8-(7-Hydroxy-3,7-dimethyl-2,5-octadienyloxy)psoralen, D-837
7-[(6-Hydroxy-3,7-dimethyl-2,7-octadienyl)oxy]-2*H*-1-benzopyran-2-one, A-491
7-Hydroxy-3,7-dimethyloctanal, H-417
6-Hydroxy-3,7-dimethyloctanoic acid, H-418
7-Hydroxy-3,8-acoranedione, H-334
4-Hydroxy-3,9,10-trimethoxypterocarpan, T-287
3′-Hydroxy-3,9-dihydroeucomin, D-404
6*a*-Hydroxy-3,9-dimethoxypterocarpan, T-700
4-Hydroxy-3,9-dimethoxypterocarpan, T-702
8-Hydroxy-3,9-dimethoxypterocarpan, T-703
ax-4′′-Hydroxy-3-′-methoxymaysin, M-83
2-Hydroxy-3-(1-methylethyl)-2-cyclopenten-1-one, I-127
2-Hydroxy-3-(1-methylethyl)pyrazine, H-526
2-Hydroxy-3-(1-methylindolyl)propanoic acid, H-518
4-Hydroxy-3-(16-methylheptadecyl)-2*H*-pyran-2-one, H-589
7-Hydroxy-3-(2,3,4-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, T-221
4-Hydroxy-3-(2-hydroxyethyl)acetophenone, H-495
1-[4-Hydroxy-3-(2-hydroxyethyl)phenyl]ethanone, H-495
2-Hydroxy-3-(2-hydroxyphenyl)propanoic acid, H-508
7-Hydroxy-3-(2-thienyl)-1(3*H*)-isobenzofuranone, C-241
3-Hydroxy-3-(3,4-dihydroxy-4-methylpentanoyl)-5-(3-methylbutyl)-1,2,4-cyclopentanetrione, H-401
2-Hydroxy-3-(3,4-dihydroxyphenyl)propanamide, D-641
4-Hydroxy-3-(3-hydroxy-3-methylbutyl)acetophenone, H-571
7-Hydroxy-3-(3-hydroxy-4-methoxybenzyl)-5-methoxy-4-chromanone, D-404
5-Hydroxy-3-(3-hydroxy-4-methoxybenzyl)-7-methoxy-4-chromanone, D-404
2-Hydroxy-3-(3-indolyl)propanoic acid, H-518
1-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]-2-(3,5-dihydroxyphenyl)ethylene, H-564
5-[2-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]ethenyl]-1,3-benzenediol, H-564

2-Hydroxy-3-(3-methyl-2-butenyl)-1,4-naphthalenedione, H-761
4-Hydroxy-3-(3-methyl-2-butenyl)acetophenone, H-571
4-Hydroxy-3-(3-methyl-2-butenyl)benzoic acid, H-572
3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenal, D-1052
3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenoic acid, D-1052
1-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]ethanone, H-571
5-Hydroxy-3-(4-hydroxy-3-methoxybenzyl)-7-methoxy-4-chromanone, D-404
5-Hydroxy-3-(4-hydroxybenzyl)-6,7,8-trimethoxy-4-chromanone, T-213
5-Hydroxy-3-(4-hydroxybenzyl)-7,8-dimethoxy-4-chromanone, T-589
7-Hydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, D-513
5-Hydroxy-3-(4-hydroxyphenyl)-7-methoxy-4*H*-1-benzopyran-4-one, D-541
2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid, H-509
7-Hydroxy-3-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, H-548
2-Hydroxy-3-(4-methoxyphenyl)propanoic acid, H-509
7-Hydroxy-3-(5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-6-yl)-4*H*-1-benzopyran-4-one, G-140
5-Hydroxy-3-(hydroxyacetyl)-1*H*-indole, H-333
2-Hydroxy-3-butenyl glucosinolate, P-464
2-Hydroxy-3-carbomethoxycarbazole, H-382
N-[3-(3-Hydroxy-3-carboxypropylamino)-3-carboxypropyl]homoserine, A-509
2-Hydroxy-3-formylcarbazole, H-382
1-Hydroxy-3-hydroxymethyl-6,8-dimethoxyanthraquinone, T-590
7-Hydroxy-3-indoleacrylic acid, I-36
2-Hydroxy-3-isopropyl-2-cyclopenten-1-one, I-127
5-(4-Hydroxy-3-isovaleryloxy-1-butynyl)-2,2′-bithiophene, B-160
8-Hydroxy-3-methoxy-1-methylanthraquinone-2-carboxylic acid, D-545
7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone, T-724
4-Hydroxy-3-methoxy-1-propenylbenzene, M-272
1-Hydroxy-3-methoxy-10-methyl-5,6-methylenedioxyacridone, T-136
1-Hydroxy-3-methoxy-10-methylacridone, D-375
4-Hydroxy-3-methoxy-2,10-bisaboladien-9-one, D-406
9-Hydroxy-3-methoxy-2-prenylpterocarpan, D-670
4-Hydroxy-3-methoxy-3′,4′-methylenedioxy-7,7′-epoxylignan, H-549
4-Hydroxy-3-methoxy-5-(3-methyl-2-butenyl)benzoic acid, D-548
4-Hydroxy-3-methoxy-5-prenylbenzoic acid, D-548
1-Hydroxy-3-methoxy-7-primeverosyloxyxanthone, T-724
6*a*-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan, T-285
4-Hydroxy-3-methoxybenzaldehyde, D-382
4-Hydroxy-3-methoxybenzenemethanol, D-400
4-Hydroxy-3-methoxybenzoic acid, D-390
4-Hydroxy-3-methoxybenzyl 7-methyloctanoate, D-400
4-Hydroxy-3-methoxybenzyl 8-methyl-6-nonenoate, D-400
4-Hydroxy-3-methoxybenzyl 8-methylnonanoate, D-400
2-(4-Hydroxy-3-methoxybenzyl)imidazole, H-363
2-Hydroxy-3-methoxycinnamic acid, D-652
4-Hydroxy-3-methoxycinnamic acid, H-554
N-(4-Hydroxy-3-methoxycinnamoyl)-1,4-butanediamine, S-256
2-(4-Hydroxy-3-methoxyphenacyl)piperidine, P-413
1-(4-Hydroxy-3-methoxyphenyl)-1,2,3-propanetriol, G-328
3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol, D-645
1-(4-Hydroxy-3-methoxyphenyl)-1,4-decadien-3-one, S-99
1-(4-Hydroxy-3-methoxyphenyl)-1,4-dodecadien-3-one, P-38
1-(4-Hydroxy-3-methoxyphenyl)-1,4-tetradecadien-3-one, P-38
1-(4-Hydroxy-3-methoxyphenyl)-2-(2-piperidinyl)ethanone, P-413
4-(4-Hydroxy-3-methoxyphenyl)-2-butanone, D-613
3-(4-Hydroxy-3-methoxyphenyl)-2-methyl-1-(2,4,6-trihydroxyphenyl)-2-propen-1-one, O-154
1-(4-Hydroxy-3-methoxyphenyl)-2-propanone, D-650
3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid, D-652
3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid, H-554
1-(4-Hydroxy-3-methoxyphenyl)-3,5-decanediol, G-116
1-(4-Hydroxy-3-methoxyphenyl)-3,5-decanedione, G-117
1-(4-Hydroxy-3-methoxyphenyl)-3,5-dodecanediol, G-116
1-(4-Hydroxy-3-methoxyphenyl)-3,5-dodecanedione, G-117
1-(4-Hydroxy-3-methoxyphenyl)-3,5-hexadecanedione, G-117
1-(4-Hydroxy-3-methoxyphenyl)-3,5-octanediol, G-116
1-(4-Hydroxy-3-methoxyphenyl)-3,5-tetradecanediol, G-116
1-(4-Hydroxy-3-methoxyphenyl)-3,5-tetradecanedione, G-117
4-(4-Hydroxy-3-methoxyphenyl)-3-buten-2-one, D-613
1-(4-Hydroxy-3-methoxyphenyl)-3-decanone, H-553
1-(4-Hydroxy-3-methoxyphenyl)-3-dodecanone, P-38
8-(4-Hydroxy-3-methoxyphenyl)-3-methoxy-6,7-dimethyl-2-naphthol, D-71
1-(4-Hydroxy-3-methoxyphenyl)-3-tetradecanone, P-38
1-(4-Hydroxy-3-methoxyphenyl)-3-undecanone, P-38
1-(4-Hydroxy-3-methoxyphenyl)-4-decen-3-one, S-99
1-(4-Hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1,4-pentadien-3-one, B-125
7-(4-Hydroxy-3-methoxyphenyl)-5-methoxy-1-phenyl-3-heptanone, H-496
2-(4-Hydroxy-3-methoxyphenyl)-6-(3,4-methylenedioxyphenyl)-3,7-dioxabicyclo[3.3.0]octane, P-393
1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, C-397
1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-4-hepten-3-one, G-118
1-(4-Hydroxy-3-methoxyphenyl)-7-phenyl-3,5-heptanedione, H-496
6-[2-(4-Hydroxy-3-methoxyphenyl)ethenyl]-4-methoxy-2*H*-pyran-2-one, D-631
α-(4-Hydroxy-3-methoxyphenyl)glycerol, G-328
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-6-methyl-4-heptenamide, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-7-methyl-5-octenamide, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-7-methyloctanamide, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-8-methyl-6-nonenamide, C-75
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-9-methyl-7-decenamide, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-9-methyldecanamide, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]nonanamide, N-132
N-[(4-Hydroxy-3-methoxyphenyl)methyl]octanamide, D-402
9-Hydroxy-3-methoxypterocarpan, D-679
6-(4-Hydroxy-3-methoxystyryl)-4-methoxy-2-pyrone, D-631
4-Hydroxy-3-methoxytoluene, M-314
6-(1-Hydroxy-3-methyl-1-butenyl)-1,3-cyclohexadiene-1-carboxylic acid γ-lactone, M-624
2-Hydroxy-3-methyl-1-prenylcarbazole, M-777
4-Hydroxy-3-methyl-2-(2-pentenyl)-2-cyclopenten-1-one, J-7
4-Hydroxy-3-methyl-2-butenenitrile, H-570
4-Hydroxy-3-methyl-2-butenoic acid, H-570
6-(4-Hydroxy-3-methyl-2-butenylamino)purine, Z-8
2-Hydroxy-3-methyl-2-cyclohexen-1-one, M-370
2-Hydroxy-3-methyl-2-cyclopenten-1-one, M-381
2-Hydroxy-3-methyl-2-cyclopentenimine, I-13
8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, A-492
8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxycoumarin, A-492
2-Hydroxy-3-methyl-4*H*-pyran-4-one, H-608
2-(3-Hydroxy-3-methyl-5-carboxypentyl)-3,5,6-trimethyl-1,4-benzoquinone, T-412
1-Hydroxy-3-methyl-9*H*-carbazole, H-574
2-Hydroxy-3-methyl-9*H*-carbazole, H-575
2-Hydroxy-3-methylbutanoic acid, H-568
3-Hydroxy-3-methylbutanoic acid, H-569
3-[4-(4-Hydroxy-3-methylbutoxy)phenyl]-2-propenal, H-745
8-(3-Hydroxy-3-methylbutyl)-7-methoxy-2*H*-1-benzopyran-2-one, O-182
8-(3-Hydroxy-3-methylbutyl)-7-methoxycoumarin, O-182
3-Hydroxy-3-methylbutyric acid, H-569
4-Hydroxy-3-methylcrotonic acid, H-570
1-Hydroxy-3-methylene-2-pentanone, H-586
6″-*O*-(3-Hydroxy-3-methylglutaroyl)cosmosiin, C-362
9′-(3-Hydroxy-3-methylglutaroyloxy)abscisic acid, A-11
2-Hydroxy-3-methylpyrazine, H-610
(4-Hydroxy-3-nitrobenzene)arsonic acid, H-626
(4-Hydroxy-3-nitrophenyl)arsonic acid, H-626
1-Hydroxy-3-nonanone, H-629
1-Hydroxy-3-nor-15-beyerene-2,12-dione, H-631
1-Hydroxy-3-octanone, H-654
2-Hydroxy-3-oxabicyclo[3.3.0]oct-1(5)-eneacetic acid, G-73
16-Hydroxy-3-oxo-1,12-oleanadien-28-oic acid, H-692
8-Hydroxy-3-oxo-12,6-eudesmanolide, H-680
2-Hydroxy-3-oxo-12-oleanen-28-oic acid, D-574
6β-Hydroxy-3-oxo-12-oleanen-28-oic acid, D-576
16-Hydroxy-3-oxo-12-oleanen-28-oic acid, D-578
7α-Hydroxy-3-oxo-12-ursen-28-oic acid, D-712
11-Hydroxy-3-oxo-12-ursen-28-oic acid, D-714
19-Hydroxy-3-oxo-12-ursen-28-oic acid, D-716
23-Hydroxy-3-oxo-12-ursen-28-oic acid, D-718
1-Hydroxy-3-oxo-4,11(13)-eudesmadien-12,6-olide, H-679
1α-Hydroxy-3-oxo-4-eudesmen-12,6α-olide, D-459
9-Hydroxy-3-oxo-4-megastigmen-13-oic acid, D-534
8-Hydroxy-3-oxo-7(11)-eremophilen-12,8-olide, H-678
6-Hydroxy-3-oxo-7,15-pimaradien-19-oic acid, H-697
28-Hydroxy-3-oxo-9,19-cyclolanost-24-en-26-oic acid, H-676
23-Hydroxy-3-oxocycloart-24-en-26-oic acid, D-418
28-Hydroxy-3-oxocycloart-24-en-26-oic acid, H-676
7-Hydroxy-3-oxolanosta-8,24-dien-26-al, H-687
1-Hydroxy-3-pentadecylbenzene, P-87
4-Hydroxy-3-penten-2-one, P-185
4-Hydroxy-3-pentenoic acid γ-lactone, M-439
2-Hydroxy-3-phenyl-2-propenoic acid, O-242
7-Hydroxy-3-phenyl-4*H*-1-benzopyran-4-one, H-519
4-Hydroxy-3-prenylbenzoic acid, H-572
4-Hydroxy-3-prenylcinnamaldehyde, D-1052
4-Hydroxy-3-prenylcinnamic acid, D-1052
2-Hydroxy-3-prenylnaphthoquinone, H-761
2-Hydroxy-3-propyl-2-cyclopenten-1-one, P-526
20-Hydroxy-3-taraxastanone, T-16
24-Hydroxy-3-ursanone, H-829

4-Hydroxy-3-[(4-sulfo-1-naphthalenyl)azo]-1-naphthalenesulfonic acid, A-529
7-Hydroxy-3-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-4*H*-1-benzopyran-4-one, T-278
3-Hydroxy-30-nor-12,20(29)-oleanadien-28-oic acid, H-636
20-Hydroxy-30-norursan-3-one, H-638
3-Hydroxy-30-oxo-12-oleanen-28-oic acid, D-587
3β-Hydroxy-4α-hydroxymethyl-4β,14α-dimethyl-7,11,15-trioxo-5α-chol-8-en-24-oic acid, L-108
3′-Hydroxy-4′,5′,7,8-tetramethoxyflavone, P-140
7-Hydroxy-4′,5′-methylenedioxypterocarpan (obsol.), M-2
3′-Hydroxy-4′,5,6,7,8-pentamethoxyflavone, H-211
4-Hydroxy-4′,5,7-trimethoxyflavan, T-185
6-Hydroxy-4′,5,7-trimethoxyflavone, T-210
8-Hydroxy-4′,5,7-trimethoxyflavone, T-211
7-Hydroxy-4′,5-dimethoxy-6-methylflavone, T-632
2′-Hydroxy-4′,6′-dimethoxy-3′-methylacetophenone, T-620
2′-Hydroxy-4′,6′-dimethoxy-3′-methylchalcone, T-627
2′-Hydroxy-4′,6′-dimethoxy-3′-methyldihydrochalcone, P-321
2′-Hydroxy-4′,6′-dimethoxyacetophenone, T-512
2′-Hydroxy-4′,6′-dimethoxychalcone, T-535
2′-Hydroxy-4′,6′-dimethoxydihydrochalcone, P-322
7-Hydroxy-4′,6-dimethoxyisoflavone, T-602
5-Hydroxy-4′,7,8-trimethoxyflavone, T-211
5-Hydroxy-4′,7-dimethoxy-6-methylflavone, T-632
2′-Hydroxy-4′,7-dimethoxyisoflavan, T-594
6-Hydroxy-4′,7-dimethoxyisoflavone, T-602
2-Hydroxy-4′-methoxyacetophenone, D-370
7-Hydroxy-4′-methoxyflavanone, D-470
3′-Hydroxy-4′-methoxyglabridin, G-135
7-Hydroxy-4′-methoxyisoflavanone, D-512
7-Hydroxy-4′-methoxyisoflavone, H-548
9-Hydroxy-4(15),10(14),11(13)-guaiatrien-12,6-olide, H-481
9-Hydroxy-4(15),10(14)-guaiadien-12,6-olide, H-476
7α-Hydroxy-4(15),11(13)-eudesmadien-12-al, E-367
7-Hydroxy-4(15),11(13)-eudesmadien-12-oic acid, E-367
2-Hydroxy-4(6)-(1-methylethyl)-2,4,6-cycloheptatrien-1-one, H-523
2-Hydroxy-4(6)-isopropyl-2,4,6-cycloheptatrien-1-one, H-523
8-Hydroxy-4(6)-lactaren-5,14-olide, H-531
8-Hydroxy-4(6)-lactarene-5,14-dial, H-530
8-Hydroxy-4(6)-lactarene-5,14-diol, H-530
9-Hydroxy-4,10(14)-oplopadien-3-one, H-667
12-Hydroxy-4,11(13)-eudesmadien-3-one, E-377
1β-Hydroxy-4,11-diepicolartin, D-458
3-Hydroxy-4,15-dinor-1(5)-xanthen-12,8-olide, H-424
2′-Hydroxy-4,4′,6′-trimethoxychalcone, T-147
2′-Hydroxy-4,4′,6′-trimethoxydihydrochalcone, H-752
5-Hydroxy-4,4′,6-trimethoxyaurone, T-139
12α-Hydroxy-4,4,14α-trimethyl-3,7,11,15-tetraoxo-5α-chol-8-en-24-oic acid, L-109
7β-Hydroxy-4,4,14-trimethyl-5α-pregn-8-ene-3,11,15,20-tetrone, L-111
3-Hydroxy-4,5′-retro-5′-apo-β-caroten-5′-one, T-10
3-Hydroxy-4,5-bis(hydroxymethyl)-2-methylpyridine, P-606
3-Hydroxy-4,5-bis(hydroxymethyl)-2-prenylphenyl 2,4-dihydroxy-6-methylbenzoate, M-770
7-Hydroxy-4,5-dimethoxy-3′,4′-methylenedioxy-2,7′-cycloligna-7,7′-dien-9′,9-olide, D-958
3-(3-Hydroxy-4,5-dimethoxyphenyl)-1,2-propanediol, T-666
3-Hydroxy-4,5-dimethyl-2(5*H*)-furanone, H-406
3-Hydroxy-4,5-methylenedioxybenzoic acid, H-584
2-(3-Hydroxy-4,5-methylenedioxyphenyl)-1-methyl-4(1*H*)-quinolinone, G-320
2-Hydroxy-4,6-dimethoxy-3′,4′-methylenedioxybenzophenone, P-91
1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, T-627
2-Hydroxy-4,6-dimethoxybenzophenone, T-521
1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-(4-hydroxyphenyl)-1-propanone, H-752
1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-(4-methoxyphenyl)-1-propanone, H-752
1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-phenyl-1-propanone, P-322
N^5-(5-Hydroxy-4,6-dimethyl-2-pyrimidinyl)ornithine, A-408
6-Hydroxy-4,6-dimethyl-3-hepten-2-one, H-408
2-Hydroxy-4,7(11)-valerenadien-12-oic acid, H-832
6-Hydroxy-4,7,22-ergostatrien-3-one, H-446
2-Hydroxy-4,7-dimethoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-399
6-Hydroxy-4,7-megastigmadiene-3,9-dione, D-531
3-Hydroxy-4,9-dimethoxycoumestan, T-539
3-Hydroxy-4,9-dimethoxypterocarpan, T-702
3-Hydroxy-4-(1-methylethyl)benzenemethanol, H-521
4-Hydroxy-4-(1*H*-indol-3-ylmethyl)glutamic acid, M-737
2-Hydroxy-4-(4-hydroxyphenyl)-1*H*-phenalen-1-one, H-506
3-Hydroxy-4-(4-hydroxyphenyl)-1*H*,3*H*-naphtho[1,8-*cd*]pyran-1-one, P-288
3-Hydroxy-4-(4-hydroxyphenyl)-6-[(4-hydroxyphenylmethylene)]-2*H*-pyran-2,5(6*H*)-dione, G-323
2-Hydroxy-4-(4-methoxyphenyl)-1*H*-phenalen-1-one, H-506
3-Hydroxy-4-(hydroxymethyl)phenyl β-D-glucopyranoside 6-benzoate, F-37
5-Hydroxy-4-(methoxymethyl)-6-methyl-3-pyridinemethanol, P-606
2-Hydroxy-4-(methylthio)butanoic acid, H-619
13-Hydroxy-4-*O*-methoxymelleolide (incorr.), P-549
8-Hydroxy-4-acoren-3-one, H-336
7-Hydroxy-4-acorene-3,8-dione, H-335
3-Hydroxy-4-butanolide, D-258
3-Hydroxy-4-deoxypaxilline, P-51
1-Hydroxy-4-eudesmen-6-one, H-460
6-Hydroxy-4-heneicosanone, H-27
5-Hydroxy-4-hexanolide, H-450
3-Hydroxy-4-hydroxymethyl-4-butanolide, D-265
2-Hydroxy-4-imino-2,5-cyclohexadienone, H-512
2-Hydroxy-4-isopropyl-1-methylbenzene, I-147
2-Hydroxy-4-isopropyl-7,8-dimethoxy-6-methyl-1-naphthalenecarboxaldehyde, T-527
3-Hydroxy-4-isopropylbenzyl alcohol, H-521
3-Hydroxy-4-isopropyltoluene, I-146
5-(3-Hydroxy-4-isovaleryloxy-1-butynyl)-2,2′-bithiophene, B-160
9-Hydroxy-4-megastigmen-3-one, H-539
6-Hydroxy-4-methoxy-3-(3-methyl-2-butenyl)-2-(2-phenylethenyl)benzoic acid, D-674
2-Hydroxy-4-methoxy-3-(3-methyl-2-butenyl)-6-(2-phenylethenyl)benzoic acid, D-673
5-Hydroxy-4-methoxy-3-methyl-2,6-canthinedione, I-31
6-Hydroxy-4-methoxy-3-prenyl-2-styrylbenzoic acid, D-674
2-Hydroxy-4-methoxy-3-prenyl-6-styrylbenzoic acid, D-673
5-Hydroxy-4-methoxy-5-(1-oxo-9,12,15-hexadecatrienyl)-2(5*H*)-furanone, H-551
4-[6-Hydroxy-4-methoxy-5-(3-methyl-2-butenyl)-2-benzofuranyl]-1,3-benzenediol, D-622
3-Hydroxy-4-methoxy-5-(3-methyl-2-butenyl)benzoic acid, D-548
3-Hydroxy-4-methoxy-5-prenylbenzoic acid, D-548
5-Hydroxy-4-methoxy-6-canthinone 3-*N*-oxide, N-58
2-Hydroxy-4-methoxy-6-styrylbenzoic acid, D-629
5-Hydroxy-4-methoxy-6*H*-indolo[3,2,1-*de*][1,5]-naphthyridin-6-one, N-58
3-Hydroxy-4-methoxy-*N,N,N*-trimethylbenzeneethanaminium, H-552
3-Hydroxy-4-methoxy-*N*-methylphenethylamine, H-552
1-(3-Hydroxy-4-methoxybenzyl)-6,7-dimethoxyisoquinoline, P-36
5-Hydroxy-4-methoxycanthin-6-one, N-58
3-Hydroxy-4-methoxycinnamic acid, D-653
8-Hydroxy-4-methoxyfuro[2,3-*b*]quinoline, F-149
9-Hydroxy-4-methoxyfuro[3,2-*g*][1]benzopyran-7-one, D-476
3-Hydroxy-4-methoxyphenethylamine, H-552
1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol, D-626
1-(2-Hydroxy-4-methoxyphenyl)-2-propanol, D-648
3-(3-Hydroxy-4-methoxyphenyl)-2-propenoic acid, D-653
2-(2-Hydroxy-4-methoxyphenyl)-5,6-methylenedioxybenzofuran, D-617
2-(2-Hydroxy-4-methoxyphenyl)-5-hydroxy-6-methoxybenzofuran, D-617
2-(2-Hydroxy-4-methoxyphenyl)-6-methoxy-3-benzofurancarboxaldehyde, D-636
3-(2-Hydroxy-4-methoxyphenyl)-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, K-13
9-Hydroxy-4-methoxypsoralen, D-476
3-Hydroxy-4-methoxystyrene, V-33
7-Hydroxy-4-methyl-1(3*H*)-isobenzofuranone, H-591
4-Hydroxy-4-methyl-2-cyclohexen-1-one, H-580
4-Hydroxy-4-methyl-2-pentanone, H-599
4-Hydroxy-4-methyl-2-propyltetrahydrofuran, T-105
7-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one, H-561
4-Hydroxy-4-methyl-7-decenoic acid γ-lactone, H-259
2-Hydroxy-4-methylbenzaldehyde, H-557
7-Hydroxy-4-methylcoumarin, H-561
4-Hydroxy-4-methyldecanoic acid lactone, H-268
2-Hydroxy-4-methylpentanoic acid, H-598
3-(2-Hydroxy-4-methylphenyl)-2-butanone, H-600
2-(2-Hydroxy-4-methylphenyl)-3-pentanone, H-602
2-(3-Hydroxy-4-methylphenyl)-5-methyl-4-hexen-3-one, H-601
2-[(2-Hydroxy-4-methylphenyl)methylene]hydrazinecarboxamide, H-557
7-Hydroxy-4-methylphthalide, H-591
2-Hydroxy-4-methylvaleric acid, H-598
6-Hydroxy-4-nonadecanone, N-93
5-Hydroxy-4-octanone, H-655
2-Hydroxy-4-oxo-12,15-heneicosadien-1-yl acetate, D-495
1-Hydroxy-4-oxo-12,15-heneicosadien-2-yl acetate, D-495
1-Hydroxy-4-oxo-2,5,10-bisabolatrien-12-al, H-673
3-Hydroxy-4-oxo-4*H*-pyran-2,6-dicarboxylic acid, H-699
2-Hydroxy-4-oxo-5,12,15-heneicosatrien-1-yl acetate, D-495
2-Hydroxy-4-oxo-5,12,15-heneicosatrien-1-yl acetate, D-496
2-Hydroxy-4-oxo-5,12-heneicosadien-1-yl acetate, D-495
2-Hydroxy-4-oxoheneicos-1-yl acetate, D-495
2-Hydroxy-4-oxopentanoic acid, H-696
2-Hydroxy-4-oxovaleric acid, H-696
8-Hydroxy-4-patchoulen-3-one, P-47
6-Hydroxy-4-pentacosanone, P-64
3-Hydroxy-4-pentenenitrile, H-707
3-Hydroxy-4-pentenoic acid, H-707
5-Hydroxy-4-pentenoic acid δ-lactone, D-348
2-Hydroxy-4-pentenyl glucosinolate, H-708
2-Hydroxy-4-phenyl-1*H*-phenalen-1-one, H-506
1-Hydroxy-4-propylbenzene, P-532
3-Hydroxy-4-pyrone-2,6-dicarboxylic acid, H-699
2-[4-[(1-Hydroxy-4-sulfo-2-naphthalenyl)azo]phenyl]-6-methyl-7-benzothiazolesulfonic acid, C-249
6-Hydroxy-4-tricosanone, T-460
3-Hydroxy-4-[(2,4,5-trimethylphenyl)azo]-2,7-naphthalenedisulfonic acid, C-254
3-Hydroxy-4-[(4-methyl-2-sulfophenyl)azo]-2-naphthalenecarboxylic acid, L-97
3-Hydroxy-4-[(4-sulfo-1-naphthalenyl)azo]-2,7-naphthalenedisulfonic acid, A-203
14*a*-Hydroxy-4*b*-deoxypaxilline, P-51

2-Hydroxy-4*H*-1-benzopyran-4-one, H-349
4-Hydroxy-4*H*-furo[3,2-*c*]pyran-2(6*H*)-one, P-49
7-Hydroxy-5′,6′-methylenedioxybenzofurano[3′,2′:3,4]coumarin, M-86
13-Hydroxy-5′-*O*-methylmelledonal, P-173
15-Hydroxy-5′-*O*-methylmelledonal, P-173
2′-Hydroxy-5′-methylacetophenone, H-556
2-Hydroxy-5,11(13)-eudesmadien-12,8-olide, H-456
1-Hydroxy-5,11(13)-eudesmadien-12,8-olide, H-459
4′-Hydroxy-5,5′-diisopropyl-2,2′-dimethyl-3,4-biphenylquinone, H-402
4′-Hydroxy-5,6,7,8-tetramethoxyflavone, P-143
4′-Hydroxy-5,6,7-trimethoxyflavone, T-210
1-Hydroxy-5,6-dimethoxy-2-methylanthraquinone, T-621
8-Hydroxy-5,6-octadienoic acid, H-650
3′-Hydroxy-5,6-seco-β,β-carotene-5,6-dione, T-810
3-Hydroxy-5,7,8-trimethoxyflavone, T-209
8-Hydroxy-5,7-dimethoxy-3-(4-methoxybenzyl)-4-chromanone, T-589
4′-Hydroxy-5,7-dimethoxyflavan, T-566
3-Hydroxy-5,7-dimethoxyflavanone, T-568
3-Hydroxy-5,7-dimethoxyflavone, T-580
3-Hydroxy-5,7-megastigmadien-9-one, H-537
3-Hydroxy-5,8-megastigmadien-7-one, M-100
4-Hydroxy-5,8-megastigmadien-7-one, M-100
7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone, H-502
3-Hydroxy-5-(hydroxyphenylmethyl)-1-methyl-4-phenyl-2-pyrrolidinone, C-302
6-Hydroxy-5-(phenylazo)-2-naphthalenesulfonic acid, H-719
3-(6-Hydroxy-5-benzofuranyl)-2-propenoic acid, H-344
1-Hydroxy-5-eudesmen-12,8-olide, H-459
3-Hydroxy-5-hexanolide, T-90
3-Hydroxy-5-hydroxymethyl-2-methyl-4-pyridinecarboxaldehyde, P-605
3-Hydroxy-5-hydroxymethyl-2-methylisonicotinic aldehyde, P-605
3-Hydroxy-5-hydroxymethyl-4-methoxymethyl-2-methylpyridine, P-606
3-Hydroxy-5-isopentenyl-4-methoxybenzoic acid, D-548
7-Hydroxy-5-isopropyl-2-methoxy-3-methyl-1,4-naphthoquinone, D-515
4-(4-Hydroxy-5-isopropyl-2-methylphenyl)-6-isopropyl-3-methyl-3,5-cyclohexadiene-1,2-dione, H-402
2-Hydroxy-5-isopropylpyrazine, H-524
7-Hydroxy-5-methoxy-2-methyl-4*H*-1-benzopyran-4-one, D-546
7-Hydroxy-5-methoxy-2-methylchromone, D-546
2-Hydroxy-5-methoxy-3-(10-pentadecenyl)-1,4-benzoquinone, D-609
2-Hydroxy-5-methoxy-3-(8,11,14-pentadecatrienyl)-1,4-benzoquinone, D-609
2-Hydroxy-5-methoxy-3-pentadecyl-1,4-benzoquinone, D-609
2-Hydroxy-5-methoxy-3-undecyl-1,4-benzoquinone, D-705
3-Hydroxy-5-methoxy-4-prenylstilbene, M-348
3-Hydroxy-5-methoxy-6,7-methylenedioxyflavanone, T-193
7-Hydroxy-5-methoxy-6,8-dimethylflavanone, D-432
3-Hydroxy-5-methoxy-6-methyl-2-pentyl-4*H*-pyran-4-one, A-180
2-Hydroxy-5-methoxybenzoic acid, D-388
3-Hydroxy-5-methoxybenzoic acid, D-391
3-Hydroxy-5-methoxybenzonitrile, D-391
3-Hydroxy-5-methoxybenzyl alcohol, D-401
7-Hydroxy-5-methoxyflavan, D-469
7-Hydroxy-5-methoxyflavanone, D-471
6-Hydroxy-5-methoxyflavone, D-472
7-Hydroxy-5-methoxyflavonol, T-580
1-(3-Hydroxy-5-methoxyphenyl)-2-(3-methoxyphenyl)ethane, D-639
2-(3-Hydroxy-5-methoxyphenyl)-5-methoxy-6-benzofuranol, D-618
2-(3-Hydroxy-5-methoxyphenyl)-6-methoxy-5-benzofuranol, D-618
8-Hydroxy-5-methoxypsoralen, D-476
9-Hydroxy-5-methoxypsoralen, D-476
3-Hydroxy-5-methoxystilbene, D-692
1-Hydroxy-5-methoxyxanthone, D-719
2-Hydroxy-5-methyl-2-cyclopenten-1-one, M-381
4-Hydroxy-5-methyl-3(2*H*)-furanone, H-588
4-Hydroxy-5-methyl-3(2*H*)-thiophenone, H-620
2-(3-Hydroxy-5-methylphenoxy)-5-methoxy-3-methylphenol, D-536
1-(2-Hydroxy-5-methylphenyl)ethanone, H-556
2-Hydroxy-5-methylpyrazine, H-611
3-Hydroxy-5-octenoic acid, H-658
3-Hydroxy-5-phenylpentanoic acid, H-730
14-Hydroxy-5-tetradecene-8,10,12-triynoic acid, H-799
6-Hydroxy-5-[(2-methoxy-5-methyl-4-sulfophenyl)azo]-2-naphthalenesulfonic acid, A-183
6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid, H-793
3-Hydroxy-5-[2-(3-methoxyphenyl)ethyl]phenol, D-639
2′-Hydroxy-6′-methoxy-4′-prenyloxychalcone, T-535
2′-Hydroxy-6′-methoxy-4′-prenyloxydihydrochalcone, P-322
2′-Hydroxy-6′-methoxyacetophenone, D-372
3-Hydroxy-6′-methyl-6′-apo-β-caroten-6′-one, R-9
2-Hydroxy-6,7-dimethoxybenzoxazole, D-738
5-Hydroxy-6,7-methylenedioxyflavone, T-582
5-Hydroxy-6,8-dimethoxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, T-634
1-(1-Hydroxy-6,8-dimethoxy-3-methyl-2-napthalenyl)ethanone, A-100
3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide, T-561
2-Hydroxy-6,8-dimethoxy-9*H*-carbazole-3-carboxaldehyde, L-48
2-Hydroxy-6-(10-pentadecenyl)benzoic acid, H-701
2-Hydroxy-6-(16-hydroxy-8-heptadecenyl)benzoic acid, H-77
5-Hydroxy-6-(2-hydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, T-419
3-Hydroxy-6-(2-hydroxyethyl)-2,2,5,7-tetramethyl-1-indanone, P-562
3-Hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone, P-561
4-Hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone, P-567
2-Hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone, P-568
3-Hydroxy-6-(2-hydroxyethyl)-2-hydroxymethyl-2,5,7-trimethyl-1-indanone, P-566
7-Hydroxy-6-(3-hydroxy-3-methyl-1-butenyl)-2*H*-1-benzopyran-2-one, H-498
5-Hydroxy-6-(4-hydroxycinnamoyl)-2,2-dimethylchromene, I-72
4-Hydroxy-6-(4-hydroxystyryl)-2-pyrone, Y-1
2-Hydroxy-6-(8,11,14-pentadecatrienyl)benzoic acid, H-701
2-Hydroxy-6-(8,11-heptadecadienyl)benzoic acid, H-77
2-Hydroxy-6-(8,11-pentadecadienyl)benzoic acid, H-701
2-Hydroxy-6-(8-pentadecenyl)benzoic acid, H-701
2-Hydroxy-6-(8-tridecenyl)benzoic acid, H-809
7-Hydroxy-6-(methoxyacetyl)-2,2-dimethyl-2*H*-1-benzopyran, H-494
8-Hydroxy-6-docosanone, D-1001
4-Hydroxy-6-docosanone, D-999
4-Hydroxy-6-eicosanone, E-12
11-Hydroxy-6-eremophilen-8-one, H-444
4-Hydroxy-6-heneicosanone, H-27
8-Hydroxy-6-heneicosanone, H-28
4-Hydroxy-6-heptacosanone, H-41
16-Hydroxy-6-hexadecenoic acid, H-492
7-Hydroxy-6-hydroxyacetyl-2,2-dimethyl-2*H*-benzopyran, H-494
8-Hydroxy-6-hydroxymethyl-1,3-dimethoxyanthraquinone, T-590
5-Hydroxy-6-isobutyryl-8,8-dimethyl-4-phenyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, M-235
2-Hydroxy-6-isopropylpyrazine, H-525
5-Hydroxy-6-isovaleryl-8,8-dimethyl-4-phenyl-2*H*,8*H*-benzo[1,2-*b*,3,4-*b*′]dipyran-2-one, M-55
7-Hydroxy-6-methoxy-α-pyrufuran, D-125
3-Hydroxy-6-methoxy-1-methyl-4,5-diphenyl-2-piperidinone, D-438
7-Hydroxy-6-methoxy-1-methylisoquinoline, D-555
3-Hydroxy-6-methoxy-2,2-dimethyl-4-chromanone, D-228
4-Hydroxy-6-methoxy-2-quinolinecarboxylic acid, D-683
7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, H-547
8-Hydroxy-6-methoxy-3,7-dimethylisochroman, D-288
1-Hydroxy-6-methoxy-3-methylanthraquinone, D-543
3-Hydroxy-6-methoxy-7(11)-eremophilen-12,8-olide, D-451
8-Hydroxy-6-methoxy-7(11)-eremophilen-12,8-olide, D-452
2-Hydroxy-6-methoxy-9*H*-carbazole-3-carboxaldehyde, L-48
7-Hydroxy-6-methoxycoumarin, H-547
5-Hydroxy-6-methoxyflavone, D-472
7-Hydroxy-6-methoxyflavone, D-474
7-Hydroxy-6-methoxyphthalide, D-511
7-Hydroxy-6-methyl-2*H*-1-benzopyran-2-one, H-562
5-Hydroxy-6-methyl-3,4-pyridinedimethanol, P-606
2-Hydroxy-6-methyl-3-(1-methylethyl)-2-cyclohexen-1-one, H-545
4-Hydroxy-6-methyl-3-(1-oxobutyl)-2*H*-pyran-2-one, H-597
4-Hydroxy-6-methyl-3-(4-methyl-1-oxopentyl)-2*H*-pyran-2-one, D-102
28-Hydroxy-6-methyl-5-tritriacontanone, H-622
7-Hydroxy-6-methylcoumarin, H-562
2-Hydroxy-6-methylpyrazine, H-612
4-Hydroxy-6-nonadecanone, N-93
8-Hydroxy-6-oxo-7(11)-eremophilen-12,8-olide, D-452
4-Hydroxy-6-pentacosanone, P-64
2-Hydroxy-6-pentadecylbenzoic acid, H-704
5-Hydroxy-6-protoilluden-14-al, H-769
4-[(2-Hydroxy-6-sulfo-1-naphthalenyl)azo]-1-naphthalenesulfonic acid, H-792
4-Hydroxy-6-tetracosanone, T-44
4-Hydroxy-6-tricosanone, T-460
8-Hydroxy-6-tricosanone, T-461
2-Hydroxy-6-tridecylbenzoic acid, H-809
2-Hydroxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, H-377
5-Hydroxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, H-378
3-Hydroxy-6*H*-[1,3]dioxolo[5,6]benzofuro[3,2-*c*][1]-benzopyran-6-one, M-86
4-Hydroxy-7(11),10(14)-guaiadien-8-one, H-480
3-Hydroxy-7(11),9-eremophiladien-8-one, H-438
4-Hydroxy-7(11),9-guaiadien-8-one, H-479
3-Hydroxy-7(11)-eremophilen-12,8-olide, H-440
6-Hydroxy-7(11)-eremophilen-12,8-olide, H-441
2-Hydroxy-7(11)-eremophilen-8-one, H-442
3-Hydroxy-7,11,15,23-tetraoxolanost-8-en-26-oic acid, T-553
12-Hydroxy-7,13-abietadien-18-oic acid, H-326
2-Hydroxy-7,15-pimaradien-19,6-olide, D-663
3-Hydroxy-7,8-didehydro-β-ionol, M-105
3-Hydroxy-7,8-dihydro-β-ionol, M-102
4′-Hydroxy-7,8-dimethoxyflavanone, T-571
5-Hydroxy-7,8-dimethoxyflavonol, T-209
5-Hydroxy-7,9,10-trimethoxy-2,2-dimethyl-2*H*,6*H*-pyrano[3,2-*b*]xanthen-6-one, D-1057
3-Hydroxy-7,9-dimethoxycoumestan, T-540
5-Hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-phenyl-3-heptanone, H-496
5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone, H-507
9-Hydroxy-7-(4-hydroxyphenyl)-8*H*-1,3-dioxolo[4,5-*g*][1]benzopyran-8-one, D-551
14-Hydroxy-7-*O*-methylrosmanol, R-54

5-Hydroxy-7-decenoic acid lactone, T-113
5-Hydroxy-7-docosanone, D-1000
O-(3-Hydroxy-7-drimen-11-yl)umbelliferone, H-436
3-Hydroxy-7-drimen-12,11-olide, H-434
5-Hydroxy-7-eicosanone, E-13
3-Hydroxy-7-isopropyl-10-methyl-1,5-dioxaspiro[5.5]undecane, M-192
9-Hydroxy-7-megastigmen-3-one, H-540
5-Hydroxy-7-methoxy-2,6-dimethyl-4*H*-1-benzopyran-4-one, D-430
5-Hydroxy-7-methoxy-2,8-dimethyl-4*H*-1-benzopyran-4-one, D-431
5-Hydroxy-7-methoxy-2-methyl-4*H*-1-benzopyran-4-one, D-546
5-Hydroxy-7-methoxy-2-methyl-6-prenylchromone, P-236
5-Hydroxy-7-methoxy-2-methylchromone, D-546
5-Hydroxy-7-methoxy-2-tritriacontyl-4*H*-1-benzopyran-4-one, D-703
5-Hydroxy-7-methoxy-2-tritriacontylchromone, D-703
2-Hydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-399
8-Hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, D-396
3-Hydroxy-7-methoxy-3′,4′-methylenedioxyflavanone, T-189
5-Hydroxy-7-methoxy-4*H*-1-benzopyran-4-one, D-394
5-Hydroxy-7-methoxy-6,8-dimethylflavanone, D-432
5-Hydroxy-7-methoxy-6,8-dimethylflavone, D-433
8-Hydroxy-7-methoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, D-668
5-Hydroxy-7-methoxy-6-methylflavone, D-554
8-Hydroxy-7-methoxy-6-prenylcoumarin, D-668
5-Hydroxy-7-methoxy-6-prenylflavanone, D-669
5-Hydroxy-7-methoxychromone, D-394
8-Hydroxy-7-methoxycoumarin, D-396
4′-Hydroxy-7-methoxyflavanone, D-470
5-Hydroxy-7-methoxyflavanone, D-471
6-Hydroxy-7-methoxyflavone, D-474
5-Hydroxy-7-methoxyflavonol, T-580
4′-Hydroxy-7-methoxyisoflavone, D-513
5-Hydroxy-7-methoxyisoflavone, D-514
6-Hydroxy-7-methoxyphthalide, D-511
3-Hydroxy-7-methyljuglone, D-558
5-Hydroxy-7-neryloxyflavanone, D-471
28-Hydroxy-7-octacosanone, H-639
12-Hydroxy-7-oxo-8,11,13-abietatrien-18-al, A-8
3-Hydroxy-7-oxociguatoxin, C-259
4-Hydroxy-7-oxociguatoxin, C-259
3-Hydroxy-7-oxolanosta-8,24-dien-26-al, D-521
4-(3-Hydroxy-7-phenyl-6-heptenyl)-1,2-benzenediol, H-733
5-Hydroxy-7-prenyloxyflavanone, D-471
5-Hydroxy-7-protoilluden-14-al, H-770
5-Hydroxy-7-tetracosanone, T-45
5-Hydroxy-7-[4-(1-hydroxyethyl)phenoxy]flavanone, D-471
4-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, B-67
9-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, X-5
3-Hydroxy-8′-apo-β-caroten-8′-al, C-283
3-Hydroxy-8′-apo-ε-caroten-8′-al, C-282
7-*O*-(3-Hydroxy-8(12)-drimen-11-yl)isofraxidin, H-435
O-(3-Hydroxy-8(12)-drimen-11-yl)umbelliferone, H-437
7-Hydroxy-8(14),15-isopimaradien-18-oic acid, H-520
7α-Hydroxy-8(14),15-isopimaradien-18-oic acid, I-109
7-Hydroxy-8(14),15-pimaradien-19-oic acid, H-755
15-Hydroxy-8(17),12*E*-labdadien-16-al, L-1
ent-3β-Hydroxy-8(17),13-labdadien-15-oic acid, L-2
15-Hydroxy-8(17),13-labdadien-16,15-olid-19-oic acid, L-12
ent-15-Hydroxy-8(17),13-labdadien-3-one, L-2
3β-Hydroxy-8(17),13*E*-labdadien-15-oic acid, L-2
ent-3β-Hydroxy-8(17),13*Z*-labdadien-15-oic acid, L-2
5-Hydroxy-8,10-dimethoxy-2-methyl-4*H*-naphtho[1,2-*b*]pyran-4-one, A-466
12-Hydroxy-8,10-octadecadienoic acid, H-641
12-Hydroxy-8,11,13-abietatrien-7-one, H-328
12-Hydroxy-8,11,13-abietatriene-6,7-dione, H-327
18-Hydroxy-8,15-isopimaradien-7-one, I-110
5-Hydroxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-404
5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]-dipyran-2-one, H-421
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-409
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-phenyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, M-235
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-412
5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-410
5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-phenyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, M-55
5-Hydroxy-8,8-dimethyl-6-(3-methyl-2-butenyl)-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-297
3-Hydroxy-8,9-dimethoxycoumestan, T-541
3-Hydroxy-8,9-dimethoxypterocarpan, T-703
3-Hydroxy-8,9-methylenedioxycoumestan, M-86
3-Hydroxy-8,9-methylenedioxypterocarpan, M-2
8-Hydroxy-8,9-seco-2(9),6-lactaradien-5,14-olide, L-23
2-Hydroxy-8-(2-octyl-1-cyclopropenyl)octanoic acid, H-786
7-Hydroxy-8-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, O-182
7-Hydroxy-8-(3-methyl-2-oxobutyl)coumarin, H-688
7-Hydroxy-8-(3-oxo-2-methylbutyl)-2*H*-1-benzopyran-2-one, H-688
7-Hydroxy-8-*O*-methylaloin A, A-190
7-Hydroxy-8-*O*-methylaloin B, A-190
10-Hydroxy-8-decene-4,6-diynoic acid, H-398
10-Hydroxy-8-decenoic acid, H-399
6-Hydroxy-8-docosanone, D-1001
6-Hydroxy-8-heneicosanone, H-28
6-Hydroxy-8-heptacosanone, H-42
6-Hydroxy-8-hexacosanone, H-148
5-Hydroxy-8-methoxy-2,2-dimethyl-7-(3-methyl-2-butenyl)-2*H*,6*H*-pyrano[3,2-*b*]xanthen-6-one, C-29
4-Hydroxy-8-methoxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-477
2-Hydroxy-8-methoxy-4-quinolinecarboxylic acid, D-682
7-Hydroxy-8-methoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, D-668
7-Hydroxy-8-methoxy-6-prenylcoumarin, D-668
6-Hydroxy-8-methoxy-7(11)-eremophilen-12,8-olide, D-452
1-Hydroxy-8-methoxyanthraquinone, D-377
3-Hydroxy-8-multifloren-29-oic acid, H-623
10-Hydroxy-8-nor-2-fenchanone, H-635
10-Hydroxy-8-norfenchone, H-635
3-Hydroxy-8-oxo-6-eremophilen-12-oic acid, H-677
6-Hydroxy-8-pentacosanone, P-65
7-Hydroxy-8-prenylcoumarin, O-182
6-Hydroxy-8-tricosanone, T-461
5-Hydroxy-8-undecenoic acid, H-823
7-Hydroxy-8-[(4-sulfo-1-naphthalenyl)azo]-1,3-naphthalenedisulfonic acid, C-314
1-Hydroxy-9(10*H*)-acridinone, H-337
3-Hydroxy-9(11),12-oleanadien-30-oic acid, H-659
3-Hydroxy-9,10-dimethoxypterocarpan, T-704
4-Hydroxy-9,11(13)-guaiadien-12,8-olide, H-475
17-Hydroxy-9,11,13,15-octadecatetraynoic acid, H-644
3-Hydroxy-9,11-eremophiladien-1-one, E-194
3-Hydroxy-9,11-eremophiladien-8-one, H-439
16-Hydroxy-9,12,14-octadecatrienoic acid, H-647
2-Hydroxy-9,12,15-octadecatrienoic acid, H-645
15-Hydroxy-9,12-octadecadienoic acid, H-642
11-Hydroxy-9,15,16-trioxooctadecanoic acid, H-816
6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3*H*,9*H*-[1,2]-dioxolo[3′,4′:4,5]furo[2,3-*f*][1]benzopyran-3-one, H-411
2-Hydroxy-9-(4-hydroxy-3-methoxyphenyl)-1*H*-phenalen-1-one, H-732
3-Hydroxy-9-(4-hydroxyphenyl)-1*H*,3*H*-naphtho[1,8-*cd*]pyran-1-one, P-288
2-Hydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, H-732
3-Hydroxy-9-calamenenone, C-33
8-Hydroxy-9-decene-4,6-diynoic acid, H-396
12-Hydroxy-9-dodecenoic acid, H-433
1-Hydroxy-9-heptadecene-4,6-diyn-3-one, H-487
13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid, D-595
3-Hydroxy-9-methoxy-10-prenylpterocarpan, D-672
3-Hydroxy-9-methoxy-4-prenylpterocarpan, D-671
3-Hydroxy-9-methoxycoumestan, C-370
3-Hydroxy-9-methoxypterocarpan, H-555
6-Hydroxy-9-methylfuro[2,3-*b*]quinolin-4(9*H*)-one, F-148
12-Hydroxy-9-octadecenoic acid, H-648
16-Hydroxy-9-oxo-10,12,14-octadecatrienoic acid, H-690
2-Hydroxy-9-phenyl-1*H*-phenalen-1-one, H-732
11-Hydroxy-9-triacontanone, H-807
11-Hydroxy-9-tridecenoic acid, H-808
1-Hydroxy-9*H*-carbazole-3-carboxaldehyde, H-379
6-Hydroxy-9*H*-carbazole-3-carboxaldehyde, H-380
8-Hydroxy-9*H*-carbazole-3-carboxaldehyde, H-381
2-Hydroxy-9*H*-carbazole-3-carboxylic acid, H-382
6-Hydroxy-9*H*-carbazole-3-carboxylic acid, H-383
2-Hydroxy-9*H*-carbazole-3-carboxaldehyde, H-382
2-Hydroxy-9*H*-xanthen-9-one, H-833
4-Hydroxy-9*H*-xanthen-9-one, H-834
8-Hydroxy-*p*-menth-1-en-7-oic acid, H-544
3-Hydroxy-*p*-menth-3-en-2-one, H-545
8-Hydroxy-*p*-menth-6-en-2-one, H-546
2-Hydroxy-*p*-mentha-1,8-dien-6-one, H-542
3-Hydroxy-*p*-mentha-1,8-dien-7-al, H-541
5-Hydroxy-*p*-mentha-6,8-dien-2-one, H-543
4-Hydroxy-*m*-xylene, D-873
2-Hydroxy-*m*-xylene, D-875
α-Hydroxy-*m*-xylene, M-321
4-Hydroxy-*N,N,N*-trimethyl-10-oxo-7-[(1-oxohexyl)oxy]-3,5,9-trioxa-4-phosphapentadecan-1-aminium inner salt 4-oxide, P-325
4-Hydroxy-*N,N,N*-trimethyl-9-oxo-7-[[(1-oxooctadecyl)oxy]methyl]-3,5,8-trioxa-4-phosphaoctacosa-13,16,19,22-tetraen-1-aminiumhydroxide, inner salt, 4-oxide, 9CI, P-325
2-Hydroxy-*N,N,N*-trimethylethanaminium(1+), C-239
4-Hydroxy-*N,N*-dimethylphenethylamine, H-302
6-Hydroxy-*N*-(2-methylpropyl)-2,4-decadienamide, D-34
4-Hydroxy-*N*-(4-hydroxycinnamoyl)anthranilic acid, A-259
5-Hydroxy-*N*-(4-hydroxycinnamoyl)anthranilic acid, A-260
6-Hydroxy-*N*-isobutyl-2,4-decadienamide, D-34
4-Hydroxy-*N*-phenylaniline, H-428
4-Hydroxy-*N*-[2-(hydroxymethyl)-1,3-butadienyl]-glutamine, P-381
5-Hydroxy-N^{ω}-methyltryptamine, H-820
α-Hydroxy-*o*-toluic acid, H-560
3-Hydroxy-*o*-xylene, D-872
4-Hydroxy-*o*-xylene, D-876
α-Hydroxy-*o*-xylene, M-320
3-Hydroxy-*p*-cymene, I-146
α-Hydroxy-*p*-cymene, M-596

8-Hydroxy-*p*-menth-1-en-6-one, H-546
3-Hydroxy-*p*-menth-4(8)-en-9,3-olide, P-224
2-Hydroxy-*p*-tolualdehyde, H-557
Hydroxy-*p*-xylene, D-874
α-Hydroxy-*p*-xylene, M-322
3′-Hydroxy-HT2 toxin, S-55
3′-Hydroxy-T2 Toxin, S-55
3′-Hydroxy-T2-triol, S-55
12-Hydroxyabietic acid, H-326
13-Hydroxyabscisic acid, A-11
Hydroxyacetaldehyde, H-329
Hydroxyacetic acid, H-330
Hydroxyacetone, H-766
2′-Hydroxyacetophenone, H-331
4′-Hydroxyacetophenone, H-332
α-Hydroxyacetosyringone, T-133
3-(Hydroxyacetyl)-1*H*-indole, H-333
6-(Hydroxyacetyl)-7-methoxy-2,2-dimethyl-2*H*-1-benzopyran, H-494
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2-Hydroxyacorenone, H-336
1-Hydroxyacridone, H-337
3-Hydroxyaflatoxin B_1, H-338
2α-Hydroxyalantolactone, H-456
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2α-Hydroxyaleuritolic acid, D-693
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13-Hydroxyanagyrine, B-7
17-Hydroxyandrost-4-en-3-one, H-340
17-Hydroxyandrost-4-ene-3,11-dione, H-339
4′-Hydroxyanigorootin, A-337
Hydroxyanigorufone, H-732
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8-Hydroxyannonacin, A-349
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4-Hydroxyanthranilic acid, A-259
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6-Hydroxyapigenin, T-210
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4-Hydroxyarginine, H-341
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6-Hydroxyasimilobine, P-2
5-Hydroxyauranetin, H-212
7-Hydroxyaustrobailignan 5, P-153
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2-Hydroxybenzeneacetic acid, H-716
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4-Hydroxybenzeneacetonitrile, H-717
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3-Hydroxybenzeneethanol, H-723
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2-Hydroxybenzenemethanol, H-355
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2-Hydroxybenzenethiol, M-226
2-Hydroxybenzoic acid, H-345
3-Hydroxybenzoic acid, H-346
4-Hydroxybenzoic acid, H-347
4′-Hydroxybenzophenone-2-carboxylic acid, H-348
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3-(4-Hydroxybenzoyl)epicatechin, P-104
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3′-(4-Hydroxybenzoyl)procyanidin B_1, P-121
3′-*O*-(4-Hydroxybenzoyl)prodelphinidin B_2, H-199
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3-Hydroxybenzyl alcohol, H-356
4-Hydroxybenzyl alcohol, H-357
4-Hydroxybenzyl cyanide, H-717
4-Hydroxybenzyl glucosinolate, H-358
4-Hydroxybenzyl isothiocyanate, H-359
α-Hydroxybenzyl phenyl ketone, B-33
1-(4-Hydroxybenzyl)-6,7-isoquinolinediol, H-364
(4-Hydroxybenzyl)aminoformic acid, H-361
(4-Hydroxybenzyl)aminothioformic acid, H-365
(4-Hydroxybenzyl)carbamic acid, H-361
2-(4-Hydroxybenzyl)imidazole, H-363
(4-Hydroxybenzyl)thiocarbamic acid, H-365
4-Hydroxybenzylamine, H-360
ω-*p*-Hydroxybenzylideneacetophenone, H-736
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8-Hydroxybergapten, D-476
9-Hydroxybergapten, D-476
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2′-Hydroxybiochanin A, T-222
2-Hydroxybiphenyl, B-92
12-Hydroxyblennin A, H-531
15-Hydroxyblennin A, H-531
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30-Hydroxybullatacin, A-450
31-Hydroxybullatacin, A-450
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12-Hydroxybullatacin, P-586
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3-Hydroxybutanethiol, M-204
3-Hydroxybutanoic acid, H-374
4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone, H-538
4-(3-Hydroxybutyl)-3,5,5-trimethyl-2-cyclohexenone, H-539
4-Hydroxybutyric acid lactone, D-253
9-Hydroxycalabaxanthone, C-29
6-Hydroxycamphor, H-373
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2-Hydroxycanthin-6-one, H-377
5-Hydroxycanthin-6-one, H-378
5-Hydroxycapric acid, H-393
3-Hydroxycaproic acid, H-493
3-Hydroxycaprylic acid, H-651
5-Hydroxycarvacrol, I-140
6-Hydroxycarvone, H-542
8-Hydroxycarvotanacetone, H-546
5′-Hydroxycastavinol, C-156
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1′-Hydroxychavicol, H-749
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13^2-Hydroxychlorophyll a, C-216
2-Hydroxychromone, H-349
2-Hydroxychrysophanol, T-622
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o-Hydroxycinnamaldehyde, H-744
p-Hydroxycinnamaldehyde, H-745
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m-Hydroxycinnamic acid, H-747
p-Hydroxycinnamic acid, H-748
α-Hydroxycinnamic acid, O-242
3β-Hydroxycinnamolide, H-434
2-*O*-(4-Hydroxycinnamoyl)-1,6-di-*O*-galloyl-β-D-glucopyranose, C-264
2-*O*-(4-Hydroxycinnamoyl)-1-*O*-galloyl-β-D-glucopyranoside, C-265
N-(4-Hydroxycinnamoyl)-3-(4-hydroxyphenyl)alanine, T-852
2-*O*-(4-Hydroxycinnamoyl)glucose, C-365
6-*O*-(4-Hydroxycinnamoyl)glucose, C-366
(4-Hydroxycinnamoyl)spermidine, C-369
N-(4-Hydroxycinnamoyl)tyrosine, T-852
4-Hydroxycinnamoylagmatine, A-221
N-*p*-Hydroxycinnamoylanthranilic acid, A-507
p-Hydroxycinnamoylferuloylmethane, C-397
1-*O*-*p*-Hydroxycinnamoylglucose, C-364
4-Hydroxycinnamoylputrescine, C-367
4-Hydroxycinnamyl alcohol, H-750
3-Hydroxycitraniaxanthin, R-9
Hydroxycitric acid, D-675
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Hydroxycitronellol, D-844
4-Hydroxycitrulline, H-387
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1α-Hydroxycolartin, D-458
1β-Hydroxycolartin, D-458
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Hydroxycoumalin, H-772
4-Hydroxycoumarin, H-349
5-Hydroxycoumarin, H-350
7-Hydroxycoumarin, H-351
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N^{α}-*p*-Hydroxycoumaroyltryptophan, T-845
4-Hydroxycoumestrol, T-539
11-Hydroxycoumestrol, T-541
17-Hydroxycryptotanshinone, E-173
5′-Hydroxycudraflavone A, C-391
8-Hydroxycumambranolide, D-487
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β-Hydroxycumene, P-307
3-Hydroxycycloart-24-en-21-al, C-423
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3-Hydroxycycloart-24-en-26-al, H-390
3-Hydroxycycloart-24-en-26-oic acid, H-390
9-Hydroxycyclocostunolide, H-481
2-Hydroxycyclohexanepropanoic acid lactone, O-64
N^5-(1-Hydroxycyclopropyl)glutamine, C-348
2-Hydroxycymene, I-147
8-Hydroxycyperotundone, P-47
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3′-Hydroxydaidzein, T-600
8-Hydroxydaidzein, T-603
19-Hydroxydeacetylnomilinic acid, H-391
19-Hydroxydeacetylnomilinic acid 17-β-D-glucopyranoside, H-391
5-Hydroxydecanoic acid, H-393
6-Hydroxydecanoic acid, H-394
9-Hydroxydecanoic acid, H-395
4-Hydroxydecanoic acid lactone, H-266
5-Hydroxydecanoic acid lactone, T-116
7-Hydroxydehydroglaucine, D-70
4-Hydroxydehydromyoporone, A-483
4-Hydroxydemethylmedicarpin, T-702
6-Hydroxydesacetyluvaricin (incorr.), H-400
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8-Hydroxydictamnine, F-149
Hydroxydihydrocitronellal dimethyl acetal, H-417
2′-Hydroxydihydrodaidzein, T-595
13-Hydroxydihydromelleolide, P-549
6-Hydroxydihydrotheaspirane, T-337
5-Hydroxydioxindole-3-acetic acid, D-239
4-Hydroxydiphenylamine, H-428
μ-Hydroxydiphenyldimercury(1+), H-429
Hydroxydivarin, P-525
1-(22-Hydroxydocosanoyl)glycerol, G-236
5-Hydroxydodecanoic acid, H-431
6-Hydroxydodecanoic acid, H-432
4-Hydroxydodecanoic acid γ-lactone, D-338
12*a*-Hydroxydolineone, D-1032
13*a*-Hydroxydolineone, D-1032
3-Hydroxydothistromin, D-1038
3-Hydroxyedulan, E-147
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ω-Hydroxyemodin, T-590
1-Hydroxyepiacorone, H-334
6-Hydroxyeremophilenolide, H-441
25-Hydroxyergocalciferol, S-68
3-Hydroxyergosta-5,8,22-trien-7-one, H-445
3-Hydroxyergostan-6-one, E-210
8-Hydroxyeriodictyol, P-111
12*a*-Hydroxyerosone, H-447

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22α-Hydroxyerythrodiol, O-140
3-Hydroxyestra-1,3,5(10)-trien-17-one, E-240
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2-Hydroxyethyl 5-methyl-2-(1-methylethyl)cyclohexyl carbonate, M-193
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1-Hydroxyethyl methyl ketone, H-376
2-Hydroxyethyl phenyl ether, P-254
2-(Hydroxyethyl) 4-hydroxyphenyl ketone, H-510
5-(2-Hydroxyethyl)-1,2,3-benzenetriol, T-664
4-(2-Hydroxyethyl)-1,2-benzenediol, D-627
5-(1-Hydroxyethyl)-2(5*H*)-furanone, H-450
6-(2-Hydroxyethyl)-2,2,5,7-tetramethyl-1-indanone, P-570
6-(1-Hydroxyethyl)-2,2-dimethyl-2*H*-1-benzopyran, A-50
6-(2-Hydroxyethyl)-2,5,7-trimethyl-1-indanone, P-560
5-(1-Hydroxyethyl)-2-(hydroxymethyl)-4*H*-pyran-4-one, H-451
6-(2-Hydroxyethyl)-2-hydroxymethyl-2,5,7-trimethyl-1-indanone, P-559
6-(1-Hydroxyethyl)-3-(hydroxymethyl)-2,7-dioxabicyclo[4.1.0]hept-3-en-5-one, E-229
5-(2-Hydroxyethyl)-4-methylthiazole, H-453
6-(2-Hydroxyethyl)-5-hydroxymethyl-2,7-dimethyl-1-indanone, P-569
2-(1-Hydroxyethyl)acrylic acid, H-582
N-(2-Hydroxyethyl)hexadecanamide, P-11
3-(2-Hydroxyethyl)indole, H-452
N-(2-Hydroxyethyl)palmitamide, P-11
2-(1-Hydroxyethyl)propenoic acid, H-582
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(2-Hydroxyethyl)trimethylammonium, C-239
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2-Hydroxyethylamine, A-249
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5-(2-Hydroxyethylidene)-4-(hydroxymethyl)-2(5*H*)-furanone, A-444
(1-Hydroxyethylidene)bisphosphonic acid, H-448
3-Hydroxyeuglenanone, D-1037
26-Hydroxyeupha-7,24-dien-3-one, E-396
9-Hydroxyfarnesol, F-10
9-Hydroxyfarnesyl oleate, F-10
5-Hydroxyfenchone, H-463
6-Hydroxyfenchone, H-464
10-Hydroxyfenchone, H-465
5-Hydroxyferulic acid, T-672
3-Hydroxyflavone, H-466
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2′-Hydroxyformononetin, T-598
2-Hydroxyfukinanolide, F-83
9β-Hydroxyfukinanolide, F-83
2-Hydroxyfuranoeremophilane, F-100
6-Hydroxyfuranoeremophilane, F-101
1α-Hydroxyfuranoeudesm-4-en-6-one, C-394
6-Hydroxyfuro[2,3-*b*]quinolin-4(9*H*)-one, F-148
8-Hydroxyfuro[2,3-*b*]quinoline-4(9*H*)-one, F-149
8-Hydroxygalangin, T-209
Hydroxygaleon, G-45
2′-Hydroxygenistein, T-222
8-Hydroxygenistein, T-226
8-Hydroxygeraniol, D-825
9-Hydroxygeraniol, D-825
16-Hydroxygeranylgeraniol, P-360
20-Hydroxygeranyllinalool, P-359
13-Hydroxygibberellin A_{15}, G-104
15β-Hydroxygibberellin A_{29}, G-97
11β-Hydroxygibberellin A_7, G-109
3-Hydroxyglabrol, D-440
24-Hydroxyglabrolide, T-661
4-Hydroxyglucobrassicin, H-517
4-Hydroxyglutamine, H-474
18α-Hydroxyglycyrrhetic acid, D-600
24-Hydroxyglycyrrhetic acid, D-604
28-Hydroxyglycyrrhetic acid, D-606
3′-Hydroxygraveoline, G-320
2α-Hydroxygypsogenin, D-597
2β-Hydroxygypsogenin, D-597
21β-Hydroxygypsogenin, T-651
7-Hydroxyharman, H-576
Hydroxyhebevinogenin, C-384
21β-Hydroxyhederagenin, T-651
4-Hydroxyheptanoic acid lactone, D-347
7-Hydroxyheptaphylline, H-100
1-(26-Hydroxyhexacosanoyl)glycerol, G-236
7-Hydroxyhexadecanedioic acid, H-488
8-Hydroxyhexadecanedioic acid, H-489
2-Hydroxyhexadecanoic acid, H-490
15-Hydroxyhexadecanoic acid, H-491
3-Hydroxyhexanoic acid, H-493
4-Hydroxyhexanoic acid lactone, E-295
5-Hydroxyhexanoic acid lactone, T-106
o-Hydroxyhippuric acid, H-354
Hydroxyhomodestruxin B, H-293
4-Hydroxyhomopterocarpin, T-702
45-Hydroxyhomoyessotoxin, Y-2
o-Hydroxyhydrocinnamic acid, H-740
p-Hydroxyhydrocinnamic acid, H-741
2-Hydroxyhydrocinnamic lactone, D-222
8-Hydroxyhyperforin 8,1-hemiacetal, H-511
6-Hydroxyiminostigmast-4-en-3-one, S-239
4-Hydroxyindol-3-ylmethyl glucosinolate, H-517
6*a*-Hydroxyinermin, T-285
N-(2-Hydroxyisobutyl)-2,4,8,10,12-tetradecapentaenamide, T-62
2-Hydroxyisobutyric acid, H-605
7-Hydroxyisoflavone, H-519
21-Hydroxyisoglabrolide, T-660
ent-17-Hydroxyisokaur-15-en-19-oic acid, K-24
4-Hydroxyisoleucine, A-263
27-Hydroxyisomangiferolic acid, D-419
6*a*-Hydroxyisomedicarpin, T-700
Hydroxyisonobilin, T-584
2′-Hydroxyisoorientin, G-201
N^6-(ω-Hydroxyisopentenyl)adenine, Z-8
4-(1-Hydroxyisopropyl)-1-cyclohexene-1-carboxylic acid, H-544
p-(Hydroxyisopropyl)toluene, M-596
2′-Hydroxyisopropyl-3′-hydroxy-2′,3′-dihydroangelicin, V-1
2′-Hydroxyisoprunetin, T-222
2-Hydroxyisovaleric acid, H-568
3-Hydroxyisovaleric acid, H-569
14α-Hydroxyixocarpanolide, I-206
2′′-Hydroxyjasminin, J-6
12-Hydroxyjasmonic acid, H-709
5′-Hydroxyjasmonic acid lactone, H-527
6-Hydroxykaempferol, P-136
8-Hydroxykaempferol, P-139
7-Hydroxykaurenolide, D-516
6-Hydroxykynurenic acid, D-683
3-Hydroxylanost-8,24-dien-21-oic acid, L-42
3-Hydroxylanosta-7,9(11),24-trien-26-oic acid, H-533
26-Hydroxylanosta-7,9(11),24*E*-trien-3-one, L-40
3-Hydroxylanosta-8,24-dien-26-oic acid, H-532
Hydroxylapatite, C-43
15-Hydroxyleptocarpin, E-185
11-Hydroxylettowianthine, L-70
α-Hydroxylevulinic acid, H-696
α-Hydroxylignoceric acid, H-796
3β-Hydroxyliguloxide, E-117
12α-Hydroxylimonin, L-90
9-Hydroxylinalool, D-826
10-Hydroxylinalyl oxide, H-534
15-Hydroxylinoleic acid, H-642
2-Hydroxylinolenic acid, H-645
24-Hydroxyliquiritic acid, D-603
4-Hydroxylonchocarpin, I-72
4-Hydroxylubimin, D-690
2′-Hydroxylupalbigenin, T-167
6-Hydroxyluteolin, P-137
8-Hydroxyluteolin, P-141
16-Hydroxylycopene, L-130
5-Hydroxylysine, D-118
Hydroxylysylpyridinoline, P-602
6*a*-Hydroxymaackiain, T-285
Hydroxymalonic acid, H-763
5-Hydroxymaltol, D-559
4′′-Hydroxymammeigin, M-55
m-Hydroxymandelic acid, H-503
p-Hydroxymandelic acid, H-504
27-Hydroxymangiferolic acid, D-419
28-Hydroxymangiferonic acid, H-676
19-Hydroxymanoyl oxide, E-141
2α-Hydroxymaprounic acid, D-693
15-Hydroxymarasmen-3-one, M-72
13-Hydroxymarasmene, M-72
14-Hydroxymarasmene, M-72
3β-Hydroxymarasmene, M-72
5-Hydroxymarmesin, C-170
3*R*-Hydroxymarmesin, D-260
10-Hydroxymatricaric acid, H-392
ax-4′′-Hydroxymaysin, M-83
eq-4′′-Hydroxymaysin, M-83
6*a*-Hydroxymedicarpin, T-700
4-Hydroxymedicarpin, T-702
9-Hydroxymegastigman-2-one, H-538
4-Hydroxymellein, D-232
6-Hydroxymellein, D-233
10-Hydroxymelleolide, P-548
Hydroxymethane, M-243
Hydroxymethyl *p*-hydroxyphenyl ketone, D-370
Hydroxymethyl indol-3-yl ketone, H-333
Hydroxymethyl methyl ketone, H-766
Hydroxymethyl methyl sulfide, M-674
2-(Hydroxymethyl)-1,2,3,4-butanetetrol, H-566
5-(Hydroxymethyl)-1,2,3-benzenetriol, H-559
4-(Hydroxymethyl)-1,2-benzenediol, D-400
5-(Hydroxymethyl)-1,3-benzenediol, D-401
6-(Hydroxymethyl)-2,4(1*H*,3*H*)-pteridinedione, H-607
1-[5-(Hydroxymethyl)-2-furanyl]-9*H*-pyrido[3,4-*b*]indole-3-carboxylic acid, F-45
3-(Hydroxymethyl)-2-heptanone, H-590
5-(Hydroxymethyl)-2-isopropylphenol, H-521
3-(Hydroxymethyl)-2-octanone, H-595
4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid, H-613
2-(Hydroxymethyl)-3,4,5-piperidinetriol, H-604
2-(Hydroxymethyl)-3,4-piperidinediol, H-603
2-(Hydroxymethyl)-3,4-pyrrolidinediol, D-508
4-(Hydroxymethyl)-3,5,5-trimethyl-2-cyclohexen-1-one, H-621
1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione, H-581
1-(Hydroxymethyl)-5,5-dimethylhydantoin, H-581
1-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol, H-577
2-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol, H-578
5-(Hydroxymethyl)-5-cyclohexene-1,2,3,4-tetrol, H-579
2-(Hydroxymethyl)-5-methyltetrahydrofuran, T-100
2-*C*-(Hydroxymethyl)-*glycero*-tetritol, H-566
3-*C*-(Hydroxymethyl)-*glycero*-tetrose, A-374
4-(Hydroxymethyl)benzenediazonium(1+), H-558
2-(Hydroxymethyl)benzoic acid, H-560
3-(Hydroxymethyl)chrysazin, D-503
3-*C*-(Hydroxymethyl)erythritol, H-566
2-(Hydroxymethyl)furan, F-96
3-(Hydroxymethyl)furan, F-97
3-[5-(Hydroxymethyl)furfurylidene]-1-pyrroline, P-631
1-[5′-(Hydroxymethyl)furfuryl]pyrrolidine, P-625
2-(Hydroxymethyl)phenyl β-D-glucopyranoside, S-15
4-(Hydroxymethyl)proline, H-613
2-*C*-(Hydroxymethyl)ribonic acid, H-615
3-*C*-(Hydroxymethyl)threitol, H-566
3-*C*-Hydroxymethyl-α-D-*erythro*-tetrofuranose, A-374
3-*C*-Hydroxymethyl-α-L-*erythro*-tetrofuranose, A-374
3-*C*-Hydroxymethyl-β-D-*erythro*-tetrofuranose, A-374
3-Hydroxymethyl-1-methoxycarbazole, H-593
6-Hydroxymethyl-1-methoxycarbazole, M-779
3-(1-Hydroxymethyl-1-propenyl)glutaric acid, F-64
3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid, F-64
3-*C*-Hydroxymethyl-2,3-*O*-isopropylidene-β-D-*erythro*-tetrofuranose, A-374
4-Hydroxymethyl-2,6-di-*tert*-butylphenol, D-147

5-Hydroxymethyl-2-furancarboxaldehyde, H-587
1-Hydroxymethyl-2-methylbenzene, M-320
4-Hydroxymethyl-2-phenyl-1,3-dioxolane, P-267
1-Hydroxymethyl-3-methylbenzene, M-321
1-Hydroxymethyl-4-isopropenylcyclohexane, M-182
1-Hydroxymethyl-4-isopropenylcyclohexene, M-129
7-Hydroxymethyl-4-methoxy-5*H*-furo[2,3-*g*][2]benzopyran-5-one, C-351
3-(2-Hydroxymethyl-4-methoxyphenyl)-6-methoxy-4(3*H*)-quinazolinone, D-168
1-Hydroxymethyl-4-methylbenzene, M-322
2-Hydroxymethyl-6-isopropyl-9-methyl-1,4-dioxaspiro[4.5]decane, M-191
3-Hydroxymethyl-7-methyl-1,6-octadien-3-ol, M-712
Hydroxymethylbenzene, B-44
5-Hydroxymethylblasticidin S, B-162
1-Hydroxymethylconduritol, H-577
1-Hydroxymethylconduritol E, H-577
8-Hydroxymethyldihydrochelerythrine, B-165
5-Hydroxymethylfurfural, H-587
3-Hydroxymethylindole, I-29
6-Hydroxymethyllumazine, H-607
o-Hydroxymethylphenol, H-355
m-Hydroxymethylphenol, H-356
p-Hydroxymethylphenol, H-357
1-Hydroxymethylpyrrolizidine, H-614
2-*C*-Hydroxymethylribose, H-616
2-Hydroxymethyltetrahydrofuran, T-85
2-Hydroxymethylthiophene, T-380
3-Hydroxymethylthiophene, T-381
5-Hydroxymethylundecane, B-254
Hydroxyminaline, H-774
ω-Hydroxymoracin N, M-756
3-Hydroxymugineic acid, M-776
12*a*-Hydroxymunduserone, G-146
6-Hydroxymusizin, A-100
4-Hydroxymyoporone, A-483
10-Hydroxymyoporone, M-831
7-Hydroxymyoporone, M-831
Hydroxymyricanone, M-833
6-Hydroxymyricetin, H-86
8-Hydroxymyricetin, H-87
10-Hydroxymyristic acid, H-798
2-Hydroxynaphthalene, N-12
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3-Methoxy-1,2-anhydridoniveusin (incorr.), E-187
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2-Methoxy-1,3-thiazino[6,5-*b*]indol-4(9*H*)-one, M-277
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2-Methoxy-1,4-dimethylbenzene, D-874
5-Methoxy-1,4-naphthoquinone, H-625
5-Methoxy-1,7-diphenyl-3-heptanone, D-950
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3-Methoxy-1-(4-methoxyphenyl)-1-propene, H-750
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7-Methoxy-1-methyl-2-phenyl-4(1*H*)-quinolinone, D-659
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4-Methoxy-2-(3,4-methylenedioxyphenyl)quinoline, M-261
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5-(6-Methoxy-3,4-methylenedioxyphenyl)-2,4-pentadienoic acid isobutylamide, P-395
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2-Methoxy-3,5-dimethylpyrimidine, H-422
5-Methoxy-3,6-bis(phenylmethyl)-2(1*H*)-pyrazinone, D-134
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2-Methoxy-3-(2-methylpropyl)pyrazine, M-264
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4-Methoxy-3-(3-methyl-1,3-butadienyl)-2(1*H*)-quinolinone, G-283
2-Methoxy-3-(4-methoxyphenyl)propanoic acid, H-509
2-Methoxy-3-(methylthio)butane, M-202
2-Methoxy-3-*sec*-butylpyrazine, M-263
2-Methoxy-3-carbomethoxycarbazole, H-382
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2-Methoxy-3-oxo-1,12,15,18-nonadecatetraene-1,4-dicarboxylic acid, M-267
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3-Methoxy-4,5-methylenedioxycinnamaldehyde, T-671
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2-(3-Methoxy-4,5-methylenedioxyphenyl)-1-methyl-4(1*H*)-quinolinone, G-320
3-(3-Methoxy-4,5-methylenedioxyphenyl)-2-propen-1-ol, T-674
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2-Methoxy-4-(1-propenyl)phenol, M-272
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1-Methoxy-4-(2-propenyl)benzene, P-513
2-Methoxy-4-(2-propenyl)phenol, M-273
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1-Methoxy-4-methylbenzene, M-573
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2-Methoxy-4-methylphenol, M-314
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3-Methoxy-4-oxo-5-(8,11,14-pentadecatrienyl)-2-hexenedioic acid, M-267
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4-Methoxy-6-(4-methoxystyryl)-α-pyrone, Y-1
7-Methoxy-6-methyl-2*H*-1-benzopyran-2-one, H-562
7-Methoxy-6-methylcoumarin, H-562
2-Methoxy-6-methylpyrazine, H-612
4-Methoxy-6-styryl-2*H*-pyran-2-one, D-72
4-Methoxy-6-[2-(3-hydroxy-4-methoxyphenyl)ethyl]-5,6-dihydro-2*H*-pyran-2-one, D-631
4-Methoxy-6-[2-(4-methoxyphenyl)ethenyl]-2*H*-pyran-2-one, Y-1
7-Methoxy-6-[2-[2-(7-methoxy-2-oxo-2*H*-1-benzopyran-6-yl)-1,4-dimethyl-3-cyclohexen-1-yl]ethenyl]-2*H*-1-benzopyran-2-one, T-326
7-Methoxy-6-[3-(1-methylethenyl)oxiranyl]-2*H*-1-benzopyran-22-one, C-291
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5-Methoxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, H-378
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4-Methoxy-7-methyl-5*H*-furo[2,3-*g*][2]benzopyran-5-one, C-351
3-Methoxy-7-methyljuglone, D-558
3β-Methoxy-7-multiflorene, M-790
5-Methoxy-7-prenyloxyflavanone, D-471
4-Methoxy-7*H*-furo[3,2-*g*]benzopyran-7-one, B-67
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5-Methoxy-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one,9CI, X-6
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7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin, C-294
7-Methoxy-8-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, O-182
7-Methoxy-8-(3-methyl-2-oxo-3-butenyl)-2*H*-1-benzopyran-2-one, A-492
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4-Methoxy-8*H*-1,3-dioxolo[4,5-*h*][1]benzopyran-8-one, T-523
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2-Methoxy-9-phenyl-1*H*-phenalen-1-one, H-732
1-Methoxy-9*H*-carbazole-3-carboxylic acid, M-257
1-Methoxy-9*H*-carbazole-3-carboxaldehyde, H-379
6-Methoxy-9*H*-carbazole-3-carboxaldehyde, H-380
8-Methoxy-9*H*-carbazole-3-carboxaldehyde, H-381
2-Methoxy-9*H*-carbazole-3-carboxaldehyde, H-382
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8-Methoxy-9*H*-carbazole-3-methanol, M-779
7-Methoxy-9*H*-pyrido[3,4-*b*]indole, M-260
5-Methoxy-*N,N*-dimethyltryptamine, B-197
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N-Methoxycarbonylanonaine, R-41
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5-Methoxycoumarin, H-350
7-Methoxycoumarin, H-351
7-Methoxycoumarin-6-carboxylic acid, H-672
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4-Methoxyhomopterocarpin, T-730
2-Methoxyhydrocinnamic acid, H-740
α-(Methoxyimino)-*N*-methyl-2-[[[1-[3-(trifluoromethyl)phenyl]ethoxy]imino]methyl]benzeneacetamide, M-259
(1-Methoxyindol-3-yl)methyl isothiocyanate, I-175
4-Methoxyindol-3-ylmethyl glucosinolate, H-517
6-Methoxyisodictamnine, F-148
6-Methoxykaempferol, T-240
8-Methoxykaempferol, T-242
6-Methoxykynurenic acid, D-683
2′-Methoxylupalbigenin, T-167
6-Methoxyluteolin, T-241
5-Methoxymarmesin, C-170
3′-Methoxymaysin(incorr.), M-83
2-Methoxymedicarpin, T-701
4-Methoxymedicarpin, T-702
10-Methoxymedicarpin, T-704
6-Methoxymellein, D-233
5-(Methoxymethyl)-1.3-benzodioxole, M-407
1-(Methoxymethyl)-2-methylbenzene, M-320
2-(Methoxymethyl)furan, F-96

3-(Methoxymethyl)thiophene, T-381
4-Methoxymethyl-1,2-methylenedioxybenzene, M-407
3-(Methoxymethylene)-2-pyrrolidinethione, M-262
3′-Methoxymucidin, S-253
4′-Methoxymucidin, S-253
7-Methoxymurrayacine, M-814
2-Methoxynaphthalene, M-266
1-Methoxynonane, N-110
2-Methoxynonane, N-111
5-Methoxynoracronycine, A-119
N-Methoxynorcepharadione A, C-178
11-Methoxynoryangonin, D-631
1-Methoxyoctadecane, O-28
2-Methoxyoctane, O-83
β-Methoxyoleuropein, O-151
2″-Methoxyoleuropein, O-151
6-Methoxypaeonol, T-512
α-Methoxypapaverine, P-35
1-Methoxypentane, P-191
1-Methoxyphaseollidin, T-695
1-Methoxyphaseollin, P-241
2′-Methoxyphaseollinisoflavan (incorr.), P-242
3-Methoxyphenethyl alcohol, H-723
N-(*p*-Methoxyphenethyl)-*N*-methylcinnamamide, H-126
2-Methoxyphenol, M-269
4-[5-(4-Methoxyphenoxy)-3-penten-1-ynyl]phenol, H-713
2-(4-Methoxyphenoxy)propanoic acid, M-270
4-Methoxyphenyl thiocyanate, T-372
1-(4-Methoxyphenyl)-1,2-ethanediol, H-722
1-(4-Methoxyphenyl)-1,2-propanediol, H-737
3-(4-Methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone, H-752
1-(4-Methoxyphenyl)-1-penten-3-one, H-731
1-(2-Methoxyphenyl)-2,4-hexadiyn-1-one, P-285
4-(4-Methoxyphenyl)-2-butanone, H-720
3-(4-Methoxyphenyl)-2-methyl-2-propenal, M-271
1-(4-Methoxyphenyl)-2-nitroethane, N-65
1-(4-Methoxyphenyl)-2-nitroethylene, H-727
3-[5-(4-Methoxyphenyl)-2-oxazolyl]pyridine, H-3
1-(4-Methoxyphenyl)-2-propanone, H-743
1-(4-Methoxyphenyl)-2-propen-1-ol, H-749
3-(4-Methoxyphenyl)-2-propen-1-ol, H-750
3-(4-Methoxyphenyl)-2-propenal, H-745
2-(4-Methoxyphenyl)-3-methyloxirane, P-512
1-(4-Methoxyphenyl)-4-methyl-1-penten-3-one, H-726
2-(3-Methoxyphenyl)ethanol, H-723
N-[2-(4-Methoxyphenyl)ethenyl]-3-phenyl-2-propenamide, M-276
2-[2-(3-Methoxyphenyl)ethenyl]-4*H*-3,1-benzoxazin-4-one, A-505
5-[2-(2-Methoxyphenyl)ethyl]-1,3-benzenediol, D-638
N-[2-(4-Methoxyphenyl)ethyl]-*N*-methyl-3-phenyl-2-propenamide, H-126
2-(4-Methoxyphenyl)naphthalic anhydride, P-288
3-(2-Methoxyphenyl)propanoic acid, H-740
4-Methoxyphthalide, H-753
6-Methoxypinobanksin, T-193
5-Methoxypiperonylic acid, H-584
6-Methoxypiperoylisobutylamine, P-395
3-Methoxypropylbenzene, P-309
8-Methoxypsoralen, X-4
9-Methoxypsoralen, X-4
5-Methoxypsoralen (obsol.), B-67
Methoxypyrazine, P-596
4′-Methoxypyridoxine, P-606
7-Methoxyrosmanol, R-54
12*a*-Methoxyrotenone, R-57
5-Methoxysalicylic acid, D-388
3-Methoxysampangine, S-26
4-Methoxysampangine, S-26
9-Methoxysampangine, S-26
5′-Methoxysativan, T-218
5-Methoxyseselin, H-404
1-Methoxyspirobrassinin, S-171
N-Methoxyspirobrassinol, S-172
N-Methoxyspirobrassinol methyl ether, S-172
7-Methoxystigmast-5-en-3-ol, S-240
9-Methoxystrobilurin A, S-253
9-Methoxystrobilurin K, S-252
2-Methoxystypandrone, M-275
o-Methoxystyrene, V-36
p-Methoxystyryl phenyl ketone, H-736
N-4-Methoxystyrylcinnamide, M-276
p-Methoxytodadiol, T-666
2-Methoxytoluene, M-571
4-Methoxytoluene, M-573
11-Methoxytubotaiwine, T-847
12-Methoxytubotaiwine, T-847
6-Methoxyvestitol, T-219
6-(2-Methoxyvinyl)-7-methyl-2*H*-1-benzopyran-2-one, M-278
6-(2-Methoxyvinyl)-7-methylcoumarin, M-278
2-Methoxyxanthone, H-833
4-Methoxyxanthone, H-834
11-Methoxyyangonin, D-631
10-Methoxyyangonin, Y-1
5-Methoxyyatein, H-216
Methyl α-D-*manno*-2-heptulopyranoside, H-118
Methyl α-L-arabinofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-β-D-xylopyranoside, A-391
Methyl α-linolenate hydroperoxides, M-284
Methyl α-maltoside, G-176
Methyl β-D-glucopyranoside, M-280
Methyl β-isomaltoside, G-176
Methyl (1-propenylthio) selenide, M-298
Methyl (1*H*-indol-3-ylmethyl)carbamodithioate, B-180
Methyl (2-propenylthio) selenide, M-299
Methyl (2-quinoxalinylmethylene)hydrazinecarboxylate *N*,*N*′-dioxide, C-84
Methyl (3-methyl-2-furyl) ketone, A-70
Methyl (3-methylpyrazinyl) ketone, A-73
Methyl (5-methyl-2-furyl) ketone, A-71
Methyl (methylsulfinyl)methyl disulfide, M-287
Methyl (methylsulfonyl)methyl disulfide, M-287
Methyl (methylthio)methyl disulfide, M-287
Methyl 1′,2,3-tri-*O*-methyl-D-*apio*-α-D-furanoside, A-374
Methyl 1′,2,3-tri-*O*-methyl-D-apio-β-D-furanoside, A-374
Methyl 1-(1-propenylsulfinyl)propyl disulfide, M-300
Methyl 1-(1-propenylthio)propyl disulfide, M-300
Methyl 1-(2-propenylsulfinyl)propyl disulfide, M-301
Methyl 1-(2-propenylthio)propyl disulfide, M-301
Methyl 1-(butylcarbamoyl)benzimidazol-2-ylcarbamate, B-14
Methyl 1-(methylsulfinyl)propyl disulfide, M-289
Methyl 1-(methylthio)propyl disulfide, M-289
Methyl 1-(propylsulfinyl)propyl disulfide, M-304
Methyl 1-(propylthio)propyl disulfide, M-304
Methyl 1-methoxy-1*H*-indole-3-carboxylate, I-27
Methyl 1-propene-1-sulfenoselenoate, M-298
S-Methyl 1-propenesulfinothioate, M-292
Methyl 1-propenyl disulfide, M-292
Methyl 1-[(butylamino)carbonyl]-1*H*-benzimidazol-2-ylcarbamate, B-14
Methyl 12,13-epoxy-11-hydroxy-9-octadecenoic acid, E-133
Methyl 15-cyanopentadecanoate, H-158
Methyl 19,20-didehydro-1-demethyl-17-hydroxyajmalan-16-carboxylate, Q-5
Methyl 1*H*-benzimidazol-2-ylcarbamate, C-88
S-Methyl 1*H*-indole-3-ylmethylcarbamothioate, B-182
Methyl 2,3,4,6-tetra-*O*-galloyl-β-D-glucopyranoside, T-73
Methyl 2,3,6-tri-*O*-galloyl-β-D-glucopyranoside, T-508
Methyl 2,3-*O*-Isopropylidene-1′-tosyl-D-apio-β-D-furanoside, A-374
Methyl 2,3-*O*-isopropylidene-3′-methyl-D-apio-β-D-furanoside, A-374
Methyl 2,4-di-*O*-acetyl-3-*O*-(2,3,4-tri-*O*-acetyl-α-L-arabinopyranosyl)-α-L-arabinopyranoside, A-394
Methyl 2,4-di-*O*-benzyl-3-*O*-(2,3,5-tri-*O*-benzyl-α-L-arabinofuranosyl)-β-D-xylopyranoside, A-392
Methyl 2,6-xylyl sulfide, D-758
Methyl 2-(difluoromethyl)-5-(4,5-dihydro-2-thiazolyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-3-pyridinecarboxylate, D-211
Methyl 2-(methoxymethylene)-3-methyl-6-phenyl-3,5-hexadienoate, S-253
Methyl 2-(methylthio)butyrate, M-199
Methyl 2-*O*-β-D-xylopyranosyl-α-L-arabinopyranoside, X-18
Methyl 2-*O*-β-D-xylopyranosyl-β-L-arabinopyranoside, X-18
Methyl 2-aminobenzoate, A-217
Methyl 2-furoate, F-94
Methyl 2-hydroxybenzoate, M-282
Methyl 2-methoxy-4-oxopropanoate, H-696
Methyl 2-methoxybenzoate, M-251
Methyl 2-methyl-3-furanyl disulfide, M-487
Methyl 2-methyl-4-pyridyl ketone, A-77
Methyl 2-methylbutyl sulfide, M-327
Methyl 2-methylpropanoate, M-605
Methyl 2-naphthyl ether, M-266
Methyl 2-nonenoate, N-120
Methyl 2-octynoate, O-116
Methyl 2-propene-1-sulfenoselenoate, M-299
S-Methyl 2-propene-1-sulfinothioate, M-293
Methyl 2-propenyl disulfide, M-293
Methyl 2-propenyl pentasulfide, M-294
Methyl 2-propenyl selenide, M-295
Methyl 2-propenyl sulfide, M-690
Methyl 2-propenyl tetrasulfide, M-296
Methyl 2-propenyl trisulfide, M-297
Methyl 2-pyridyl ketone, A-87
Methyl 2-pyrrolyl ketone, A-89
Methyl 2-thenyl sulfide, T-379
Methyl 2-thenyl sulfone, T-379
Methyl 2-thiazolin-2-yl ketone, A-47
Methyl 2-thiazolyl ketone, A-95
Methyl 2-thienyl ketone, A-97
Methyl 2-thiofuroate, F-92
Methyl 3,4,5,6-tetrahydro-2-pyridyl ketone, A-93
Methyl 3,4,5-trimethoxycinnamate, T-672
Methyl 3,4,6-tri-*O*-galloyl-β-D-glucopyranoside, T-509
Methyl 3-(2-quinoxalinylmethylene)carbazate N^1,N^4-dioxide, C-84
Methyl 3-(methylsulfinyl)-1-propenyl disulfide, M-288
Methyl 3-(methylthio)-1-propenyl disulfide, M-288
Methyl 3-*C*-(methoxymethyl)-2,3-di-*O*-methyl-α-D-*erythro*-tetrofuranoside, A-374
Methyl 3-*C*-(methoxymethyl)-2,3-di-*O*-methyl-β-D-*erythro*-tetrofuranoside, A-374
Methyl 3-*O*-α-L-arabinofuranosyl-β-D-xylopyranoside, A-392
Methyl 3-*O*-α-L-arabinopyranosyl-α-L-arabinopyranoside, A-394
Methyl 3-*O*-α-L-arabinopyranosyl-β-L-arabinopyranoside, A-394
Methyl 3-*O*-β-L-arabinopyranosyl-α-L-arabinopyranoside, A-395
Methyl 3-carbazolecarboxylate, C-87
Methyl 3-formyl-1*H*-indole-2-sulfinate, B-179
Methyl 3-hydroxy-11-oxo-12-oleanen-29,22α-olid-27-oate, D-596
Methyl 3-methyl-1-butenyl disulfide, M-285
Methyl 3-methyl-2-thienyl ketone, A-80
Methyl 3-methyl-4-pyridyl ketone, A-78
Methyl 3-methylbutanoate, M-331
S-Methyl 3-methylthiobutyrate, M-326
Methyl 3-pyridyl ketone, A-88
Methyl 3-thienyl ketone, A-98
Methyl 3-thienyl sulfide, T-383
Methyl 3-thienyl sulfone, T-383
Methyl 3-[5-(1-hydroxy-4-hepten-2-ynyl)-2-furanyl]-2-propenoate, W-17
Methyl 4,6-di-*O*-galloyl-β-D-glucopyranoside, D-216
Methyl 4,9-dihydro-β-hydroperoxy-α-[(methoxycarbonyl)amino]-4,6-dimethyl-9-oxo-1*H*-imidazo[1,2-*a*]purine-7-butanoate, W-16
Methyl 4-(methylthio)butyrate, M-201
Methyl 4-hydroxybenzoate, H-347
Methyl 4-methoxy-2-(methoxymethylene)-3-methyl-6-phenyl-5-hexenoate, O-185

Methyl 4-methoxy-2-(methoxymethylene)-6-(4-methoxyphenyl)-3-methyl-5-hexenoate, O-185
Methyl 4-methoxybenzoate, M-253
Methyl 4-methyl-2-pyridyl ketone, A-74
S-Methyl 4-methylpentanethioate, M-545
Methyl 4-methylpentanoate, M-548
Methyl 5-aminopentasulfide 1-sulfinate, A-212
Methyl 5-methyl-2-pyridyl ketone, A-75
Methyl 5-methyl-2-thienyl ketone, A-81
Methyl 5-phenylthio-1*H*-benzimidazol-2-ylcarbamate, F-23
Methyl 6′-apo-γ-carotenoate, A-378
Methyl 6′-apo-9′*Z*-lycopen-6′-oate, A-378
Methyl 6-(4-chloro-3-methoxyphenyl)-4-methoxy-2-(methoxymethylene)-3-methyl-5-hexenoate, O-185
Methyl 6-*O*-digalloyl-β-D-glucopyranoside, G-49
Methyl 6-*O*-galloyl-β-D-glucopyranoside, G-49
Methyl 6-butyl-1,4-dihydro-4-oxo-7-(phenylmethoxy)-3-quinolinecarboxylate, N-50
Methyl 6-hydroxy-*m*-tolyl ketone, H-556
Methyl 6-methoxy-9*H*-carbazole-3-carboxylate, H-383
Methyl 6-methyl-2-pyridyl ketone, A-76
Methyl 7-(benzyloxy)-6-butyl-1,4-dihydro-4-oxo-3-quinolinecarboxylate, N-50
Methyl 8-methoxy-2-carbazolecarboxylate (obsol.), H-383
Methyl *ent*-16α-acetoxy-19-oxo-17-kauranoate, K-20
Methyl *N*-(2-methoxyacetyl)-*N*-(2,6-dimethylphenyl)alaninate, M-236
S-Methyl *N*-(methylcarbamoyloxy)thioacetimidate, M-246
Methyl *N*-methylanthranilate, M-307
Methyl *N*-[[(methylamino)carbonyl]oxy]ethanimidothioate, M-246
Methyl *o*-tolyl ether, M-571
Methyl *p*-anisate, M-253
Methyl *p*-cumyl ketone, I-117
Methyl *p*-tolyl ether, M-573
Methyl *p*-tolyl ketone, M-305
Methyl acetate, M-279
Methyl acrylate, P-487
Methyl alcohol, M-243
Methyl apo-6′-lycopenate, A-378
Methyl aspartylphenylalanine, A-461
S-Methyl benzenecarbothioate, B-18
Methyl benzoate, B-31
Methyl benzoquate, N-50
S-Methyl benzothioate, B-18
Methyl benzoyl ketoxime, P-303
Methyl brevifolincarboxylate, B-188
Methyl bromide, B-193
S-Methyl butanethioate, B-215
Methyl butyl ketone, H-237
Methyl butyrate, B-218
Methyl caprate, D-41
Methyl caproate, H-234
Methyl caprylate, O-80
Methyl carbonate, D-740
Methyl cellulose, C-173
Methyl chlorooxoacetate, O-189
Methyl cinnamate, P-312
Methyl cyperenoate, P-46
Methyl decanoate, D-41
Methyl diantilis, D-400
Methyl dihydrojasmonate, O-241
Methyl diselenide, D-741
Methyl disulfide, D-742
Methyl dodecanoate, D-1016
Methyl ethyl ketone, B-221
Methyl galbanate, G-44
Methyl glucooleoside, O-149
Methyl glucosinolate, M-281
Methyl heptanoate, H-93
Methyl heptyne carbonate, O-116
S-Methyl hexanethioate, H-232
Methyl hexanoate, H-234
Methyl hydrogen fumarate, F-86
Methyl hydrogen phenylphosphonate, M-745
Methyl hydroperoxidooctadecatrienoates, M-284
Methyl isobutyrate, M-605
Methyl isopropenyl ketone, M-347
Methyl isothiocyanate, M-283
Methyl isovalerate, M-331
Methyl jasmonate, J-8
Methyl laurate, D-1016
Methyl linoleate, O-22
Methyl linolelaidate, O-22
Methyl lucidenate F, L-110
Methyl melitrate A, S-20
Methyl mercaptan, M-242
SeS-Methyl methanesulfeno(selenothioperoxoate), B-149
Methyl methanesulfenoselenoate, M-286
S-Methyl methanesulfinothioate, D-742
Methyl methanethiosulfinate, D-742
Methyl methanethiosulfonate, M-241
Methyl methylthio selenide, M-286
S-Methyl methylthiomethanesulfonothioate, M-287
Methyl mustard oil, M-283
Methyl nomilinate 17-glucoside, N-76
Methyl nonyl ketone, U-18
Methyl octa-*O*-methyl-D-lactonate, L-29
Methyl octa-*O*-methylmaltobionate, M-38
Methyl octadecanoate, O-26
Methyl octanoate, O-80
Methyl octynecarboxylate, N-140
Methyl pamplemousse, T-782
Methyl parasept, H-347
Methyl penta-*O*-acetyl-α-D-*manno*-2-heptulopyranoside, H-118
Methyl pentanoate, P-190
Methyl pentyl diketone, O-77
Methyl pentyl disulfide, P-186
Methyl pentyl ether, P-191
Methyl pentyl ketone, H-97
Methyl phaeophorbide b, P-237
Methyl phenethyl ether, P-273
Methyl phenyl diketone, P-303
Methyl phenyl disulfide, M-290
Methyl phenyl ether, M-250
Methyl phenyl glyoxime, P-303
Methyl phenyl ketone, A-27
Methyl phenyl phenylphosphonate, M-745
Methyl phenyl sulfide, M-291
Methyl phenyl sulfone, M-291
Methyl phenylacetate, P-258
Methyl phenylmethyl disulfide, B-50
Methyl propenyl ketone, P-206
Methyl propionate, P-478
Methyl propyl diketone, H-229
Methyl propyl disulfide, M-302
Methyl propyl glyoxal, H-229
Methyl propyl glyoxime, H-229
Methyl propyl ketone, P-193
Methyl propyl sulfide, P-475
Methyl propyl trisulfide, M-303
Methyl pyrazinyl ketone, A-86
Methyl rosmarinate, D-641
Methyl salicylate, M-282
Methyl selenide, D-744
Methyl sorbate, H-172
Methyl stearate, O-26
Methyl styryl ketone, P-265
Methyl succinate, S-261
Methyl sulfate sodium salt, S-137
Methyl sulfoxide, D-745
Methyl tetradecanoate, T-59
Methyl tetradecyl ketone, H-161
Methyl tetrasulfide, D-746
S-Methyl thioacetate, E-244
Methyl thioalcohol, M-242
S-Methyl thiobenzoate, B-18
Methyl thiocyanate, T-374
Methyl trisulfide, D-747
Methyl undecanoate, U-15
Methyl valerate, P-190
Methyl vanillyl ketone, D-650
Methyl viologen, D-768
Methyl yellow, D-750
Methyl [5-(phenylsulfinyl)-1*H*-benzimidazol-2-yl]-carbamate, O-192
2-[Methyl(3-phenylpropanoyl)amino]benzoic acid, M-307
4-*O*-Methyl-α-D-glucopyranosyl-(1 → 2)-β-D-xylopyranosyl-(1 → 4)-D-xylose, G-194
2-*O*-(4-*O*-Methyl-α-D-glucopyranuronosyl)-D-xylose, G-195
3-*O*-(4-*O*-Methyl-α-D-glucopyranuronosyl)-D-xylose, G-196
3-*O*-(4-*O*-Methyl-α-D-glucopyranuronosyl)-L-arabinose, G-188
4-*O*-(4-*O*-Methyl-α-D-glucopyranuronosyl)-L-arabinose, G-189
O-Methyl-α-clusin, C-310
O-Methyl-α-cubebin, C-380
3-Methyl-α-ionol, M-707
3-Methyl-α-ionone, M-707
1-Methyl-α-ionone, T-758
n-Methyl-α-ionone, T-758
3-Methyl-α-ionyl acetate, M-707
4-Methyl-α-methylene-3-cyclohexeneethanol, M-130
(+)-*N*-Methyl-α-narcotine, N-17
1-Methyl-β-carboline, M-357
O-Methyl-β-clusin, C-310
O-Methyl-β-cubebin, C-380
3-Methyl-β-ionone, M-706
1-Methyl-β-ionone, T-757
α-Methyl-β-mercaptopropyl-α′-methyl-β′-hydroxypropyl sulfide, M-218
β-Methyl-β-phenylglycidic acid, M-586
α-Methyl-δ-oxo-3-furanpentanoic acid, B-9
5-Methyl-δ-valerolactone, T-106
α-Methyl-γ-butyrolactone, D-299
3-Methyl-γ-butyrolactone, D-300
5-Methyl-γ-thiobutyrolactone, D-331
3-*O*-Methyl-(±)-*cis*-fustin, T-189
3-*O*-Methyl-(±)-*trans*-fustin, T-189
3-*O*-Methyl-(+)-*trans*-fustin, T-189
N-Methyl-(+)-coniine, P-533
N-Methyl-(-)-coniine, P-533
5-Methyl-1,2,3-benzenetriol, M-316
6-Methyl-1,2,3-oxathiazin-4(3*H*)-one 2,2-dioxide, A-18
5-Methyl-1,2,4-triazolo[3,4-*b*]benzothiazole, T-465
3-Methyl-1,2,4-trithiane, M-708
3-Methyl-1,2-anhydridoniveusin, E-187
4-Methyl-1,2-benzenediol, M-314
3-Methyl-1,2-cyclohexanedione, M-370
3-Methyl-1,2-cyclopentanedione, M-381
6-Methyl-1,3,8,9-anthracenetetrol, T-245
1-Methyl-1,3-cyclohexadiene, M-369
4-(4-Methyl-1,3-dioxolan-2-yl)-1,2-benzenediol, D-642
2-Methyl-1,3-dioxolane-2-acetaldehyde, O-197
2-Methyl-1,3-dithiolane, M-398
2-Methyl-1,3-oxathiane, M-526
2-(4-Methyl-1,3-pentadienyl)-9,10-anthracenedione, M-542
2-(4-Methyl-1,3-pentadienyl)anthraquinone, M-542
7-Methyl-1,4,5-naphthalenetriol, M-507
2-*C*-Methyl-1,4-erythronolactone, M-433
2-Methyl-1,4-naphthalenediol, M-506
2-Methyl-1,4-naphthalenedione, M-508
2-Methyl-1,4-naphthoquinol, M-506
2-Methyl-1,4-naphthoquinone, M-508
4-Methyl-1-(1-methylethenyl)-3-cyclohexen-1-ol, M-127
4-Methyl-1-(1-methylethyl)-3-cyclohexen-1-ol, M-172
4-Methyl-1-(1-methylethyl)bicyclo[3.1.0]hexan-3-one, T-391
4-Methyl-1-(1-methylethyl)cyclohexanol, M-150
4-Methyl-1-(1-methylethyl)cyclohexene, M-158
2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone, M-703
3-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone, M-704
2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-propanone, M-705
2-Methyl-1-(2,4,6-trimethoxyphenyl)-1-propanone, M-705
3-Methyl-1-(3-methyl-2-butenyl)-9*H*-carbazol-2-ol, M-777

2-Methyl-1-(methylsulfinyl)propane, M-604
2-Methyl-1-(methylthio)butane, M-327
3-Methyl-1-(methylthio)butane, M-328
2-Methyl-1-(methylthio)propane, M-604
3-Methyl-1-butanamine, M-350
2-Methyl-1-butanethiol, M-327
3-Methyl-1-butanethiol, M-328
2-Methyl-1-butanol, M-332
3-Methyl-1-butanol, M-334
4-(3-Methyl-1-butenyl)-3,3′,4′,5-tetrahydroxystilbene, H-714
4-(3-Methyl-1-butenyl)-3,4′,5-trihydroxystilbene, H-714
3-Methyl-1-butylamine, M-350
N-Methyl-1-deoxynojirimycin, H-604
25-Methyl-1-hexacosanol, M-472
4-(5-Methyl-1-methylene-4-hexenyl)-1-(4-methyl-3-pentenyl)cyclohexene, C-69
3-Methyl-1-pentanol, M-549
2-Methyl-1-phenyl-1*H*-pyrrole, M-639
4-Methyl-1-phenyl-2-pentanol, M-589
4-Methyl-1-phenyl-2-pentanone, M-590
2-Methyl-1-phenyl-2-propanol, M-594
3-Methyl-1-phenyl-3-pentanol, M-588
1-Methyl-1-phenylethyl isobutyrate, P-308
4-Methyl-1-piperazinecarbodithioic acid, P-385
2-Methyl-1-propanamine, M-618
2-Methyl-1-propanethiol, M-604
2-Methyl-1-propanol, M-606
2-Methyl-1-propenethiol, M-607
2-Methyl-1-propylamine, M-618
3-Methyl-1-[2,4,6-trihydroxy-3,5-bis(3-methyl-2-butenyl)phenyl]-1-butanone, D-85
2-Methyl-1-[2,4,6-trihydroxy-3-(3-methyl-2-butenyl)phenyl]-1-propanone, M-702
4-Methyl-1-[tetrahydro-5-(3-hydroxy-1-methylpropyl)-2-methyl-2-furanyl]-2-pentanone, I-48
25-Methyl-10-triacontanone, M-695
12-Methyl-13-tridecanolide, M-701
N-Methyl-14-*O*-demethylepiporphyroxine, G-143
3-Methyl-1*H*-indole, M-483
3-Methyl-1*H*-pyrrolo[3,2-*b*]pyridine, M-646
4-Methyl-1*H*-1-aza-2,9,10-anthracenetrione, M-74
N-Methyl-1*H*-indole-3-ethanamine, M-710
N-Methyl-1*H*-indole-3-propanamide, I-30
1-Methyl-1H-indole-3-methanamine, I-28
3-Methyl-2(1*H*)-pyrazinethione, M-634
5-Methyl-2(1*H*)-pyrazinethione, M-635
6-Methyl-2(1*H*)-pyrazinethione, M-636
3-Methyl-2(1*H*)-pyrazinone, H-610
5-Methyl-2(1*H*)-pyrazinone, H-611
6-Methyl-2(1*H*)-pyrazinone, H-612
5-Methyl-2(3*H*)-furanone, M-439
4-Methyl-2,3,5-trithiaheptane, E-353
5-Methyl-2,3-bis(1-methylethyl)phenol, D-725
5-Methyl-2,3-hexanedione, M-476
4-Methyl-2,3-pentanedione, M-544
5-Methyl-2,3:7,8-bis(methylenedioxy)benzo[*c*]phenanthridinium(1+), S-36
3-Methyl-2,4-bis(1-methylethyl)phenol, D-726
5-Methyl-2,4-bis(1-methylethyl)phenol, D-727
3-Methyl-2,4-nonanedione, M-512
3-Methyl-2,5-bis(1-methylethyl)phenol, D-728
4-Methyl-2,5-bis(1-methylethyl)phenol, D-729
5-Methyl-2,5-di-1-pyrrolidinyl-2-cyclopenten-1-one, M-397
3-Methyl-2,5-dioxopiperazine, M-600
3-Methyl-2,5-piperazinedione, M-600
8-Methyl-2,6,7-trithia-3-decene, M-616
3-Methyl-2,6-bis(1-methylethyl)phenol, D-730
1-Methyl-2-(1,1,2,2-tetrafluoroethoxy)benzene, M-571
5-Methyl-2-(1-methylethenyl)-4-hexen-1-ol, L-55
5-Methyl-2-(1-methylethenyl)cyclohexanol, M-181
5-Methyl-2-(1-methylethenyl)cyclohexanone, M-188
5-Methyl-2-(1-methylethyl)-1,3-cyclohexadiene, M-120
5-Methyl-2-(1-methylethyl)-2-cyclopenten-1-one, I-143
5-Methyl-2-(1-methylethyl)-2-hexenal, I-145
1-Methyl-2-(1-methylethyl)benzene, I-137
5-Methyl-2-(1-methylethyl)cyclohexanecarboxylic acid, I-142
5-Methyl-2-(1-methylethyl)cyclohexanethione, M-165
5-Methyl-2-(1-methylethyl)cyclohexanol, M-149
5-Methyl-2-(1-methylethyl)cyclohexanone, M-153
3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-1,2-propanediol, M-499
5-Methyl-2-(1-methylethyl)phenol, I-146
4-Methyl-2-(1-methylethyl)thiazole, D-110
5-Methyl-2-(1-methylethylidene)cyclohexanone, M-186
4-Methyl-2-(1-phenylethyl)-1,3-dioxolane, M-584
3-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, M-641
5-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, M-642
3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one, M-562
2-Methyl-2-(2-phenylethenyl)-1,3-dithiolane, P-265
N-Methyl-2-(3,4-dihydroxyphenyl)ethylamine, E-57
1-Methyl-2-(3,4-methylenedioxyphenyl)-4(1*H*)-quinolinone, G-320
5-Methyl-2-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,3-benzenediol, G-325
4-Methyl-2-(3-methyl-1,3-butadienyl)oxepane, Q-9
2-Methyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-6-chromanol, D-333
6-Methyl-2-(4-methyl-3-cyclohexen-1-yl)-5-hepten-2-ol, B-99
1-Methyl-2-(5-undecenyl)-4(1*H*)-quinolinone, U-31
1-Methyl-2-(6-undecenyl)-4(1*H*)-quinolinone, U-31
7-Methyl-2-(7-oxo-1,3,5-nonatrienyl)-3*H*-azepine, C-182
7-Methyl-2-(7-oxo-1,3-nonadienyl)-3*H*-azepine, C-182
1-Methyl-2-(8-oxononyl)-4(1*H*)-quinolinone, N-139
5-Methyl-2-(*N*-pyrrolidinomethyl)furan, M-445
2-Methyl-2-(methyldithio)propanal, M-488
1-Methyl-2-(phenylmethyl)-4(1*H*)-quinazolinone, B-61
S-Methyl-2-(propionyloxy)propanethioate, M-664
1-Methyl-2-(trifluoromethoxy)benzene, M-571
7-Methyl-2-benzofurancarboxaldehyde, M-317
2-Methyl-2-bornanol, T-300
3-Methyl-2-butanethiol, M-329
2-Methyl-2-butanol, M-333
3-Methyl-2-butanol, M-335
2-Methyl-2-buten-1-ol, M-342
3-Methyl-2-buten-1-ol, M-344
2-Methyl-2-butenal, M-336
3-Methyl-2-butenal, M-337
2-Methyl-2-butene-1,4-diol, M-338
3-Methyl-2-butene-1-thiol, M-339
2-Methyl-2-butenoic acid, M-340
3-Methyl-2-butenoic acid, M-341
2-Methyl-2-butenoic acid 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, T-398
3-Methyl-2-butenyl caffeate, M-344
S-(3-Methyl-2-butenyl) 2-methylpropanethioate, M-339
S-(3-Methyl-2-butenyl) 3-methylbutanethioate, M-339
S-(3-Methyl-2-butenyl) ethanethioate, M-339
2-(3-Methyl-2-butenyl)-5-(2-phenylethenyl)-1,3-benzenediol, M-348
10-(3-Methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,6,9(11*a H*)-triol, T-693
2-(3-Methyl-2-butenyl)-6*H*-benzofuro[3,2-*c*][1]benzopyran-3,6*a*,9(11*a H*)-triol, T-691
N^6-(3-Methyl-2-butenyl)agmatine, A-221
7-*O*-(3-Methyl-2-butenyl)limocitrin, T-157
1-[(3-Methyl-2-butenyl)oxy]-4-(2-propenyl)benzene, P-513
9-[(3-Methyl-2-butenyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, I-14
3-[5-[4-[(3-Methyl-2-butenyl)oxy]phenyl]-2-oxazolyl]pyridine, H-3
N-[2-[4-[(3-Methyl-2-butenyl)oxy]phenyl]ethyl]-3-phenyl-2-propenamide, H-712
6-(3-Methyl-2-butenylamino)purine, Z-8
9-(3-Methyl-2-butenyloxy)-7-oxofuro[3,2-*g*]chromene, I-14
3-Methyl-2-cyclohexen-1-one, M-377
2-Methyl-2-cyclopenten-1-one, M-383
3-Methyl-2-cyclopenten-1-one, M-384
α-Methyl-2-furanacrolein, F-118
5-Methyl-2-furancarboxaldehyde, M-437
5-Methyl-2-furancarboxaldehyde thiosemicarbazone, M-437
α-Methyl-2-furanmethanethiol, M-208
5-Methyl-2-furanmethanethiol, M-438
5-Methyl-2-furanthiol, M-441
1-(5-Methyl-2-furanyl)-1,2-propanedione, M-448
2-(5-Methyl-2-furanyl)-3-piperidinol, M-447
3-(5-Methyl-2-furanyl)butanal, M-443
1-(3-Methyl-2-furanyl)ethanone, A-70
1-(5-Methyl-2-furanyl)ethanone, A-71
3-[(5-Methyl-2-furanyl)methyl]-1*H*-pyrrole, M-444
1-[(5-Methyl-2-furanyl)methyl]pyrrolidine, M-445
2-(5-Methyl-2-furanyl)piperidine, M-446
2-[2-(5-Methyl-2-furanyl)propyl]-1,3-dioxane, M-443
2-[2-(5-Methyl-2-furanyl)propyl]-1,3-dioxolane, M-443
2-(5-Methyl-2-furanyl)pyrrolidine, M-449
5-Methyl-2-furfurylmercaptan, M-438
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2-(5-Methyl-2-furyl)-3,4,5,6-tetrahydropyridine, T-103
4-Methyl-2-heptanol, M-463
6-Methyl-2-heptanol, M-465
5-Methyl-2-hepten-4-one, M-468
5-Methyl-2-hexanone, M-479
5-Methyl-2-methylene-3-vinyl-4-hexen-1-ol, M-497
6-Methyl-2-methylene-6-octene-1,3,8-triol, M-495
1-Methyl-2-nonyl-4(1*H*)-quinolinone, N-139
2-Methyl-2-octenal, M-521
5-Methyl-2-octyl-3(2*H*)-furanone, M-523
2-(3-Methyl-2-oxiranyl)-1,4-benzenediol, M-528
3-Methyl-2-oxobutanoic acid, M-529
3-Methyl-2-oxopentanoic acid, M-532
4-Methyl-2-oxopentanoic acid, M-533
1-Methyl-2-oxopropyl butyrate, H-376
3-Methyl-2-oxovaleric acid, M-532
4-Methyl-2-pentanone, M-550
2-Methyl-2-pentenal, M-551
4-Methyl-2-pentenal, M-553
2-Methyl-2-pentenoic acid, M-554
4-Methyl-2-pentenoic acid, M-557
5-(4-Methyl-2-pentyl)tetrahydro-2-oxo-3-furancarboxylic acid, A-173
4-Methyl-2-pentyl-1,3-dioxolane, M-567
3-Methyl-2-pentyl-2-cyclopentenone, M-566
4-Methyl-2-phenyl-1,3-dioxolane, M-581
5-Methyl-2-phenyl-2-hexenal, M-585
4-Methyl-2-phenyl-2-pentenal, M-592
3-Methyl-2-phenylbutanal, M-577
2-Methyl-2-propen-1-ol, M-608
1-Methyl-2-propylbenzene, M-619
3-Methyl-2-pyrazinethiol, M-634
5-Methyl-2-pyrazinethiol, M-635
6-Methyl-2-pyrazinethiol, M-636
6-Methyl-2-pyrazinyl 2-furfuryl sulfide, F-123
1-(4-Methyl-2-pyridinyl)ethanone, A-74
1-(5-Methyl-2-pyridinyl)ethanone, A-75
1-(6-Methyl-2-pyridinyl)ethanone, A-76
1-Methyl-2-pyrrolecarboxaldehyde, P-617
1-Methyl-2-pyrrolidineacetic acid, P-619
4-Methyl-2-pyrrolidinecarboxylic acid, M-640
4-Methyl-2-pyrroline, D-316
2-Methyl-2-thiazoline, D-322
Methyl-2-thienyl sulfide, T-382
1-(5-Methyl-2-thienyl)-1-propanone, M-663
5-(5-Methyl-2-thienyl)-2,4-pentadien-4-olide, M-661
5-(5-Methyl-2-thienyl)-2-penten-4-ynoic acid, M-662
1-(3-Methyl-2-thienyl)ethanone, A-80
1-(5-Methyl-2-thienyl)ethanone, A-81
5-[(5-Methyl-2-thienyl)methylene]-2(5*H*)-furanone, M-661
5-Methyl-2-thiophenethiol, M-684

1-Methyl-2-undecyl-4(1*H*)-quinolinone, U-31
6-Methyl-2-vinyl-5-heptene-1,2-diol, M-712
2-Methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid, M-535
25-Methyl-21-tritriacontene-1,9,11-triol, M-709
14-Methyl-24-methylene-9,19-cyclocholestan-3-ol, M-366
25-Methyl-24-methylenecholest-5-en-3-ol, M-490
4-Methyl-24-methylenecholest-7-en-3-ol, M-427
4-Methyl-24-methylenecholest-8-en-3-ol, M-428
14-Methyl-24-methylenecholest-9(11)-ene-3,7-diol, M-423
25-Methyl-24-methylenecholesterol, M-490
28-Methyl-27-nonacosenoic acid, M-511
24-Methyl-28,29-dinorcycloart-25-en-3-ol, M-367
24-Methyl-28-norcycloart-25-en-3-ol, D-775
24-Methyl-28-norcycloart-25-en-3-one, D-775
24-Methyl-29-norcycloart-25-en-3-ol, D-775
24-Methyl-29-norcycloart-25-en-3-one, D-775
24-Methyl-29-norcycloartan-3-ol, C-450
24-Methyl-29-norcycloartan-3-one, C-450
5-Methyl-3(13-oxotriacontyl)-2(5*H*)-furanone, R-8
5-Methyl-3,4,6-trithiaoctane, E-263
2-Methyl-3,4-dithiaoctane, B-235
2-Methyl-3,4-pentadienoic acid, M-541
2-Methyl-3,4-piperidinediol, M-601
2-Methyl-3,5-dinitrobenzamide, M-396
2-Methyl-3,5-dinitrobenzoic acid, M-396
6-Methyl-3,5-heptadien-2-one, M-459
5-Methyl-3,7-diphenyl-2-oxo-5-azabicyclo[2.2.1]-heptan-6-one, C-442
4′-*O*-Methyl-3,9-dihydropunctatin, T-589
7-*O*-Methyl-3,9-dihydropunctatin, T-589
1-Methyl-3-(1-methylethenyl)cyclohexanol, M-170
1-Methyl-3-(1-methylethyl)benzene, I-138
6-Methyl-3-(1-methylethylidene)-7-oxabicyclo[4.1.0]heptan-2-one, E-170
1-Methyl-3-(1-methylethylidene)cyclohexene, M-112
2-Methyl-3-(1-propenyl)pyrazine, M-609
5-Methyl-3-(11,15,19-triacontatrienyl)-2(5*H*)-furanone, M-697
5-Methyl-3-(11,15-triacontadienyl)-2(5*H*)-furanone, M-697
5-Methyl-3-(13,17-triacontadienyl)-2(5*H*)-furanone, M-696
5-Methyl-3-(2,8,13,14-tetrahydroxytriacontyl)-2(5*H*)-furanone, D-1034
2-Methyl-3-(2-methylphenyl)propanal, M-502
2-Methyl-3-(2-methylpropyl)pyrazine, M-504
2-Methyl-3-(2-pentenyl)-2-cyclopenten-1-one, M-561
2-Methyl-3-(2-propenyl)pyrazine, M-610
1-Methyl-3-(2-thiazolyl)-1*H*-indole, T-355
2-Methyl-3-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-naphthalenedione, V-44
2-Methyl-3-(3,7,11,15-tetramethylhexadecyl)-1,4-naphthalenedione, V-44
3-Methyl-3-(4-methylphenyl)oxiranecarboxylic acid, M-501
2-Methyl-3-(4-methylphenyl)propanal, M-503
5-Methyl-3-(9,13,17-triacontatrienyl)-2(5*H*)-furanone, M-696
2-Methyl-3-(*p*-tolyl)propionaldehyde, M-503
2-Methyl-3-(methyldithio)furan, M-487
2-Methyl-3-(methylthio)furan, M-440
2-Methyl-3-(methylthio)pyrazine, M-634
2-Methyl-3-(phenylthio)furan, M-440
2-Methyl-3-(propyldithio)furan, M-623
2-Methyl-3-(thioacetoxy)-4,5-dihydrofuran, D-302
3-Methyl-3-buten-1-ol, M-345
2-Methyl-3-buten-2-ol, M-343
3-Methyl-3-buten-2-ol, M-346
3-Methyl-3-buten-2-one, M-347
O-(3-Methyl-3-butenyl)halfordinol, H-3
Methyl-3-cyano-2-hydroxy-2-methylpropanoate, H-565
3-Methyl-3-cyclohexen-1-ol, M-376
1-(4-Methyl-3-cyclohexen-1-yl)ethanone, A-69
2-(4-Methyl-3-cyclohexenyl)-2-propanol, M-175
3-(4-Methyl-3-cyclohexenyl)butanal, M-378
2-(4-Methyl-3-cycohexen-1-yl)-1-propanol, M-176
3-Methyl-3-decen-1-ol, M-393
3-Methyl-3-decenoic acid, M-391
α-Methyl-3-furanacrolein, F-119
2-Methyl-3-furanthiol, M-440
5-Methyl-3-furanthiol, M-442
3-[(2-Methyl-3-furanyl)thio]-4-heptanone, M-450
4-[(2-Methyl-3-furanyl)thio]-5-nonanone, M-451
2-Methyl-3-furyl propyl disulfide, M-623
8-Methyl-3-hentriacontene, M-455
5-Methyl-3-heptanol, M-464
5-Methyl-3-hepten-2-one, M-467
5-Methyl-3-hexen-2-one, M-480
7-Methyl-3-methylene-1,2,6,7-octanetetrol, M-493
7-Methyl-3-methylene-1,6,7-octanetriol, M-494
7-Methyl-3-methylene-1,6-octadiene, M-491
2-Methyl-3-methylene-2-norbornanol, M-489
2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol, M-489
2-Methyl-3-nonacosanone, M-510
7-Methyl-3-octen-2-one, M-522
4-Methyl-3-oxa-6-thiabicyclo[3.3.0]octa-1,4-diene, D-323
N-(5-Methyl-3-oxohexyl)alanine, A-151
4-Methyl-3-penten-2-one, M-558
2-Methyl-3-pentenoic acid, M-555
3-(4-Methyl-3-pentenoyl)furan, E-6
6-(4-Methyl-3-pentenyl)-1,2,3,4-tetrathia-6-cyclooctene, D-312
5-(4-Methyl-3-pentenyl)-1,2,3-trithia-5-cycloheptene, D-313
4-(4-Methyl-3-pentenyl)-1,2-dithia-4-cyclohexene, D-311
4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde, M-560
2-(4-Methyl-3-pentenyl)anthraquinone, M-542
3-(4-Methyl-3-pentenyl)thiophene, M-563
2-Methyl-3-phenoxy-1-butene, M-346
2-Methyl-3-phenoxy-1-propene, M-608
2-Methyl-3-phenyl-2-propenal, M-597
N-Methyl-3-phenyl-*N*-(2-phenylethenyl)-2-propenamide, L-45
2-Methyl-3-phenylacrolein, M-597
N-Methyl-3-phenyloxiranecarboxamide, P-292
3-Methyl-3-phenyloxiranecarboxylic acid, M-586
2-Methyl-3-phytyl-1,4-naphthoquinone, V-44
2-Methyl-3-propylpyrazine, M-626
1-(5-Methyl-3-pyridinyl)-1-decanone, M-637
5-Methyl-3-thiomorpholinecarboxylic acid 1-oxide, C-416
2-Methyl-3-thiophenethiol, M-683
5-Methyl-3-thiophenethiol, M-685
2-Methyl-3-vinylpyrazine, M-713
5-Methyl-3-[10-[3-(3-octadecenyl)oxiranyl]decyl]-2(5*H*)-furanone, E-58
24-Methyl-31-norlanost-9(11)-en-3-ol, T-740
3-Methyl-3*H*-imidazo[4,5-*f*]quinoxalin-2-amine, A-268
6-Methyl-4,5-dithia-2-octene, M-617
9-Methyl-4,8-sphingadienine, A-275
1-Methyl-4-(1-methylethenyl)-1,3-cyclohexadiene, M-155
1-Methyl-4-(1-methylethenyl)-2-cyclohexen-1-ol, M-131
1-Methyl-4-(1-methylethenyl)-3-cyclohexen-1-ol, M-132
1-Methyl-4-(1-methylethenyl)-7-oxabicyclo[4.1.0]-heptan-2-one, E-171
1-Methyl-4-(1-methylethenyl)-7-oxabicyclo[4.1.0]-heptane, E-164
1-Methyl-4-(1-methylethenyl)benzene, M-154
1-Methyl-4-(1-methylethenyl)cyclohexanol, M-179
1-Methyl-4-(1-methylethenyl)cyclohexene, L-88
1-Methyl-4-(1-methylethyl)-1,3-cyclohexadiene, M-114
1-Methyl-4-(1-methylethyl)-1,3-cyclohexanediol, M-136
1-Methyl-4-(1-methylethyl)-1,4-cyclohexadiene, M-115
1-Methyl-4-(1-methylethyl)-2,3-dioxabicyclo[2.2.2]oct-5-ene, A-443
1-Methyl-4-(1-methylethyl)-2-cyclohexene-1,4-diol, M-162
1-Methyl-4-(1-methylethyl)-3-cyclohexen-1-ol, M-177
1-Methyl-4-(1-methylethyl)-7-oxabicyclo[2.2.1]heptane, E-153
1-Methyl-4-(1-methylethyl)benzene, I-139
α-Methyl-4-(1-methylethyl)benzenepropanal, I-153
1-Methyl-4-(1-methylethyl)cyclohexanol, M-147
2-Methyl-4-(1-methylethyl)thiazole, D-110
1-Methyl-4-(1-methylethylidene)cyclohexanol, M-178
1-Methyl-4-(1-methylethylidene)cyclohexene, M-116
2-Methyl-4-(1*H*-purin-6-ylamino)-2-buten-1-ol, Z-8
3-Methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one, M-706
3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-ol, M-707
3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, M-707
1-Methyl-4-(2-methyloxiranyl)-7-oxabicyclo[4.1.0]-heptane, L-88
5-Methyl-4-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,2,3-benzenetriol, N-34
1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)cyclohexene, B-109
4-Methyl-4-(methylthio)-2-pentanone, M-217
1-Methyl-4-(trifluoromethoxy)benzene, M-573
2-Methyl-4-butanolide, D-299
3-Methyl-4-butanolide, D-300
3-Methyl-4-decanolide, H-267
4-Methyl-4-decanolide, H-268
3-Methyl-4-decen-1-ol, M-394
3-Methyl-4-decenoic acid, M-392
N-(1-Methyl-4-hydroxy-3-imidazolin-2-ylidene)alanine, D-310
1-Methyl-4-isopropenylbenzene, M-154
3-Methyl-4-octanolide, B-246
3-Methyl-4-oxo-2-pentenal, M-534
2-Methyl-4-oxoglutaric acid, M-531
2-Methyl-4-oxopentanedioic acid, M-531
4-Methyl-4-penten-2-one, M-559
2-Methyl-4-pentenal, M-552
2-Methyl-4-pentenoic acid, M-556
2-Methyl-4-phenyl-2-butanol, M-578
3-Methyl-4-phenyl-3-buten-2-one, M-580
2-Methyl-4-phenylbutanal, M-576
2-Methyl-4-propyl-1,3-oxathiane, M-625
1-(2-Methyl-4-pyridinyl)ethanone, A-77
1-(3-Methyl-4-pyridinyl)ethanone, A-78
1-(2-Methyl-4-pyrimidinyl)ethanone, A-79
3-Methyl-4-tetradecanoyloxy-2-butenenitrile, H-570
14α-Methyl-5α-cholesta-8,24-diene-3β,6α-diol, S-220
4α-Methyl-5α-stigmast-8(14)-en-3β-ol, M-650
5′-*S*-Methyl-5′-thioadenosine, T-365
25-Methyl-5,24(28)-ergostadien-3-ol, M-490
2-Methyl-5,6-dithia-3-heptene, M-285
7-[[3-Methyl-5-(1,3,3-trimethyl-7-oxabicyclo[2.2.1]-hept-2-yl)-2-pentenyl]oxy]-2*H*-1-benzopyran-2-one, F-15
2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-ol, M-128
2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one, M-135
2-Methyl-5-(1-methylethenyl)cyclohexanol, M-180
2-Methyl-5-(1-methylethenyl)cyclohexanone, M-187
2-Methyl-5-(1-methylethenyl)cyclopentanecarboxaldehyde, I-115
2-Methyl-5-(1-methylethyl)-1,3-benzenediol, I-140
2-Methyl-5-(1-methylethyl)-1,3-cyclohexadiene, M-117
2-Methyl-5-(1-methylethyl)-1-nitro-1,3-cyclohexadiene, N-69
2-Methyl-5-(1-methylethyl)-2,5-cyclohexadiene-1,4-dione, M-122
2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-one, M-185
2-Methyl-5-(1-methylethyl)bicyclo[3.1.0.]hex-2-ene, T-392
2-Methyl-5-(1-methylethyl)bicyclo[3.1.0]hexan-2-ol, T-390
2-Methyl-5-(1-methylethyl)cyclohexanol, M-148

2-Methyl-5-(1-methylethyl)cyclohexanone, M-152
2-Methyl-5-(1-methylethyl)furan, I-144
2-Methyl-5-(1-methylethyl)pyrazine, I-149
1-Methyl-5-(1-methylethylidene)cyclohexene, M-113
2-Methyl-5-(1-propenyl)pyrazine, M-611
2-Methyl-5-(2-piperidinyl)furan, M-446
2-Methyl-5-(2-propenyl)pyrazine, M-612
3-Methyl-5-(2-pyrrolidinyl)-2(5*H*)-furanone, P-24
2-Methyl-5-(2-pyrrolidinyl)furan, M-449
7-[[3-Methyl-5-(3-hydroxy-2,2-dimethyl-6-methylene)cyclohexyl-2-pentenyl]oxy]-2*H*-1-benzopyran-2-one, F-14
2-Methyl-5-(3-pyrrolylmethyl)furan, M-444
2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-benzenediol, M-539
2-Methyl-5-(8,11-pentadecadienyl)-1,3-benzenediol, M-539
2-Methyl-5-(8-pentadecenyl)-1,3-benzenediol, M-539
2-Methyl-5-(methylthio)furan, M-441
2-Methyl-5-(methylthio)pyrazine, M-635
2-Methyl-5-(methylthio)thiophene, M-684
6-Methyl-5-hepten-2-ol, M-466
5-Methyl-5-hepten-2-one, M-469
6-Methyl-5-hepten-2-one, M-470
4-Methyl-5-hexanolide, T-83
5-Methyl-5-hexen-2-one, M-481
6-Methyl-5-methylene-2-heptene, I-135
1-[4-(4-Methyl-5-oxo-2(5*H*)-furanylidene)butyl]-2-pyrrolidinone, P-20
5-Methyl-5-pentacosanol, M-537
3-Methyl-5-pentyl-1,2,4-trithiolane, M-570
3-Methyl-5-pentyl-2-furannonanoic acid, M-568
3-Methyl-5-pentyl-2-furanundecanoic acid, M-569
2-Methyl-5-propanoylthiophene, M-663
3-Methyl-5-propyl-2-cyclohexen-1-one, M-621
2-Methyl-5-propylpyrazine, M-627
4-Methyl-5-thiazoleethanol, H-453
2-Methyl-5-thiazolol, H-618
2-(4-Methyl-5-thiazolyl)ethanol, H-453
9-(5-*S*-Methyl-5-thio-β-D-xylofuranosyl)adenine, T-365
2-Methyl-5-vinylpyrazine, M-714
4-Methyl-5-vinylthiazole, M-715
2-Methyl-5-[5-(2-methylpropyl)-3-furanyl]-2-cyclohexen-1-one, B-88
7-Methyl-5*H*-benzo[*g*]-1,3-benzodioxolo[6,5,4-*de*]-quinoline-5,6(7*H*)-dione, C-178
1-Methyl-5*H*-pyrido[3,4-*b*]indol-1-amine, A-276
6′-Methyl-6′-apo-β-caroten-6′-one, C-281
1-Methyl-6,7-isoquinolinediol, D-555
3-Methyl-6-(1-methylethenyl)-3-cyclohexen-1-ol, M-123
3-Methyl-6-(1-methylethyl)-1,2-cyclohexanediol, M-138
9-Methyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decane-2-methanol, M-191
3-Methyl-6-(1-methylethyl)-2,5-piperazinedione, C-415
3-Methyl-6-(1-methylethyl)-2-cyclohexen-1-ol, M-171
3-Methyl-6-(1-methylethyl)-2-cyclohexen-1-one, M-184
3-Methyl-6-(1-methylethyl)-3-cyclohexen-1-ol, M-173
3-Methyl-6-(1-methylethylidene)-2-cyclohexen-1-one, M-134
2-Methyl-6-(1-propenyl)pyrazine, M-613
2-Methyl-6-(2-propenyl)pyrazine, M-614
2-Methyl-6-(3,7,11,15-tetramethyl-2-hexadecenyl)-1,4-benzenediol, M-599
5-Methyl-6-(3,7,11-trimethyl-2,6,10-dodecatrienyl)-1,3-benzenediol, N-34
2-Methyl-6-(4-methyl-2,4-cyclohexadien-1-yl)-2-hepten-4-ene, B-112
2-Methyl-6-(4-methyl-3-cyclohexen-1-yl)-2,5-heptadien-4-one, B-114
2-Methyl-6-(4-methylenebicyclo[3.1.0]hex-1-yl)-2-heptenal, S-94
2-Methyl-6-(4-methylphenyl)-1-hepten-3-one, B-103
2-Methyl-6-(4-methylphenyl)-2-hepten-4-one, B-102
2-Methyl-6-(4-methylphenyl)-3-heptanone, B-103
2-Methyl-6-(4-methylphenyl)-4-heptanone, B-102
6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one, M-500
2-Methyl-6-(methylthio)pyrazine, M-636
2-Methyl-6-methylene-2,7-octadien-1-ol, M-492
2-Methyl-6-methylene-7-octen-2-ol, M-496
2-Methyl-6-oxo-2,4-heptadienoic acid, M-530
14-Methyl-6-pentadecenoic acid, M-540
1-Methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridin-2-amine, A-293
2-Methyl-6-phytylhydroquinone, M-599
4-Methyl-6-[(2-oxo-2*H*-1-benzopyran-7-yl)oxy]-4-hexenal, H-351
2-[[9-Methyl-6-[(phenylmethyl)amino]-9*H*-purin-2-yl]amino]ethanol, O-155
4-Methyl-7-(1-methylethenyl)-1-azulenecarboxaldehyde, M-498
4-Methyl-7-(1-methylethenyl)-1-azulenemethanol, M-498
10-Methyl-7-(1-methylethyl)-1,5-dioxaspiro[5.5]undecan-3-ol, M-192
4-Methyl-7-(1-methylethyl)-2-oxepanone, H-418
2-Methyl-7-(7-oxo-1,3-nonadienyl)-2*H*-azepine, C-182
11-Methyl-7-oxatetracyclo[6.3.1.$0^{1,6}$.$0^{4,11}$]dodecane, M-525
4-Methyl-8(14)-cholesten-3-ol, M-362
8-Methyl-8-azabicyclo[3.2.1]octan-1-ol, P-356
8-Methyl-8-azabicyclo[3.2.1]octane-3,6,7-triol, M-309
10-Methyl-9(10*H*)-acridinone, M-306
14α-Methyl-9,19-cyclo-5α,9β-cholestane-3β,6α-diol, C-505
14-Methyl-9,19-cycloergost-24(28)-en-3-ol, M-366
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14-Methyl-9,19-cycloergost-25-en-3-ol, M-367
14-Methyl-9,19-cycloergost-25-en-3-one, M-367
24-Methyl-9,19-cyclolanost-25-en-3-ol, M-364
10-Methyl-9-acridanone, M-306
9-Methyl-9-azabicyclo[3.3.1]nonan-3-one, A-516
1-*O*-(10-Methyl-9-octadecenoyl)glycerol, G-236
3-Methyl-9*H*-carbazole, M-356
3-Methyl-9*H*-carbazol-1-ol, H-574
3-Methyl-9*H*-carbazol-2-ol, H-575
3-Methyl-9*H*-carbazole-9-carboxaldehyde, M-356
1-Methyl-9*H*-pyrido[3,4-*b*]indol-7-ol, H-576
1-Methyl-9*H*-pyrido[3,4-*b*]indole, M-357
3-*O*-Methyl-D-*chiro*-inositol, I-40
6-*O*-Methyl-D-*myo*-inositol, M-485
2-*O*-Methyl-D-rhamnose, R-20
2-*O*-Methyl-L-*chiro*-inositol, I-40
3-*O*-Methyl-L-*chiro*-inositol, I-40
3-*O*-Methyl-L-*erythro*-hex-2-enono-1,4-lactone, I-70
1-*O*-Methyl-L-*myo*-inositol, M-485
2-*O*-Methyl-L-fucose, F-81
3-(*N*-Methyl-L-isoleucine)destruxin B, H-293
2-*O*-Methyl-L-rhamnose, R-20
3-*O*-Methyl-L-rhamnose, R-20
4-*O*-Methyl-L-rhamnose, R-20
5-*O*-Methyl-L-rhamnose, R-20
4-*O*-Methyl-*myo*-inositol, M-485
N-Methyl-*N*-(2-phenylethenyl)-3-phenyl-2-oxiranecarboxamide, M-583
1-*C*-Methyl-*scyllo*-inositol, M-484
N-Methyl-*N*-*cis*-styrylcinnamamide, L-45
O-Methyl-*N*-depropionylaspidolimine, P-607
4′-Methyl-*N*-methylcoclaurine, H-282
N-Methyl-*N*-nitrosomethanamine, N-73
N-Methyl-*N*-phenylethylcinnamamide, P-278
2-Methyl-*N*-propyl-1-propylamine, M-618
3-Methyl-*N*-propylbutylamine, M-350
N-Methyl-*N*-styrylcinnamamide, L-45
7-Methyl-*N*-vanillyl-5-octenamide, D-402
9-Methyl-*N*-vanillyl-7-decenamide, D-402
1-Methyl-*N*-[3-(1-methylethyl)-5,8-dioxo-7-(phenylmethyl)-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-2-pyrrolidinecarboxamide, C-163
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(Methyl-*ONN*-azoxy)methanol, M-310
Methyl-*p*-tolylcarbinol, M-582
Methyl-*p*-tolylglycidic acid, M-501
4′-Methylacetophenone, M-305
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10-Methylacridone, M-306
N-Methylacridone, M-306
3-Methylacrylic acid, B-223
N-Methylactinodaphnine, D-154
β-Methylaesculetin, H-547
N^6-Methylagmatine, A-221
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2-Methylallyl butyrate, M-608
Methylallylacetic acid, M-556
N^5-(Methylamidino)ornithine, M-308
N^5-[(Methylamino)(methylimino)methyl]ornithine, D-754
2-(Methylamino)benzoic acid, M-307
2-(Methylamino)butanoic acid, A-219
N-[[(Methylamino)carbonyl]oxy]-2-(methylthio)ethanimine, M-246
4-(Methylamino)cycloheptanone, P-356
4-[2-(Methylamino)ethyl]-1,2-benzenediol, E-57
4-[2-(Methylamino)ethyl]phenol, H-712
4-[2-(Methylamino)ethyl]pyrocatechol, E-57
2-Methylamino-3-phenylpropanoic acid, P-259
N-Methylaminodithioformic acid, M-355
3-(2-Methylaminoethyl)-1*H*-indol-5-ol, H-820
4-(β-Methylaminoethyl)catechol, E-57
3-(2-Methylaminoethyl)indole, M-710
3-(Methylaminomethyl)indole, I-28
o-Methylanisole, M-571
N-Methylanonaine, R-41
N-Methylanthranilic acid, M-307
6-Methylapigenin, T-632
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N^ω-Methylarginine, M-308
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4-*O*-Methylarmillaridin, D-677
6-*O*-Methylarmillaridin, D-677
N-Methylasimilobine, D-379
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O-Methylatheroline, O-215
N-Methylatherosperminium, A-484
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3′-*O*-Methylbatatasin III, D-639
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3-Methylbenzaldehyde, M-312
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4-Methylbenzeneacetaldehyde, M-575
α-Methylbenzeneacetaldehyde, P-301
α-Methylbenzenebutanal, M-576
α-Methylbenzeneethanol, P-306
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3-Methylbenzenemethanol, M-321
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α-Methylbenzenepropanol, P-261
2-Methylbenzenethiol, M-315
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2-Methylbenzothiazole, M-319
4-Methylbenzo[*g*]quinoline-2,5,10(1*H*)-trione, M-74
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3-Methylbenzyl alcohol, M-321
4-Methylbenzyl alcohol, M-322
α-Methylbenzyl alcohol, P-272
α-Methylbenzyl butyrate, P-272
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4-Methylbiphenyl, M-323
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O-Methylbufotenine *N*-oxide, B-197
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3-Methylbutanal, M-325
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3-Methylbutanethioic acid, M-326
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3-Methylbutanoic acid, M-331
3-*O*-(2*S*-Methylbutanoyl)pinobanksin, T-568
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3-Methylbutyl 2-furanbutanoate, F-91
3-Methylbutyl 2-hydroxybenzoate, H-345
2-Methylbutyl 2-methylbutanoate, M-330
3-Methylbutyl 2-methylbutanoate, M-330
3-Methylbutyl 2-methylpropanoate, M-334
3-Methylbutyl 2-oxopropanoate, P-632
2-Methylbutyl 3-methylbutanoate, M-331
3-Methylbutyl 3-methylbutanoate, M-331
3-Methylbutyl 3-oxobutanoate, O-199
3-Methylbutyl 4-methoxybenzoate, M-253
3-Methylbutyl benzoate, M-334
1-Methylbutyl butanoate, P-192
3-Methylbutyl decanoate, D-41
3-Methylbutyl dodecanoate, D-1016
3-Methylbutyl formate, M-334
3-Methylbutyl glucosinolate, M-349
3-Methylbutyl hexanoate, H-234
2-Methylbutyl isovalerate, M-331
3-Methylbutyl nonanoate, N-109
3-Methylbutyl octanoate, O-80
3-Methylbutyl pentanoate, P-190
3-Methylbutyl phenylacetate, P-258
3-Methylbutyl propanoate, M-334
1-(3-Methylbutyl)-β-carboline, M-351
2-(3-Methylbutyl)-1*H*-pyrrolo[2,3-*b*]pyridine, M-354
N-(2-Methylbutyl)-2,4-undecadiene-8,10-diynamide, U-11
1-(3-Methylbutyl)-9*H*-pyrido[3,4-*b*]indole, M-351
N-(3-Methylbutyl)acetamide, M-350
3-[(3-Methylbutyl)nitrosoamino]-2-butanone, M-353
3-(3-Methylbutylidene)-1(3*H*)-isobenzofuranone, M-352
α-(3-Methylbutylidene)benzeneacetaldehyde, M-585
2-Methylbutyraldehyde, M-324
3-Methylbutyraldehyde, M-325
γ-Methylbutyrolactone, D-301
(2-Methylbutyryl)phloroglucinol, M-703
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2′-*O*-Methylcajanone, C-28
3-*O*-Methylcalopocarpin, D-670
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4′-*O*-Methylcatechin, P-104
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24-Methylcholest-5-ene-3,7,22-triol, E-222
4-Methylcholest-7-en-3-ol, M-361
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24-Methylcholesta-5,22-dien-3-ol, M-359
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24-Methylcholesta-5,23-dien-3-ol, E-206
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24-Methylcholesta-5,7-dien-3-ol, E-205
24-Methylcholesta-5,8,22-triene-3,7-diol, E-216
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24-Methylcholesta-7,23-dien-3-ol, E-208
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24-Methylcholesta-7,9(11),22-triene-3,5,6-triol, E-219
24-Methylcholesta-8,22-diene-3,5,6,7-tetrol, E-201
14-Methylcholesta-9(11),24-diene-3,7-diol, M-358
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24-Methylcholestane-2,3,22,23-tetrol, E-211
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6-Methylchrysin, D-554
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O-Methylcorypalline, T-78
3-*O*-Methylcoumestrol, C-370
9-*O*-Methylcoumestrol, C-370
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3-Methylcrotonic acid, M-341
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24-Methylcycloart-23-en-3β-yl acetate, C-497
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3-Methylcyclohexanone, M-374
4-Methylcyclohexanone, M-375
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8-Methyldihydrochelerythrine, B-165
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4-Methyldiphenyl ether, M-573
6-Methyldipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, A-269
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2-(Methyldithio)propanoic acid, M-399
Methyldithiocarbamic acid, M-355
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3-Methyldodecane, M-401
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1,1′-(1-Methylene-1,3-propanediyl)bisbenzene, D-946
4-Methylene-1-(1-methylethyl)-2-cyclohexen-1-ol, M-124
4-Methylene-1-(1-methylethyl)-7-oxabicyclo[4.1.0]-heptane, E-165
4-Methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane, T-393
4-Methylene-1-(1-methylethyl)cyclohexene, M-119
3-Methylene-2-octanone, M-419
4-Methylene-2-pyrrolidinecarboxylic acid, M-421
4-Methylene-2-tetradecenal, M-422
24-Methylene-28,29-dinorcycloartan-3-one, M-368
24-Methylene-28-norcycloartan-3-one, C-450
24-Methylene-29-norcycloartan-3-ol, C-450
24-Methylene-29-norcycloartan-3-one, C-450
2-Methylene-4-oxoglutaric acid, M-420
2-Methylene-4-oxopentanedioic acid, M-420
2-Methylene-5-(1-methylethenyl)cyclohexanol, M-126
2-Methylene-5-(1-methylethyl)-3-cyclohexen-1-ol, M-125
3-Methylene-6-(1-methylethyl)-4-nitrocyclohexene, N-70
3-Methylene-6-(1-methylethyl)cyclohexene, M-118
24-Methylene-9,19-cyclolanostan-3-ol, M-404
3,3′-Methylenebis-4-hydroxycoumarin, D-165
8,8′-Methylenebiscatechin, M-402
S,*S*′-Methylenebiscysteine, D-997
2,2′-Methylenebisfuran, D-212
Methylenebis[2,5-dihydroxy-4-geranylgeranyl-3,6-benzoquinone], A-308
8,8′-Methylenebis[3,3′,4′,5,7-pentahydroxyflavan], M-402
2,2′-Methylenebis[3,6-dihydroxy-5-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)]-2,5-cyclohexadiene-1,4-dione, A-308
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3,3′-Methylenebis[4-hydroxy-5-methyl-2*H*-1-benzopyran-2-one], G-80
3,3′-Methylenebis[6-ethyl-4-hydroxy-5-methyl-2*H*-pyran-2-one], H-21
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24-Methylenecholest-5-en-3-ol, E-207
24-Methylenecholesta-5,7-diene-3,20-diol, E-215
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1,2-(Methylenedioxy)-4-(1-propenyl)benzene, I-160
6-[(3,4-Methylenedioxy)phenyl]-3,3-dimethyl-1-hexene, M-410
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3,4-Methylenedioxybenzoic acid, M-406
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3,4-Methylenedioxycinnamaldehyde, M-417
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7,8-Methylenedioxycoumarin, D-396
1,2-Methylenedioxynoraporphine, R-41
3,4-Methylenedioxyphenol, M-408
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3-(3,4-Methylenedioxyphenyl)-1,2-propanediol, M-416
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9-(3,4-Methylenedioxyphenyl)-2,4,8-nonatrienoic acid pyrrolidide, M-412
1-[9-(3,4-Methylenedioxyphenyl)-2,4,8-nonatrienoyl]pyrrolidine, M-412
5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoic acid, M-413
5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoic acid isobutylamide, P-395
5-(3,4-Methylenedioxyphenyl)-2,4-pentadienoic acid piperidide, P-402
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5-(3,4-Methylenedioxyphenyl)-2-pentenoic acid pyrrolidide, M-415
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2-(3,4-Methylenedioxyphenyl)-4(1*H*)-quinolinone, G-320
7-(3,4-Methylenedioxyphenyl)-6-heptenoic acid pyrrolidide, M-411
1-[7-(3,4-Methylenedioxyphenyl)-6-heptenoyl]piperidine, P-401
1-[7-(3,4-Methylenedioxyphenyl)-6-heptenoyl]pyrrolidine, M-411
1-[8-(3,4-Methylenedioxyphenyl)-7-octadecenoyl]-piperidine, P-403
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1-[7-(3,4-Methylenedioxyphenyl)heptadienoyl]piperidine, P-388
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Tetrahydro-5-methyl-2-furanone, D-301
2,3,4,5-Tetrahydro-5-methyl-5-(4-methyl-2-oxopentyl)-[2,3′-bifuran]-2′(5′*H*)-one, I-47
2,3,4,5-Tetrahydro-5-methyl-5-[(4-methyl-2-furanyl)methyl]-2,3′-bifuran, I-45
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1,2,3,4-Tetrahydro-6,7-dihydroxy-1-methylisoquinoline, T-77
1,2,3,4-Tetrahydro-6,7-dimethoxy-1-[(4-methoxyphenyl)methyl]-5-isoquinolinol, A-355
1,2,3,4-Tetrahydro-6,7-dimethoxy-2,2-dimethylisoquinolinium, T-78
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1,2,3,4-Tetrahydro-6,7-dimethoxy-2-methylisoquinoline, T-78
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2,3,6,7-Tetrahydro-6,7-dimethylcyclopent[*b*]azepin-8(1*H*)-one, T-79
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2,3,4,5-Tetrahydro-6-(5-methyl-2-furanyl)pyridine, T-103
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1,2,12,12*a*-Tetrahydro-6*a*-hydroxy-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano[3,4-*b*]furo[2,3-*h*]benzopyran-6(6*aH*)-one, R-57
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3,4,5,6-Tetrahydro-7,9,11-trihydroxy-2-methyl-2,6-epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, A-512
1,2,3,4-Tetrahydro-7-hydroxy-1-methyl-β-carboline, H-576
6,7,7*a*,8-Tetrahydro-7-methyl-5*H*-benzo[*g*]-1,3-benzodioxolo[6,5,4-*de*]quinoline, R-41
2,3,6,7-Tetrahydro-7-methylcyclopent[*b*]azepin-8(1*H*)-one, T-99
5,6,7,8-Tetrahydro-8,8-dimethyl-2-(1-methylethyl)-3,4-phenanthrenedione, M-722
1,2,12,12*a*-Tetrahydro-8,9-dimethoxy-2-(1-methylethenyl)-[1]benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6(6*aH*)-one, R-58
5,6,7,8-Tetrahydro-8-(4-hydroxy-3-methoxyphenyl)-3-methoxy-6,7-dimethyl-2-naphthalenol, G-327
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1,2,3,4-Tetrahydro-8-methoxy-2-methyl-6,7-methylenedioxyisoquinoline, H-320
1,2,3,4-Tetrahydro-8-methoxy-6-methyl-1,3-dioxolo[4,5-*g*]isoquinoline, H-320
4,6,7,13-Tetrahydro-9,10-dimethoxy-5-methylbenzo[*e*]1,3-dioxolo[4,5-*l*][2]benzazecin-12(5*H*)-one, C-375
1,2,3,4-Tetrahydro-9,11-dimethoxy-2-methylnaphth[2,1-*f*]isoquinoline-8,12-diol, L-96
6*a*,7,12,12*a*-Tetrahydro-9,11-dimethoxy-6,6-dimethyl-8-(3-methyl-2-butenyl)-6*H*-benzo[*b*]-naphtho[2,3-*d*]pyran-3-ol, H-139
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2,3,6,8-Tetrahydroxy-1-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, T-284
3,4,5,6-Tetrahydroxy-1-cyclohexene-1-methanol, H-579
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2,3,6,23-Tetrahydroxy-12-ursen-28-oic acid, T-291
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1,3,5,8-Tetrahydroxy-2,4-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one, T-172
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1,3,5,8-Tetrahydroxy-2,4-diprenylxanthone, T-172
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3,5,7,8-Tetrahydroxy-2-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, H-87
1,3,5,6-Tetrahydroxy-2-(3-methyl-2-butenyl)-9*H*-acridin-9-one, T-260
1,3,5,8-Tetrahydroxy-2-(3-methyl-2-butenyl)-xanthone, T-282
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3,5,6,7-Tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, P-136
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3,5,7,8-Tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, P-139
3,6,7,8-Tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, P-142
5,6,7,8-Tetrahydroxy-2-(4-hydroxyphenyl)-4*H*-1-

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4,4′,5,5′-Tetrahydroxy-2-(hydroxymethyl)-2′-methyl-[9,9′-bianthracene]-10,10′(9*H*,9′*H*)-dione, P-9
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1,3,5,8-Tetrahydroxy-2-prenylxanthone, T-282
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1,3,20,24-Tetrahydroxy-24-(hydroxymethyl)cycloartan-28-oic acid, T-215
1,3,22,24-Tetrahydroxy-24-(hydroxymethyl)cycloartan-28-oic acid, T-216
2,3,22,23-Tetrahydroxy-24-methyl-*B*-homo-7-oxacholestan-6-one, B-181
2,3,14,22-Tetrahydroxy-24-methylcholest-7-en-6-one, T-179
1,3,11,22-Tetrahydroxy-24-methylcholesta-5,24-dien-26-oic acid, T-175
2,3,14,22-Tetrahydroxy-24-methylcholesta-7,20-dien-6-one, T-176
3,5,9,14-Tetrahydroxy-24-methylcholesta-7,22-dien-6-one, T-178
1,3,24,31-Tetrahydroxy-24-methylcycloartan-28-oic acid, T-591
2,3,14,22-Tetrahydroxy-24-methylenecholest-7-en-6-one, T-177
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3,4′,5,7-Tetrahydroxy-3′,6,8-trimethoxyflavone, H-88
3,4′,5,7-Tetrahydroxy-3′,6-dimethoxyflavone, T-156
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3′,5,5′,7-Tetrahydroxy-4′-methoxyflavonol, P-159
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1,3,5,6-Tetrahydroxy-4-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, T-281
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3,6,8,9-Tetrahydroxy-7(11)-eremophilen-12,8-olide, T-174
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2′,4′,5,7-Tetrahydroxy-8-(4-hydroxy-3-methyl-2-butenyl)isoflavone, T-277
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1,3,5,6-Tetrahydroxy-9*H*-xanthen-9-one, T-296
1,3,6,7-Tetrahydroxy-9*H*-xanthen-9-one, T-297
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3′,4′,7-Trihydroxy-3,5-dimethoxyflavone, T-546
3′,4′,5-Trihydroxy-3,7-dimethoxy-6-prenylflavone, P-170
3′,4′,5-Trihydroxy-3,7-dimethoxyflavone 5-glucoside, P-134
5,6,7-Trihydroxy-3-(2,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one, H-214
5,6,7-Trihydroxy-3-(2-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-223
2,5,8-Trihydroxy-3-(3-methyl-2-butenyl)-1,4-naphthalenedione, T-690
1,4,5-Trihydroxy-3-(3-methyl-2-butenyl)-9*H*-xanthen-9-one, T-699
5,7,8-Trihydroxy-3-(4-hydroxybenzyl)-4-chromanone, T-589

5,7,8-Trihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, T-226
2,3,4-Trihydroxy-3-(hydroxymethyl)butanal, A-374
3′,4′,7-Trihydroxy-3-flavanol, T-181
3′,4,5′-Trihydroxy-3-isopentadienylstilbene, H-564
1,5,6-Trihydroxy-3-methoxy-2,4-diprenylxanthone, T-170
1,5,6-Trihydroxy-3-methoxy-4-prenylxanthone, T-281
4′,5,7-Trihydroxy-3-methoxy-6-prenylflavone, T-270
3′,4′,5-Trihydroxy-3-methoxy-7,8-methylenedioxyflavone, H-209
4′,5,6-Trihydroxy-3-methoxy-8-methylflavone, T-249
3′,4′,7-Trihydroxy-3-methoxyflavanone, T-189
3′,4′,7-Trihydroxy-3-methoxyflavanone, T-189
4′,5,7-Trihydroxy-3-methoxyflavanone, T-190
4′,6,7-Trihydroxy-3-methoxyflavone, T-207
4′,7,8-Trihydroxy-3-methoxyflavone, T-208
5,7,8-Trihydroxy-3-methoxyflavone, T-209
1,6,7-Trihydroxy-3-methoxyxanthone, T-297
1-(1,6,8-Trihydroxy-3-methyl-2-naphthalenyl)ethanone, A-100
1,5,8-Trihydroxy-3-methyl-2-prenylxanthone, T-282
1,2,8-Trihydroxy-3-methyl-9,10-anthracenedione, T-622
1,2,8-Trihydroxy-3-methylanthraquinone, T-622
2′,4′,6′-Trihydroxy-3-methylbutyrophenone, M-704
1,5,8-Trihydroxy-3-methylnaphthalene, M-507
1-(2,4,6-Trihydroxy-3-methylphenyl)ethanone, T-620
8,10,15-Trihydroxy-3-oxo-1,4,11(13)-germacratrien-12,6-olide, T-658
2,5,8-Trihydroxy-3-prenyl-1,4-naphthoquinone, T-690
2′,4,4′-Trihydroxy-3-prenylchalcone, T-679
1,4,5-Trihydroxy-3-prenylxanthone, T-699
2,4,6-Trihydroxy-3-[1-hydroxy-3-(4-hydroxyphenyl)-2-propenyl]phenyl β-D-glucopyranoside, P-455
1,4,5-Trihydroxy-3-[[3-(4-hydroxyphenyl)-1-oxo-2-propenyl]oxy]cyclohexanecarboxylic acid, C-368
3′,5,7-Trihydroxy-4′,5′,8-trimethoxyflavone, H-210
3′,5,7-Trihydroxy-4′,5′-dimethoxyflavone, P-135
3′,5′,7-Trihydroxy-4′,5,8-trimethoxyflavone, H-210
3′,5,7-Trihydroxy-4′,6,8-trimethoxyflavone, T-709
3,5,7-Trihydroxy-4′,6-dimethoxyflavanone, P-110
5,7,8-Trihydroxy-4′,6-dimethoxyflavone, P-143
3,3′,5-Trihydroxy-4′,7-dimethoxy-6-prenylflavone, P-170
2′,5,6′-Trihydroxy-4′,7-dimethoxy-8-prenylflavanone, P-167
3,3′,5-Trihydroxy-4′,7-dimethoxyflavan, P-104
3,3′,5-Trihydroxy-4′,7-dimethoxyflavanone, P-109
3,5,7-Trihydroxy-4′,8-dimethoxyflavone, T-548
2′,5,7-Trihydroxy-4′-methoxy-3′,8-diprenylisoflavanone, T-166
2′,4,6′-Trihydroxy-4′-methoxy-3′-prenylchalcone, T-263
2′,5,7-Trihydroxy-4′-methoxy-6-prenylisoflavone, T-276
3′,5,7-Trihydroxy-4′-methoxy-6-prenylisoflavone, T-279
3′,5,7-Trihydroxy-4′-methoxy-8-(4-hydroxyprenyl)isoflavone, G-55
2′,5,7-Trihydroxy-4′-methoxy-8-prenylisoflavanone, T-274
2,3′,6-Trihydroxy-4′-methoxybenzylcoumaranone, D-403
2′,4,6′-Trihydroxy-4′-methoxychalcone, T-147
3′,5,7-Trihydroxy-4′-methoxydihydroflavonol, P-109
3′,5′,7-Trihydroxy-4′-methoxyflavan, T-183
3′,5,7-Trihydroxy-4′-methoxyflavanone, T-614
5,7,3′-Trihydroxy-4′-methoxyflavanone, T-614
3,3′,7-Trihydroxy-4′-methoxyflavone, T-204
3,6,7-Trihydroxy-4′-methoxyflavone, T-207
3,5,7-Trihydroxy-4′-methoxyflavone, T-616
3′,5,7-Trihydroxy-4′-methoxyflavone, T-617
5,7,8-Trihydroxy-4′-methoxyflavone, T-619
3′,5,7-Trihydroxy-4′-methoxyflavonol, T-236
2′,5,7-Trihydroxy-4′-methoxyisoflavanone, T-220
2′,5,7-Trihydroxy-4′-methoxyisoflavone, T-222
3′,5,7-Trihydroxy-4′-methoxyisoflavone, T-224
3,3′,5-Trihydroxy-4′-methoxystilbene, D-621
2′,4,6′-Trihydroxy-4′-prenyloxychalcone, T-147
3,11,13-Trihydroxy-4(15),10(14)-guaiadien-12,6-olide, T-586
1,3,8-Trihydroxy-4,10(14),11(13)-germacratrien-12,6-olide, T-584
3β,7α,15α-Trihydroxy-4,4,14α-trimethyl-11-oxo-5α-chol-8-en-24-oic acid, L-109
3,6,12-Trihydroxy-4,4,8,14-tetramethyl-18-norpregnan-20-one, T-588
3,4′,5-Trihydroxy-4-, H-714
3,4′,5-Trihydroxy-4-(3-methyl-1-butenyl)stilbene, A-398
1,3,5-Trihydroxy-4-(3-methyl-2-butenyl)-9(10*H*)-acridinone, T-677
4′,5,7-Trihydroxy-4-flavanol, T-185
2,7,8-Trihydroxy-4-isopropyl-6-methyl-1-naphthalenecarboxaldehyde, T-527
1,3,5-Trihydroxy-4-methoxy-10-methylacridone, T-135
2′,4′,6′-Trihydroxy-4-methoxychalcone, T-147
2′,4′,6′-Trihydroxy-4-methoxydihydrochalcone, H-752
1,3,8-Trihydroxy-4-methyl-2,7-bis(3-methyl-2-butenyl)-9*H*-xanthen-9-one, T-629
1,3,8-Trihydroxy-4-methyl-2,7-diprenylxanthone, T-629
1,3,5-Trihydroxy-4-prenylacridone, T-677
3,6*a*,9-Trihydroxy-4-prenylpterocarpan, T-692
3,4′,5-Trihydroxy-4-prenylstilbene, A-399
3β,16β,20*S*-Trihydroxy-5α-pregnane-20-carboxylic acid 22,16-lactone, L-129
2′,3,5-Trihydroxy-5′,7-dimethoxyflavanone, P-107
3′,5,7-Trihydroxy-5′-methoxyflavanone, T-192
2,3,23-Trihydroxy-5,12-oleanadien-28-oic acid, T-642
3,4,4′-Trihydroxy-5,5′-diisopropyl-2,2′-dimethylbiphenyl, T-154
3′,4′,7-Trihydroxy-5,5′-dimethoxyflavone, P-135
1,7,13-Trihydroxy-5,6,11,12,17,18-trinaphthylenehexone, T-816
3,4,5-Trihydroxy-5-(3-methyl-2-butenyl)-2-(3-methyl-1-oxobutyl)-2-cyclopenten-1-one, O-258
3,5,6-Trihydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-one, T-593
1,3,6-Trihydroxy-5-methoxy-10-methyl-2-prenylacridone, T-260
1,3,6-Trihydroxy-5-methoxy-10-methylacridine, T-136
2′,4′,7-Trihydroxy-5-methoxy-3′,6-diprenylisoflavan, T-164
1,3,6-Trihydroxy-5-methoxy-4-prenylxanthone, T-281
1,4,6-Trihydroxy-5-methoxy-7-prenylxanthone, T-283
2′,4′,7-Trihydroxy-5-methoxy-8-prenylisoflavone, T-277
3′,4′,7-Trihydroxy-5-methoxyflavonol, T-235
2′,4′,7-Trihydroxy-5-methoxyisoflavone, T-222
1,3,6-Trihydroxy-5-methoxyxanthone, T-296
2′,4,4′-Trihydroxy-6′-methoxy-3′,5′-diprenylchalcone, T-161
2′,4,4′-Trihydroxy-6′-methoxy-3′-prenylchalcone, T-263
2′,4,4′-Trihydroxy-6′-methoxy-3′-prenyldihydrochalcone, T-263
2′,4′,7-Trihydroxy-6′-methoxy-3′-prenylisoflavone, T-278
2′,4,4′-Trihydroxy-6′-methoxychalcone, T-147
2′,4,4′-Trihydroxy-6′-methoxydihydrochalcone, H-752
3,4′,5-Trihydroxy-6′-methyldibenzo-α-pyrone, A-192
3′,4′,5-Trihydroxy-6,7,8-trimethoxyflavanone, H-203
3′,4′,5-Trihydroxy-6,7,8-trimethoxyflavone, H-211
1,3,5-Trihydroxy-6,7-dimethoxy-2-methylanthraquinone, P-162
4′,5,7-Trihydroxy-6,8-dimethoxyflavone, P-143
4′,5,7-Trihydroxy-6-(2-hydroxy-3-methyl-3-butenyl)isoflavone, T-688
3,8,10-Trihydroxy-6-(2-methyl-1-propenyl)-6*H*,7*H*-[1]benzopyrano[4,3-*b*]benzopyran-7-one, C-443
4′,5,7-Trihydroxy-6-(4-hydroxy-3-methyl-2-butenyl)isoflavone, T-688
1,3,8-Trihydroxy-6-hydroxymethylanthraquinone, T-590
1,2,8-Trihydroxy-6-methoxy-3-methylanthraquinone, T-246
3′,4′,6-Trihydroxy-6-methoxyaurone, T-137
3,5,7-Trihydroxy-6-methoxyflavanone, T-193
4′,5,7-Trihydroxy-6-methoxyflavonol, T-240
1,3,7-Trihydroxy-6-methoxyxanthone, T-297
2,3,4-Trihydroxy-6-methyl-5-(3,7,11-trimethyl-2,6,10-dodecatrienyl)benzaldehyde, S-60
1,3,8-Trihydroxy-6-methyl-9(10*H*)-anthracenone, T-245
1,2,5-Trihydroxy-6-methyl-9,10-anthracenedione, T-621
1,3,7-Trihydroxy-6-methyl-9,10-anthracenedione, T-623
1,3,8-Trihydroxy-6-methyl-9,10-anthracenedione, T-624
1,2,5-Trihydroxy-6-methylanthraquinone, T-621
1,3,7-Trihydroxy-6-methylanthraquinone, T-623
1,3,8-Trihydroxy-6-methylanthraquinone, T-624
4′,5,7-Trihydroxy-6-methylflavone, T-632
1,3,4-Trihydroxy-6-oxabicyclo[3.2.1]octan-7-one, Q-10
4′,5,7-Trihydroxy-6-prenylflavanone, T-682
4′,5,7-Trihydroxy-6-prenylflavonol, T-270
4′,5,7-Trihydroxy-6-prenylisoflavone, T-688
1,3,9-Trihydroxy-6*H*-benzofuro[3,2-*c*]benzopyran-6-one, T-537
2,3,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, T-538
3,4,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, T-539
3,7,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, T-540
3,8,9-Trihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, T-541
15α,26,27-Trihydroxy-7α-methoxy-8,24-lanostadien-3-one, T-229
24,25,26-Trihydroxy-7α-methoxy-8-lanosten-3-one, T-230
3,6,8-Trihydroxy-7(11)-eremophilen-12,8-olide, T-561
3,6,9-Trihydroxy-7(11)-eremophilen-12,8-olide, T-562
3β,12β,28-Trihydroxy-7,11,15-trioxo-25,26,27-trisnorlanost-8-en-24-oic acid, L-108
3,12,23-Trihydroxy-7,11,15-trioxolanosta-8,24-dien-26-oic acid, T-159
2′,4′,5-Trihydroxy-7,8-[2-(1-methylethenyl)furo]isoflavone, D-615
13,14,15-Trihydroxy-7-labdene, L-16
3,5,6-Trihydroxy-7-megastigmen-9-one, T-613
1,3,6-Trihydroxy-7-methoxy-2,5,8-triprenylxanthone, T-289
1,3,6-Trihydroxy-7-methoxy-2,8-diprenylxanthone, T-173
2′,4′,5-Trihydroxy-7-methoxy-3′,6-diprenylisoflavanone, T-165
2′,4′,5-Trihydroxy-7-methoxy-3′,6-diprenylisoflavone, T-167
2′,4′,5-Trihydroxy-7-methoxy-3-prenylflavone, T-266
11,12,14-Trihydroxy-7-methoxy-8,11,13-abietatrien-20,6-olide, R-54
2′,4′,5-Trihydroxy-7-methoxy-8-prenylflavone, T-268
2′,4′,5-Trihydroxy-7-methoxyflavanone, T-186
3,3′,4′-Trihydroxy-7-methoxyflavanone, T-189
3′,5,5′-Trihydroxy-7-methoxyflavanone, T-192
2′,4′,5-Trihydroxy-7-methoxyflavone, T-202
3,5,8-Trihydroxy-7-methoxyflavone, T-209
4′,5,6-Trihydroxy-7-methoxyflavone, T-210
4′,5,8-Trihydroxy-7-methoxyflavone, T-211
3′,4′,5-Trihydroxy-7-methoxyflavone, T-615
4′,5,8-Trihydroxy-7-methoxyflavonol, P-139
3′,4′,5-Trihydroxy-7-methoxyflavonol, T-234

2′,4′,5-Trihydroxy-7-methoxyisoflavanone, T-220
2′,4′,5-Trihydroxy-7-methoxyisoflavone, T-222
3′,4′,5-Trihydroxy-7-methoxyisoflavone, T-224
1,3,6-Trihydroxy-7-methoxyxanthone, T-297
1,4,6-Trihydroxy-7-methylanthraquinone, T-625
3,4,5-Trihydroxy-7-oxabicyclo[4.1.0]heptane-2-methanol, C-494
3′,4′,6-Trihydroxy-7-prenylaurone, T-678
7,11,12-Trihydroxy-8,11,13-abietatrien-20,6-olide, R-54
6,11,12-Trihydroxy-8,11,13-abietatrien-20,7-olide, C-117
4′,5,7-Trihydroxy-8-(2-hydroxy-3-methyl-3-butenyl)flavone, T-685
4′,5,7-Trihydroxy-8-(3-hydroxy-3-methylbutyl)isoflavone, T-689
4′,5,7-Trihydroxy-8-(4-hydroxyprenyl)isoflavone, G-55
13,14,15-Trihydroxy-8-labdene, L-17
3,5,7-Trihydroxy-8-methoxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one, T-548
3,5,7-Trihydroxy-8-methoxyflavone, T-209
4′,5,7-Trihydroxy-8-methoxyflavone, T-211
4′,5,7-Trihydroxy-8-methoxyflavonol, T-242
4′,5,7-Trihydroxy-8-methylflavanone, T-631
4′,5,6-Trihydroxy-8-methylflavonol, T-249
4′,5,7-Trihydroxy-8-methylisoflavanone, T-633
2′,4′,7-Trihydroxy-8-prenylflavan, T-680
4′,5,7-Trihydroxy-8-prenylflavanone, T-683
4′,5,7-Trihydroxy-8-prenylflavone, T-685
4′,5,7-Trihydroxy-8-prenylflavonol, T-272
2′,4′,7-Trihydroxy-8-prenylisoflavanone, T-274
4′,5,7-Trihydroxy-8-prenylisoflavone, T-689
3,7,15-Trihydroxy-8-scirpenone, T-706
1,2,3-Trihydroxy-9(10*H*)-acridinone, T-513
1,3,5-Trihydroxy-9(10*H*)-acridinone, T-514
1,3,6-Trihydroxy-9(10*H*)-acridinone, T-515
11,12,13-Trihydroxy-9,15-octadecadienoic acid, T-637
2,6,7-Trihydroxy-9-methyl-4-dibenzofurancarboxylic acid, T-628
5,8,12-Trihydroxy-9-octadecenoic acid, T-640
1,3,7-Trihydroxy-9*H*-xanthen-9-one, T-724
α,3,4-Trihydroxyacetophenone, T-511
2,3′,4′-Trihydroxyacetophenone, T-511
2′,4′,6′-Trihydroxyacetophenone, T-512
1,2,3-Trihydroxyacridone, T-513
1,3,5-Trihydroxyacridone, T-514
1,3,6-Trihydroxyacridone, T-515
1,2,10-Trihydroxyaporphine, T-516
2,4,5-Trihydroxybenzaldehyde, T-517
3,4,5-Trihydroxybenzaldehyde, T-518
1,2,3-Trihydroxybenzene, B-24
1,3,5-Trihydroxybenzene, B-25
α,3,4-Trihydroxybenzenepropanoic acid, D-641
3,4,5-Trihydroxybenzenepropanoic acid, T-667
2,4,6-Trihydroxybenzoic acid, T-519
3,4,5-Trihydroxybenzoic acid, T-520
2,4,6-Trihydroxybenzophenone, T-521
3,4,5-Trihydroxybenzoyl glucoside, G-46
3,4,5-Trihydroxybenzyl alcohol, H-559
2′,3,5-Trihydroxybibenzyl, D-638
3,3′,5-Trihydroxybibenzyl, D-639
3,4′,5-Trihydroxybiphenyl, B-93
3,12,14-Trihydroxybufa-4,20,22-trienolide, T-526
1-(1,3,4-Trihydroxybutyl)-9*H*-pyrido[3,4-*b*]indole, P-603
1-[5-(2,3,4-Trihydroxybutyl)pyrazinyl]-1,2,3,4-butanetetrol, T-140
1-[6-(2,3,4-Trihydroxybutyl)pyrazinyl]-1,2,3,4-butanetetrol, T-141
2′,4′,5′-Trihydroxybutyrophenone, T-663
3,5,14-Trihydroxycard-20(22)-enolide, T-528
3,11,14-Trihydroxycard-20(22)-enolide, T-529
3,14,19-Trihydroxycard-20(22)-enolide, T-530
2,4,4′-Trihydroxychalcone, T-533
2′,4,4′-Trihydroxychalcone, T-534
2′,4′,6′-Trihydroxychalcone, T-535
3,7,12-Trihydroxycholan-24-oic acid, T-536
N-(3,7,12-Trihydroxycholan-24-oyl)taurine, T-29
3,4,5-Trihydroxycinnamaldehyde, T-671
3,4,5-Trihydroxycinnamic acid, T-672
3′,4′,5′-Trihydroxycinnamyl alcohol, T-674
5,6,7-Trihydroxycoumarin, T-522
6,7,8-Trihydroxycoumarin, T-523
1,3,9-Trihydroxycoumestan, T-537
2,3,9-Trihydroxycoumestan, T-538
6,7,12-Trihydroxycoumestan, T-538
3,4,9-Trihydroxycoumestan, T-539
3,7,9-Trihydroxycoumestan, T-540
7,10,12-Trihydroxycoumestan, T-540
3,8,9-Trihydroxycoumestan, T-541
7,11,12-Trihydroxycoumestan, T-541
16,20,25-Trihydroxycucurbit-5-ene-2,3,11,22-tetrone, T-151
3,7,25-Trihydroxycucurbita-5,23-dien-19-al, T-543
16,20,25-Trihydroxycucurbita-5,23-diene-2,3,11,22-tetrone, T-151
3,7,23-Trihydroxycucurbita-5,24-dien-19-al, T-542
3β,11α,15α-Trihydroxycycloart-24*E*-en-26-oic acid, A-326
3,6,20-Trihydroxydammar-24-en-12-one, D-18
2,3,4-Trihydroxydibenzofuran, D-130
1,2,3-Trihydroxydibenz[*cd,f*]indol-4(5*H*)-one, T-544
1,2,10-Trihydroxydihydro-*trans*-linalyl oxide 7-*O*-β-D-glucopyranoside, H-534
2′,4′,6′-Trihydroxydihydrochalcone, P-322
3,4,5-Trihydroxydihydrocinnamic acid, T-667
3′,4′,7-Trihydroxydihydroflavonol, T-189
4′,5,7-Trihydroxydihydroflavonol, T-190
5,6,7-Trihydroxydihydroflavonol, T-193
3,5,9-Trihydroxyergost-7-en-6-one, E-200
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid, T-563
3,5,9-Trihydroxyergosta-7,22-dien-6-one, E-200
3,22,23-Trihydroxyergostan-6-one, T-564
3,4,4′-Trihydroxyflavan, T-565
4′,5,7-Trihydroxyflavan, T-566
4′,5,7-Trihydroxyflavanol, T-184
3,4′,7-Trihydroxyflavanone, T-567
3,5,7-Trihydroxyflavanone, T-568
4′,5,7-Trihydroxyflavanone, T-569
4′,5,8-Trihydroxyflavanone, T-570
4′,7,8-Trihydroxyflavanone, T-571
5,6,7-Trihydroxyflavanone, T-572
5,7,8-Trihydroxyflavanone, T-573
5,7,8-Trihydroxyflavanone 7-glucoside, T-573
4′,5,7-Trihydroxyflavanone(3 → 8)-3,4′,5,7-tetrahydroxyflavanone, H-83
2′,5,6-Trihydroxyflavone, T-574
3,3′,4′-Trihydroxyflavone, T-575
3′,4′,5′-Trihydroxyflavone, T-576
3,4′,7-Trihydroxyflavone, T-577
3′,4′,7-Trihydroxyflavone, T-578
3′,5,6-Trihydroxyflavone, T-579
3,5,7-Trihydroxyflavone, T-580
4′,5,7-Trihydroxyflavone, T-581
5,6,7-Trihydroxyflavone, T-582
4′,5,7-Trihydroxyflavone(3′ → 8)-4′,5,7-trihydroxyflavone, A-206
3′,4′,7-Trihydroxyflavonol, T-204
4′,5,7-Trihydroxyflavonol, T-206
4′,6,7-Trihydroxyflavonol, T-207
4′,7,8-Trihydroxyflavonol, T-208
5,7,8-Trihydroxyflavonol, T-209
3,22,26-Trihydroxyfurostan-12-one, T-583
2,4,6-Trihydroxyisobutyrophenone, M-705
2′,4′,7-Trihydroxyisoflavan, T-594
2′,4′,7-Trihydroxyisoflavanone, T-595
3′,4′,7-Trihydroxyisoflavanone, T-596
4′,5,7-Trihydroxyisoflavanone, T-597
2′,4′,7-Trihydroxyisoflavone, T-598
2′,5,7-Trihydroxyisoflavone, T-599
3′,4′,7-Trihydroxyisoflavone, T-600
4′,5,7-Trihydroxyisoflavone, T-601
4′,6,7-Trihydroxyisoflavone, T-602
4′,7,8-Trihydroxyisoflavone, T-603
2,4,6-Trihydroxyisovalerophenone, M-704
3,15,22-Trihydroxylanosta-7,9(11),24-trien-26-oic acid, T-611
15,26,27-Trihydroxylanosta-7,9(11),24-trien-3-one, T-612
24,25,26-Trihydroxylanosta-7,9(11)-dien-3-one, L-37
3,7,15-Trihydroxylanosta-8,24-dien-26-oic acid, T-608
3,7,22-Trihydroxylanosta-8,24-dien-26-oic acid, T-609
3,26,27-Trihydroxylanosta-8,24-dien-7-one, T-610
1,4,5-Trihydroxynaphthalene, N-9
1,2,3-Trihydroxynortropane, A-521
1,2,4-Trihydroxynortropane, A-522
1,2,7-Trihydroxynortropane, A-523
9,10,13-Trihydroxyoctadecanoic acid, T-638
9,10,18-Trihydroxyoctadecanoic acid, T-639
3,4,5-Trihydroxypentanoic acid 1,4-lactone, D-265
3,4,5-Trihydroxyphenacyl alcohol, T-133
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3,4,6-Trihydroxyphenanthrene, P-250
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Crassostrea Secocarotenoid, S-63
7,7′,8,8′-Tetrahydro-β,β-carotene-3,3′-diol, Z-9
7,7′,8,8′-Tetrahydro-β,β-carotene, C-119
2,6,11,15-Tetramethyl-2,4,6,8,10,12,14,16-octadecaoctaenedioic acid; (all-*E*)-*form*; 18-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenoyl) ester, 1-Me ester, T-306
Valenciachrome, V-3
Valenciaxanthin; (9*E*)-*form*, V-4
Valenciaxanthin; (9*Z*)-*form*, V-4
Xantofyl palmitate, INN, L-124
α-Zeacarotene, Z-4
Zeaxanthin; (3*R*,3′*R*, *all-E*)-*form*, Z-9

Natural food colourants (chlorophylls)

Chlorophyll a, C-216
Chlorophyll b, C-217
Chlorophyll c, C-218
Chlorophyll d, C-219
Brassica napus Fluorescent chlorophyll catabolite, F-51
Capsicum annuum Fluorescent chlorophyll catabolite, F-51
Bn-NCC-1, N-18

Bn-NCC-2, N-18
So-NCC-2, R-60
Bn-NCC-3, N-18
Phaeophorbide b, P-237
Pyrophaeophorbide a, P-613
RP 14, R-60

Food lipids (saturated fatty acids)

Arachidonic acid, E-17
Butanoic acid, B-218
Butter acids, B-232
Butyl pentanoate, P-190
2-*O*-Caffeoylhydroxycitric acid, D-675
Catelaidic acid, D-1007
Cetoleic acid, D-1007
2-*O*-*p*-Coumaroylhydroxycitric acid, D-675
Cyclohexaneundecanoic acid, C-464
4,6-Decadiyn-1-ol isovalerate, D-38
Decanoic acid, D-41
1,5-Dibutyl methyl hydroxycitrate, D-675
1,2-Dihydroxy-1,2,3-propanetricarboxylic acid; (1*S*,2*S*)-*form*; γ-Lactone, dibutyl ester, D-675
10,20-Dihydroxyeicosanoic acid, D-448
15,16-Dihydroxyoctadecanoic acid; (+)-*form*, D-566
Dodecanoic acid, D-1016
Eicosanoic acid, E-15
Ethyl 2-methylbutyrate, M-330
Ethyl octanoate, O-80
Ethyl pentanoate, P-190
2-Ethylheptanoic acid; (ξ)-*form*, E-309
2-Ethylhexanoic acid, E-314
4-Ethyloctanoic acid; (ξ)-*form*, E-345
FEMA 2719, M-330
2-*O*-Feruloylhydroxycitric acid, D-675
Garcinia acid, D-675
10,12-Heptacosanedione, H-44
9-Heptadecenoic acid; (*Z*)-*form*, H-74
Heraclenol; (*R*)-*form*; 2′-*O*-(3-Methyl-2-butenoyl), H-125
Heraclenol; (*R*)-*form*; 2′-*O*-(3-Methylbutanoyl), H-125
Hexadecanamide, 9CI, H-159
Hexadecanoic acid, H-159
Hexanedioic acid, H-227
2-Hydroxy-22-methyltetracosanoic acid, H-617
4-Hydroxy-3-methoxybenzyl 7-methyloctanoate, D-400
4-Hydroxy-3-methoxybenzyl 8-methylnonanoate, D-400
12-Hydroxy-8,10-octadecadienoic acid, H-641
11-Hydroxy-9,15,16-trioxooctadecanoic acid; (-)-*form*, H-816
13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid, D-595
3-Hydroxybutanoic acid; (*R*)-*form*; *O*-[α-L-Arabinopyranosyl-(1 → 6)-β-D-glucopyranoside], butyl ester, H-374
3-Hydroxybutanoic acid; (*S*)-*form*; *O*-[α-L-Arabinopyranosyl-(1 → 6)-β-D-glucopyranoside], butyl ester, H-374
9-Hydroxydecanoic acid, H-395
7-Hydroxyhexadecanedioic acid; (ξ)-*form*, H-488
8-Hydroxyhexadecanedioic acid; (ξ)-*form*, H-489
2-Hydroxyhexadecanoic acid; (*R*)-*form*, H-490
3-Hydroxynonanoic acid; (±)-*form*, H-627
3-Hydroxyoctanoic acid; (ξ)-*form*; Et ester, *O*-[β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranoside], H-651
3-Hydroxyoctanoic acid; (*R*)-*form*, H-651
6-Hydroxypentadecanedioic acid, H-702
10-Hydroxytetradecanoic acid; Me ester, H-798
Mangiferic acid, O-23
Methyl 15-cyanopentadecanoate, H-158
Methyl octanoate, O-80
Methyl pentanoate, P-190
4-Methyl-2-oxopentanoic acid, M-533
2-Methylbutanoic acid; (±)-*form*, M-330
2-Methylbutanoic acid; (*S*)-*form*, M-330
3-Methylbutanoic acid, M-331
2-Methylbutyl 2-methylbutanoate, M-330
8-Methyldecanoic acid; (ξ)-*form*, M-389
9-Methyldecanoic acid, M-390
16-Methylheptadecanoic acid, M-458
11-Methylhexadecanoic acid; (±)-*form*, M-473
14-Methylhexadecanoic acid; (*S*)-*form*, M-474
16-Methyloctadecanoic acid; (ξ)-*form*, M-516
17-Methyloctadecanoic acid; (ξ)-*form*, M-517
14-Methylpentadecanoic acid, M-538
12-Methyltridecanoic acid, M-700
Octadecanamide, O-26
Octadecanoic acid, O-26
Octanoic acid, O-80
Oryzarol, M-273
2-Oxo-4-methylenepentanedioic acid, O-228
3-Oxodecanoic acid glycerides, O-194
3-Oxododecanoic acid glycerides, O-194
3-Oxohexadecanoic acid glycerides, O-194
2-Oxohexanedioic acid, O-224
3-Oxohexanoic acid glycerides, O-194
3-Oxooctanoic acid glycerides, O-194
3-Oxotetradecanoic acid glycerides, O-194
Paullinic acid, E-24
9-Pentadecenoic acid, P-83
2,3,7,11,15-Pentamethylhexadecanoic acid, P-179
2,2,6,10,14-Pentamethylpentadecanoic acid, P-180
Pentanoic acid, P-190
Petroselinic acid, O-41
Phaseolic acid, P-240
2-Phenylethyl 2-methylbutanoate, P-273
Phloionolic acid, T-639
1-Phytanoic acid; (3*R*,7*R*,11*R*)-*form*, P-357
Tetradecanoic acid, T-59
Tetrahydro-6-nonyl-2*H*-pyran-2-one, 9CI, H-797
Tetrahydro-6-propyl-2*H*-pyran-2-one; (ξ)-*form*, T-122
2,6,10,14-Tetramethylpentadecanoic acid, T-311
Triacontanoic acid, T-442

Food lipids (unsaturated fatty acids)

AF Toxin II, A-133
Anacardic acid, H-701
Angelic acid, M-340
6′-Apo-ψ-caroten-6′-al; (7*Z*,9*Z*,9′*Z*)-*form*; 6′-Carboxylic acid, Me ester, A-378
6′-Apo-ψ-caroten-6′-al; (*all-E*)-*form*, A-378
Araliacerebroside, A-284
AS 1-1, A-281
AS 1-2, A-281
Asclepic acid, O-46
Butter acids, B-232
Butyl heptanoate, H-93
Calendic acid, O-33
Capsianoside I, D-662
Capsianoside IV, H-754
Capsianoside V, T-675
Cibaric acid, D-593
Cinnatriacetin A, H-799
Cinnatriacetin B, H-799
Clupanodonic acid, D-998
Colneleic acid; (2′*E*,4′*Z*,8*E*)-*form*, C-327
Colnelenic acid; (2′*E*,4′*Z*,7′*Z*,8*E*)-*form*, C-328
Corchorifatty acid F, T-636
Coronaric acid, E-174
Corticrocin, T-57
Crotonic acid, B-223
7-Cyano-2-heptene-4,6-diynoic acid, O-94
2-Decene-4,6,8-triynoic acid; (*Z*)-*form*; Me ester, D-55
3-Decenoic acid, D-58
4-Decenoic acid, D-59
9-Decenoic acid, D-62
Dihydro-5-(2-octenyl)-2(3*H*)-furanone, D-337
2,3-Dihydroxy-4-decynoic acid, D-424
9,10-Dihydroxy-8-oxo-12-octadecenoic acid; (9*R*,10*S*,12*Z*)-*form*, D-594
4,8-Dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoic acid; (2*E*,4*Z*,6*E*,8*E*,10*E*)-*form*; Me ester, D-865
α-Dimorphecolic acid, H-640
4,8,12,15,19-Docosapentaenoic acid, D-1003
7,10,13-Docosatrienoic acid; (*all-Z*)-*form*, D-1004
13,16,19-Docosatrienoic acid; (*all-Z*)-*form*, D-1005
3,6-Dodecadien-1-ol; (*Z*,*Z*)-*form*, D-1013
8-Dotriacontenoic acid, D-1048
Elaidic acid, O-44
12,13-Epoxy-11-hydroxy-9,15-octadecadienoic acid; (9*Z*,11*R*,12*S*,13*S*,15*Z*)-*form*, E-133
Ethyl heptanoate, H-93
1,3,6,10-Farnesatetraene; (3*E*,6*E*)-*form*, F-6
1,3,6,10-Farnesatetraene; (3*Z*,6*E*)-*form*, F-6
1,3(15),6,10-Farnesatetraene; (*E*)-*form*, F-7
FEMA 2709, H-249
FEMA 3169, H-249
FEMA 3342, H-250
FEMA 3364, H-250
FEMA 3954, N-120
Gondoic acid, E-23
Goshuyic acid, T-55
Heptanoic acid, H-93
3-Hexadecenoic acid; (*E*)-*form*, H-162
11-Hexadecenoic acid; (*E*)-*form*, H-166
3-Hexenoic acid, H-250
Hydroxy-α-sanshool, D-1021
Hydroxy-γ-isosanshool, T-62
Hydroxy-γ-sanshool, T-62
9-Hydroxy-10,12,15-octadecatrienoic acid; (9*S*,10*E*,12*Z*,15*Z*)-*form*, H-646
8-Hydroxy-2,4,6-octatriynamide, H-656
10-Hydroxy-2,8-decadiene-4,6-diynoic acid; (*E*,*E*)-*form*, H-392
10-Hydroxy-2,8-decadiene-4,6-diynoic acid; (*Z*,*Z*)-*form*; Me ester, H-392
10-Hydroxy-2-decene-4,6-diynoic acid; (*E*)-*form*, H-397
8-Hydroxy-2-octene-4,6-diynoic acid; (*E*)-*form*, H-657
2-(5-Hydroxy-2-pentenyl)-3-oxocyclopentaneacetic acid; (3ξ,7ξ)-*form*; *O*-β-D-Glucopyranoside, Et ester, H-709
2-(5-Hydroxy-2-pentenyl)-3-oxocyclopentaneacetic acid; (3*R*,7*S*)-*form*; *O*-β-D-Glucopyranoside, Me ester, H-709
2-(5-Hydroxy-2-pentenyl)-3-oxocyclopentaneacetic acid; (3*R*,7*S*)-*form*; *O*-β-D-Glucopyranoside, H-709
4-Hydroxy-3-methoxybenzyl 8-methyl-6-nonenoate, D-400
2-Hydroxy-6-(8,11,14-pentadecatrienyl)benzoic acid, 9CI, H-701
2-Hydroxy-6-(8-pentadecenyl)benzoic acid, 9CI, H-701
2-Hydroxy-6-tridecylbenzoic acid, H-809
10-Hydroxy-8-decene-4,6-diynoic acid; (*Z*)-*form*, H-398
10-Hydroxy-8-decenoic acid; (*E*)-*form*, H-399
17-Hydroxy-9,11,13,15-octadecatetraynoic acid; (*S*)-*form*, H-644
11-Hydroxy-9-tridecenoic acid, H-808
15-Hydroxylinoleic acid, H-642
2-Hydroxylinolenic acid, H-645
3-(4-Hydroxyphenyl)-2-propenoic acid; (*Z*)-*form*; *O*-(3,7-Dimethyl-2,6-octadienyl), Me ester, H-748
N-Isobutyl-2,4,8,10,12-tetradecapentaenamide, T-62
N-Isobutyl-2,8-dodecadienamide, D-1012
Isotriglochinin, T-510
Linoleic acid, O-22
Linolenelaidic acid, O-35
γ-Linolenic acid, O-32
α-Linolenic acid, O-35
Lumequic acid, T-443
Methyl 6′-apo-9′*Z*-lycopen-6′-oate, A-378
Methyl apo-6′-lycopenate, A-378
14-Methyl-6-pentadecenoic acid; (*Z*)-*form*, M-540
2-Methylene-4-oxopentanedioic acid, M-420
Myristoleic acid, T-67

Neoherculin, D-1021
Nervonic acid, T-51
3-Nonenoic acid; (ξ)-*form*, N-121
2-Nonenoic acid, N-120
11,13-Octadecadien-9-ynoic acid; (*E,E*)-*form*, O-24
4,8,12,15-Octadecatetraenoic acid, O-29
10,14,16-Octadecatrien-12-ynoic acid; (10*Z*,14*E*,16*E*)-*form*, O-36
15-Octadecene-9,11,13-triynoic acid, O-39
13-Octadecenoic acid; (*Z*)-*form*, O-48
5-Octadecynoic acid, O-53
2,4,6-Octatriynoic acid, O-87
Oleic acid, O-44
15-Oxo-11-eicosenoic acid; (*Z*)-*form*, O-209
10′-Oxo-6,10′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-205
6′-Oxo-6,5′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-202
6′-Oxo-6,6′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-203
8′-Oxo-6,8′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-204
10-Oxo-8-decenoic acid; (*E*)-*form*, O-201
4-Oxo-9,11,13,15-octadecatetraenoic acid; (9*Z*,11*E*,13*E*,15*Z*)-*form*, O-234
13-Oxo-9,11-tridecadienoic acid, O-253
13-Oxo-9-octadecenoic acid; (*Z*)-*form*, O-235
Palmitoleic acid, H-165
Punicic acid, O-34
Raphanusol B, T-672
Ricinoleic acid, H-648
Sanshoamide, D-1020
Sciadonic acid, E-21
Soyacerebroside I, A-281
Soyacerebroside II, A-281
Stearidonic acid, O-30
5,8-Tetradecadienoic acid; (*Z,Z*)-*form*; Et ester, T-55
5,8-Tetradecadienoic acid; (*Z,Z*)-*form*; Me ester, T-55
2,6,11,15-Tetramethyl-2,4,6,8,10,12,14,16-octadecaoctaenedioic acid; (all-*E*)-*form*; 18-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenoyl) ester, 1-Me ester, T-306
Traumatin, O-208
Triglochinin, T-510
9,12,13-Trihydroxy-10-octadecenoic acid; (9*S*,10*E*,12*S*,13*S*)-*form*, T-641
9,12,13-Trihydroxy-10-octadecenoic acid, T-641
Tuberceramide, A-282
Vaccenic acid, O-46
Ximenic acid, H-154

Food lipids (oxidation products)

Cryptocapsone, C-122
α-Dimorphecolic acid, H-640
3-(3-Ethyloxiranyl)-2-propenal, 9CI, H-80
Fabatin, F-1
13-Hydroxy-10-oxo-11-octadecenoic acid; (±)-(*E*)-*form*, H-691
4-Hydroxy-2-nonenal, H-630
2-Hydroxy-6-(8-tridecenyl)benzoic acid, H-809
Methyl α-linolenate hydroperoxides, M-284
2,4-Nonadienal; (2*E*,4*E*)-*form*, N-96
8-Nonen-2-one, N-130
8-Nonen-3-one, N-131
6-Pentyl-2*H*-pyran-2-one, P-218
2-Pentylfuran, P-214
14-Pentyloxacyclotetradec-11-ene-2,11-dione, H-691
Sissotrin, D-542
Tetrahydro-6-nonyl-2*H*-pyran-2-one, 9CI, H-797
Tetrahydro-6-pentyl-2*H*-pyran-2-one, T-116
3′,4′,5-Trihydroxy-3,7-dimethoxyflavone 5-glucoside, P-134

Food lipids (diacylglycerols)

1,2-Di-*O*-(8-hexadecenoyl)-3-*O*-(6-sulfoquinovopyranosyl)glycerol, G-239
1,2-Di-*O*-myristoyl-3-*O*-(6-sulfoquinovopyranosyl)glycerol, G-239
1,2-Di-*O*-palmitoyl-3-*O*-(6-sulfoquinovopyranosyl)glycerol, G-239
1-*O*-β-D-Glucopyranosyl-2,3-di-*O*-(8-hexadecenoyl)glycerol, G-239
1-*O*-β-D-Glucopyranosyl-2,3-di-*O*-palmitoylglycerol, G-239
Glycerol 1,2-di-(9*Z*-octadecenoate), G-239
Glycerol 1,2-dioctadecanoate, G-239
Glycerol 2-(9*Z*,12*Z*-octadecadienoate) 1-hexadecanoate; 3-*O*-[α-D-Galactopyranosyl-(1 → 6)-β-D-galactopyranoside], G-239

Food lipids (monoacylglycerols)

Glycerol 1-octadecanoate, G-236
Glycerol 1-propanoate, G-236
Glycerol 2-alkanoates, G-237

Food lipids (triacylglycerols)

Asclepic acid, O-46
Capsianoside E, C-77
Glycerol 1,2-di-(9*Z*,11*E*,13*Z*-octadecatrienoate) 3-(8*Z*,11*Z*,13*E*-octadecatrienoate), G-244
Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-(9*Z*-octadecenoate), G-244
Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-hexadecanoate, G-244
Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate) 3-octadecanoate, G-244
Glycerol 1,2-di-(9*Z*-octadecenoate) 3-octadecanoate, G-244
Glycerol 1,2-di-(9*Z*-octadecenoate) 3-tetradecanoate, G-244
Glycerol 1,2-didodecanoate 3-tetradecanoate, G-244
Glycerol 1,2-dihexadecanoate 3-(9*Z*,12*Z*-octadecadienoate), G-244
Glycerol 1,2-dihexadecanoate 3-(9*Z*-octadecenoate), G-244
Glycerol 1,2-dioctadecanoate 3-(9*Z*-octadecenoate), G-244
Glycerol 1,3-di-(9*Z*,12*Z*-octadecadienoate) 2-(9*Z*-octadecenoate), G-243
Glycerol 1,3-di-(9*Z*,12*Z*-octadecadienoate) 2-hexadecanoate, G-243
Glycerol 1,3-di-(9*Z*,12*Z*-octadecadienoate) 2-octadecanoate, G-243
Glycerol 1,3-di-(9*Z*-octadecenoate) 2-(9*Z*,12*Z*-octadecadienoate), G-243
Glycerol 1,3-di-(9*Z*-octadecenoate) 2-hexadecanoate, G-243
Glycerol 1,3-di-(9*Z*-octadecenoate) 2-octadecanoate, G-243
Glycerol 1,3-didodecanoate 2-decanoate, G-243
Glycerol 1,3-dihexadecanoate 2-(9*Z*,12*Z*-octadecadienoate), G-243
Glycerol 1,3-dihexadecanoate 2-(9*Z*-octadecenoate), G-243
Glycerol 1,3-dioctadecanoate 2-(9*Z*-octadecenoate), G-243
Glycerol 1,3-dioctadecanoate 2-hexadecanoate, G-243
Glycerol 1,3-ditetradecanoate 2-(9*Z*-octadecenoate), G-243
Glycerol 1-(9*Z*-octadecenoate) 2-hexadecanoate 3-octadecanoate, G-245
Glycerol 1-(9*Z*-octadecenoate) 2-octanoate 3-tetradecanoate, G-245
Glycerol 1-dodecanoate 2-tetradecanoate 3-octanoate, G-245
Glycerol 1-eicosanoate 2-(9*Z*-octadecenoate) 3-octadecanoate, G-245
Glycerol 1-hexadecanoate, G-236
Glycerol 1-octadecanoate 2-(9*Z*-octadecenoate) 3-hexadecanoate, G-245
Glycerol 1-propanoate; Di-Ac, G-236
Glycerol 2,3-di-(9*Z*-octadecenoate) 1-hexadecanoate, G-244
Glycerol tri-9,11,13,15-octadecatetraenoate, G-260
Glycerol triacetate, G-242
Glycerol trialkanoates (diacid, symmetrical), G-243
Glycerol trialkanoates (diacid, unsymmetrical), G-244
Glycerol trialkanoates (triacid), G-245
Glycerol tributanoate, G-246
Glycerol tridecanoate, G-247
Glycerol tridocosanoate, G-248
Glycerol trieicosanoate, G-251
Glycerol triheneicosanoate, G-252
Glycerol triheptadecanoate, G-253
Glycerol trihexadecanoate, G-254
Glycerol trihexanoate, G-255
Glycerol trilinoleate, G-258
Glycerol trinonadecanoate, G-257
Glycerol trioctanoate, G-264
Glycerol trioleate, G-263
Glycerol tripentadecanoate, G-265
Glycerol tritetracosanoate, G-268
Glycerol tritridecanoate, G-270
Glycerol triundecanoate, G-271
Omega-3 Marine Triglycerides, O-156
3-Phosphatidylinositol, P-326
Quinoside A, D-582
Trierucin, G-249
Tripetroselinin, G-262
Triricinolein, G-256
Vaccenic acid, O-46

Food lipids (phospholipids)

Bis(diacylglycero)phosphonic acids, B-123
Dehydrophytosphingosine, A-284
Glycerol 1,2-di-(9*Z*,12*Z*-octadecadienoate); 3-Phosphate, G-239
Glycerol 1-(9*Z*-octadecenoate) 2-tetradecanoate; 3-Phosphate, G-239
Glycerylphosphoinositol, G-272
9,12,15-Octadecatrienoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester, G-239
9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester, 9CI, G-239
9-Octadecenoic acid 1-[[(1-oxohexadecyl)oxy]methyl]-2-(phosphonoxy)ethyl ester, G-239
1-Phenyl-1,3-docosanedione, P-268

Food lipids (steroids)

3α-Acetoxy-15α,22*S*-dihydroxylanosta-7,9(11),24*E*-trien-26-oic acid, T-611
3α-Acetoxy-15α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, D-592
3-Acetoxy-15-hydroxy-7-methoxylanosta-8,24-dien-26-oic acid, T-608
22*S*-Acetoxy-3α,15α-dihydroxylanosta-7,9(11),24-trien-26-oic acid, T-611
15α-Acetoxy-3α-hydroxy-23-oxo-7,9(11),24*E*-lanostatrien-26-oic acid, D-592
22-Acetoxy-3α-hydroxy-7α-methoxylanosta-8,24*E*-dien-26-oic acid, T-609
22*S*-Acetoxy-3β,15α-dihydroxylanosta-7,9(11),24-trien-26-oic acid, T-611
12-Acetoxy-3,7,11,15,23-pentaoxolanost-8-en-26-oic acid, T-714
12-Acetoxy-3-hydroxy-7,11,15,23-tetraoxolanost-8-en-26-oic acid, T-714
15-Acetoxy-3-oxolanosta-7,9(11),24-trien-26-oic acid, D-524
12β-Acetoxy-4,4,14-trimethyl-3,7,11,15-tetraoxochol-8-en-24-oic acid, 9CI, L-106
15-Acetoxy-7-hydroxy-3-oxolanosta-8,24-dien-26-oic acid, T-608
Acetylsoyasaponin A_1, O-134
Acetylsoyasaponin A_2, O-134
Acetylsoyasaponin A_3, O-134
Acetylsoyasaponin A_4, O-134
Acetylsoyasaponin A_5, O-134

Acetylsoyasaponin A_6, O-134
Agavasaponin C′, H-782
Agavasaponin C, H-782
Agavasaponin D, H-782
Agavasaponin E, H-782
Agavasaponin H, T-583
Agavoside A, H-782
Agavoside B, H-782
Agavoside F, H-782
Agavoside G, T-583
Aginoside progenin, S-185
Alliofuroside A, F-157
Alliospiroside C, S-196
Alliospiroside D, S-196
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1-(4-Hydroxyphenyl)-1,2-propanediol; (1*R*,2*S*)-*form*; 4′-Me ether, H-737
1-(4-Hydroxyphenyl)-1,2-propanediol; (1*RS*,2*RS*)-*form*; 4′-*O*-β-D-Glucopyranoside, H-737
1-(4-Hydroxyphenyl)-1,2-propanediol; (1*RS*,2*SR*)-*form*; 4′-Me ether, H-737
1-(4-Hydroxyphenyl)-1,2-propanediol; (1*S*,2*R*)-*form*; 4′-Me ether, 1-*O*-β-D-glucopyranoside, H-737
1-(4-Hydroxyphenyl)-1,2-propanediol; (1*S*,2*R*)-*form*; 4′-Me ether, 2-*O*-β-D-glucopyranoside, H-737
3-(4-Hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)-1-propanone; 2′-*O*-[Xylosyl-(1→?)-β-D-glucopyranoside], H-752
7-(4-Hydroxyphenyl)-1-phenyl-4-hepten-3-one, H-734
1-(4-Hydroxyphenyl)-2-propen-1-ol; (±)-*form*; Di-Ac, H-749
3-(4-Hydroxyphenyl)-2-propen-1-ol; (*E*)-*form*; 1-Me ether, 4′-*O*-β-D-glucopyranoside, H-750
3-(2-Hydroxyphenyl)-2-propenal; (*E*)-*form*, H-744
3-(4-Hydroxyphenyl)-2-propenal; (*E*)-*form*, H-745
3-(4-Hydroxyphenyl)-2-propenoic acid; (ξ)-*form*; *O*-β-D-Glucopyranoside, H-748
3-(4-Hydroxyphenyl)-2-propenoic acid; (*E*)-*form*, H-748
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2-(4-Hydroxyphenyl)naphthalic anhydride, P-288
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4-Hydroxyphenylacetic acid, H-717
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2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol; 1-*O*-β-D-Xylopyranoside, H-768
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Hyperin; 6″-*O*-(4-Carboxy-3-hydroxy-3-methylbutanoyl), H-837
Hyperin; 6″-*O*-[β-D-Glucopyranosyl-(1→3)-α-L-rhamnopyranosyl], H-837
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p-Mentha-1,8-diene-6,7-diol; (4*S*,6*R*)-*form*; 7-*O*-β-D-Glucopyranoside, M-121
p-Mentha-2,4(8)-dien-9,3-olide; (ξ)-*form*, M-133
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p-Menthane-1,2,8,9-tetrol; (1*R**,2*R**,4*R**,8*S**)-*form*; 9-*O*-β-D-Glucopyranoside, M-141
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p-Menthane-1,2,8,9-tetrol; (1*S*,2*S*,4*R*,8*S*)-*form*; 2-*O*-β-D-Glucopyranoside, M-141
p-Menthane-1,2,8,9-tetrol; (1*S*,2*S*,4*R*,8*S*)-*form*, M-141
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5-[(5-Methyl-2-thienyl)methylene]-2(5*H*)-furanone; (*Z*)-*form*, M-661
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2-Hydroxy-2-phenylethyl glucosinolate; (2*S*)-*form*, H-725
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3-Mercapto-2-methylpentanal, M-215
3-Mercapto-2-methylpentanol, M-216
3-Mercapto-2-pentanone, M-225
1-Mercapto-2-propanone, M-230
2-Mercapto-3-methyl-1-butanol; (ξ)-*form*, M-213
3-Mercapto-3-methyl-1-butanol; *O*-Ac, M-214
3-Mercapto-3-methyl-1-butanol, M-214
3-Mercapto-3-methylbutyl formate, M-214
2-Mercapto-3-pentanone, M-224
4-Mercapto-4-methyl-2-pentanone, M-217
8-Mercapto-*p*-menthan-3-one; (1*S*,4*S*)-*form*; *S*-Ac, M-211
2-(1-Mercaptoethyl)furan, M-208
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2-Methoxy-1,3-thiazino[6,5-*b*]indol-4(9*H*)-one, M-277
5-Methoxy-2-(methylthio)-1,3-thiazino[6,5-*b*]indole, M-265
4-Methoxy-2-methyl-2-butanethiol, 9CI, M-214
6-Methoxy-3-(2-thiazolyl)-1*H*-indole, T-355
8-Methoxy-8*H*-isothiazolo[5,4-*b*]indole, I-169
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Methyl (methylthio)methyl disulfide, M-287
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Methyl 2-(methylthio)butyrate, M-199
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Methyl 2-propenyl disulfide, M-293
Methyl 2-propenyl pentasulfide, M-294
Methyl 2-propenyl tetrasulfide, M-296
Methyl 2-propenyl trisulfide, M-297
Methyl 3-(methylsulfinyl)-1-propenyl disulfide, M-288
Methyl 3-(methylthio)-1-propenyl disulfide; (*Z*)-*form*; 7-Oxide, M-288
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3-Methyl-1-butanethiol, M-328
2-Methyl-1-propenethiol, M-607
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3-Methylbutyl glucosinolate, M-349
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S-Methylmethionine; (*S*)-*form*, M-486
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[3-(Methylsulfinyl)-1-propenyl] 2-propenyl disulfide; (*Z*)-*form*, M-654
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1-(Methylsulfinyl)propyl 2-propenyl disulfide, M-693
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2-(5-Methylsulfinyl-2-pentyn-4-enylidene)-1,6-dioxaspiro[4.4]non-3-ene; (7*Z*,11*E*)-*form*, M-653
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3-(Methylthio)-1-hexanol, M-210
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3-(Methylthio)-1-propene, M-690
2-(Methylthio)-1*H*-indole-3-carboxaldehyde, M-673
4-(Methylthio)-2-butanol, 9CI, M-204
1-(Methylthio)-2-butanone, M-205
4-(Methylthio)-2-oxobutanoic acid, M-222
1-(Methylthio)-2-propanone, 9CI, M-230
5-(Methylthio)-2-[(methylthio)methyl]-2-pentenal, M-678
2-(Methylthio)-3*H*-phenoxazin-3-one, M-686
5-[5-(Methylthio)-4-penten-2-ynyl]-2-furanacrolein; (2*E*,11*Z*)-*form*, M-679
1-(Methylthio)-5-phenyl-1-penten-3-yne; (*Z*)-*form*, M-687
4-(Methylthio)butyl glucosinolate, M-668
1-(Methylthio)ethyl 2-propenyl disulfide, M-670
2-(Methylthio)ethyl glucosinolate, M-669
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9-(Methylthio)nonanenitrile, 9CI, M-220
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3-(Methylthio)propyl acetate, M-229
1-(Methylthio)propyl propyl disulfide, M-694
2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene; (2*Z*,4′*Z*)-*form*, M-680
2-(5-Methylthio-4-penten-2-ynylidene)-1,6-dioxaspiro[4.4]non-3-ene; (2Z,4′*E*)-*form*, M-680
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2-Propenyl 1-(1-propenylsulfinyl)propyl disulfide, P-494
1-Propenyl 1-(1-propenylthio)propyl disulfide, P-492
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2-Propenyl 1-(2-propenylsulfinyl)propyl disulfide, P-495
1-Propenyl 1-(propylsulfinyl)propyl disulfide, P-499
2-Propenyl 1-(propylsulfinyl)propyl disulfide, P-500
1-Propenyl 1-(propylthio)propyl disulfide; (*E*)-*form*, P-499
1-Propenyl 1-(propylthio)propyl disulfide; (*Z*)-*form*, P-499
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S-2-Propenyl 1-propanesulfinothioate, P-497
S-2-Propenyl 1-propenesulfinothioate, P-490
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1-Propenyl 2-propenyl disulfide; (*Z*)-*form*, P-490
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S-1-Propenyl thiosulfate; (*Z*)-*form*, P-501
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S-(1-Propenyl)cysteine; (*R*)-(*E*)-*form*, P-510
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Propyl 1-(propylthio)propyl disulfide, P-521
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S-Propylcysteine sulfoxide; $(R)_C(R)_S$-*form*, P-527
S-Propylcysteine sulfoxide; $(R)_C(S)_S$-*form*, P-527
1-(Propylthio)-1-propanethiol; (ξ)-*form*, P-537
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5-(1-Propynyl)-2-thiophenepropanoic acid; Me ester, P-541
5-(1-Propynyl)-5′-vinyl-2,2′-bithiophene, P-517
Protogonyautoxin I, G-297
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Raphanusanin; (*Z*)-*form*, R-2
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S-Propyl 1-propanesulfinothioate, 9CI, D-975
Selenocysteine, S-80
Selenomethionine; (*S*)-*form*, S-81
Sinalbine, H-358
6-Sinapoylglucoraphenin, M-667
Spirobrassinin; (*S*)-*form*, S-171
1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-β-carboline-3-carboxylic acid; (1*R*,3*R*,3′*S*)-*form*, T-129
1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-β-carboline-3-carboxylic acid; (1*R*,3*S*,3′*R*)-*form*, T-129
Tetrahydro-2-methylthiophen-3-ol, T-111
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3,7,7,10-Tetramethyl-12-thiabicyclo[9.1.0]dodeca-3,7-diene, 9CI, H-310
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3-(2-Thiazolyl)-1*H*-indole, T-355
1-(2-Thienyl)-1-heptanone, T-359
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1,1′-Thiobisethanethiol, T-367
3-Thiocyanato-1-propene, T-373
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4′,5,7-Trihydroxyflavone; 7-*O*-Sulfate, T-581
1,2,3-Trithiane, T-821
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Apigenin 7-*O*-(2″-*O*-acetylglucoside), C-362
Apigenin 7-*O*-(6″-*O*-acetylglucoside), C-362
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Betavulgarin xyloside, T-223
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Betavulgaroside VIII, H-636
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Canavalioside, P-152
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Carthamone, C-130
Castamollissin, T-518
Celereoside, C-170
6-Cinnamoyl-1,2-digalloylglucose, C-268
2-Cinnamoyl-1,6-digalloylglucose; β-D-Pyranose-*form*, C-264
2-Cinnamoyl-1-galloylglucose; β-D-Pyranose-*form*, C-265
6-Cinnamoyl-1-galloylglucose, C-268
1-*O*-Cinnamoylglucose; β-D-(*E*)-*form*, C-266
2-*O*-Cinnamoylglucose; β-D-Pyranose-(*E*)-*form*, C-267
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Cosmosiin; 2″,3″-Di-Ac, C-362
Cosmosiin; 3″,4″-Di-Ac, C-362
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1-*O*-*p*-Coumaroylglucose; β-D-*form*; 2′-Hydroxy, 4′-Me ether, C-364
1-*O*-*p*-Coumaroylglucose; β-D-*form*, C-364
6-*O*-*p*-Coumaroylglucose; D-*form*, C-366
6″-*p*-Coumaroylprunin, T-569
Daucic acid, D-26
6-*C*-(6-Deoxygalactopyranosyl)-3′,4′,5,7-tetrahydroxyflavone, G-28
1-Deoxyglucitol; D-*form*, D-82
6-*C*-(6-Deoxyglucopyranosyl)-3′,4′,5,7-tetrahydroxyflavone, D-83
1-Deoxyribitol; D-*form*, D-88
1-Deoxyxylitol; D-*form*, D-90
3″,6″-Di-*O*-*p*-coumaroyltrifolin, T-502
1,3-Di-*O*-galloyl-4,6-(*S*)-hexahydroxydiphenoyl-α-D-glucopyranose, H-193
1,2′-Di-*O*-galloylhamamelofuranose, H-616
1,2-Digalloylglucose; β-D-Pyranose-*form*, D-213
1,6-Digalloylglucose; β-D-Pyranose-*form*, D-214
2,6-Digalloylglucose, D-215
2′,5-Digalloylhamamelofuranose, H-616
2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (*S*)-*form*; *O*-α-L-Rhamnopyranoside, D-270
2,3-Dihydro-3-hydroxy-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (2*S*,3*R*)-*form*; 1′-*O*-β-D-Glucopyranoside, D-260
2-(1,2-Dihydroxy-1-methylethyl)-2,3-dihydro-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (1′ξ,2*S*)-*form*; 2′-*O*-β-D-Glucopyranoside, D-552
1,3-Dihydroxy-12,6-eudesmanolide; (1β,4α,6α,11α*H*)-*form*; 3-Ketone, 1-*O*-β-D-glucopyranoside, D-457
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), Me ester, D-542
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), D-542
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*S*)-(*E*)-*form*; 3‴-*O*-β-D-Glucopyranoside, D-619
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*S*)-(*E*)-*form*; 3‴-*O*-β-D-Glucopyranoside, D-619
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Elatoside G, T-650
Eleutheroside C, E-267
Epilotaustralin, H-567
Estragonoside, H-211
Ethyl glucoside; β-D-Pyranose-*form*, E-268
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1-*O*-Feruloylglucose, C-364
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Fucose; L-*form*, F-81
8-Galactopyranosyl-6-glucopyranosyl-4′,5-dihydroxy-7-methoxyflavone, G-21
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Galactose; D-*form*, G-36
Galactose; L-*form*, G-36
Galacturonic acid; D-*form*, G-42
Galangin 7-rhamnoside, T-580
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Gallic acid 4-*O*-(6-galloylglucoside), G-48
1-*O*-Galloyl-β-D-glucopyranose, G-46
1-*O*-Galloyl-2,3;4,6-bis-(*S*)-hexahydroxydiphenoyl-α-D-glucopyranose, B-134
1-*O*-Galloyl-2,3;4,6-bis-(*S*)-hexahydroxydiphenoyl-β-D-glucopyranose, B-134
1-*O*-Galloylfructose, F-75
2-Galloylglucose, G-47
6-Galloylglucose, G-49
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Genistein 7-glucoside, T-601
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1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6α)-*form*; 11,13-Dihydro, β-D-glucopyranosyl ester, G-87
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Gladiatoside C_2, R-17
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4-Glucogallic acid, G-48
3-Glucogallic acid, T-520
6-*O*-α-D-Glucopyranosyl-D-glucitol, G-157

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N-Glycolylneuraminic acid, G-284
Gynocardin, G-358
4,6-Heptadiyne-1,3-diol; 1-*O*-β-D-Glucopyranoside, H-82
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Hydrojuglone glucoside, N-9
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6″-*O*-(3-Hydroxy-3-methylglutaroyl)cosmosiin, C-362
2-*O*-(4-Hydroxycinnamoyl)-1,6-di-*O*-galloyl-β-D-glucopyranose, C-264
2-*O*-(4-Hydroxycinnamoyl)-1-*O*-galloyl-β-D-glucopyranoside, C-265
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myo-Inositol, I-41
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7-Megastigmene-3,6,9-triol; (3*S*,5*R*,6*S*,7*E*,9ξ)-*form*; 9-*O*-β-D-Glucopyranoside, M-104
p-Menth-1-en-8-ol; (*R*)-*form*; *O*-β-D-Glucopyranoside, M-175
p-Menth-1-en-8-ol; (*S*)-*form*; *O*-β-D-Glucopyranoside, M-175
2-Methoxy-4-(2-propenyl)phenol; *O*-[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside], M-273
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Methyl 2,3,6-tri-*O*-galloyl-β-D-glucopyranoside, T-508
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Methyl 6-*O*-digalloyl-β-D-glucopyranoside, G-49
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2-*C*-Methyl-1,4-erythronolactone; D-*form*, M-433
2-Methyl-2-butene-1,4-diol; (*Z*)-*form*; 4-*O*-β-D-Glucopyranoside, M-338
4-*O*-Methyl-*myo*-inositol; D-*form*, M-485
1-*C*-Methyl-*scyllo*-inositol, M-484
2-*O*-Methylxylose; D-*form*, M-716
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1,4,5-Naphthalenetriol; 4-*O*-β-D-Glucopyranoside, N-9
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D-*glycero*-D-*ido*-3-Octulose, O-113
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12-Oleanene-3,22,24-triol; (3β,22β)-*form*; 3-*O*-β-D-Glucuronopyranoside, O-139
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3,4′,5,6,7-Pentahydroxyflavone; 3-*O*-β-D-Glucopyranoside, P-136
2′,4′,5,5′,7-Pentahydroxyisoflavanone; (ξ)-*form*; 4′,5′-Methylene, 2′-Me ether, 7-*O*-(6-*O*-malonyl-β-D-glucopyranoside), P-149
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1,2,4,6-Tetragalloylglucose; β-D-Pyranose-*form*, T-72
3′,5,7,8-Tetrahydroxy-4′-methoxyflavone; 8-*O*-β-D-Glucopyranoside, 3′-*O*-sulfate, T-243
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3-(3,4-Dihydroxyphenyl)-2-propenoic acid; (*E*)-*form*; [β-D-Apiofuranosyl-(1→6)-β-D-glucopyranosyl] ester, D-653
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2-*O*-α-D-Galactopyranosyl-D-*chiro*-inositol, I-40
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Maysin, M-83
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Spirostane-3,6-diol; (3β,5β,6α,25*S*)-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 4)-β-D-glucopyranoside], S-182
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4′,5,7-Trihydroxy-3′,5′-dimethoxyflavone; 7-*O*-[4-Hydroxy-3,5-dimethoxy-*E*-cinnamoyl-(→ 2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-549
4′,5,7-Trihydroxy-3′,5′-dimethoxyflavone; 7-*O*-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→ 2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-549
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4-*O*-β-D-Xylopyranosyl-D-xylose, X-28
3-*O*-α-D-Xylopyranosyl-L-arabinose, X-17
2-*O*-β-D-Xylopyranosyl-L-arabinose, X-18
3-*O*-β-D-Xylopyranosyl-L-arabinose, X-19
4-*O*-β-D-Xylopyranosyl-L-arabinose, X-20
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3,16-Dihydroxy-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-β-D-Glucopyranoside, 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)]-α-L-arabinopyranosyl] ester, D-578
3,23-Dihydroxy-12-oleanene-28,30-dioic acid; 3β-*form*; 3-*O*-[α-L-Arabinopyranosyl-(1 → 3)-β-D-glucuronopyranoside], 28-*O*-β-D-glucopyranosyl ester, 30-Me ester, D-573
3,23-Dihydroxy-12-oleanene-28,30-dioic acid; 3β-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 2)-β-D-glucopyranoside], 28-*O*-β-D-glucopyranosyl ester, 30-Me ester, D-573
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Furostane-2,3,6,22,26-pentol; (2α,3β,5α,6α,22*R*,25*R*)-*form*; 22-Me ether, 3-*O*-[β-D-glucopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucopyranosyl-(1 → 4)-β-D-galactopyranoside], 26-*O*-β-D-glucopyranoside, F-153
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β-D-Galactopyranosyl-(1 → 3)-β-D-galactopyranosyl-(1 → 4)-D-glucose, G-15
β-D-Galactopyranosyl-(1 → 3)-β-D-galactopyranosyl-(1 → 6)-D-galactose, G-10
β-D-Galactopyranosyl-(1 → 3)-2-acetamido-2-deoxy-β-D-glucopyranosyl-(1 → 3)-β-D-galactopyranosyl-(1 → 4)-D-glucose, G-3
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1,2,3,4,5,6-Hexahydro-6-methyl-7*H*-cyclopenta[*b*]pyridin-7-one, H-185
2,3,4,5,6,7-Hexahydro-7-methylcyclopent[*b*]azepin-8(1*H*)-one, T-99
1,2,3,4,5,6-Hexahydro-7*H*-cyclopenta[*b*]pyridin-7-one, H-174
2,3,4,5,6,7-Hexahydrocyclopent[*b*]azepin-8(1*H*)-one, H-175
2-Hexyl-4,5-dimethylthiazole, T-445
5-Imino-2-methyl-1-cyclopenten-1-ol, I-13
4-Isopropyl-2-methylthiazole, D-110
2-Isopropyl-4,5-dimethylthiazole, T-445
2-Isopropyl-4-methylthiazole, D-110
2-Isopropyl-4-propylthiazole, D-110
2-Isopropyl-5-methyl-2-hexenal, I-145
Maltoxazine, M-46
3-Mercapto-2-pentanone, M-225
2-Mercapto-3-pentanone, M-224
2-(1-Mercaptoethyl)furan, M-208
3-Methyl-1,2,4-trithiane, M-708
2-Methyl-1,3-dithiolane, M-398
5-Methyl-2,5-di-1-pyrrolidinyl-2-cyclopenten-1-one, M-397
4-Methyl-2,5-dipropylthiazole, T-445
3-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, M-641
5-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, M-642
5-Methyl-2-furanmethanethiol, M-438
2-(5-Methyl-2-furanyl)-3-piperidinol, M-447
3-[(5-Methyl-2-furanyl)methyl]-1*H*-pyrrole, M-444
1-[(5-Methyl-2-furanyl)methyl]pyrrolidine, M-445
2-(5-Methyl-2-furanyl)piperidine, M-446
2-(5-Methyl-2-furanyl)pyrrolidine, M-449
4-Methyl-2-pentylthiazole, D-110
5-Methyl-2-pentylthiazole, D-111
1-Methyl-2-pyrrolecarboxaldehyde, P-617
5-Methyl-3-furanthiol, M-442
2-Methyl-3-thiophenethiol, M-683
5-Methyl-3-thiophenethiol, M-685
2-Methyl-5-(1-propenyl)pyrazine, M-611
2-Methylfuran, M-436
1-Methylpyrrole, M-638
2-Methylpyrrole, M-639
1-Methylpyrrolo[1,2-*a*]pyrazine, M-643
3-(Methylthio)thiophene, 9CI, T-383
2-Methylthiophene, M-681
3-Methylthiophene, M-682
2-Octyl-4-propylthiazole, D-110
2-Pentyl-4-propylthiazole, D-110
2-Pentylpyridine, P-219
2-Pentylthiophene, P-223
2-Propanoylthiazole, P-481
2-Propanoylthiophene, P-482
1-Propenylpyrazine, P-514
Pyrazine, P-592
4-(9*H*-Pyrido[3,4-*b*]indol-1-yl)-1,2,4-butanetriol; (2*S*,4*R*)-*form*, P-603
1-(9*H*-Pyrido[3,4-*b*]indol-1-yl)-1,4-butanediol, 9CI, P-603
Pyrraline, A-253
5-[2*H*-Pyrrol-4-(3*H*)-ylidenemethyl]-2-furanmethanol, P-631
1-Pyrrolidinecarboxaldehyde, P-620
1-(1-Pyrrolidinyl)-2-butanone, P-622
3-(1-Pyrrolidinyl)-2-butanone, P-623
2-(1-Pyrrolidinyl)-2-cyclopenten-1-one, P-624
3-(1-Pyrrolidinyl)-2-pentanone, P-627
1-(1-Pyrrolidinyl)-2-propanone, P-628
2-(1-Pyrrolidinyl)-3-pentanone, P-626
5-(1-Pyrrolidinylmethyl)-2-furanmethanol, P-625
1*H*-Pyrrolo[2,1-*c*][1,4]thiazine, P-630
1,2,3,4-Tetrahydro-β-carboline-1,3-dicarboxylic acid, T-75
1,2,3,4-Tetrahydro-1-methyl-β-carboline-1,3-dicarboxylic acid; (1ξ,3*S*)-*form*, T-98
2,3,6,7-Tetrahydro-6,7-dimethylcyclopent[*b*]azepin-8(1*H*)-one, T-79
2,3,4,5-Tetrahydro-6-(5-methyl-2-furanyl)pyridine, T-103
2,3,6,7-Tetrahydro-7-methylcyclopent[*b*]azepin-8(1*H*)-one, T-99
2,3,6,7-Tetrahydrocyclopent[*b*]azepin-8(1*H*)-one, T-76
2-(1,2,3,4-Tetrahydroxybutyl)-6-(2,3,4-trihydroxybutyl)pyrazine, T-141
Thiacremonone, T-349
Thieno[2,3-*b*]thiophene, T-356
Thiophene, T-376
2-Thiophenecarboxylic acid; Me ester, T-378
2-Thiophenemethanol, T-380
3-Thiophenemethanol, T-381
1,2,5-Trimethyl-1*H*-pyrrole, D-898
Trimethylpropylpyrazine, T-794
2-Vinylthiophene, V-39

Nucleosides and nucleotides

Acadesine; 5′-Phosphate, A-16
Adenosine 5′-diphosphate glucose, A-123
Agrocin 84, A-143
Agrocin C58, A-144
Arecoline, T-107
Clitocine, C-307
Cytarabine, BAN, INN, JAN, USAN, C-521
Cytidine 5′-triphosphate, C-518
5′-Deoxy-5′-(methylsulfinyl)adenosine, 9CI, T-365
Deoxyeritadenine, E-231
Disodium inosinate, I-39
Eritadenine; (2*R*,3*R*)-*form*, E-231
Guanosine diphosphate mannose, G-345
5′-Guanylic acid, G-346
Homoarecoline, T-107
N-[(5-Hydroxy-2-pyridinyl)methyl]adenosine, H-773
Inosine, I-38
Nebularine, N-19
Pseudouridine C, P-554
3-Ribofuranosyluric acid; β-D-*form*, R-33
1,2,5,6-Tetrahydro-1-methyl-3-pyridinecarboxylic acid, T-107
5′-Thioadenosine; *S*-Me, *S*-oxide(*S*-), T-365

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Food processing agents

Acetic anhydride, A-24
Benzene, B-17
Calcium lactate, JAN, USAN, H-765
Phosphoryl chloride, P-332
Potassium lactate, H-765
1,2-Propanediol, P-471
2-Propenal, P-483
Pyroligneous acid, P-612
Sodium lactate, JAN, USAN, H-765
Starch; 2-Hydroxypropyl ether, S-219
Starch; Phosphate, S-219
Starch; Unbranched-*form*; Per-Ac, S-219

Food processing aids

2-Aminoethanol, A-249
Ammonium chloride ($(NH_4)Cl$), A-313
Ammonium phosphate ($(NH_4)_2HPO_4$), A-316
Ammonium sulfate, S-278
2-Butoxyethanol, B-230
Calcium chloride ($CaCl_2$), C-39
Calcium sulfate, C-54
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Cordycepic acid, M-66
Diethylenetriamine, D-201
Dimethylamine, D-749
Docusate sodium, BAN, INN, B-130
Ficin, F-36
Heptanoic acid, H-93
Hydrocyanite, C-347
Hydrogen chloride, H-323
Magnesium hydroxide, M-21
Magnesium octadecanoate, O-27
Magnesium sulfate heptahydrate, M-28
Oxirane, O-193
Pentanedial, P-183
Polyethylene glycol, P-417
Potassium bromide (KBr), P-428
Potassium carbonate (K_2CO_3), P-429
Potassium hydrogen carbonate, P-433
Potassium hydroxide (KOH), P-435
Sodium carbonate (Na_2CO_3), S-122
Sodium chloride (NaCl), S-123
Sodium hypochlorite, S-134
Sodium octyl sulfate, O-82
Sodium silicate (Na_2SiO_3), S-143
Sodium stearoyl 2-lactylate, L-34
Sodium sulfide (Na_2S), S-146

Acids/bases

Acetic acid sodium salt (2:1), 9CI, S-119
Ammonium bicarbonate, C-93
Ammonium phosphate ($(NH_4)(H_2PO_4)$), A-315
Calcium carbonate, C-38
Fumaric acid, F-86
Hydrogen chloride, H-323
Malic acid; (±)-*form*, M-36
Potassium phosphate (K_3PO_4), P-444
Sodium aluminium phosphate, S-120

Anticaking agents

Aluminium calcium silicate, A-195
Aluminium dodecanoate, D-1017
Aluminium octanoate, O-81
Aluminium potassium silicate, A-197
Aluminium sodium silicate, A-200
Calcium chloride ($CaCl_2$), C-39
Calcium dodecanoate, D-1017
Calcium gluconate, USAN, G-152
Calcium hydroxide phosphate ($Ca_5(OH)(PO_4)_3$),

C-43
Calcium metasilicate ($CaSiO_3$), C-45
Calcium octadecanoate, O-27
Calcium octanoate, O-81
Calcium oxide (CaO), C-46
Calcium oxide silicate ($Ca_3O(SiO_4)$), C-47
Calcium phosphate ($Ca_3(PO_4)_2$), C-51
Calcium silicate (Ca_2SiO_4), C-53
Calcium sulfate, C-54
Cellulose, C-173
Cordycepic acid, M-66
Decanoic acid, D-41
Iron(*III*) ammonium citrate, I-52
Magnesium carbonate, M-18
Magnesium dodecanoate, D-1017
Magnesium octadecanoate, O-27
Magnesium octanoate, O-81
Magnesium oxide (MgO), M-23
Magnesium silicate (Mg_2SiO_4), M-27
Magnesium trisilicate, M-29
9-Octadecenoic acid; (*Z*)-*form*; Na salt, O-44
Potassium dodecanoate, D-1017
Potassium octadecanoate, O-27
Potassium octanoate, O-81
1,2-Propanediol, P-471
Silica gel, S-102
Sodium dodecanoate, D-1017
Sodium magnesium aluminosilicate, S-135
Sodium octadecanoate, O-27
Sodium octanoate, O-81
Yellow prussiate of soda, H-221

Antifoaming agents

Butyl octadecanoate, O-26
Cordycepic acid, M-66
Decanoic acid, D-41
Hexadecanoic acid, H-159
Magnesium octadecanoate, O-27
Methyl octadecanoate, O-26
Octadecanoic acid, O-26
Octanoic acid, O-80
Oleyl alcohol, O-51
Polysorbate 40, S-159
Polysorbate 65, S-159
Potassium octadecanoate, O-27
Propylene glycol stearate, P-471
Silica gel, S-102
Sorbitan monolaurate, BAN, USAN, A-335
Sorbitan monostearate, BAN, USAN, A-335
Tetradecanoic acid, T-59

Antimicrobial agents

Bacitracin A, B-3
Bacitracin, B-3
Benzoic acid, B-31
2-Biphenylol, B-92
Butyl 4-hydroxybenzoate, H-347
Calcium chloride ($CaCl_2$), C-39
Calcium propionate, P-478
Cyanocarbamodithioic acid; Di-Na salt, C-410
2,2-Dibromo-2-cyanoacetamide, 9CI, D-139
Dimethyl carbonate, D-740
Dowicide A, B-92
1,2-Ethanediamine, E-241
Ethylparaben, INN, USAN, H-347
Hydrogen peroxide (H_2O_2), H-324
1-Hydroxy-1,1-ethanediphosphonic acid, H-448
Methyl 4-hydroxybenzoate, H-347
Methylcarbamodithioic acid; K salt, M-355
Nabam, BSI, ISO, E-303
Nisin, N-63
Ozone, 11CI, O-257
Pentanedial, P-183
Peracetic acid, P-226
Peroxyoctanoic acid, P-232
ε-Polylysine, P-419
Potassium propionate, P-478
Potassium sorbate, H-172
Propanoic acid, P-478
Propyl 4-hydroxybenzoate, H-347
2,6-Pyridinedicarboxylic acid, P-600
Sodium benzoate, B-32
Sodium chloride (NaCl), S-123
Sodium chlorite, S-124
Sodium dimethyldithiocarbamate, S-125
Sodium disulfite, S-127
Sodium erythorbate, I-70
Sodium hydrogen sulfite, S-132
Sodium hydroxide (NaOH), S-133
Sodium propionate, P-478
Sodium sorbate, H-172
Sodium sulfite (Na_2SO_3), S-147
Sulfur dioxide, S-277
1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane, T-36
Thiolutin, A-247
Virginiamycin, BAN, INN, USAN, O-183

Antioxidants

Alfacol, T-406
Ascorbyl palmitate, USAN, A-447
Ascorbyl stearate, A-447
2-*tert*-Butyl-1,4-benzenediol, B-242
2-Butyl-4-methylphenol, B-253
Butylated hydroxyanisole, B-241
Calcium ascorbate, A-447
Calcium lactate, JAN, USAN, H-765
3-[3-Carboxy-2,3-dihydro-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-5-benzofuranyl]-2-propenoic acid, 9CI, E-63
Citric acid; 1-Isopropyl ester, C-290
Citric acid; 2-Isopropyl ester, C-290
2,6-Di-*tert*-butyl-4-hydroxymethylphenol, D-147
2,6-Di-*tert*-butyl-4-methylphenol, D-148
2-(1,2-Diamino-1-propenyl)phenol, D-120
Didodecyl thiobispropanoate, T-370
3,4-Dihydro-2,2,5,7,8-pentamethyl-2*H*-1-benzopyran-6-ol, D-340
3,4-Dihydro-6-hydroxy-2,5,7,8-tetramethyl-2*H*-1-benzopyran-2-carboxylic acid, D-283
2′,5′-Dihydroxychalcone, D-413
3′,4′-Dihydroxychalcone, D-414
Dilauryl 3,3′-thiodipropionate, D-993
Dodecyl gallate, T-520
E315, I-70
6-Ethoxy-1,2-dihydro-2,2,4-trimethylquinoline, 9CI, 8CI, D-364
2-Ethyl-4-hydroxy-5-methyl-3(2*H*)-furanone, E-318
Fumaric acid, F-86
4-Hexyl-1,3-benzenediol, H-262
3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid; (*E*)-*form*, H-554
Malic acid; (±)-*form*, M-36
5-(Methylthio)-2-[(methylthio)methyl]-2-pentenal, M-678
Octyl gallate, T-520
Paralactic acid, H-765
1,2-Propanediol, P-471
Propyl 3,4,5-trihydroxybenzoate, T-520
Sodium ascorbate, INN, A-447
Sodium carbonate (Na_2CO_3), S-122
Sodium erythorbate, I-70
Sodium hydrogen sulfite, S-132
Sodium sulfite (Na_2SO_3), S-147
Sodium triphosphate ($Na_5(P_3O_{10})$), S-149
2-Stearyl citrate, C-290
Sucrose, S-263
3,3′,4,4′-Tetrahydroxylignan, T-231
L-Threaric acid, T-27
Tin chloride ($SnCl_4$), T-400
Tin(*II*) chloride ($SnCl_2$), T-399
α-Tocopherol succinate, T-406
δ-Tocopherol, T-408
γ-Tocopherol, T-409
Tocophersolan, USAN, T-406
13,15-Triacontanedione, T-441
3,4,5-Trihydroxybenzoic acid, T-520
1-(2,4,5-Trihydroxyphenyl)-1-butanone, T-663
Vitamin C, A-447

Binders

Aluminium dodecanoate, D-1017
Aluminium octanoate, O-81
Calcium dodecanoate, D-1017
Calcium octadecanoate, O-27
Calcium octanoate, O-81
Cellulose, C-173
Decanoic acid, D-41
Dextrin, D-101
Guar gum, G-347
Hexasodium metaphosphate ($P_6O_{18}^{6\ominus}$), H-239
Hydroxypropyl methyl cellulose, C-173
Magnesium dodecanoate, D-1017
Magnesium octadecanoate, O-27
Magnesium octanoate, O-81
9-Octadecenoic acid; (*Z*)-*form*; Na salt, O-44
Octanoic acid, O-80
Polyethylene glycol, P-417
Potassium dodecanoate, D-1017
Potassium octadecanoate, O-27
Potassium octanoate, O-81
Sodium dodecanoate, D-1017
Sodium octadecanoate, O-27
Sodium octanoate, O-81
Zein, Z-11

Bleaching/decolourising agents

Ammonium peroxydisulfate, P-231
Azoformamide, D-123
Calcium peroxide (CaO_2), C-48
Calcium phosphate ($Ca_3(PO_4)_2$), C-51
Calcium sulfate, C-54
Chlorine oxide (ClO_2), C-195
Chlorine, C-194
Dibenzoyl peroxide, D-131
2,2-Dihydroperoxypropane, D-343
Hydrogen peroxide (H_2O_2), H-324
Nitrogen chloride (NCl_3), N-67
Nitrosyl chloride ((NO)Cl), N-74
Nitrosylsulfuric acid, N-75
Peracetic acid, P-226
Potassium alum, A-198
Potassium permanganate, P-441
Sodium chlorite, S-124
Sodium dithionite ($Na_2S_2O_4$), S-128
Sodium hypochlorite, S-134

Buffering/pH control agents

Acetic acid sodium salt (2:1), 9CI, S-119
Acetic acid, A-23
Aluminium hydroxide, A-196
Aluminium octadecanoate, O-27
Ammonium alum, A-194
Ammonium bicarbonate, C-93
Ammonium citrate, C-290
Ammonium hydroxide ($(NH_4)(OH)$), A-314
Ammonium phosphate ($(NH_4)(H_2PO_4)$), A-315
Ammonium phosphate ($(NH_4)_2HPO_4$), A-316
Calcium acetate, C-36
Calcium chloride ($CaCl_2$), C-39
Calcium diphosphate ($Ca_2P_2O_7$), C-40
Calcium ferrocyanide, H-221
Calcium hydroxide ($Ca(OH)_2$), C-42
Calcium lactate, JAN, USAN, H-765
Calcium oxide (CaO), C-46
Calcium phosphate ($Ca(H_2PO_4)_2$), C-49
Calcium phosphate ($Ca(HPO_4)$), C-50
Calcium sulfate, C-54
Citric acid, C-290
Dipotassium phosphate, D-965
Disodium phosphate, D-980
FEMA 2655, M-36
Fujiglucon, G-153
Fumaric acid, F-86
Gluconic acid; D-*form*, G-152
Hexanedioic acid, H-227
Hydrogen chloride, H-323
2-Hydroxypropanoic acid, H-765
Magnesium carbonate, M-18
Magnesium hydroxide, M-21

Magnesium lactate, M-22
Magnesium phosphate ($Mg(HPO_4)$), M-25
Magnesium phosphate ($Mg_3(PO_4)_2$), M-26
Malic acid; (±)-*form*, M-36
Malic acid, M-36
Metatartaric acid, M-238
Phosphoric acid, P-331
Potassium bitartrate, T-27
Potassium carbonate (K_2CO_3), P-429
Potassium chloride, P-430
Potassium citrate, C-290
Potassium diphosphate ($K_4(P_2O_7)$), P-431
Potassium ferrocyanide, H-221
Potassium hydrogen carbonate, P-433
Potassium hydrogen sulfate ($KHSO_4$), P-434
Potassium hydroxide (KOH), P-435
Potassium lactate, H-765
Potassium metaphosphate; Polymeric-*form*, P-438
Potassium phosphate ($K(H_2PO_4)$), P-443
Potassium phosphate (K_3PO_4), P-444
Quinic acid; (-)-*form*, Q-10
Sodium acetate, S-119
Sodium alum, A-201
Sodium carbonate (Na_2CO_3), S-122
Sodium chloride (NaCl), S-123
Sodium citrate, C-290
Sodium diphosphate ($Na_4(P_2O_7)$), S-126
Sodium hydrogen carbonate, S-130
Sodium hydrogen sulfate, S-131
Sodium hydroxide (NaOH), S-133
Sodium lactate, JAN, USAN, H-765
Sodium phosphate ($Na(H_2PO_4)$), S-140
Sodium phosphate (Na_3PO_4), S-141
Sodium potassium tartrate, T-27
Sodium sulfate decahydrate, S-145
Sodium sulfate, S-144
Sodium tartrate, T-27
Sodium triphosphate ($Na_5(P_3O_{10})$), S-149
Succinic acid, S-261
Sulfuric acid, S-278
Tannin, T-12
L-Threaric acid, T-27
Trona, T-818
Vitamin C, A-447
Yellow prussiate of soda, H-221

Catalysts

Nickel, N-52
Trifluoromethanesulfonic acid, T-500

Clarifying agents

Acrylamide, P-487
β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 3)-D-glucose, G-168
Gum arabic, A-385
Octadecanoic acid, O-26
Palygorskite, P-12
Papain, P-33
Polyvidone, P-422
Sodium chloride (NaCl), S-123
Sodium hydroxide (NaOH), S-133
Sodium sulfate decahydrate, S-145
Sorbitan monooleate, BAN, USAN, A-335
Tannin, T-12

Coatings

Butyl oleate sulfate, B-238
Decanoic acid, D-41
Dodecanoic acid, D-1016
β-D-Fructofuranosyl α-D-glucopyranoside monohexadecanoate, 9CI, S-263
Glycerol 1-octadecanoate 2-(9*Z*-octadecenoate) 3-hexadecanoate, G-245
Glycerol 1-octadecanoate, G-236
Hexadecanoic acid, H-159
Morpholine, M-764
Octadecanoic acid, O-26
Oleic acid, O-44
Paraffin wax, P-39
Polyethylene glycol, P-417
Polysorbate 40, S-159
Polysorbate 60, S-159
Polyvidone, P-422
Potassium persulfate ($K_2S_2O_8$), P-442
Sorbitan monostearate, BAN, USAN, A-335

Colourants (artificial)

2-Acetyl-4(5)-(1,2,3,4-tetrahydroxybutyl)imidazole; (1*R*,2*S*,3*R*)-*form*, A-94
Allura red AC, A-183
Amaranth, A-203
5-Amino-4-hydroxy-3-(phenylazo)-2,7-naphthalenedisulfonic acid, A-266
Azorhodine 2G, A-528
Azorubine, A-529
C.I. Acid Blue 3, S-281
C.I. Acid Green 3, C-244
C.I. Acid Green 50, C-246
C.I. Acid Green 5, C-245
C.I. Acid Violet 49, C-247
C.I. Acid Yellow 17, C-248
C.I. Direct Red 45, C-249
C.I. Food Black 1, C-250
C.I. Food Black 2, C-251
C.I. Food Brown 3, C-252
C.I. Food Red 1, C-253
C.I. Food Red 6, C-254
C.I. Pigment Blue 63, I-21
C.I. Pigment red 172, E-237
C.I. Pigment Yellow 100, 9CI, T-28
C.I. Pigment Yellow 104, H-793
C.I. Solvent Red 80, C-257
9-(2-Carboxyphenyl)-3,6-bis(diethylamino)xanthylium(1+), 9CI, R-27
Cochineal Red A, C-314
4,11-Dichloro-5,12-dihydroquino[2,3-*b*]acridine-7,14-dione, D-157
4-[(2,4-Dihydroxyphenyl)azo]benzenesulfonic acid, D-610
1-[(2,5-Dimethylphenyl)azo]-2-naphthalenol, D-878
Erioglaucine A, E-230
Erythrosine, E-237
Fast green FCF; Al salt, F-18
Fast green FCF, F-18
Ferrous gluconate, USAN, G-152
Gold, G-294
4-[(2-Hydroxy-1-naphthalenyl)azo]benzenesulfonic acid, H-624
6-Hydroxy-5-(phenylazo)-2-naphthalenesulfonic acid; Na salt, H-719
6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid; Di-Na salt, H-793
6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid, H-793
4-[(2-Hydroxy-6-sulfo-1-naphthalenyl)azo]-1-naphthalenesulfonic acid, H-792
Indigotin disulfonate sodium, USAN, I-21
Iron(*III*) oxide (Fe_2O_3), I-60
Lithol Rubine, L-97
Orange B, O-164
Orange I, O-163
Quinacridone, Q-8
Quinoline yellow, Q-13
Rose bengal sodium, INN, R-50
Rose bengal, R-50
Sulforhodamine B, S-276
Tartrazine; Ca lake, T-28
Tartrazine; Tri-Na salt, T-28

Colourants (natural or nature-identical)

5-(4-Acetoxy-3-oxo-1-butynyl)-2,2′-bithiophene, B-160
Amaranthussaponin I, D-574
Amaranthussaponin II, D-597
Americanin A, A-207
Americanin D, A-209
Americanol, A-210
α-Amyrin, U-44
8′-Apo-β-caroten-8′-al, A-377
6′-Apo-ψ-caroten-6′-al; (7*Z*,9*Z*,9′*Z*)-*form*; 6′-Carboxylic acid, Me ester, A-378
(-)-Aromadendrene, A-417
Artemisiatriene, T-778
Astaxanthin; (3′*RS*,3′*SR*)-*form*, A-474
Bentonite, B-15
Betanidin; 5-*O*-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside], B-70
Betanin, B-70
1,7-Bis(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, 9CI, C-397
Bixin, N-146
α-Bixin, N-146
C.I. Natural green 5, C-255
C.I. Natural red 20, D-507
3′′-*O*-Caffeoylcosmosiin, C-362
Canthaxanthin, I-199
Carmine red, C-111
β-Carotene, C-119
Chlorophyll, C-215
Crosatoside B, H-724
Cucurbic acid; 6,7-Diepimer, *O*-β-D-glucopyranoside, C-383
Curcumin, C-397
Cyanidin 3-(6-caffeoylglucoside) 5-glucoside, P-144
2-Decene-4,6,8-triynoic acid; (*Z*)-*form*; Me ester, D-55
Dehydroroemerine, D-74
Dihydro-4-hydroxy-2(3*H*)-furanone; (*S*)-*form*; *O*-β-D-Glucopyranoside, D-258
3,8-Dihydroxy-1-methylanthraquinone-2-carboxylic acid, D-545
6,8-Dihydroxy-3-methoxy-1-methylanthraquinone-2-carboxylic acid, T-626
2,3-Dihydroxy-30-nor-23-oxo-12,20(29)-oleanadien-28-oic acid; (2β,3β)-*form*; 23-Carboxylic acid, 3-*O*-β-D-glucuronopyranoside, 28-*O*-β-D-glucopyranosyl ester, D-565
2-(3,4-Dihydroxyphenyl)ethenol; (*Z*)-*form*; 1-*O*-3,4-Dihydroxycinnamoyl(*E*-), D-628
4,8-Dimethyl-12-oxo-2,4,6,8,10-dodecapentaenoic acid; (2*E*,4*Z*,6*E*,8*E*,10*E*)-*form*; Me ester, D-865
2,5-Dimethyl-3-vinyl-5-hexene-2,4-diol; 2-Ac, D-919
2,5-Dimethyl-3-vinyl-5-hexene-2,4-diol; 4-Ketone, 2-Ac, D-919
Dopaquinone; (*S*)-*form*, D-1036
Egomaketone, E-6
Epijasminoside A, H-621
5,6-Epoxy-3,3,6-trimethyl-1-hepten-4-one, T-777
Esculentic acid, D-573
Esculentoside E, T-646
5-Ethynyl-5′-(1-propynyl)-2,2′-bithiophene, E-358
Fernenol, F-33
1,7,9-Heptadecatriene-11,13,15-triyne; (*all-E*)-*form*, H-66
1-Hydroxy-2,4(18),11(13)-eudesmatrien-12-oic acid; 1α-*form*, H-458
2-Hydroxy-3-(2-hydroxyphenyl)propanoic acid; (*S*)-*form*, H-508
8-Hydroxy-3-methoxy-1-methylanthraquinone-2-carboxylic acid, D-545
1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, 9CI, C-397
3-Hydroxy-5-phenylpentanoic acid; (ξ)-*form*;

O-β-D-Glucopyranoside, H-730
3-Hydroxy-*p*-mentha-1,8-dien-7-al, H-541
Isobetanidin, B-70
Isobetanin, B-70
4-Isopropylbenzoic acid, I-121
Isozeaxanthin, I-199
Lutein, L-124
Luteolin 7-(caffeoylglucoside), T-205
Luteolin 7-sulfate, T-205
Lycopene, L-127
Lyratol; (*S,E*)-*form*; Ac, L-131
Lyratol; (*S,E*)-*form*; Propanoyl, L-131
Lyratol; (*S,Z*)-*form*; Ac, L-131
Mangicrocin, M-62
p-Menth-8-en-7-ol; (1*RS*,4*SR*)-*form*, M-182
p-Menth-8-en-7-yl caffeate, M-182
8-Methoxy-6,7-methylenedioxycoumarin, T-523
Methyl 6′-apo-9′*Z*-lycopen-6′-oate, A-378
Methyl apo-6′-lycopenate, A-378
5-Methyl-2-methylene-3-vinyl-4-hexen-1-ol; (*S*)-*form*; Ac, M-497
4-Methyl-2-oxopentanoic acid, M-533
5-(5-Methyl-2-thienyl)-2-penten-4-ynoic acid; (*Z*)-*form*; Me ester, M-662
2-Methyl-6-oxo-2,4-heptadienoic acid; (2*E*,4*E*)-*form*; [β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl] ester, M-530
cis-Methylbixin, N-146
trans-Methylbixin, N-146
Monascin, M-736
Neobetanin, B-70
Norbixin; (9*E*)-*form*; 6-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-6′-Me ester, N-146
Norbixin; (9*Z*)-*form*; 6-(3,7,11,5-Tetramethyl-2,6,10,14-hexadecatetraenyl)-6′-Me ester, N-146
Norbixin; (9*Z*,9′*Z*)-*form*; Di-Me ester, N-146
Norbixin, N-146
Orcein, O-165
3-Oxo-1,4,11(13)-eudesmatrien-12-oic acid, O-212
10′-Oxo-6,10′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-205
6′-Oxo-6,5′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-202
6′-Oxo-6,6′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-203
8′-Oxo-6,8′-diapo-6-carotenoic acid; (9*Z*)-*form*; Me ester, O-204
2-Oxopentanoic acid, O-238
3,4′,5,6,7-Pentahydroxyflavone; 7-*O*-β-D-Allopyranoside, P-136
3,4′,5,6,7-Pentahydroxyflavone; 7-*O*-β-D-Glucopyranoside, P-136
3′,4′,5,7,8-Pentahydroxyflavone; 8-*O*-Sulfate, P-141
Perilloside A, M-129
Perilloside C, M-182
Perilloside D, M-182
Perilloside E, P-506
Phytolaccasaponin B, T-646
Phytolaccasaponin E, T-646
Phytolaccasaponin G, T-646
Phytolaccinic acid, D-573
Phytolaccoside A, D-573
Phytolaccoside D, D-573
Phytolaccoside D_2, D-573
Phytolaccoside I, D-573
Picrocrocin, H-811
Pokeberrygenin, D-572
Prebetanin, B-70
5-(1-Propynyl)-5′-vinyl-2,2′-bithiophene, P-517
Protodioscin 22-methyl ether, F-160
Pyruvic acid, P-632
Quercetagitrin, H-207
Quercimeritrin; 3-*O*-α-L-Arabinopyranoside, Q-6
Riboflavine, R-32
Santolina alcohol; (*S*)-*form*; Ac, S-43
Tagetiin, H-207
2′,3′,4′,6′-Tetrahydroxyacetophenone; 6′-Me ether, 3′-*O*-β-D-glucopyranoside, T-134
4′,5,6,7-Tetrahydroxyflavone; 7-*O*-[β-D-Glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-210
2,6,11,15-Tetramethyl-2,4,6,8,10,12,14,16-octadecaoctaenedioic acid; (all-*E*)-*form*; 18-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenoyl) ester, 1-Me ester, T-306
Tomentosic acid, T-253
12-Tricosanol, T-463
1,3,5-Tridecatriene-7,9,11-triyne; (3*E*,5*Z*)-*form*, T-485
2,3,23-Trihydroxy-12-oleanen-28-oic acid; (2β,3β)-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 3)-β-D-glucuronopyranoside], 28-*O*-β-D-glucopyranosyl ester, T-647
2′,4′,6′-Trihydroxyacetophenone; 2′-Me ether, 6′-*O*-β-D-glucopyranoside, T-512
4′,5,7-Trihydroxyflavone; 7-*O*-Sulfate, T-581
2,4,6-Trimethylbenzaldehyde, T-734
12-Ursen-3-ol; 3β-*form*; Ac, U-44
Vinyl caffeate, D-653
Vulgarin, H-681
Vulgarole, B-170
Vulgaxanthin I, V-58
Xantofyl palmitate, INN, L-124

Colourant aids

Calcium phosphate ($Ca(HPO_4)$), C-50
Calcium sulfate, C-54
Chlorophyll a, C-216
Cyclohexane, C-456
Diethylene glycol distearate, O-255
E315, I-70
2-Ethoxyethanol, E-252
Ethyl acetate, E-259
Poly(vinyl alcohol), P-423
Polyethylene glycol, P-417
Polyvidone, P-422
Silica gel, S-102
Sodium chloride (NaCl), S-123
Sodium citrate, C-290
Sodium hydroxide (NaOH), S-133
Sodium nitrate ($NaNO_3$), S-138
Sodium nitrite, S-139
Titanium(*IV*) oxide (TiO_2), T-403

Cooling agents

4-(Butoxymethyl)-2-methoxyphenol, 9CI, D-400
Carbon dioxide, C-90
Dichlorodifluoromethane, D-156
Ethyl menthane carboxamide, I-142
Helium, H-22
Menthadienyl acetate, M-126
Menthone 1,2-glyceryl ketal, M-191
Menthyl ethylene glycol carbonate, M-193
3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-1,2-propanediol, M-499
1,1,2-Trichloro-1,2,2-trifluoroethane, T-455
N,2,3-Trimethyl-2-(1-methylethyl)butanamide, 9CI, I-130

Curing agents

Calcium chloride ($CaCl_2$), C-39
Fujiglucon, G-153
Sodium carbonate (Na_2CO_3), S-122
Sodium chloride (NaCl), S-123
Sodium erythorbate, I-70

Dough conditioners

Ammonium bicarbonate, C-93
Ammonium chloride ($(NH_4)Cl$), A-313
Ammonium phosphate ($(NH_4)(H_2PO_4)$), A-315
Ammonium phosphate ($(NH_4)_2HPO_4$), A-316
Ammonium sulfate, S-278
Calcium iodate(*V*) ($Ca(IO_3)_2$), C-44
Calcium lactate, JAN, USAN, H-765
Calcium oxide (CaO), C-46
Calcium stearoyl 2-lactylate, L-34
Calcium sulfate, C-54
Cysteine hydrochloride, USAN, C-514
Cysteine; (*R*)-*form*, C-514
2,2-Dihydroperoxypropane, D-343
Ficin, F-36
β-D-Fructofuranosyl α-D-glucopyranoside monooctadecanoate, 9CI, S-263
Magnesium lactate, M-22
Octadecyl fumarate, F-86
Oxirane, O-193
Polysorbate 60, S-159
Potassium bromate(*V*) ($KBrO_3$), P-427
Potassium iodate(*V*) (KIO_3), P-436
1,2-Propanediol, P-471
Sodium stearoyl 2-lactylate, L-34
Sorbitan monolaurate, BAN, USAN, A-335
Subtilisins, S-260
Vitamin C, A-447

Drying agents

Butyl oleate sulfate, B-238
Calcium phosphate ($Ca(HPO_4)$), C-50
Calcium sulfate, C-54
Iron octanoate, O-81
Magnesium carbonate, M-18

Emulsifiers

Alginic acid, A-167
Aluminium dodecanoate, D-1017
Aluminium octanoate, O-81
Ammonium alginate, A-167
Ammonium citrate, C-290
Arabinogalactan, A-393
Calcium alginate, A-167
Calcium citrate, C-290
Calcium dodecanoate, D-1017
Calcium octadecanoate, O-27
Calcium octanoate, O-81
Calcium phosphate ($Ca(HPO_4)$), C-50
Calcium stearoyl 2-lactylate, L-34
1-Carboxyethyl stearate, H-765
Cholic acid, T-536
Crill 43, A-335
Croscarmellose, BAN, INN, C-173
γ-Cyclodextrin, C-447
Decanoic acid, D-41
Deoxycholic acid, D-415
Dihydro-3-(1-octenyl)-2,5-furandione, D-335
Disodium phosphate, D-980
Disodium pyrophosphate, D-981
Docusate sodium, BAN, INN, B-130
β-D-Fructofuranosyl α-D-glucopyranoside monohexadecanoate, 9CI, S-263
β-D-Fructofuranosyl α-D-glucopyranoside monooctadecanoate, 9CI, S-263
Furcelleran, F-142
Ghatti gum, G-89
Glycerol 1,2-di-(9*Z*-octadecenoate), G-239
Glycerol 1,2-dialkanoates, G-239
Glycerol 1,2-dioctadecanoate, G-239
Glycerol 1-octadecanoate, G-236
Graham's salt, S-136
Guar gum, G-347
Gum arabic, A-385
Gum karaya, G-350
Gum tragacanth, G-351
Hexasodium metaphosphate ($P_6O_{18}^{6\ominus}$), H-239
Magnesium dodecanoate, D-1017
Magnesium octadecanoate, O-27
Magnesium octanoate, O-81
Methyl cellulose, C-173
9-Octadecenoic acid; (*Z*)-*form*; Na salt, O-44
Oleic acid, O-44
Pectic acid, P-53
Phosphatidylcholine, P-325
Polysorbate 20, S-159
Polysorbate 40, S-159
Polysorbate 60, S-159
Polysorbate 65, S-159
Polysorbate 80, S-159
Polysorbate 85, S-159
Potassium alginate, A-167

Potassium dodecanoate, D-1017
Potassium octadecanoate, O-27
Potassium octanoate, O-81
Potassium phosphate (K_3PO_4), P-444
1,2-Propanediol, P-471
Propylene glycol alginate, A-167
Propylene glycol stearate, P-471
Sodium alginate, A-167
Sodium aluminium phosphate, S-120
Sodium chloride (NaCl), S-123
Sodium citrate, C-290
Sodium dodecanoate, D-1017
Sodium lactate, JAN, USAN, H-765
Sodium lauryl sulfate, D-1024
Sodium octadecanoate, O-27
Sodium octanoate, O-81
Sodium phosphate ($Na(H_2PO_4)$), S-140
Sodium phosphate (Na_3PO_4), S-141
Sodium phosphinate, S-142
Sodium potassium tartrate, T-27
Sodium stearoyl 2-lactylate, L-34
Sodium tartrate, T-27
Sodium triphosphate ($Na_5(P_3O_{10})$), S-149
Sorbitan monolaurate, BAN, USAN, A-335
Sorbitan monooleate, BAN, USAN, A-335
Sorbitan monopalmitate, BAN, USAN, A-335
Sorbitan monostearate, BAN, USAN, A-335
Sorbitan trioleate, BAN, USAN, A-335
Sorbitan tristearate, BAN, USAN, A-335
2-Stearyl citrate, C-290
Taurocholic acid; Na salt, T-29
Taurocholic acid, T-29
Xanthan, X-1

Encapsulants

Gum arabic, A-385
Maltodextrin, M-39

Enzymes

α-Amylase, A-323
β-Amylase, A-324
Bacillolysin, B-2
Bromelains, B-190
Catalase, C-159
Cellulase, C-172
Ficin, F-36
β-Fructofuranosidase, F-70
β-Galactosidase, G-38
endo-1,3(4)-β-Glucanase, G-148
Glucoamylase, G-151
Glucose oxidase, G-198
Glutaminase, G-210
Lysozyme, L-135
Mannan *endo*-1,4-β-mannosidase, M-65
Pancreatin, P-19
Papain, P-33
Pepsin, P-225
3-Phytase, P-358
Polygalacturonase, P-418
Prophospholipase A_2, P-519
Rennin, R-6
Rizolipase, R-38
Subtilisins, S-260
Tannase, T-11
Trypsin, T-833
endo-1,4-β-Xylanase, X-11

Fat replacers

Glycerol tridecanoate, G-247
Maltodextrin, M-39
Olestra, S-263

Fermentation aids

Ammonium phosphate ($(NH_4)(H_2PO_4)$), A-315
Ammonium phosphate ($(NH_4)_2HPO_4$), A-316
α-Amylase, A-323
Dipotassium phosphate, D-965
Formic acid, F-60
D-*glycero*-D-*manno*-Heptose, H-116
Hydrogen chloride, H-323
Methyl octadecanoate, O-26
Zinc sulfate, Z-17

Filter aids

Acrylamide, P-487
Dextranase, D-98
Fuller's earth, M-748
Sodium chloride (NaCl), S-123
Talc, T-4

Firming agents

Aluminium hydroxide, A-196
Aluminium octadecanoate, O-27
Aluminium sulfate, A-202
Ammonium phosphate ($(NH_4)_2HPO_4$), A-316
Ammonium sulfate, S-278
Amylose, S-219
Calcium acetate, C-36
Calcium chloride ($CaCl_2$), C-39
Calcium gluconate, USAN, G-152
Calcium hydroxide ($Ca(OH)_2$), C-42
Calcium lactate, JAN, USAN, H-765
Calcium lactobionate, L-29
Calcium oxide (CaO), C-46
Calcium phosphate ($Ca(H_2PO_4)_2$), C-49
Calcium sulfate, C-54
Cordycepic acid, M-66
Guar gum, G-347
Gum arabic, A-385
Magnesium gluconate, G-152
Magnesium oxide (MgO), M-23
Sodium alum, A-201
Sodium chloride (NaCl), S-123
Starch; 2-Hydroxypropyl ether, S-219
Starch; Phosphate, S-219
Starch; Unbranched-*form*; Per-Ac, S-219
L-Threaric acid, T-27

Flocculants

Acrylamide, P-487
Fuller's earth, M-748
Palygorskite, P-12
Sodium chloride (NaCl), S-123
Sodium hydroxide (NaOH), S-133
Sodium sulfate decahydrate, S-145

Flour treatment agents

Amylose, S-219
Calcium bromate, C-37
Calcium peroxide (CaO_2), C-48
Chlorine oxide (ClO_2), C-195
Chlorine, C-194
Nitrogen chloride (NCl_3), N-67
Nitrosyl chloride ((NO)Cl), N-74
Nitrosylsulfuric acid, N-75
Polysorbate 40, S-159
Polysorbate 60, S-159
1,2-Propanediol, P-471
Thiamine mononitrate, USAN, T-350

Formulation aids

Acetic acid, A-23
Calcium sulfate, C-54
Cordycepic acid, M-66
γ-Cyclodextrin, C-447
Glycerol 1,2-dialkanoates, G-239
Glycerol triacetate, G-242
Guar gum, G-347
Gum arabic, A-385
2-Hydroxyhexadecanoic acid; (*R*)-*form*, H-490
Potassium hydrogen carbonate, P-433
Potassium hydroxide (KOH), P-435
1,2-Propanediol, P-471
Propylene glycol alginate, A-167
Sodium stearoyl 2-lactylate, L-34
Sodium thiosulfate, S-148
Urea, U-33

Humectants

Calcium chloride ($CaCl_2$), C-39
Erythritol, E-236
FEMA 3029, G-150
Glucose; D-*form*, G-197
Glycerol triacetate, G-242
Glycerol, G-235
Gum arabic, A-385
1,2-Propanediol, P-471
Sodium lactate, JAN, USAN, H-765
Tagatose; D-*form*, T-2
L-Threaric acid, T-27

Leavening/raising agents

Acetophenone, A-27
Ammonium bicarbonate, C-93
Ammonium carbonate, A-312
Ammonium chloride ($(NH_4)Cl$), A-313
Ammonium hydroxide ($(NH_4)(OH)$), A-314
Ammonium phosphate ($(NH_4)(H_2PO_4)$), A-315
Ammonium phosphate ($(NH_4)_2HPO_4$), A-316
Calcium carbonate, C-38
Calcium phosphate ($Ca(H_2PO_4)_2$), C-49
Calcium phosphate ($Ca(HPO_4)$), C-50
Calcium sulfate, C-54
Carbon dioxide, C-90
Coenzyme Q_6, C-317
Cysteine; (*R*)-*form*, C-514
Disodium pyrophosphate, D-981
Fujiglucon, G-153
Fumaric acid, F-86
Magnesium phosphate ($Mg(HPO_4)$), M-25
Potassium bitartrate, T-27
Potassium bromate(*V*) ($KBrO_3$), P-427
Potassium phosphate ($K(H_2PO_4)$), P-443
Sodium alum, A-201
Sodium aluminium phosphate, S-120
Sodium chloride (NaCl), S-123
Sodium hydrogen carbonate, S-130
Sodium phosphate ($Na(H_2PO_4)$), S-140
L-Threaric acid, T-27

Lubricants/release/antisticking agents

Amylose, S-219
Calcium octadecanoate, O-27
Cordycepic acid, M-66
Decanoic acid, D-41
Dodecanoic acid, D-1016
Glycerol 1,2-di-(9*Z*-octadecenoate), G-239
Glycerol 1,2-dialkanoates, G-239
Glycerol 1-octadecanoate, G-236
Guar gum, G-347
Hexadecanoic acid, H-159
Magnesium octadecanoate, O-27
Magnesium oxide (MgO), M-23
Octadecanoic acid, O-26
Octanoic acid, O-80
Oleyl alcohol, O-51
Phosphatidylcholine, P-325
Starch; 2-Hydroxypropyl ether, S-219
Starch; Phosphate, S-219
Starch; Unbranched-*form*; Per-Ac, S-219
Tetradecanoic acid, T-59

Masticatory aids

Calcium phosphate ($Ca(HPO_4)$), C-50
1,3-Di-*O*-methyl-*myo*-inositol, D-812
Gellan gum, G-72
Mutastein, M-819
Octadecanoic acid, O-26
Potassium octadecanoate, O-27
Talc, T-4

Modified starches

2-Chloro-1-propanol; (±)-*form*, C-221
(Chloromethyl)oxirane, C-211

Ethenyl acetate, 9CI, E-246
Methyloxirane, M-527
2,7-Oxepanedione, 9CI, H-227
Starch; 2-Hydroxypropyl ether, S-219
Starch; Carboxymethyl ether, S-219
Starch; Phosphate, S-219
Starch; Unbranched-*form*; Per-Ac, S-219

Oxidising agents

Calcium peroxide (CaO_2), C-48
Hydrogen peroxide (H_2O_2), H-324
Magnesium perchlorate, M-24
Sodium hydroxide (NaOH), S-133

Plasticisers

2-Biphenylol, B-92
Dowicide A, B-92
2-Hydroxy-22-methyltetracosanoic acid, H-617
Polyethylene glycol, P-417

Preservatives

Acetic acid sodium salt (2:1), 9CI, S-119
Acetic acid, A-23
3-Acetyl-4-hydroxy-6-methyl-2*H*-pyran-2-one; Na salt, A-64
3-Acetyl-4-hydroxy-6-methyl-2*H*-pyran-2-one, A-64
Acetylbalchanolide, H-469
8-Acetylegelolide, E-5
Achillicin, D-486
Achimilic acid, A-103
Achimillic acid A, A-104
Achimillic acid B, A-104
Achimillic acid C, A-104
Airbron, A-35
4-Amino-2-methyl-1-naphthol, A-274
Ammonium benzoate, B-32
8-Angeloylegelolide, E-5
Argon, A-407
Ascorbyl palmitate, USAN, A-447
Ascorbyl stearate, A-447
Benzoic acid, B-31
Betonicine, H-423
Biphenyl, B-91
2-Biphenylol, B-92
Boric acid (H_3BO_3), B-169
Boric acid (HBO_2), B-168
Butyl 4-hydroxybenzoate, H-347
Butyl nitrite, B-237
Calcium benzoate, B-32
Calcium hydrogen sulfite, C-41
Calcium lactate, JAN, USAN, H-765
Calcium propionate, P-478
Calcium sorbate, H-172
Calcium sulfite, C-55
Carbon dioxide, C-90
Citric acid, C-290
Cysteine; (*R*)-*form*, C-514
2,4-Decadienoic isobutylamide; (*E*,*E*)-*form*, D-34
2,4,6,8-Decatetraenoic acid dehydropiperidide, D-50
2,4,6-Decatrienoic acid dehydropiperidide; (2*E*,4*E*,6*Z*)-*form*, D-50
Diethyl dicarbonate, D-153
Diethyl fumarate, F-86
1-(2,4-Dihydroxyphenyl)-1-butanone, D-612
Dimethyl carbonate, D-740
Dimethyl dicarbonate, D-153
Dimethyl fumarate, F-86
Disodium ethylenediaminetetraacetate, D-979
Disodium hydrogen citrate, C-290
Disodium pyrophosphate, D-981
Dowicide A, B-92
Edetate disodium, USAN, E-305
Edetate trisodium, USAN, E-305
1,4-Epoxy-5-hydroxy-10(14)-germacren-12,6-olide; (1α,4α,5β,6α,11β*H*)-*form*, E-128
Ethanol, E-245
6-Ethoxy-1,2-dihydro-2,2,4-trimethylquinoline, 9CI, 8CI, D-364
Ethyl hydrogen fumarate, F-86
Ethylparaben, INN, USAN, H-347
Formic acid, F-60
Garbogiol, P-18
Garcinia acid, D-675
Guttiferone E; (-)-*form*, G-356
4-Hexyl-1,3-benzenediol, H-262
Homostachydrine; (*S*)-*form*, H-296
2-Hydroxybenzoic acid, H-345
2-Hydroxypropanoic acid, H-765
Isoachifolidiene, D-490
N-Isobutyl-2,4,8-decatrienamide, D-49
Isocrotonic acid, B-223
Isogarcinol, I-197
Lysozyme, L-135
Manganese hypophosphite, M-59
Methyl 4-hydroxybenzoate, H-347
Millefin, D-480
Millefolide, M-721
Nisin, N-63
2-Nonenoic acid; (*E*)-*form*; Et ester, N-120
1,3-Octanediol; (±)-*form*, O-76
Octanoic acid, O-80
Panosorb, H-172
Paralactic acid, H-765
α-Peroxyachifolide, E-51
Pimaricin, P-371
Potassium benzoate, B-32
Potassium dihydrogen citrate, C-290
Potassium disulfite, P-432
Potassium nitrate (KNO_3), P-439
Potassium nitrite (KNO_2), P-440
Potassium propionate, P-478
Potassium sorbate, H-172
1,2-Propanediol, P-471
Propanoic acid, P-478
Prophenin 1, P-518
Propyl 4-hydroxybenzoate, H-347
Sodium benzoate, B-32
Sodium calcium edetate, BAN, INN, E-305
Sodium chloride (NaCl), S-123
Sodium citrate, C-290
Sodium dihydrogen citrate, C-290
Sodium disulfite, S-127
Sodium hydrogen sulfite, S-132
Sodium nitrate ($NaNO_3$), S-138
Sodium nitrite, S-139
Sodium propionate, P-478
Sodium sorbate, H-172
Sodium sulfite (Na_2SO_3), S-147
Subtilin, S-259
Sucrose, S-263
Sulfur dioxide, S-277
1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane, T-36
2,4-Undecadiene-8,10-diynoic acid 2,3-dehydropiperidide, U-11
2,4-Undecadiene-8,10-diynoic acid isobutylamide, U-11
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Propellants/aerating/whipping agents

Butane, B-208
Carbon dioxide, C-90
Chloropentafluoroethane, C-212
Hydrogen, H-322
2-Methylpropane, M-603
Nitrogen oxide (N_2O), N-68
Nitrogen, N-66
Octafluorocyclobutane, O-63
Propane, P-468
Sodium lauryl sulfate, D-1024
Sodium nitrate ($NaNO_3$), S-138

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1-Hydroxy-1,1-ethanediphosphonic acid, H-448
Sodium borohydride, S-121
Sodium hydroxide (NaOH), S-133
Sodium thiosulfate, S-148
Sorenson's sodium phosphate, D-980

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Calcium acetate, C-36
Calcium gluconate, USAN, G-152
Calcium phosphate ($Ca(H_2PO_4)_2$), C-49
Citric acid; 1-Isopropyl ester, C-290
Citric acid; 2-Isopropyl ester, C-290
Dipotassium phosphate, D-965
Disodium ethylenediaminetetraacetate, D-979
Disodium phosphate; Dodecahydrate, D-980
Disodium phosphate, D-980
Edetate disodium, USAN, E-305
Edetate sodium, USAN, E-305
Fujiglucon, G-153
Gluconic acid; D-*form*; NH_4 salt, G-152
Graham's salt, S-136
Hexasodium metaphosphate ($P_6O_{18}^{6\ominus}$), H-239
myo-Inositol hexakis(phosphate), I-41
Metaphosphoric acid ($H_6P_6O_{18}$); Tri-Ca salt, M-237
[Nitrilotris(methylene)]trisphosphonic acid, N-64
Phosphoric acid, P-331
Potassium diphosphate ($K_4(P_2O_7)$), P-431
Potassium gluconate, G-152
Potassium triphosphate ($K_5(P_3O_{10})$), P-449
Sodium calcium edetate, BAN, INN, E-305
Sodium diphosphate ($Na_4(P_2O_7)$), S-126
Sodium gluconate, G-152
Sodium phosphate ($Na(H_2PO_4)$), S-140
Sodium phosphate (Na_3PO_4), S-141
Sodium triphosphate ($Na_5(P_3O_{10})$), S-149
2-Stearyl citrate, C-290
Tannin, T-12
L-Threaric acid, T-27

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Docusate sodium, BAN, INN, B-130
β-D-Fructofuranosyl α-D-glucopyranoside monooctadecanoate, 9CI, S-263
Oxirane, O-193
Polysorbate 40, S-159
Polysorbate 85, S-159
Sorbitan monolaurate, BAN, USAN, A-335

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Acetic acid, A-23
Acetone, A-25
1,3-Butanediol, B-209
2-Butoxyethanol, B-230
Carbon dioxide, C-90
Citric acid; 1-Isopropyl ester, C-290
1,2-Dichloroethane, D-160
Dichloromethane, D-161
Ethanol, E-245
Ethyl acetate, E-259
Glycerol 1,2-diacetate; (±)-*form*, G-238
Glycerol triacetate, G-242
Glycerol trioctanoate, G-264
Glycerol triundecanoate, G-271
Glycerol, G-235
Hexane, H-226
Methanol, M-243
1,2-Propanediol, P-471
2-Propanol, P-480
Trichloroethylene, T-452
Tridodecylamine, T-495
Triethyl citrate, C-290
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Stabilisers

Agar, A-139
Alginic acid, A-167
2-Aminoheptanedioic acid, A-255
Ammonium alginate, A-167
Amylose, S-219
Arabinogalactan, A-393
Bentonite, B-15
Calcium acetate, C-36
Calcium alginate, A-167

Calcium chloride ($CaCl_2$), C-39
Calcium gluconate, USAN, G-152
Calcium octadecanoate, O-27
Calcium phosphate ($Ca(H_2PO_4)_2$), C-49
Calcium phosphate ($Ca(HPO_4)$), C-50
Calcium sulfate, C-54
Carrageenan, C-128
Cordycepic acid, M-66
Croscarmellose, BAN, INN, C-173
γ-Cyclodextrin, C-447
Dihydro-3-(1-octenyl)-2,5-furandione, D-335
Disodium phosphate, D-980
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4-Ethoxy-3-methoxybenzaldehyde, D-382
Ethyl cellulose, C-173
Furcelleran, F-142
Gelatin, G-71
Gellan gum, G-72
Glycerol 1,2-di-(9*Z*-octadecenoate), G-239
Glycerol 1,2-dialkanoates, G-239
Glycerol 1,2-dioctadecanoate, G-239
Guar gum, G-347
Gum arabic, A-385
Gum tragacanth, G-351
3,3′,4′,5,5′,7-Hexahydroxyflavone; 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-α-L-rhamnopyranoside], 7-*O*-[α-L-rhamnopyranosyl-(1 → 2)-β-D-glucopyranoside], H-205
3-Hydroxy-12-oleanen-29-oic acid; 3α-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 2)[α-L-rhamnopyranosyl-(1 → 4)]-β-D-glucopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 29-*O*-[β-D-glucopyranosyl-(1 → 2)-β-D-glucopyranosyl] ester, H-664
Isoschaftoside 4′-glucoside, I-162
Locust bean gum, L-98
Maltodextrin, M-39
Methyl cellulose, C-173
4-Methyl-2-phenyl-1,3-dioxolane, M-581
Monotropein, M-746
Octadecyl fumarate, F-86
Oleyl alcohol, O-51
Oxirane, O-193
Pectic acid, P-53
3-Phenyl-2-propen-1-ol; (*E*)-*form*, P-313
Phosphoric acid, P-331
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Polysorbate 65, S-159
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Potassium alginate, A-167
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Potassium hydroxide (KOH), P-435
Potassium phosphate (K_3PO_4), P-444
1,2-Propanediol, P-471
Propylene glycol alginate, A-167
Propylene glycol stearate, P-471
Schaftoside 4′-glucoside, S-51
Sodium alginate, A-167
Sodium phosphate (Na_3PO_4), S-141
Sodium phosphinate, S-142
Sodium stearoyl 2-lactylate, L-34
Sodium triphosphate ($Na_5(P_3O_{10})$), S-149
Sorbitan monolaurate, BAN, USAN, A-335
Sorbitan monopalmitate, BAN, USAN, A-335
Sorbitan monostearate, BAN, USAN, A-335
Sorbitan tristearate, BAN, USAN, A-335
Starch; 2-Hydroxypropyl ether, S-219
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Tagatose; D-*form*, T-2
Tetradecanoic acid; Li salt, T-59
1,2,3,6-Tetragalloylglucose; β-D-Pyranose-*form*, T-71
L-Threaric acid, T-27
2,2,6-Trimethylcyclohexanone; (ξ)-*form*, T-747
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Surface finishing agents/coatings/glazes/waxes

Ammonium hydroxide ($(NH_4)(OH)$), A-314
Betavulgaroside VII, H-12
Cordycepic acid, M-66
Dimeticone, D-922
Docusate sodium, BAN, INN, B-130
Gelatin, G-71
Glycerol 1,2-dialkanoates, G-239
Gum arabic, A-385
Paraffin wax, P-39
Zein, Z-11

Surfactants/dispersants/suspending agents/foam stabilisers

1,2,3,5-Benzenetetrol; 1,2,3-Tri-Me ether, 5-*O*-β-D-glucopyranoside, B-22
Calcium chloride ($CaCl_2$), C-39
Calcium stearoyl 2-lactylate, L-34
Cobalt(*II*) sulfate ($CoSO_4$), C-312
Crill 43, A-335
3,16-Dihydroxy-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 2)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-578
3,23-Dihydroxy-12-oleanene-28,30-dioic acid; 3β-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 28-*O*-[α-L-rhamnopyranosyl-(1 → 2)-[β-D-glucopyranosyl-(1 → 3)]-[2*R*-methylbutanoyl-(→ 4)]-β-D-fucopyranosyl] ester, 30-Me ester, D-573
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 3)-[β-D-galactopyranosyl-(1 → 2)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-[β-D-glucopyranosyl-(1 → 3)]-α-L-rhamnopyranosyl-(1 → 2)-3-*O*-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 3)-[β-D-galactopyranosyl-(1 → 2)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-[β-D-glucopyranosyl-(1 → 3)]-α-L-rhamnopyranosyl-(1 → 2)-4-*O*-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 3)-[β-D-galactopyranosyl-(1 → 2)]-β-D-glucuronopyranoside], 28-*O*-[β-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)-4-*O*-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 28-*O*-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[α-L-rhamnopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-[β-D-glucopyranosyl-(1 → 3)]-α-L-rhamnopyranosyl-(1 → 2)-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-[β-D-glucopyranosyl-(1 → 3)]-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
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3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 28-*O*-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598
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3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[6-*O*-acetyl-β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[6-*O*-acetyl-β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[α-L-rhamnopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-[β-D-glucopyranosyl-(1 → 3)]-α-L-rhamnopyranosyl-(1 → 2)-3-*O*-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-[β-D-glucopyranosyl-(1 → 3)]-α-L-rhamnopyranosyl-(1 → 2)-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-apiofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-[β-D-glucopyranosyl-(1 → 3)]-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-xylopyranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[6-*O*-acetyl-β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[6-*O*-acetyl-β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-xylopyranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-4-*O*-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)-4-*O*-[5-[[5-(α-L-arabinofuranosyloxy)-3-hydroxy-6-methyl-1-oxooctyl]oxy]-3-hydroxy-6-methyl-1-oxooctyl]-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 3)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[6-*O*-acetyl-β-D-glucopyranosyl-(1 → 3)-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)]-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Galactopyranosyl-(1 → 2)-[β-D-xylopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], 28-*O*-[6-*O*-acetyl-β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)]-4-*O*-acetyl-β-D-fucopyranosyl] ester, D-598

3,16-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Xylopyranosyl-(1 → 3)-[β-D-galactopyranosyl-(1 → 2)]-β-D-glucuronopyranoside], D-598

Docusate sodium, BAN, INN, B-130

Dodecanoic acid, D-1016

4-Dodecylbenzenesulfonic acid; Na salt, D-1027

β-D-Fructofuranosyl α-D-glucopyranoside monohexadecanoate, 9CI, S-263

β-D-Fructofuranosyl α-D-glucopyranoside monooctadecanoate, 9CI, S-263

Glycocholic acid; Na salt, G-282

7-Hydroxy-4-methyl-1(3*H*)-isobenzofuranone; *O*-[β-L-Arabinopyranosyl-(1 → 6)-β-D-glucopyranoside], H-591

Oxirane, O-193

Polyethylene glycol, P-417

Polysorbate 20, S-159

Polysorbate 40, S-159

Polysorbate 60, S-159

Polysorbate 80, S-159

Polysorbate 85, S-159

Potassium diphosphate ($K_4(P_2O_7)$), P-431

Prosapogenin, D-598

QS 18, Q-1

QS 21, Q-1

Quillajasaponin, D-598

Saponin S13, D-573

Sodium diphosphate ($Na_4(P_2O_7)$), S-126

Sodium lauryl sulfate, D-1024

Sodium stearoyl 2-lactylate, L-34

Triethyl citrate, C-290

Triton X 305, T-825

β-D-Xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-D-fucose, X-26

Sweeteners

Acesulfame K, A-18

Acesulfame, A-18

7β-Acetoxy-12,14-labdadiene-6α,8β-diol, L-8

6α-Acetoxy-12,14-labdadiene-7β,8β-diol, L-8

6-Acetyl-5-hydroxy-4-methyl-2*H*-1-benzopyran-2-one, A-63

6″-Acetylliquiritin, D-470

Achyranthoside D, O-146

Alitame, A-168

2-Amino-*N*-(2,2,4,4-tetramethyl-3-thietanyl)-propanamide; (*R*)-*form*, A-305

Ammonium glycyrrhizinate, G-291

Aspartame, A-461

N^{α}-Aspartylphenylalanine; L-L-*form*, A-464

Australigenin, S-194

Austroinulin, L-8

N-Benzoyl-β-alanine, 9CI, A-295

Betavulgarin glucoside, T-223

Betavulgarin xyloside, T-223

Betavulgaroside I, B-71

Betavulgaroside II, B-71

Betavulgaroside IV, O-147

Betavulgaroside IX, O-146

Betavulgaroside VI, H-11

Betavulgaroside VII, H-12

Betavulgaroside VIII, H-636

Betavulgaroside X, H-636

Calenduloside E, O-147

6-Chlorotryptophan; (±)-*form*, C-225

Cordycepic acid, M-66

Cyclohexylsulfamic acid, C-472

Cyclotetradecane, C-506

11-Deoxoglycyrrhetinic acid, H-665

Dhurrin 6′-glucoside, H-504

2,6-Diamino-5-hydroxyhexanoic acid; (2*S*,5*S*)-*form*; N^6-Ac, D-118

5,7-Dihydro-2-methylthieno[3,4-*d*]pyrimidine, D-324

7,8-Dihydro-3-methylpyrrolo[1,2-*a*]pyrimidin-2(6*H*)-one, D-321

3,4-Dihydro-8-hydroxy-3-(3-hydroxy-4-methoxyphenyl)-1*H*-2-benzopyran-1-one, D-614

3,9-Dihydroxy-1-methoxy-2-prenylpterocarpene, T-694

3,9-Dihydroxy-1-methoxycoumestan, T-537

3β,24-Dihydroxy-11,13(18)-oleanadien-30,22β-olide, T-643

3,24-Dihydroxy-11,13(18)-oleanadien-30-oic acid; 3β-*form*; Me ester, D-569

3,21-Dihydroxy-11-oxo-12-oleanen-29,18-olide, T-660

3β,24-Dihydroxy-11-oxo-12-oleanen-30,22β-olide, T-661

6′,7-Dihydroxy-2′,4′-dimethoxy-3′-prenylflavanone, T-264

3-(3,4-Dihydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)-2-propen-1-one, T-146

2′,7-Dihydroxy-3′,4′-dimethoxyisoflavan, T-217

2′,7-Dihydroxy-3′,4′-methylenedioxyisoflavone, T-221

2′,7-Dihydroxy-4′,5-dimethoxy-3′-prenylisoflavan, T-273

2′,7-Dihydroxy-4′,6′-dimethoxy-3′-prenylisoflavone, T-278

5,7-Dihydroxy-4′-methoxy-6-prenylisoflavone, T-688

2′,7-Dihydroxy-4′-methoxyisoflavan; (*R*)-*form*; 7-*O*-β-D-Glucopyranoside, D-540

2′,4′-Dihydroxy-5,7-dimethoxy-3′,6-diprenylisoflavan, T-164

5,7-Dihydroxy-6-prenylflavanone; (*S*)-*form*, D-669

4′,5-Dihydroxy-7-methoxy-6-prenylisoflavone, T-688

4′,5-Dihydroxy-7-methoxyisoflavone, D-541

3,24-Dihydroxy-9(11),12-oleanadien-30-oic acid; 3β-*form*, D-568

3,4-Dihydroxybenzoyl β-D-xylopyranoside, D-390

4′,7-Dihydroxyflavanone; (*S*)-*form*; 4′-*O*-[3-*O*-Acetyl-β-D-apiofuranosyl-(1 → 2)-β-D-glucopyranoside], D-470

4′,7-Dihydroxyflavanone; (*S*)-*form*; 7-*O*-[β-D-Apiofuranosyl-(1 → 2)-β-D-glucopyranoside], D-470

2-(3,4-Dihydroxyphenyl)-4,6-dimethoxy-5-prenylbenzofuran, D-622

2-(3,4-Dihydroxyphenyl)-6-hydroxy-4-methoxy-5-prenylbenzofuran, D-622

2′,5-Dimethoxy-6,7-methylenedioxyflavanone, T-188

E953, G-179

Erythritol, E-236
(4-Ethoxyphenyl)urea, E-258
5-Ethoxysorgoleone 358, D-609
2-Ethyl-3-hydroxy-4*H*-pyran-4-one, E-320
Fagopyritol B_2, I-40
FEMA 3029, G-150
β-D-Fructofuranosyl β-D-galactopyranosyl-(1 → 4)-α-D-glucopyranoside, F-71
Fructose; D-*form*, F-75
α-D-Galactopyranosyl-(1 → 4)-β-D-galactopyranosyl-(1 → 4)-D-glucose, G-14
Gancaonin C, G-55
Gancaonin D, G-55
Gancaonin R, G-56
Gancaonin U, G-57
Gancaonin V, G-54
Gancaonin X, N-40
Glabrene, G-134
Glabric acid, D-601
Glabridin; (*R*)-*form*, G-135
Glabrone, G-140
Glicophenone, L-84
Glucoliquiritin apioside, D-470
1-*O*-α-D-Glucopyranosyl-D-fructose, G-154
5-*O*-α-D-Glucopyranosyl-D-fructose, G-155
4-*O*-α-D-Glucopyranosyl-D-glucitol, G-156
6-*O*-α-D-Glucopyranosyl-D-glucitol, G-157
Glucose; D-*form*, G-197
Glycyrrhizaflavonol A, G-289
Glycyrrhizaisoflavone C, G-290
Glyinflanin H, G-292
Glypallidifloric acid, H-660
Glyphoside, I-158
Glyzarin, G-293
Hernandulcin, H-368
Hispaglabridin A; (*R*)-*form*, H-284
Hispaglabridin B; (*R*)-*form*, H-285
9-Hydroxy-1,3-dimethoxy-2-prenylpterocarpan, T-694
3β-Hydroxy-11-oxo-12-oleanen-29,18α-olide, D-599
3-Hydroxy-11-oxo-12-oleanen-30-oic acid; (3β,18β)-*form*; Me ester, H-694
3β-Hydroxy-12-oleanen-30,22β-olide, O-141
7-Hydroxy-2-methylisoflavone; Ac, H-592
7-Hydroxy-2-methylisoflavone, H-592
3′-Hydroxy-4′-methoxyglabridin, G-135
5-Hydroxy-4-methoxy-5-(1-oxo-9,12,15-hexadecatrienyl)-2(5*H*)-furanone, H-551
3-(2-Hydroxy-4-methoxyphenyl)-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, 9CI, K-13
2-Hydroxy-5-methoxy-3-(8,11,14-pentadecatrienyl)-1,4-benzoquinone, D-609
3-Hydroxy-9-methoxy-4-prenylpterocarpan, D-671
3-Hydroxyglabrol, D-440
18α-Hydroxyglycyrrhetic acid, D-600
24-Hydroxyglycyrrhetic acid, D-604
28-Hydroxyglycyrrhetic acid, D-606
24-Hydroxyliquiritic acid, D-603
3-(4-Hydroxyphenyl)-1-phenyl-2-propen-1-one, H-736
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Isoglycycoumarin, I-91
Isoliquiritin, T-534
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Kanzonol H, K-7
Kanzonol I, K-4
Kanzonol J, K-8
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Kanzonol M, K-10
Kanzonol N, K-10
Kanzonol O, K-11
Kanzonol Q, X-6
Kanzonol T, I-78
Kanzonol U, K-12
Kanzonol V, K-5
Kanzonol W, K-13
Kanzonol Y; (*R*)-*form*, K-14
Kanzonol Z, K-15
Kenposide B, L-55
Lactitol, L-24
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Licoagrochalcone D, L-76
Licoagrodin, L-77
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Licoagrone, L-79
Licoagroside A, P-150
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Licocoumarin A, L-81
Licofuranocoumarin, L-82
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3-Lupanol; 3β-*form*, L-115
Maltoheptaose, M-40
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Maltopentaose, M-42
Maltose, M-43
Maltotetraose, M-44
Maltotriose, M-45
Melizame, M-110
7-Methoxy-2-methylisoflavone, H-592
3-Methoxy-4-oxo-5-(8,11,14-pentadecatrienyl)-2-hexenedioic acid; Di-Me ester, M-267
4′-Methoxybenzophenone-2-carboxylic acid, H-348
1-Methoxyphaseollin, P-241
Methyl 3-hydroxy-11-oxo-12-oleanen-29,22α-olid-27-oate, D-596
3-Methyl-3-hepten-2-one, M-467
2′-*O*-Methylglabridin, G-135
4′-*O*-Methylglabridin, G-135
4′-*O*-Methylglucoliquiritigenin, D-470
Monatin; (2*S*,4*S*)-*form*, M-737
Monoglucuronylglycyrrhetinic acid, H-694
Neohesperidin dihydrochalcone, N-35
Neoisoliquiritin, T-534
Neokestose, N-36
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Neotame, A-464
5-Nitro-2-propoxyaniline, A-278
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3,3′,4′,5,7-Pentahydroxy-5′-prenylflavone, P-169
3,3′,4′,5,7-Pentahydroxy-6-prenylflavone, P-170
3′,4,4′,5,7-Pentahydroxyflavan, P-105
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8-Prenylphaseollinisoflavan; (*S*)-*form*, P-460
Rhamnoisoliquiritin, T-534
Saccharin calcium, USAN, S-2
Saccharin sodium, USAN, S-2
Saccharin; NH_4 salt (1:1), S-2
Saccharin, S-2
Shinflavanone, E-361
Shinpterocarpin; (-)-*form*, S-98
Sodium cyclamate, BAN, C-472
Sorghumol, A-401
Sorgolactone, S-161
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Sterebin G, L-4
Sterebin H, L-4
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Tagatose; D-*form*, T-2
Talc, T-4
5,6,7,8-Tetrahydro-2,4-dimethylquinoline, T-84
5,6,7,8-Tetrahydro-4-methylquinoline, T-108
3,3′,4,4′-Tetrahydroxy-2-methoxychalcone, P-93
2′,4′,5,7-Tetrahydroxy-3′,6-diprenylisoflavanone; (±)-*form*, T-165
2′,4′,5,7-Tetrahydroxy-3′,6-diprenylisoflavanone, T-165
2′,4′,5,7-Tetrahydroxy-3′,8-diprenylisoflavanone; (±)-*form*, T-166
3,4′,5,7-Tetrahydroxy-3′-methoxy-6-prenylflavone, P-170
3,4′,5,7-Tetrahydroxy-3′-prenylflavone, T-269
4′,5,5′,6-Tetrahydroxy-3-methoxy-2′-prenylflavone, P-172
3′,4′,5,7-Tetrahydroxy-3-methoxy-5′-prenylflavone, P-169
3′,4′,5,7-Tetrahydroxy-5′,6-diprenylisoflavone, T-168
3′,4′,5,7-Tetrahydroxy-5′,8-diprenylflavanone; (*S*)-*form*, T-162
3′,4′,5,7-Tetrahydroxy-5′,8-diprenylisoflavone, T-169
3,4′,5,7-Tetrahydroxy-6-prenylflavone, T-270
3′,4′,5,7-Tetrahydroxy-6-prenylflavone, T-271
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Thaumatin, T-327
α,α-Trehalose, T-430
1,2,3-Tri-*O*-galloyl-4,6-(*S*)-hexahydroxydiphenoyl-β-D-glucopyranose, H-193
2,3,23-Trihydroxy-12-oleanen-28-oic acid; (2β,3β)-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 3)-β-D-glucuronopyranoside], 28-*O*-β-D-glucopyranosyl ester, T-647
6α,7β,8α-Trihydroxy-14,15-dinor-11-labden-13-one, D-435
3′,4,4′-Trihydroxy-2-methoxy-3-prenylchalcone, T-262
4′,5,7-Trihydroxy-3′,6-diprenylflavone, T-556
2′,4′,7-Trihydroxy-3′,8-diprenylisoflavan; (*R*)-*form*, T-557
4′,5,7-Trihydroxy-3′-prenylflavanone; (*S*)-*form*, T-681
2′,4,4′-Trihydroxy-3-prenylchalcone; (*E*)-*form*, T-679
2′,5,7-Trihydroxy-4′-methoxy-6-prenylisoflavone, T-276
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2′,4′,7-Trihydroxy-5-methoxy-3′,6-diprenylisoflavan, T-164
2′,4′,7-Trihydroxy-6′-methoxy-3′-prenylisoflavone, T-278
2′,4′,5-Trihydroxy-7-methoxy-3′,6-diprenylisoflavanone, T-165
2′,4′,5-Trihydroxy-7-methoxy-3′,6-diprenylisoflavone, T-167
3′,4′,6-Trihydroxy-7-prenylaurone, T-678
2,4,4′-Trihydroxychalcone; (*E*)-*form*, T-533
Glycyrrhiza Triterpene, T-819
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Xylitol, X-12
Xylose; D-*form*, X-29

Tenderisers/tissue softening agents

Bromelains, B-190
Ficin, F-36

Papain, P-33
Subtilisins, S-260
Trypsin, T-833

Texturisers

Alginic acid, A-167
Ammonium bicarbonate, C-93
Calcium chloride ($CaCl_2$), C-39
Calcium gluconate, USAN, G-152
Calcium oxide (CaO), C-46
Calcium stearoyl 2-lactylate, L-34
Calcium sulfate, C-54
Cordycepic acid, M-66
β-D-Fructofuranosyl α-D-glucopyranoside monohexadecanoate, 9CI, S-263
Glycerol 1,2-dialkanoates, G-239
Glycerol 1-octadecanoate, G-236
Graham's salt, S-136
Gum arabic, A-385
Hexasodium metaphosphate ($P_6O_{18}^{6\ominus}$), H-239
Mannan, M-64
Potassium triphosphate ($K_5(P_3O_{10})$), P-449
Sodium chloride (NaCl), S-123
Sodium stearoyl 2-lactylate, L-34
Sodium triphosphate ($Na_5(P_3O_{10})$), S-149
Sulfur dioxide, S-277
Tagatose; D-*form*, T-2

Thickeners/viscosity modifiers/gelling/stiffening agents

Agar, A-139
Albafuran C, A-154
Albanin F, A-158
Alginic acid, A-167
2-Aminoheptanedioic acid, A-255
Ammonium alginate, A-167
Amylose, S-219
Calcium acetate, C-36
Calcium alginate, A-167
Calcium chloride ($CaCl_2$), C-39
Calcium octadecanoate, O-27
Calcium phosphate ($Ca(H_2PO_4)_2$), C-49
Calcium phosphate ($Ca(HPO_4)$), C-50
Calcium sulfate, C-54
Carrageenan, C-128
Cellulose sulfate, C-173
Cordycepic acid, M-66
Croscarmellose, BAN, INN, C-173
Dextrin, D-101
3′,7-Dihydroxy-2′,4′-dimethoxyisoflavan; (±)-*form*, D-429
3-Epikatonic acid, H-664
Erythritol, E-236
Ethyl cellulose, C-173
Fucose; L-*form*, F-81
Furcelleran, F-142
2-*O*-β-D-Galactopyranosyl-D-xylose, G-29
Gelatin, G-71
Gellan gum, G-72
4-*O*-α-D-Glucopyranuronosyl-D-galactose, G-192
4-*O*-β-D-Glucopyranuronosyl-L-fucose, G-190
Guar gum, G-347
Gum karaya, G-350
Gum tragacanth, G-351
3,3′,4′,5,5′,7-Hexahydroxyflavone; 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-α-L-rhamnopyranoside], 7-*O*-[α-L-rhamnopyranosyl-(1 → 2)-β-D-glucopyranoside], H-205
3-Hydroxy-12-oleanen-29-oic acid; 3α-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 2)[α-L-rhamnopyranosyl-(1 → 4)]-β-D-glucopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 29-*O*-[β-D-glucopyranosyl-(1 → 2)-β-D-glucopyranosyl] ester, H-664
Hydroxyethyl methyl cellulose, C-173
Hydroxypropyl methyl cellulose, C-173
Isoschaftoside 4′-glucoside, I-162
Lanosterol, L-44
Locust bean gum, L-98
Maltodextrin, M-39
Maltoheptaose, M-40
Maltohexaose, M-41
Maltopentaose, M-42
Maltotetraose, M-44
Maltotriose, M-45
Mannan, M-64
Methyl cellulose, C-173
1-Octadecanol, O-28
Pectic acid, P-53
Phosphoric acid, P-331
Potassium alginate, A-167
Potassium chloride, P-430
Potassium diphosphate ($K_4(P_2O_7)$), P-431
Potassium hydroxide (KOH), P-435
Propylene glycol alginate, A-167
Rennin, R-6
Schaftoside 4′-glucoside, S-51
Scleroglucan, S-52
Sodium alginate, A-167
Sodium diphosphate ($Na_4(P_2O_7)$), S-126
Sodium triphosphate ($Na_5(P_3O_{10})$), S-149
Soyasapogenol B, O-139
Starch; 2-Hydroxypropyl ether, S-219
Starch; Carboxymethyl ether, S-219
Starch; Phosphate, S-219
Starch; Unbranched-*form*; Per-Ac, S-219
Sucrose, S-263
1,2,3,6-Tetragalloylglucose; β-D-Pyranose-*form*, T-71
2,2,6-Trimethylcyclohexanone; (ξ)-*form*, T-747
Xanthan, X-1
Xenognosin A, X-7

Unspecified food additives

7-Acetoxy-6-methoxycoumarin, H-547
2,3-Dihydroxy-5-undecyl-1,4-benzoquinone, D-704
1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-3-phenyl-2-propen-1-one, T-627
4-*O*-α-D-Galactopyranuronosyl-D-galactose, G-32
3,3′,4′,5,5′,7-Hexahydroxyflavone; 3-*O*-(3,4-Di-*O*-acetyl-α-L-rhamnopyranoside), H-205
2-Hydroxy-5-methoxy-3-undecyl-1,4-benzoquinone, D-705
7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, H-547
Maltobionic acid, M-38
Myricetin 7-rhamnoside, H-205
2,4-Nonadien-1-ol, N-99
6-Octenal, O-92
Quercitrin; 4′′-*O*-Glucopyranosyl, 7-*O*-[α-L-rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], Q-7
Riboflavine 2′,3′,4′,5′-tetrabutanoate, 9CI, R-32
1,2,8-Trihydroxy-3-methylanthraquinone, T-622

Food flavours and odours

Astringent flavours

Acetic acid sodium salt (2:1), 9CI, S-119
Chrysaloin, A-190
1-*O*-Cinnamoylglucose; β-D-(*E*)-*form*, C-266
Epicatechin(4β → 8)epicatechin(2β → 7,4β → 8)epicatechin(4β → 8)epicatechin(4β → 8)catechin, P-131
Epicatechin(4β → 8)epicatechin(2β → 7,4β → 8)epicatechin(4β → 8)epicatechin(4β → 8)epicatechin, P-131
Epicatechin-(4β → 8)-epicatechin-(2β → 7,4β → 8)-catechin, P-127
Fumaric acid, F-86
Hexanoic acid, H-234
3-Hydroxy-2-methyl-4*H*-pyran-4-one, H-609
4-Hydroxy-2-oxobutanoic acid, H-675
4-Hydroxybenzyl isothiocyanate, H-359
9-(Methylthio)nonanenitrile, 9CI, M-220
8-(Methylthio)octanenitrile, 9CI, M-221
Procyanidin B_6, P-120
Procyanidin B_7, P-120
Procyanidin B_8, P-120
Quinine, Q-11
Sodium acetate, S-119
Tannin, T-12
Tetronasin, T-323

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Aloin, A-190
Aloinoside A, A-190
Aloinoside B, A-190
Amygdalin, H-718
Benzaldehyde, B-16
Benzyl acetate, B-43
Butyl levulinate, O-239
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Cascaroside B, A-190
Cascaroside C, A-190
Cascaroside D, A-190
Cascaroside E, A-190
Cascaroside F, A-190
Clerosterol, S-227
Cucurbita-5,24-diene-3,7,23-triol; (3β,7β,22ξ)-*form*; 7-*O*-β-D-Glucopyranoside, C-385
Cyclo(alanylvalyl); (3ξ,6ξ)-*form*, C-415
Cyclo(leucylprolyl); (3*S*,8*aS*)-*form*, C-476
Cyclo(prolylalanyl); (3*S*,8*aS*)-*form*, C-495
4-Deoxycohumulone, D-80
11-Dihydro-12-norneoquassin, N-56
3,4-Dihydro-2*H*-1-benzopyran-2-one, D-222
1,8-Dihydroxy-3-hydroxymethylanthraquinone; 8-*O*-β-D-Glucopyranoside, D-503
1,8-Dihydroxy-3-hydroxymethylanthraquinone, D-503
1,2-Dimethoxy-4-(1-propenyl)benzene, 9CI, P-503
1,2-Dimethoxy-4-(2-propenyl)benzene, P-504
1,4-Dimethoxybenzene, D-737
3,7-Dimethyl-1-octanol; (*R*)-*form*, D-845
α-Eleostearic acid, O-34
Epicatechin-(2β → 5,4β → 6)*ent*-epicatechin, P-118
13β,28-Epoxy-11-ursen-3-one, E-191
5,6-Epoxy-7-megastigmene-3,9-diol; (3α,5α,6α,7*E*,9ξ)-*form*; 3-*O*-β-D-Glucopyranoside, E-148
Ethyl glucoside; β-D-Pyranose-*form*, E-268
4-Ethylbenzaldehyde, E-284
FEMA 2423, O-243
FEMA 3038, S-263
Frangulin A, T-624
11-α-*O*-β-D-Glucopyranosyl-16α-*O*-methylneoquassin, N-55
7-Glucosyloxy-5-hydroxy-6-methoxycoumarin, T-522
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Goyaglycoside c, E-71
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Goyaglycoside e, E-69
Goyaglycoside f, E-70
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Goyasaponin II, H-695
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Higenamine; (*R*)-*form*, H-282
12α-Hydroxy-13,18-dehyroparain, N-57
5-Hydroxy-4-methoxy-3-methyl-2,6-canthinedione, I-31
5-Hydroxy-4-methoxy-6-canthinone 3-*N*-oxide, N-58
7-Hydroxy-8-*O*-methylaloin A, A-190
7-Hydroxy-8-*O*-methylaloin B, A-190
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Isoliensinine, N-21
Kaempferol 3-*O*-α-L-rhamnofuranoside, T-206
Kaempferol 3-arabinofuranoside 7-rhamnofuranoside, T-206
Liensinine, N-21
Lotusine, H-282
Menthyl isovalerate, M-149
2-Methoxy-6*H*-indolo[3,2,1-*de*][1,5]naphthyridin-6-one, 9CI, H-377
Methyl 3-methylbutanoate, M-331
3-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one, M-641
(4-Methylphenyl)acetaldehyde, M-575
2-Methylpropyl 2-hydroxybenzoate, H-345
1α-*O*-Methylquassin, Q-2
Momorcharaside A, C-389
Momorcharaside B, C-389
Momordenol, H-787
Momordicilin, H-829
Momordicin I, T-542
Momordicin II, T-542
Momordicoside A, C-389
Momordicoside B, C-389
Momordicoside C, C-390
Momordicoside D, C-386
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Momordicoside F_2, E-69
Momordicoside G, E-69
Momordicoside I, E-69
Momordicoside K, T-543
Momordicoside L, T-543
Momordin a, M-734
Momordol, M-735
Momoridcin, D-715
Neferine, N-21
Neohesperidin, T-614
Nigakihemiacetal B; 16-Epimer, 16-Me ether, N-55
Nigakihemiacetal B, N-55
Nigakinone, N-58
Nonyl octanoate, N-110
Palmidin A, P-9
Palmidin B, P-9
Palmidin C, P-9
Pavetannin A_2, P-461
2,3,4,5,6-Penta-*O*-acetyl-D-glucose, G-197
2-Phenyl-2-butenal; (*E*)-*form*, P-262
2-Phenylethanol, P-273
Proanthocyanidin $A_{5'}$, P-461
Quassimarin, S-107
Quassin, Q-2
Quassinol, Q-3
Quinine bisulfate, Q-11
Quinine sulfate, JAN, USAN, Q-11
α-Rhamnorobin, T-206
β-Sinensal, F-5
Stigmast-4-en-3-one, S-247
Stigmasta-5,25-dien-3-ol; (3β,24*S*)-*form*; 3-*O*-β-D-Glucopyranoside, S-227
Stigmasta-7,22,25-trien-3-ol; (3β,5α,22*E*,24*S*)-*form*; *O*-β-D-Glucopyranoside, S-238
Stigmasta-7,22,25-trien-3-ol; (3β,5α,22*E*,24*S*)-*form*, S-238
Stigmasta-7,25-dien-3-ol; (3β,5α,24*S*)-*form*, S-231
α-Terpinyl anthranilate, M-175
1,2,3,4-Tetrahydro-6,7-dihydroxy-1-methylisoquinoline; (ξ)-*form*, T-77
2,3,6,7-Tetrahydro-7-methylcyclopent[*b*]azepin-8(1*H*)-one, T-99
3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,3′,5,5′,7-pentahydroxyflavan; (2*S*,2′*R*,3*S*,3′*R*,4*S*)-*form*, T-196
Theobromine, T-342
Thiamine hydrochloride, USAN, T-350
Tolualdehyde glyceryl acetal, T-422
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1,3,8-Trihydroxy-6-methylanthraquinone, T-624
3,7,25-Trihydroxycucurbita-5,23-dien-19-al; (3β,7β,23*E*)-*form*; 25-Me ether, T-543
1,3,3-Trimethylbicyclo[2.2.1]heptan-2-ol, T-737
Momordica charantia Trypsin inhibitor I, T-837
Momordica charantia Trypsin inhibitor II, T-840
Momordica charantia Trypsin inhibitor III, T-841

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Acetaldehyde, A-20
Aceteugenol, M-273
Acetophenone, A-27
3-Acetoxy-3-methyl-1-phenylbutane, M-578
Acetyl tributyl citrate, C-290
3-Acetyl-2,7-naphthyridine, A-83
1-[1-(Acetyloxy)-1-cyclohexyl]ethanone, 9CI, A-34
S-[1-[2-(Acetyloxy)ethyl]butyl] ethanethioate, M-210
5-Acetyltetrahydro-2(3*H*)-furanone; (ξ)-*form*, A-91
Acetylvalerenolic acid, H-832
Acevaltrate, INN, V-11
1-α-Acevaltrate, V-11
Aconitic acid; (*E*)-*form*, A-108
Actinidine; (*S*)-*form*, A-120
Allyl 3-cyclohexylpropionate, C-463
Allyl butyrate, B-218
Allyl cinnamate, P-312
Allyl cyclohexylacetate, C-457
Allyl phenoxyacetate, P-253
Allyl propionate, P-478
Allyl tiglate, M-340
Allyl undecylenate, U-27
α-Amylcinnamyl acetate, B-58
α-Amylcinnamyl formate, B-58
α-Amylcinnamyl isovalerate, B-58
Anapear, O-58
Anisoxide; (±)-*form*, A-338
Anisyl acetate, H-357
Benzoin; (±)-*form*, B-33
Benzophenone, B-34
Benzyl 3-methylbutanoate, M-331
Benzyl ethyl ether, B-46
Benzyl formate, B-47
Benzyl propanoate, P-478
Benzyl salicylate, H-345
Benzyl tiglate, M-340
2-Benzyl-4,5-dimethyl-1,3-dioxolane, B-54
3-Benzyl-4-heptanone, B-56
2-Benzylidene-1-heptanol, B-58
1-Benzyloxy-1-(2-methoxyethoxy)ethane, B-60
[2,2-Bis(2-methylpropoxy)ethyl]benzene, 9CI, P-257
1,6-Bis(4-methoxyphenyl)-1,5-hexadiene; (*E*,*E*)-*form*, B-147
2,4-Bis(4-methoxyphenyl)-5-methyl-1,3-dioxolane, H-737
2,6,10-Bisabolatriene, B-107
2,7,10-Bisabolatriene, B-108
2,7(14),10-Bisabolatriene, B-109
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Bornyl formate, B-171
Bornyl isovalerate, B-171
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Butyl 2-aminobenzoate, A-217
Butyl 2-decenoate, D-57
Butyl 2-methylbutanoate, M-330
Butyl 2-methylpropanoate, M-605
Butyl 3-methylbutanoate, M-331
Butyl acetate, B-219
Butyl acetoacetate, O-199
Butyl butyrate, B-218
Butyl cinnamate, P-312
Butyl dodecanoate, D-1016
Butyl formate, F-60
Butyl heptanoate, H-93
Butyl hexanoate, H-234
Butyl lactate, H-765
Butyl octadecanoate, O-26
Butyl pentanoate, P-190
Butyl propionate, P-478
Butyl undecylenate, U-27
3-Butyl-1(3*H*)-isobenzofuranone; (*S*)-*form*, B-252
5(6)-Butyl-1,4-dioxan-2-one, B-248
2-Butyl-3-phenyl-2-propen-1-al, B-260
4(15),5,11-Cadinatriene, C-11
3′′-*O*-Caffeoylcosmosiin, C-362
Campholenic alcohol; (ξ)-*form*, C-68
3-Carene, C-105
Carvyl propionate, M-128
β-Caryophyllene alcohol; Ac, C-137
Cinnamyl acetate, P-313
Cinnamyl butyrate, P-313
Cinnamyl cinnamate, P-312
Cinnamyl formate, P-313
Cinnamyl isobutyrate, P-313
Cinnamyl isovalerate, P-313
Cinnamyl propionate, P-313
Citronellyl butyrate, D-857
Citronellyl formate, D-857
Citronellyl phenylacetate, D-857
Citronellyl propionate, D-857
Clarycet, T-105
Cucurbic acid; 6,7-Diepimer, *O*-β-D-glucopyranoside, C-383
Cuelure, H-720
Cyclohexyl 2-aminobenzoate, A-217
Cyclohexyl 3-methylbutanoate, C-465
Cyclohexyl butanoate, C-465
Cyclohexyl cinnamate, P-312
Cyclohexyl pentanoate, C-465
Deacetylisovaltrate, V-11
2,4-Decadienoic acid; (2*Z*,4*E*)-*form*; Et ester, D-32
Decanal, D-39
1-Decanol, D-42
3-Decen-2-one; (*E*)-*form*, D-64
2-Decenal, D-51
2-Decenoic acid; (*E*)-*form*; Me ester, D-57
Decyl acetate, D-42
8,9-Dehydrotheaspirone; (ξ)-*form*, D-75
5-Deoxymyricanone, M-833
3,3′-Di-*O*-galloylprodelphinidin B_5, P-120
Dibenzyl ether, D-133
Dibutyl decanedioate, D-40
8,8-Diethoxy-2,6-dimethyl-2-octanol, 9CI, H-417
1,1-Diethoxy-3,7-dimethyl-2,6-octadiene, D-822
1,1-Diethoxyethane, D-192
Diethyl malonate, D-194
2,5-Diethyltetrahydrofuran, D-208
3,3′-Digalloylprodelphinidin B_1, H-199
4,5-Dihydro-1-benzoxepin-3(2*H*)-one, D-223
6,7-Dihydro-4-(hydroxymethyl)-2-(*p*-hydroxyphenethyl)-7-methyl-5*H*-2-pyrindinium, D-271
Dihydro-5-methyl-2(3*H*)-furanone, D-301
Dihydro-5-octyl-2(3*H*)-furanone; (ξ)-*form*, D-338
Dihydro-5-propyl-2(3*H*)-furanone; (±)-*form*, D-347
5,6-Dihydro-6-pentyl-2*H*-pyran-2-one, D-342
Dihydrocarveol acetate, M-180
Dihydrovaltrate, V-11
3′,7-Dihydroxy-4′,8-dimethoxyisoflavone, T-225
3′,7-Dihydroxy-4′-methoxyisoflavanone, T-596
4′,7-Dihydroxyflavanone; (*S*)-*form*, D-470
2-(3,4-Dihydroxyphenyl)-1,3-benzodioxole-5-carboxaldehyde; (±)-*form*, D-611
3-(3,4-Dihydroxyphenyl)-1-propanol; 3′-*O*-β-D-Glucopyranoside, D-649
2-(2,4-Dihydroxyphenyl)-5,6-dimethoxybenzofuran, D-617
2-(3,4-Dihydroxyphenyl)ethenol; (*Z*)-*form*; 1-*O*-3,4-Dihydroxycinnamoyl(*E*-), D-628
Diisopropyl disulfide, D-722
6,7-Dimethoxy-1-methylisoquinoline, 9CI, D-555
6,6-Dimethoxy-2,5,5-trimethyl-2-hexene, 9CI, T-782
8,8-Dimethoxy-2,6-dimethyl-2-octanol, H-417
1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene, 9CI, D-822
3,4-Dimethoxybenzaldehyde, D-734
1,1-Dimethoxydecane, D-39
(2,2-Dimethoxyethyl)benzene, 9CI, P-257

[2-(Dimethoxymethyl)-1-heptenyl]benzene, 9CI, P-217
1,1-Dimethoxyoctane, 9CI, O-73
3,7-Dimethyl-1,3,7-octatriene; (*Z*)-*form*, D-847
2-(2,6-Dimethyl-1,5-heptadienyl)-4-methyl-1,3-dioxolane, D-799
3,7-Dimethyl-1,6-octadien-3-ol; (*R*)-*form*, D-832
3,7-Dimethyl-1,6-octadien-3-ol, D-832
3,7-Dimethyl-1,7-octanediol; (±)-*form*, D-844
7,7-Dimethyl-2-methylenebicyclo[2.2.1]heptane; (-)-*form*, D-814
3,7-Dimethyl-3,6-octadienal, D-823
3,7-Dimethyl-3-octanol; (±)-*form*, D-846
2,6-Dimethyl-4-heptanone, D-802
2,6-Dimethyl-5-heptenal; (±)-*form*, D-803
2,6-Dimethyl-6-hepten-1-ol; (±)-*form*, D-804
3,7-Dimethyl-6-octen-1-ol; (*S*)-*form*, D-857
3,7-Dimethyl-6-octen-1-ol, D-857
3,7-Dimethyl-6-octenal; (*R*)-*form*, D-850
3,7-Dimethyl-6-octenal, D-850
3,7-Dimethyl-6-octenoic acid, D-856
[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde, D-860
3,7-Dimethyl-7-octen-1-ol, D-858
2′,4′-Dimethylacetophenone, D-748
2,4-Dimethylbenzaldehyde, D-756
2,6-Dimethyloctanal, D-843
Diphenyl ether, D-944
1,3-Diphenyl-2-propanone, D-955
2-Dodecenal; (*E*)-*form*, D-1022
Dodecyl 2-methylpropanoate, M-605
Dodecyl acetate, D-1018
Egomaketone, E-6
Epimyricanol 5-glucoside, M-833
7,10-Epoxy-2-guaianone, E-120
1(10),11-Eremophiladien-2-one, E-195
1-Ethenylhexyl butanoate, O-98
1-Ethoxy-2-methoxy-4-(1-propenyl)benzene, P-503
2-Ethoxy-6-methylpyrazine, H-612
4-Ethoxybenzaldehyde, H-343
1-(1-Ethoxyethoxy)-3-hexene; (*Z*)-*form*, E-253
2-Ethoxynaphthalene, E-256
Ethyl 2-aminobenzoate, A-217
Ethyl 2-decenoate, D-57
Ethyl 2-hydroxybenzoate, H-345
Ethyl 2-methylbutyrate, M-330
Ethyl 2-methylpropanoate, 9CI, M-605
Ethyl 3-methylbutanoate, M-331
Ethyl 4-decenoate, D-59
Ethyl *p*-anisate, M-253
Ethyl acetate, E-259
Ethyl acetoacetate, E-260
Ethyl aconitate, A-108
Ethyl benzoate, B-31
Ethyl butyrate, B-218
Ethyl cinnamate, P-312
Ethyl crotonate, B-223
Ethyl decanoate, D-41
Ethyl dodecanoate, D-1016
Ethyl formate, E-266
Ethyl heptanoate, H-93
Ethyl hexanoate, H-234
Ethyl lactate, H-765
Ethyl octadecanoate, O-26
Ethyl octanoate, O-80
Ethyl oleate, O-44
Ethyl pentanoate, P-190
Ethyl phenylglycidate, P-292
Ethyl propionate, P-478
6-Ethyl-2,10,10-trimethyl-1-oxaspiro[4.5]deca-3,6-diene, E-357
2-Ethyl-4-hydroxy-5-methyl-3(2*H*)-furanone, E-318
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2,4,6,10-Farnesatetraene; (2*Z*,4*E*,6*E*)-*form*, F-8
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7-Hydroxy-4′-methoxyisoflavanone, D-512
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1-(2-Hydroxy-4-methoxyphenyl)-2-propanol, D-648
3-Hydroxy-5-phenylpentanoic acid; (ξ)-*form*; *O*-β-D-Glucopyranoside, H-730
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3-Mercapto-1-hexanol; (*R*)-*form*, M-210
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3-Mercapto-1-hexanol; (*S*)-*form*; *S*-Me, *O*-hexanoyl, M-210
3-Mercapto-1-hexanol; (*S*)-*form*; *S*-Me, M-210
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2-Methoxy-4-(2-propenyl)phenol, M-273
1-Methoxy-4-methylbenzene, M-573
2-Methoxy-4-methylphenol, 9CI, M-314
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Methyl 3-methylbutanoate, M-331
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3-Methyl-1*H*-indole, M-483
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3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one; (±)-(*E*)-*form*, M-707
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2-Methyl-4-propyl-1,3-oxathiane, M-625
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3-Methylbutyl 3-methylbutanoate, M-331
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3-Methylbutyl octanoate, O-80
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Myricanol; 11-Deoxy, 11*E*,12-didehydro, 5-*O*-[α-L-arabinofuranosyl-(1 → 6)-β-D-glucopyranoside], M-833
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3,3′,4′,5,7-Pentahydroxyflavylium(1+); 3-*O*-[β-D-Xylopyranosyl-(1 → 2)-(4-hydroxycinnamoyl)-(→ 6)-β-D-glucopyranoside](*E*-), 5-*O*-β-D-glucopyranoside, P-144
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2-Phenylethyl propanoate, P-273
Phenylmethyl 2-methylpropanoate, M-605
Phenylmethyl butanoate, B-218
Phenylmethylglycidic ester, M-586
2-Phenylpropanal; (±)-*form*, P-301
1-Phenylpropyl butyrate, P-305
2-Phenylpropyl butyrate, P-307
3-Phenylpropyl hexanoate, P-309
2-Phenylpropyl isobutyrate, P-307
3-Phenylpropyl isovalerate, P-309
3-Phenylpropyl propanoate, P-309
Prexanthoperol, H-327
1-Propanol, P-479
2-Propanol, P-480
2-Propenyl 2-aminobenzoate, A-217
2-Propenyl 2-ethylbutanoate, E-291
2-Propenyl 3-methylbutanoate, M-331
2-Propenyl cyclohexanebutanoate, C-458
2-Propenyl cyclohexanepentanoate, C-462
2-Propenyl heptanoate, H-93
2-Propenyl hexanoate, H-234
2-Propenyl octanoate, O-80
Propyl 2,4-decadienoate, D-32
Propyl 2-furanacrylate, F-137
Propyl 2-methylpropanoate, M-605
Propyl 3-methylbutanoate, M-331
Propyl acetate, P-479
Propyl benzoate, B-31
Propyl butyrate, B-218
Propyl cinnamate, P-312
Propyl formate, F-60
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Propyl hexanoate, H-234
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Prunasin, H-718
Rhodinyl acetate, D-858
Rhodinyl butyrate, D-858
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Rhodinyl isobutyrate, D-858
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Rose oxide, R-51
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Salfredin B_{11}, S-14
β-Santalyl acetate, S-39
α-Santalyl acetate, S-41
β-Santalyl phenylacetate, S-39
α-Santalyl phenylacetate, S-41
3,4-Secocycloarta-4(28),24-diene-3,26-dioic acid; (24*Z*)-*form*; 26-Me ester, S-65
Styrene, S-255
Tamariscene; (-)-*form*, T-6
α-Terpinyl anthranilate, M-175
α-Terpinyl cinnamate, M-175
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Tetradecanal, T-58
Tetrahydro-2,2-dimethyl-5-(1-methyl-1-propenyl)furan, T-81
Tetrahydro-2,4-dimethyl-4-phenylfuran, T-82
Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran, T-94
Tetrahydro-6-pentyl-2*H*-pyran-2-one, T-116
Tetrahydrofurfuryl butyrate, T-85
Tetrahydrofurfuryl cinnamate, T-85
4′,5,6,7-Tetrahydroxyflavone; 7-*O*-[β-D-Glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-210
2,6,9,10-Tetramethyl-1-oxaspiro[4.5]deca-3,6-diene, T-307
2,6,10,10-Tetramethyl-1-oxaspiro[4.5]decan-6-ol, 9CI, T-337
Theaspirane, T-337
Toluene, T-423
p-Tolyl acetate, M-573
1-Tridecene-3,5,7,9,11-pentayne, T-489
5,7,8-Trihydroxy-4′,6-dimethoxyflavone, P-143
3′,4′,7-Trimethoxyisoflavone, T-600
4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanol, T-742
2,2,4-Trimethyl-1,3-dioxolane; (±)-*form*, T-772
1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one, T-757
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone, 9CI, M-96
1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1,6-heptadien-3-one, T-756
1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one, T-758
4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-butanone, 9CI, 8CI, M-94
2,3,4-Trimethyl-3-pentanol, T-790
2,4,6-Trimethyl-4-phenyl-1,3-dioxane, T-792
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1-Undecanol, U-16
2-Undecanol, U-17
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Valdiate, T-324
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4,7(11)-Valeradien-12-al, V-6
Valeranone; (-)-*form*, V-5
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Valerianol, E-197
Valtrate; 11-De-Ac, 11-*O*-(3-hydroxy-3-methylbutanoyl), V-11
Valtrate; 7,11-Bisdeacyl, 7-*O*-(3-methylpentanoyl), 11-*O*-(3-hydroxy-3-methylbutanoyl), V-11
Valtrate, V-11
Vanillin isobutyrate, D-382
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Veranisatin B, V-15
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Verimol B, H-737
Verimol D, V-16
Verimol E, V-16
Verimol F; (*S*)-*form*, V-17
Verimol G, V-18
Verimol H, V-19
Verimol I, H-750
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Violet-leaf aldehyde, N-97
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Meaty flavours and odours

4-Acetoxy-2,5-dimethyl-3(2H)furanone, H-407
3-Acetyl-1,2-dithiolane, A-58
4-Acetyl-2-methylpyrimidine, A-79
2-Acetyl-4,5-dihydrothiazole, A-47
2-Acetylpyridine, A-87
2-Acetylthietane; (ξ)-*form*, A-96
Allithiamine, A-179
Bis(2,5-dimethyl-3-furanyl) disulfide, B-126
Bis(2-methyl-3-furanyl)tetrasulfide, B-148
1,2-Butanedithiol; (±)-*form*, B-212
1,3-Butanedithiol; (±)-*form*, B-213
2,4,7-Decatrienal; (2*E*,4*Z*,7*Z*)-*form*, D-47
3-Decenoic acid, D-58
Di-2-thienyl disulfide, D-990
3,5-Diethyl-2-methylpyrazine, D-204
3,4-Diethylthiophene, D-209
N-(4,5-Dihydro-1-methyl-4-oxo-1*H*-imidazol-2-yl)alanine; (*S*)-*form*, D-310
2,5-Dihydro-2,4,5-trimethyloxazole, D-363
2,5-Dihydro-2,4,5-trimethylthiazole, D-365
Dihydro-2,4,6-trimethyl-4*H*-1,3,5-dithiazine; (2α,4α,6α)-*form*, D-361
Dihydro-2-methoxy-2-methyl-3(2*H*)-thiophenone, D-290
Dihydro-2-methyl-3(2*H*)-furanthione, D-302
S-(4,5-Dihydro-2-methyl-3-furanyl) ethanethioate, 9CI, D-302
4,5-Dihydro-2-methyl-3-thiophenethiol, D-328
2,5-Dihydro-4,5-dimethyl-2-(2-methylpropyl)thiazole, D-247
Dihydro-4,6-dimethyl-4*H*-1,3,5-dithiazine, D-244
Dihydro-4-mercapto-3(2*H*)-furanone, D-286
Dihydro-4-mercapto-5-methyl-3(2*H*)-thiophenone, D-287
2,3-Dihydro-5-methyl-3-thiophenethiol, D-327
4,5-Dihydro-5-methyl-3-thiophenethiol, D-329
3,5-Dimethyl-1,2,4-trithiolane, D-917
2,5-Dimethyl-3-furanthiol, D-794
S-(2,5-Dimethyl-3-furanyl) 2-furancarbothioate, D-795
2,6-Dimethyl-3-[(2-methyl-3-furanyl)thio]-4-heptanone, D-819
1,3-Dimethylpyrrolo[1,2-*a*]pyrazine, D-902
1,4-Dimethylpyrrolo[1,2-*a*]pyrazine, D-903
3,4-Dimethylpyrrolo[1,2-*a*]pyrazine, D-904
1,4-Dithiane-2,5-diol, D-988
3,3′-Dithiobis[2-methylfuran], D-992
3,3′-Dithiobis[4,5-dihydro-2-methylfuran], D-991
2,6-Dodecadienal, D-1009
Ethyl methyl trisulfide, E-273
2-Ethyl-2,5-dihydro-4,5-dimethylthiazole, E-294
4-Ethyl-2-methoxyphenol, E-286
2-Ethyl-5-methylpyrazine, E-335
2-Ethyl-6-methylpyrazine, E-336
FEMA 3574, M-513
FEMA 3638, T-483
FEMA 3670, D-1008
(2-Furanylmethyl) methyl disulfide, F-113
Furfuryl thioacetate, F-95
Glutamic acid; (*S*)-*form*; Hydrochloride, G-209
Glutamic acid; (*S*)-*form*, G-209
Hexahydro-2′,3*a*-dimethylspiro[1,3-dithiolo[4,5-*b*]furan-2,3′(2′*H*)-furan], H-178
Hexahydro-2′,4-dimethylspiro[1,3-dithiolo[4,5-*c*]furan-2,3′(2′*H*)-furan], H-179
1-Hexanethiol, H-233
4-Hydroxy-5-methyl-3(2*H*)-furanone, H-588
4-Hydroxy-5-methyl-3(2*H*)-thiophenone, H-620
L-Lysine, L-132
3-[(2-Mercapto-1-methylpropyl)thio]-2-butanol, M-218
3-Mercapto-2-pentanone, M-225
1-Mercapto-2-propanone, M-230
2-Mercapto-3-pentanone, M-224
4-Mercapto-5-methyl-3(2*H*)-thiophenone, M-219
2-Methyl-2-(methyldithio)propanal, M-488
3-Methyl-2-butanethiol, M-329
2-Methyl-3-(methyldithio)furan, M-487
2-Methyl-3-(methylthio)furan, M-440
2-Methyl-3-(propyldithio)furan, M-623
2-Methyl-3-furanthiol, M-440
5-Methyl-3-furanthiol, M-442
3-[(2-Methyl-3-furanyl)thio]-4-heptanone, M-450
4-[(2-Methyl-3-furanyl)thio]-5-nonanone, M-451
2-Methyl-3-thiophenethiol, M-683
5-Methyl-3-thiophenethiol, M-685
2-Methyl-5-(methylthio)thiophene, M-684
4-Methyl-5-vinylthiazole, M-715
8-Methyldecanoic acid; (ξ)-*form*, M-389
9-Methyldecanoic acid, M-390
1-(Methylthio)-1-butene, M-666
5-(Methylthio)-2-[(methylthio)methyl]-2-pentenal, M-678
3-(Methylthio)propanal, M-688
Monosodium glutamate, G-209
1,8-Octanedithiol, O-78
Oleic aldehyde, O-37
1,2-Propanedithiol; (±)-*form*, P-472
1,3-Propanedithiol, P-473
Pyrazinemethanethiol, P-594
Pyrrolo[1,2-*a*]pyrazine, P-629
1*H*-Pyrrolo[2,1-*c*][1,4]thiazine, P-630
Tetrahydro-2-methyl-2-thiophenethiol, T-109
Tetrahydro-2-methyl-3-furanol, T-101
Tetrahydro-2-methyl-3-thiophenethiol, T-110
Tetrahydro-2-thiophenethiol; (ξ)-*form*, T-128
1,2,3,4-Tetrahydro-6-propanoylpyridine, T-119
2-(2-Thienyl)furan, T-358
1,1′-Thiobisethanethiol, T-367
2,2,4-Trimethyl-1,3-dioxolane; (±)-*form*, T-772
2,5-Undecadienal; (2*E*,5*Z*)-*form*, U-7

Pungent flavours and odours

Acetal R; (±)-*form*, A-19
Acetaldehyde butyl phenethyl acetal, A-21
Aceteugenol, M-273
4-Acetoxy-2,5-dimethyl-3(2H)furanone, H-407
6″-Acetylapiin, C-362
2-Amino-5-(methylthio)pentanoic acid; (*S*)-*form*, A-277
2-Aminoethanesulfonic acid, A-248
Ammonium isovalerate, M-331
Apiin, C-362
Apional, A-373
Benzenethiol, B-23
1-[5-(1,3-Benzodioxol-5-yl)-1-oxo-2-pentenyl]piperidine, P-402
Benzyl benzoate, USAN, B-31
Bis(methylthio)methane, B-150
Butanoic acid, B-218
3-Butenenitrile, 9CI, B-224
Capsaicin, C-75
Chavicine, P-402
Crispane, C-371
Crispanone, C-371
Cysteine; (*R*)-*form*, C-514
Di-2-propenyl disulfide, D-967
Di-2-propenyl sulfide, D-972
Di-2-propenyl tetrasulfide, D-973
Di-2-propenyl trisulfide, D-974
1,2:3,4-Diepoxy-*p*-menth-8-ene, D-190
Diethyl disulfide, D-193
Diethyl sulfide, D-195
Dimethyl disulfide, D-742
Dimethyl trisulfide, D-747
Dipropyl disulfide, D-975
Dipropyl trisulfide, D-976
1,4-Dithiane-2,5-diol, D-988
1,4-Dithiane, D-987
1,4-Epidioxy-*p*-mentha-2,8-diene, E-55
Ethyl 4-(methylthio)butyrate, M-201
Ethyl methyl trisulfide, E-273
2-Ethylbenzenethiol, E-287
Feruloylcholine, C-239
2-Furanmethanethiol, F-95
Graveobioside A, T-205
Heptanal, H-90
3-Heptanol; (±)-*form*, H-96
1-Heptanol, H-94
4-Heptanone, H-99
2-Heptenal, H-101
6-Hexadecenoic acid; (*E*)-*form*, H-164
4-(4-Hydroxy-3-methoxyphenyl)-2-butanone, 9CI, 8CI, D-613
2-Hydroxybenzaldehyde, H-342
Isochavicine, P-402
Isopiperine, P-402
4-Isopropyl-3-cyclohexene-1-carboxylic acid; (ξ)-*form*, I-125
4-Isopropylbenzaldehyde, I-118
4-Isothiocyanato-1-(methylthio)-1-butene; (*E*)-*form*, I-181
3-Isothiocyanato-1-propene, I-194
1-Isothiocyanato-3-(methylthio)propane, I-188
1-Isothiocyanato-6-(methylsulfinyl)hexane, 9CI, I-185
1-Isothiocyanato-6-(methylthio)hexane, I-185
1-Isothiocyanato-7-(methylsulfinyl)heptane, I-184
1-Isothiocyanato-7-(methylthio)heptane, I-184
1-Isothiocyanato-8-(methylthio)octane, I-186
6″-Malonylapiin, C-362
6″-Malonylcosmosiin, C-362
p-Menth-1-en-3-ol, M-171
p-Mentha-1,3,8-triene, M-155
3-Mercapto-2-methylpentanal, M-215
Methanethiol, M-242
5-Methoxy-2-methylthiazole, 9CI, H-618
2-Methoxy-4-(2-propenyl)phenol, M-273
1-Methoxy-4-methylbenzene, M-573
4-Methoxybenzaldehyde, M-249
Methyl 1-propenyl disulfide; (*E*)-*form*, M-292
Methyl 2-propenyl disulfide, M-293
Methyl 3-methyl-1-butenyl disulfide, M-285
S-Methyl 3-methylthiobutyrate, M-326
S-Methyl hexanethioate, H-232
Methyl phenyl sulfide, M-291
Methyl propyl disulfide, M-302
Methyl propyl trisulfide, M-303
2-Methyl-1,3-dithiolane, M-398
2-Methyl-1-propenethiol, M-607
4-Methyl-2,3-pentanedione, M-544
3-Methyl-2,4-nonanedione, M-512
2-Methyl-2-pentenal, M-551
3-Methylbutanal, M-325
2-Methylbutanoic acid; (±)-*form*, M-330
3-Methylbutanoic acid, M-331
4-Methylphenol, M-573
2-(4-Methylphenyl)propanal, M-593
2-Methylpropanoic acid, M-605
1-(Methylthio)-1-hexanethiol, M-671
Nonivamide, N-132
Norchalciporyl propionate, N-147
Nuatigenin; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 2)-β-D-glucopyranoside], N-157
Octanoic acid, O-80
Pentanoic acid, P-190
1-Penten-3-one, P-205
1-Phenyl-1,2-propanedione, P-303
3-Phenyl-1-propanol, P-309
3-Phenyl-2-propenal; (*E*)-*form*, P-311
4-Phenyl-3-buten-2-one, P-265
Phenylmethanethiol, P-287
3-Phenylpropanal, P-302
3-Phenylpropyl acetate, P-309
Piperidine, P-389
Piperine, P-402
Propanal, P-467
1-Propanethiol, P-475
1-Propene-1-thiol; Thial-*form*; *S*-Oxide, P-485
1-Propene-1-thiol, P-485
2-Propene-1-thiol, P-486
2-Propenyl glucosinolate, P-489
1-Propenyl propyl disulfide, P-496
2-Propenyl propyl disulfide, P-497
1-(Propylthio)-1-propanethiol; (ξ)-*form*, P-537
Spirost-5-ene-3,25-diol; (3β,25*S*)-*form*; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 2)-β-D-glucopyra-

noside], S-192
1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene, T-299
2,4,6-Triethyl-1,3,5-oxadithiane, T-497
2,4,6-Triethyl-1,3,5-trioxane, T-498
2,4,6-Triethyl-1,3,5-trithiane, T-499
4′,5,7-Trihydroxy-3′-methoxyflavone; 7-*O*-(Malonyl-β-D-glucopyranoside), T-618
Vaginatin, D-423

Sour flavours

Acetic acid, A-23
Capsianoside F, C-78
Citric acid, C-290
Deoxymorellin, M-759
Dihydromorelloflavone, M-760
Gambogic acid, G-53
α-Guttiferin, G-352
δ-Guttiferinic acid, G-353
γ-Guttiferinic acid, G-354
3-Hydroxy-28,13-lupanolide, D-527
Isomorellic acid, M-759
Malic acid; (±)-*form*, M-36
3-Methylbutanoic acid, M-331
2-Methylpentanoic acid; (±)-*form*, M-546
3-Methylpentanoic acid; (±)-*form*, M-547
Morellic acid, M-759
Morellin, M-759
Morellinol, M-759
Moreollin, M-761
4-Oxopentanoic acid, O-239
4-Pentenoic acid, P-202
3-(3-Pentyloxiranyl)-2-propenal, 9CI, D-30
Propyl benzoate, B-31
Pyruvic acid, P-632
L-Threaric acid, T-27
3,5,7-Trihydroxy-3′,4′-dimethoxyflavone, T-547

Sweet flavours and odours

4,4a,5,6-Tetrahydro-7-methyl-2(3*H*)-naphthalenone; (±)-*form*, A-482
2-Acetyl-3-methylthiophene, A-80
6″-Acetylliquiritin, D-470
Afzelechin 7-apioside, T-184
Alanine; (±)-*form*, A-151
Alanine; (*S*)-*form*, A-151
2-Aminoheptanedioic acid, A-255
Anisyl acetate, H-357
Australigenin, S-194
7-Baueren-3-ol; 3β-*form*; Me ether, B-10
2-Benzyl-5-hydroxymethyl-1,3-dioxolane, B-57
7-Butyl-2-oxepanone, 9CI, 8CI, H-394
Carvyl propionate, M-128
Cyclopentanone, C-492
4,9-Dihydro-7-methoxy-1-methyl-3*H*-pyrido[3,4-*b*]indole, H-9
4′,7-Dihydroxyflavanone; (*S*)-*form*; 4′-*O*-[3-*O*-Acetyl-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside], D-470
4′,7-Dihydroxyflavanone; (*S*)-*form*; 7-*O*-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside], D-470
3-(2,4-Dihydroxyphenyl)-7-hydroxy-5-methoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, 9CI, G-288
3,4-Dimethyl-1,2-cyclopentanedione, D-777
3,7-Dimethyl-2,6-octadien-1-ol; (*Z*)-*form*; *O*-β-D-Glucopyranoside, D-833
S-2,5-Dimethyl-3-furanyl 3-methylbutanethioate, D-796
Dulcoside A, H-528
E315, I-70
2-Ethoxy-4-(methoxymethyl)phenol, 9CI, D-400
Ethyl phenylacetate, P-258
3-Ethyl-1,2-cyclopentanedione, E-293
4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one, E-317
2-Ethyl-3-hydroxy-4*H*-pyran-4-one, E-320
2-Ethyl-4-hydroxy-5-methyl-3(2*H*)-furanone, E-318
2-Ethylidenehexanal, E-324
FEMA 2751, U-32
FEMA 3255, A-397
FEMA 3355, H-418
β-D-Fructofuranosyl β-D-galactopyranosyl-(1→4)-α-D-glucopyranoside, F-71
3-(2-Furanyl)-2-phenyl-2-propenal, F-130
Glucoliquiritin apioside, D-470
6-β-D-Glucopyranosyl-8-β-D-ribopyranosylapigenin, S-51
Glycyrin, G-288
Guaiol acetate, G-340
Harmalol, H-9
5-Hexyl-1,4-dioxan-2-one, H-270
3-Hexylpyridine, H-278
7-Hydroxy-1-methyl-β-carboline, H-576
5-Hydroxy-2-benzyl-1,3-dioxane, H-362
3-Hydroxy-2-methyl-4*H*-pyran-4-one, H-609
2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one, H-812
4-Hydroxy-3-methoxybenzenemethanol, 9CI, D-400
3-Hydroxy-4,5-dimethyl-2(5*H*)-furanone, H-406
Hydroxyacetic acid, H-330
Isobutyl cinnamate, P-312
Isodulcitol, R-20
Isoeugenol acetate, M-272
Isopropyl cinnamate, P-312
Isopropyl phenylacetate, P-258
3-Isopropyl-1,2-cyclopentanedione, I-127
Isoschaftoside 4′-glucoside, I-162
Licorice glycoside C1, D-470
Licorice glycoside C2, D-470
Licorice glycoside D1, D-470
Licorice glycoside D2, D-470
Licorice glycoside E, D-470
Linalool acetate, D-832
Liquiritigenin 4′,7-diglucoside, D-470
Liquiritin, D-470
p-Mentha-1,8-dien-6-ol; (4*R*,6*R*)-*form*, M-128
p-Mentha-1,8-dien-6-ol; (4*R*,6*S*)-*form*, M-128
(-)-Menthone, M-153
3-Methoxy-14-taraxerene, T-26
4-Methoxy-2,5-dimethyl-3(2*H*)-furanone, H-407
1-Methoxy-4-(1-propenyl)benzene, 9CI, P-512
3β-Methoxy-7-multiflorene, M-790
1-(4-Methoxyphenyl)-4-methyl-1-penten-3-one, 9CI, H-726
Methyl phenylacetate, P-258
3-Methyl-α-ionyl acetate, M-707
3-Methyl-1,2-cyclopentanedione, M-381
4-Methyl-1-phenyl-2-pentanone, M-590
5-Methyl-2,3-hexanedione, M-476
5-Methyl-2-furancarboxaldehyde, M-437
4-Methyl-3-penten-2-one, M-558
3-Methylbutyl phenylacetate, P-258
4′-*O*-Methylglucoliquiritigenin, D-470
4-Methylphenyl phenylacetate, P-258
2-Methylpropyl phenylacetate, P-258
Neoliquiritin, D-470
Neryl butyrate, D-833
Nystose, N-159
Orientin, O-167
2-Oxopropanal, O-245
Periandrin I, D-586
Periandrin III, D-586
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2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*R*,6*S*)-*form*; 3′,3″-Di-Me ether, 4-Ac, D-632
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*R*,6*S*)-*form*; 3′,3″-Di-Me ether, D-632
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*S*,6*S*)-*form*; 3′,3″-Di-Me ether, 4-Ac, D-632
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*S*,6*S*)-*form*; 3′,3″-Di-Me ether, D-632
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3-Hydroxy-2-methylenebutanoic acid; (ξ)-*form*; 2-Methylpropyl ester, H-582
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4(10)-Thujene; (-)-*form*, T-393
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3β,24-Dihydroxy-11-oxo-12-oleanen-30,22β-olide, T-661
3,23-Dihydroxy-12,19(29)-ursadien-28-oic acid; 3β-*form*; 3-*O*-α-L-Arabinopyranoside, 28-*O*-β-D-glucopyranosyl ester, D-707
3,30-Dihydroxy-12-oleanen-11-one, H-694
3,16-Dihydroxy-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-β-D-Glucopyranoside, 28-*O*-[β-D-glucopyranosyl-(1 → 3)-[β-D-xylopyranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)]-α-L-arabinopyranosyl] ester, D-578
3,19-Dihydroxy-12-oleanen-28-oic acid; (3β,19α)-*form*; 3-*O*-α-L-Arabinopyranoside, 28-*O*-β-D-glucopyranosyl ester, D-580
3,11-Dihydroxy-12-ursen-28-oic acid; (3β,11α)-*form*; 11-Me ether, 3-Ac, Me ester, D-714
3,19-Dihydroxy-12-ursen-28-oic acid; (3β,19α)-*form*; 28-*O*-β-D-Glucopyranosyl ester, D-716
3,19-Dihydroxy-12-ursen-28-oic acid; (3β,19α)-*form*; 3-*O*-α-L-Arabinopyranoside, 28-*O*-[3,4,5-trihydroxybenzoyl-(→ 6)-β-D-glucopyranosyl] ester, D-716
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11,12-Dihydroxy-20-nor-5(10),8,11,13-abietatetraen-1-one, D-561
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O-(3,6-Dihydroxy-7-drimen-11-yl)umbelliferone; (3′ξ,5′α,9′ξ,10′β)-*form*; 6′-Ketone, D-447
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2,5-Dimethylpyrazine, D-895
2,6-Dimethylpyrazine, D-896
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3-Ethoxy-4-hydroxybenzaldehyde, D-382
7-Ethoxy-4-methyl-2*H*-1-benzopyran-2-one, H-561
2-Ethoxy-5-(1-propenyl)phenol, 9CI, P-503
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2,4,6-Decatrienoic acid dehydropiperidide; (2*E*,4*E*,6*Z*)-*form*, D-50
1-Decen-3-ol; (±)-*form*, D-63
9-Decenal, D-53
2-Decene-4,6,8-triynoic acid; (*Z*)-*form*; Me ester, D-55
5-Decenoic acid, D-60
6-Decenoic acid, D-61
Decyl butanoate, D-42
Decyl propionate, D-42
Dehydroanonaine, D-74
12-Dehydroporson, M-833
Dehydroroemerine, D-74
2,3-Dehydrosilybin, S-103
1-Deoxy-L-erythritol, B-217
$\Delta^{3,5}$-Deoxyneotigogenin, S-180
4,4′-Diaminodibutylamine, D-116

Diasesartemin, S-91
Dibenzyl disulfide, D-132
1,5-Dibutyl methyl hydroxycitrate, D-675
Dibutyl sulfide, D-142
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2,5-Diethyl-3-methylpyrazine, D-203
2,3-Diethyl-5-methylpyrazine, D-202
2,3-Diethylpyrazine, D-205
2,5-Diethylpyrazine, D-206
2,6-Diethylpyrazine, D-207
2,3-Dihydro-1*H*-pyrrole; *N*-Ac, D-349
Dihydro-2(3*H*)-furanone, D-253
6,7-Dihydro-2,3-dimethyl-5*H*-cyclopentapyrazine, D-241
Dihydro-2-isopropyl-4,6-dimethyl-4*H*-1,3,5-dithiazine, D-106
Dihydro-2-methyl-3(2*H*)-thiophenone; (ξ)-*form*, D-330
3,4-Dihydro-2*H*-pyrrole, D-350
Dihydro-3(2*H*)-thiophenone, D-359
3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2*H*-pyran; (ξ)-*form*, D-308
Dihydro-5-(2-octenyl)-2(3*H*)-furanone, D-337
Dihydro-5-octyl-2(3*H*)-furanone; (±)-*form*, D-338
Dihydro-6-isopropyl-2,4-dimethyl-4*H*-1,3,5-dithiazine, D-106
Dihydroaspidospermatine, A-469
2,9-Dihydroxy-1,10-dimethoxynoraporphine, B-166
4,9-Dihydroxy-10(14)-oplopen-3-one; (4*S*,9α)-*form*; 9-(3-Methyl-2*E*-butenoyl), 4-Ac, D-589
4,9-Dihydroxy-10(14)-oplopen-3-one; (4*S*,9α)-*form*; 9-(3-Methyl-2*E*-pentenoyl), D-589
4,9-Dihydroxy-10(14)-oplopen-3-one; (4*S*,9α)-*form*; 9-(3-Methylbutanoyl), D-589
4,9-Dihydroxy-10(14)-oplopen-3-one; (4*S*,9α)-*form*; 9-Angeloyl, 4-Ac, D-589
1,3-Dihydroxy-12,6-eudesmanolide; (1β,4α,6α,11α*H*)-*form*; 3-Ketone, 1-*O*-β-D-glucopyranoside, D-457
2,3-Dihydroxy-2,4-cyclopentadien-1-one, D-420
2′,4′-Dihydroxy-2-biphenylcarboxylic acid, D-405
4,10-Dihydroxy-2-oxo-1(5)-guaien-12,6-olide, T-587
5,7-Dihydroxy-3′,4′,6-trimethoxyflavone, D-699
1,8-Dihydroxy-3,7(11)-eudesmadien-12,8-olide; (1β,8β)-*form*, D-456
1,7-Dihydroxy-3-methoxyxanthone, T-724
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2′,7-Dihydroxy-4′-methoxyisoflavanone, T-595
5,7-Dihydroxy-4′-methoxyisoflavone, D-542
2′,7-Dihydroxy-4′-methoxyisoflavone, T-598
2,9-Dihydroxy-4,10(14)-oplopadien-3-one; (2β,4*Z*,9α)-*form*; 2,9-Bis(3-methyl-2*E*-pentenoyl), D-588
2,9-Dihydroxy-4,10(14)-oplopadien-3-one; (2β,4*Z*,9α)-*form*; 9-(3-Methyl-2*E*-pentenoyl), 2-(2-methylbutanoyl), D-588
2,9-Dihydroxy-4,10(14)-oplopadien-3-one; (2β,4*Z*,9α)-*form*; 9-(3-Methyl-2*E*-pentenoyl), 2-angeloyl, D-588
1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone, P-320
1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-2-propen-1-one, 9CI, T-550
1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
4′,5-Dihydroxy-7-methoxy-6-methylflavone, T-632
1,3-Dihydroxy-7-methoxyxanthone, T-724
2β,9ξ-Dihydroxy-8-oxo-1(10),4,11(13)-germacratrien-12,6α-olide, T-585
3,7-Dihydroxy-9-methoxycoumestan, T-540
2′,3′-Dihydroxyacetophenone, D-368
2′,4′-Dihydroxyacetophenone, D-369
2,4′-Dihydroxyacetophenone, D-370
2′,5′-Dihydroxyacetophenone, D-371
2′,6′-Dihydroxyacetophenone, D-372
3′,4′-Dihydroxyacetophenone, D-373
3′,5′-Dihydroxyacetophenone, D-374
2,3-Dihydroxybenzoic acid, D-386
2,4-Dihydroxybenzoic acid, D-387
3,5-Dihydroxystilbene; (*E*)-*form*; Di-Me ether, D-692
Diisopropyl disulfide, D-722
4,4-Dimethoxy-2-butanone, 9CI, O-197
3,4-Dimethoxy-3,4-desmethylenecubebin, P-101
2,6-Dimethoxy-4-(1-propenyl)phenol, P-507
2,6-Dimethoxy-4-methylphenol, 9CI, M-316
1,2-Dimethoxy-4-vinylbenzene, V-33
1,1-Dimethoxyethane, 9CI, A-20
2,6-Dimethoxyphenol, B-24
Dimethyl sulfoxide, D-745
3,5-Dimethyl-1,2-cyclopentanedione, D-778
2,5-Dimethyl-1,4-dithiane-2,5-diol, D-781
3,7-Dimethyl-1,5,7-octatrien-3-ol; (*S*,*E*)-*form*, D-849
2,6-Dimethyl-1,7-octadien-3-one, D-834
3,6-Dimethyl-2(3*H*)-benzofuranone; (±)-*form*, D-760
2,6-Dimethyl-2,4-heptadiene, D-797
2,3-Dimethyl-2-cyclohexen-1-one, D-776
2,4-Dimethyl-2-pentenoic acid, D-868
2,5-Dimethyl-3-vinyl-5-hexene-2,4-diol; 2-Ac, D-919
2,5-Dimethyl-3-vinyl-5-hexene-2,4-diol; 4-Ketone, 2-Ac, D-919
2,6-Dimethyl-4-heptanol, D-801
1-(1,9-Dimethyl-5-methylene-8-decenyl)-4-methylbenzene, D-815
2,3-Dimethyl-5-propylpyrazine, D-891
2,4-Dimethyl-5-vinylthiazole, D-921
3,7-Dimethyl-6-octenoic acid; (ξ)-*form*; Me ester, D-856
1,4-Dimethyl-7-ethylazulene, D-789
2,6-Dimethyl-7-octen-3-one, D-859
6,10-Dimethyl-9-undecen-2-one, D-918
2,6-Dimethylbenzenethiol, D-758
2,3-Dimethylbenzofuran, D-759
2,3-Dimethylbicyclo[2.2.1]hept-2-ene, D-765
5,6-Dimethylbicyclo[2.2.1]hept-5-en-2-ol; (1*R**,2*S**)-*form*, D-766
2,3-Dimethylbicyclo[2.2.1]heptan-2-ol, D-764
2,4-Dimethylfuran, D-790
3,4-Dimethylheptane, D-800
3,3-Dimethylhexane, D-808
2,5-Dimethylphenol, D-874
2,6-Dimethylphenol, D-875
3,4-Dimethylphenol, D-876
2,3-Dimethylpyrazine, D-894
2,6-Dimethylpyridine, D-897
4,5-Dimethylthiazole, D-910
2,3-Dimethylthiirane; (2*RS*,3*SR*)-*form*, D-911
2,3-Dimethylthiophene, D-912
2,4-Dimethylthiophene, D-913
2,5-Dimethylthiophene, D-914
3,4-Dimethylthiophene, D-915
Diphenyl disulfide, D-943
2,3-Diphenylpyrazine, D-956
2,2′-Dithenyl sulfide, D-985
Djenkolic acid; (*R*,*R*)-*form*; *N*-Ac, D-997
Dodecanoic acid, D-1016
N-(2,14-Eicosadienoyl)piperidine, E-9
2,4,8-Eicosatrienoic acid isobutylamide, E-18
2,4,14-Eicosatrienoic acid isobutylamide, E-19
1,3-Elemadien-6-ol; 6β-*form*; Ac, E-29
1,3,7(11)-Elematrien-8-one, E-33
1-Epi-α-gurjunene, A-415
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3-Epiarmefolin, D-454
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(+)-Episyringaresinol, S-292
3,4-Epoxy-1,5,8-trihydroxy-7(14),10-bisabola-dien-2-one; (1*R*,3*R*,4*R*,5*S*,6*S*,8ξ)-*form*; 8-Angeloyl, 1-Ac, E-183
3,4-Epoxy-1,5,8-trihydroxy-7(14),10-bisabola-dien-2-one; (1*S*,3*S*,4*S*,5*R*,6ξ,8ξ)-*form*; 8-Angeloyl, 1,5-di-Ac, E-183
5,6-Epoxy-3,3,6-trimethyl-1-hepten-4-one, T-777
4,7′-Epoxy-3,8′-bilign-7-ene-3′,4′,5,9,9′-pentol; (7′ξ,8′ξ)-*form*; 3′,5-Di-Me ether, E-63
6,7-Epoxy-5,20-dihydroxy-1-oxowitha-2,24-dienolide, E-134
1,4-Epoxy-5-hydroxy-10(14)-germacren-12,6-olide; (1α,4α,5β,6α,11β*H*)-*form*, E-128
4,5-Epoxy-*p*-menth-1-en-3-ol; (3β,4β,5β)-*form*; 3-*O*-β-D-Glucopyranoside, E-169
1,2-Epoxy-*p*-menth-4(8)-en-3-one, E-170
Epoxypseudoisoeugenol 2-methylbutanoate, M-528
11-Eremophilen-1-one, E-199
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1,2-Ethanedithiol, E-243
4-(1-Ethenyl-1,5,9-trimethyl-4,8-decadienyl)-1,2-benzenediol, E-247
1-Ethenyl-2-methoxybenzene, 9CI, V-36
2-Ethoxy-1-methyl-4-(1-methylethyl)benzene, 9CI, I-147
4-Ethoxy-3-methoxybenzaldehyde, D-382
1-Ethoxy-3-methyl-2-butene, 9CI, M-344
2-(Ethoxymethyl)phenol, 9CI, H-355
4-Ethoxyphenol, B-21
2-Ethoxythiazole, T-353
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Ethyl 4-methylphenoxyacetate, M-574
Ethyl *N*-ethylanthranilate, A-217
Ethyl acrylate, P-487
Ethyl levulinate, O-239
Ethyl nitrite, E-277
Ethyl tetradecanoate, T-59
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Ethyl undecanoate, U-15
Ethyl vanillin isobutyrate, D-382
2-Ethyl-1-hexanethiol; (±)-*form*, E-313
5-Ethyl-2,4-dimethylthiazole, T-445
2-Ethyl-2-heptenal, E-310
3-Ethyl-2-hydroxy-4-methyl-2-cyclopenten-1-one, E-316
5-Ethyl-2-methylpyridine, E-338
2-Ethyl-3,4-dihydroxyfuran, E-297
2-Ethyl-3,5-dimethylpyrazine, E-298
7-Ethyl-3,6-dihydro-1,4-dimethylazulene, D-789
5-Ethyl-3-hydroxy-4-methyl-2(5*H*)-furanone; (±)-*form*, E-319
2-Ethyl-3-methylpyrazine, E-334
2-Ethyl-4,5-dimethyloxazole, T-444
2-Ethyl-4-(2-furanyl)-2-propenal, E-308
7-Ethyl-5,6-dihydro-1,4-dimethylazulene, D-789
2-Ethylbutanal, E-290
2-Ethylbutanoic acid, E-291
5-Ethyldihydro-2(3*H*)-furanone; (±)-*form*, E-295
3-Ethylidenehexahydropyrrolo[1,2-*a*]pyrazine-1,4-dione; (*S*)-*form*, E-323
4-Ethyloctanoic acid; (ξ)-*form*, E-345
2-Ethylpyrazine, E-347
3-Ethylpyridine, E-348
2-Ethylthiazole, E-352
Ethylvanillin glucoside, D-382
4,11-Eudesmanediol; (4α,5α)-*form*; 11-*O*-α-L-Rhamnopyranoside, E-379
1,4,11-Eudesmatrien-3-one, E-377
4-Eudesmen-11-ol; 7β-*form*; *O*-α-L-Rhamnopyranoside, E-383
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2-Furancarboxaldehyde, F-93
2-Furanmethanol, F-96
3-(2-Furanyl)-2-methyl-2-propenal, F-118
1-(2-Furanyl)-2-propanone, F-135
3-(2-Furanyl)-2-propenal, F-136
4-(2-Furanyl)-3-buten-2-one, F-108
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S-(2-Furanylmethyl) propanethioate, F-95
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Galeon; (-)-*form*, G-45
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1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6α)-*form*; β-D-Glucopyranosyl ester, G-87
1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6α)-*form*; 11,13-Dihydro, β-D-glucopyranosyl ester, G-87
β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 4)-D-glucose, G-169
2-(β-D-Glucopyranosyloxy)-2-methylpropanenitrile, 9CI, H-605
3-Glucopyranosyloxy-4′,5,7-trihydroxy-3′-methoxyflavone; 6″-*O*-β-L-Rhamnofuranosyl, G-182
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1(5),6-Guaiadiene; (4α,10α)-*form*, G-329
1(5),6-Guaiadiene; (4β,10α)-*form*, G-329
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1,7,9-Heptadecatriene-11,13,15-triyne; (*all-E*)-*form*, H-66
1,8,15-Heptadecatriene-11,13-diyne; (8*E*,15*E*)-*form*, H-62
1,8,15-Heptadecatriene-11,13-diyne; (8*Z*,15*Z*)-*form*, H-62
2,9,16-Heptadecatriene-4,6-diyn-8-ol; (*Z,Z*)-*form*, H-65
1,5,8-Heptadecatriene; (5*Z*,8*Z*)-*form*, H-61
Heptanoic acid, H-93
3-Hepten-2-one, H-109
2-Hepten-4-one, H-108
2-Heptylfuran, H-123
1,1,1,3,3,3-Hexachloro-2-propanone, H-143
1-Hexadecanol, H-160
11-Hexadecenoic acid; (*E*)-*form*, H-166
2-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4.5]dec-3-ene; (*E*)-*form*, H-173
3,3′,4′,5,5′,7-Hexahydroxyflavone; 3,3′-Di-*O*-galactoside, H-205
3,3′,4′,5,7,8-Hexahydroxyflavone; 3-*O*-β-D-Glucopyranoside, 8-*O*-β-D-glucuronopyranoside, H-209
3,3′,4′,5,5′,7-Hexahydroxyflavone; 7-*O*-[3,4,5-Trihydroxybenzoyl-(→ 6)-β-D-glucopyranoside], H-205
3,3′,4′,5,7,8-Hexahydroxyflavone; 8-*O*-β-D-Glucuronopyranoside, 3-*O*-sulfate, H-209
2,2,4,4,6,6-Hexamethyl-1,3,5-trithiane, H-224
3,4-Hexanedione, H-230
1,6-Hexanedithiol, H-231
3-Hexanol; (±)-*form*, H-236
3-Hexanone, H-238
4-Hexen-1-ol, H-254
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3-Hexenal; (*E*)-*form*, H-247
2-Hexenoic acid; (*Z*)-*form*, H-249
cis-3-Hexenyl 2-aminobenzoate, A-217
6-(3-Hexenyl)tetrahydro-2*H*-pyran-2-one, 9CI, 8CI, H-823
Hexyl 2-furoate, F-94
2-Hexyl-1,3-dioxan-5-ol, H-269
2-Hexyl-1,3-dioxolane-4-methanol, H-272
6-Hexyltetrahydro-2*H*-pyran-2-one; (±)-*form*, H-281
Homostachydrine; (*S*)-*form*, H-296
9-Hydroxy-1,2,10-trimethoxynoraporphine, L-54
2-Hydroxy-1-methoxyaporphine, D-379
3-Hydroxy-12-ursen-28-oic acid; 3β-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-xylopyranoside], H-830
10-Hydroxy-16-hentriacontanone, H-486
3-Hydroxy-18-lupen-21-one; 3β-*form*, H-536
1-Hydroxy-2,4(18),11(13)-eudesmatrien-12-oic acid; 1α-*form*, H-458
2-Hydroxy-2,6,6-trimethylcyclohexanone, H-810
4-Hydroxy-2,6-dimethyl-7-octen-3-one, H-419
5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)-benzofuran, H-499
N-[[3-Hydroxy-2-(2-pentenyl)cyclopentyl]acetyl]isoleucine, J-9
5-Hydroxy-2-(5-methyl-1-oxo-4-hexenyl)benzofuran, H-499
4′-Hydroxy-2-biphenylcarboxylic acid, H-366
3-Hydroxy-2-butanone, H-376
3-Hydroxy-2-oxopropanoic acid, H-698
3-Hydroxy-2-pentanone; (±)-*form*, H-705
5-Hydroxy-2-phenyl-1,3-dioxane, H-721
1-Hydroxy-3,7-dimethoxyxanthone, T-724
2-Hydroxy-3-(2-hydroxyphenyl)propanoic acid; (*S*)-*form*, H-508
7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone, T-724
1-Hydroxy-3-methoxy-7-primeverosyloxyxanthone, T-724
5-Hydroxy-4′,7-dimethoxy-6-methylflavone, T-632
9-Hydroxy-4,10(14)-oplopadien-3-one; (4*E*,9α)-*form*; 9-(3-Methyl-2*E*-pentenoyl), H-667
9-Hydroxy-4,10(14)-oplopadien-3-one; (4*Z*,9α)-*form*; 9-(3-Methyl-2-butenoyl), H-667
9-Hydroxy-4,10(14)-oplopadien-3-one; (4*Z*,9α)-*form*; 9-Angeloyl, H-667
1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
3-Hydroxy-4,9-dimethoxypterocarpan, T-702
2-Hydroxy-4-methylbenzaldehyde, H-557
5-Hydroxy-4-octanone; (±)-*form*, H-655
7-Hydroxy-6-methoxyflavone, D-474
7-Hydroxy-8(14),15-isopimaradien-18-oic acid; 7α-*form*, H-520
3-Hydroxy-*p*-menth-3-en-2-one, H-545
2′-Hydroxyacetophenone, H-331
1α-Hydroxyarbusculin A, D-460
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3-(2-Hydroxyethyl)indole; *O*-[β-D-Xylopyranosyl-(1 → 6)-β-D-glucopyranoside], H-452
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3-(Hydroxymethyl)-2-octanone, H-595
Hydroxymyricanone, M-833
Hydroxypelenolide, H-472
p-Hydroxyphenethyl *trans*-ferulate, H-724
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Trigoneoside X_b, F-154
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Trigoneoside XIIa, F-159
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2,4,9-Trihydroxy-10(14)-oplopen-3-one; (*ent*-2β,4*S*,9α)-*form*; 9-(3-Methyl-2*E*-pentenoyl), 2-(2-methylbutanoyl), T-654
4′,5,6-Trihydroxy-3′,7,8-trimethoxyflavone, T-710
2,3′,6-Trihydroxy-4′-methoxybenzylcoumaranone, D-403
3′,5,7-Trihydroxy-4′-methoxyflavone; 7-*O*-β-D-Glucuronopyranoside, T-617
3,6,9-Trihydroxy-7(11)-eremophilen-12,8-olide; (3β,6β,8β,9α,10β)-*form*; 6-Angeloyl, T-562
3,6,9-Trihydroxy-7(11)-eremophilen-12,8-olide; (3β,6β,8β,9β,10β)-*form*; 6-Angeloyl, T-562
3,7,9-Trihydroxycoumestan, T-540
4′,5,7-Trihydroxyflavone; 7-*O*-[α-L-Rhamnopyranosyl-(1 → 2)-β-D-galacturonopyranoside], T-581
3-(3,4,5-Trihydroxyphenyl)-1,2-propanediol; 3′,4′-Di-Me ether, 1-*O*-β-D-glucopyranoside, T-666
1,3,7-Trihydroxyxanthone, T-724
3-(3,4,5-Trimethoxyphenyl)propanoic acid, T-667
4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanone, T-743
2,6,6-Trimethyl-1-cyclohexene-1-carboxaldehyde, T-749
3,5,5-Trimethyl-1-hexanol; (±)-*form*, T-781
3,5,5-Trimethyl-2-cyclohexen-1-one, T-752
2,6,6-Trimethyl-2-cyclohexene-1,4-dione, T-751
2,6,6-Trimethyl-2-cyclohexene-1-carboxaldehyde, T-750
3,5,5-Trimethyl-2-cyclopenten-1-one, T-763
3,4,7-Trimethyl-2*H*-1-benzopyran-2-one, T-736
2,2,3-Trimethyl-3-cyclopenten-1-ylacetaldehyde, C-68
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3-(5,6,6-Trimethylbicyclo[2.2.1]hept-1-yl)cyclohexanol, T-738
3,3,5-Trimethylcyclohexanol, T-746
2,2,6-Trimethylcyclohexanone; (±)-*form*, T-747
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3,5,5-Trimethylhexanal; (±)-*form*, T-779
2,3,6-Trimethylphenol, T-791
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11,12,13-Trinor-1,3,5-bisabolatrien-10-oic acid, T-805
1,3,5-Trithiane, T-822
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2,4-Undecadiene-8,10-diynoic acid 2,3-dehydropiperidide, U-11
2,4-Undecadiene-8,10-diynoic acid isobutylamide, U-11
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1,5-Undecadiene; (*Z*)-*form*, U-9
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6-Undecanone, U-19
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2-Undecenal; (*E*)-*form*, U-21
10-Undecenoic acid, U-27
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12-Ursen-3-ol; 3β-*form*; Ac, U-44
12-Ursene-3,16,21-triol; (3ξ,16ξ,21ξ)-*form*, U-42
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2-Bromo-1*H*-indole-3-carboxaldehyde, B-191
3-Bromosulfolane, B-196
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Conen; (±)-*form*, C-337
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2,6-Diethylaniline, D-197
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2,3-Dihydro-2,2-dimethyl-3,7-benzofurandiol 7-(methylcarbamate), C-89
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2,2-Dimethyl-7-[[(methylamino)carbonyl]oxy]-3(2*H*)-benzofuranone, 9CI, C-89
3,5-Dimethylphenyl methylcarbamate, D-877
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2-(Ethylsulfinylmethyl)phenyl methylcarbamate, E-248
2-(Ethylsulfonylmethyl)phenyl methylcarbamate, E-248
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2-Methyl-3,5-dinitrobenzamide, 9CI, M-396
1-Methylmocimycin, 9CI, M-726
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1-Naphthaleneacetic acid; Et ester, N-6
1-Naphthaleneacetic acid, N-6
(2-Naphthalenyloxy)acetic acid, N-10
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1,2,5,6-Tetrahydro-4*H*-pyrrolo[3,2,1-*ij*]quinolin-4-one, T-124
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1,3,5-Trichloro-(2-methylsulfonyl)benzene, T-450
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20-Deoxynarasin, N-14
Diflubenzuron, D-210
6-Ethoxy-1,2-dihydro-2,2,4-trimethylquinoline, 9CI, 8CI, D-364
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Gizzerosine; (*S*)-*form*, G-131
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2-Hydroxy-4-(methylthio)butanoic acid; (±)-*form*, H-619
3-Iodopropanoic acid, I-44
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3,3-Dichloro-4-(dichloromethylene)-2,5-pyrrolidinedione, D-155
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3,4-Dihydro-8-hydroxy-6-methoxy-3-methyl-1*H*-2-benzopyran-1-one, D-233
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1-(3-Furanyl)-1,4-pentanedione, F-128
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5-(3-Furanyl)-5-hydroxy-2-pentanone, 9CI, F-127
Fusarin C, F-162
Gizzerosine; (*S*)-*form*, G-131
Gyromitrin, G-360
3-[(3-Methylbutyl)nitrosoamino]-2-butanone, M-353
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Muscarine; (2*S*,4*R*,5*S*)-*form*, M-817
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3,4-Dichloro-2,5-pyrrolidinedione, D-163
2,6-Diethylaniline; *N*-Ac, D-197
2,6-Diethylaniline; *N*-Chloroacetyl, D-197
2,6-Diethylaniline, D-197
2,2′,3,4,4′,5′,6-Heptabromodiphenyl ether, H-38
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2,2′,4,4′,5-Pentabromodiphenyl ether, P-61
2,2′,4,4′,6-Pentabromodiphenyl ether, P-61
Pentabromodiphenyl ethers, P-61
2-Propenal, P-483
2,2′,4,4′-Tetrabromodiphenyl ether, T-37
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3,3′,4,4′-Tetrachloroazobenzene, T-38
3*a*,4,7,7*a*-Tetrahydro-4-hydroxy-1*H*-isoindole-1,3(2*H*)-dione, T-89
3*a*,4,5,7*a*-Tetrahydro-5-hydroxy-1*H*-isoindole-1,3(2*H*)-dione, T-88
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Tribromodiphenyl ethers, T-448
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3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole, A-244
2-Amino-1,6-dimethylfuro[3,2-*e*]imidazo[4,5-*b*]pyridine, A-241
3-Amino-1-methyl-5*H*-pyrido[4,3-*b*]indole, A-276
2-Amino-3,4,8-trimethyl-3*H*-imidazo[4,5-*f*]quinoxaline, A-307
2-Amino-3,8-dimethyl-3*H*-imidazo[4,5-*f*]quinoxaline, A-243
2-Amino-5-phenylpyridine, A-294
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2-Aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole, A-246
Cycasin, M-310
Dihydro-2,4,6-trimethyl-4*H*-1,3,5-dithiazine; (2α,4α,6α)-*form*; *N*-Nitroso, D-361
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3-Methyl-3*H*-imidazo[4,5-*f*]quinoxalin-2-amine, A-268
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Aluminium sodium oxide ($AlNaO_2$), A-199
2-Amino-*N*-(2,2,4,4-tetramethyl-3-thietanyl)-propanamide; (*R*)-*form*, A-305
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2,2′-Bis(4-hydroxyphenyl)propane, B-141
2,2-Bis[4-(2,3-epoxypropoxy)phenyl]propane, B-128
3-Chloro-1,2-propanediol, C-220
(Chloromethyl)oxirane, C-211
Cyclohexylamine, C-467
3-(Dichloromethylene)-2,5-pyrrolidinedione, D-162
2-Diethylaminoethanol, 9CI, A-249
Dihydro-3-(2-octenyl)-2,5-furandione, D-336
1-(3,4-Dihydroxyphenyl)-2-propanone, D-650
1,1′-Ethylidenebistryptophan, E-322
Gizzerosine; (*S*)-*form*, G-131
Hydrazine, H-319
4-Hydroxyphenethylamine, H-712
Lysinoalanine, L-133
Methionine sulfoximine, M-245
Morpholine, M-764
Octadecylamine, O-52
Orthoperiodic acid, O-174
Potassium triphosphate ($K_5(P_3O_{10})$), P-449
Sodium methyl sulfate, S-137
Sodium silicate (Na_2SiO_3), S-143
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15-Acetoxy-12,13-epoxy-3,7-dihydroxy-9-trichothecen-8-one, S-56
3′-*N*-Acetyl-4′-*O*-(10,12-octadecadienoyl)fusarochromanone, F-163
3′-*N*-Acetyl-4′-*O*-(14-methylheptadecanoyl)fusarochromanone, F-163
3′-*N*-Acetyl-4′-*O*-(14-methylpentadecanoyl)fusarochromanone, F-163
3′-*N*-Acetyl-4′-*O*-(9-octadecenoyl)fusarochromanone, F-163
4-Acetyl-*cis*-zearalenone, Z-7
8-Acetyl-T2 tetrol, S-55
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Aflatoxin GM_2, A-136
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Aflatoxin M_2, A-137
Aflatoxin M_4, A-134
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5-Amino-2,3-dihydro-6-(3-hydroxy-4-methoxy-1-oxobutyl)-2,2-dimethyl-4*H*-1-benzopyran-4-one, A-235
α-Amino-4-carboxy-3-furanpropanoic acid; (*S*)-*form*, A-226
5-Amino-6-(4-hydroxy-2-butenoyl)-2,2-dimethyl-4-chromanone, F-163
5-Amino-6-(4-hydroxybutanoyl)-2,2-dimethyl-4-chromanone, F-163
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Apotrichothecene, A-382
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3-[(Cyanophenylmethyl)amino]-3-oxopropanoic acid; (*S*)-*form*, C-412
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Diacetylfusarochromanone, F-163
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1′,2′-Dihydro-1,1′-dimethyl-2′-oxo-4,4′-bipyridinium(1+), D-249
2,3-Dihydro-2,3-dihydroxy-4-(4-hydroxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-4-(4-methoxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-9-phenyl-1*H*-phenalen-1-one, D-279
2,3-Dihydro-4-(4-hydroxyphenyl)-1*H*-phenalene-1,2,3-triol; (1*R*,2*R*,3*R*)-*form*; 3-Ketone, D-279
2,3-Dihydro-4-(4-hydroxyphenyl)-1*H*-phenalene-1,2,3-triol; (1*S*,2*R*,3*S*)-*form*, D-279
2,3-Dihydro-4-(4-methoxyphenyl)-1*H*-phenalene-1,2,3-triol, D-279
5,6-Dihydro-4-methoxy-2*H*-pyran-2-one, D-291
3,4-Dihydro-6-methoxy-3,7-dimethyl-1*H*-2-benzopyran-8-ol, D-288
7,8-Dihydro-7,8-dihydroxy-3,5,7-trimethyl-6*H*-2-benzopyran-6-one, D-240
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Dihydrohydroxy-*O*-methylsterigmatocystin, S-222
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11,12-Dihydroxy-1(10)-spirovetiven-2-one; (4*R*,5*S*,7*R*,11ξ)-*form*; 12-*O*-β-D-Glucopyranoside, D-691
11,12-Dihydroxy-1(10)-spirovetiven-2-one; (4*R*,5*S*,7*R*,11ξ)-*form*, D-691
11,12-Dihydroxy-1(10)-spirovetiven-2-one; (4*R*,5*S*,7*R*,11*R*)-*form*, D-691
11,12-Dihydroxy-1(10)-spirovetiven-2-one; (4*R*,5*S*,7*R*,11*S*)-*form*; 11-*O*-β-D-Glucopyranoside, D-691
11,12-Dihydroxy-1(10)-spirovetiven-2-one; (4*R*,5*S*,7*R*,11*S*)-*form*, D-691
2,7-Dihydroxy-1,3,4-trimethoxydibenzofuran, D-127
2,3-Dihydroxy-11-spirovetiven-14-al, D-690
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2,3-Dihydro-3,5-dihydroxy-2-oxo-1*H*-indole-3-acetic acid; (*R*)-*form*; 5-*O*-β-D-Glucopyranoside, D-237
2,3-Dihydro-3,5-dihydroxy-2-oxo-1*H*-indole-3-acetic acid; (*R*)-*form*; 5-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-glucopyranoside], D-237
2,3-Dihydro-3,5-dihydroxy-2-oxo-1*H*-indole-3-acetic acid; (*S*)-*form*; 5-*O*-β-D-Glucopyranoside, D-237
2,3-Dihydro-3,5-dihydroxy-2-oxo-1*H*-indole-3-acetic acid; (*S*)-*form*; 5-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-glucopyranoside], D-237
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2,3-Dihydro-3,5-dihydroxy-2-oxo-3-indoleacetic acid; (*R*)-*form*; 5-*O*-β-D-Glucopyranoside, D-239
2,3-Dihydro-3,5-dihydroxy-2-oxo-3-indoleacetic acid; (*R*)-*form*; 5-*O*-[β-D-Glucopyranosyl-(1 → 4)-β-D-glucopyranoside], D-239
2,3-Dihydro-3,5-dihydroxy-2-oxo-3-indoleacetic acid; (*R*)-*form*, D-239
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2,3-Dihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-*form*; 3-*O*-β-D-Glucopyranoside, 28-*O*-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-α-L-arabinopyranosyl] ester, D-571
2,3-Dihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-*form*; 3-*O*-β-D-Glucopyranoside, D-571
2,3-Dihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-*form*; 3-*O*-β-D-Glucuronopyranoside, 28-*O*-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-α-L-arabinopyranosyl] ester, D-571
2,3-Dihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-*form*; 3-*O*-β-D-Glucuronopyranoside, D-571
2,3-Dihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-β-D-glucopyranoside], 28-*O*-[β-D-xylopyranosyl-(1 → 4)-α-L-rhamnopyranosyl-(1 → 2)-α-L-arabinopyranosyl] ester, D-571
2,3-Dihydroxy-12-oleanene-23,28-dioic acid; (2β,3β)-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 3)-β-D-glucopyranoside], D-571
3,23-Dihydroxy-12-oleanene-28,30-dioic acid; 3β-*form*; 3-*O*-[α-L-Arabinopyranosyl-(1 → 3)-β-D-glucuronopyranoside], 28-*O*-β-D-glucopyranosyl ester, 30-Me ester, D-573
3,23-Dihydroxy-12-oleanene-28,30-dioic acid; 3β-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 3)-β-D-xylopyranosyl-(1 → 2)-β-D-glucopyranoside], 28-*O*-β-D-glucopyranosyl ester, 30-Me ester, D-573
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1,26-Hexacosanediol diferulate, H-145
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1-Hydroxy-12,15-cassadiene-3,11-dione, D-411
3-Hydroxy-12-oleanene-28,30-dioic acid; 3β-*form*; 3-*O*-[α-L-Arabinopyranosyl-(1 → 3)-β-D-glucuronopyranoside], 28-*O*-β-D-glucopyranosyl ester, 30-Me ester, H-662
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5-Hydroxy-2-oxo-1*H*-indole-3-acetic acid; Me ester, H-685
4-Hydroxy-2-pyrrolidinecarboxylic acid; (2*S*,4*R*)-*form*; β-D-Galactopyranosyl ester, H-776
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2-Hydroxy-2*H*-1,4-benzoxazin-3(4*H*)-one; (*R*)-*form*, H-353
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5,6,8-Trihydroxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one; 8-Me ether, 6-*O*-[β-D-glucopyranosyl-(1 → 3)-β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranoside], T-634
5,6,8-Trihydroxy-2-methyl-4*H*-naphtho[2,3-*b*]pyran-4-one, T-634
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3,22,23-Trihydroxy-24-methyl-*B*-homo-7-oxacholestan-6-one, B-181
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4′,5,7-Trihydroxy-3′,5′-dimethoxyflavone; 7-*O*-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-549
4′,5,7-Trihydroxy-3′,5′-dimethoxyflavone; 7-*O*-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1 → 2)-[β-D-glucuronopyranosyl-(1 → 3)]-β-D-glucuronopyranoside], T-549
4′,5,7-Trihydroxy-3′,5′-dimethoxyflavone; 7-*O*-[4-Hydroxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-549
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4′,5,7-Trihydroxy-3′-methoxyflavone; 7-*O*-[β-D-Glucuronopyranosyl-(→?)-β-D-glucuronopyranosyl-(→?)-β-D-glucuronopyranoside], T-618
4′,5,7-Trihydroxy-3′-methoxyflavone; 7-*O*-[β-D-Glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-618
4′,5,7-Trihydroxy-3′-methoxyflavone; 7-*O*-[4-Hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], T-618
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4′,5,7-Trihydroxyflavone; 4′-*O*-[4-Hydroxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 7-*O*-β-D-glucuronopyranoside, T-581
4′,5,7-Trihydroxyflavone; 7-*O*-[β-D-Glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 4′-*O*-β-D-glucuronopyranoside, T-581
4′,5,7-Trihydroxyflavone; 7-*O*-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranosyl-(1 → 2)-β-D-glucuronopyranoside], 4′-*O*-β-D-glucuronopyranoside, T-581
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3-(3,4,5-Trihydroxyphenyl)-2-propenoic acid; (*Z*)-*form*; 3,5-Di-Me ether, T-672
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Furanojaponin, F-100
S-Furanopetasitin, F-99
Furoeremophilone 1, F-102
Furostane-3,22,26-triol; (3β,5β,22α,25*R*)-*form*; 22-Me ether, 3-*O*-[β-D-glucopyranosyl-(1 → 2)-β-D-glucopyranoside], 26-*O*-β-D-glucopyranoside, F-156
2*H*-Furo[2,3-*h*][1]benzopyran-2-one, F-144
Gallic acid 3-*O*-(6-galloylglucoside), T-520
Gallic acid 4-*O*-(6-galloylglucoside), G-48
1-*O*-Galloyl-β-D-glucopyranose, G-46
3-*O*-Galloylepicatechin, P-104
1-*O*-Galloylfructose, F-75
2-Galloylglucose, G-47
6-Galloylglucose, G-49
1-*O*-Galloylglycerol, G-50
3-Galloylprocyanidin B_1, P-121
1′-*O*-Galloylsucrose, S-263
2-*O*-Galloylsucrose, S-263
4′-*O*-Galloylsucrose, S-263
6′-*O*-Galloylsucrose, S-263
6-*O*-Galloylsucrose, S-263
Genistein 7-*O*-(2-*p*-coumaroylglucoside), T-601
Geranyl butyrate, D-833
O-Geranylvanillin, D-382
Gibberellin A_{19}, G-96
Gibberellin A_{44}, G-104
Gibberellin A_{50}, G-103
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Glucoemodin, T-624
4-Glucogallic acid, G-48
3-Glucogallic acid, T-520
Glucohesperetin, T-614
β-D-Glucopyranosyl 2,6-dimethylbenzoate, D-761
β-D-Glucopyranosyl-(1 → 4)-β-D-glucopyranosyl-(1 → 4)-D-mannose, G-172
ω-*O*-β-D-Glucopyranosylaloeemodin, D-503
1-*O*-β-D-Glucopyranosylaloeemodin, D-503
2-(β-D-Glucopyranosyloxy)-2-methylpropanenitrile, 9CI, H-605
6-Glucopyranosylprocyanidin B_1, G-185
8-Glucopyranosylprocyanidin B_1, G-186
6-Glucopyranosylprocyanidin B_2, G-185
8-Glucopyranosylprocyanidin B_2, G-186
β-D-Glucopyranuronosyl-(1 → 3)-α-D-galactopyranuronosyl-(1 → 2)-α-L-rhamnopyranosyl-(1 → 4)-[β-D-glucopyranuronosyl-(1 → 3)]-α-D-galactopyranuronosyl-(1 → 2)-L-rhamnopyranose, G-191
Glucorhein, D-378
β-D-Glucuronopyranosyl-(1 → 3)-α-D-galacturonopyranosyl-(1 → 2)-L-rhamnose, G-207
γ-L-Glutamyl-L-pipecolic acid, P-391
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1,8,15-Heptadecatriene-11,13-diyne; (8*E*,15*E*)-*form*, H-62
1,8,15-Heptadecatriene-11,13-diyne; (8*Z*,15*Z*)-*form*, H-62
2,9,16-Heptadecatriene-4,6-diyn-8-ol; (*Z*,*Z*)-*form*, H-65
2,5-Heptadien-1-ol, H-81
3,3′,4,4′,5,5′,7-Heptahydroxyflavan; 3-*O*-[β-D-Galactopyranosyl-(1 → 4)-β-D-glucopyranoside], H-85
3,3′,4′,5,5′,6,7-Heptahydroxyflavone; 6,7-Methylene, 4′-Me ether, 3-*O*-β-D-glucuronopyranoside, H-86
3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate, H-113
2-Heptylfuran, H-123
Heraclenol; (*R*)-*form*; 2′-*O*-(3-Methyl-2-butenoyl), H-125
Heraclenol; (*R*)-*form*; 2′-*O*-(3-Methylbutanoyl), H-125
1-Hexacosene, H-153
N-Hexadecanoylpyrrolidine, P-618
3-Hexadecenoic acid; (*E*)-*form*, H-162
3,3′,4′,5,6,7-Hexahydroxyflavone; 3′,4′,7-Tri-Me ether, 3-*O*-β-D-glucuronopyranoside, H-207
3,3′,4′,5,6,7-Hexahydroxyflavone; 3′,7-Di-Me ether, 3-*O*-β-D-glucuronopyranoside, H-207
3,3′,4′,5,7,8-Hexahydroxyflavone; 3-*O*-β-D-Glucopyranoside, 8-*O*-β-D-glucuronopyranoside, H-209
3,3′,4′,5,6,7-Hexahydroxyflavone; 4′,7-Di-Me ether, 3-*O*-β-D-glucuronopyranoside, H-207
3,3′,4′,5,6,7-Hexahydroxyflavone; 6,7-Methylene, 3′,4′-di-Me ether, 3-*O*-β-D-glucuronopyranoside, H-207
3,3′,4′,5,6,7-Hexahydroxyflavone; 6,7-Methylene, 3,3′-di-Me ether, 4′-*O*-β-D-glucuronopyranoside, H-207
3,3′,4′,5,6,7-Hexahydroxyflavone; 6,7-Methylene, 3-Me ether, 4′-*O*-β-D-glucuronopyranoside, H-207
3,3′,4′,5,6,7-Hexahydroxyflavone; 6,7-Methylene, 4′-Me ether, 3-*O*-β-D-glucuronopyranoside, H-207
3,3′,4′,5,7,8-Hexahydroxyflavone; 8-*O*-β-D-Glucuronopyranoside, 3-*O*-sulfate, H-209
3,3′,4′,5,5′,7-Hexahydroxyflavylium(1+); 3-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), 5-*O*-β-D-glucopyranoside, H-213
2-Hexen-1-ol; (*E*)-*form*, H-252
Homofukinolide, F-84
8-Hydroxy-1-methoxy-3-methylanthraquinone, D-544
ent-8α-Hydroxy-1-oxo-7(11)-eremophilen-12,8-olide, D-450
9-Hydroxy-10-undecenoic acid; (*S*)-*form*, H-824
11-Hydroxy-13-nor-6-eremophilen-8-one; (10β*H*,11ξ)-*form*, H-634
ent-17-Hydroxy-15-kauren-19-oic acid, K-24
7-Hydroxy-2,5-dimethyl-4*H*-1-benzopyran-4-one, H-405
3-Hydroxy-2,9-dimethoxypterocarpan, T-701
4′-Hydroxy-2-biphenylcarboxylic acid, H-366
7-Hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-acetic acid, 9CI, D-275
7-Hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-carboxylic acid; 7-*O*-β-D-Glucopyranoside, H-596
7-Hydroxy-2-methyl-4-oxo-4*H*-1-benzopyran-5-carboxylic acid, H-596
2-Hydroxy-2-methylbutyl glucosinolate, H-573
8-Hydroxy-3,9-dimethoxypterocarpan, T-703
4-Hydroxy-3-(16-methylheptadecyl)-2*H*-pyran-2-one, H-589
9-Hydroxy-3-methoxy-2-prenylpterocarpan, D-670
3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid; (*E*)-*form*, H-554
2-Hydroxy-3-methyl-4*H*-pyran-4-one; *O*-(6*E*-Cinnamoyl-β-D-glucopyranoside), H-608
8-Hydroxy-3-oxo-7(11)-eremophilen-12,8-olide; (8βOH,10β)-*form*, H-678
3-Hydroxy-4,9-dimethoxypterocarpan, T-702
7-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one; Ac, H-561
7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone; 7-*O*-β-D-Glucopyranoside, H-502
5-Hydroxy-6,7-methylenedioxyflavone, T-582
3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide, T-561
11-Hydroxy-6-eremophilen-8-one, H-444
7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, H-547
3-Hydroxy-6-methoxy-7(11)-eremophilen-12,8-olide, D-451
3-Hydroxy-7(11)-eremophilen-12,8-olide; (3β,8β)-*form*, H-440
6-Hydroxy-7(11)-eremophilen-12,8-olide; (6β,8α)-*form*, H-441
5-Hydroxy-7-methoxy-2-tritriacontyl-4*H*-1-benzopyran-4-one, 9CI, D-703
8-Hydroxy-7-methoxy-2*H*-1-benzopyran-2-one, 9CI, D-396
7-Hydroxy-8(14),15-pimaradien-19-oic acid; (*ent*-7α)-*form*, H-755
7-Hydroxy-8(14),15-pimaradien-19-oic acid; (*ent*-7β)-*form*, H-755
7-Hydroxy-8-methoxy-6-(3-methyl-2-butenyl)-2*H*-1-benzopyran-2-one, D-668
6-Hydroxy-8-methoxy-7(11)-eremophilen-12,8-olide, D-452
3-Hydroxy-8-oxo-6-eremophilen-12-oic acid; (3β,11ξ)-*form*; Me ester, H-677
4-Hydroxybenzyl glucosinolate; 4-(4-*O*-Acetyl-α-L-rhamnopyranoside), H-358
(4-Hydroxybenzyl)carbamic acid; *O*-α-L-Rhamnopyranoside, Et ester, H-361
(4-Hydroxybenzyl)carbamic acid; *O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), Et ester, H-361
(4-Hydroxybenzyl)carbamic acid; *O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), Me ester, H-361
(4-Hydroxybenzyl)thiocarbamic acid; 4′-*O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), *O*-Et ester (*Z*-), H-365
(4-Hydroxybenzyl)thiocarbamic acid; 4′-*O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), *O*-Et ester, H-365
(4-Hydroxybenzyl)thiocarbamic acid; 4′-*O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), *O*-Me ester (*E*-), H-365
2-*O*-(4-Hydroxycinnamoyl)-1,6-di-*O*-galloyl-β-D-glucopyranose, C-264

2-*O*-(4-Hydroxycinnamoyl)-1-*O*-galloyl-β-D-glucopyranoside, C-265
6-(Hydroxymethyl)-2,4(1*H*,3*H*)-pteridinedione, H-607
2-(Hydroxymethyl)benzoic acid, H-560
6-Hydroxypentadecanedioic acid, H-702
4-[5-(4-Hydroxyphenoxy)-3-penten-1-ynyl]phenol; (*E*)-*form*, H-713
4-(4-Hydroxyphenyl)-2-butanone; *O*-β-D-Glucopyranoside, H-720
4-(4-Hydroxyphenyl)-2-butanone; *O*-[2,6-Bis(3,4,5-trihydroxybenzoyl)-β-D-glucopyranoside], H-720
4-(4-Hydroxyphenyl)-2-butanone; *O*-[3,4,5-Trihydroxybenzoyl-(→2)-6-*O*-cinnamoyl-β-D-glucopyranoside], H-720
4-(4-Hydroxyphenyl)-2-butanone; *O*-[4-Hydroxy-*E*-cinnamoyl-(→6)-[3,4,5-trihydroxybenzoyl-(→2)]-β-D-glucopyranoside], H-720
3-(2-Hydroxyphenyl)-2-propenoic acid; (*E*)-*form*, H-746
4-Hydroxyphenylthiocarbamic acid; *OH*-*form*; Et ester, H-751
3-Hydroxyspirostan-12-one; (3β,5β,25*R*)-*form*; 3-*O*-[β-D-Glucopyranosyl-(1→2)-[α-L-arabinopyranosyl-(1→6)]-β-D-glucopyranoside], H-782
Indocentoic acid, I-22
1*H*-Indole-3-acetic acid, I-25
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Isobyakangelicin; (*R*)-*form*; 3′-*O*-β-D-Glucopyranoside, I-76
Isolindleyin, H-720
Isomultiflorenyl acetate, M-791
Isopetasoside, H-438
2-Isopropyl-5-methoxypyrazine, H-524
7-Isopropyl-5-methylbicyclo[2.2.2]oct-5-en-2-one, I-141
2-Isopropyl-6-methoxypyrazine, H-525
Isoquercitrin; *O*′′-(4-Hydroxy-3-methoxycinnamoyl), 4′-*O*-β-D-glucopyranoside, I-158
Isorhamnetin 3-β-laminaribioside, G-182
Isoscoparin; 2′′-*O*-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→6)-β-D-glucopyranosyl], 4′-*O*-β-D-glucopyranoside, I-164
Isosilybin, I-165
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Isoswertiajaponin, O-167
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1-(Isothiocyanatomethyl)-4-methoxybenzene, 9CI, H-359
Isotriglochinin, T-510
Isowertin 2′′-rhamnoside, V-46
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Jaceidin 4′-glucuronide, T-711
S-Japonin, H-442
Kaempferol 3-(6-acetylgalactoside), T-502
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20(29)-Lupene-2,3,28-triol; (2α,3β)-*form*; 3,28-Dihexadecanoyl, L-118
20(29)-Lupene-2,3,28-triol; (2α,3β)-*form*, L-118
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Melilotussaponin O_2, D-605
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Melongoside P, F-156
p-Mentha-1(7),5-dien-2-ol; (2*S*,4*R*)-*form*; Ac, M-125
p-Mentha-1,8-dien-6-ol, M-128
3-Mercapto-2-(mercaptomethyl)propanoic acid; *S*-Ac, M-212
3-Mercapto-2-(mercaptomethyl)propanoic acid, M-212
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Methoxatin, M-247
2-Methoxy-3-(1-methylpropyl)pyrazine, M-263
3-Methoxy-4,5-methylenedioxybenzoic acid, H-584
2-Methoxy-4-(2-propenyl)phenol; *O*-[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside], M-273
1-Methoxy-4-[5-(4-methoxyphenoxy)-3-penten-1-ynyl]benzene, H-713
4-Methoxy-7*H*-furo[3,2-*g*]benzopyran-7-one, B-67
6β-Methoxyfuranoeremophilane, F-101
4-[5-(4-Methoxyphenoxy)-3-penten-1-ynyl]phenol, H-713
2-Methoxystypandrone, M-275
Methyl 15-cyanopentadecanoate, H-158
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Methyl 6-*O*-digalloyl-β-D-glucopyranoside, G-49
Methyl 6-*O*-galloyl-β-D-glucopyranoside, G-49
3-Methyl-1-butylamine, M-350
12-Methyl-13-tridecanolide, M-701
3-Methyl-2-oxobutanoic acid, M-529
3-Methyl-2-oxopentanoic acid, M-532
4-Methyl-2-oxopentanoic acid, M-533
4-Methyl-2-phenyl-2-pentenal, M-592
2-Methyl-5-(1-propenyl)pyrazine, M-611
2-Methyl-5-propylpyrazine, M-627
2-Methyl-5-vinylpyrazine, M-714
2-Methyl-6-(1-propenyl)pyrazine, M-613
6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one; (*E*)-*form*, M-500
2-Methyl-6-phytylhydroquinone, M-599
4′-Methylacetophenone, M-305
3-Methylbutanoic acid, M-331
3-(3-Methylbutylidene)-1(3*H*)-isobenzofuranone, M-352
9-*O*-Methylcoumestrol, C-370
N-(14-Methylhexadecanoyl)pyrrolidine, P-618
S-Methylmethionine; (*S*)-*form*, M-486
4-Methylphenol, M-573
1-(4-Methylphenyl)ethanol; (ξ)-*form*, M-582
1-Methylpropyl 1-propenyl disulfide; (-)-*form*, M-617
1-Methylpropyl 3-(methylthio)-2-propenyl disulfide; (+)-*form*, M-616
3-(2-Methylpropylidene)-1(3*H*)-isobenzofuranone; (*E*)-*form*, M-624
3-(2-Methylpropylidene)-3*a*,4-dihydro-1(3*H*)-isobenzofuranone, M-624
4-Methylthiazole, M-658
3-(Methylthio)-1-propanol, M-229
9-(Methylthio)nonanenitrile, 9CI, M-220
8-(Methylthio)octanenitrile, 9CI, M-221
3-(Methylthio)propanal, M-688
1-(Methylthio)propyl 1-propenyl disulfide; (-)-*form*, M-692
Mollupentin; 7-Me ether, 2′′-*O*-α-L-rhamnopyranoside, M-731
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Morphine; (-)-*form*, M-763
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Niazimin A, H-361
Niazimin B, H-361
Niaziminin A, H-365
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Niazinin A, H-365
Niazinin B, H-365
6-Nitro-*p*-mentha-1(7),2-diene; (4*R*∗,6*R*∗)-*form*, N-70
6-Nitro-*p*-mentha-1(7),2-diene; (4*R*∗,6*S*∗)-*form*, N-70
2-Nitro-*p*-mentha-1,5-diene; (*R*)-*form*, N-69
2,4-Nonadienal; (2*E*,4*E*)-*form*, N-96
3,6-Nonadienal; (3*Z*,6*Z*)-*form*, N-98
2-Nonanol, N-111
2-Nonanone, N-113
3-Nonen-1-ol; (*Z*)-*form*, N-124
1-Nonen-3-ol; (ξ)-*form*; Ac, N-122
1-Nonen-3-ol, N-122
2-Nonenal; (*E*)-*form*, N-116
13-Nor-6-eremophilene-8,11-dione, H-634
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Octacosyl (*E*)-isoferulate, D-653
9,17-Octadecadiene-12,14-diyne-1,11,16-triol; (9*Z*,11*S*,16*S*)-*form*; 1-Ac, O-20
3-Octen-2-one, O-107
Octopamine; (*R*)-*form*, O-111
Oleacein, O-119
12-Oleanene-3,21,28-triol; (3β,21β)-*form*; 28-*O*-[β-D-Arabinopyranosyl-(1→3)-β-D-arabinopyranosyl-(1→3)-β-D-arabinopyranoside], O-138
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5-Oxo-2-pyrrolidinecarboxylic acid; (*S*)-*form*, O-249
ent-7-Oxo-8(14),15-pimaradien-19-oic acid, H-755
4-Oxopentanoic acid, O-239
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5,10-Pentadecadien-1-ol, P-73
2-Pentadecanone, P-77
3-Pentadecenal, P-79
Pentaglycosides; 3-*O*-[β-D-Glucopyranosyl-(1→3)-[α-L-arabinopyranosyl-(1→4)]-β-D-glucuronopyranoside], 28-*O*-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester, O-146
3,3′,4′,5,7-Pentahydroxy-6-methoxyflavone; 3-*O*-[β-D-Apiofuranosyl-(1→2)-[β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside], P-157
3,3′,4′,5,7-Pentahydroxy-6-methoxyflavone; 3-*O*-[β-D-Apiofuranosyl-(1→2)-[4-hydroxy-3-methoxycinnamoyl-(→2)-β-D-glucopyranosyl-(1→6)]-β-D-glucopyranoside], P-157
3,3′,4′,5,7-Pentahydroxyflavan(4→8)-3,3′,4′,5,7-pentahydroxyflavan(4→6)-

3,3′,4′,5,7-pentahydroxyflavan; (2*R*,2′*R*,2″*R*,3*R*,3′*R*,3″*S*,4*R*,4′*R*)-*form*; 3,3′-Bis(3,4,5-trihydroxybenzoyl), P-128
3′,4′,5,7,8-Pentahydroxyflavone; 3′,7-Di-Me ether, 8-*O*-β-D-glucopyranoside, P-141
3,4′,5,6,7-Pentahydroxyflavone; 6,7-Methylene, 3-Me ether, 4′-*O*-β-D-glucuronopyranoside, P-136
3′,4′,5,7,8-Pentahydroxyflavone; 8-*O*-β-D-Glucopyranoside, 3′-*O*-sulfate, P-141
3,3′,4′,5,7-Pentahydroxyflavone, P-134
3′,4′,5,6,7-Pentahydroxyflavone, P-137
1,2,3,5,6-Pentathiepane, P-196
1,2,4,5,7-Pentathiocane, P-197
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Petasitenine, P-235
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1-Phenyl-1-pentanone, P-298
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Piscidic acid; (2*R*,3*S*)-*form*, P-407
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Dammar-24-ene-3,6,12,17,20-pentol; (3β,6α,12β,17α,20*S*)-*form*; 20-*O*-[β-D-Glucopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside], 3-*O*-[β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranoside], 6-*O*-β-D-xylopyranoside, D-12
Dammar-24-ene-3,6,12,17,20-pentol; (3β,6α,12β,17α,20*S*)-*form*; 20-*O*-[β-D-Glucopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside], 6-*O*-β-D-glucopyranoside, D-12
Dammar-24-ene-3,6,12,17,20-pentol; (3β,6α,12β,17α,20*S*)-*form*; 20-*O*-[β-D-Glucopyranosyl-(1 → 2)-[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside], 6-*O*-β-D-xylopyranoside, D-12
Debenzoylzucchini factor B, M-788
Decanoic acid, D-41
1-Decanol, D-42
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Sambucus nigra Degraded cyanogenic glycosides; 2′-Epimer, D-67
Sambucus nigra Degraded cyanogenic glycosides; 2-Epimer, D-67
Sambucus nigra Degraded cyanogenic glycosides, D-67
Dehydrocarpaine I, C-127
Dehydrocarpaine II, C-127
25-Dehydrofungisterol, E-209
8,9-Dehydrotheaspirone; (ξ)-*form*, D-75
Delphin, H-213
Delphinidin 3-(6-coumaroylglucoside), H-213
Delphinidin 3-(acetylglucoside), H-213
Delphinidin 3-arabinoside, H-213
Delphinidin 3-gentiobioside, H-213
Delphinidin 3-sophoroside, H-213
Demethylcalabaxanthone, C-29
O-Demethylforbexanthone, F-59
Demethyloleuropein, O-151
4-Deoxy-6-hydroxysquamotacin, S-214
4-Deoxyannoreticuin, A-352
cis-4-Deoxyannoreticuin, A-352
6-*C*-(6-Deoxygalactopyranosyl)-3′,4′,5,7-tetrahydroxyflavone, G-28
6-*C*-(6-Deoxyglucopyranosyl)-3′,4′,5,7-tetrahydroxyflavone, D-83
Deoxymorellin, M-759
5-Deoxymyricanone, M-833
3′-Deoxyoleacein, O-119
4-Deoxyphysalolactone, P-350
$\Delta^{3,5}$-Deoxytigogenin, S-180
Di-4-coumaroylputrescine, D-166
1,2-Di-*O*-(8-hexadecenoyl)-3-*O*-(6-sulfoquinovopyranosyl)glycerol, G-239
3,5-Di-*O*-caffeoylquinic acid, D-151
3,5-Di-*O*-galloyl-1,4-galactarolactone, G-1
1,4-Di-*O*-galloyl-3,6-(*R*)-hexahydroxydiphenoyl-β-D-glucopyranose, H-192
3,3′-Di-*O*-galloylprodelphinidin B_5, P-120
2,8-Di-*O*-methylellagic acid, E-36
1,2-Di-*O*-myristoyl-3-*O*-(6-sulfoquinovopyranosyl)glycerol, G-239
1,2-Di-*O*-palmitoyl-3-*O*-(6-sulfoquinovopyranosyl)glycerol, G-239
2,6-Di-*tert*-butyl-4-ethylphenol, D-146

24,25-Diacetylvulgaroside, V-57
Dibutyl malate, M-36
1,5-Dibutyl methyl hydroxycitrate, D-675
10′,11′-Didehydro-5,8,11′,12′-tetrahydro-10′-apo-β-carotene-3,5,8-triol, D-176
4,7-Didehydroneophysalin B, D-175
5,6-Didehydropersin, D-496
1,4-Dideoxy-1,4-imino-D-ribitol, D-508
1,5-Dideoxy-1,5-(methylimino)-D-glucitol, 9CI, H-604
1,5-Dideoxy-1,5-imino-D-glucitol, 9CI, H-604
Diellagilactone, D-177
5,6-Diepikarpoxanthin, D-224
Diepomuricanin A, E-172
Dieporeticanin, D-178
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5,9:6,9-Diepoxy-3-megastigmene, D-188
5,5′,6,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-caroten-3-ol, 9CI, V-40
3,6:5′,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3′,5-diol, C-388
5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-caroten-3-ol, A-495
1,1-Diethoxypentane, P-181
Diethyl disulfide, D-193
Diethyl malonate, D-194
Diethyl trisulfide, D-196
Diferuloylputrescine, D-166
N^1,N^{10}-Diferuloylspermidine, D-167
Diferuloylspermine, S-165
3,3′-Digalloylprodelphinidin B_1, H-199
3,3′-Digalloylprodelphinidin B_2, H-199
6,8-Diglucopyranosyl-4′,5,7-trihydroxyflavanone; (2*R*)-*form*, D-218
6,8-Diglucopyranosyl-4′,5,7-trihydroxyflavanone; (2*S*)-*form*, D-218
3,6-Diglucopyranosyl-5,7-dihydroxy-4′-methoxyflavone, D-219
1,1-Dihexyloxyethane, D-221
1,2-Dihydro-1,1,6-trimethylnaphthalene, D-362
5,7*a*-Dihydro-1,4,4,7*a*-tetramethyl-4*H*-indene, D-356
3,4-Dihydro-1-methyl-β-carboline, D-293
Dihydro-2(3*H*)-furanone, D-253
2,3-Dihydro-2,3-dihydroxy-4-(4-hydroxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-4-(4-methoxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-9-(4-hydroxy-3-methoxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2,3-dihydroxy-9-phenyl-1*H*-phenalen-1-one, D-279
2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (*S*)-*form*; *O*-α-L-Rhamnopyranoside, D-270
6,7-Dihydro-2-methyl-5*H*-cyclopenta[*b*]pyrazine, D-294
2,3-Dihydro-2-oxo-1*H*-indole-3-acetic acid; (ξ)-*form*, D-339
Dihydro-3-methyl-2(3*H*)-furanone, D-299
25,27-Dihydro-4,7-didehydro-7-deoxyphysalin A, D-227
2,3-Dihydro-4-(4-hydroxyphenyl)-1*H*-phenalene-1,2,3-triol; (1*R*,2*R*,3*R*)-*form*; 3-Ketone, D-279
2,3-Dihydro-4-(4-hydroxyphenyl)-1*H*-phenalene-1,2,3-triol; (1*S*,2*R*,3*S*)-*form*, D-279
2,3-Dihydro-4-(4-methoxyphenyl)-1*H*-phenalene-1,2,3-triol, D-279
3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2*H*-pyran; (ξ)-*form*, D-308
2,3-Dihydro-5,5′,7,7′-tetrahydroxy-2-(4-hydroxyphenyl)[3,8′-bi-4*H*-1-benzopyran]-4,4′-dione, D-355
7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, D-231
7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(2-methyl-1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, D-229
7,8-Dihydro-5,7-dihydroxy-8,8-dimethyl-10-(3-methyl-1-oxobutyl)-4-propyl-2*H*,6*H*-benzo[1,2-*b*:5,4-*b*′]dipyran-2-one, D-230
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(1-oxobutyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-263
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(1-oxobutyl)-4-propyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-264
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(2-methyl-1-oxopropyl)-4-phenyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-262
8,9-Dihydro-5-hydroxy-8-(1-hydroxy-1-methylethyl)-6-(3-methyl-1-oxobutyl)-4-propyl-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, D-261
Dihydro-5-methyl-2(3*H*)-furanone, D-301
Dihydro-5-octyl-2(3*H*)-furanone; (ξ)-*form*, D-338
Dihydro-5-pentyl-2(3*H*)-furanone, D-341
Dihydro-5-propyl-2(3*H*)-furanone; (ξ)-*form*, D-347
5,6-Dihydro-6-pentyl-2*H*-pyran-2-one, D-342
4,9-Dihydro-7-methoxy-1-methyl-3*H*-pyrido[3,4-*b*]indole, H-9
7′,8′-Dihydro-8′-hydroxyreticulataxanthin, R-9
9,10-Dihydroabscisic alcohol, A-12
Dihydrobrassicasterol, E-223
Dihydrocycloartomunin, D-226
22,23-Dihydroergosterol, E-205
N-Dihydroferuloyltyramine, H-712
Dihydroisocycloartomunin, C-488
7,8-Dihydrolycopene, D-285
Dihydromorelloflavone, M-760
Dihydroprudomenin, P-112
Dihydroroseoside, D-533
Dihydrosuberenol, H-498
4,5-Dihydrovomifoliol, D-533
2,3-Dihydrowithanolide E, W-7
1,2-Dihydroxy-1,2,3-propanetricarboxylic acid; (1*S*,2*S*)-*form*; γ-Lactone, dibutyl ester, D-675
6,8-Dihydroxy-1,7-diprenylxanthone-2-carboxylic acid, D-443
2,7-Dihydroxy-1-(3-methyl-2-butenyl)-9*H*-carbazole-3-carboxaldehyde, 9CI, H-100
3,6-Dihydroxy-1-methyl-4,5-diphenyl-2-piperidinone, D-438
3,9-Dihydroxy-10-prenylpterocarpan, D-672
3,13-Dihydroxy-11-oleanen-28-oic acid; (3β,13β)-*form*; 11α,12α-Epoxide, 28 → 13 lactone, 3-Ac, D-577
9,10-Dihydroxy-12-octadecenoic acid; (9ξ,10ξ,12ξ)-*form*, D-567
2,3-Dihydroxy-12-oleanen-28-oic acid; (2α,3β)-*form*; 3-*O*-β-D-Glucopyranoside, D-574
2,3-Dihydroxy-12-oleanen-28-oic acid; (2α,3β)-*form*; 3-*O*-(4-*E*-Hydroxycinnamoyl), D-574
2,3-Dihydroxy-12-oleanen-28-oic acid; (2α,3β)-*form*; 3-*O*-(4-*Z*-Hydroxycinnamoyl), D-574
3,16-Dihydroxy-12-oleanen-28-oic acid; (3β,16α)-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 2)-α-L-arabinopyranoside], 28-*O*-[α-L-rhamnopyranosyl-(1 → 4)-β-D-glucopyranosyl-(1 → 4)-β-D-glucopyranosyl] ester, D-578
2,3-Dihydroxy-12-ursen-28-oic acid; (2α,3α)-*form*; 3-(4-Hydroxy-3-methoxy-*E*-cinnamoyl), D-710
1,2-Dihydroxy-16-heptadecyn-4-one; 1-Ac, D-500
ent-7α,12β-Dihydroxy-16-kauren-19,6β-olide, T-606
6,7-Dihydroxy-16-kauren-19-oic acid; (*ent*-6α,7α)-*form*, D-516
5,7-Dihydroxy-2′,4′,6′-trimethoxy-8-prenylflavanone, P-167
4′,5-Dihydroxy-2′,7-dimethoxy-8-prenylflavone, T-268
1,11-Dihydroxy-2,10-dimethoxynoraporphine, C-361
1,9-Dihydroxy-2,10-dimethoxynoraporphine, I-74
6,11-Dihydroxy-2,2-dimethylpyrano[3,2-*c*]xanthen-7(2*H*)-one, D-434
3,4-Dihydroxy-2-hydroxymethyl-1-pyrrolidinepropanamide, D-508
1,5-Dihydroxy-2-methoxy-6-methylanthraquinone, T-621
2,3-Dihydroxy-23-oxo-12-oleanen-28-oic acid; (2α,3β)-*form*; 3-*O*-β-D-Glucopyranoside, D-597
3,21-Dihydroxy-23-oxo-12-oleanen-28-oic acid, T-651
20,26-Dihydroxy-24-dammaren-3-one; (20*S*,24*E*)-*form*, D-422
2′,8-Dihydroxy-3′,4′,5′,7-tetramethoxyflavan, H-196
5′,8-Dihydroxy-3′,4′,7-trimethoxyflavan, P-106
2,4′-Dihydroxy-3′,5′-dimethoxyacetophenone, T-133
3′,5-Dihydroxy-3,4′,6,7-tetramethoxyflavone, D-694
1,8-Dihydroxy-3,5-dimethoxy-2-prenylxanthone, T-282
1,7-Dihydroxy-3,6-dimethoxy-2,8-diprenylxanthone, T-173
1,5-Dihydroxy-3,6-dimethoxy-4,8-diprenylxanthone, T-171
1,6-Dihydroxy-3,7-dimethoxy-2,8-diprenylxanthone, T-173
1,5-Dihydroxy-3-methoxy-2-prenylxanthone, T-696
1,6-Dihydroxy-3-methoxy-2-prenylxanthone, T-697
1,7-Dihydroxy-3-methoxy-2-prenylxanthone, T-698
6*a*,9-Dihydroxy-3-methoxypterocarpan, T-700
6,11-Dihydroxy-3-methyl-3-(4-methyl-3-pentenyl)-3*H*,7*H*-pyrano[2,3-*c*]xanthen-7-one, D-557
3′,8-Dihydroxy-4′,5′,7-trimethoxyflavone, P-140
2′,5-Dihydroxy-4′,7-dimethoxyflavanone, T-186
2′,7-Dihydroxy-4′-methoxy-8-prenylflavan, T-680
2′,6′-Dihydroxy-4′-methoxyacetophenone, T-512
5,7-Dihydroxy-4′-methoxyflavanone; (*S*)-*form*; 7-*O*-β-D-Xylopyranoside, D-537
6,9-Dihydroxy-4,7-megastigmadien-3-one; (6ξ,7*E*,9ξ)-*form*; 9-*O*-β-D-Glucopyranoside, D-531
6,9-Dihydroxy-4,7-megastigmadien-3-one; (6ξ,7*E*,9ξ)-*form*; 9-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside], D-531
6,9-Dihydroxy-4,7-megastigmadien-3-one; (6*S*,7*E*,9*R*)-*form*; 7,8-Dihydro, 9-*O*-[α-L-rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], D-531
6,9-Dihydroxy-4,7-megastigmadien-3-one; (6*S*,7*E*,9*R*)-*form*; 7,8-Dihydro, 9-*O*-[β-D-apiofuranosyl-(1 → 6)-β-D-glucopyranoside], D-531
6,9-Dihydroxy-4,7-megastigmadien-3-one; (6*S*,7*E*,9*R*)-*form*; 9-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside], D-531
6,11-Dihydroxy-4-eudesmen-3-one; 6α-*form*, D-463
6,11-Dihydroxy-4-eudesmen-3-one; 6β-*form*, D-463
5,7-Dihydroxy-6,8-dimethylflavanone; (*S*)-*form*, D-432
5,7-Dihydroxy-6-methoxyflavanone, T-572
5,7-Dihydroxy-6-methoxyflavone; 5-*O*-α-L-Rhamnopyranoside, D-539
2′,4′-Dihydroxy-7-methoxy-8-prenylflavan, T-680
4′,5-Dihydroxy-7-methoxy-8-prenylflavone, T-685
14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid; (14*S*)-*form*, D-518
5,7-Dihydroxy-8-methoxyflavanone, T-573
3,29-Dihydroxy-8-multifloren-7-one; 3α-*form*; Bis(4-methoxybenzoyl), D-560
2,2′-Dihydroxy-9,9′-bis(4-hydroxyphenyl)-[3,3′-bi-1*H*-phenalene]-1,1′-dione, B-140
2,3-Dihydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, H-732
3,6*a*-Dihydroxy-9-methoxypterocarpan, T-700

Dihydroxyacidissiminol, A-105
4′,4″-Dihydroxyanigorootin, A-337
2,6-Dihydroxybenzoic acid; Benzyl ester, 2-*O*-β-D-glucopyranoside, D-389
2,4-Dihydroxybenzoic acid, D-387
3,14-Dihydroxycard-20(22)-enolide; (3β,5α,14β,17β)-*form*; 3-*O*-[β-D-Xylopyranosyl-(1 → 2)-α-L-rhamnopyranoside], D-410
2,4-Dihydroxychalcone, D-412
3,23-Dihydroxycycloart-24-en-26-oic acid; (3β,23ξ)-*form*; 23-Epimer, D-418
3,23-Dihydroxycycloart-24-en-26-oic acid; (3β,23ξ)-*form*, D-418
3,22-Dihydroxycycloart-24-en-26-oic acid, C-426
10,20-Dihydroxyeicosanoic acid, D-448
3,22-Dihydroxyergost-5-en-7-one, E-222
4′,7-Dihydroxyflavanone; (*S*)-*form*; 4′-Me ether, 7-*O*-α-L-rhamnopyranoside, D-470
5,7-Dihydroxyflavone; 7-*O*-[α-L-Rhamnopyranosyl-(1 → 4)-β-D-glucopyranoside], D-473
3β,6β-Dihydroxynortropane, A-517
3,4-Dihydroxyphenethyl glucoside, D-627
1-(3,4-Dihydroxyphenyl)-1,2-ethanediol; (ξ)-*form*, D-626
4-(3,4-Dihydroxyphenyl)-2,3-dihydro-2,3-dihydroxy-1*H*-phenalen-1-one, D-279
1-(3,5-Dihydroxyphenyl)-2-(3,4,5-trihydroxyphenyl)ethylene; (*Z*)-*form*; 4″-Me ether, D-661
1-(2,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene; (*E*)-*form*; 3′-*O*-β-D-Glucopyranoside, D-620
1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene; (*E*)-*form*, D-640
1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene; (*Z*)-*form*; 3,4′-Di-*O*-β-D-glucopyranoside, D-640
1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene; (*Z*)-*form*; 4′-*O*-β-D-Glucopyranoside, D-640
4-(3,4-Dihydroxyphenyl)-2-hydroxy-1*H*-phenalen-1-one, H-506
3-(3,4-Dihydroxyphenyl)-2-propenoic acid; (*E*)-*form*, D-653
3-(3,5-Dihydroxyphenyl)-2-propenoic acid, D-654
1-(2,4-Dihydroxyphenyl)-3-[8-hydroxy-2-methyl-2-(4-methyl-3-pentenyl)-2*H*-1-benzopyran-5-yl]-1-propanone, D-637
2-(3,5-Dihydroxyphenyl)-5,6-dimethoxybenzofuran, D-618
2-(3,5-Dihydroxyphenyl)-5-hydroxy-6-methoxybenzofuran, D-618
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*R*)-(*E*)-*form*, D-619
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*S*)-(*E*)-*form*; 3‴-*O*-β-D-Glucopyranoside, D-619
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*S*)-(*E*)-*form*; 3‴-*O*-β-D-Glucopyranoside, D-619
2-(3,5-Dihydroxyphenyl)-6-hydroxybenzofuran, D-635
2-(3,4-Dihydroxyphenyl)ethanol, D-627
5-[2-(3,5-Dihydroxyphenyl)ethenyl]-2-methoxy-1,3-benzenediol, D-661
N-(2,5-Dihydroxyphenyl)pyridinium(1+), D-657
3,22-Dihydroxystigmast-5-en-7-one, S-243
7-(2,4-Dihydroxystyryl)-5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran, D-630
1,5-Dihydroxyxanthone, D-719
1,7-Dihydroxyxanthone, D-720
Diisopropyl disulfide, D-722
2,4-Dimethoxy-3-dibenzofuranol, 9CI, D-130
1,2-Dimethoxy-4-(2-propenyl)benzene, P-504
1,6-Dimethoxy-9*H*-carbazole-3-carboxaldehyde, 9CI, D-407
3,4-Dimethoxybenzaldehyde, D-734
1,2-Dimethoxybenzene, D-735
4,8-Dimethoxyfuro[2,3-*b*]quinoline, F-149
9-(3,4-Dimethoxyphenyl)-2-methoxy-1*H*-phenalen-1-one, H-732
Dimethyl *ent*-16α-kaurane-17,19-dioate, K-19
Dimethyl disulfide, D-742
Dimethyl trisulfide, D-747
3,7-Dimethyl-1,6-octadien-3-ol; (ξ)-*form*; *O*-[α-L-Arabinofuranosyl-(1 → 6)-β-D-glucopyranoside], D-832
3,7-Dimethyl-1,6-octadien-3-ol; (ξ)-*form*; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], D-832
3,7-Dimethyl-1,6-octadien-3-ol; (*R*)-*form*; *O*-β-D-Glucopyranoside, D-832
3,7-Dimethyl-1,6-octadien-3-ol, D-832
2,7-Dimethyl-2,4-octadiene-1,8-diol; (2*E*,4*E*,7*R*)-*form*; 8-*O*-β-D-Glucopyranoside, D-829
2,6-Dimethyl-2,5-heptadienoic acid; (*E*)-*form*; β-D-Glucopyranosyl ester, D-798
2,6-Dimethyl-2,5-heptadienoic acid; (*E*)-*form*, D-798
3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-*form*; *O*-β-D-Glucopyranoside, D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-*form*; *O*-[α-L-Arabinofuranosyl-(1 → 6)-β-D-glucopyranoside], D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-*form*; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*Z*)-*form*; *O*-β-D-Glucopyranoside, D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*Z*)-*form*; *O*-[α-L-Arabinofuranosyl-(1 → 6)-β-D-glucopyranoside], D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*Z*)-*form*; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], D-833
4-(3,7-Dimethyl-2,6-octadienyl)-1,3,5-trihydroxyxanthone; (*E*)-*form*, D-842
2′-(3,6-Dimethyl-2-heptenyl)-3′,4′,7-trihydroxyflavanone; (*S*)-(*E*)-*form*, D-805
4-(1,1-Dimethyl-2-propenyl)-1,3,5,6-tetrahydroxy-7-prenylxanthone, D-889
2,6-Dimethyl-3,7-octadiene-2,6-diol, D-827
3,7-Dimethyl-3-octene-1,2,6,7-tetrol, D-853
2,6-Dimethyl-5,7-octadiene-2,3-diol; (*S,E*)-*form*, D-828
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8-Heptadecenal, 9CI, H-60
16-Heptadecene-1,2,4-triol; (2*S*,4*S*)-*form*; 1-Ac, H-73
16-Heptadecene-1,2,4-triol; (2*S*,4*S*)-*form*; 2-Ac, H-73
16-Heptadecene-1,2,4-triol; (2*S*,4*S*)-*form*; 4-Ac, H-73
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16-Heptadecyne-1,2,4-triol; (2*S*,4*S*)-*form*; 2-Ac, H-79
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2-Heptanol; (ξ)-*form*, H-95
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3,3′,4′,5,5′,7-Hexahydroxyflavanone; (2*R*,3*R*)-*form*, H-201
3,3′,4′,5,5′,7-Hexahydroxyflavone; 3-*O*-(3,4-Di-*O*-acetyl-α-L-rhamnopyranoside), H-205
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5-Hydroxy-2-piperidinecarboxylic acid; (2*S*,5*S*)-*form*, H-757
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4-Hydroxy-3-methoxybenzyl 8-methylnonanoate, D-400
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2-Hydroxy-4(6)-isopropyl-2,4,6-cycloheptatrien-1-one, H-523
3-Hydroxy-4-(4-hydroxyphenyl)-1*H*,3*H*-naphtho[1,8-*cd*]pyran-1-one, P-288
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2-Hydroxy-4-(4-methoxyphenyl)-1*H*-phenalen-1-one, H-506
9-Hydroxy-4-megastigmen-3-one; (6*R*,9*R*)-*form*; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], H-539
9-Hydroxy-4-megastigmen-3-one; (6*R*,9*R*)-*form*; *O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside], H-539
1-(2-Hydroxy-4-methoxyphenyl)-2-propanol, D-648
4-Hydroxy-4-methyl-2-pentanone, H-599
2-Hydroxy-4-oxo-12,15-heneicosadien-1-yl acetate, D-495
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2-Hydroxy-4-oxo-5,12-heneicosadien-1-yl acetate, D-495
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3-(6-Hydroxy-5-benzofuranyl)-2-propenoic acid; (*Z*)-*form*; *O*-β-D-Glucopyranoside, H-344
7-Hydroxy-5-methoxy-6,8-dimethylflavanone, D-432
2-(3-Hydroxy-5-methoxyphenyl)-6-methoxy-5-benzofuranol, D-618
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3-Hydroxy-6-methoxy-1-methyl-4,5-diphenyl-2-piperidinone, D-438
9-Hydroxy-7-megastigmen-3-one; *O*-β-D-Glucopyranoside, H-540
28-Hydroxy-7-octacosanone, H-639
7-Hydroxy-8(14),15-isopimaradien-18-oic acid; 7α-*form*, H-520
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5-Hydroxy-8,8-dimethyl-6-(1-oxobutyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]-dipyran-2-one, H-421
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-409
5-Hydroxy-8,8-dimethyl-6-(2-methyl-1-oxopropyl)-4-propyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-412
5-Hydroxy-8,8-dimethyl-6-(3-methyl-1-oxobutyl)-4-pentyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, H-410
11-Hydroxy-9,15,16-trioxooctadecanoic acid; (-)-*form*, H-816
6-Hydroxy-9,9-dimethyl-5-(3-methyl-1-oxobutyl)-1-propyl-3*H*,9*H*-[1,2]-dioxolo[3′,4′:4,5]furo[2,3-*f*][1]benzopyran-3-one, H-411
2-Hydroxy-9-(4-hydroxy-3-methoxyphenyl)-1*H*-phenalen-1-one, H-732
3-Hydroxy-9-(4-hydroxyphenyl)-1*H*,3*H*-naphtho[1,8-*cd*]pyran-1-one, P-288
2-Hydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one, H-732
2-Hydroxy-9-phenyl-1*H*-phenalen-1-one, H-732
11-Hydroxy-9-tridecenoic acid, H-808
4′-Hydroxyanigorootin, A-337
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2-Hydroxybenzoic acid; *O*-β-D-Glucopyranoside, Me ester, H-345
2-Hydroxybenzoic acid; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], Me ester, H-345
3-Hydroxybenzyl alcohol; α-*O*-β-D-Glucopyranoside, H-356
4-Hydroxybenzyl alcohol, H-357
27-Hydroxybullatacin, A-450
3-Hydroxybutanoic acid; (*R*)-*form*; *O*-[α-L-Arabinopyranosyl-(1 → 6)-β-D-glucopyranoside], butyl ester, H-374
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3-Hydroxybutanoic acid; (*S*)-*form*; Butyl ester, *O*-β-D-glucopyranoside, H-374
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7-Hydroxyhexadecanedioic acid; (ξ)-*form*, H-488
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4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid; (2*R*,4*S*)-*form*, H-613
4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid; (2*S*,4*S*)-*form*, H-613
3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid, F-64
ω-Hydroxymoracin N, M-756
3-Hydroxyoctanoic acid; (ξ)-*form*; Et ester, *O*-[β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranoside], H-651
3-Hydroxyoctanoic acid; (*R*)-*form*, H-651
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4-(4-Hydroxyphenyl)-2-butanone, H-720
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2-(3-Hydroxyphenyl)ethanol; 1′-*O*-β-D-Glucopyranoside, H-723
2-(4-Hydroxyphenyl)naphthalic anhydride, P-288
2-Hydroxyphenylacetic acid; *O*-β-D-Glucopyranoside, H-716
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4,7-Megastigmadiene-3,6,9-triol; (3β,6α,7*E*,9ξ)-*form*; 9-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside], M-91
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p-Menth-1-en-8-ol; (*S*)-*form*; *O*-β-D-Glucopyranoside, M-175
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7-Methyl-1,4,5-naphthalenetriol; 4-*O*-[β-D-Xylopyranosyl-(1 → 6)-β-D-glucopyranoside], M-507
2-Methyl-1-(2,4,6-trihydroxyphenyl)-1-butanone; (*S*)-*form*; 2-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside], M-703
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2-Methyl-4-propyl-1,3-oxathiane, M-625
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24-Methylene-29-norcycloartan-3-one, C-450
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Tetrahydroharmol, H-576
Tetrahydropentoxyline, T-114
3,19,23,24-Tetrahydroxy-12-oleanen-28-oic acid; (3β,19α)-*form*, T-256
1,3,5,8-Tetrahydroxy-2,4-diprenylxanthone, T-172
1,3,6,7-Tetrahydroxy-2,5,8-triprenylxanthone, T-289
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{1''}$-Isomer(*E*-), 3″-hydroxy, 3,6,7-tri-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{1''}$-Isomer(*E*-), 3″-hydroxy, 3,7-di-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{3''}$-Isomer, 2″ξ-hydroxy, 3,6,7-tri-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{3''}$-Isomer, 2″ξ-hydroxy, 3,7-di-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{3''}$-Isomer, 2″-oxo, 3,7-di-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 3,6,7-tri-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 3,7-di-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone; $\Delta^{3'}$-Isomer, 2′ξ-hydroxy, 6,7-di-Me ether, T-173
1,3,6,7-Tetrahydroxy-2,8-diprenylxanthone, T-173
1,3,5,8-Tetrahydroxy-2-prenylxanthone, T-282
5′,5‴,8,8″-Tetrahydroxy-3′,3‴,4′,4‴,7′,7″-hexamethoxy-5,5″-biflavan, P-123
3,4′,5,7-Tetrahydroxy-3′,5′-dimethoxyflavylium(1+), T-158
3,4′,5,7-Tetrahydroxy-3′-methoxyflavanone, P-109
3,4′,5,7-Tetrahydroxy-3′-methoxyflavone; 7-*O*-α-L-Rhamnopyranoside, 3-*O*-α-L-arabinopyranoside, T-238
3,4′,5,7-Tetrahydroxy-3′-methoxyflavylium(1+); 3-*O*-[4-Hydroxycinnamoyl-(→6)-β-D-glucopyranoside], 5-*O*-β-D-glucopyranoside, T-244
3,4′,5,7-Tetrahydroxy-3′-methoxyflavylium(1+); 3-*O*-[4-Hydroxycinnamoyl-(→?)-β-D-glucopyranoside], T-244
3,4′,5,7-Tetrahydroxy-3′-methoxyflavylium(1+), T-244
2′,4′,5,7-Tetrahydroxy-3,8-diprenylflavone, T-163
2′,4′,5,7-Tetrahydroxy-3-prenylflavone, T-266
2′,5,5′,7-Tetrahydroxy-4′-methoxy-3,3′-diprenylflavone, P-97
2′,3,4′,5-Tetrahydroxy-4-(3-methyl-1-butenyl)-stilbene, A-398
2′,3,4′,5-Tetrahydroxy-4-prenylstilbene, A-399
1,3,5,6-Tetrahydroxy-4-prenylxanthone, T-281
2′,4′,5,7-Tetrahydroxy-6-(3-methyl-1-butenyl)-flavone, T-267
3′,4′,5,7-Tetrahydroxy-6-*C*-sophorosylflavone, I-105
1,3,5,8-Tetrahydroxy-6-methoxy-2-methylanthraquinone, P-164
3,4′,5,7-Tetrahydroxy-6-methoxyflavone, T-240
2′,4′,5,7-Tetrahydroxy-6-prenylflavone, T-267
3′,4′,5,7-Tetrahydroxy-8-methylisoflavone; 3′,4′,7-Tri-Me ether, 5-*O*-[α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside], T-250
3,4′,5,7-Tetrahydroxy-8-prenylflavone; 4′-Me ether, 3-*O*-[α-L-rhamnopyranosyl-(1→6)-β-D-galactopyranoside], 7-*O*-β-D-galactopyranoside, T-272
2′,4′,5,7-Tetrahydroxy-8-prenylisoflavanone, T-274
1,3,11,22-Tetrahydroxyergosta-5,24-dien-26-oic acid; (1α,3β,11β,22*R*,24*E*)-*form*; 26-*O*-β-D-Glucopyranosyl ester, T-175
1,3,11,22-Tetrahydroxyergosta-5,24-dien-26-oic acid; (1α,3β,11β,22*R*,24*E*)-*form*; 26-*O*-[β-D-Glucopyranosyl-(1→2)-6-acetyl-β-D-glucopyranosyl] ester, T-175
3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,3′,4′,5,7-pentahydroxyflavan, T-200
3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,3′,5,5′,7-pentahydroxyflavan; (2*S*,2′*R*,3*S*,3′*R*,4*S*)-*form*, T-196
3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,4′,5,7-tetrahydroxyflavan; (2*S*,2″*R*,3*S*,3″*R*,4*S*)-*form*; 3-*O*-(4-Hydroxybenzoyl), T-200
3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,4′,5,7-tetrahydroxyflavan; (2*S*,2″*R*,3*S*,3″*S*,4*S*)-*form*, T-200
3,4′,5,7-Tetrahydroxyflavan(2→7,4→8)-3,4′,5,7-tetrahydroxyflavan; (2*S*,2″*S*,3*S*,3″*R*,4*S*)-*form*, T-200
3,4′,5,7-Tetrahydroxyflavan(4→8)-3,4′,5,7-tetrahydroxyflavan(4→8)-3,4,4′,5,7-pentahydroxyflavan, T-201
3,4,4′,7-Tetrahydroxyflavan; (2*S*,3*R*,4*R*)-*form*, T-182
3,4,4′,7-Tetrahydroxyflavan; (2*S*,3*S*,4*R*)-*form*, T-182
3,3′,4′,7-Tetrahydroxyflavanone; (2*R*,3*R*)-*form*; 7-*O*-α-L-Rhamnopyranoside, T-189
2′,4′,5,7-Tetrahydroxyflavanone; (*S*)-*form*, T-186
2,4′,5,7-Tetrahydroxyflavanone, T-187
4′,5,6,7-Tetrahydroxyflavone; 4′,5,6-Tri-Me ether, 7-*O*-β-D-glucopyranoside, T-210
4′,5,6,7-Tetrahydroxyflavone; 6-*O*-β-D-Xylopyranoside, T-210
3′,4′,5,7-Tetrahydroxyflavone; 7-*O*-(Disulfoglucoside), T-205
2′,4′,5,7-Tetrahydroxyflavone, T-202
3,4′,5,7-Tetrahydroxyflavone, T-206
3,4′,5,7-Tetrahydroxyflavylium(1+), T-212
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2′,4′,5,7-Tetrahydroxyisoflavone, T-222
1,3,14,20-Tetrahydroxywitha-5,24-dienolide; (1α,3β,14α,20*R*,22*R*)-*form*; 3-*O*-β-D-Glucopyranoside, 1-Ac, T-294
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1,3,4,6-Tetramethoxy-2-dibenzofuranol, D-126
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1,2,4-Trigalloylglucose; β-D-Pyranose-*form*, T-504
1,2,6-Trigalloylglucose; β-D-Pyranose-*form*, T-505
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2,4,5-Trihydroxy-1-methoxyxanthone, T-295
3,20,27-Trihydroxy-1-oxowitha-5,24-dienolide; (3β,20*R*,22*R*)-*form*; 3-*O*-β-D-Glucopyranoside, T-662
2,3,23-Trihydroxy-12-oleanen-28-oic acid; (2α,3β)-*form*; 3-*O*-β-D-Glucopyranoside, T-647
3,6,19-Trihydroxy-12-ursen-28-oic acid; (3β,6α,19α)-*form*, T-721
6,7,12-Trihydroxy-16-kauren-19-oic acid; (*ent*-6α,7α,12α)-*form*, T-606
4′,5,7-Trihydroxy-2′-methoxyisoflavanone, T-220
1,3,5-Trihydroxy-2,4-diprenylxanthone, T-559
1,3,7-Trihydroxy-2,8-diprenylxanthone, T-560
3,6,8-Trihydroxy-2-methoxy-1-prenylxanthone, T-284
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3,12,13-Trihydroxy-28-oleanaoic acid; (3β,12α,13β)-*form*; 28→13 Lactone, 3-Ac, T-644
5′,8,8″-Trihydroxy-3′,3‴,4′,4‴,5‴,7′,7″-heptamethoxy-5,5″-biflavan, P-123
3,5,7-Trihydroxy-3′,4′-dimethoxyflavone, T-547
4′,5,7-Trihydroxy-3′-methoxyflavone; 7-*O*-(Di-*O*-sulfo-β-D-glucopyranoside), T-618
4′,5,7-Trihydroxy-3′-prenylflavone; 7-*O*-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], T-684
4′,5,7-Trihydroxy-3,3′,6-trimethoxyflavone, T-711
2,7-Trihydroxy-3,4,6-trimethoxydibenzofuran, D-128
1,5,6-Trihydroxy-3-methoxy-2,4-diprenylxanthone, T-170
1,5,6-Trihydroxy-3-methoxy-4-prenylxanthone, T-281
4′,5,7-Trihydroxy-3-methoxyflavanone, T-190
1,5,8-Trihydroxy-3-methyl-2-prenylxanthone, T-282
1,4,5-Trihydroxy-3-prenylxanthone, T-699
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3,5,7-Trihydroxy-4′,8-dimethoxyflavone, T-548
3′,5,7-Trihydroxy-4′-methoxyflavanone; (*S*)-*form*; 5-*O*-β-D-Glucopyranoside, T-614
3,5,7-Trihydroxy-4′-methoxyflavone; 3-*O*-[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside], 7-*O*-α-L-rhamnopyranoside, T-616
3,5,7-Trihydroxy-4′-methoxyflavone; 3-*O*-[β-D-Glucopyranosyl-(1→?)-β-D-glucopyranoside], T-616
1,3,8-Trihydroxy-4-methyl-2,7-diprenylxanthone, T-629
1,3,6-Trihydroxy-5-methoxyxanthone, T-296
1,3,6-Trihydroxy-7-methoxy-2,8-diprenylxanthone, T-173
2′,4′,5-Trihydroxy-7-methoxy-3-prenylflavone, T-266
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1,3,6-Trihydroxy-7-methoxyxanthone, T-297
2′,4′,7-Trihydroxy-8-prenylflavan; (*S*)-*form*; 4′-Me ether, 2′,7-di-*O*-β-D-glucopyranoside, T-680
2′,4′,6′-Trihydroxyacetophenone, T-512
3,12,14-Trihydroxybufa-4,20,22-trienolide; (3β,12β,14β)-*form*; 3-*O*-[β-D-Glucopyrano-

syl-(1 → 2)-α-L-rhamnopyranoside], T-526
3,7,25-Trihydroxycucurbita-5,23-dien-19-al; (3β,7β,23*E*)-*form*; 25-Me ether, T-543
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid; (1α,3β,22*R*,24*E*)-*form*; 22-Ac, 3-*O*-β-D-glucopyranoside, 26-*O*-[β-D-glucopyranosyl-(1 → 4)-β-D-glucopyranosyl-(1 → 2)-6-acetyl-β-D-glucopyranosyl] ester, T-563
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid; (1α,3β,22*R*,24*E*)-*form*; 22-Ac, 3-*O*-β-D-glucopyranoside, 26-*O*-[β-D-glucopyranosyl-(1 → 4)-6-acetyl-β-D-glucopyranosyl-(1 → 2)-6-acetyl-β-D-glucopyranosyl] ester, T-563
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid; (1α,3β,22*R*,24*E*)-*form*; 3-*O*-β-D-Glucopyranoside, 26-*O*-β-D-glucopyranosyl ester, T-563
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid; (1α,3β,22*R*,24*E*)-*form*; 3-*O*-β-D-Glucopyranoside, 26-*O*-[β-D-glucopyranosyl-(1 → 2)-β-D-glucopyranosyl] ester, T-563
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid; (1α,3β,22*R*,24*E*)-*form*; 3-*O*-β-D-Glucopyranoside, 26-*O*-[β-D-glucopyranosyl-(1 → 2)-6-acetyl-β-D-glucopyranosyl] ester, T-563
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid; (1α,3β,22*R*,24*E*)-*form*; 3-*O*-β-D-Glucopyranoside, 26-*O*-[β-D-glucopyranosyl-(1 → 4)-β-D-glucopyranosyl-(1 → 2)-6-acetyl-β-D-glucopyranosyl] ester, T-563
1,3,22-Trihydroxyergosta-5,24-dien-26-oic acid; (1α,3β,22*R*,24*E*)-*form*; 3-*O*-β-D-Glucopyranoside, 26-*O*-[β-D-glucopyranosyl-(1 → 4)-6-acetyl-β-D-glucopyranosyl-(1 → 2)-6-acetyl-β-D-glucopyranosyl] ester, T-563
3,4,4′-Trihydroxyflavan; (2*S*,3*R*,4*R*)-*form*, T-565
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3,5,7-Trihydroxyflavanone; (2*R*,3*R*)-*form*; 5-*O*-[β-D-Galactopyranosyl-(1 → 4)-β-D-glucopyranoside], T-568
3,4′,7-Trihydroxyflavanone; (2*R*,3*R*)-*form*, T-567
4′,5,7-Trihydroxyflavanone; (*S*)-*form*; 5-*O*-α-L-Rhamnopyranoside, T-569
3,3′,4′-Trihydroxyflavone; 3-*O*-[α-L-Rhamnopyranosyl-(1 → 2)[α-L-rhamnopyranosyl-(1 → 6)]-β-D-glucopyranoside], T-575
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2-(3,4,5-Trihydroxyphenyl)ethanol; 3′,5′-Di-Me ether, 4′-*O*-β-D-glucopyranoside, T-664
1,3,27-Trihydroxywitha-5,24-dienolide; (1α,3β)-*form*; 1-Ac, 3-*O*-β-D-glucopyranoside, T-723
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2,4-*cis*-Trilobacinone, T-725
2,4-*trans*-Trilobacinone, T-725
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2,3,4-Trimethyl-3-pentanol, T-790
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4,14,24-Trimethylcholesta-8,25-dien-3-ol; (3β,4α,5α,14α,24*R*)-*form*, T-739
2,2,6-Trimethylcyclohexanone; (ξ)-*form*, T-747
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1,2,3,4-Tetrahydro-1-methyl-β-carboline-3-carboxylic acid; (1ξ,3ξ)-*form*, T-97
24,25,26-Tetrahydroxy-8-lanostene-3,7-dione, T-230
3,5,9,14-Tetrahydroxyergosta-7,22-dien-6-one; (3β,5α,9α,14α,22*E*,24*R*)-*form*, T-178
3,5,9,14-Tetrahydroxyergosta-7,22-dien-6-one; (3β,5α,9α,14β,22*E*,24*R*)-*form*, T-178
3-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-1,2,4-benzenetriol; (*all-E*)-*form*; 2-Ac, T-303
3-(3,7,11,15-Tetramethyl-2,6,10,14-hexadecatetraenyl)-1,2,4-benzenetriol; (*all-E*)-*form*; 4-Me ether, T-303
1,2,4,5-Tetrathiane, T-317
1,2,4,6-Tetrathiepane, T-318
Theanine; (*S*)-*form*, T-335
Thelephoric acid, T-340
5′-Thioadenosine; *S*-Me, *S*-oxide(*S*-), T-365
Threitol; (2*R*,3*R*)-*form*, T-386
TML 1, T-404
Trametenolic acid, L-42
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3α,7α,22-Triacetoxy-15α-hydroxylanosta-8,24*E*-dien-26-oic acid, T-228
3α,15α,22-Triacetoxy-7α-hydroxylanosta-8,24*E*-dien-26-oic acid, T-228
3α,15α,22*S*-Triacetoxy-7α-hydroxylanosta-8,24*E*-dien-26-oic acid, T-228
3α,15α,22*S*-Triacetoxy-7α-methoxylanosta-8,24*E*-dien-26-oic acid, T-228
3α,15α,22*S*-Triacetoxylanosta-7,9(11),24-trien-26-oic acid, T-611
3β,15α,22*S*-Triacetoxylanosta-7,9(11),24*E*-trien-26-oic acid, T-611
Tricholomic acid, T-457
5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol; (2*S*,3*S*,4*S*)-*form*, T-482
2,4,6,8-Tridecatetrayne, T-481
2-Tridecene-4,6,8-triyn-1-ol; (*E*)-*form*, T-491
3,7,23-Trihydroxy-11,15-dioxolanosta-8,24-dien-26-oic acid, T-552
3,5,9-Trihydroxy-23-methylergosta-7,22-dien-6-one; (3β,5α,9α,22*E*,24*R*)-*form*, T-630
15α,26,27-Trihydroxy-7α-methoxy-8,24-lanostadien-3-one, T-229
24,25,26-Trihydroxy-7α-methoxy-8-lanosten-3-one, T-230
3,12,23-Trihydroxy-7,11,15-trioxolanosta-8,24-dien-26-oic acid, T-159
3,5,9-Trihydroxyergost-7-en-6-one, E-200
3,15,22-Trihydroxylanosta-7,9(11),24-trien-26-oic acid; (3α,15α,22*R*,24*E*)-*form*, T-611
3,15,22-Trihydroxylanosta-7,9(11),24-trien-26-oic acid; (3β,15α,22*S*,24*E*)-*form*, T-611
24,25,26-Trihydroxylanosta-7,9(11)-dien-3-one, L-37
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4,4,14-Trimethyl-3,7,11,15-tetraoxochol-8-en-24-oic acid, L-110
1,2,4-Trithiolane, T-823
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5-Acetyl-2,3-dihydro-1*H*-pyrrolizine, A-45
5-Acetyl-2,3-dihydro-6-methyl-1*H*-pyrrolizine, A-41
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5-Carboxy-3,8-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)pyrano[4,3,2-*de*]-1-benzopyrylium; 3-*O*-β-D-Glucopyranoside, C-96
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3,6-Dihydro-4-(4-methyl-3-pentenyl)-1,2-dithiin, D-311
3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2*H*-pyran; (ξ)-*form*, D-308
Dihydro-5-(1-hydroxyethyl)-2(3*H*)-furanone, H-450
4,7-Dihydro-5-(4-methyl-3-pentenyl)-1,2,3-trithiepin, D-313
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Dihydro-5-octyl-2(3*H*)-furanone; (ξ)-*form*, D-338
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5,8-Dihydro-6-(4-methyl-3-pentenyl)-1,2,3,4-tetrathiocin, D-312
2,3-Dihydro-6-methyl-1*H*-pyrrolizine-5-carboxaldehyde, D-319
22,23-Dihydroergosterol, E-205
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4,5-Dihydrovomifoliol, D-533
2,3-Dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone, D-623

1,3-Dihydroxy-12,6-eudesmanolide; (1β,4α,6α,11α*H*)-*form*; 3-Ketone, 1-*O*-β-D-glucopyranoside, D-457
4,4′-Dihydroxy-2′,6′-dimethoxychalcone, T-147
10,11-Dihydroxy-2,6-farnesadien-1-oic acid; (2*E*,6*E*,10ξ)-*form*; β-D-Glucopyranosyl ester, D-464
2,3-Dihydroxy-2-methylbutanoic acid, D-547
4,10-Dihydroxy-2-oxo-1(5)-guaien-12,6-olide, T-587
1,7-Dihydroxy-3-methoxyxanthone, T-724
5-(2,3-Dihydroxy-3-methylbutyl)-4-(3,4-epoxy-4-methylpentanoyl)-3,4-dihydroxy-2-isopentanoyl-2-cyclopenten-1-one, D-549
2′,4-Dihydroxy-4′,6′-dimethoxy-3′-prenylchalcone, T-263
6,9-Dihydroxy-4,7-megastigmadien-3-one; (6ξ,7*E*,9ξ)-*form*; 9-*O*-β-D-Glucopyranoside, D-531
6,9-Dihydroxy-4,7-megastigmadien-3-one; (6ξ,7*E*,9ξ)-*form*; 9-*O*-[β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranoside], D-531
4′,7-Dihydroxy-5-methoxy-8-prenylflavanone, T-683
3,4-Dihydroxy-5-methoxybenzoic acid, T-520
1,3-Dihydroxy-7-methoxyxanthone, T-724
2,3-Dihydroxybenzoic acid, D-386
2,4-Dihydroxybenzoic acid, D-387
3,4-Dihydroxybenzoic acid, D-390
1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene; (*E*)-*form*, D-640
1-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene; (*Z*)-*form*; 4′-*O*-β-D-Glucopyranoside, D-640
3-(3,4-Dihydroxyphenyl)-2-propenoic acid; (*E*)-*form*, D-653
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*R*)-(*E*)-*form*, D-619
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*S*)-(*E*)-*form*; 3‴-*O*-β-D-Glucopyranoside, D-619
3-(3,5-Dihydroxyphenyl)-5-[2-(3,5-dihydroxyphenyl)ethenyl]-2,3-dihydro-2-(4-hydroxyphenyl)benzofuran; (2*S*,3*S*)-(*E*)-*form*; 3‴-*O*-β-D-Glucopyranoside, D-619
3,5-Dimethoxy-1*H*-inden-1-one, H-513
Dimethyl *ent*-16α-kaurane-17,19-dioate, K-19
3,7-Dimethyl-1,6-octadien-3-ol; (ξ)-*form*; *O*-[α-L-Arabinofuranosyl-(1 → 6)-β-D-glucopyranoside], D-832
3,7-Dimethyl-1,6-octadien-3-ol; (ξ)-*form*; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], D-832
3,7-Dimethyl-1,6-octadien-3-ol; (*R*)-*form*; *O*-β-D-Glucopyranoside, D-832
2,4-Dimethyl-1-hexanol; (2ξ,4ξ)-*form*, D-809
3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-*form*; *O*-β-D-Glucopyranoside, D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-*form*; *O*-[α-L-Arabinofuranosyl-(1 → 6)-β-D-glucopyranoside], D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*E*)-*form*; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*Z*)-*form*; *O*-[α-L-Arabinofuranosyl-(1 → 6)-β-D-glucopyranoside], D-833
3,7-Dimethyl-2,6-octadien-1-ol; (*Z*)-*form*; *O*-[α-L-Rhamnopyranosyl-(1 → 6)-β-D-glucopyranoside], D-833
8,8-Dimethyl-2-methylene-6-oxabicyclo[3.2.1]octan-7-one, D-816
2,6-Dimethyl-3,7-octadiene-2,6-diol, D-827
2,5-Dimethyl-4-(1-pyrrolidinyl)-3(2*H*)-furanone, D-901
1-(1,9-Dimethyl-5-methylene-8-decenyl)-4-methylbenzene, D-815
3,7-Dimethyl-6-octen-1-ol; (*R*)-*form*; *O*-β-D-Glucopyranoside, D-857
3,7-Dimethyl-6-octen-1-ol; (*S*)-*form*; *O*-β-D-Glucopyranoside, D-857
2,6-Dimethyl-7-octene-2,3,6-triol, D-855
2,6-Dimethyl-7-octene-2,6-diol, D-827
2,5-Dimethylphenol, D-874
2,6-Dimethylphenol, D-875
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2-Dodecanone, D-1019
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Epicatechin(6′ → 8)epicatechin, P-122
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6,7-Epoxy-2,9-humuladiene, E-125
4,7′-Epoxy-3′,4′,5,9,9′-lignanepentol; (7′*R*,8′*R*)-*form*; 3′,5-Di-Me ether, 9′-*O*-β-D-glucopyranoside, E-144
4,7′-Epoxy-3′,4′,5,9,9′-lignanepentol; (7′*R*,8′*R*)-*form*; 3′-Me ether, 9′-*O*-β-D-glucopyranoside, E-144
6,9-Epoxy-4-megastigmene-3,9-diol, E-149
2,3-Epoxy-6,9-humuladiene, E-124
5,6-Epoxy-7-megastigmene-3,9-diol; (3α,5α,6α,7*E*,9ξ)-*form*; 3-*O*-β-D-Glucopyranoside, E-148
10,14-Epoxyaromadendrane, A-417
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5-Ethoxy-4,5-dihydro-2(3*H*)furanone, E-251
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Ethyl 2-methylpropanoate, 9CI, M-605
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Ethyl crotonate, B-223
Ethyl decanoate, D-41
Ethyl dodecanoate, D-1016
Ethyl glucoside; β-D-Pyranose-*form*, E-268
Ethyl heptanoate, H-93
Ethyl hexadecanoate, H-159
Ethyl hexanoate, H-234
Ethyl hydrogen sulfate, E-269
Ethyl lactate, H-765
Ethyl octanoate, O-80
Ethyl pentanoate, P-190
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Ethyl undecanoate, U-15
2-Ethyl-1-hexanol; (ξ)-*form*, E-315
3-Ethyl-2-methoxypyrazine, E-321
5-Ethyl-2-methylpyridine, E-338
7-Ethyl-3,6-dihydro-1,4-dimethylazulene, D-789
7-Ethyl-5,6-dihydro-1,4-dimethylazulene, D-789
N-Ethylacetamide, E-282
4-Ethylbenzaldehyde, E-284
5-Ethyldihydro-2(3*H*)-furanone; (ξ)-*form*, E-295
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3,7(11)-Eudesmadiene, E-363
4(15),7(11)-Eudesmadiene, E-365
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3-(2-Furanyl)-2-propenal, F-136
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Gentioside, T-724
Geranyl pentanoate, D-833
3′-Geranyl-2′,4,4′,6′-tetrahydroxychalcone, D-839
1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6α)-*form*; β-D-Glucopyranosyl ester, G-87
1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6α)-*form*; 11,13-Dihydro, β-D-glucopyranosyl ester, G-87
Glabracin A, G-132
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Glabranin, G-133
Glabrin A, G-136
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α-D-Glucopyranosyl-(1 → 4)-α-D-glucopyranosyl-(1 → 6)-D-glucose, G-162
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Glucose; D-*form*, G-197
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2-Glucosyl-3,4′,5-trihydroxystilbene; (*Z*)-*form*, G-206
7-Glucosyloxy-5-hydroxy-6-methoxycoumarin, T-522
3-Glucosyloxy-8-hydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-5-(4-hydroxyphenyl)pyrano[4,3,2-*de*]-1-benzopyrylium(1+); 3″-Methoxy, G-199
3-Glucosyloxy-8-hydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-5-(4-hydroxyphenyl)pyrano[4,3,2-*de*]-1-benzopyrylium(1+); 6‴-*O*-(4-Hydroxy-*E*-cinnamoyl), G-199
3-Glucosyloxy-8-hydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-5-(4-hydroxyphenyl)pyrano[4,3,2-*de*]-1-benzopyrylium(1+), G-199
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1-Heptanol, H-94
2-Heptanone, H-97
2-Heptenoic acid; Me ester, H-103
4-Heptenoic acid, H-104
Heptyl 2-methylpropanoate, M-605
Heptyl acetate, H-94
6-Heptyltetrahydro-2*H*-pyran-2-one; (ξ)-*form*, H-124
N^b-Hexacosanoyltryptamine, T-844
2-Hexadecanone, H-161
N^b-Hexadecanoyltryptamine, T-844
Hexahydro-1,1-dimethyl-4-methylene-1*H*-cyclopenta[*c*]furan, H-177
2,3,5,6,8,8*a*-Hexahydro-2,5,5,8*a*-tetramethyl-7*H*-1-benzopyran-7-one, H-186
1,2,3,4,5,6-Hexahydro-7*H*-cyclopenta[*b*]pyridin-7-one, H-174
3,3′,4′,5,5′,7-Hexahydroxyflavylium(1+), H-213
2,3-Hexanedione, H-229
1-Hexanol, H-235
2-Hexanone, H-237
2-Hexen-1-ol; (*E*)-*form*, H-252
3-Hexenoic acid, H-250
cis-3-Hexenyl lactate, H-765
Hexyl acetate, H-235
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HMBOA-Glc, D-399
Hotrienol, D-849
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2,9-Humuladien-6-one, H-309
2,9-Humuladien-7-ol, H-308
2,7(14),9-Humulatriene, H-311
Humulinic acid A, H-315
Humulinic acid B, H-315
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6,7-Dihydro-2,5-dimethyl-5*H*-cyclopentapyrazine, D-242
6,7-Dihydro-2-methyl-5*H*-cyclopenta[*b*]pyrazine, D-294
6,7-Dihydro-5-methyl-5*H*-cyclopenta[*b*]pyrazine, D-295
Dimethyl disulfide, D-742
3,5-Dimethyl-2-propylpyrazine, D-893
3,7-Dimethyl-6-octenal, D-850
Docusate sodium, BAN, INN, B-130
(-)-Epicatechin 8-*C*-galactoside, G-39
Epicatechin-(2β → 5,4β → 6)*ent*-epicatechin, P-118
4-Ethyl-2-isopropyl-5-methyloxazole, T-444
4-Ethyl-2-methyl-5-propyloxazole, T-444
5-Ethyl-2-methylpyridine, E-338
2-Ethyl-5-methylpyrazine, E-335
2-Ethyl-6-methylpyrazine, E-336
2-Ethylpyrazine, E-347
FEMA 2490, F-96
FEMA 3526, H-376
FEMA 3721, O-54
2-Furanmethanol, F-96
1-(2-Furanyl)-1-butanone, F-107
α-D-Galactopyranosyl-(1 → 6)-α-D-galactopyranosyl-(1 → 6)-D-glucose, G-13
3-*O*-β-D-Galactopyranosylcinnamtannin B_1, P-124
3-*O*-β-D-Galactopyranosylproanthocyanidin $A_{5'}$, P-461
Glycerol 1,2-dioctadecanoate 3-(9*Z*-octadecenoate), G-244
Glycerol 1,3-didodecanoate 2-decanoate, G-243
Glycerol 1,3-dihexadecanoate 2-(9*Z*,12*Z*-octadecadienoate), G-243
Glycerol 1,3-dihexadecanoate 2-(9*Z*-octadecenoate), G-243
Glycerol 1,3-dioctadecanoate 2-(9*Z*-octadecenoate), G-243
Glycerol 1,3-dioctadecanoate 2-hexadecanoate, G-243
Glycerol 1-(9*Z*-octadecenoate) 2-hexadecanoate 3-octadecanoate, G-245
Glycerol 1-octadecanoate 2-(9*Z*-octadecenoate) 3-hexadecanoate, G-245
Glycerol 2,3-di-(9*Z*-octadecenoate) 1-hexadecanoate, G-244
3-Hexenoic acid, H-250
3-Hydroxy-2-butanone, H-376
3-Hydroxy-2-methyl-4*H*-pyran-4-one, H-609
3-Hydroxy-2-oxopropanoic acid, H-698
2′-Hydroxyacetophenone, H-331
5-(2-Hydroxyethyl)-4-methylthiazole, H-453
N-[2-(1*H*-Indol-3-yl)ethyl]docosanamide, T-844
Indole, I-23
Isopropyl benzoate, B-31
2-Isopropyl-4,5-dimethyloxazole, T-444
2-Isopropyl-4,5-dimethylthiazole, T-445
2-Isopropyl-4-methylthiazole, D-110
2-Isopropyl-5-methyl-2-hexenal, I-145
2-Isopropyl-5-methylpyrazine, I-149
p-Menth-3-en-1-ol; (ξ)-*form*, M-177
Methoxypyrazine, P-596
Methyl 2-aminobenzoate, A-217
Methyl 2-furoate, F-94
Methyl phenyl disulfide, M-290
Methyl phenylacetate, P-258
Methyl propyl trisulfide, M-303
2-Methyl-1-phenyl-2-propanol, M-594
3-Methyl-2,5-piperazinedione; (*S*)-*form*, M-600
3-Methyl-2-butenal, M-337
3-Methyl-2-oxobutanoic acid, M-529
3-Methyl-2-oxopentanoic acid, M-532
4-Methyl-2-oxopentanoic acid, M-533
5-Methyl-2-phenyl-2-hexenal, M-585
2-Methyl-5-propylpyrazine, M-627
2-Methyl-5-vinylpyrazine, M-714
4-Methyl-5-vinylthiazole, M-715
4-Methylbiphenyl, M-323
3-Methylbutyl benzoate, M-334
8,8′-Methylenebiscatechin, M-402
(1-Methylethenyl)pyrazine, M-435
2-Methylpropyl benzoate, M-606
Methylpyrazine, M-633
3-(Methylthio)propanal, M-688
2,3-Pentanedione, P-184
3-Penten-2-one, P-206
2-Pentylthiazole, P-221
Phenoxyacetic acid, P-253
1-Phenylethanol, P-272
2-Phenylethylamine, P-277
Procyanidin B_5, P-120
Propanoic acid, P-478
1-Propenylpyrazine, P-514
Quinoline, Q-12
Styrene, S-255
1,2,3,4-Tetrahydro-6,7-dihydroxy-1-methylisoquinoline; (ξ)-*form*, T-77
5,6,7,8-Tetrahydroquinoxaline, T-125
Tetramethylpyrazine, T-314
Theobromine, T-342
Trimethylamine, T-731
Trimethylpropylpyrazine, T-794
2-Undecanol; (*S*)-*form*, U-17

Coffee

Abietin, D-656
2-Acetyl-1,6,8-trihydroxy-3-methylnaphthalene; 6-Me ether, 8-*O*-[β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 3)-β-D-glucopyranosyl-(1 → 6)-β-D-glucopyranoside], A-100
2-Acetyl-1,8-dihydroxy-6-methoxy-3-methylnaphthalene, A-100
1-Acetyl-1-hydroxy-3,5-dimethoxy-1*H*-indene, A-99
5-Acetyl-2,4-dimethyloxazole, A-53
4-Acetyl-2-methylpyridine, A-77
2-Acetyl-3,5-dimethylpyrazine, A-54
2-Acetyl-3,6-dimethylpyrazine, A-55
4-Acetyl-3-methylpyridine, A-78
2-Acetyl-5-methylfuran, A-71
2-Acetyl-5-methylpyridine, A-75
2-Acetyl-5-methylthiophene, A-81
2-Acetyl-6-methylpyridine, A-76
2-Acetylpyrrole, A-89
Allantoic acid, A-175
2-Amino-4,8-octadecadiene-1,3-diol; (2*S*,3*R*,4*E*,8*Z*)-*form*; *N*-Hexadecanoyl, 1-*O*-β-D-glucopyranoside, A-281
2-Amino-4-hydroxybutanoic acid; (*S*)-*form*, A-262
6-*O*-β-D-Apiofuranosyl-D-glucose; β-D-Pyranose-*form*; 1-*O*-(3-Methyl-2-butenoyl), A-371
6-*O*-β-D-Apiofuranosyl-D-glucose; β-D-Pyranose-*form*; 1-*O*-(3-Methylbutanoyl), A-371
Arnidenediol, T-18
Astragalin; 2″,4″-Bis-*O*-(4-hydroxycinnamoyl), A-478
Astragalin; 2″,6″-Bis-*O*-(4-hydroxycinnamoyl), A-478
Baptifoline, B-7
1,3-Benzenediol, B-20
Benzofuran, B-29
Benzyl formate, B-47
Biphenyl, B-91
Bis(2-furanylmethyl) disulfide, B-131
Bis(2-furanylmethyl) sulfide, B-132
2,3-Butanedione, B-211
Butanoic acid, B-218
Cafamarine, C-15
Cafestol, C-17
Caffeine, C-18
4-*O*-Caffeoyl-3-*O*-feruloylquinic acid, D-150
3-*O*-Caffeoylquinic acid; (*E*)-*form*, C-20
5-*O*-Caffeoylquinic acid; (*E*)-*form*, C-22
1-*O*-Caffeoylquinic acid, C-19
4-*O*-Caffeoylquinic acid, C-21
N-Caffeoyltryptophan, T-845
Calystegine A_6, A-523
Calystegine C_1, A-518
Calystegine C_2, A-518
3-Carboxy-1-methylpyridinium betaine, C-100
Cassiaside B, T-634
Cassiaside B_2, T-634
Cassiaside C, T-424
Cassiaside, T-634
Cassitoroside, A-82
Chrysophanol 1-tetraglucoside, D-544
Chrysophanol 1-triglucoside, D-544
Chrysophanol 8-gentiobioside, D-544
Cofaryloside, T-605
Coffeasterene, C-318
Cyclopentanone, C-492
De-*O*-methylsimmondsin, S-108
Dehydroanonaine, D-74
Dehydronuciferine, D-73
Dehydroroemerine, D-74
2,3-Dehydrosilybin, S-103
10-*O*-Demethylflavasperone 10-gentiobioside, A-466
DHBOA-Glc, D-399
Di-2-furanylmethane, D-212
3,4-Di-*O*-caffeoylquinic acid, D-150
3,5-Di-*O*-caffeoylquinic acid, D-151
4,5-Di-*O*-caffeoylquinic acid, D-152
Dide-*O*-methyl-4-*O*-α-D-glucopyranosylsimmondsin, S-108
Dide-*O*-methylsimmondsin, S-108
3,5-Diethyl-2-methylpyrazine, D-204
2,6-Diethyl-3,5-dimethylpyrazine, D-200
2,5-Diethyl-3,6-dimethylpyrazine, D-199
2,5-Diethyl-3-methylpyrazine, D-203
2,3-Diethyl-5,6-dimethylpyrazine, D-198
2,5-Diethylpyrazine, D-206
2,6-Diethylpyrazine, D-207
2,4-Diethylthiazole, D-110
2,5-Diethylthiazole, D-111
Dihydro-2(3*H*)-thiophenone, D-358
6,7-Dihydro-2,3-dimethyl-5*H*-cyclopentapyrazine, D-241

6,7-Dihydro-2,5-dimethyl-5*H*-cyclopentapyrazine, D-242
6,7-Dihydro-2,6-dimethyl-5*H*-cyclopentapyrazine, D-243
Dihydro-2-methyl-3(2*H*)-furanone; (ξ)-*form*, D-298
Dihydro-2-methyl-3(2*H*)-thiophenone; (ξ)-*form*, D-330
6,7-Dihydro-2-methyl-5*H*-cyclopenta[*b*]pyrazine, D-294
Dihydro-3(2*H*)-thiophenone, D-359
Dihydro-5-methyl-2(3*H*)-furanone, D-301
6,7-Dihydro-5-methyl-5*H*-cyclopenta[*b*]pyrazine, D-295
2,3-Dihydro-6-methylthieno[2,3-*c*]furan, D-323
1,3-Dihydroxy-12,6-eudesmanolide; (1β,4α,6α,11α*H*)-*form*; 3-Ketone, 1-*O*-β-D-glucopyranoside, D-457
8,15-Dihydroxy-2-oxo-1(10),3,11(13)-guaiatrien-12,6-olide; (5α,6α,8α)-*form*; 11α,13-Dihydro, 15-aldehyde, 8-(4-hydroxyphenylacetyl), D-590
16,17-Dihydroxy-9(11)-kauren-19-oic acid; (*ent*-16β*OH*)-*form*, D-517
3′,4′-Dihydroxyacetophenone, D-373
2,4-Dihydroxybenzoic acid, D-387
3-(3,4-Dihydroxyphenyl)-2-propenoic acid; (*E*)-*form*, D-653
3,5-Dimethoxy-1*H*-inden-1-one, H-513
1,2-Dimethoxy-4-vinylbenzene, V-33
3,4-Dimethyl-1,2-cyclopentanedione, D-777
3,5-Dimethyl-1,2-cyclopentanedione, D-778
3,3-Dimethyl-1,2-dithiolane, D-782
4,5-Dimethyl-2-propyloxazole, T-444
3,5-Dimethyl-2-vinylpyrazine, D-920
2,5-Dimethyl-3-(methyldithio)furan, D-813
2,5-Dimethyl-3-(methylthio)furan, D-794
2,3-Dimethylbenzofuran, D-759
2,4-Dimethyloxazole, D-861
2,5-Dimethyloxazole, D-862
4,5-Dimethyloxazole, D-863
2,5-Dimethylphenol, D-874
2,6-Dimethylphenol, D-875
3,4-Dimethylphenol, D-876
11-Eicosen-1-ol; (*Z*)-*form*, E-25
4,7′-Epoxy-3,8′-bilign-7-ene-3′,4′,5,9,9′-pentol; (7′ξ,8′ξ)-*form*; 3′,5-Di-Me ether, E-63
Ergostanol, E-212
Ethyl acetoacetate, E-260
Ethyl formate, E-266
Ethyl methyl sulfide, E-272
Ethyl methyl trisulfide, E-273
3-Ethyl-1,2-benzenediol, E-285
4-Ethyl-1,2-benzenediol, E-286
3-Ethyl-1,2-cyclopentanedione, E-293
4-Ethyl-1,2-dimethoxybenzene, E-286
5-Ethyl-2,4-dimethyloxazole, T-444
5-Ethyl-2,4-dimethylthiazole, T-445
4-Ethyl-2,5-dimethyloxazole, T-444
3-Ethyl-2,5-dimethylpyrazine, E-299
4-Ethyl-2,5-dimethylthiazole, T-445
4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one, E-317
4-Ethyl-2-methyloxazole, D-107
5-Ethyl-2-methyloxazole, D-108
4-Ethyl-2-methylphenol, E-333
5-Ethyl-2-methylthiazole, D-111
4-Ethyl-2-methylthiazole, E-340
2-Ethyl-3,5-dimethylpyrazine, E-298
2-Ethyl-4,5-dimethyloxazole, T-444
2-Ethyl-4,5-dimethylthiazole, T-445
2-Ethyl-4-methyloxazole, D-107
5-Ethyl-4-methyloxazole, D-109
2-Ethyl-4-methylphenol, E-329
2-Ethyl-4-methylthiazole, E-339
5-Ethyl-4-methylthiazole, E-341
3-Ethyl-5-methyl-1,2-cyclopentanedione, E-327
3-Ethyl-5-methyl-2-vinylpyrazine, E-344
2-Ethyl-5-methyloxazole, D-108
2-Ethyl-5-methylpyrazine, E-335
2-Ethyl-5-methylpyridine, E-337
4-Ethyl-5-methylthiazole, D-112
2-Ethyl-6-methylpyrazine, E-336
2-Ethylfuran, E-306
3-Ethylfuran, E-307
2-Ethylpyrazine, E-347
3-Ethylpyridine, E-348
2-[(Ethylthio)methyl]furan, 9CI, F-95
1,4,11-Eudesmatrien-3-one, E-377
Falcarinone, H-54
FEMA 2490, F-96
FEMA 3709, P-599
3-*O*-Feruloylquinic acid, C-20
Flavoxanthin, E-85
Fructose; D-*form*, F-75
2-Furancarboxaldehyde, F-93
2-Furanmethanethiol, F-95
2-Furanmethanol, F-96
1-(2-Furanyl)-1,2-butanedione, F-105
1-(2-Furanyl)-1,2-propanedione, F-133
1-(2-Furanyl)-1-butanone, F-107
1-(2-Furanyl)-2-propanone, F-135
3-(2-Furanyl)-2-propenal, F-136
4-(2-Furanyl)-3-buten-2-one, F-108
(2-Furanylmethyl) methyl disulfide, F-113
1-(2-Furanylmethyl)-1*H*-pyrrole, F-120
4-[(2-Furanylmethyl)thio]-2-pentanone, F-124
Furfuryl isovalerate, F-96
Furfuryl thioacetate, F-95
2-*O*-α-D-Galactopyranosyl-D-*chiro*-inositol, I-40
4-*O*-α-D-Galactopyranosyl-D-galactose, G-17
6-*O*-α-D-Galactopyranosyl-D-glucose, G-22
2-*O*-α-D-Galactopyranuronosyl-L-rhamnose, G-35
1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6α)-*form*; β-D-Glucopyranosyl ester, G-87
1(10),4,11(13)-Germacratrien-12,6-olid-14-oic acid; (1(10)*Z*,4*E*,6α)-*form*; 11,13-Dihydro, β-D-glucopyranosyl ester, G-87
Glucocaffeic acid, D-653
Glucoobtusifolin, T-622
β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 4)-D-mannose, G-173
2-(β-D-Glucopyranosyloxy)-2-methylpropanenitrile, 9CI, H-605
β-D-Glucuronopyranosyl-(1 → 3)-α-D-galacturonopyranosyl-(1 → 2)-L-rhamnose, G-207
HDMBOA-Glc, D-399
9-Hentriacontanone, H-35
1,8,15-Heptadecatriene-11,13-diyne; (8*E*,15*E*)-*form*, H-62
1,8,15-Heptadecatriene-11,13-diyne; (8*Z*,15*Z*)-*form*, H-62
3,4-Heptanedione, H-92
3,3′,4′,5,5′,8-Hexahydroxyflavone, H-206
3,3′,4′,5,5′,7-Hexahydroxyflavylium(1+); 3-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), 5-*O*-β-D-glucopyranoside, H-213
2,3-Hexanedione, H-229
Higenamine; (*R*)-*form*, H-282
HMBOA-Glc, D-399
6′-HMG SDG, S-71
2-Hydroxy-1,6,7,8-tetramethoxy-3-methylanthraquinone, P-163
2-Hydroxy-1-methoxyaporphine, D-379
3-Hydroxy-18-lupen-21-one; 3β-*form*, H-536
4-Hydroxy-2,6-dimethoxyphenyl glucoside, B-22
4′-Hydroxy-2-(1-methylpiperidin-2-yl)acetophenone, P-413
1-Hydroxy-2-butanone, H-375
3-Hydroxy-2-butanone, H-376
3-Hydroxy-2-methyl-4*H*-pyran-4-one, H-609
2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one, H-812
3-Hydroxy-4,5-dimethyl-2(5*H*)-furanone, H-406
2′-Hydroxy-5′-methylacetophenone, H-556
2-Hydroxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one, D-399
2′-Hydroxyacetophenone, H-331
N^{α}-*p*-Hydroxycoumaroyltryptophan, T-845
3-(2-Hydroxyethyl)indole; *O*-[β-D-Xylopyranosyl-(1 → 6)-β-D-glucopyranoside], H-452
23-Hydroxytormentic acid, T-292
Isoliensinine, N-21
Isopropyl formate, P-480
3-Isopropyl-1,2-cyclopentanedione, I-127
2-Isopropyl-4,5-dimethyloxazole, T-444
2-Isopropyl-5-methoxypyrazine, H-524
2-Isopropyl-5-methylpyrazine, I-149
2-Isopropyl-6-methoxypyrazine, H-525
2-Isopropylfuran, I-133
Isosilybin, I-165
Isosilychristin, I-166
Kahweol, C-17
Lactucin, D-590
Lactupicrin, D-590
Liensinine, N-21
Linocinnamarin, H-748
Linusitamarin, D-654
Lotusine, H-282
Lucenin 2; 7-*O*-α-L-Rhamnopyranoside, L-102
Lyciumin B, L-126
Lyciumin C, L-126
Lyciumin D, L-126
Lyciumoside I, P-359
Lyciumoside II, P-359
Lyciumoside III, P-363
Lyciumoside IV, P-359
Lyciumoside IX, P-359
Lyciumoside VI, P-359
Lyciumoside VII, P-359
Lyciumoside VIII, P-361
Mascaroside, M-80
3-Mercapto-3-methyl-1-butanol, M-214
3-Mercapto-3-methylbutyl formate, M-214
Methanethiol, M-242
6-Methoxy-2(3*H*)-benzoxazolone, M-254
2-(Methoxymethyl)furan, 9CI, F-96
Methyl 2-furoate, F-94
Methyl butyrate, B-218
Methyl hexanoate, H-234
Methyl pentanoate, P-190
Methyl phenyl sulfide, M-291
Methyl phenylacetate, P-258
S-Methyl thioacetate, E-244
3-Methyl-1,2-cyclohexanedione, M-370
3-Methyl-1,2-cyclopentanedione, M-381
5-Methyl-2,3-hexanedione, M-476
4-Methyl-2,3-pentanedione, M-544
3-Methyl-2-butene-1-thiol, M-339
5-Methyl-2-furanmethanethiol, M-438
1-(5-Methyl-2-furanyl)-1,2-propanedione, M-448
2-Methyl-2-pentenal, M-551
5-Methyl-2-propyloxazole, D-108
2-Methyl-3-(2-methylpropyl)pyrazine, M-504
2-Methyl-3-(methyldithio)furan, M-487
2-Methyl-3-(methylthio)furan, M-440
2-Methyl-3-(methylthio)pyrazine, M-634
2-Methyl-5-(1-propenyl)pyrazine, M-611
2-Methyl-5-(methylthio)furan, 9CI, M-441
2-Methyl-5-propylpyrazine, M-627
2-Methyl-5-vinylpyrazine, M-714
2-Methyl-6-(1-propenyl)pyrazine, M-613
2-Methylbenzaldehyde, M-311
3-Methylbenzaldehyde, M-312
4-Methylbenzaldehyde, M-313
2-Methylbutanal; (*S*)-*form*, M-324
2-Methylbutanoic acid; (±)-*form*, M-330
(1-Methylethenyl)pyrazine, M-435
5-Methylquinoxaline, M-648
4-Methylthiazole, M-658
4-(Methylthio)-1-butanol, 9CI, M-203
3-(Methylthio)-1-propanol, M-229
1-(Methylthio)-2-butanone, M-205
2-[(Methylthio)methyl]-2-butenal, M-676
2-(Methylthio)phenol, 9CI, M-226
2-(Methylthiomethyl)furan, F-95
2-Methylthiophene, M-681
3-Methylthiophene, M-682
Mozambioside, M-80
Neferine, N-21
Neosilyhermin A, N-41
Neosilyhermin B, N-41
2-Nonenal; (*E*)-*form*, N-116
Norrubrofusarin 6-β-gentiobioside, T-634
2,3-Octanedione, O-77

2-Octanone, O-85
Orientin; 7-*O*-α-L-Rhamnopyranoside, O-167
2,3-Pentanedione, P-184
2-Pentylfuran, P-214
1-Phenyl-1,2-propanedione, P-303
1-Phenyl-1-propanone, P-310
Pronuciferine; (*R*)-*form*, P-466
Propanal, P-467
1-Propenylpyrazine, P-514
3-Propyl-1,2-cyclopentanedione, P-526
Propylpyrazine, P-534
1*H*-Pyrrole-2-carboxaldehyde, P-617
Pyrrolidine, P-618
Quercilicoside A, T-292
Quinic acid; (-)-*form*, Q-10
Roemerine; (*R*)-*form*, R-41
Rubrofusarin 6-gentiobioside, T-634
Scorzonoside, E-62
Scorzoside, H-476
Secoisolariciresinol 9,9′-diglucoside, S-71
Secoisolariciresinol; (8*R*,8′*R*)-*form*; 9,9′-Bis-*O*-[4-carboxy-3-hydroxy-3-methylbutanoyl-(→6)-β-D-glucopyranoside], S-71
Sericic acid, T-254
Sericoside, T-254
Silandrin, S-101
Silybin, S-103
Silychristin, S-104
Silydianin, S-105
Silyhermin, S-106
Silymonin, S-105
Simmondsin 2′-ferulate, S-108
Simmondsin; 3-*O*-De-Me, 2′-(4-hydroxy-3-methoxy-*Z*-cinnamoyl), S-108
Simmondsin; 4-*O*-De-Me, 2′-(4-hydroxy-3-methoxy-*E*-cinnamoyl), S-108
Simmondsin, S-108
Styrene, S-255
Syringoylglycerol; (1*R*∗,2*R*∗)-*form*, S-294
Syringoylglycerol; (1*R*∗,2*S*∗)-*form*, S-294
Taraxacoside, T-15
20-Taraxasten-3-one, T-23
20(30)-Taraxasten-3-one, T-24
ψ-Taraxasterol, T-23
Taraxasterol, T-24
Taraxerol, T-26
5,6,7,7*a*-Tetrahydro-4,4,7*a*-trimethyl-2(4*H*)-benzofuranone, T-130
Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran, T-94
1,2,3,4-Tetrahydro-6,7-dimethoxy-2-methylisoquinoline, T-78
5,6,7,8-Tetrahydroquinoxaline, T-125
4,11,13,15-Tetrahydroridentin B, D-457
2,3,19,24-Tetrahydroxy-12-oleanen-28-oic acid; (2α,3β,19α)-*form*; 2,3,23-Tri-Ac, T-254
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2,8-Decadiene-4,6-diyn-1-ol; (2*E*,8*Z*)-*form*; 3-Methylbutanoyl, D-31
2,4-Decadienoic isobutylamide; (*E*,*E*)-*form*, D-34
4,6-Decadiyn-1-ol isovalerate, D-38
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1,4-Di-*O*-caffeoylquinic acid, D-149
1,6-Di-*O*-galloyl-2,3-(*S*)-hexahydroxydiphenoyl-α-D-glucopyranose, H-191
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1,3-Diacetoxy-4,6,12-tetradecatriene-8,10-diyne, T-64
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3,5-Dicaffeoyl-4-succinoylquinic acid, D-151
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3,5-Didecanoyl-1,4-dihydro-4-nonylpyridine, D-105
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3,6:5′,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-carotene-3′,5-diol, C-388
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2,5-Diethyltetrahydrofuran, D-208
2,3-Dihydro-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (*S*)-*form*; *O*-β-D-Galactopyranoside, D-270
2,3-Dihydro-3-hydroxy-2-(1-hydroxy-1-methylethyl)-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (2*S*,3*R*)-*form*; 1′-*O*-β-D-Glucopyranoside, D-260
2,3-Dihydro-3-methyl-1*H*-pyrrole, D-316
2,3-Dihydro-3-methylpyrrole; (+)(HCl)-*form*, D-317
7,8-Dihydro-3-methylpyrrolo[1,2-*a*]pyrimidin-2(6*H*)-one, D-321
3,4-Dihydro-4,8-dihydroxy-3-methyl-1*H*-2-benzopyran-1-one; (3*R**,4*S**)-*form*, D-232
6,7-Dihydro-4-(hydroxymethyl)-2-(*p*-hydroxyphenethyl)-7-methyl-5*H*-2-pyrindinium, D-271
Dihydro-4-hydroxy-2(3*H*)-furanone; (*S*)-*form*; *O*-β-D-Glucopyranoside, D-258
Dihydro-5-octyl-2(3*H*)-furanone; (ξ)-*form*, D-338
2,3-Dihydro-7-hydroxy-2,2-dimethyl-4-oxo-4*H*-1-benzopyran-6-propanoic acid; *O*-β-D-Glucopyranoside, D-257
4,9-Dihydro-7-methoxy-1-methyl-3*H*-pyrido[3,4-*b*]indole, H-9
2,3-Dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(1-propenyl)benzofuran, D-289
3,4-Dihydro-8-hydroxy-3-(6-pentadecenyl)-1*H*-2-benzopyran-1-one; (3*R*, 6′*Z*)-*form*, D-278
3,4-Dihydro-8-hydroxy-3-tridecyl-1*H*-2-benzopyran-1-one; (*R*)-*form*, D-284
(-)-Dihydrocarveol, M-180
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1,2-Dihydrodehydroguaiaretic acid, D-71
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10,11-Dihydropipercide, R-14
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2-[1,2-Dihydroxy-1-(hydroxymethyl)ethyl]-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one, R-69
3,9-Dihydroxy-1-methoxy-2-prenylpterocarpene, T-694
3,9-Dihydroxy-1-methoxycoumestan, T-537
2-(1,2-Dihydroxy-1-methylethyl)-1,11-dihydro-5-hydroxy-11-methylfuro[2,3-*c*]acridin-6(2*H*)-one, R-69
2-(1,2-Dihydroxy-1-methylethyl)-2,3-dihydro-7*H*-furo[3,2-*g*][1]benzopyran-7-one; (1′ξ,2*S*)-*form*; 2′-*O*-β-D-Glucopyranoside, D-552
3β,24-Dihydroxy-11,13(18)-oleanadien-30,22β-olide, T-643
3,24-Dihydroxy-11,13(18)-oleanadien-30-oic acid; 3β-*form*; Me ester, D-569
3,21-Dihydroxy-11-oxo-12-oleanen-29,18-olide, T-660
3β,24-Dihydroxy-11-oxo-12-oleanen-30,22β-olide, T-661
3,23-Dihydroxy-12,19(29)-ursadien-28-oic acid; 3β-*form*; 3-*O*-α-L-Arabinopyranoside, 28-*O*-β-D-glucopyranosyl ester, D-707
3,30-Dihydroxy-12-oleanen-11-one, H-694
3,19-Dihydroxy-12-oleanen-28-oic acid; (3β,19α)-*form*; 3-*O*-α-L-Arabinopyranoside, 28-*O*-β-D-glucopyranosyl ester, D-580
2,3-Dihydroxy-12-ursen-24-oic acid; (2α,3α)-*form*, D-709
3,11-Dihydroxy-12-ursen-24-oic acid; (3α,11α)-*form*; 11-Ketone, 3-Ac, Me ester, D-713
3,11-Dihydroxy-12-ursen-24-oic acid; (3α,11α)-*form*; 11-Ketone, 3-Ac, D-713
3,19-Dihydroxy-12-ursen-28-oic acid; (3β,19α)-*form*; 28-*O*-β-D-Glucopyranosyl ester, D-716
3,19-Dihydroxy-12-ursen-28-oic acid; (3β,19α)-*form*; 3-*O*-α-L-Arabinopyranoside, 28-*O*-[3,4,5-trihydroxybenzoyl-(→6)-β-D-glucopyranosyl] ester, D-716
6′,7-Dihydroxy-2′,4′-dimethoxy-3′-prenylflavanone, T-264
2,3-Dihydroxy-2,4-cyclopentadien-1-one, D-420
5,7-Dihydroxy-2,6-dimethyl-4*H*-1-benzopyran-4-one, D-430
5,7-Dihydroxy-2,8-dimethyl-4*H*-1-benzopyran-4-one, D-431
2′,4′-Dihydroxy-2-biphenylcarboxylic acid, D-405
9,10-Dihydroxy-2-fenchanone, D-465
1,3-Dihydroxy-2-methoxy-8,9-methylenedioxypterocarpan, P-175
3-(3,4-Dihydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)-2-propen-1-one, T-146
8,15-Dihydroxy-2-oxo-1(10),3,11(13)-guaiatrien-12,6-olide; (5α,6α,8α)-*form*; 11α,13-Dihydro, 15-aldehyde, 8-(4-hydroxyphenylacetyl), D-590
4,10-Dihydroxy-2-oxo-1(5)-guaien-12,6-olide, T-587
11,12-Dihydroxy-20-nor-5(10),8,11,13-abietatetraen-1-one, D-561
4,7-Dihydroxy-2*H*-1-benzopyran-2-one, D-392
5,7-Dihydroxy-3′,4′,6,8-tetramethoxyflavone, D-695
5,7-Dihydroxy-3′,4′,6-trimethoxyflavone, D-699
5,6-Dihydroxy-3′,4′,7,8-tetramethoxyflavone, H-211
5,7-Dihydroxy-3′,4′-dimethoxy-5′-prenylflavanone, T-265
2′,7-Dihydroxy-3′,4′-dimethoxyisoflavan, T-217
2′,7-Dihydroxy-3′,4′-methylenedioxyisoflavone, T-221
4′,7-Dihydroxy-3′,8-diprenylflavanone; (*S*)-*form*, D-440
4,10-Dihydroxy-3,10-dimethoxypterocarpan, T-287
4,9-Dihydroxy-3,10-dimethoxypterocarpan, T-287
4,4′-Dihydroxy-3,3′,5,5′-tetramethoxy-7,7′-epoxylignan, H-194
4,4′-Dihydroxy-3,3′,5-trimethoxy-7,7′-epoxylignan, P-99
3′,5-Dihydroxy-3,4′,6,7-tetramethoxyflavone, D-694
9,9′-Dihydroxy-3,4,5-trimethoxy-3′,4′-methylenedioxylignan, H-89
5,7-Dihydroxy-3,8-dimethoxyflavone, T-209
5,7-Dihydroxy-3-(3-hydroxy-4-methoxybenzyl)-4-chromanone, D-404
5,7-Dihydroxy-3-(4-hydroxybenzyl)-4-chromanone; (-)-*form*, D-502
5,8-Dihydroxy-3-(4-hydroxybenzyl)-6,7-dimethoxy-4-chromanone, T-213
5,8-Dihydroxy-3-(4-hydroxybenzyl)-7-methoxy-4-chromanone, T-589
4,9-Dihydroxy-3-methoxy-3′,4′-methylenedioxy-7,9′-epoxylignan, P-100
5,7-Dihydroxy-3-methoxyflavone, T-580
4,9-Dihydroxy-3-methoxypterocarpan, T-702
1,7-Dihydroxy-3-methoxyxanthone, T-724
1,6-Dihydroxy-3-methylanthraquinone, D-543
3,3′-Dihydroxy-4′,5,7-trimethoxyflavan, P-104
2′,7-Dihydroxy-4′,5-dimethoxy-3′-prenylisoflavan, T-273
2′,7-Dihydroxy-4′,6′-dimethoxy-3′-prenylisoflavone, T-278
5,7-Dihydroxy-4′-methoxy-6-prenylisoflavone, T-688
5,7-Dihydroxy-4′-methoxy-8-prenylisoflavone, T-689
5,7-Dihydroxy-4′-methoxyflavone; 7-*O*-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside], D-538
2′,7-Dihydroxy-4′-methoxyisoflavan; (*R*)-*form*; 7-*O*-β-D-Glucopyranoside, D-540
2′,7-Dihydroxy-4′-methoxyisoflavanone, T-595
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), Me ester, D-542
5,7-Dihydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), D-542
5,7-Dihydroxy-4′-methoxyisoflavone, D-542
2′,7-Dihydroxy-4′-methoxyisoflavone, T-598
5,7-Dihydroxy-4′-prenyloxyflavanone, T-569
(11α)-1β,5α-Dihydroxy-4(15)-eudesmen-12,6α-olide, D-455
1-(2,6-Dihydroxy-4-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone, P-320
1-(2,6-Dihydroxy-4-methoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
4,4′-Dihydroxy-5,5′-diisopropyl-2,2′-dimethyl-3,6-biphenyldione, D-426
2′,4′-Dihydroxy-5,7-dimethoxy-3′,6-diprenylisoflavan, T-164
2′,4′-Dihydroxy-6′-methoxyacetophenone, T-512
4′,5-Dihydroxy-6,7,8-trimethoxyflavone, P-143
4′,5-Dihydroxy-6,7-methylenedioxyisoflavone, D-551
1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-2-propen-1-one, 9CI, T-550
1-(2,4-Dihydroxy-6-methoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
5,7-Dihydroxy-6-prenylflavanone; (*S*)-*form*, D-669
11,12-Dihydroxy-7,14-dimethoxy-8,11,13-abietatrien-20,6-olide, R-54
3,5-Dihydroxy-7,8-dimethoxyflavone, T-209
O-(3,6-Dihydroxy-7-drimen-11-yl)umbelliferone; (3′ξ,5′α,9′ξ,10′β)-*form*; 3′-Deoxy, 6′-ketone, D-447
O-(3,6-Dihydroxy-7-drimen-11-yl)umbelliferone; (3′ξ,5′α,9′ξ,10′β)-*form*; 6′-Ketone, D-

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4′,5-Dihydroxy-7-methoxy-6-methylflavone, T-632
4′,5-Dihydroxy-7-methoxy-6-prenylisoflavone, T-688
4′,5-Dihydroxy-7-methoxyisoflavone, D-541
1,3-Dihydroxy-7-methoxyxanthone, T-724
11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid, A-9
11,12-Dihydroxy-8,11,13-icetexatrien-20-one, D-509
3,6*a*-Dihydroxy-8,9-methylenedioxypterocarpan, T-285
2β,9ξ-Dihydroxy-8-oxo-1(10),4,11(13)-germacratrien-12,6α-olide, T-585
3,24-Dihydroxy-9(11),12-oleanadien-30-oic acid; 3β-*form*, D-568
3,7-Dihydroxy-9-methoxycoumestan, T-540
3,4-Dihydroxy-9-methoxypterocarpan, T-702
8,9-Dihydroxy-*p*-menth-1(6)-en-2-one; (4*S*,8*R*)-*form*, D-535
8,9-Dihydroxy-*p*-menth-1(6)-en-2-one; (4*S*,8*S*)-*form*, D-535
1,3-Dihydroxyanthraquinone, D-376
2,3-Dihydroxybenzoic acid, D-386
3,4-Dihydroxybenzoyl β-D-xylopyranoside, D-390
3-(3,4-Dihydroxybenzyl)-7-hydroxy-5-methoxy-4-chromanone, D-404
3-(1,2-Dihydroxybutyl)-1*H*-2-benzopyran-1-one, B-228
3,14-Dihydroxycard-20(22)-enolide; (3β,5β,14β,17β)-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 6)-β-D-glucopyranosyl-(1 → 4)-2,6-dideoxy-β-D-*ribo*-hexopyranoside], D-410
3,14-Dihydroxycarda-4,20(22)-dienolide; (3β,14β)-*form*; 3-*O*-[β-D-Glucopyranosyl-(1 → 4)-6-deoxy-β-D-allopyranoside], D-408
6-*O*-(3,4-Dihydroxycinnamoyl)glucose; β-D-Pyranose-*form*; 3′-Me ether, 2,3,4-trihydroxy-3-methylbutyl glycoside, D-417
6,9-Dihydroxyfenchone; (1*R*,3*S*,4*S*,6*R*)-*form*; 6-*O*-β-D-Glucopyranoside, D-466
8,10-Dihydroxyfenchone; (1*S*,3*R*,4*R*)-*form*; 10-*O*-β-D-Glucopyranoside, D-467
9,10-Dihydroxyfenchone; (1*S*,3*S*,4*R*)-*form*; 10-*O*-β-D-Glucopyranoside, D-468
4′,7-Dihydroxyflavanone; (*S*)-*form*; 4′-*O*-[3-*O*-Acetyl-β-D-apiofuranosyl-(1 → 2)-β-D-glucopyranoside], D-470
4′,7-Dihydroxyflavanone; (*S*)-*form*; 7-*O*-[β-D-Apiofuranosyl-(1 → 2)-β-D-glucopyranoside], D-470
1-(3,4-Dihydroxyphenyl)-1,2-ethanediol; (*R*)-*form*; 3′,4′-Di-Me ether, 1-*O*-β-D-glucopyranoside, D-626
1-(3,4-Dihydroxyphenyl)-1,2-ethanediol; (*R*)-*form*; 3′,4′-Di-Me ether, 2-*O*-β-D-glucopyranoside, D-626
1-(3,4-Dihydroxyphenyl)-1,2-ethanediol; (*R*)-*form*; 4′-Me ether, 3′-*O*-β-D-glucopyranoside, D-626
3-(3,4-Dihydroxyphenyl)-1,2-propanediol; (ξ)-*form*; 3′-Me ether, 2-*O*-[(3,4,5-trihydroxybenzoyl)(→ 6)-β-D-glucopyranoside], D-645
2-(3,4-Dihydroxyphenyl)-1,3-benzodioxole-5-carboxaldehyde; (±)-*form*, D-611
2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3-methyl-5-(1-propenyl)benzofuran; (7′*S*,8′*S*)-*form*; 3′-Me ether, D-616
3-(3,4-Dihydroxyphenyl)-2-propenoic acid; (*E*)-*form*; [β-D-Apiofuranosyl-(1 → 6)-β-D-glucopyranosyl] ester, D-653
2-(3,4-Dihydroxyphenyl)-4,6-dimethoxy-5-prenylbenzofuran, D-622
2-(3,4-Dihydroxyphenyl)-6-hydroxy-4-methoxy-5-prenylbenzofuran, D-622
1-(3,4-Dihydroxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, C-397
2-(3,4-Dihydroxyphenyl)ethenol; (*Z*)-*form*; 1-*O*-3,4-Dihydroxycinnamoyl(*E*-), D-628
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*R*,6*S*)-*form*; 3′,3″,5″-Tri-Me ether, D-632
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*R*,6*S*)-*form*; 3′,3″-Di-Me ether, 4-Ac, D-632
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*R*,6*S*)-*form*; 3′,3″-Di-Me ether, D-632
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*S*,6*S*)-*form*; 3′,3″-Di-Me ether, 4-Ac, D-632
2-[2-(3,4-Dihydroxyphenyl)ethyl]tetrahydro-6-(3,4,5-trihydroxyphenyl)-2*H*-pyran-4-ol; (2*S*,4*S*,6*S*)-*form*; 3′,3″-Di-Me ether, D-632
15,20-Dihydroxypregn-4-en-3-one; (15α,20*R*)-*form*; 20-*O*-[β-D-Glucopyranosyl-(1 → 4)-6-*O*-acetyl-β-D-glucopyranoside], D-667
15,20-Dihydroxypregn-4-en-3-one; (15α,20*R*)-*form*, D-667
Diisopropyl disulfide, D-722
5,5-Diisopropyl-2,2′-dimethylbiphenyl-3,3′,4,4′-tetrone, D-724
2,4-Diisopropyl-3-methylphenol, D-726
2,5-Diisopropyl-3-methylphenol, D-728
2,6-Diisopropyl-3-methylphenol, D-730
2,5-Diisopropyl-4-methylphenol, D-729
2,3-Diisopropyl-5-methylphenol, D-725
2,4-Diisopropyl-5-methylphenol, D-727
2,5-Diisopropylphenol, D-731
Dillapiol, D-732
Dillapional, D-733
2,5-Dimethoxy-1,4-benzoquinone, D-397
6,7-Dimethoxy-1-methylisoquinoline, 9CI, D-555
3,4-Dimethoxy-3,4-desmethylenecubebin, P-101
6,7-Dimethoxy-3-methyl-1*H*-carbazole-1,4(9*H*)-dione, K-40
1,2-Dimethoxy-4-(2-propenyl)benzene, P-504
2,6-Dimethoxy-4-(2-propenyl)phenol, 9CI, P-508
2,5-Dimethoxy-4-(2-propenyl)phenol, 9CI, P-509
α-[1-[2,6-Dimethoxy-4-(2-propenyl)phenoxy]ethyl]-4-hydroxy-3-methoxybenzenemethanol, 9CI, A-184
6,7-Dimethoxy-7-epirosmanol, T-132
11,12-Dimethoxy-8,11,13-abietatrien-20,7-olide, C-117
1,2-Dimethoxy-9,10-methylenedioxynoraporphine, N-4
1,2-Dimethoxy-9,10-methylenedioxyoxoaporphine, O-244
1,3-Dimethoxyanthraquinone, D-376
3,4-Dimethoxybenzaldehyde, D-734
5,8-Dimethoxychalepensin, C-184
4,6-Dimethoxyfuro[2,3-*b*]quinoline, 9CI, F-148
4,8-Dimethyl-1,3,7-nonatriene; (*E*)-*form*, D-821
3,7-Dimethyl-1,3,7-octatriene; (*Z*)-*form*, D-847
3,7-Dimethyl-1,6-octadien-3-ol; (*R*)-*form*, D-832
3,7-Dimethyl-1,6-octadien-3-ol; (*S*)-*form*; 3-*O*-β-D-Glucopyranoside, D-832
3,7-Dimethyl-1,6-octadien-3-ol; (*S*)-*form*; *O*-(6-*O*-Malonyl-β-D-glucopyranoside), D-832
3,7-Dimethyl-1,6-octadien-3-ol; (*S*)-*form*, D-832
3,7-Dimethyl-1,6-octadien-3-ol, D-832
2,6-Dimethyl-1,7-octadien-3-one, D-834
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3β-Hydroxy-11-oxo-12-oleanen-30,22β-olide, D-602
3-Hydroxy-11-oxo-12-oleanen-30-oic acid; (3β,18β)-*form*; Me ester, H-694
3-Hydroxy-11-oxo-12-ursen-24-oic acid, D-713
3-Hydroxy-12,18-ursadien-28-oic acid; 3β-*form*; 3-*O*-α-L-Arabinopyranoside, H-825
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3-Hydroxy-13(18)-oleanen-28-oic acid; 3β-*form*; Ac, Me ester, H-666
1-Hydroxy-14,16-epoxy-20-nor-5(10),6,8,13,15-abietapentaene-11,12-dione, T-13
6′-Hydroxy-2′,4′-dimethoxy-3′-methylacetophenone, T-620
1-Hydroxy-2,3-dimethoxydibenz[*cd,f*]indol-4(5*H*)-one, 9CI, T-544
4-Hydroxy-2,6,6-trimethyl-3-oxo-1,4-cyclohexadiene-1-carboxaldehyde, H-813
4-Hydroxy-2,6-dimethyl-7-octen-3-one, H-419
5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)-benzofuran, H-499
5-Hydroxy-2-(5-methyl-1-oxo-4-hexenyl)benzofuran, H-499
4′-Hydroxy-2-biphenylcarboxylic acid, H-366
6-Hydroxy-2-bornanone; (1*R*,4*R*,6*S*)-*form*; *O*-β-D-Glucopyranoside, H-373
3-(4-Hydroxy-2-methoxyphenyl)-2-propenal, D-651
2-Hydroxy-2-methylbutyl glucosinolate, H-573
3-Hydroxy-2-methylenebutanoic acid; (ξ)-*form*; 2-Methylbutyl ester, H-582
3-Hydroxy-2-methylenebutanoic acid; (ξ)-*form*; 2-Methylpropyl ester, H-582
3-Hydroxy-2-methylenebutanoic acid; (ξ)-*form*; 3-Methylbutyl ester, H-582
3-Hydroxy-2-methylenebutanoic acid; (ξ)-*form*; Butyl ester, H-582
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7-Hydroxy-2-methylisoflavone, H-592
2-(5-Hydroxy-2-pentenyl)-3-oxocyclopentaneacetic acid; (3ξ,7ξ)-*form*; *O*-β-D-Glucopyranoside, Et ester, H-709
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7-Hydroxy-2*H*-1-benzopyran-2-one, H-351
5-Hydroxy-3′,4′,6,7,8-pentamethoxyflavone, H-211
5-Hydroxy-3′,4′,7,8-tetramethoxyflavone, P-141
9-Hydroxy-3′,4′-dimethoxy-3,4-methylenedioxy-9,9′-epoxylignan, P-101
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4′-Hydroxy-3,3′,4,5-tetramethoxy-7,7′-epoxylignan, P-99
7-(4-Hydroxy-3,5-dimethoxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one, G-118
1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[2-methoxy-4-(1-propenyl)phenoxy]-1-propanol, V-41
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7-Hydroxy-3,8-acoranedione, H-334
4-Hydroxy-3,9,10-trimethoxypterocarpan, T-287
6*a*-Hydroxy-3,9-dimethoxypterocarpan, T-700
4-Hydroxy-3,9-dimethoxypterocarpan, T-702
4-Hydroxy-3-(16-methylheptadecyl)-2*H*-pyran-2-one, H-589
4-Hydroxy-3-(2-hydroxyethyl)acetophenone; 4-*O*-β-D-Glucopyranoside, H-495
2-Hydroxy-3-(2-hydroxyphenyl)propanoic acid; (*S*)-*form*, H-508
2-Hydroxy-3-(3,4-dihydroxyphenyl)propanamide, D-641
7-Hydroxy-3-(3-hydroxy-4-methoxybenzyl)-5-methoxy-4-chromanone, D-404
4-Hydroxy-3-(3-methyl-2-butenyl)acetophenone; *O*-β-D-Glucopyranoside, H-571
5-Hydroxy-3-(4-hydroxybenzyl)-7,8-dimethoxy-4-chromanone, T-589
7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone, T-724
1-Hydroxy-3-methoxy-10-methylacridone, D-375
4-Hydroxy-3-methoxy-2,10-bisaboladien-9-one, D-406
1-Hydroxy-3-methoxy-7-primeverosyloxyxanthone, T-724
6*a*-Hydroxy-3-methoxy-8,9-methylenedioxypterocarpan, T-285
4-Hydroxy-3-methoxybenzaldehyde, D-382
4-Hydroxy-3-methoxybenzenemethanol, 9CI, D-400
4-Hydroxy-3-methoxybenzyl 7-methyloctanoate, D-400
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3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol, D-645
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3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid; (*E*)-*form*, H-554
1-(4-Hydroxy-3-methoxyphenyl)-3-decanone, H-553
1-(4-Hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1,4-pentadien-3-one, B-125
7-(4-Hydroxy-3-methoxyphenyl)-5-methoxy-1-phenyl-3-heptanone, 9CI, H-496
1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione, 9CI, C-397
1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-4-hepten-3-one, G-118
1-(4-Hydroxy-3-methoxyphenyl)-7-phenyl-3,5-heptanedione, 9CI, H-496
2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]-5-octylfuran, A-172
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N-[(4-Hydroxy-3-methoxyphenyl)methyl]-7-methyl-5-octenamide, 9CI, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-7-methyloctanamide, 9CI, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-9-methyl-7-decenamide, 9CI, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]-9-methyldecanamide, 9CI, D-402
N-[(4-Hydroxy-3-methoxyphenyl)methyl]octanamide, 9CI, D-402
1-Hydroxy-3-methyl-9*H*-carbazole, H-574
2-Hydroxy-3-methyl-9*H*-carbazole, H-575
2-Hydroxy-3-methylbutanoic acid; (*R*)-*form*; 3-Methylbutanoyl, H-568
6′′-*O*-(3-Hydroxy-3-methylglutaroyl)cosmosiin, C-362
2-Hydroxy-3-oxo-12-oleanen-28-oic acid, D-574
1α-Hydroxy-3-oxo-4-eudesmen-12,6α-olide, D-459
2′-Hydroxy-4′,6′-dimethoxyacetophenone, T-512
5-Hydroxy-4′,7-dimethoxy-6-methylflavone, T-632
3′-Hydroxy-4′-methoxyglabridin, G-135
7-Hydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), Me ester, H-548
7-Hydroxy-4′-methoxyisoflavone; 7-*O*-(6-*O*-Malonyl-β-D-glucopyranoside), H-548
7-Hydroxy-4′-methoxyisoflavone, H-548
3-Hydroxy-4,5-dimethyl-2(5*H*)-furanone, H-406
1-(2-Hydroxy-4,6-dimethoxy-3-methylphenyl)-3-phenyl-1-propanone, P-321
6-Hydroxy-4,6-dimethyl-3-hepten-2-one, H-408
3-Hydroxy-4,9-dimethoxypterocarpan, T-702
8-Hydroxy-4-acoren-3-one; Ac, H-336
8-Hydroxy-4-acoren-3-one, H-336
7-Hydroxy-4-acorene-3,8-dione, H-335
1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol, D-626
3-(2-Hydroxy-4-methoxyphenyl)-8,8-dimethyl-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, 9CI, K-13
4-Hydroxy-4-methyl-2-cyclohexen-1-one; (ξ)-*form*, H-580
7-Hydroxy-4-methyl-2*H*-1-benzopyran-2-one; Ac, H-561
3-(2-Hydroxy-4-methylphenyl)-2-butanone, H-600
2-(2-Hydroxy-4-methylphenyl)-3-pentanone, H-602
2-(3-Hydroxy-4-methylphenyl)-5-methyl-4-hex-

en-3-one, H-601
1-Hydroxy-5,11(13)-eudesmadien-12,8-olide, H-459
4′-Hydroxy-5,5′-diisopropyl-2,2′-dimethyl-3,4-biphenylquinone, H-402
2-Hydroxy-5-methoxybenzoic acid, D-388
3-Hydroxy-5-phenylpentanoic acid; (ξ)-*form*; *O*-β-D-Glucopyranoside, H-730
7-Hydroxy-6-methoxyflavone, D-474
7-Hydroxy-6-methyl-2*H*-1-benzopyran-2-one, H-562
4-Hydroxy-6-methyl-3-(1-oxobutyl)-2*H*-pyran-2-one, H-597
4-Hydroxy-7(11),10(14)-guaiadien-8-one; (1α,4β,5β)-*form*, H-480
5-Hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-phenyl-3-heptanone, H-496
5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone, H-507
O-(3-Hydroxy-7-drimen-11-yl)umbelliferone; (3′α,5′α,9′ξ,10′β)-*form*, H-436
O-(3-Hydroxy-7-drimen-11-yl)umbelliferone; (3′β,5′α,9′ξ,10′β)-*form*, H-436
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5-Hydroxy-7-methoxy-2,8-dimethyl-4*H*-1-benzopyran-4-one, D-431
5-Hydroxy-7-methoxy-2-methyl-4*H*-1-benzopyran-4-one, D-546
12-Hydroxy-7-oxo-8,11,13-abietatrien-18-al, A-8
4-(3-Hydroxy-7-phenyl-6-heptenyl)-1,2-benzenediol, 9CI, H-733
10-Hydroxy-8-nor-2-fenchanone; *O*-β-D-Glucopyranoside, H-635
3-Hydroxy-9-methoxy-4-prenylpterocarpan, D-671
11-Hydroxy-9-triacontanone; (+)-*form*, H-807
2-Hydroxy-9*H*-carbazole-3-carboxaldehyde, 9CI, H-382
8-Hydroxy-*p*-menth-1-en-7-oic acid; (*S*)-*form*, H-544
8-Hydroxy-*p*-menth-6-en-2-one; (*R*)-*form*; Ac, H-546
2-Hydroxy-*p*-mentha-1,8-dien-6-one, H-542
3-Hydroxy-*p*-mentha-1,8-dien-7-al, H-541
5-Hydroxy-*p*-mentha-6,8-dien-2-one, H-543
4′-Hydroxyacetophenone; *O*-[4-Hydroxy-3,5-dimethoxybenzoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside], H-332
4′-Hydroxyacetophenone; *O*-[4-Hydroxybenzoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside], H-332
2′-Hydroxyacetophenone, H-331
2α-Hydroxyalantolactone, H-456
1α-Hydroxyarbusculin A, D-460
7-Hydroxyaustrobailignan 5, P-153
4-Hydroxybenzaldehyde; *O*-(4-*O*-Acetyl-α-L-rhamnopyranoside), H-343
2-Hydroxybenzaldehyde, H-342
4-Hydroxybenzeneacetonitrile, H-717
4-Hydroxybenzoic acid; [β-D-Apiofuranosyl-(1→6)-β-D-glucopyranosyl] ester, H-347
(4-Hydroxybenzoyl)choline, C-239
4-Hydroxybenzyl alcohol; 4-Me ether, α-*O*-(2-*O*-sulfo-β-D-glucopyranoside), H-357
4-Hydroxybenzyl glucosinolate; 4-(4-*O*-Acetyl-α-L-rhamnopyranoside), H-358
4-Hydroxybenzyl isothiocyanate; *O*-α-L-Rhamnopyranoside, H-359
4-Hydroxybenzyl isothiocyanate; *O*-(4-*O*-Acetyl-α-L-rhamnopyranoside), H-359
4-Hydroxybenzyl isothiocyanate, H-359
(4-Hydroxybenzyl)carbamic acid; *O*-α-L-Rhamnopyranoside, Et ester, H-361
(4-Hydroxybenzyl)carbamic acid; *O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), Et ester, H-361
(4-Hydroxybenzyl)carbamic acid; *O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), Me ester, H-361
(4-Hydroxybenzyl)thiocarbamic acid; 4′-*O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), *O*-Et ester (*Z*-), H-365
(4-Hydroxybenzyl)thiocarbamic acid; 4′-*O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), *O*-Et ester, H-365
(4-Hydroxybenzyl)thiocarbamic acid; 4′-*O*-(Tri-*O*-acetyl-α-L-rhamnopyranoside), *O*-Me ester (*E*-), H-365
4-Hydroxybenzylamine, H-360
1′-Hydroxychavicol acetate, H-749
1β-Hydroxycolartin, D-458
Hydroxydestruxin B, D-95
3-(2-Hydroxyethyl)indole; *O*-[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside], H-452
5-Hydroxyfenchone; (1*R*,4*R*,5*S*)-*form*; *O*-β-D-Glucopyranoside, H-463
6-Hydroxyfenchone; (1*R*,4*S*,6*R*)-*form*; *O*-β-D-Glucopyranoside, H-464
10-Hydroxyfenchone; (1*S*,4*R*)-*form*; *O*-β-D-Glucopyranoside, H-465
Hydroxygaleon, G-45
9-Hydroxygeraniol, D-825
3-Hydroxyglabrol, D-440
18α-Hydroxyglycyrrhetic acid, D-600
24-Hydroxyglycyrrhetic acid, D-604
28-Hydroxyglycyrrhetic acid, D-606
Hydroxyhomodestruxin B, H-293
8-Hydroxyhyperforin 8,1-hemiacetal, H-511
Hydroxyisonobilin, T-584
5′-Hydroxyjasmonic acid lactone, H-527
10-Hydroxylinalyl oxide; (3*R*,6*R*)-*form*; 7-*O*-β-D-Glucopyranoside, H-534
10-Hydroxylinalyl oxide; (3*R*,6*S*)-*form*; 7-*O*-β-D-Glucopyranoside, H-534
2-Hydroxylinolenic acid, H-645
24-Hydroxyliquiritic acid, D-603
2-(Hydroxymethyl)-1,2,3,4-butanetetrol; (*R*)-*form*, H-566
3-Hydroxymethyl-1-methoxycarbazole, H-593
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1-(4-Hydroxyphenyl)-1,2-propanediol; (1*S*,2*R*)-*form*; 4′-Me ether, 2-*O*-β-D-glucopyranoside, H-737
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6-Methoxy-3-(2-thiazolyl)-1*H*-indole, T-355
1-Methoxy-4-(2-propenyl)benzene, 9CI, P-513
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12-Methyl-13-tridecanolide, M-701
3-Methyl-2,4-nonanedione, M-512
3-Methyl-2-buten-1-ol, M-344
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Dictionary of Food Compounds on CD-ROM

This CD-ROM allows users to search the entire contents of the Dictionary in a highly sophisticated manner. Food compounds can be searched by structure, name, CAS number, molecular formula and food use. There is a user manual and an extensive, intuitive help system.

INSTALLATION

Insert the CD in the CD-ROM drive and click on the Start button and select Run. In the command line, type D:\setup.exe (where D is your CD-ROM drive letter), then click OK. If you would like a shortcut added to your start menu (includes a shortcut to the help text, manual and introduction), check the appropriate box.

You have two installation options:

- Standard installation
  The default installation copies the program files only to your computer's hard drive. Use this option if your computer has limited hard disk space. You will need to insert the CD every time you use the *Dictionary of Food Compounds*.
- Hard disk installation
  If you would like to copy the entire database to your hard drive, please check the option Copy Database to HD. This will require approximately 125 MB of hard disk space and is the best option for computers with ample hard disk space. (Due to Windows® requirements, we recommend only using this option if you have at least 300 MB free hard disk space, otherwise system performance may be affected).

INSTALL

If you do not already have Adobe Acrobat Reader® installed on your PC, you may install it at this point to access this manual and the database introduction in PDF format.

Check that the path to your CD-ROM drive is correct and then press OK.

You will be prompted to select a folder in which to install the software. If you wish the program to be installed to the default folder C:\Dictionary of Food Compounds, just click Install Dictionary of Food Compounds. Otherwise, type a new folder location and then click Install Dictionary of Food Compounds.

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